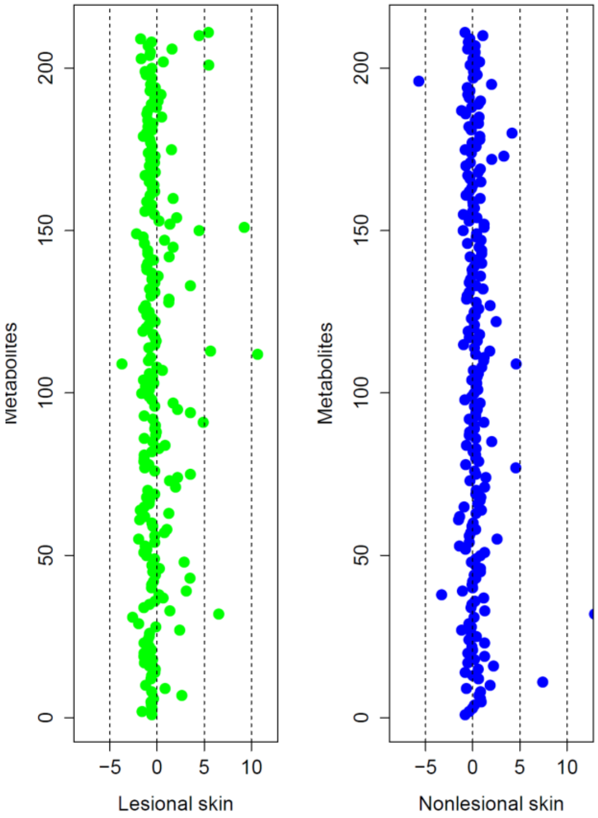
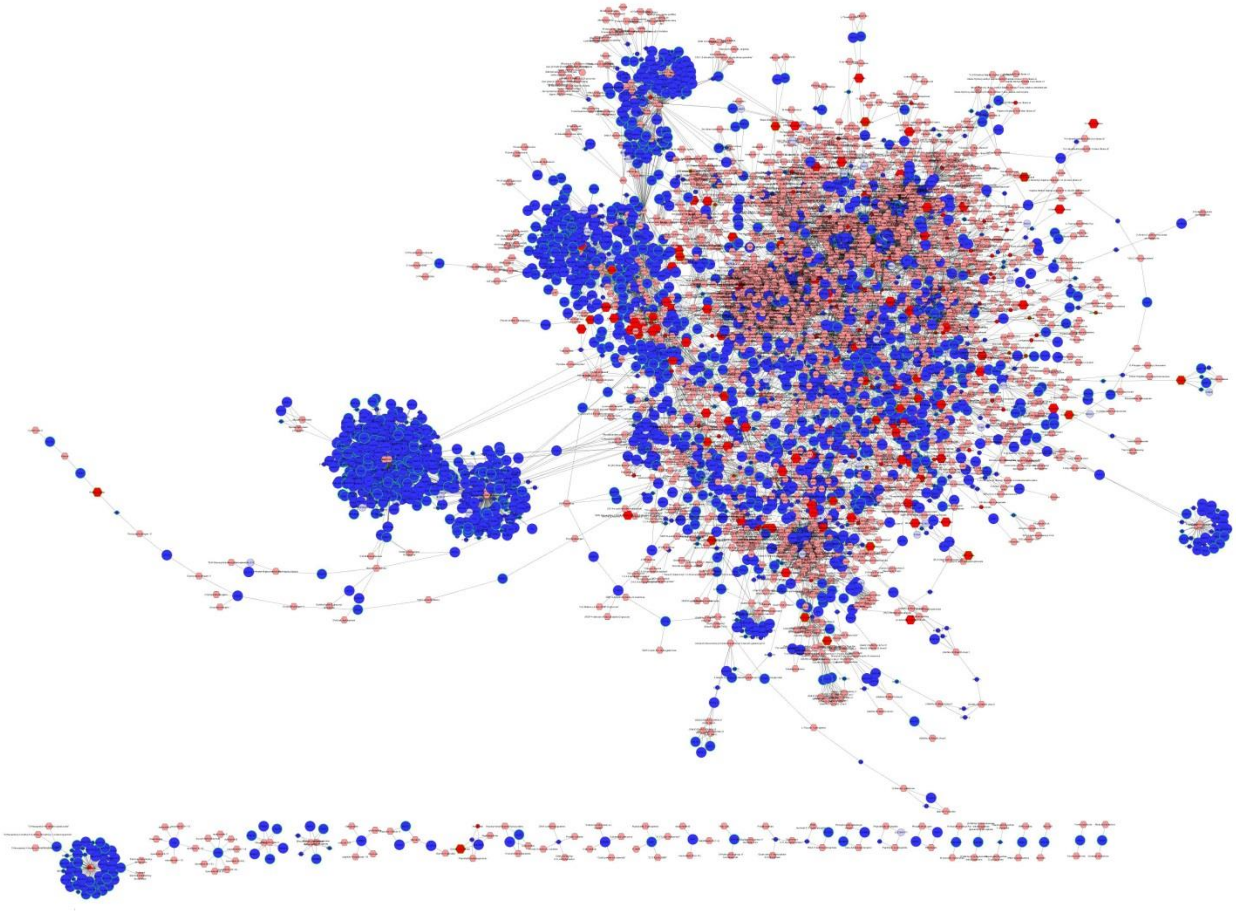
Supplementary Materials:

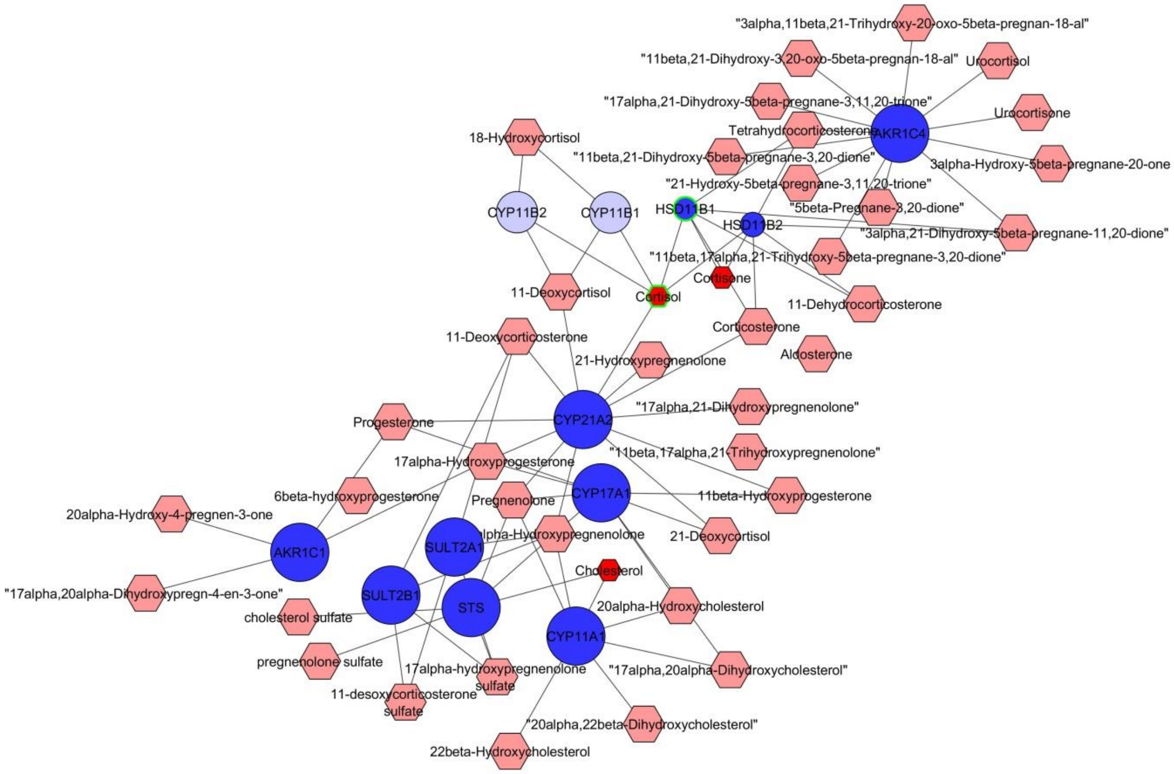
Supplementary Figures



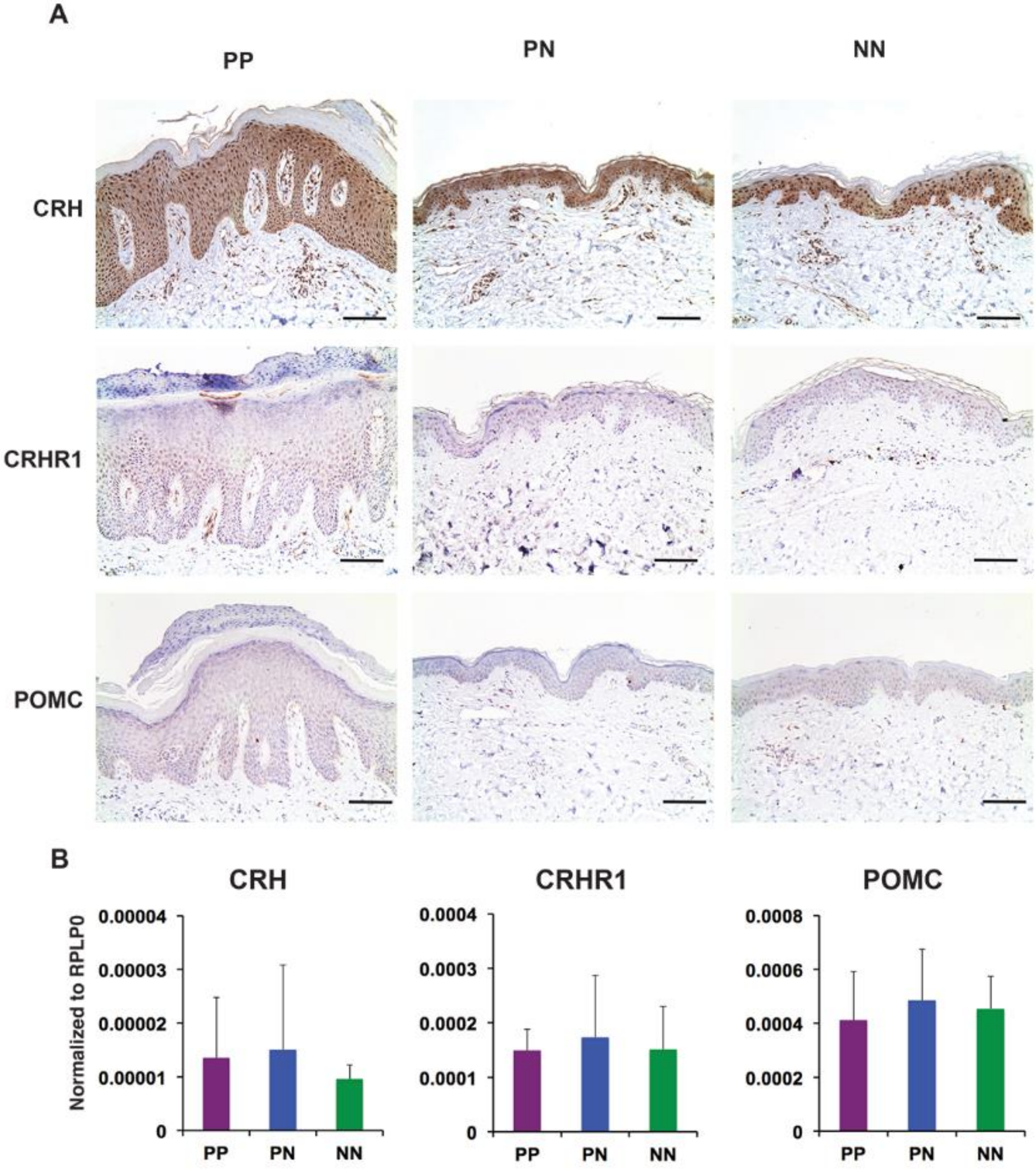
Supplementary Figure 1. Z-scores for negatively charged metabolites



Supplementary Figure 2. Global view of transcriptional and metabolomic changes in psoriatic skin. Genome wide expression analysis of mRNA expression by RNA-seq in psoriasis vs normal skin (blue) against metabolomic profiling of psoriatic vs normal skin (red). Smaller circles represent decreased expression, smaller hexagons represents decreased levels of compound in psoriatic skin.

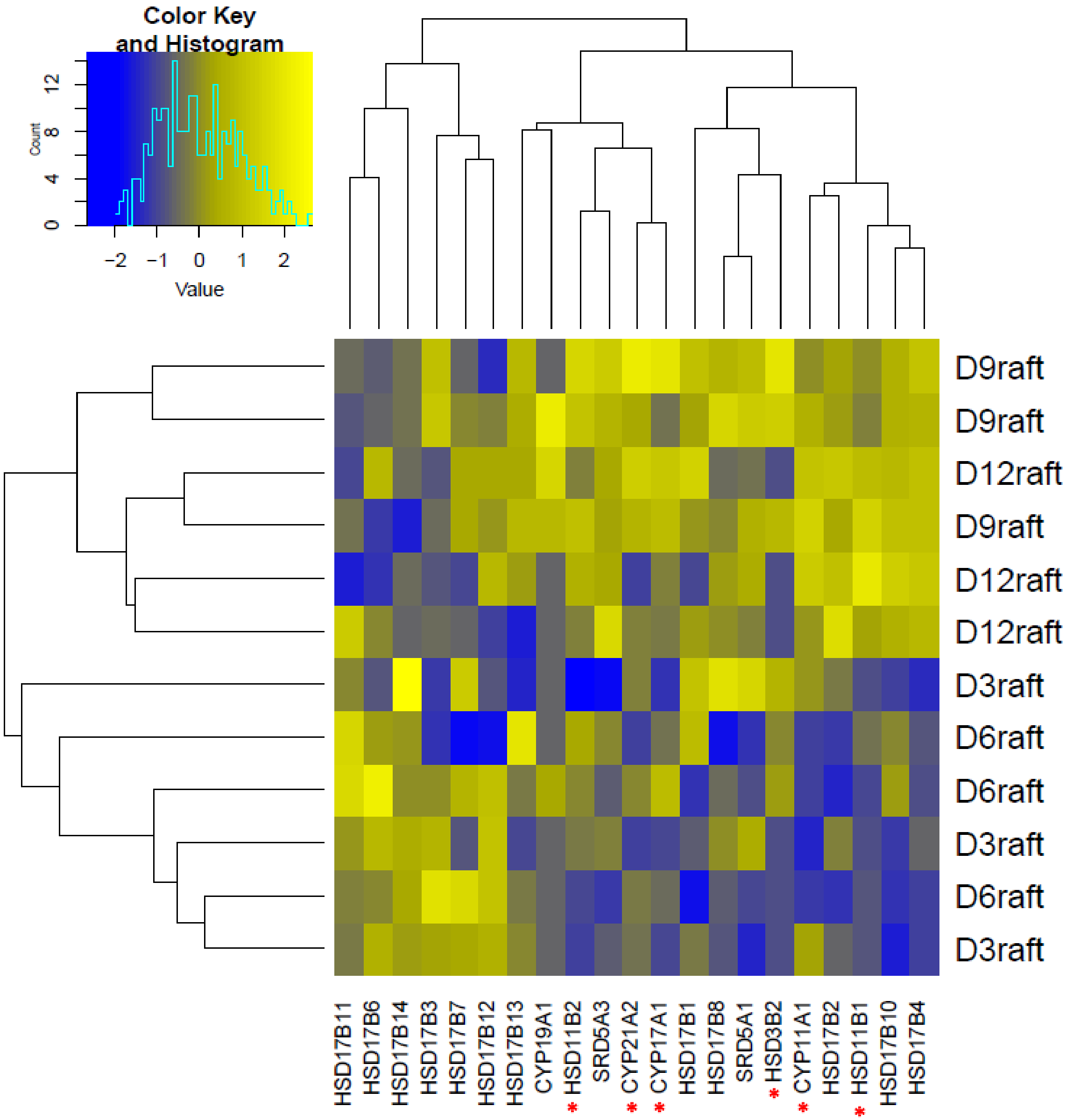


Supplementary Figure 3: Steroid biosynthetic pathway. Cross-analysis of mRNA expression by RNA-seq in psoriasis vs normal skin (blue) against metabolomic profiling of psoriatic vs normal skin (red). Smaller circles represent decreased expression, smaller hexagons represents decreased levels of compound in psoriatic skin.

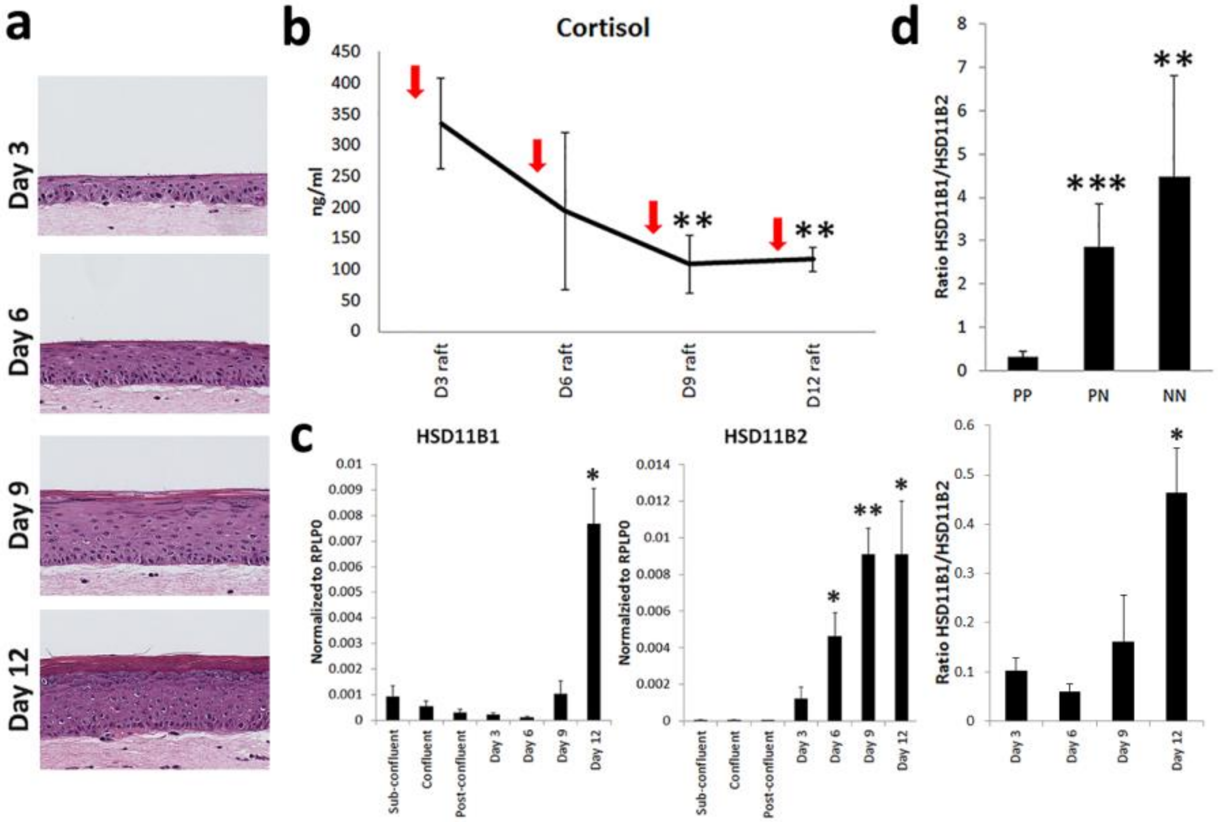


Supplementary Figure 4: HPA axis in psoriasis. We were unable to detect differences in the protein (A) or mRNA expression of the HPA axis members CRH, CRHR1 and POMC in psoriatic skin. Data are shown with SEM, n=4 for each experiment. For IHC representative figures are shown (n=3).

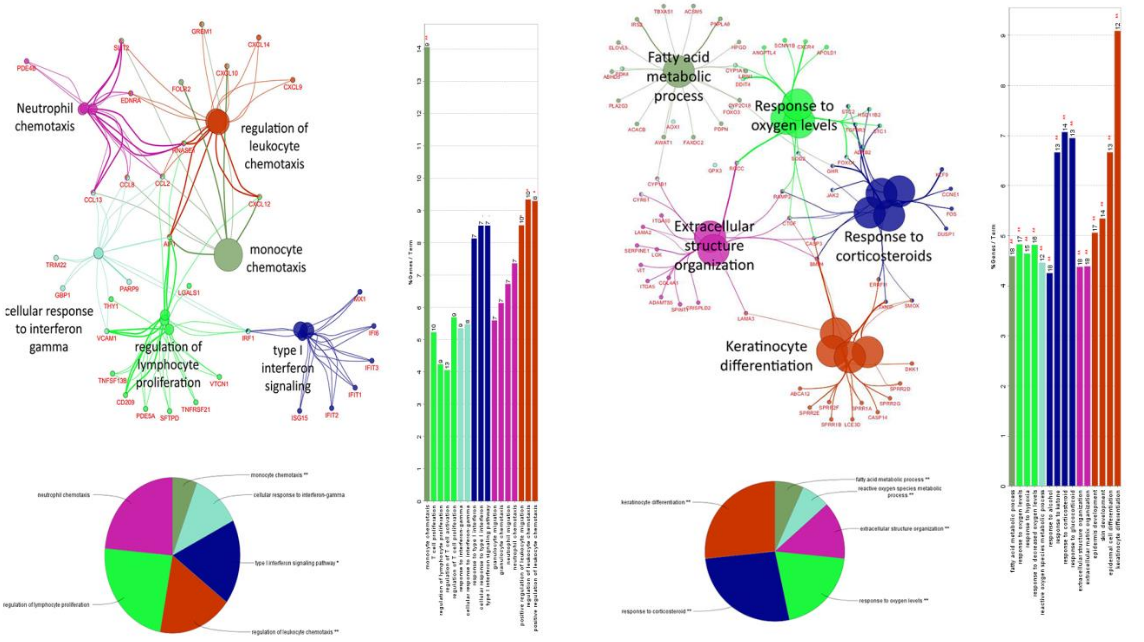
Supplementary Figure 5 – related to Figure 3. **HSD11B1 expression across skin disease datasets.** Geo accession numbers (http://www.ncbi.nlm.nih.gov/gds) are listed in parentheses.



Supplementary Figure 6. **Expression of steroid biosynthesis genes in 3D skin cultures** is dependent upon the differentiation stage of the epidermal rafts. Using hierarchical clustering the rafts grouped according to differentiation stage. The majority of critical enzymes in glucocorticoid biosynthesis (red asterix) are more highly expressed in in differentiated (Day9-Day12 rafts) compared to less differentiated rafts (Day 3-Day6).



Supplementary Figure 7. **Steroid biosynthesis and utilization is dependent upon differentiation state of the epidermis**. (**a**) In the 3-D human epidermal tissue culture model the keratinocyte monolayer is rebuilt into a fully stratified epidermis in 12 days. (**b**) Cortisol levels in culture supernatants progressively decrease with progression of epidermal development. (Note that these cultures are supplemented with 1000nM of hydrocortisone; red arrows indicate time of supplementation). (**c**) Differentiation was closely associated with increased gene expression of HSD11B1 and HSD11B2. (**d**) As HSD11B1 regulates synthesis of cortisol and HSD11B2 facilitates conversion of biologically active cortisol to inactive cortisone we determined the ratio between HSD11B1 and HSD11B2 in both psoriatic (PP), uninvolved (PN) and normal skin (NN)(D) and at different stages of epidermal development, with the ratio in fully developed rafts trending toward a pattern seen in normal skin. (Data are shown with SEM, n=3 for each experiment, *$p<0.05$, **$p<0.01$).



Supplementary Figure 8. **Genes suppressed (left) and induced (right) with topical application of steroids in normal skin.** The analysis was performed using Cytoscape and ClueGo on 328 genes suppressed and 427 genes induced in normal skin following topical application of glucocorticoid for 24 hours ($p<0.05$). The figures shows enriched biologic categories along with associated genes amongst glucocorticoid suppressed (left) and induced (right) genes.

Supplementary Data Files.

Supplementary data file 1. Compounds identified in positive mode (positively charged compounds

Supplementary data file 2. Compounds identified in negative mode (negatively charged compounds

Supplementary data file 3. Gene ontology of genes expressed in psoriatic and normal skin against # of TF binding sites.

SUPPLEMENTARY MATERIALS AND METHODS

Patient cohort

Nine patients with moderate chronic plaque psoriasis were enrolled for this study. Patients were off all systemic treatment at least 4 weeks and off all topical treatments 2 weeks prior to enrollment. Two biopsies were taken under local anesthesia from each psoriatic patient and each healthy control, with one biopsy submitted for RNA-sequencing and the other matching biopsy for metabolomic profiling. For the steroid treated cohort (n=3) patients underwent a single six millimeter punch biopsy prior to initiation of treatment and after 7 days of topical steroid use (triamcinolone acetate 0.1%). For healthy subjects, clobetasol propionate was applied topically as a 0.05% cream to the skin of right arm of healthy human volunteers once as described (Baida *et al.*, 2015). Untreated left arm skin was used as control. Biopsies were taken 24h after treatment.

3-D human epidermal tissue cultures

Normal human epidermal keratinocytes were isolated from a pool of neonatal foreskins (n=3) and grown using a J2-3T3 mouse fibroblasts as feeder layer as originally described by Rheinwald and Green (Nature, 1977). 3-D human epidermal raft cultures seeded in collagen hydrogels were prepared using three distinct donor pools as described previously (Arnette Getsios et al. 2016) and grown at air-liquid interface for 12 days in E-Medium (DMEM/DMEM-F12 (1:1), 5% Fetal Bovine Serum, , adenine (180µM), Bovine pancreatic insulin (5µg/ml), Human apo-transferrin (5µg/ml), triiodothyronine (5µg/ml), L-Glutamine (4mM), Cholera toxin (10ng/ml), Gentamicin (10μg/ml), Amphotericin B (0.25μg/ml)) supplemented with various concentrations of hydrocortisone or cortisol as indicated in the text. In some experiments, the cultures were treated with an HSD11B1 inhibitor PF915275 (10μM). For cytokine stimulations the 3-D RHE cultures were established as previously described (Simpson *et al.*, 2010). After 9 days at an air-liquid-interface to allow for epidermal maturation, the RHEs were treated with 0.1% BSA/phosphate-buffered saline (Sigma Aldrich, St Louis, MO) as a vehicle control or 10.0 ng/ml TNF-a, IL-17A, IL-22 (R&D Systems, Minneapolis, MN) alone or as a combination for 72 h, harvested, and analyzed for changes in gene expression as described (Gordon *et al.*, 2013). At harvest, culture medium conditioned for 24hr media was collected and stored at -80 for further analysis. Epidermal tissues were separated from the collagen scaffold and lysed in QIAzol for RNA isolation. For histological analysis, rafts were fixed in 10% neutral buffered formalin for 24hr and embedded in paraffin (Arnette *et al.*, 2016).

Serum analyses and ELISAs

Serum was obtained from 37 patients with moderate-to-severe psoriasis and 43 healthy non-psoriatic controls. These samples were obtained at evaluation of patients recruited into our psoriasis genetic cohort database (Li *et al.*, 2014) and stored at -80°C until analysis. Serum and culture supernatants cortisol levels were measured using a competitive enzyme immunoassay (R&D Systems, cat# KGE008). ELISA kit for CXCL9 and CXCL10 was obtained from R&D Systems (cat# DY392 and DY266).

RNA-seq processing, QRT-PCR, statistical and bioinformatics analyses

Six millimeter punch biopsies from six psoriatic patients (both lesional, and non-lesional skin) and six healthy normal controls were obtained. Skin was anaesthetized with lidocaine with epinephrine (1:10,000). Matching biopsies were taken and snap frozen in liquid nitrogen. Biopsy tissue was stored at -80°C until processing. At processing, tissue was homogenized and RNA isolated with RNeasy Plus Mini kit (Qiagen). RNA was isolated from epidermal rafts in a similar manner as described above. RNA quality was assessed using the Agilent 2100 Bioanalyzer (Agilent) and only samples with RNA-quality above RIN of 7 were subjected to RNA-sequencing. 50 nucleotide single-end read was performed using Illumina Hi-Seq 2000 Genome Analyzer (Illumina). The reads were mapped by Cufflinks (Trapnell *et al.*, 2010) and TopHat (Trapnell *et al.*, 2009) and gene expression levels were expressed as fragments per kilobase of region per million mapped reads (FPKM). Genomic location binding sites for NR3C1 were identified using HOMER (http://homer.salk.edu/homer/). For skin from healthy individuals treated with topical clobetasol RNA was hybridized with the Human Whole-Genome Gene Expression BeadChips HT-12v4.0 (Illumina). Data processing was performed using the Limma package and differentially expressed probes were identified using the linear model implemented in Limma. For QRT-PCR RNA was reverse transcribed using a High Capacity cDNA Transcription kit (Applied Biosystems). qRT-PCR was performed using the 7900HT Fast Real-Time PCR system (Applied Biosystems) with Taqman primers purchased from Applied Biosystems (CXCL1: Hs00236937_m1; CXCL8: Hs00174103; CXCL9: Hs0017065; CXCL10: Hs01124251; RPLP0: Hs99999902; HSD11B1: Hs01547870; HSD11B2: Hs00388669; IVL: Hs00846307_s1; LOR: Hs01894962; FLG: Hs00856927; DEFB4: HS00175474; IL36G: Hs00219742; CRH: Hs01921237_s1; CRHR1: Hs00366363_m1; POMC: Hs01596743_m1.

Immunohistochemistry and immunofluorescence

Immunhistochemistry was performed on 5 µm thick paraffin sections from skin and epidermal rafts using antibodies against CYP21A2 (LifeSpan Biosciences # LS-B9758), HSD3B2 (Fisher Scientific # PIPA527791), HSD11B1 (LifeSpan Biosciences # LS-C172267), NR3C1 (Abnova Corp # MAB0119), Cortisol (Sigma-Aldrich # c8409), CRH (Abcam # ab8901), CRHR1 (ThermoFisher # 720290), POMC (Santa Cruz # Sc-20148), hBD2 (PeproTech Inc # 500-P161G), CXCL9 (Novus Biologicals # NBP1-31155), CXCL10 (PeproTech Inc # 500-P93), FLG (LifeSpan Biosciences # LS-C153448), E-cadherin (HECD1; Gift from M. Takeichi and O. Abe, RIKEN Center for Developmental Biology, Kobe, Japan), DSG1/2 (4B2 supernatant, anti–Dsg1 cytodomain (Dusek *et al.*, 2006); LOR (BioLegend). Secondary antibodies for immunofluorescence were obtained from (Life technologies, Alexa Flour 555 and 488).

Metabolomic profiling

For untargeted metabolomic profiling tissue was homogenized and cell pellet was resuspended in a 1.5ml microcentrifuge tube with 500µl of extraction solvent composed of methanol, chloroform and water at 8:1:1 ratios. Samples were kept on ice and sonicated briefly and then centrifuged for 10 min at 15,000 rpm at 4°C. 250µl of supernatant was transferred to another 1.5ml microcentrifuge tube and dried under nitrogen stream at room temperature. Sample was then reconstituted in 100µl of reconstitution solvent composed of methanol and water at 1:1 ratio. Samples were subsequently vortexed for 5 minutes and then centrifuged for 5 min at 15,000 rpm. Supernatants were then transferred to autosampler vials. Chromatography was performed on 1290 Infinity Binary LC System from Agilent together with Waters Acquity UPLC HSST3 1.8µm 2.1 x 100 mm column in connection with a Water Acquity UPLC HSS T3 1.8µm VanGuard Pre-column. Mass spectrometry was performed using Agilent Technologies 6530 Accurate-Mass Q-Tof with a dual ASJ ESI ion source.

For targeted steroid profiling samples were prepared for analysis by protein precipitation followed by liquid-liquid extraction. Protein was precipitated with 300 µl acetonitrile and methanol (2:1 ratio). The mixture was spiked with internal standard solution and then centrifuged for 10 minutes at 14,000 rpm. The supernatant was transferred to a 2 ml vial for extraction. 1 ml of methyl- t-butyl ether (MTBE) was added to the 2 ml vial and the steroid analytes extracted via vigorous mixing with a vortex mixer. After extraction, 0.5 ml of deionized water which was added to the 2 ml vial and vigorously stirred on a vortex mixer to wash the organic phase and to enhance phase separation. The MTBE organic phase was transferred to a clean 2 ml vial and the MTBE dried down with highly purified $N_{2.}$ The dried extract was reconstituted with 100 µl of 50:50 methanol: deionized water, transferred to an autosampler vial, and analyzed by LC/MS (MRM mode). Samples were analyzed with an Agilent 1290 HPLC and 6490 QqQ LC/MS using ESI with positive/negative polarity switching ionization mode. The steroids were resolved on a Phenomenex Biphenyl 50 x 2.1 mm column. A methanol-Di H_2O gradient was used for elution of the steroids from the reversed phase column. Mobile phase A was Di H_2O with 0.25 µM ammonium fluoride and mobile phase B was methanol with 0.20µM ammonium fluoride.

Statistics

For all experiments described, 2-tailed Student's t tests were performed. Graphs are presented as mean ± SEM. P-values less than 0.05 were considered statistically significant. Raw data processing of metabolomic data was done using Agilent software (MassHunter Qual, and ProFinder). Quality of analysis was performed by visual inspection of the chromatographic traces and relative quantification of internal standards. Analysis reproducibility was also evaluated using comparison of multiple injections of the pooled sample created by combining aliquots of all the samples included in the set and pooled human blood sample plasma samples. Data analysis was performed with Agilent MassProfiler Pro package using recursive analysis workflow. Data were processed using MassHunter Quantitative analysis version B.07.00. Steroids were identified by compound-specific MRM, normalized to a the nearest isotope labeled internal standard, and quantitated using 2 replicated injections of 10 standards to create a linear calibration curve with accuracy better than 80% for each standard.

Study approval

Informed consent was obtained from all patients and controls, under protocols approved by the Institutional Review Board of the University of Michigan Medical School, and Northwestern University Institutional Review Board. This study was conducted according to the Declaration of Helsinki Principles.

Sample ID	Name	GROUP	FILE
S00001201		POOLED PLASMA	Neg_Human Plasma Extraction_0
S00001201		POOLED PLASMA	Neg_Human Plasma Extraction_1
S00001201		POOLED PLASMA	Neg_Human Plasma Extraction_2
S00001201		POOLED PLASMA	Neg_Human Plasma Extraction_3
S00001201		POOLED PLASMA	Neg_Human Plasma Extraction_4
S00001201		POOLED PLASMA	Neg_Human Plasma Extraction_5
S00001201		POOLED PLASMA	Neg_Human Plasma Extraction_6
S00016763		POOLED	Neg Pool QC 1
S00016763		POOLED	Neg Pool QC 2
S00016763		POOLED	Neg Pool QC 3
S00016763		POOLED	Neg Pool QC 4
S00015447	5022PP	Lesional	Neg_S00015447_1
S00015448	5258PP	Lesional	Neg_S00015448_2
S00015449	5311PP	Lesional	Neg_S00015449_3
S00015450	5397PP	Lesional	Neg_S00015450_4
S00015451	TR PP	Lesional	Neg_S00015451_5
S00015452	KB PP	Lesional	Neg_S00015452_6
S00015453	5022PN	Nonlesional	Neg_S00015453_7
S00015454	5258PN	Nonlesional	Neg_S00015454_8
S00015455	5311PN	Nonlesional	Neg_S00015455_9
S00015456	5397PN	Nonlesional	Neg_S00015456_10
S00015457	TR PN	Nonlesional	Neg_S00015457_11
S00015458	KB PN	Nonlesional	Neg_S00015458_12
S00015459	6108 C	Healthy	Neg_S00015459_13
S00015460	5660 C	Healthy	Neg_S00015460_14
S00015461	4480 C	Healthy	Neg_S00015461_15
S00015462	6609 C	Healthy	Neg_S00015462_16
S00015463	6998 C	Healthy	Neg_S00015463_17
S00015464	DM NN	Healthy	Neg_S00015464_18

Compound	Alignment Value	Annotations	CAS Number	ChEBI ID	CompositeSpectrum	Compound Name	KEGG ID	CompoundAlgo	Frequency	Ionization mode	Mass	METLIN ID	PubChem ID	Retention Time
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1-METHYLADENOSINE (CAS# 15763-06-1); (M	1-METHYLADENOSINE (CAS# 15763-06-1); (M	1-METHYLADENOSINE (CAS# 15763-06-1); (M+HCOO)- [,	15763-06-1		(326.1114, 416.82)(327.1111, 88.257996)	1-METHYLADENOSINE (CAS# 15763-06-1); (M+HCOO)-		FindByFormula	5	-	281.1145			3.0081959
1-METHYLURIC ACID (CAS# 708-79-2); (2M-H	1-METHYLURIC ACID (CAS# 708-79-2); (2M-H	1-METHYLURIC ACID (CAS# 708-79-2); (2M-H)- [, tgt=72.	708-79-2		(363.08096, 566.64166)(364.07907, 147.14166)	1-METHYLURIC ACID (CAS# 708-79-2); (2M-H)-		FindByFormula	6	-	182.0436			2.2023296
1-METHYLURIC ACID (CAS# 708-79-2); (M-H)	1-METHYLURIC ACID (CAS# 708-79-2); (M-H)-	1-METHYLURIC ACID (CAS# 708-79-2); (M-H)- [, tgt=85.2	708-79-2		(181.0362, 898.365)(182.03693, 65.585)	1-METHYLURIC ACID (CAS# 708-79-2); (M-H)-		FindByFormula	6	-	182.044			2.2054987
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+HCOO)- [	111-03-5		(401.28973, 507.03998)(402.30188, 192.05)	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+HCOO)-		FindByFormula	2	-	356.2919			22.731297
2',3'-CYCLIC CMP (CAS# 15718-51-1); (M-H)-	2',3'-CYCLIC CMP (CAS# 15718-51-1); (M-H)-	2',3'-CYCLIC CMP (CAS# 15718-51-1); (M-H)- [, tgt=60.90,	15718-51-1		(304.03558, 952.23)(305.03165, 217.71834)	2',3'-CYCLIC CMP (CAS# 15718-51-1); (M-H)-		FindByFormula	6	-	305.0408			0.7186671
2,3-DIHYDROXY-2-PHOSPHONOPROPANOIC A	2,3-DIHYDROXY-2-PHOSPHONOPROPANOIC A	2,3-DIHYDROXY-2-PHOSPHONOPROPANOIC ACID (CAS# 2	2553-59-5		(184.9871, 609.04)(185.9833, 22.87)	2,3-DIHYDROXY-2-PHOSPHONOPROPANOIC ACID (CAS# 2553-59-5); (M-H)-		FindByFormula	1	-	185.9941			0.869
2,3-DIHYDROXYBENZOATE (CAS# 303-38-8); (	2,3-DIHYDROXYBENZOATE (CAS# 303-38-8); (	2,3-DIHYDROXYBENZOATE (CAS# 303-38-8); (M-H)- [, tgt	303-38-8		(153.01894, 2774.7803)(154.01941, 144.43364)(155.02534,	2,3-DIHYDROXYBENZOATE (CAS# 303-38-8); (M-H)-	C00196	FindByFormula	11	-	154.0266			4.873888
2',4'-DIHYDROXYACETOPHENONE (CAS# 89-8	2',4'-DIHYDROXYACETOPHENONE (CAS# 89-8	2',4'-DIHYDROXYACETOPHENONE (CAS# 89-84-9); (M-H)-	89-84-9		(151.03966, 1281.4633)(152.04222, 106.44999)	2',4'-DIHYDROXYACETOPHENONE (CAS# 89-84-9); (M-H)-	C03663	FindByFormula	6	-	152.0469			7.436485
2,5-DIOXOPIPERAZINE (CAS# 106-57-0); (M-H	2,5-DIOXOPIPERAZINE (CAS# 106-57-0); (M-H	2,5-DIOXOPIPERAZINE (CAS# 106-57-0); (M-H)- [, tgt=83.	106-57-0		(113.0351, 8448.36)(114.0463, 654.15)	2,5-DIOXOPIPERAZINE (CAS# 106-57-0); (M-H)-	C02777	FindByFormula	1	-	114.043			0.72399896
20:0 LYSO PC (CAS# 108341-80-6); (M+Cl)-	20:0 LYSO PC (CAS# 108341-80-6); (M+Cl)-	20:0 LYSO PC (CAS# 108341-80-6); (M+Cl)- [, tgt=20.97, o	108341-80-6		(586.36273, 300.37668)(587.36304, 167.51)	20:0 LYSO PC (CAS# 108341-80-6); (M+Cl)-		FindByFormula	3	-	551.3929			22.717962
24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M	24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M	24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M+HCOO)- [,	60037-60-7		(859.69226, 653.77374)(860.6939, 227.12668)(861.69366, 8	24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M+HCOO)-		FindByFormula	21	-	814.6953			27.899458
265.2973@22.820448					(310.29462, 471.65967)(264.2898, 28153.832)(265.29303, 4	265.2973@22.820448		FindByFormula	28	-	265.2973			22.820448
2-AMINOETHYL DIHYDROGEN PHOSPHATE (C	2-AMINOETHYL DIHYDROGEN PHOSPHATE (C	2-AMINOETHYL DIHYDROGEN PHOSPHATE (CAS# 1071-2	1071-23-4		(140.01192, 2453.664)(141.01253, 71.442635)(142.01299, 1	2-AMINOETHYL DIHYDROGEN PHOSPHATE (CAS# 1071-23-4); (M-H)-		FindByFormula	19	-	141.0195			0.78752667
2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+C	2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Cl	2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Cl)- [, tgt=49.	154-17-6		(199.03676, 21567.576)(200.04205, 1505.14)(201.03456, 83	2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Cl)-	C00586	FindByFormula	12	-	164.0673			0.7944166
2'-DEOXYINOSINE (CAS# 890-38-0); (M-H)-	2'-DEOXYINOSINE (CAS# 890-38-0); (M-H)-	2'-DEOXYINOSINE (CAS# 890-38-0); (M-H)- [, tgt=70.94, c	890-38-0		(251.0805, 1160.5911)(252.07721, 145.71555)(253.0719, 30.	2'-DEOXYINOSINE (CAS# 890-38-0); (M-H)-		FindByFormula	9	-	252.0869			2.0829997
2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 4	2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 4	2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 4026-18-0); (	4026-18-0		(117.055565, 15349.582)(118.05573, 885.34436)(119.05514,	2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 4026-18-0); (M-H)-		FindByFormula	25	-	118.0627			3.4881525
2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (	2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (	2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91	583-91-5		(149.0265, 815.095)(150.021, 31.765)(151.0282, 37.335)	2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-5); (M-H)-		FindByFormula	2	-	150.0337			3.3519962
2-HYDROXYBUTYRATE (CAS#); (M-H)-	2-HYDROXYBUTYRATE (CAS#); (M-H)-	2-HYDROXYBUTYRATE (CAS#); (M-H)- [, tgt=86.41, overall=86.41]			(103.04042, 969.2825)(104.04213, 32.147503)	2-HYDROXYBUTYRATE (CAS#); (M-H)-		FindByFormula	4	-	104.0478			1.7777481
2-METHYLGLUTARIC ACID (CAS# 18069-17-5)	2-METHYLGLUTARIC ACID (CAS# 18069-17-5);	2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M-H)- [, t	18069-17-5		(145.05101, 4373.947)(146.04979, 233.2075)(147.05185, 61.	2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M-H)-		FindByFormula	24	-	146.0582			3.5413687
2-METHYLMALEATE (CAS# 498-23-7); (M-H)-	2-METHYLMALEATE (CAS# 498-23-7); (M-H)-	2-METHYLMALEATE (CAS# 498-23-7); (M-H)- [, tgt=56.32	498-23-7		(129.01971, 931.8344)(130.02019, 48.15333)	2-METHYLMALEATE (CAS# 498-23-7); (M-H)-	C02226	FindByFormula	9	-	130.0273			1.939443
2-OXOADIPATE (CAS# 3184-35-8); (M-H)-	2-OXOADIPATE (CAS# 3184-35-8); (M-H)-	2-OXOADIPATE (CAS# 3184-35-8); (M-H)- [, tgt=42.49, ov	3184-35-8		(159.0287, 651.09)(160.0209, 24.07)	2-OXOADIPATE (CAS# 3184-35-8); (M-H)-	C00322	FindByFormula	1	-	160.0356			1.6060001
3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-	3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-9	3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M-H)	6482-98-0		(181.05063, 3403.1184)(182.05168, 370.546)(183.05458, 13	3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M-H)-	C03672	FindByFormula	25	-	182.0576			3.7870307
3,3'-DITHIODIVALINE (PENICILLAMINE SS DIM	3,3'-DITHIODIVALINE (PENICILLAMINE SS DIM	3,3'-DITHIODIVALINE (PENICILLAMINE SS DIMER) (CAS# 2	20902-45-8		(295.0839, 816.26)(296.0822, 51.8)(297.0694, 329.67)	3,3'-DITHIODIVALINE (PENICILLAMINE SS DIMER) (CAS# 20902-45-8); (M-H)-		FindByFormula	1	-	296.0877			1.2929988
3,4-DIHYDROXYBENZOATE (CAS# 99-50-3); (	3,4-DIHYDROXYBENZOATE (CAS# 99-50-3); (	3,4-DIHYDROXYBENZOATE (CAS# 99-50-3); (M-H)- [, tgt=	99-50-3		(153.01894, 2774.7803)(154.01941, 144.43364)(155.02534,	3,4-DIHYDROXYBENZOATE (CAS# 99-50-3); (M-H)-	C00230	FindByFormula	11	-	154.0266			4.873888
3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-	3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-	3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-92-7); (M-H	59-92-7		(196.06454, 3219.415)(197.05795, 418.04498)(198.06549, 1	3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-92-7); (M-H)-		FindByFormula	2	-	197.0704			0.6704993
3,4-DIHYDROXYPHENYLACETATE (CAS# 102-3	3,4-DIHYDROXYPHENYLACETATE (CAS# 102-3	3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+Cl	102-32-9		(203.0107, 635.94)(204.0193, 164.26)(205.0077, 117.99)	3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+Cl)-		FindByFormula	1	-	168.0422			3.5270038
3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CA	3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CA	3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CAS# 28822-7	28822-73-3		(151.03946, 1107.4299)(152.03915, 339.225)	3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CAS# 28822-73-3); (M-H)-[-H2O]		FindByFormula	2	-	170.0564			1.2264997
3',5'-CYCLIC AMP (CAS# 60-92-4); (M-H)-	3',5'-CYCLIC AMP (CAS# 60-92-4); (M-H)-	3',5'-CYCLIC AMP (CAS# 60-92-4); (M-H)- [, tgt=68.07, ov	60-92-4		(328.04614, 653.7425)(329.04718, 114.2975)	3',5'-CYCLIC AMP (CAS# 60-92-4); (M-H)-		FindByFormula	4	-	329.0539			2.0245006
3,5-DIBROMO-4-HYDROXYBENZONITRILE (CA	3,5-DIBROMO-4-HYDROXYBENZONITRILE (CA	3,5-DIBROMO-4-HYDROXYBENZONITRILE (CAS# 1689-84-	1689-84-5		(275.8523, 330.95)(276.8485, 22.58)(277.8466, 200.25)	3,5-DIBROMO-4-HYDROXYBENZONITRILE (CAS# 1689-84-5); (M-H)-	C04178	FindByFormula	1	-	274.86			12.529693
317.9225@19.306116					(317.7696, 23273.66)(318.7719, 1697.1886)(319.761, 25929.	317.9225@19.306116		FindByFormula	7	-	317.9225			19.306116
370.1825@23.004324					(369.1747, 5548.4165)(370.1787, 2499.1833)(371.18054, 90	370.1825@23.004324		FindByFormula	24	-	370.1825			23.004324
3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE	3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (	3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (CAS# 516-5	516-55-2		(335.21783, 213.52998)(336.21924, 54.918)(337.20813, 361.	3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (CAS# 516-55-2); (M+Cl)-[-H2O]		FindByFormula	5	-	318.2539			21.089184
3BETA-HYDROXYANDROST-5-EN-17-ONE 3-SU	3BETA-HYDROXYANDROST-5-EN-17-ONE 3-SU	3BETA-HYDROXYANDROST-5-EN-17-ONE 3-SULFATE (CAS#); (M-H)- [, tgt=52.97, ov			(367.16003, 13494.344)(368.16025, 2919.8694)(369.1611, 2	3BETA-HYDROXYANDROST-5-EN-17-ONE 3-SULFATE (CAS#); (M-H)-		FindByFormula	25	-	368.1669			15.516088
3'-CMP (CAS# 63-37-6); (M-H)-	3'-CMP (CAS# 63-37-6); (M-H)-	3'-CMP (CAS# 63-37-6); (M-H)- [, tgt=60.31, overall=60.3	63-37-6		(322.04602, 1797.3595)(323.0427, 340.69467)(324.03906, 1	3'-CMP (CAS# 63-37-6); (M-H)-	C00055	FindByFormula	17	-	323.0518			0.88070637
3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M	3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M	3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M-H)- [, tgt=	2922-42-1		(171.03038, 929.746)(172.02866, 198.526)	3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M-H)-	C02637	FindByFormula	5	-	172.036			0.9125991
3-HYDROXY-3-METHYLGLUTARATE (CAS# 503	3-HYDROXY-3-METHYLGLUTARATE (CAS# 503	3-HYDROXY-3-METHYLGLUTARATE (CAS# 503-49-1); (M-	503-49-1		(161.04483, 2770.5378)(162.04314, 78.70588)(163.04274, 8	3-HYDROXY-3-METHYLGLUTARATE (CAS# 503-49-1); (M-H)-	C03761	FindByFormula	17	-	162.0517			1.6098232
3-HYDROXYBENZALDEHYDE (CAS# 100-83-4);	3-HYDROXYBENZALDEHYDE (CAS# 100-83-4);	3-HYDROXYBENZALDEHYDE (CAS# 100-83-4); (M-H)- [, t	100-83-4		(121.02974, 57991.727)(122.029236, 8441.99)(123.030235,	3-HYDROXYBENZALDEHYDE (CAS# 100-83-4); (M-H)-	C03067	FindByFormula	20	-	122.0365			4.928725
3-HYDROXYKYNURENINE (CAS# 2147-61-7); (	3-HYDROXYKYNURENINE (CAS# 2147-61-7); (	3-HYDROXYKYNURENINE (CAS# 2147-61-7); (M-H)- [, tgt	2147-61-7		(223.07314, 887.84595)(224.07228, 131.28801)(225.0666, 7	3-HYDROXYKYNURENINE (CAS# 2147-61-7); (M-H)-		FindByFormula	15	-	224.0807			1.0785338
3-HYDROXYPHENYLACETATE (CAS# 621-37-4)	3-HYDROXYPHENYLACETATE (CAS# 621-37-4);	3-HYDROXYPHENYLACETATE (CAS# 621-37-4); (M-H)- [, t	621-37-4		(151.03966, 1271.6483)(152.04222, 105.28666)	3-HYDROXYPHENYLACETATE (CAS# 621-37-4); (M-H)-	C05593	FindByFormula	6	-	152.0469			7.436485
3-METHOXY-4-HYDROXYMANDELATE (CAS# 5	3-METHOXY-4-HYDROXYMANDELATE (CAS# 5	3-METHOXY-4-HYDROXYMANDELATE (CAS# 55-10-7); (M	55-10-7		(197.0439, 869.81)(198.0367, 24.88)	3-METHOXY-4-HYDROXYMANDELATE (CAS# 55-10-7); (M-H)-		FindByFormula	1	-	198.0509			1.6900008
3-METHOXYTYROSINE (CAS# 4214-13-5); (M-	3-METHOXYTYROSINE (CAS# 4214-13-5); (M-	3-METHOXYTYROSINE (CAS# 4214-13-5); (M-H)- [, tgt=6	4214-13-5		(210.0762, 226.72)(211.0726, 43.75)	3-METHOXYTYROSINE (CAS# 4214-13-5); (M-H)-		FindByFormula	1	-	211.0824			1.934
3-METHYGLUTARIC ACID (CAS# 626-51-7); (	3-METHYGLUTARIC ACID (CAS# 626-51-7); (	3-METHYGLUTARIC ACID (CAS# 626-51-7); (M-H)- [, tgt=	626-51-7		(145.05101, 4430.9727)(146.04973, 232.79387)(147.05116,	3-METHYGLUTARIC ACID (CAS# 626-51-7); (M-H)-		FindByFormula	26	-	146.0582			3.5393395
3-METHYLADIPIC ACID (CAS# 3058-01-3); (M	3-METHYLADIPIC ACID (CAS# 3058-01-3); (M	3-METHYLADIPIC ACID (CAS# 3058-01-3); (M-H)- [, tgt=8	1/3/3058		(159.06609, 1147.4896)(160.06697, 103.704994)(161.066, 4	3-METHYLADIPIC ACID (CAS# 3058-01-3); (M-H)-		FindByFormula	24	-	160.073			5.661709
3-NITRO-L-TYROSINE (CAS# 621-44-3); (M-H)	3-NITRO-L-TYROSINE (CAS# 621-44-3); (M-H)	3-NITRO-L-TYROSINE (CAS# 621-44-3); (M-H)- [, tgt=34.4	621-44-3		(225.0524, 615.795)(226.05261, 96.590004)	3-NITRO-L-TYROSINE (CAS# 621-44-3); (M-H)-		FindByFormula	2	-	226.0611			2.4955008
3-OXALOMALATE (CAS# 89304-26-7); (M-H)-	3-OXALOMALATE (CAS# 89304-26-7); (M-H)-[	3-OXALOMALATE (CAS# 89304-26-7); (M-H)-[-H2O] [, tgt	89304-26-7		(186.9932, 1175.04)(187.9919, 5452.49)	3-OXALOMALATE (CAS# 89304-26-7); (M-H)-[-H2O]	C01990	FindByFormula	1	-	206.0072			0.9569996
3-PHOSPHOGLYCERATE (CAS#); (M-H)-	3-PHOSPHOGLYCERATE (CAS#); (M-H)-	3-PHOSPHOGLYCERATE (CAS#); (M-H)- [, tgt=54.32, overall=54.32]			(184.9871, 609.04)(185.9833, 22.87)	3-PHOSPHOGLYCERATE (CAS#); (M-H)-		FindByFormula	1	-	185.9941			0.869
3-SULFINO-L-ALANINE (CAS# 1115-65-7); (M-	3-SULFINO-L-ALANINE (CAS# 1115-65-7); (M-	3-SULFINO-L-ALANINE (CAS# 1115-65-7); (M-H)- [, tgt=6	1115-65-7		(152.00153, 1897.02)(153.00275, 155.9175)(153.9987, 72.74	3-SULFINO-L-ALANINE (CAS# 1115-65-7); (M-H)-	C00606	FindByFormula	4	-	153.0086			0.68725026
3-UREIDOPROPIONIC ACID (CAS# 462-88-4);	3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (	3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (M-H)- [, tgt	462-88-4		(131.04565, 3545.7002)(132.03854, 66.13)(133.0431, 49.78)	3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (M-H)-	C02642	FindByFormula	2	-	132.0527			0.6375007
410.2124@23.249462					(409.2057, 1135.37)(410.2072, 595.36)	410.2124@23.249462		FindByFormula	1	-	410.2124			23.249462
427.8849@19.306257					(463.1402, 14131.067)(464.14633, 1552.2157)(465.13702, 3	427.8849@19.306257		FindByFormula	7	-	427.8849			19.306257
468.2923@24.718874					(467.28485, 2531.363)(468.28848, 1407.986)(469.2871, 662.	468.2923@24.718874		FindByFormula	19	-	468.2923			24.718874
486.3341@22.79494					(485.32733, 2474.4187)(486.32797, 814.9624)(487.3403, 29	486.3341@22.79494		FindByFormula	8	-	486.3341			22.79494
498.3864@23.170763					(498.3749, 1621.2367)(499.3693, 400.05002)(499.37827, 16	498.3864@23.170763		FindByFormula	6	-	498.3864			23.170763
4-ACETAMIDOBUTANOATE (CAS# 3025-96-5)	4-ACETAMIDOBUTANOATE (CAS# 3025-96-5);	4-ACETAMIDOBUTANOATE (CAS# 3025-96-5); (M-H)- [, t	3025-96-5		(144.0663, 520.48)(145.0612, 61.02)	4-ACETAMIDOBUTANOATE (CAS# 3025-96-5); (M-H)-	C02946	FindByFormula	1	-	145.0727			1.9370009
4-ACETAMINOPHEN SULFATE (CAS# 32113-41	4-ACETAMINOPHEN SULFATE (CAS# 32113-41	4-ACETAMINOPHEN SULFATE (CAS# 32113-41-0); (M-H)-	32113-41-0		(230.0127, 10573.382)(231.01566, 1046.824)(232.01312, 53	4-ACETAMINOPHEN SULFATE (CAS# 32113-41-0); (M-H)-		FindByFormula	17	-	231.0202			2.4080563
4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-	4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-	4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-KRYNURENI	492-27-3		(188.0362, 362.12)(189.0362, 80.83)	4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-KRYNURENIC ACID (CAS# 492-27-3); (M-H)-		FindByFormula	1	-	189.0429			4.9339843
4-HYDROXYBENZALDEHYDE (CAS# 123-08-0);	4-HYDROXYBENZALDEHYDE (CAS# 123-08-0);	4-HYDROXYBENZALDEHYDE (CAS# 123-08-0); (M-H)- [, t	123-08-0		(121.02974, 57638.98)(122.029236, 8419.261)(123.030235,	4-HYDROXYBENZALDEHYDE (CAS# 123-08-0); (M-H)-	C00633	FindByFormula	20	-	122.0365			4.928725
4-HYDROXYBENZOATE (CAS# 99-96-7); (M-H)	4-HYDROXYBENZOATE (CAS# 99-96-7); (M-H)	4-HYDROXYBENZOATE (CAS# 99-96-7); (M-H)- [, tgt=98.6	99-96-7		(137.02472, 41715.992)(138.02614, 3335.7053)(139.0281, 5	4-HYDROXYBENZOATE (CAS# 99-96-7); (M-H)-	C00156	FindByFormula	27	-	138.0319			4.05162
4-HYDROXYPHENYLACETATE (CAS# 156-38-7)	4-HYDROXYPHENYLACETATE (CAS# 156-38-7);	4-HYDROXYPHENYLACETATE (CAS# 156-38-7); (M-H)- [, t	156-38-7		(151.0402, 588.77)(152.0353, 29.77)	4-HYDROXYPHENYLACETATE (CAS# 156-38-7); (M-H)-		FindByFormula	1	-	152.0471			4.672963
4-METHYL-2-OXOPENTANOATE (CAS# 816-66	4-METHYL-2-OXOPENTANOATE (CAS# 816-66	4-METHYL-2-OXOPENTANOATE (CAS# 816-66-0); (M-H)-	816-66-0		(129.05585, 25087.197)(130.05823, 1698.5269)(131.06168,	4-METHYL-2-OXOPENTANOATE (CAS# 816-66-0); (M-H)-		FindByFormula	26	-	130.0632			4.8252854
4-METHYL-2-OXOVALERIC ACID (CAS# 816-66	4-METHYL-2-OXOVALERIC ACID (CAS# 816-66	4-METHYL-2-OXOVALERIC ACID (CAS# 816-66-0); (M-H)-	816-66-0		(129.05583, 24211.332)(130.05823, 1632.7843)(131.06212,	4-METHYL-2-OXOVALERIC ACID (CAS# 816-66-0); (M-H)-		FindByFormula	26	-	130.0632			4.8157086
4-NITROBENZOIC ACID (CAS# 62-23-7); (M-H	4-NITROBENZOIC ACID (CAS# 62-23-7); (M-H)	4-NITROBENZOIC ACID (CAS# 62-23-7); (M-H)- [, tgt=85.	62-23-7		(166.01463, 9353.692)(167.01787, 864.71954)(168.02054, 7	4-NITROBENZOIC ACID (CAS# 62-23-7); (M-H)-		FindByFormula	20	-	167.0219			8.4284725
4-NITROPHENOL (CAS# 100-02-7); (M-H)-	4-NITROPHENOL (CAS# 100-02-7); (M-H)-	4-NITROPHENOL (CAS# 100-02-7); (M-H)- [, tgt=94.57, ov	100-02-7		(138.01974, 3359.3208)(139.0207, 235.77356)(140.02335, 3	4-NITROPHENOL (CAS# 100-02-7); (M-H)-	C00870	FindByFormula	28	-	139.0269			6.9920697
4-PYRIDOXATE (CAS# 82-82-6); (M-H)-	4-PYRIDOXATE (CAS# 82-82-6); (M-H)-	4-PYRIDOXATE (CAS# 82-82-6); (M-H)- [, tgt=70.61, over	82-82-6		(182.04588, 7058.763)(183.04408, 1112.4899)(184.04964, 1	4-PYRIDOXATE (CAS# 82-82-6); (M-H)-	C00847	FindByFormula	12	-	183.0523			1.864665
518.3953@22.578754					(517.3933, 336.81497)(518.39197, 117.02251)(519.3982, 84.	518.3953@22.578754		FindByFormula	4	-	518.3953			22.578754
518.3984@22.878284					(517.3912, 5696.015)(518.39685, 2081.7788)(519.40186, 38	518.3984@22.878284		FindByFormula	8	-	518.3984			22.878284
520.4115@23.179062					(519.4044, 2844.58)(520.40857, 1023.6)(521.41907, 2325.41	520.4115@23.179062		FindByFormula	2	-	520.4115			23.179062
520.4118@22.931578					(519.4051, 5838.74)(520.4056, 2029.7484)(521.4179, 3326.4	520.4118@22.931578		FindByFormula	6	-	520.4118			22.931578
520.4139@22.747055					(519.4045, 302.645)(520.41064, 106.495)(521.4081, 63.44)	520.4139@22.747055		FindByFormula	2	-	520.4139			22.747055
539.3401@22.711172					(538.3431, 74.41)(539.3295, 46.47)	539.3401@22.711172		FindByFormula	1	-	539.3401			22.711172
539.3414@22.447004					(538.3338, 3266.0627)(539.34906, 2040.0907)(540.3426, 12	539.3414@22.447004		FindByFormula	19	-	539.3414			22.447004
546.4274@22.924608					(545.4191, 1759.2583)(546.42, 627.63336)(547.43, 1192.868	546.4274@22.924608		FindByFormula	6	-	546.4274			22.924608
548.4426@23.1736					(547.4358, 2200.065)(548.4386, 856.5384)(549.4497, 1599.9	548.4426@23.1736		FindByFormula	6	-	548.4426			23.1736
548.4469@22.920895					(547.4484, 406.46002)(548.4431, 112.26)(549.4423, 211.355	548.4469@22.920895		FindByFormula	2	-	548.4469			22.920895
564.4392@22.893457					(565.44824, 209.22667)(566.44147, 82.85333)(567.4561, 14	564.4392@22.893457		FindByFormula	3	-	564.4392			22.893457
592.4735@23.019382					(593.4789, 489.575)(594.4796, 194.21251)	592.4735@23.019382		FindByFormula	4	-	592.4735			23.019382
592.4751@23.119793					(593.4792, 4460.996)(594.48096, 1818.0267)	592.4751@23.119793		FindByFormula	21	-	592.4751			23.119793
5ALPHA-ANDROSTANE-3ALPHA,17BETA-DIOL	5ALPHA-ANDROSTANE-3ALPHA,17BETA-DIOL	5ALPHA-ANDROSTANE-3ALPHA,17BETA-DIOL (CAS# 1852-	1852-53-5		(309.1938, 443.7)(310.19955, 107.86)(311.19873, 964.025)(	5ALPHA-ANDROSTANE-3ALPHA,17BETA-DIOL (CAS# 1852-53-5); (M+Cl)-[-H2O]		FindByFormula	2	-	292.2429			19.037003
5-AMINOPENTANOATE (CAS# 660-88-8); (M-	5-AMINOPENTANOATE (CAS# 660-88-8); (M-	5-AMINOPENTANOATE (CAS# 660-88-8); (M-H)- [, tgt=58	660-88-8		(116.07103, 1711.5287)(117.0716, 90.44429)	5-AMINOPENTANOATE (CAS# 660-88-8); (M-H)-	C00431	FindByFormula	21	-	117.0783			0.8793337
5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+	5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+	5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+HCOO)- [, t	4754-39-6		(296.09955, 1334.1654)(297.09857, 222.20001)(298.09738,	5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+HCOO)-	C05198	FindByFormula	13	-	251.1017			2.595999
5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3)	5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3);	5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M-H)- [, t	92340-57-3		(360.10278, 3823.9685)(361.10596, 894.7134)(362.10287, 3	5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M-H)-		FindByFormula	6	-	361.1099			12.295391
5-HYDROXYINDOLEACETATE (CAS# 54-16-0);	5-HYDROXYINDOLEACETATE (CAS# 54-16-0);	5-HYDROXYINDOLEACETATE (CAS# 54-16-0); (M-H)- [, tg	54-16-0		(190.0538, 1123.8049)(191.05246, 116.29)(192.0438, 139.66	5-HYDROXYINDOLEACETATE (CAS# 54-16-0); (M-H)-		FindByFormula	2	-	191.0601			4.047504
5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8);	5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (	5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (M-H)- [, tgt	9/8/4350		(219.07697, 871.6048)(220.0768, 148.71048)(221.0678, 312.	5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (M-H)-		FindByFormula	21	-	220.0842			1.7712854
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9)	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+Cl)- [,	2457-80-9		(332.06067, 438.1291)(333.05927, 125.38453)(334.0554, 18	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+Cl)-	C00170	FindByFormula	11	-	297.091			4.4177136
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9)	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+HCOO	2457-80-9		(342.0888, 555.5923)(343.08908, 120.165306)(344.08398, 6	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+HCOO)-	C00170	FindByFormula	17	-	297.0915			4.446628
5-OXOPROLINE (CAS# 4042-36-8); (M-H)-	5-OXOPROLINE (CAS# 4042-36-8); (M-H)-	5-OXOPROLINE (CAS# 4042-36-8); (M-H)- [, tgt=98.89, ov	4042-36-8		(128.03558, 601968.75)(129.03793, 36607.785)(130.04053,	5-OXOPROLINE (CAS# 4042-36-8); (M-H)-	C02237	FindByFormula	22	-	129.0429			1.1928643
5-VALEROLACTONE (CAS# 542-28-9); (M+HC	5-VALEROLACTONE (CAS# 542-28-9); (M+HC	5-VALEROLACTONE (CAS# 542-28-9); (M+HCOO)- [, tgt=5	542-28-9		(145.0505, 30574.45)(146.05365, 2306.65)	5-VALEROLACTONE (CAS# 542-28-9); (M+HCOO)-	C02240	FindByFormula	2	-	100.0522			2.0715003
663.4302@22.925947					(662.42334, 2342.7751)(663.4248, 1600.9742)(664.4334, 12	663.4302@22.925947		FindByFormula	19	-	663.4302			22.925947
6-CARBOXYHEXANOATE (CAS# 111-16-0); (M	6-CARBOXYHEXANOATE (CAS# 111-16-0); (M	6-CARBOXYHEXANOATE (CAS# 111-16-0); (M-H)- [, tgt=8	111-16-0		(159.06609, 1147.4896)(160.06697, 103.704994)(161.066, 4	6-CARBOXYHEXANOATE (CAS# 111-16-0); (M-H)-	C02656	FindByFormula	24	-	160.073			5.661709
706.3872@22.69812					(705.3798, 1684.9268)(706.38934, 1205.7026)(707.398, 762.	706.3872@22.69812		FindByFormula	19	-	706.3872			22.69812
743.8369@21.5465					(746.8291, 372.43)(747.8249, 298.78)(748.8148, 327.88)	743.8369@21.5465		FindByFormula	1	-	743.8369			21.5465
743.84@22.061306					(746.8285, 320.14502)(747.82996, 242.13)(748.8187, 254.12	743.84@22.061306		FindByFormula	2	-	743.84			22.061306
743.8414@21.734903					(742.83417, 1703.1487)(743.83264, 586.50714)(744.83075,	743.8414@21.734903		FindByFormula	7	-	743.8414			21.734903
745.5704@23.833296					(744.5633, 2002.5325)(745.56116, 1512.2988)(746.559, 564.	745.5704@23.833296		FindByFormula	8	-	745.5704			23.833296
751.5512@25.219986					(750.5447, 6386.377)(751.547, 3110.5093)(752.5491, 981.07	751.5512@25.219986		FindByFormula	27	-	751.5512			25.219986
752.1517@22.943537					(751.14417, 8557.565)(752.1474, 2552.7952)(753.1494, 891.	752.1517@22.943537		FindByFormula	28	-	752.1517			22.943537
752.4377@23.038685					(751.4329, 1681.6711)(752.4376, 654.8438)(753.4346, 955.0	752.4377@23.038685		FindByFormula	8	-	752.4377			23.038685
752.445@22.738989					(751.4484, 261.73)(752.4302, 198.78)	752.445@22.738989		FindByFormula	1	-	752.445			22.738989
754.1354@22.516384					(753.1306, 1547.1824)(754.1323, 477.38)	754.1354@22.516384		FindByFormula	16	-	754.1354			22.516384
754.167@23.181934					(753.16003, 10006.78)(754.16315, 2970.761)(755.1646, 952.	754.167@23.181934		FindByFormula	28	-	754.167			23.181934
754.4549@23.16386					(753.45087, 1453.4155)(754.4541, 660.1521)	754.4549@23.16386		FindByFormula	9	-	754.4549			23.16386
756.1528@22.731094					(755.1452, 4809.2383)(756.14874, 1466.1903)(757.1505, 49	756.1528@22.731094		FindByFormula	28	-	756.1528			22.731094
756.3416@15.243095					(755.3344, 1532.6533)(756.34064, 681.86334)	756.3416@15.243095		FindByFormula	6	-	756.3416			15.243095
756.3914@6.6580634					(755.38385, 3510.6846)(756.38226, 1651.0299)(757.38293,	756.3914@6.6580634		FindByFormula	9	-	756.3914			6.6580634
757.5168@24.177675					(756.50757, 1198.493)(757.51013, 669.68445)(758.5134, 28	757.5168@24.177675		FindByFormula	20	-	757.5168			24.177675
757.8295@0.5829288					(756.82074, 6207.488)(757.8232, 1169.8933)(758.8243, 202	757.8295@0.5829288		FindByFormula	28	-	757.8295			0.5829288
758.1685@22.93772					(757.16077, 6683.486)(758.1646, 2031.0116)(759.1655, 675.	758.1685@22.93772		FindByFormula	28	-	758.1685			22.93772
760.1843@23.183365					(759.1768, 6247.9653)(760.1805, 1889.3021)(761.1808, 623.	760.1843@23.183365		FindByFormula	28	-	760.1843			23.183365
763.2823@22.120653					(762.2754, 904.80493)(763.2781, 376.4841)	763.2823@22.120653		FindByFormula	22	-	763.2823			22.120653
763.5161@24.211672					(762.51074, 1042.4)(763.5159, 534.4614)	763.5161@24.211672		FindByFormula	14	-	763.5161			24.211672
765.3026@22.42728					(764.2938, 1086.1201)(765.2905, 545.02747)	765.3026@22.42728		FindByFormula	8	-	765.3026			22.42728
765.5312@24.455208					(764.5297, 3404.0088)(765.53174, 1715.5498)(766.5256, 11	765.5312@24.455208		FindByFormula	23	-	765.5312			24.455208
766.091@22.448961					(765.0848, 2865.1672)(766.0883, 805.90436)	766.091@22.448961		FindByFormula	28	-	766.091			22.448961
766.4387@22.702051					(765.4309, 3599.7268)(766.4353, 1918.1913)(767.4377, 756.	766.4387@22.702051		FindByFormula	25	-	766.4387			22.702051
769.2969@22.135288					(768.29407, 539.49)(769.2821, 57.54)(770.2773, 100.55)	769.2969@22.135288		FindByFormula	2	-	769.2969			22.135288
769.2982@22.117897					(768.2934, 2221.6345)(769.2956, 847.7866)(770.29755, 296.	769.2982@22.117897		FindByFormula	27	-	769.2982			22.117897
769.3001@22.014704					(768.29297, 1068.4119)(769.2965, 456.48523)(770.2897, 10	769.3001@22.014704		FindByFormula	25	-	769.3001			22.014704
769.5533@25.231102					(768.54517, 2083.88)(769.54663, 1124.1449)(770.5518, 604.	769.5533@25.231102		FindByFormula	26	-	769.5533			25.231102
771.3164@22.434029					(770.30963, 1779.6289)(771.31195, 803.11035)(772.31464,	771.3164@22.434029		FindByFormula	24	-	771.3164			22.434029
772.1086@22.449924					(771.1021, 2035.0316)(772.1056, 594.4154)	772.1086@22.449924		FindByFormula	28	-	772.1086			22.449924
773.3314@22.663164					(772.3281, 1385.15)(773.3243, 542.63776)(774.31256, 30.77	773.3314@22.663164		FindByFormula	9	-	773.3314			22.663164
773.3329@22.743011					(772.32776, 3048.8245)(773.3295, 1123.0691)(774.337, 471.	773.3329@22.743011		FindByFormula	11	-	773.3329			22.743011
773.335@22.795414					(772.3296, 350.31)(773.3218, 46.37)	773.335@22.795414		FindByFormula	1	-	773.335			22.795414
773.5369@24.573845					(772.5295, 1021.17944)(773.52985, 545.8129)(774.53345, 3	773.5369@24.573845		FindByFormula	24	-	773.5369			24.573845
774.1318@22.694763					(773.1245, 2233.797)(774.1269, 787.2559)	774.1318@22.694763		FindByFormula	27	-	774.1318			22.694763
774.1361@22.876322					(773.1239, 316.14)(774.1436, 160.19)	774.1361@22.876322		FindByFormula	1	-	774.1361			22.876322
774.5898@24.286057					(773.586, 1273.5309)(774.5853, 607.2084)(775.5822, 223.66	774.5898@24.286057		FindByFormula	25	-	774.5898			24.286057
775.5406@23.993422					(774.5316, 1059.6333)(775.5341, 542.53094)	775.5406@23.993422		FindByFormula	23	-	775.5406			23.993422
775.5501@25.273186					(774.5426, 373.23)(775.547, 162.38)	775.5501@25.273186		FindByFormula	1	-	775.5501			25.273186
775.5523@25.12754					(774.54376, 2375.0315)(775.5469, 1227.0286)(776.5536, 69	775.5523@25.12754		FindByFormula	22	-	775.5523			25.12754
776.1531@13.099658					(775.14606, 2769.4722)(776.14935, 976.3661)	776.1531@13.099658		FindByFormula	28	-	776.1531			13.099658
776.602@24.71119					(775.5951, 1202.5294)(776.59595, 616.2937)	776.602@24.71119		FindByFormula	22	-	776.602			24.71119
777.5507@24.352367					(776.5446, 1977.005)(777.54785, 976.5313)(778.54803, 407.	777.5507@24.352367		FindByFormula	26	-	777.5507			24.352367
779.5681@24.801208					(778.56055, 2362.7754)(779.56335, 1153.515)(780.55725, 4	779.5681@24.801208		FindByFormula	27	-	779.5681			24.801208
780.4092@22.723911					(779.4009, 4070.9207)(780.4084, 1898.3126)(781.40674, 71	780.4092@22.723911		FindByFormula	25	-	780.4092			22.723911
782.2537@8.460257					(781.24603, 6815.9365)(782.2499, 3014.248)(783.25287, 93	782.2537@8.460257		FindByFormula	28	-	782.2537			8.460257
783.5687@25.759329					(782.5611, 2681.7668)(783.5641, 1608.9302)(784.5617, 704.	783.5687@25.759329		FindByFormula	20	-	783.5687			25.759329
784.4399@22.926924					(783.4322, 5793.6304)(784.4356, 2652.1208)(785.436, 937.2	784.4399@22.926924		FindByFormula	27	-	784.4399			22.926924
785.5021@8.227946					(784.4941, 2729.9597)(785.4965, 1241.5776)(786.4985, 367.	785.5021@8.227946		FindByFormula	22	-	785.5021			8.227946
785.5479@24.86617					(784.5363, 2486.2407)(785.5393, 1483.4741)(786.5464, 772.	785.5479@24.86617		FindByFormula	27	-	785.5479			24.86617
785.5833@26.954992					(784.5754, 1815.5071)(785.5785, 1077.7991)(786.5731, 418.	785.5833@26.954992		FindByFormula	20	-	785.5833			26.954992
786.4252@22.721195					(831.4356, 894.82294)(785.4189, 6571.2007)(786.4225, 292	786.4252@22.721195		FindByFormula	26	-	786.4252			22.721195
787.5625@25.745083					(786.55634, 2281.8455)(787.5579, 1406.4812)(788.55707, 5	787.5625@25.745083		FindByFormula	20	-	787.5625			25.745083
787.5717@24.559904					(786.5628, 399.88)(787.5697, 310.6)	787.5717@24.559904		FindByFormula	1	-	787.5717			24.559904
787.5729@24.754206					(786.5655, 2610.4133)(787.56903, 1371.2183)	787.5729@24.754206		FindByFormula	6	-	787.5729			24.754206
788.4697@23.181292					(787.4626, 2177.6956)(788.4693, 1048.3408)(789.4624, 534.	788.4697@23.181292		FindByFormula	28	-	788.4697			23.181292
788.5303@23.708025					(787.521, 1138.3645)(788.52435, 573.2836)	788.5303@23.708025		FindByFormula	25	-	788.5303			23.708025
789.5494@24.23396					(788.54156, 773.3506)(789.54584, 416.58386)	789.5494@24.23396		FindByFormula	18	-	789.5494			24.23396
789.5799@24.9088					(788.5757, 661.1359)(789.5847, 363.44333)	789.5799@24.9088		FindByFormula	12	-	789.5799			24.9088
789.5848@25.24628					(788.5764, 399.125)(789.5819, 243.20999)	789.5848@25.24628		FindByFormula	2	-	789.5848			25.24628
789.9816@24.124975					(788.97656, 2385.8254)(789.9749, 515.88446)	789.9816@24.124975		FindByFormula	9	-	789.9816			24.124975
789.982@23.816015					(788.97595, 9171.935)(789.97675, 1780.6387)	789.982@23.816015		FindByFormula	7	-	789.982			23.816015
789.9827@24.123894					(788.976, 3376.5334)(789.9751, 709.8117)	789.9827@24.123894		FindByFormula	17	-	789.9827			24.123894
789.9832@23.233425					(788.9765, 12394.954)(789.97595, 2319.6284)(790.9766, 35	789.9832@23.233425		FindByFormula	28	-	789.9832			23.233425
789.9837@23.188755					(788.9764, 7697.646)(789.97656, 1494.8044)	789.9837@23.188755		FindByFormula	28	-	789.9837			23.188755
789.9851@23.19702					(788.9765, 5232.1504)(789.97577, 1080.8456)	789.9851@23.19702		FindByFormula	22	-	789.9851			23.19702
789.9853@23.433258					(788.9755, 11939.21)(789.977, 2267.61)	789.9853@23.433258		FindByFormula	6	-	789.9853			23.433258
790.4564@22.92349					(835.44556, 965.0757)(836.46075, 682.91315)(789.4495, 92	790.4564@22.92349		FindByFormula	26	-	790.4564			22.92349
790.4627@23.183979					(789.4562, 249.25)(790.4606, 107.36)	790.4627@23.183979		FindByFormula	1	-	790.4627			23.183979
791.5117@24.541157					(790.5048, 3973.0588)(791.5088, 1946.8822)(792.5183, 977.	791.5117@24.541157		FindByFormula	26	-	791.5117			24.541157
791.5359@24.590044					(790.534, 641.58)(791.5293, 357.09)(792.5229, 129.16)	791.5359@24.590044		FindByFormula	1	-	791.5359			24.590044
791.5372@24.788036					(790.5313, 1734.6315)(791.5297, 786.8086)(792.5313, 961.6	791.5372@24.788036		FindByFormula	7	-	791.5372			24.788036
792.1075@22.582975					(791.1007, 1908.429)(792.1034, 610.40295)(793.10443, 516.	792.1075@22.582975		FindByFormula	28	-	792.1075			22.582975
793.3004@22.121735					(792.2926, 894.41)(793.2973, 490.75903)	793.3004@22.121735		FindByFormula	19	-	793.3004			22.121735
793.4574@25.23036					(792.4487, 848.033)(793.45074, 476.0621)(794.457, 227.998	793.4574@25.23036		FindByFormula	23	-	793.4574			25.23036
794.1233@22.874426					(793.1159, 4363.125)(794.11975, 1303.6184)(795.11914, 52	794.1233@22.874426		FindByFormula	28	-	794.1233			22.874426
794.4872@23.182186					(793.48004, 2386.932)(794.4838, 1154.1095)(795.4813, 443.	794.4872@23.182186		FindByFormula	28	-	794.4872			23.182186
795.4708@25.864923					(794.4641, 647.914)(795.46564, 324.7496)	795.4708@25.864923		FindByFormula	25	-	795.4708			25.864923
796.17@1.0048324					(795.16473, 2393.9482)(796.1662, 809.0816)	796.17@1.0048324		FindByFormula	6	-	796.17			1.0048324
796.3649@22.58109					(795.358, 1347.4166)(796.3567, 683.39056)(797.36005, 394.	796.3649@22.58109		FindByFormula	24	-	796.3649			22.58109

796.3704@22.851322	(795.3615, 348.64)(796.3703, 166.91)	796.3704@22.851322	FindByFormula	1 -	796.3704	22.851322
797.5844@26.244934	(796.5774, 5829.427)(797.57947, 3468.4202)(798.5803, 143	797.5844@26.244934	FindByFormula	22 -	797.5844	26.244934
798.126@22.58789	(797.1194, 2033.7666)(798.12085, 631.6571)	798.126@22.58789	FindByFormula	27 -	798.126	22.58789
798.6694@16.161427	(843.66583, 1583.6914)(797.662, 1181.0614)	798.6694@16.161427	FindByFormula	7 -	798.6694	16.161427
799.5634@25.208157	(798.5562, 5477.1807)(799.5588, 3203.9646)(800.56116, 12	799.5634@25.208157	FindByFormula	20 -	799.5634	25.208157
799.5993@27.654818	(798.5909, 2344.9792)(799.5944, 1355.5072)(800.5968, 527.	799.5993@27.654818	FindByFormula	21 -	799.5993	27.654818
800.1383@22.869429	(799.13293, 4511.7905)(800.13654, 1419.0702)(801.1323, 5	800.1383@22.869429	FindByFormula	28 -	800.1383	22.869429
800.3695@15.587159	(799.3609, 1971.7035)(800.36237, 845.30664)	800.3695@15.587159	FindByFormula	6 -	800.3695	15.587159
800.3953@22.848757	(799.38806, 10750.257)(800.3917, 4477.6406)(801.3957, 14	800.3953@22.848757	FindByFormula	28 -	800.3953	22.848757
801.5529@24.113777	(800.5462, 1560.1603)(801.5441, 836.6996)(802.5453, 315.5	801.5529@24.113777	FindByFormula	23 -	801.5529	24.113777
801.58@26.247076	(800.57196, 3091.5933)(801.57385, 1829.0701)(802.5747, 7	801.58@26.247076	FindByFormula	20 -	801.58	26.247076
803.5704@24.495302	(802.5611, 49165.152)(803.5646, 23492.887)(804.5655, 655	803.5704@24.495302	FindByFormula	26 -	803.5704	24.495302
803.6027@22.72572	(802.59656, 5094.2295)(803.599, 2705.4314)(804.59717, 85	803.6027@22.72572	FindByFormula	7 -	803.6027	22.72572
804.2994@13.099768	(803.2919, 3249.0344)(804.29535, 1454.1038)(805.2969, 49	804.2994@13.099768	FindByFormula	28 -	804.2994	13.099768
804.4079@22.715647	(803.4, 2005.2289)(804.40625, 998.3585)(805.4043, 380.284	804.4079@22.715647	FindByFormula	27 -	804.4079	22.715647
804.4124@22.867323	(803.4074, 424.78)(804.3979, 96.55)	804.4124@22.867323	FindByFormula	1 -	804.4124	22.867323
805.5843@24.927763	(804.57623, 15452.713)(805.5803, 7479.321)(806.5828, 226	805.5843@24.927763	FindByFormula	27 -	805.5843	24.927763
806.412@22.846617	(805.40546, 8288.139)(806.4087, 3660.4746)(807.4128, 125	806.412@22.846617	FindByFormula	28 -	806.412	22.846617
806.6577@22.847794	(805.65283, 1103.3629)(806.6567, 760.8868)	806.6577@22.847794	FindByFormula	28 -	806.6577	22.847794
807.2674@22.275352	(806.2591, 1214.7908)(807.2669, 446.76654)	807.2674@22.275352	FindByFormula	26 -	807.2674	22.275352
807.2695@22.306526	(806.2592, 1491.6752)(807.2672, 547.35516)	807.2695@22.306526	FindByFormula	27 -	807.2695	22.306526
809.4521@22.830763	(808.44635, 2099.688)(809.451, 985.5087)	809.4521@22.830763	FindByFormula	28 -	809.4521	22.830763
809.843@0.58403724	(808.8332, 10088.627)(809.83594, 1969.5814)(810.83563, 1	809.843@0.58403724	FindByFormula	27 -	809.843	0.58403724
810.3161@13.099784	(809.30896, 1302.0195)(810.3121, 594.5558)	810.3161@13.099784	FindByFormula	26 -	810.3161	13.099784
810.4253@22.712088	(809.41907, 4026.2803)(810.4227, 1973.1384)(811.41943, 7	810.4253@22.712088	FindByFormula	25 -	810.4253	22.712088
811.5413@24.925144	(810.536, 1349.7872)(811.5364, 734.8776)(812.5474, 274.56	811.5413@24.925144	FindByFormula	21 -	811.5413	24.925144
811.5424@25.074976	(810.5393, 360.75)(811.542, 260.58)(812.5553, 112.4)	811.5424@25.074976	FindByFormula	1 -	811.5424	25.074976
811.5692@24.689384	(810.5628, 1682.0834)(811.5667, 900.41144)(812.5715, 782.	811.5692@24.689384	FindByFormula	20 -	811.5692	24.689384
812.3241@22.450232	(811.31415, 1530.4523)(812.31335, 716.9226)	812.3241@22.450232	FindByFormula	27 -	812.3241	22.450232
812.683@22.848618	(811.6768, 2515.5503)(812.6799, 1436.889)(813.6806, 532.8	812.683@22.848618	FindByFormula	28 -	812.683	22.848618
813.2876@22.269299	(812.2812, 1630.4451)(813.287, 657.5411)(814.2781, 223.24	813.2876@22.269299	FindByFormula	26 -	813.2876	22.269299
813.2878@22.306946	(812.2811, 2871.232)(813.28674, 1074.4547)(814.2909, 447.	813.2878@22.306946	FindByFormula	26 -	813.2878	22.306946
813.5792@25.59589	(812.5716, 9710.091)(813.5742, 5824.0283)(814.5766, 2194.	813.5792@25.59589	FindByFormula	20 -	813.5792	25.59589
813.5891@24.8463	(812.5791, 3444.1685)(813.58246, 1745.1271)(814.58606, 7	813.5891@24.8463	FindByFormula	7 -	813.5891	24.8463
814.546@23.81533	(813.5411, 1586.1577)(814.5436, 777.0373)(815.54297, 267.	814.546@23.81533	FindByFormula	25 -	814.546	23.81533
815.4733@22.83448	(814.4656, 1524.6704)(815.46185, 761.3896)	815.4733@22.83448	FindByFormula	24 -	815.4733	22.83448
815.5134@24.467724	(814.5032, 2392.5679)(815.5115, 1280.5496)(816.517, 728.3	815.5134@24.467724	FindByFormula	25 -	815.5134	24.467724
815.5943@26.812017	(814.5872, 3715.2065)(815.5883, 2263.7773)(816.58905, 87	815.5943@26.812017	FindByFormula	23 -	815.5943	26.812017
816.1082@22.516327	(815.1021, 1230.2535)(816.1034, 391.93753)	816.1082@22.516327	FindByFormula	20 -	816.1082	22.516327
816.1365@23.182901	(815.1298, 2489.0571)(816.13367, 826.0508)(817.1344, 532.	816.1365@23.182901	FindByFormula	28 -	816.1365	23.182901
816.5609@24.13103	(815.5534, 6854.925)(816.5557, 3299.3823)(817.5585, 1033.	816.5609@24.13103	FindByFormula	27 -	816.5609	24.13103
817.5255@24.673075	(816.5254, 2054.8145)(817.5274, 1040.1512)(818.5293, 481.	817.5255@24.673075	FindByFormula	26 -	817.5255	24.673075
817.5743@24.801659	(816.5672, 1607.5176)(817.5706, 852.38257)(818.56647, 44	817.5743@24.801659	FindByFormula	12 -	817.5743	24.801659
818.1219@22.739376	(817.1153, 3335.1902)(818.1182, 1103.8923)(819.1195, 434.	818.1219@22.739376	FindByFormula	28 -	818.1219	22.739376
819.5442@25.223696	(818.53705, 1562.7429)(819.5398, 824.4527)(820.5463, 487.	819.5442@25.223696	FindByFormula	26 -	819.5442	25.223696
820.1395@22.945572	(819.131, 5275.1704)(820.134, 1679.1393)(821.13605, 643.3	820.1395@22.945572	FindByFormula	28 -	820.1395	22.945572
820.4259@23.03401	(819.4204, 1394.6671)(820.42126, 598.8685)	820.4259@23.03401	FindByFormula	7 -	820.4259	23.03401
822.1261@22.515121	(821.1167, 1545.12)(822.11725, 508.89917)	822.1261@22.515121	FindByFormula	12 -	822.1261	22.515121
822.1552@23.183685	(821.147, 6354.8315)(822.14996, 2012.97)(823.1507, 706.44	822.1552@23.183685	FindByFormula	28 -	822.1552	23.183685
824.1386@22.73434	(823.13226, 3486.6548)(824.13367, 1157.5271)	824.1386@22.73434	FindByFormula	28 -	824.1386	22.73434
825.554@24.128143	(824.54333, 3409.331)(825.5457, 1749.6298)(826.5543, 185	825.554@24.128143	FindByFormula	11 -	825.554	24.128143
825.6151@27.624212	(824.6076, 3527.9485)(825.61066, 2204.9937)(826.6121, 93	825.6151@27.624212	FindByFormula	20 -	825.6151	27.624212
825.8165@0.5850002	(824.8094, 5720.07)(825.81244, 1299.2029)(826.81476, 162	825.8165@0.5850002	FindByFormula	25 -	825.8165	0.5850002
826.1555@22.940037	(825.148, 4510.37)(826.1512, 1419.3998)(827.1506, 523.040	826.1555@22.940037	FindByFormula	28 -	826.1555	22.940037
827.5669@24.455841	(826.5613, 790.0351)(827.56274, 471.0925)(828.562, 184.37	827.5669@24.455841	FindByFormula	4 -	827.5669	24.455841
827.5673@24.247963	(826.56036, 4840.492)(827.56323, 2495.1604)(828.5655, 79	827.5673@24.247963	FindByFormula	22 -	827.5673	24.247963
827.5687@24.43402	(826.5611, 22145.447)(827.5636, 11102.083)(828.5661, 330	827.5687@24.43402	FindByFormula	26 -	827.5687	24.43402
827.5949@26.126913	(826.5874, 4072.1265)(827.58997, 2519.234)(828.5917, 970.	827.5949@26.126913	FindByFormula	20 -	827.5949	26.126913
827.6032@22.714869	(826.5949, 1980.5825)(827.59924, 1184.4601)	827.6032@22.714869	FindByFormula	8 -	827.6032	22.714869
827.6418@25.125055	(826.63995, 803.7641)(827.6354, 634.8771)	827.6418@25.125055	FindByFormula	17 -	827.6418	25.125055
828.1705@23.183365	(827.1641, 4743.7954)(828.1673, 1491.6357)	828.1705@23.183365	FindByFormula	28 -	828.1705	23.183365
829.5868@24.66468	(828.578, 8731.473)(829.58105, 4417.38)(830.5807, 1348.47	829.5868@24.66468	FindByFormula	26 -	829.5868	24.66468
830.6569@25.71992	(829.65045, 806.12787)(830.64307, 309.98218)	830.6569@25.71992	FindByFormula	14 -	830.6569	25.71992
831.2707@22.120157	(830.2656, 1134.9535)(831.26855, 477.54395)	831.2707@22.120157	FindByFormula	20 -	831.2707	22.120157
831.5205@23.83582	(830.5101, 2246.47)(831.51794, 1565.3629)(832.5208, 635.7	831.5205@23.83582	FindByFormula	21 -	831.5205	23.83582
831.5993@25.1719	(830.5923, 16380.398)(831.5953, 8245.653)(832.5961, 2533.	831.5993@25.1719	FindByFormula	27 -	831.5993	25.1719
833.2875@22.428438	(832.2807, 1330.3729)(833.2807, 597.3257)	833.2875@22.428438	FindByFormula	7 -	833.2875	22.428438
833.5208@24.428453	(832.515, 1106.7634)(833.5175, 664.8726)(834.51733, 366.5	833.5208@24.428453	FindByFormula	22 -	833.5208	24.428453
833.6146@25.746096	(832.6069, 1767.5981)(833.6075, 897.7767)(834.6105, 307.1	833.6146@25.746096	FindByFormula	26 -	833.6146	25.746096
834.0804@22.447712	(833.07227, 1644.9167)(834.0748, 509.701)	834.0804@22.447712	FindByFormula	28 -	834.0804	22.447712
834.4263@22.703411	(833.42, 2140.811)(834.42114, 1106.2368)(835.41974, 439.4	834.4263@22.703411	FindByFormula	25 -	834.4263	22.703411
835.5342@24.885294	(834.527, 1393.5331)(835.5292, 743.71265)(836.5203, 276.3	835.5342@24.885294	FindByFormula	26 -	835.5342	24.885294
837.2864@22.020664	(836.28046, 1040.996)(837.2858, 450.3585)	837.2864@22.020664	FindByFormula	20 -	837.2864	22.020664
837.2881@22.129385	(836.28406, 618.096)(837.2816, 255.58598)(838.2804, 108.8	837.2881@22.129385	FindByFormula	5 -	837.2881	22.129385
837.2883@22.120522	(836.28186, 1746.2076)(837.2843, 706.5655)(838.2838, 262.	837.2883@22.120522	FindByFormula	26 -	837.2883	22.120522
839.3039@22.433565	(838.29694, 1331.1166)(839.3015, 636.16724)(840.3019, 23	839.3039@22.433565	FindByFormula	25 -	839.3039	22.433565
839.6043@24.974514	(838.5931, 1048.571)(839.597, 573.12756)(840.5913, 192.53	839.6043@24.974514	FindByFormula	20 -	839.6043	24.974514
840.3183@3.597034	(875.272, 806.0906)(839.3107, 4271.403)(840.31256, 2338.6	840.3183@3.597034	FindByFormula	23 -	840.3183	3.597034
841.3184@22.74658	(840.314, 2718.9211)(841.3227, 1144.7)	841.3184@22.74658	FindByFormula	8 -	841.3184	22.74658
841.611@26.701244	(840.60315, 5135.6216)(841.6054, 3198.2966)(842.60767, 1	841.611@26.701244	FindByFormula	22 -	841.611	26.701244
841.7751@21.406652	(840.7684, 6464.4873)(841.7747, 1955.7413)(842.766, 1786	841.7751@21.406652	FindByFormula	7 -	841.7751	21.406652
841.7887@0.5935558	(840.78564, 3369.21)(841.7927, 850.45337)(842.786, 877.68	841.7887@0.5935558	FindByFormula	18 -	841.7887	0.5935558
842.5799@24.28314	(841.5698, 718.1925)(842.5689, 409.0072)	842.5799@24.28314	FindByFormula	21 -	842.5799	24.28314
843.5413@25.124508	(842.5345, 771.14044)(843.5374, 443.45856)(844.5469, 358.	843.5413@25.124508	FindByFormula	21 -	843.5413	25.124508
843.6257@28.317738	(842.61896, 2049.683)(843.6211, 1281.246)(844.6208, 515.9	843.6257@28.317738	FindByFormula	20 -	843.6257	28.317738
843.6809@24.930634	(888.6737, 662.89453)(889.6795, 387.45056)(842.6713, 184	843.6809@24.930634	FindByFormula	19 -	843.6809	24.930634
844.1401@13.100767	(843.1326, 1694.4608)(844.13544, 638.49615)	844.1401@13.100767	FindByFormula	28 -	844.1401	13.100767
844.225@8.460042	(843.2167, 2458.7927)(844.22125, 1159.7324)(845.22253, 4	844.225@8.460042	FindByFormula	28 -	844.225	8.460042
845.5317@24.049585	(844.5226, 159.19)(845.5286, 135.44)	845.5317@24.049585	FindByFormula	1 -	845.5317	24.049585
845.5383@24.346788	(844.53204, 997.0148)(845.53326, 523.5218)	845.5383@24.346788	FindByFormula	23 -	845.5383	24.346788
847.5115@23.699986	(846.5041, 3037.08)(847.5068, 1790.1443)(848.50995, 743.6	847.5115@23.699986	FindByFormula	21 -	847.5115	23.699986
847.5537@24.80091	(846.5482, 1159.0792)(847.54913, 565.7165)(848.54535, 24	847.5537@24.80091	FindByFormula	26 -	847.5537	24.80091
848.3947@22.723244	(847.3879, 5516.494)(848.3926, 2599.6084)(849.39526, 889.	848.3947@22.723244	FindByFormula	25 -	848.3947	22.723244
850.2403@8.458829	(849.2334, 2054.536)(850.2378, 984.4518)(851.2386, 342.25	850.2403@8.458829	FindByFormula	28 -	850.2403	8.458829
851.5602@24.372017	(850.5547, 520.77)(851.553, 311.39)	851.5602@24.372017	FindByFormula	1 -	851.5602	24.372017
851.566@24.185974	(850.5586, 555.0425)(851.5643, 321.23)(852.5469, 71.1)	851.566@24.185974	FindByFormula	4 -	851.566	24.185974
851.5676@24.191595	(850.5591, 1793.7477)(851.56177, 986.0132)(852.5607, 359.	851.5676@24.191595	FindByFormula	19 -	851.5676	24.191595
851.571@24.327486	(850.5578, 11173.284)(851.56085, 5954.2397)(852.56836, 2	851.571@24.327486	FindByFormula	15 -	851.571	24.327486
852.4268@22.929146	(851.42035, 8857.33)(852.42303, 4081.4604)(853.42633, 14	852.4268@22.929146	FindByFormula	27 -	852.4268	22.929146
853.5806@24.555206	(852.57404, 3466.9573)(853.5756, 1857.8516)(854.5844, 78	853.5806@24.555206	FindByFormula	24 -	853.5806	24.555206
854.4134@22.721003	(853.4059, 4746.9375)(854.41095, 2204.301)(855.4111, 961.	854.4134@22.721003	FindByFormula	25 -	854.4134	22.721003
855.5999@25.083378	(854.5934, 9589.799)(855.5958, 5101.696)(856.5986, 1631.6	855.5999@25.083378	FindByFormula	26 -	855.5999	25.083378
856.4573@23.18165	(855.4511, 4397.2007)(856.45496, 2063.1274)(857.4556, 77	856.4573@23.18165	FindByFormula	28 -	856.4573	23.18165
856.5126@23.707132	(855.50604, 961.0762)(856.5111, 462.4534)	856.5126@23.707132	FindByFormula	18 -	856.5126	23.707132
856.6719@25.828072	(855.66583, 1394.842)(856.6654, 711.79236)	856.6719@25.828072	FindByFormula	25 -	856.6719	25.828072
857.6144@25.13311	(856.60864, 407.425)(857.6043, 164.355)	857.6144@25.13311	FindByFormula	2 -	857.6144	25.13311
857.6148@25.444185	(856.6092, 2370.6177)(857.608, 1273.6733)(858.5968, 579.2	857.6148@25.444185	FindByFormula	21 -	857.6148	25.444185
858.4442@22.92771	(857.43665, 7589.6733)(858.4412, 3472.1362)(859.44336, 1	858.4442@22.92771	FindByFormula	25 -	858.4442	22.92771
859.5004@24.543152	(858.4932, 1269.4932)(859.49677, 679.8426)(860.5035, 338.	859.5004@24.543152	FindByFormula	19 -	859.5004	24.543152
860.0948@22.581999	(859.08765, 1420.8047)(860.0872, 500.46445)	860.0948@22.581999	FindByFormula	27 -	860.0948	22.581999
862.1093@22.87621	(861.1027, 2293.8696)(862.1061, 759.40393)	862.1093@22.87621	FindByFormula	28 -	862.1093	22.87621
862.3615@22.861217	(861.3547, 1966.6356)(862.3599, 904.6407)(863.36395, 564.	862.3615@22.861217	FindByFormula	28 -	862.3615	22.861217
862.4706@22.896145	(861.4717, 435.915)(862.4741, 305.685)(863.48, 155.16)	862.4706@22.896145	FindByFormula	2 -	862.4706	22.896145
862.4753@23.181692	(861.46924, 2162.6687)(862.4833, 1568.9475)(863.4863, 75	862.4753@23.181692	FindByFormula	20 -	862.4753	23.181692
864.353@22.580797	(863.34705, 1026.0543)(864.3427, 529.01526)	864.353@22.580797	FindByFormula	23 -	864.353	22.580797
868.1262@22.870573	(867.1201, 1793.4174)(868.1212, 614.78534)	868.1262@22.870573	FindByFormula	28 -	868.1262	22.870573
868.3824@22.852972	(867.3751, 6698.1196)(868.3792, 2880.3792)(869.3832, 108	868.3824@22.852972	FindByFormula	28 -	868.3824	22.852972
869.2725@3.5984445	(868.2629, 3950.422)(869.2654, 2246.9858)(870.25916, 375	869.2725@3.5984445	FindByFormula	22 -	869.2725	3.5984445
871.5551@24.4953	(870.5481, 12689.553)(871.551, 6264.204)(872.5508, 1974.3	871.5551@24.4953	FindByFormula	26 -	871.5551	24.4953
871.5902@22.725449	(870.584, 3945.6785)(871.5872, 2215.7)(872.5894, 764.6667	871.5902@22.725449	FindByFormula	6 -	871.5902	22.725449
872.2861@13.0997305	(871.27924, 3090.3088)(872.2834, 1413.4735)(873.28595, 5	872.2861@13.0997305	FindByFormula	28 -	872.2861	13.0997305
872.3943@22.709047	(871.3878, 2657.4028)(872.3936, 1345.7231)(873.3977, 531.	872.3943@22.709047	FindByFormula	26 -	872.3943	22.709047
873.5701@24.92519	(872.5626, 6575.131)(873.5658, 3316.134)(874.567, 1060.67	873.5701@24.92519	FindByFormula	26 -	873.5701	24.92519
874.4002@22.849009	(873.393, 6909.8975)(874.39685, 3055.1265)(875.40234, 10	874.4002@22.849009	FindByFormula	28 -	874.4002	22.849009
874.651@22.847902	(873.6458, 2424.8223)(874.6494, 1407.9664)(875.6494, 610.	874.651@22.847902	FindByFormula	28 -	874.651	22.847902
875.258@22.252308	(874.2523, 1014.51105)(875.2547, 414.97046)	875.258@22.252308	FindByFormula	20 -	875.258	22.252308
875.26@22.325977	(874.2549, 402.21497)(875.244, 126.36)	875.26@22.325977	FindByFormula	2 -	875.26	22.325977
877.4398@22.829332	(876.4319, 1359.4226)(877.43646, 660.8993)	877.4398@22.829332	FindByFormula	26 -	877.4398	22.829332
877.5748@24.456886	(876.5679, 1185.485)(877.5723, 701.14667)	877.5748@24.456886	FindByFormula	6 -	877.5748	24.456886
877.8291@0.5838698	(876.82184, 8424.337)(877.82556, 1830.9552)(878.8243, 12	877.8291@0.5838698	FindByFormula	23 -	877.8291	0.5838698
878.4136@22.711048	(877.40533, 2698.5098)(878.40857, 1373.0225)(879.39996,	878.4136@22.711048	FindByFormula	25 -	878.4136	22.711048
878.5307@24.134247	(877.52386, 1039.1981)(878.526, 556.46)	878.5307@24.134247	FindByFormula	26 -	878.5307	24.134247
879.5989@24.969696	(878.5914, 5957.9453)(879.5942, 3350.2747)(880.59326, 17	879.5989@24.969696	FindByFormula	6 -	879.5989	24.969696
880.3095@22.448568	(879.3026, 1688.4011)(880.3007, 813.9903)(881.30457, 359.	880.3095@22.448568	FindByFormula	28 -	880.3095	22.448568
880.6714@22.84751	(879.66425, 3087.8928)(880.6681, 1759.5011)(881.66766, 6	880.6714@22.84751	FindByFormula	28 -	880.6714	22.84751
881.2764@22.30472	(880.26935, 2271.14)(881.2762, 910.3787)(882.27136, 349.5	881.2764@22.30472	FindByFormula	24 -	881.2764	22.30472
881.2784@22.259848	(880.26904, 1520.198)(881.27576, 629.25714)	881.2784@22.259848	FindByFormula	21 -	881.2784	22.259848
881.28@22.323523	(880.2692, 1062.44)(881.2824, 474.82)(882.2728, 236.75)	881.28@22.323523	FindByFormula	1 -	881.28	22.323523
881.5753@24.849968	(880.5666, 1259.2555)(881.5687, 577.0856)	881.5753@24.849968	FindByFormula	9 -	881.5753	24.849968
881.6139@25.22479	(880.6054, 951.2158)(881.60815, 524.2076)(882.60144, 424.	881.6139@25.22479	FindByFormula	12 -	881.6139	25.22479
882.4112@16.984701	(881.4013, 1431.415)(882.4035, 694.13336)	882.4112@16.984701	FindByFormula	6 -	882.4112	16.984701
882.5337@23.808203	(881.5242, 1119.0446)(882.52673, 577.6841)	882.5337@23.808203	FindByFormula	22 -	882.5337	23.808203
884.1239@23.18904	(883.1168, 1857.6729)(884.11993, 673.1383)	884.1239@23.18904	FindByFormula	28 -	884.1239	23.18904
884.5485@24.132364	(883.5407, 4558.5215)(884.5438, 2261.4482)(885.54694, 92	884.5485@24.132364	FindByFormula	26 -	884.5485	24.132364
884.6832@22.728521	(883.6763, 2046.1683)(884.67883, 1262.7881)(885.6734, 56	884.6832@22.728521	FindByFormula	25 -	884.6832	22.728521
886.1106@22.738554	(885.10223, 2011.3654)(886.1045, 720.7079)	886.1106@22.738554	FindByFormula	28 -	886.1106	22.738554
888.126@22.948214	(887.118, 2921.6812)(888.12115, 1000.7592)	888.126@22.948214	FindByFormula	28 -	888.126	22.948214
888.4174@23.04077	(887.40967, 1375.0948)(888.4135, 654.99335)	888.4174@23.04077	FindByFormula	6 -	888.4174	23.04077
888.5404@22.979513	(887.5332, 984.8289)(888.53424, 602.8144)	888.5404@22.979513	FindByFormula	27 -	888.5404	22.979513
889.5122@24.501265	(888.50854, 2495.763)(889.50696, 1526.96)(890.50635, 732.	889.5122@24.501265	FindByFormula	21 -	889.5122	24.501265
890.14@23.186148	(889.134, 3782.607)(890.13715, 1290.3632)	890.14@23.186148	FindByFormula	28 -	890.14	23.186148
890.7308@22.92085	(889.7241, 3114.2703)(890.72815, 1903.3971)(891.73047, 7	890.7308@22.92085	FindByFormula	27 -	890.7308	22.92085
891.5227@24.915838	(890.521, 709.33997)(891.5247, 441.91122)	891.5227@24.915838	FindByFormula	17 -	891.5227	24.915838
893.5414@24.138895	(892.53217, 2234.8284)(893.5356, 1213.85)(894.5456, 1725.	893.5414@24.138895	FindByFormula	6 -	893.5414	24.138895
893.5472@23.895632	(892.5471, 196.69)(893.5575, 59.48)(894.5329, 152.9)	893.5472@23.895632	FindByFormula	1 -	893.5472	23.895632
893.8083@0.5906194	(892.7979, 4769.54)(893.8029, 1220.4514)(894.8074, 1129.5	893.8083@0.5906194	FindByFormula	21 -	893.8083	0.5906194
894.1401@22.941717	(893.13416, 1980.4037)(894.1368, 710.41815)	894.1401@22.941717	FindByFormula	28 -	894.1401	22.941717
895.4517@5.7646427	(894.44403, 3031.1582)(895.44806, 1500.7666)	895.4517@5.7646427	FindByFormula	6 -	895.4517	5.7646427
895.5529@24.245691	(894.5469, 2549.5754)(895.54736, 1393.4413)(896.5509, 47	895.5529@24.245691	FindByFormula	17 -	895.5529	24.245691
895.5542@24.443047	(894.54553, 874.83624)(895.5466, 510.97125)(896.54486, 2	895.5542@24.443047	FindByFormula	8 -	895.5542	24.443047
895.5547@24.433441	(894.5465, 6809.506)(895.5475, 3619.306)(896.5475, 1221.4	895.5547@24.433441	FindByFormula	26 -	895.5547	24.433441
896.1574@23.18372	(895.1506, 2134.194)(896.15216, 745.4443)	896.1574@23.18372	FindByFormula	28 -	896.1574	23.18372
896.534@10.775598	(895.52545, 5907.42)(896.52826, 2998.5718)(897.5302, 939.	896.534@10.775598	FindByFormula	22 -	896.534	10.775598
896.6366@22.722181	(895.62805, 1115.9604)(896.6356, 688.06006)(897.63025, 6	896.6366@22.722181	FindByFormula	21 -	896.6366	22.722181
897.5714@24.652512	(896.56146, 4281.031)(897.56323, 2278.7202)(898.5591, 76	897.5714@24.652512	FindByFormula	25 -	897.5714	24.652512
899.2533@22.1221	(898.2539, 908.31433)(899.25464, 431.23557)	899.2533@22.1221	FindByFormula	18 -	899.2533	22.1221
899.5875@25.17249	(898.57825, 6608.4995)(899.5821, 3453.0637)(900.5821, 11	899.5875@25.17249	FindByFormula	26 -	899.5875	25.17249
900.4308@13.097647	(899.4239, 1693.6409)(900.42474, 995.7892)(901.4289, 462.	900.4308@13.097647	FindByFormula	26 -	900.4308	13.097647
902.6853@22.925789	(901.67975, 1164.3373)(902.6824, 734.4752)(903.6767, 709.	902.6853@22.925789	FindByFormula	25 -	902.6853	22.925789
903.4596@10.270146	(902.45276, 1387.4419)(903.45496, 757.984)	903.4596@10.270146	FindByFormula	5 -	903.4596	10.270146
905.2745@22.047352	(904.2699, 1015.49335)(905.2701, 488.41934)	905.2745@22.047352	FindByFormula	15 -	905.2745	22.047352
905.2751@22.121227	(904.2704, 1357.4406)(905.2715, 610.8578)	905.2751@22.121227	FindByFormula	27 -	905.2751	22.121227
905.28@22.128592	(904.2708, 691.5308)(905.2732, 365.58582)	905.28@22.128592	FindByFormula	12 -	905.28	22.128592
907.2904@22.43314	(906.284, 1329.4154)(907.28827, 635.7874)	907.2904@22.43314	FindByFormula	19 -	907.2904	22.43314
908.6825@22.715044	(907.675, 1740.2383)(908.6791, 1166.6393)	908.6825@22.715044	FindByFormula	25 -	908.6825	22.715044
910.5611@24.28466	(909.55396, 599.0088)(910.5506, 323.9488)	910.5611@24.28466	FindByFormula	17 -	910.5611	24.28466
912.2129@8.460721	(911.20447, 1256.7949)(912.2086, 619.0101)	912.2129@8.460721	FindByFormula	28 -	912.2129	8.460721
913.5176@24.37286	(912.51044, 1251.3892)(913.51404, 758.2376)(914.51575, 2	913.5176@24.37286	FindByFormula	21 -	913.5176	24.37286
913.5596@8.419434	(912.5512, 1575.4171)(913.5541, 846.15137)(914.55273, 28	913.5596@8.419434	FindByFormula	22 -	913.5596	8.419434
914.4015@22.935183	(913.3949, 1497.8618)(914.3995, 782.47656)(915.4005, 490.	914.4015@22.935183	FindByFormula	26 -	914.4015	22.935183
914.5233@22.523075	(913.5138, 2248.1057)(914.5204, 1321.2056)	914.5233@22.523075	FindByFormula	9 -	914.5233	22.523075
915.5349@24.771643	(914.5313, 910.5358)(915.5328, 503.89584)	915.5349@24.771643	FindByFormula	24 -	915.5349	24.771643
915.5364@24.828178	(914.5331, 849.275)(915.5353, 385.115)	915.5364@24.828178	FindByFormula	2 -	915.5364	24.828178
916.3827@22.726923	(915.3753, 3393.9377)(916.3808, 1643.3438)(917.3818, 676.	916.3827@22.726923	FindByFormula	25 -	916.3827	22.726923
917.5408@25.1594	(916.53784, 1180.35)(917.54047, 751.25543)(918.5388, 369.	917.5408@25.1594	FindByFormula	11 -	917.5408	25.1594
917.5432@24.807274	(916.53613, 380.53)(917.5379, 171.715)	917.5432@24.807274	FindByFormula	2 -	917.5432	24.807274
919.5464@24.195518	(918.5448, 571.09)(919.5361, 505.29)	919.5464@24.195518	FindByFormula	1 -	919.5464	24.195518
919.5533@24.193195	(918.54626, 1421.048)(919.54364, 953.10596)(920.5596, 31	919.5533@24.193195	FindByFormula	10 -	919.5533	24.193195
919.5547@24.310604	(918.5474, 8430.691)(919.54736, 4670.723)(920.5562, 2044.	919.5547@24.310604	FindByFormula	8 -	919.5547	24.310604
919.5599@23.847548	(918.5582, 563.255)(919.5416, 429.19)	919.5599@23.847548	FindByFormula	2 -	919.5599	23.847548
920.2356@0.827666	(919.2277, 8966.575)(920.2305, 3295.682)(921.23096, 1120.	920.2356@0.827666	FindByFormula	6 -	920.2356	0.827666
920.4147@22.931295	(919.40814, 5621.36)(920.411, 2703.5088)(921.41296, 1004.	920.4147@22.931295	FindByFormula	27 -	920.4147	22.931295
921.5694@24.390371	(920.5539, 413.82)(921.57, 230.23)(922.5601, 166.77)	921.5694@24.390371	FindByFormula	1 -	921.5694	24.390371
921.5741@24.54876	(920.5598, 3024.3398)(921.56415, 1737.7379)(922.5632, 89	921.5741@24.54876	FindByFormula	9 -	921.5741	24.54876
922.3991@22.722313	(921.39185, 3540.3762)(922.397, 1756.9873)(923.39746, 70	922.3991@22.722313	FindByFormula	25 -	922.3991	22.722313
923.5869@25.089668	(922.5767, 4181.7)(923.58057, 2325.24)(924.57764, 831.428	923.5869@25.089668	FindByFormula	25 -	923.5869	25.089668

924.4461@23.183435				(923.4382, 3361.8508)(924.4421, 1682.3551)(925.443, 668.7	924.4461@23.183435		FindByFormula	28	-	924.4461	23.183435
924.65@25.827486				(923.65204, 1119.2714)(924.652, 623.11127)	924.65@25.827486		FindByFormula	15	-	924.65	25.827486
925.5929@25.445068				(924.59155, 1509.3707)(925.59436, 840.31537)(926.58636,	925.5929@25.445068		FindByFormula	15	-	925.5929	25.445068
926.4317@22.929146				(925.42456, 5596.9585)(926.42834, 2723.7002)(927.4322, 9	926.4317@22.929146		FindByFormula	26	-	926.4317	22.929146
927.4878@24.544098				(926.4776, 1240.4921)(927.48035, 698.6564)(928.48285, 37	927.4878@24.544098		FindByFormula	19	-	927.4878	24.544098
928.0811@22.579584				(927.07385, 1163.4337)(928.0726, 460.71567)	928.0811@22.579584		FindByFormula	28	-	928.0811	22.579584
930.0965@22.88042				(929.08997, 1669.8195)(930.0932, 622.6407)	930.0965@22.88042		FindByFormula	28	-	930.0965	22.88042
930.3513@22.86497				(929.3431, 1953.904)(930.34735, 918.56995)(931.35205, 59	930.3513@22.86497		FindByFormula	28	-	930.3513	22.86497
930.4617@23.18279				(929.4547, 2248.6382)(930.45953, 1150.6926)(931.455, 512.	930.4617@23.18279		FindByFormula	28	-	930.4617	23.18279
932.3407@22.582136				(931.3338, 1182.0862)(932.3323, 617.3763)	932.3407@22.582136		FindByFormula	24	-	932.3407	22.582136
932.6817@22.702452				(931.6746, 1655.644)(932.6774, 1113.4872)(933.6746, 487.9	932.6817@22.702452		FindByFormula	25	-	932.6817	22.702452
933.5284@24.497889				(932.51764, 850.29663)(933.51794, 464.40134)	933.5284@24.497889		FindByFormula	23	-	933.5284	24.497889
933.7588@23.180662				(932.75244, 952.24115)(933.7539, 714.95886)	933.7588@23.180662		FindByFormula	27	-	933.7588	23.180662
933.7776@21.858654				(932.77216, 2055.89)(933.77386, 786.6262)(934.7695, 5742.	933.7776@21.858654		FindByFormula	8	-	933.7776	21.858654
933.7777@21.93379				(932.77094, 2229.8784)(933.7765, 857.57)(934.7677, 6194.1	933.7777@21.93379		FindByFormula	7	-	933.7777	21.93379
933.7836@21.68482				(932.7786, 405.96)(933.7738, 235.62)(934.7771, 518.43)(93	933.7836@21.68482		FindByFormula	1	-	933.7836	21.68482
935.5416@24.914215				(934.5298, 814.23474)(935.5345, 450.16354)	935.5416@24.914215		FindByFormula	17	-	935.5416	24.914215
936.2052@0.8363326				(935.19806, 2103.78)(936.20074, 810.7583)	936.2052@0.8363326		FindByFormula	6	-	936.2052	0.8363326
936.3699@22.860899				(935.3627, 6664.247)(936.3666, 2976.1653)(937.36914, 107	936.3699@22.860899		FindByFormula	28	-	936.3699	22.860899
937.5204@24.107702				(936.5086, 319.9773)(937.5035, 228.8082)	937.5204@24.107702		FindByFormula	11	-	937.5204	24.107702
937.521@24.351555				(936.508, 946.9566)(937.51044, 639.4583)	937.521@24.351555		FindByFormula	6	-	937.521	24.351555
939.5417@24.50164				(938.5341, 6263.7)(939.53705, 3241.6611)(940.5378, 1089.9	939.5417@24.50164		FindByFormula	26	-	939.5417	24.50164
939.5801@22.726946				(938.57227, 3336.5315)(939.5755, 1899.4033)(940.5795, 67	939.5801@22.726946		FindByFormula	6	-	939.5801	22.726946
940.2718@13.098411				(939.26715, 1390.3431)(940.2704, 700.00287)	940.2718@13.098411		FindByFormula	28	-	940.2718	13.098411
940.3804@22.708122				(939.37494, 1736.7888)(940.3803, 906.4196)	940.3804@22.708122		FindByFormula	26	-	940.3804	22.708122
940.3898@22.853197				(939.385, 509.07)(940.3857, 287.51)	940.3898@22.853197		FindByFormula	1	-	940.3898	22.853197
941.4597@10.364922				(940.4524, 3044.1016)(941.4559, 1640.4066)(942.45703, 55	941.4597@10.364922		FindByFormula	6	-	941.4597	10.364922
941.5576@24.924244				(940.5467, 3759.2603)(941.5516, 1998.3119)(942.55444, 74	941.5576@24.924244		FindByFormula	25	-	941.5576	24.924244
942.2172@0.7988327				(941.21, 22231.398)(942.2127, 8039.562)(943.2119, 2849.00	942.2172@0.7988327		FindByFormula	6	-	942.2172	0.7988327
942.3879@22.852045				(941.3803, 5010.618)(942.384, 2316.3284)(943.38837, 786.6	942.3879@22.852045		FindByFormula	28	-	942.3879	22.852045
942.641@22.846617				(941.6337, 2927.6135)(942.641, 1802.9296)(943.64545, 778.	942.641@22.846617		FindByFormula	28	-	942.641	22.846617
943.2475@22.245485				(942.23895, 987.8305)(943.2449, 447.74835)	943.2475@22.245485		FindByFormula	18	-	943.2475	22.245485
943.7652@21.867544				(942.75745, 2226.53)(943.7668, 862.2643)(944.7624, 888.53	943.7652@21.867544		FindByFormula	7	-	943.7652	21.867544
945.8182@0.58300024				(944.8096, 6546.7656)(945.8133, 1584.1223)	945.8182@0.58300024		FindByFormula	22	-	945.8182	0.58300024
946.3981@22.709084				(945.39294, 1836.2825)(946.3967, 976.90533)(947.3932, 48	946.3981@22.709084		FindByFormula	26	-	946.3981	22.709084
946.519@24.131824				(945.5098, 1187.4154)(946.5123, 646.82495)(947.51306, 24	946.519@24.131824		FindByFormula	26	-	946.519	24.131824
946.6513@22.727638				(945.64526, 2164.325)(946.64703, 1326.6664)(947.64514, 6	946.6513@22.727638		FindByFormula	25	-	946.6513	22.727638
947.5838@24.97403				(946.576, 2839.4348)(947.5799, 1666.1266)(948.5744, 974.3	947.5838@24.97403		FindByFormula	6	-	947.5838	24.97403
948.6596@22.84815				(947.65216, 3560.0728)(948.6558, 2089.4456)(949.65765, 8	948.6596@22.84815		FindByFormula	28	-	948.6596	22.84815
949.2609@22.270824				(948.2563, 1330.6305)(949.2645, 622.69305)(950.2583, 123.	949.2609@22.270824		FindByFormula	23	-	949.2609	22.270824
949.2633@22.307463				(948.2569, 1704.5078)(949.26514, 758.4805)(950.26654, 33	949.2633@22.307463		FindByFormula	25	-	949.2633	22.307463
949.567@24.811762				(948.5618, 940.6886)(949.5602, 472.20285)	949.567@24.811762		FindByFormula	7	-	949.567	24.811762
950.5183@23.81049				(949.5105, 936.8969)(950.5108, 498.94583)	950.5183@23.81049		FindByFormula	19	-	950.5183	23.81049
952.5352@24.13251				(951.5271, 3121.4575)(952.5293, 1608.1866)(953.532, 620.9	952.5352@24.13251		FindByFormula	27	-	952.5352	24.13251
952.6676@22.725416				(951.6634, 2639.2017)(952.6675, 1661.3539)(953.6581, 936.	952.6676@22.725416		FindByFormula	23	-	952.6676	22.725416
952.7013@22.91744				(951.6939, 2234.6711)(952.69464, 1425.3011)(953.6948, 65	952.7013@22.91744		FindByFormula	28	-	952.7013	22.91744
954.0963@22.742481				(953.08844, 1496.3372)(954.08997, 597.0347)	954.0963@22.742481		FindByFormula	28	-	954.0963	22.742481
954.4813@12.198559				(953.47394, 1516.9784)(954.4754, 891.615)	954.4813@12.198559		FindByFormula	6	-	954.4813	12.198559
956.1108@22.95032				(955.10486, 2042.587)(956.10187, 856.9478)	956.1108@22.95032		FindByFormula	28	-	956.1108	22.95032
956.9781@0.67696446				(955.9721, 14630.851)(956.9751, 3080.2615)(957.96985, 51	956.9781@0.67696446		FindByFormula	28	-	956.9781	0.67696446
958.1287@23.18668				(957.1204, 2662.1453)(958.1221, 992.5798)	958.1287@23.18668		FindByFormula	28	-	958.1287	23.18668
958.1891@0.80716604				(957.18243, 8670.87)(958.18463, 3288.6648)(959.1817, 184	958.1891@0.80716604		FindByFormula	6	-	958.1891	0.80716604
958.7182@22.927029				(957.7113, 3649.9666)(958.71423, 2438.2375)(959.716, 100	958.7182@22.927029		FindByFormula	25	-	958.7182	22.927029
961.5246@24.127699				(960.5174, 1248.1901)(961.52057, 694.91425)	961.5246@24.127699		FindByFormula	7	-	961.5246	24.127699
961.5559@25.16651				(960.54846, 725.70703)(961.5492, 413.31747)	961.5559@25.16651		FindByFormula	20	-	961.5559	25.16651
961.7809@0.58430463				(960.78314, 3411.6404)(961.7887, 1104.6832)(962.7918, 10	961.7809@0.58430463		FindByFormula	23	-	961.7809	0.58430463
963.5356@24.451153				(962.5313, 962.1828)(963.5313, 541.5671)(964.5304, 216.62	963.5356@24.451153		FindByFormula	7	-	963.5356	24.451153
963.5419@24.244617				(962.5331, 1849.3342)(963.5347, 1024.0623)(964.53644, 38	963.5419@24.244617		FindByFormula	14	-	963.5419	24.244617
963.5438@24.433931				(962.53253, 4812.178)(963.5341, 2554.2686)(964.5335, 890.	963.5438@24.433931		FindByFormula	21	-	963.5438	24.433931
964.1985@0.77649945				(963.1914, 9970.6455)(964.19476, 3639.327)(965.19165, 14	964.1985@0.77649945		FindByFormula	6	-	964.1985	0.77649945
965.5593@24.655502				(964.54706, 3535.2217)(965.55, 1938.2175)(966.5469, 888.6	965.5593@24.655502		FindByFormula	19	-	965.5593	24.655502
967.5749@25.17143				(966.56323, 4254.3496)(967.56635, 2302.818)(968.5648, 82	967.5749@25.17143		FindByFormula	25	-	967.5749	25.17143
968.4186@13.099865				(967.4109, 1835.5057)(968.4112, 1113.3923)(969.4151, 500.	968.4186@13.099865		FindByFormula	26	-	968.4186	13.099865
969.5907@25.74866				(968.58, 849.63745)(969.58563, 492.07535)	969.5907@25.74866		FindByFormula	24	-	969.5907	25.74866
970.0489@22.452425				(969.04236, 1331.6052)(970.0435, 482.97995)	970.0489@22.452425		FindByFormula	28	-	970.0489	22.452425
970.6544@22.714334				(969.6464, 1278.1978)(970.6489, 812.8377)	970.6544@22.714334		FindByFormula	23	-	970.6544	22.714334
973.1458@0.8071661				(972.13947, 5970.0747)(973.1469, 3734.718)(974.1525, 143	973.1458@0.8071661		FindByFormula	6	-	973.1458	0.8071661
973.2642@22.120821				(972.25714, 1275.3774)(973.2578, 604.7957)	973.2642@22.120821		FindByFormula	24	-	973.2642	22.120821
975.2786@22.430065				(974.27057, 1017.9291)(975.27386, 517.6909)	975.2786@22.430065		FindByFormula	22	-	975.2786	22.430065
976.6711@22.716951				(975.6641, 1944.9254)(976.6687, 1364.2205)(977.66406, 76	976.6711@22.716951		FindByFormula	24	-	976.6711	22.716951
980.1707@0.77266604				(979.1646, 5253.24)(980.16705, 2002.3568)(981.1592, 1414.	980.1707@0.77266604		FindByFormula	6	-	980.1707	0.77266604
981.5181@24.339703				(980.5085, 1004.0641)(981.51154, 600.438)	981.5181@24.339703		FindByFormula	5	-	981.5181	24.339703
984.3693@22.730658				(983.36273, 3396.513)(984.36786, 1693.3698)(985.3704, 66	984.3693@22.730658		FindByFormula	24	-	984.3693	22.730658
986.4176@23.184006				(985.40906, 1388.0627)(986.41364, 771.1708)	986.4176@23.184006		FindByFormula	28	-	986.4176	23.184006
987.536@24.185728				(986.532, 1378.23)(987.5342, 841.6601)	987.536@24.185728		FindByFormula	6	-	987.536	24.185728
987.5417@24.357668				(986.5352, 5851.63)(987.5386, 3313.7473)(988.54535, 1306.	987.5417@24.357668		FindByFormula	7	-	987.5417	24.357668
988.4018@22.932953				(987.3943, 5866.3027)(988.39844, 2849.1177)(989.4011, 11	988.4018@22.932953		FindByFormula	26	-	988.4018	22.932953
989.5563@24.561628				(988.5447, 1425.535)(989.5494, 786.5259)(990.5482, 552.74	989.5563@24.561628		FindByFormula	12	-	989.5563	24.561628
990.3873@22.72658				(989.3799, 2628.8333)(990.3858, 1312.5463)(991.3882, 554.	990.3873@22.72658		FindByFormula	24	-	990.3873	22.72658
991.5681@25.086418				(990.56415, 2576.4316)(991.56714, 1491.5833)(992.56635,	991.5681@25.086418		FindByFormula	25	-	991.5681	25.086418
992.4333@23.181005				(991.42487, 4157.11)(992.42957, 2107.8572)(993.43146, 82	992.4333@23.181005		FindByFormula	28	-	992.4333	23.181005
993.5878@25.416513				(992.58105, 2112.9265)(993.58325, 1227.9333)(994.57916,	993.5878@25.416513		FindByFormula	6	-	993.5878	25.416513
994.4194@22.931183				(993.41144, 3896.1406)(994.4163, 1982.8374)(995.4182, 77	994.4194@22.931183		FindByFormula	26	-	994.4194	22.931183
995.1276@0.79599935				(994.12115, 4096.9995)(995.1281, 2897.4001)(996.13116, 1	995.1276@0.79599935		FindByFormula	6	-	995.1276	0.79599935
996.054@22.584139				(995.0505, 1975.3514)(996.0413, 713.9184)	996.054@22.584139		FindByFormula	13	-	996.054	22.584139
996.6188@22.10788				(995.6103, 1821.9175)(996.6108, 1097.1975)(997.6129, 440.	996.6188@22.10788		FindByFormula	8	-	996.6188	22.10788
998.4517@23.18197				(997.44183, 1997.028)(998.4461, 1059.1013)	998.4517@23.18197		FindByFormula	28	-	998.4517	23.18197
ACETAMINOPHEN (TN TYLENOL) (CAS# 103-9	ACETAMINOPHEN (TN TYLENOL) (CAS# 103-9	ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M-H)-	103-90-2	(150.05568, 1074.4893)(151.05449, 108.08929)	ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M-H)-	C06804	FindByFormula	14	-	151.0625	3.0774937
ADENOSINE (CAS# 58-61-7); (M+HCOO)-	ADENOSINE (CAS# 58-61-7); (M+HCOO)-	ADENOSINE (CAS# 58-61-7); (M+HCOO)- [, tgt=83.73, ov	58-61-7	(312.09454, 1059.1605)(313.0941, 151.7643)(314.0918, 130.	ADENOSINE (CAS# 58-61-7); (M+HCOO)-	C00212	FindByFormula	21	-	267.0961	1.765572
ADENOSINE 2',3'-CYCLIC MONOPHOSPHATE (	ADENOSINE 2',3'-CYCLIC MONOPHOSPHATE (	ADENOSINE 2',3'-CYCLIC MONOPHOSPHATE (CAS# 634-01	634-01-5	(328.0426, 509.1)(329.0529, 136.46)	ADENOSINE 2',3'-CYCLIC MONOPHOSPHATE (CAS# 634-01-5); (M-H)-		FindByFormula	1	-	329.0515	1.4580019
ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-	ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-	ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-73-2); (M-H	1053-73-2	(426.0256, 501.10165)(427.02444, 116.6)(428.0085, 25.59)	ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-73-2); (M-H)-	C00054	FindByFormula	6	-	427.0323	1.2408347
ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-1	ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-1	ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-19-8); (M-H)	61-19-8	(346.05518, 1820.3699)(347.05896, 248.66)(348.05765, 97.1	ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-19-8); (M-H)-		FindByFormula	4	-	347.0636	1.1850009
ADENOSINE 5'-PHOSPHOSULFATE (CAS# 485-	ADENOSINE 5'-PHOSPHOSULFATE (CAS# 485-	ADENOSINE 5'-PHOSPHOSULFATE (CAS# 485-84-7); (M-H	485-84-7	(426.01123, 851.719)(427.01007, 219.51454)(428.0088, 64.5	ADENOSINE 5'-PHOSPHOSULFATE (CAS# 485-84-7); (M-H)-	C00224	FindByFormula	11	-	427.0176	0.5995457
ADIPIC ACID (CAS# 124-04-9); (M-H)-	ADIPIC ACID (CAS# 124-04-9); (M-H)-	ADIPIC ACID (CAS# 124-04-9); (M-H)- [, tgt=82.69, overa	124-04-9	(145.05101, 4430.9727)(146.04973, 232.79387)(147.05116,	ADIPIC ACID (CAS# 124-04-9); (M-H)-	C06104	FindByFormula	26	-	146.0582	3.5393395
ALLANTOIN (CAS# 97-59-6); (M-H)-	ALLANTOIN (CAS# 97-59-6); (M-H)-	ALLANTOIN (CAS# 97-59-6); (M-H)- [, tgt=72.12, overall=	97-59-6	(157.03647, 2142.0544)(158.03671, 262.71286)(159.03717,	ALLANTOIN (CAS# 97-59-6); (M-H)-		FindByFormula	14	-	158.0429	0.6887862
ALLOSE (CAS# 2595-97-3); (M-H)+[-H2O]	ALLOSE (CAS# 2595-97-3); (M-H)+[-H2O]	ALLOSE (CAS# 2595-97-3); (M-H)+[-H2O] [, tgt=84.53, ov	2595-97-3	(161.04466, 2531.196)(162.04382, 84.457504)(163.0411, 67.	ALLOSE (CAS# 2595-97-3); (M-H)+[-H2O]	C01487	FindByFormula	20	-	180.0634	1.6113994
ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 2	ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 22	ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 2255-14-3); (	2255-14-3	(259.0233, 3648.1812)(260.02444, 614.36)(261.0225, 608.64	ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 2255-14-3); (M-H)-		FindByFormula	13	-	260.0289	0.74800026
ALPHA-HYDROXYISOBUTYRIC ACID (CAS# 594	ALPHA-HYDROXYISOBUTYRIC ACID (CAS# 594	ALPHA-HYDROXYISOBUTYRIC ACID (CAS# 594-61-6); (M-I	594-61-6	(103.04042, 969.2825)(104.04213, 32.147503)	ALPHA-HYDROXYISOBUTYRIC ACID (CAS# 594-61-6); (M-H)-		FindByFormula	4	-	104.0478	1.7777481
ALPHA-KETO-GLUTARATE (CAS# 328-50-7); (	ALPHA-KETO-GLUTARATE (CAS# 328-50-7); (M	ALPHA-KETO-GLUTARATE (CAS# 328-50-7); (M-H)- [, tgt=	328-50-7	(145.01434, 4069.3823)(146.02551, 122.38)	ALPHA-KETO-GLUTARATE (CAS# 328-50-7); (M-H)-		FindByFormula	4	-	146.022	0.94199944
ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M	ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+	ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+HCOO)- [, t	463-40-1	(323.2211, 78457.055)(324.22437, 14621.172)(325.22064, 1	ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+HCOO)-		FindByFormula	28	-	278.2229	22.851686
ARABITOL (CAS# 7643-75-6); (M+Cl)-	ARABITOL (CAS# 7643-75-6); (M+Cl)-	ARABITOL (CAS# 7643-75-6); (M+Cl)- [, tgt=68.61, overall	7643-75-6	(187.03821, 757.44446)(188.04263, 80.17556)(189.03429, 6	ARABITOL (CAS# 7643-75-6); (M+Cl)-	C00532	FindByFormula	9	-	152.0671	0.6824447
ARABITOL (CAS# 7643-75-6); (M+HCOO)-	ARABITOL (CAS# 7643-75-6); (M+HCOO)-	ARABITOL (CAS# 7643-75-6); (M+HCOO)- [, tgt=53.04, ov	7643-75-6	(197.06555, 1192.485)(198.0701, 295.4)	ARABITOL (CAS# 7643-75-6); (M+HCOO)-	C00532	FindByFormula	2	-	152.0675	0.7364992
ARACHIDIC ACID (CAS# 506-30-9); (M-H)-	ARACHIDIC ACID (CAS# 506-30-9); (M-H)-	ARACHIDIC ACID (CAS# 506-30-9); (M-H)- [, tgt=82.77, o	506-30-9	(311.2947, 2559.1099)(312.29727, 594.6778)(313.29803, 10	ARACHIDIC ACID (CAS# 506-30-9); (M-H)-	C06425	FindByFormula	27	-	312.3017	23.579536
ARACHIDONATE (CAS# 506-32-1); (M-H)-	ARACHIDONATE (CAS# 506-32-1); (M-H)-	ARACHIDONATE (CAS# 506-32-1); (M-H)- [, tgt=97.09, ov	506-32-1	(303.23383, 426050.72)(304.2372, 92981.99)(305.23993, 11	ARACHIDONATE (CAS# 506-32-1); (M-H)-		FindByFormula	28	-	304.2413	22.700317
ASPARAGINE (CAS# 70-47-3); (M-H)-	ASPARAGINE (CAS# 70-47-3); (M-H)-	ASPARAGINE (CAS# 70-47-3); (M-H)- [, tgt=80.24, overall	70-47-3	(131.04565, 3545.7002)(132.03854, 66.13)(133.0431, 49.78)	ASPARAGINE (CAS# 70-47-3); (M-H)-		FindByFormula	2	-	132.0527	0.6375007
ASPARTATE (CAS# 56-84-8); (M-H)-	ASPARTATE (CAS# 56-84-8); (M-H)-	ASPARTATE (CAS# 56-84-8); (M-H)- [, tgt=89.36, overall=	56-84-8	(132.02979, 10134.772)(133.02962, 487.85333)(134.03276,	ASPARTATE (CAS# 56-84-8); (M-H)-		FindByFormula	21	-	133.0367	0.6420479
AZELAIC ACID (CAS# 123-99-9); (M-H)-	AZELAIC ACID (CAS# 123-99-9); (M-H)-	AZELAIC ACID (CAS# 123-99-9); (M-H)- [, tgt=96.57, over	123-99-9	(187.09763, 14757.177)(188.10095, 1535.3376)(189.10541,	AZELAIC ACID (CAS# 123-99-9); (M-H)-	C08261	FindByFormula	28	-	188.1049	10.678747
BEHENIC ACID (CAS# 112-85-6); (M-H)-	BEHENIC ACID (CAS# 112-85-6); (M-H)-	BEHENIC ACID (CAS# 112-85-6); (M-H)- [, tgt=94.76, over	112-85-6	(339.32632, 3728.59)(340.32953, 929.08954)(341.33157, 16	BEHENIC ACID (CAS# 112-85-6); (M-H)-		FindByFormula	25	-	340.3342	24.084297
BENZALDEHYDE (CAS# 100-52-7); (M+HCOO)	BENZALDEHYDE (CAS# 100-52-7); (M+HCOO)	BENZALDEHYDE (CAS# 100-52-7); (M+HCOO)- [, tgt=81.8	100-52-7	(151.0402, 588.77)(152.0353, 29.77)	BENZALDEHYDE (CAS# 100-52-7); (M+HCOO)-	C00261	FindByFormula	1	-	106.0416	4.672963
BENZOATE (CAS# 65-85-0); (M-H)-	BENZOATE (CAS# 65-85-0); (M-H)-	BENZOATE (CAS# 65-85-0); (M-H)- [, tgt=73.07, overall=7	65-85-0	(121.02974, 57638.98)(122.029236, 8419.261)(123.030235,	BENZOATE (CAS# 65-85-0); (M-H)-	C00180	FindByFormula	20	-	122.0365	4.928725
BETA-ALANINE (CAS# 107-95-9); (M-H)-	BETA-ALANINE (CAS# 107-95-9); (M-H)-	BETA-ALANINE (CAS# 107-95-9); (M-H)- [, tgt=83.49, ove	107-95-9	(88.03999, 9497.932)(89.038376, 325.11804)(90.041565, 42.	BETA-ALANINE (CAS# 107-95-9); (M-H)-		FindByFormula	10	-	89.047	0.6941005
BETA-MALTOSE (CAS# 69-79-4); (2M+Cl)-[-H	BETA-MALTOSE (CAS# 69-79-4); (2M+Cl)-[-H2	BETA-MALTOSE (CAS# 69-79-4); (2M+Cl)-[-H2O] [, tgt=9	69-79-4	(701.19147, 10831.811)(702.195, 3127.9875)(703.19006, 43	BETA-MALTOSE (CAS# 69-79-4); (2M+Cl)-[-H2O]	C00208	FindByFormula	22	-	342.1171	0.7156367
BETA-MALTOSE (CAS# 69-79-4); (2M-H)-[-H2	BETA-MALTOSE (CAS# 69-79-4); (2M-H)-[-H2	BETA-MALTOSE (CAS# 69-79-4); (2M-H)-[-H2O] [, tgt=46.	69-79-4	(665.2148, 423.73627)(666.2159, 123.968414)(667.21014, 6	BETA-MALTOSE (CAS# 69-79-4); (2M-H)-[-H2O]	C00208	FindByFormula	19	-	342.1157	0.7932636
BETA-MALTOSE (CAS# 69-79-4); (M+Cl)-	BETA-MALTOSE (CAS# 69-79-4); (M+Cl)-	BETA-MALTOSE (CAS# 69-79-4); (M+Cl)- [, tgt=97.82, ove	69-79-4	(377.08475, 25323.936)(378.08945, 4187.432)(379.08237, 1	BETA-MALTOSE (CAS# 69-79-4); (M+Cl)-	C00208	FindByFormula	24	-	342.116	0.7031669
BETA-MALTOSE (CAS# 69-79-4); (M+HCOO)-	BETA-MALTOSE (CAS# 69-79-4); (M+HCOO)-	BETA-MALTOSE (CAS# 69-79-4); (M+HCOO)- [, tgt=73.99	69-79-4	(387.11395, 959.8128)(388.11154, 277.31714)(389.1217, 11	BETA-MALTOSE (CAS# 69-79-4); (M+HCOO)-	C00208	FindByFormula	7	-	342.1152	0.7178578
BIOTIN (CAS# 58-85-5); (M-H)-	BIOTIN (CAS# 58-85-5); (M-H)-	BIOTIN (CAS# 58-85-5); (M-H)- [, tgt=76.88, overall=76.8	58-85-5	(243.08134, 605.13196)(244.07878, 77.23399)(245.07874, 4	BIOTIN (CAS# 58-85-5); (M-H)-		FindByFormula	5	-	244.0887	6.227297
C10 H10 Cl3 N8 O3 P3 S	C10 H10 Cl3 N8 O3 P3 S	[C10 H10 Cl3 N8 O3 P3 S, tgt=80.17, overall=80.17]		(554.85864, 420.4025)(555.8624, 85.96)(556.8664, 1212.937	C10 H10 Cl3 N8 O3 P3 S		FindByFormula	6	-	519.8876	20.970896
C10 H10 N6 O3	C10 H10 N6 O3	[C10 H10 N6 O3, tgt=83.68, overall=83.68]		(297.05585, 160.41501)(298.0512, 46.98)(299.0438, 42.47)(	C10 H10 N6 O3		FindByFormula	14	-	262.0825	15.632241
C10 H11 N5	C10 H11 N5	[C10 H11 N5, tgt=99.69, overall=99.69]		(236.0654, 55.46)(246.09773, 73.40428)(200.09416, 6414.24	C10 H11 N5		FindByFormula	28	-	201.1014	3.8769908
C10 H11 N5 O4	C10 H11 N5 O4	[C10 H11 N5 O4, tgt=94.93, overall=94.93]		(300.0475, 652.9437)(301.0464, 141.90929)(302.0466, 916.6	C10 H11 N5 O4		FindByFormula	19	-	265.0813	1.1459478
C10 H12 N4 O5	C10 H12 N4 O5	[C10 H12 N4 O5, tgt=98.78, overall=98.78]		(303.05072, 13325.942)(304.05573, 2154.4114)(305.04822,	C10 H12 N4 O5		FindByFormula	27	-	268.0815	1.8237039
C10 H12 N6 O4	C10 H12 N6 O4	[C10 H12 N6 O4, tgt=88.18, overall=88.18]		(315.0699, 56.4)(325.0917, 90.566)(279.08527, 7968.5522)(	C10 H12 N6 O4		FindByFormula	6	-	280.0926	4.3029866
C10 H13 Cl N6 O	C10 H13 Cl N6 O	[C10 H13 Cl N6 O, tgt=95.95, overall=95.95]		(313.08215, 88.8)(314.07983, 41.05)(267.07788, 3914.8174)	C10 H13 Cl N6 O		FindByFormula	27	-	268.0849	13.105981
C10 H13 N5 O	C10 H13 N5 O	[C10 H13 N5 O, tgt=99.83, overall=99.83]		(254.08186, 86539.13)(255.08427, 11143.851)(256.07898, 2	C10 H13 N5 O		FindByFormula	28	-	219.1125	3.8769913
C10 H13 N5 O5	C10 H13 N5 O5	[C10 H13 N5 O5, tgt=96.99, overall=96.99]		(318.06155, 2601.762)(319.06262, 329.47498)(320.05856, 1	C10 H13 N5 O5		FindByFormula	23	-	283.0917	1.8198265
C10 H16 N2 O4	C10 H16 N2 O4	[C10 H16 N2 O4, tgt=99.53, overall=99.53]		(263.0798, 1186.7847)(264.08774, 197.10583)(265.07523, 5	C10 H16 N2 O4		FindByFormula	25	-	228.1115	4.1578684
C10 H16 N2 O8	C10 H16 N2 O8	[C10 H16 N2 O8, tgt=39.92, overall=39.92]		(327.06036, 268.90155)(328.0547, 203.245)(329.05707, 49.0	C10 H16 N2 O8		FindByFormula	17	-	292.0912	0.77452934
C10 H18 Cl3 N4 O7 P3 S2	C10 H18 Cl3 N4 O7 P3 S2	[C10 H18 Cl3 N4 O7 P3 S2, tgt=77.71, overall=77.71]		(604.8591, 192.0)(605.8734, 116.855)(606.8559, 379.77)(60	C10 H18 Cl3 N4 O7 P3 S2		FindByFormula	7	-	567.8876	20.925045
C10 H19 N4 O4 P	C10 H19 N4 O4 P	[C10 H19 N4 O4 P, tgt=94.27, overall=94.27]		(325.0838, 519.4766)(326.08383, 92.18667)(327.0778, 181.8	C10 H19 N4 O4 P		FindByFormula	9	-	290.1143	18.64101
C10 H20 N2 O P2 S	C10 H20 N2 O P2 S	[C10 H20 N2 O P2 S, tgt=96.89, overall=96.89]		(313.04105, 1804.6967)(314.04544, 331.15997)(315.04047,	C10 H20 N2 O P2 S		FindByFormula	8	-	278.0748	9.856897
C10 H20 O6 P2 S	C10 H20 O6 P2 S	[C10 H20 O6 P2 S, tgt=93.22, overall=93.22]		(365.0172, 225.3)(366.0272, 38.1)(367.0063, 42.93)(375.045	C10 H20 O6 P2 S		FindByFormula	9	-	330.0462	0.81222194
C10 H5 N5	C10 H5 N5	[C10 H5 N5, tgt=93.57, overall=93.57]		(194.04736, 4474.118)(195.0512, 425.26334)(196.05174, 82.	C10 H5 N5		FindByFormula	6	-	195.055	6.1876388
C10 H6 S2	C10 H6 S2	[C10 H6 S2, tgt=78.51, overall=78.51]		(234.99152, 116.715004)(188.9854, 45308.87)(189.98909, 3	C10 H6 S2		FindByFormula	6	-	189.9927	2.4389956
C10 H8 N2 O19 P2	C10 H8 N2 O19 P2	[C10 H8 N2 O19 P2, tgt=98.57, overall=98.57]		(556.87714, 203.038)(557.88293, 71.5175)(558.8732, 74.853	C10 H8 N2 O19 P2		FindByFormula	22	-	521.9185	0.581773
C10 H8 N3 O9 P	C10 H8 N3 O9 P	[C10 H8 N3 O9 P, tgt=60.53, overall=60.53]		(379.9758, 97.80334)(380.9688, 108.74)(381.98, 22.08)(389.	C10 H8 N3 O9 P		FindByFormula	20	-	345.002	0.7776501
C10 H9 N O2	C10 H9 N O2	[C10 H9 N O2, tgt=93.03, overall=93.03]		(220.0618, 73.95)(174.05566, 1912.0499)(175.05269, 246.34	C10 H9 N O2		FindByFormula	7	-	175.0626	6.838254
C10 H9 N3	C10 H9 N3	[C10 H9 N3, tgt=88.71, overall=88.71]		(216.0714, 61.81)(170.07343, 4528.2026)(171.07593, 726.33	C10 H9 N3		FindByFormula	8	-	171.0807	15.69971
C11 H10 N10	C11 H10 N10	[C11 H10 N10, tgt=96.89, overall=96.89]		(317.08002, 1066.1599)(318.07462, 268.57004)(319.07434,	C11 H10 N10		FindByFormula	9	-	282.1088	4.2390976
C11 H10 N6 O2	C11 H10 N6 O2	[C11 H10 N6 O2, tgt=96.48, overall=96.48]		(293.05356, 114.381424)(294.04498, 28.329998)(295.0509,	C11 H10 N6 O2		FindByFormula	10	-	258.0865	13.0329685
C11 H11 N O3	C11 H11 N O3	[C11 H11 N O3, tgt=59.90, overall=59.90]		(204.06648, 3522.6355)(205.06638, 501.54218)(206.07188,	C11 H11 N O3		FindByFormula	14	-	205.074	7.355265
C11 H13 N3 O5	C11 H13 N3 O5	[C11 H13 N3 O5, tgt=71.16, overall=71.16]		(302.05933, 323.63202)(303.0633, 323.32)(312.0846, 182.63	C11 H13 N3 O5		FindByFormula	15	-	267.0858	0.96993375
C11 H13 N7 O3 P2	C11 H13 N7 O3 P2	[C11 H13 N7 O3 P2, tgt=82.42, overall=82.42]		(388.02155, 181.38)(389.02612, 52.17)(390.0176, 413.14502	C11 H13 N7 O3 P2		FindByFormula	8	-	353.0546	3.5289946
C11 H13 N8 O2 P3	C11 H13 N8 O2 P3	[C11 H13 N8 O2 P3, tgt=50.04, overall=50.04]		(427.03775, 143.145)(381.0302, 4826.81)(382.0342, 961.965	C11 H13 N8 O2 P3		FindByFormula	8	-	382.0383	1.0341246
C11 H14 N6 O S3	C11 H14 N6 O S3	[C11 H14 N6 O S3, tgt=71.89, overall=71.89]		(377.01492, 107.285)(378.0203, 45.17)(379.0244, 21.8)(387.	C11 H14 N6 O S3		FindByFormula	18	-	342.0403	1.3553894
C11 H14 O19 P4 S	C11 H14 O19 P4 S	[C11 H14 O19 P4 S, tgt=97.06, overall=97.06]		(640.8401, 751.0178)(641.83936, 303.66833)(642.83325, 72	C11 H14 O19 P4 S		FindByFormula	25	-	605.8798	0.58600014
C11 H14 O3	C11 H14 O3	[C11 H14 O3, tgt=91.01, overall=91.01]		(229.0587, 55.47)(239.08708, 73.10167)(193.08705, 2988.24	C11 H14 O3		FindByFormula	28	-	194.0936	15.073958
C11 H16 O3	C11 H16 O3	[C11 H16 O3, tgt=53.54, overall=53.54]		(231.07764, 75.64111)(241.10696, 824.58856)(242.1079, 10	C11 H16 O3		FindByFormula	20	-	196.1082	15.479227
C11 H17 O20 P3 S4	C11 H17 O20 P3 S4	[C11 H17 O20 P3 S4, tgt=86.41, overall=86.41]		(724.81635, 419.68127)(725.81213, 213.23141)(726.82324,	C11 H17 O20 P3 S4		FindByFormula	28	-	689.8414	0.5847502
C11 H18 N2 O S2	C11 H18 N2 O S2	[C11 H18 N2 O S2, tgt=82.89, overall=82.89]		(293.05548, 131.30333)(294.06143, 177.78333)(303.0801, 1	C11 H18 N2 O S2		FindByFormula	24	-	258.0856	1.4993753
C11 H18 N2 O4	C11 H18 N2 O4	[C11 H18 N2 O4, tgt=99.43, overall=99.43]		(277.0966, 206.17667)(278.09506, 52.49583)(279.08978, 15	C11 H18 N2 O4		FindByFormula	28	-	242.1268	6.5225134
C11 H19 N3 O3	C11 H19 N3 O3	[C11 H19 N3 O3, tgt=89.38, overall=89.38]		(276.11182, 1063.4781)(277.11105, 157.93666)(278.10858,	C11 H19 N3 O3		FindByFormula	21	-	241.142	5.0091166
C11 H19 N7 O	C11 H19 N7 O	[C11 H19 N7 O, tgt=95.22, overall=95.22]		(300.13577, 612.2709)(301.13843, 141.44211)(302.13254, 2	C11 H19 N7 O		FindByFormula	28	-	265.1656	15.762439
C11 H19 P3	C11 H19 P3	[C11 H19 P3, tgt=99.66, overall=99.66]		(279.04025, 155004.17)(280.04376, 17048.238)(281.0368, 5	C11 H19 P3		FindByFormula	28	-	244.0702	1.3647501
C11 H20 Cl P3	C11 H20 Cl P3	[C11 H20 Cl P3, tgt=98.23, overall=98.23]		(315.0191, 76.35285)(316.0132, 31.12)(317.0274, 98.85)(32	C11 H20 Cl P3		FindByFormula	28	-	280.0472	1.3471432
C11 H22 N2 O3	C11 H22 N2 O3	[C11 H22 N2 O3, tgt=86.08, overall=86.08]		(265.1302, 481.2046)(266.13278, 141.32666)(267.1261, 147.	C11 H22 N2 O3		FindByFormula	24	-	230.1627	3.6009905
C11 H22 O2 S4	C11 H22 O2 S4	[C11 H22 O2 S4, tgt=93.02, overall=93.02]		(349.01428, 1059.5074)(350.0163, 133.42499)(351.0135, 46	C11 H22 O2 S4		FindByFormula	6	-	314.0496	3.5108242
C11 H9 Cl N8 O	C11 H9 Cl N8 O	[C11 H9 Cl N8 O, tgt=58.71, overall=58.71]		(339.0272, 95.02779)(340.0221, 59.649998)(341.01398, 65.2	C11 H9 Cl N8 O		FindByFormula	28	-	304.0588	1.6595358
C12 H12 N8 O4	C12 H12 N8 O4	[C12 H12 N8 O4, tgt=81.66, overall=81.66]		(367.06967, 138.755)(368.07007, 33.098)(377.0956, 76.4185	C12 H12 N8 O4		FindByFormula	23	-	332.0992	5.198663
C12 H14 Cl O12 P	C12 H14 Cl O12 P	[C12 H14 Cl O12 P, tgt=73.65, overall=73.65]		(450.96207, 1420.4337)(451.9631, 220.86)(452.95956, 1353.	C12 H14 Cl O12 P		FindByFormula	12	-	415.9927	0.69774985
C12 H14 N6 O2	C12 H14 N6 O2	[C12 H14 N6 O2, tgt=97.58, overall=97.58]		(319.10886, 81.763336)(273.11118, 6441.6055)(274.11465,	C12 H14 N6 O2		FindByFormula	6	-	274.1184	18.851236
C12 H14 N8 O9	C12 H14 N8 O9	[C12 H14 N8 O9, tgt=98.20, overall=98.20]		(449.05194, 80.74571)(450.0673, 30.1)(459.07593, 516.075)	C12 H14 N8 O9		FindByFormula	28	-	414.0881	13.100551
C12 H14 O4	C12 H14 O4	[C12 H14 O4, tgt=94.26, overall=94.26]		(257.06384, 69.009995)(267.0829, 67.380005)(221.08232, 3	C12 H14 O4		FindByFormula	27	-	222.089	14.446555
C12 H15 N O4	C12 H15 N O4	[C12 H15 N O4, tgt=87.89, overall=87.89]		(272.07266, 747.4443)(273.07126, 117.49334)(274.07236, 3	C12 H15 N O4		FindByFormula	24	-	237.1004	8.659585
C12 H15 N3 O2 P2	C12 H15 N3 O2 P2	[C12 H15 N3 O2 P2, tgt=78.56, overall=78.56]		(330.02853, 70.26)(294.056, 4769.675)(295.05954, 655.0666	C12 H15 N3 O2 P2		FindByFormula	6	-	295.0635	8.581113
C12 H16	C12 H16	[C12 H16, tgt=91.06, overall=91.06]		(205.12347, 2838.825)(206.12683, 448.885)(159.11772, 187	C12 H16		FindByFormula	6	-	160.1252	18.842905
C12 H16 Cl N O S	C12 H16 Cl N O S	[C12 H16 Cl N O S, tgt=75.14, overall=75.14]		(292.027, 57.25)(293.0455, 318.0)(302.06186, 621.2233)(30	C12 H16 Cl N O S		FindByFormula	23	-	257.0664	0.7011305
C12 H16 O2	C12 H16 O2	[C12 H16 O2, tgt=99.73, overall=99.73]		(227.08751, 609.5062)(228.08894, 89.18)(237.1103, 151.547	C12 H16 O2		FindByFormula	8	-	192.1151	12.961586
C12 H16 O5	C12 H16 O5	[C12 H16 O5, tgt=83.45, overall=83.45]		(275.0696, 53.51)(285.098, 59.174)(239.0933, 22965.766)(2	C12 H16 O5		FindByFormula	17	-	240.1	15.625771
C12 H16 O6	C12 H16 O6	[C12 H16 O6, tgt=70.89, overall=70.89]		(291.0672, 63.934998)(255.08792, 8061.854)(256.08932, 11	C12 H16 O6		FindByFormula	17	-	256.095	9.885918
C12 H18 O3	C12 H18 O3	[C12 H18 O3, tgt=99.61, overall=99.61]		(245.09491, 564.6967)(246.09442, 79.44703)(247.0893, 213.	C12 H18 O3		FindByFormula	28	-	210.126	13.099695
C12 H20 O3	C12 H20 O3	[C12 H20 O3, tgt=98.53, overall=98.53]		(257.13898, 64.41471)(211.13374, 3127.8464)(212.13696, 4	C12 H20 O3		FindByFormula	28	-	212.1413	14.720131
C12 H23 Cl O11	C12 H23 Cl O11	[C12 H23 Cl O11, tgt=97.96, overall=97.96]		(413.06622, 65.655)(423.09256, 132.49667)(424.10626, 59.0	C12 H23 Cl O11		FindByFormula	24	-	378.0927	0.7028335
C12 H23 N O3	C12 H23 N O3	[C12 H23 N O3, tgt=99.25, overall=99.25]		(264.1347, 125.806435)(265.13593, 34.694286)(266.13007,	C12 H23 N O3		FindByFormula	26	-	229.1678	14.119108
C12 H24 O2	C12 H24 O2	[C12 H24 O2, tgt=98.77, overall=98.77]		(245.17613, 93.99777)(199.17044, 6812.3364)(200.17395, 9	C12 H24 O2		FindByFormula	28	-	200.1779	21.744308
C12 H27 N4 O P3 S	C12 H27 N4 O P3 S	[C12 H27 N4 O P3 S, tgt=87.05, overall=87.05]		(403.07877, 143.46858)(404.0759, 20.56)(405.0558, 23.86)(	C12 H27 N4 O P3 S		FindByFormula	28	-	368.1137	0.6706788
C12 H3 Cl N3 P	C12 H3 Cl N3 P	[C12 H3 Cl N3 P, tgt=97.89, overall=97.89]		(289.94394, 10326.29)(290.94513, 1704.0797)(291.9409, 65	C12 H3 Cl N3 P		FindByFormula	28	-	254.9754	2.5028205
C12 H3 Cl O4	C12 H3 Cl O4	[C12 H3 Cl O4, tgt=67.78, overall=67.78]		(244.96387, 4844.6787)(245.9641, 1457.2645)(246.96156, 1	C12 H3 Cl O4		FindByFormula	11	-	245.9702	0.5513637
C12 H6 N6 O4	C12 H6 N6 O4	[C12 H6 N6 O4, tgt=97.16, overall=97.16]		(333.01422, 74.51)(343.0424, 51.48)(297.03876, 23511.691)	C12 H6 N6 O4		FindByFormula	7	-	298.046	8.18007
C12 H8 N5 P	C12 H8 N5 P	[C12 H8 N5 P, tgt=87.70, overall=87.70]		(252.0451, 4374.112)(253.04948, 680.98505)(254.0537, 167.	C12 H8 N5 P		FindByFormula	6	-	253.0524	6.5013022
C13 H11 N2 O2 P	C13 H11 N2 O2 P	[C13 H11 N2 O2 P, tgt=81.43, overall=81.43]		(293.02512, 72.50888)(294.03394, 21.185001)(295.01556, 5	C13 H11 N2 O2 P		FindByFormula	25	-	258.0561	18.328394
C13 H12 N10	C13 H12 N10	[C13 H12 N10, tgt=98.66, overall=98.66]		(353.1244, 68.56)(307.11755, 4806.029)(308.12033, 759.153	C13 H12 N10		FindByFormula	27	-	308.1247	16.893229
C13 H13 N7 O4	C13 H13 N7 O4	[C13 H13 N7 O4, tgt=66.72, overall=66.72]		(366.07355, 80.291435)(376.09604, 79.423996)(330.09796,	C13 H13 N7 O4		FindByFormula	14	-	331.1039	4.8006988
C13 H13 O28 P3 S	C13 H13 O28 P3 S	[C13 H13 O28 P3 S, tgt=94.22, overall=94.22]		(776.81775, 280.20746)(777.8198, 245.35417)(778.81964, 2	C13 H13 O28 P3 S		FindByFormula	22	-	741.8528	0.5845457
C13 H14 O	C13 H14 O	[C13 H14 O, tgt=90.30, overall=90.30]		(221.0763, 118.095)(222.0775, 37.85)(223.0663, 22.36)(231.	C13 H14 O		FindByFormula	8	-	186.1048	15.708082
C13 H14 O P2	C13 H14 O P2	[C13 H14 O P2, tgt=89.07, overall=89.07]		(283.0259, 61.42)(284.02835, 23.285)(285.0176, 21.6)(247.0	C13 H14 O P2		FindByFormula	24	-	248.0523	4.4078565
C13 H16 N2 O4	C13 H16 N2 O4	[C13 H16 N2 O4, tgt=85.27, overall=85.27]		(299.0776, 86.518745)(300.06992, 197.63335)(309.11038, 8	C13 H16 N2 O4		FindByFormula	27	-	264.1113	5.2273407
C13 H16 N4 O5 S	C13 H16 N4 O5 S	[C13 H16 N4 O5 S, tgt=94.21, overall=94.21]		(385.0802, 110.32294)(339.07687, 8714.869)(340.08057, 14	C13 H16 N4 O5 S		FindByFormula	28	-	340.0843	13.103872
C13 H16 O4	C13 H16 O4	[C13 H16 O4, tgt=98.04, overall=98.04]		(271.0688, 98.58)(281.1052, 589.94)(282.10385, 98.59667)(	C13 H16 O4		FindByFormula	7	-	236.1051	12.97862
C13 H18 N2 O9	C13 H18 N2 O9	[C13 H18 N2 O9, tgt=99.37, overall=99.37]		(381.0672, 72.26857)(382.0758, 44.89)(383.061, 43.02)(391.	C13 H18 N2 O9		FindByFormula	28	-	346.1003	13.0997305
C13 H19 N2 P S	C13 H19 N2 P S	[C13 H19 N2 P S, tgt=91.51, overall=91.51]		(301.0683, 157.33667)(311.09985, 283.66998)(312.09818, 1	C13 H19 N2 P S		FindByFormula	18	-	266.1	0.7088336
C13 H19 N5 O4	C13 H19 N5 O4	[C13 H19 N5 O4, tgt=89.40, overall=89.40]		(344.12045, 71.479996)(354.1428, 210.99916)(355.14297, 9	C13 H19 N5 O4		FindByFormula	25	-	309.1434	3.878429
C13 H20 N2 P2 S	C13 H20 N2 P2 S	[C13 H20 N2 P2 S, tgt=68.23, overall=68.23]		(333.04672, 77.75)(334.0416, 23.693335)(335.04932, 40.77)	C13 H20 N2 P2 S		FindByFormula	12	-	298.0823	15.695149
C13 H20 O2	C13 H20 O2	[C13 H20 O2, tgt=99.52, overall=99.52]		(243.12122, 82.44)(244.1371, 21.96)(245.1088, 27.36)(253.1	C13 H20 O2		FindByFormula	28	-	208.1467	14.839072
C13 H20 O4	C13 H20 O4	[C13 H20 O4, tgt=97.61, overall=97.61]		(285.1321, 50.23)(239.12878, 6484.643)(240.13193, 972.944	C13 H20 O4		FindByFormula	28	-	240.136	16.891094
C13 H21 Cl3 N12 O S	C13 H21 Cl3 N12 O S	[C13 H21 Cl3 N12 O S, tgt=69.17, overall=69.17]		(534.7923, 108.1275)(535.64014, 36.232002)(536.04175, 10	C13 H21 Cl3 N12 O S		FindByFormula	23	-	498.0741	3.6023822
C13 H22 O3	C13 H22 O3	[C13 H22 O3, tgt=90.65, overall=90.65]		(271.1552, 66.74077)(225.1497, 7480.236)(226.15305, 1111.	C13 H22 O3		FindByFormula	28	-	226.1569	14.55287

C13 H23 Cl N O5 P	C13 H23 Cl N O5 P	[C13 H23 Cl N O5 P, tgt=76.67, overall=76.67]	(374.06894, 373.774)(375.07788, 204.43001)(376.07092, 33	C13 H23 Cl N O5 P	FindByFormula	13 -	339.1001	10.485076
C13 H23 N2 O P S	C13 H23 N2 O P S	[C13 H23 N2 O P S, tgt=86.76, overall=86.76]	(321.09268, 269.72064)(322.0954, 43.00071)(323.08948, 13	C13 H23 N2 O P S	FindByFormula	21 -	286.127	1.4394292
C13 H24 N6 O2	C13 H24 N6 O2	[C13 H24 N6 O2, tgt=88.76, overall=88.76]	(331.1653, 88.61667)(332.16492, 27.323334)(333.1457, 63.8	C13 H24 N6 O2	FindByFormula	28 -	296.1972	22.448032
C13 H25 N O3	C13 H25 N O3	[C13 H25 N O3, tgt=99.46, overall=99.46]	(278.15146, 410.0848)(279.15085, 95.24387)(280.1461, 163.	C13 H25 N O3	FindByFormula	28 -	243.1838	15.760689
C13 H28 O6 S2	C13 H28 O6 S2	[C13 H28 O6 S2, tgt=51.63, overall=51.63]	(379.10556, 103.05399)(380.1091, 45.116665)(381.1009, 71.	C13 H28 O6 S2	FindByFormula	23 -	344.1319	3.5870783
C13 H3 Cl O5	C13 H3 Cl O5	[C13 H3 Cl O5, tgt=80.72, overall=80.72]	(318.9625, 242.29333)(272.95972, 20188.72)(273.96063, 62	C13 H3 Cl O5	FindByFormula	27 -	273.9663	0.5491853
C13 H3 N2 O5 P	C13 H3 N2 O5 P	[C13 H3 N2 O5 P, tgt=86.95, overall=86.95]	(332.94205, 62.861664)(333.93646, 218.7725)(334.9355, 43.	C13 H3 N2 O5 P	FindByFormula	14 -	297.9768	8.653025
C13 H31 N4 O3 P	C13 H31 N4 O3 P	[C13 H31 N4 O3 P, tgt=80.15, overall=80.15]	(357.17685, 193.85333)(358.1709, 44.3)(359.1771, 50.36)(3	C13 H31 N4 O3 P	FindByFormula	27 -	322.213	22.58755
C13 H32 N10	C13 H32 N10	[C13 H32 N10, tgt=44.60, overall=44.60]	(363.25092, 412.40768)(364.25394, 124.33099)(365.25107,	C13 H32 N10	FindByFormula	17 -	328.283	23.009085
C13 H33 N4 O3 P	C13 H33 N4 O3 P	[C13 H33 N4 O3 P, tgt=88.27, overall=88.27]	(359.1996, 84.0)(369.22046, 472.54642)(370.2285, 29.87)(3	C13 H33 N4 O3 P	FindByFormula	28 -	324.2284	22.851725
C13 H33 N4 O4 P	C13 H33 N4 O4 P	[C13 H33 N4 O4 P, tgt=91.50, overall=91.50]	(375.19037, 53.8525)(385.22293, 98.937775)(386.2429, 36.8	C13 H33 N4 O4 P	FindByFormula	28 -	340.2238	22.400873
C13 H7 P S3	C13 H7 P S3	[C13 H7 P S3, tgt=87.75, overall=87.75]	(324.9124, 55.92)(334.9356, 79.59)(288.93683, 29334.879)(	C13 H7 P S3	FindByFormula	27 -	289.9445	0.54577786
C13 H9 Cl O2	C13 H9 Cl O2	[C13 H9 Cl O2, tgt=91.22, overall=91.22]	(231.02205, 5329.4985)(232.02602, 783.00507)(233.01958,	C13 H9 Cl O2	FindByFormula	6 -	232.0296	18.466747
C14 H13 N2 O2 P	C14 H13 N2 O2 P	[C14 H13 N2 O2 P, tgt=80.81, overall=80.81]	(317.06726, 110.29314)(318.07135, 41.422855)(271.06476,	C14 H13 N2 O2 P	FindByFormula	28 -	272.0719	19.82244
C14 H13 N3 O4 S2	C14 H13 N3 O4 S2	[C14 H13 N3 O4 S2, tgt=98.59, overall=98.59]	(350.0283, 33901.098)(351.03104, 6032.828)(352.0261, 376	C14 H13 N3 O4 S2	FindByFormula	6 -	351.0355	15.548823
C14 H14 O22 P4	C14 H14 O22 P4	[C14 H14 O22 P4, tgt=94.22, overall=94.22]	(692.8465, 237.30333)(693.8492, 218.68666)(694.8452, 96.3	C14 H14 O22 P4	FindByFormula	22 -	657.8933	0.57804567
C14 H16 N12 O P4	C14 H16 N12 O P4	[C14 H16 N12 O P4, tgt=92.02, overall=92.02]	(527.01526, 82.00833)(528.01697, 37.855)(537.0389, 70.424	C14 H16 N12 O P4	FindByFormula	27 -	492.052	18.321089
C14 H16 N2 O4	C14 H16 N2 O4	[C14 H16 N2 O4, tgt=97.45, overall=97.45]	(311.08176, 141.449)(312.0858, 33.08636)(313.0823, 64.854	C14 H16 N2 O4	FindByFormula	23 -	276.1111	7.4955964
C14 H16 N2 O5	C14 H16 N2 O5	[C14 H16 N2 O5, tgt=97.81, overall=97.81]	(327.07446, 151.32443)(328.07693, 49.10455)(329.07385, 8	C14 H16 N2 O5	FindByFormula	23 -	292.1067	4.2849
C14 H17 N O8	C14 H17 N O8	[C14 H17 N O8, tgt=98.28, overall=98.28]	(362.0646, 62.916668)(372.0946, 169.3)(373.0967, 75.04)(3	C14 H17 N O8	FindByFormula	18 -	327.0959	2.2654982
C14 H18 O4	C14 H18 O4	[C14 H18 O4, tgt=97.51, overall=97.51]	(295.1166, 62.30818)(249.11288, 3443.2192)(250.11536, 43	C14 H18 O4	FindByFormula	28 -	250.12	18.611658
C14 H20 O P2 S	C14 H20 O P2 S	[C14 H20 O P2 S, tgt=94.34, overall=94.34]	(333.03528, 72.439995)(334.03046, 34.49)(335.0241, 34.9)(	C14 H20 O P2 S	FindByFormula	28 -	298.0719	5.3295426
C14 H21 N O3	C14 H21 N O3	[C14 H21 N O3, tgt=97.90, overall=97.90]	(296.14542, 128.00874)(250.1452, 9174.21)(251.14809, 157	C14 H21 N O3	FindByFormula	27 -	251.1525	21.059086
C14 H21 O3 P3	C14 H21 O3 P3	[C14 H21 O3 P3, tgt=97.31, overall=97.31]	(375.0599, 112.175)(376.0501, 53.69)(329.06293, 5433.2656	C14 H21 O3 P3	FindByFormula	7 -	330.0697	15.634928
C14 H22 N2 O5 S	C14 H22 N2 O5 S	[C14 H22 N2 O5 S, tgt=99.22, overall=99.22]	(329.11826, 52138.0)(330.12125, 8745.283)(331.11823, 340	C14 H22 N2 O5 S	FindByFormula	22 -	330.1257	4.546574
C14 H22 O4 S	C14 H22 O4 S	[C14 H22 O4 S, tgt=99.25, overall=99.25]	(321.09436, 56.88667)(322.0933, 23.09)(285.11713, 4983.12	C14 H22 O4 S	FindByFormula	9 -	286.1242	19.259483
C14 H23 N6 O8 P S2	C14 H23 N6 O8 P S2	[C14 H23 N6 O8 P S2, tgt=0.20, overall=0.20]	(533.0494, 89.520004)(543.0762, 118.450005)(497.06647, 2	C14 H23 N6 O8 P S2	FindByFormula	9 -	498.0749	1.0768883
C14 H23 N6 O9 P3 S	C14 H23 N6 O9 P3 S	[C14 H23 N6 O9 P3 S, tgt=75.27, overall=75.27]	(579.0078, 135.61269)(580.00616, 34.297142)(581.00757, 4	C14 H23 N6 O9 P3 S	FindByFormula	28 -	544.044	13.107979
C14 H23 O5 P S	C14 H23 O5 P S	[C14 H23 O5 P S, tgt=92.27, overall=92.27]	(369.07404, 329.53476)(370.07175, 184.31999)(371.0792, 6	C14 H23 O5 P S	FindByFormula	25 -	334.1014	1.3715601
C14 H24 N2 S4	C14 H24 N2 S4	[C14 H24 N2 S4, tgt=72.36, overall=72.36]	(383.0629, 122.4)(384.0645, 55.26)(393.08667, 220.06625)(	C14 H24 N2 S4	FindByFormula	19 -	348.0819	0.73531586
C14 H26 N6 O2	C14 H26 N6 O2	[C14 H26 N6 O2, tgt=72.46, overall=72.46]	(345.1818, 119.088745)(346.1957, 47.765)(347.18427, 32.09	C14 H26 N6 O2	FindByFormula	24 -	310.2124	22.66245
C14 H26 O2	C14 H26 O2	[C14 H26 O2, tgt=80.13, overall=80.13]	(225.18639, 2336.4946)(226.18898, 386.42688)	C14 H26 O2	FindByFormula	26 -	226.1932	22.090343
C14 H28 O2	C14 H28 O2	[C14 H28 O2, tgt=99.74, overall=99.74]	(263.1734, 122.174995)(264.173, 33.49)(273.21204, 886.102	C14 H28 O2	FindByFormula	28 -	228.2093	22.448605
C14 H28 O3	C14 H28 O3	[C14 H28 O3, tgt=99.45, overall=99.45]	(279.16977, 157.09334)(280.16534, 43.85)(281.1519, 22.5)(	C14 H28 O3	FindByFormula	28 -	244.2039	21.465591
C14 H30 N6 O	C14 H30 N6 O	[C14 H30 N6 O, tgt=82.83, overall=82.83]	(333.21686, 237.76265)(334.21768, 71.141426)(335.2135, 1	C14 H30 N6 O	FindByFormula	28 -	298.2503	21.981737
C14 H33 N6 O9 P	C14 H33 N6 O9 P	[C14 H33 N6 O9 P, tgt=83.69, overall=83.69]	(495.17017, 112.881676)(496.1438, 106.5)(505.19202, 706.3	C14 H33 N6 O9 P	FindByFormula	28 -	460.2041	22.84601
C14 H5 N4 O2 P S4	C14 H5 N4 O2 P S4	[C14 H5 N4 O2 P S4, tgt=71.37, overall=71.37]	(454.8744, 53.7)(464.89368, 168.00667)(465.9021, 40.6)(46	C14 H5 N4 O2 P S4	FindByFormula	11 -	419.9025	0.56527275
C14 H6 Cl2 N O5 P	C14 H6 Cl2 N O5 P	[C14 H6 Cl2 N O5 P, tgt=95.33, overall=95.33]	(403.90524, 3089.5234)(404.9116, 452.86847)(405.90253, 2	C14 H6 Cl2 N O5 P	FindByFormula	20 -	368.9366	0.9502004
C14 H9 Cl2 N2 P3 S2	C14 H9 Cl2 N2 P3 S2	[C14 H9 Cl2 N2 P3 S2, tgt=81.29, overall=81.29]	(466.8533, 1308.35)(467.8557, 263.81143)(468.84857, 672.6	C14 H9 Cl2 N2 P3 S2	FindByFormula	7 -	431.8801	18.923565
C15 H12 N2 O6 S	C15 H12 N2 O6 S	[C15 H12 N2 O6 S, tgt=98.38, overall=98.38]	(347.03433, 17616.867)(348.03757, 2935.26)(349.03235, 13	C15 H12 N2 O6 S	FindByFormula	6 -	348.0416	5.334646
C15 H14 O3	C15 H14 O3	[C15 H14 O3, tgt=71.14, overall=71.14]	(277.06494, 253.526)(278.06583, 62.948334)(279.06094, 56.	C15 H14 O3	FindByFormula	14 -	242.0941	15.768389
C15 H15 N7 O5	C15 H15 N7 O5	[C15 H15 N7 O5, tgt=97.05, overall=97.05]	(408.08542, 211.03471)(409.0845, 134.87555)(418.10825, 1	C15 H15 N7 O5	FindByFormula	28 -	373.1133	1.2065002
C15 H15 N9 O	C15 H15 N9 O	[C15 H15 N9 O, tgt=97.37, overall=97.37]	(372.11676, 63.7825)(373.1219, 39.22)(382.1487, 72.13)(33	C15 H15 N9 O	FindByFormula	28 -	337.1405	10.379736
C15 H16 N10	C15 H16 N10	[C15 H16 N10, tgt=99.03, overall=99.03]	(371.12518, 1278.1252)(372.12695, 272.69678)(373.12375,	C15 H16 N10	FindByFormula	28 -	336.1565	5.692571
C15 H16 N4 O	C15 H16 N4 O	[C15 H16 N4 O, tgt=98.02, overall=98.02]	(303.1018, 122.4725)(304.0962, 52.38)(305.1096, 88.79)(31	C15 H16 N4 O	FindByFormula	10 -	268.1322	18.555048
C15 H16 N4 O S	C15 H16 N4 O S	[C15 H16 N4 O S, tgt=84.51, overall=84.51]	(345.09927, 221.03421)(346.09683, 48.831875)(299.0969, 1	C15 H16 N4 O S	FindByFormula	28 -	300.1044	21.7437
C15 H17 N12 O7 P5	C15 H17 N12 O7 P5	[C15 H17 N12 O7 P5, tgt=91.42, overall=91.42]	(666.9676, 89.72833)(667.96277, 28.064001)(668.9687, 25.7	C15 H17 N12 O7 P5	FindByFormula	8 -	632.0022	15.702835
C15 H18 N6 P2	C15 H18 N6 P2	[C15 H18 N6 P2, tgt=91.08, overall=91.08]	(379.07254, 77.778336)(380.0703, 24.82)(381.0631, 39.98)(	C15 H18 N6 P2	FindByFormula	28 -	344.1066	13.096411
C15 H20 N6 O11	C15 H20 N6 O11	[C15 H20 N6 O11, tgt=94.08, overall=94.08]	(495.08932, 338.57144)(496.09348, 100.221436)(497.0781,	C15 H20 N6 O11	FindByFormula	7 -	460.1183	0.98714244
C15 H20 O5	C15 H20 O5	[C15 H20 O5, tgt=97.02, overall=97.02]	(315.09872, 72.35333)(279.1241, 5050.365)(280.12732, 914.	C15 H20 O5	FindByFormula	6 -	280.1314	17.489107
C15 H21 N10 O3 P3	C15 H21 N10 O3 P3	[C15 H21 N10 O3 P3, tgt=97.89, overall=97.89]	(517.0679, 52.65)(481.0934, 20538.08)(482.09607, 4034.433	C15 H21 N10 O3 P3	FindByFormula	6 -	482.1011	0.7229996
C15 H22 O2	C15 H22 O2	[C15 H22 O2, tgt=99.80, overall=99.80]	(269.13223, 691.58966)(270.13232, 96.79714)(271.12714, 2	C15 H22 O2	FindByFormula	28 -	234.1622	19.67431
C15 H22 O6	C15 H22 O6	[C15 H22 O6, tgt=97.96, overall=97.96]	(333.11185, 964.4965)(334.1146, 200.36346)(335.1094, 381.	C15 H22 O6	FindByFormula	28 -	298.142	9.92434
C15 H24 N3 O6 P S	C15 H24 N3 O6 P S	[C15 H24 N3 O6 P S, tgt=86.43, overall=86.43]	(440.08054, 122.94499)(441.0683, 2564.66)(442.0722, 316.5	C15 H24 N3 O6 P S	FindByFormula	24 -	405.113	0.7103753
C15 H24 N5 O3 P3	C15 H24 N5 O3 P3	[C15 H24 N5 O3 P3, tgt=96.11, overall=96.11]	(450.08008, 127.93333)(451.08316, 39.653336)(452.0826, 3	C15 H24 N5 O3 P3	FindByFormula	28 -	415.1086	3.8667762
C15 H24 O4 S3	C15 H24 O4 S3	[C15 H24 O4 S3, tgt=24.78, overall=24.78]	(399.05173, 70.344284)(400.0587, 119.5)(401.04755, 30.82)	C15 H24 O4 S3	FindByFormula	9 -	364.0814	0.7839997
C15 H25 O4 P3	C15 H25 O4 P3	[C15 H25 O4 P3, tgt=83.48, overall=83.48]	(397.0635, 54.41)(407.09296, 186.62881)(408.09058, 123.19	C15 H25 O4 P3	FindByFormula	24 -	362.0967	1.341792
C15 H26 N3 O4 P S3	C15 H26 N3 O4 P S3	[C15 H26 N3 O4 P S3, tgt=64.17, overall=64.17]	(474.0647, 65.35)(484.08716, 111.82875)(485.08334, 142.63	C15 H26 N3 O4 P S3	FindByFormula	11 -	439.0825	3.6027193
C15 H28 N4 S2	C15 H28 N4 S2	[C15 H28 N4 S2, tgt=96.97, overall=96.97]	(363.14456, 4597.701)(364.14676, 842.6)(365.1427, 1645.92	C15 H28 N4 S2	FindByFormula	22 -	328.1754	4.5758915
C15 H30 O2	C15 H30 O2	[C15 H30 O2, tgt=98.26, overall=98.26]	(277.19357, 196.18182)(278.1988, 65.35)(287.22314, 248.16	C15 H30 O2	FindByFormula	28 -	242.225	22.66305
C15 H31 N4 O3 P	C15 H31 N4 O3 P	[C15 H31 N4 O3 P, tgt=78.26, overall=78.26]	(391.2087, 29116.865)(392.2123, 5983.1665)(393.2107, 203	C15 H31 N4 O3 P	FindByFormula	27 -	346.2122	22.59514
C15 H31 N4 P S2	C15 H31 N4 P S2	[C15 H31 N4 P S2, tgt=87.50, overall=87.50]	(407.17142, 73.434)(361.16412, 4160.659)(362.16748, 876.7	C15 H31 N4 P S2	FindByFormula	28 -	362.1721	17.351126
C15 H33 Cl N4 O2	C15 H33 Cl N4 O2	[C15 H33 Cl N4 O2, tgt=77.69, overall=77.69]	(371.19894, 148.885)(372.2048, 47.14)(381.22766, 604.5666	C15 H33 Cl N4 O2	FindByFormula	25 -	336.2315	22.774744
C15 H33 N4 O3 P	C15 H33 N4 O3 P	[C15 H33 N4 O3 P, tgt=98.35, overall=98.35]	(383.18784, 318.25333)(384.1878, 41.56)(385.1837, 353.52)	C15 H33 N4 O3 P	FindByFormula	28 -	348.2285	22.73045
C15 H35 N4 O3 P	C15 H35 N4 O3 P	[C15 H35 N4 O3 P, tgt=98.00, overall=98.00]	(395.24307, 735.0752)(396.2484, 85.081116)(349.23703, 99	C15 H35 N4 O3 P	FindByFormula	28 -	350.2445	22.927792
C15 H37 N4 O3 P	C15 H37 N4 O3 P	[C15 H37 N4 O3 P, tgt=98.26, overall=98.26]	(387.23743, 56.338)(351.2527, 64934.492)(352.25586, 1362	C15 H37 N4 O3 P	FindByFormula	28 -	352.26	23.185507
C15 H9 N8 P	C15 H9 N8 P	[C15 H9 N8 P, tgt=76.53, overall=76.53]	(367.0379, 570.6891)(368.04077, 129.07706)(369.02722, 41	C15 H9 N8 P	FindByFormula	21 -	332.0671	4.2046037
C16 H11 Cl N6 O4	C16 H11 Cl N6 O4	[C16 H11 Cl N6 O4, tgt=0.44, overall=0.44]	(431.062, 53.97)(385.0436, 3336.5044)(386.04892, 755.4267	C16 H11 Cl N6 O4	FindByFormula	7 -	386.0528	18.507746
C16 H12 N8 O4	C16 H12 N8 O4	[C16 H12 N8 O4, tgt=96.55, overall=96.55]	(415.06702, 63.0475)(416.0767, 22.53)(379.0918, 3056.0818	C16 H12 N8 O4	FindByFormula	6 -	380.0994	4.78815
C16 H16 N2 O3	C16 H16 N2 O3	[C16 H16 N2 O3, tgt=97.85, overall=97.85]	(329.1178, 81.32)(283.10925, 18852.744)(284.11234, 3652.8	C16 H16 N2 O3	FindByFormula	6 -	284.1166	23.246927
C16 H16 O3 S3	C16 H16 O3 S3	[C16 H16 O3 S3, tgt=58.24, overall=58.24]	(386.99997, 564.535)(387.99713, 89.45778)(388.98984, 336.	C16 H16 O3 S3	FindByFormula	14 -	352.0288	0.6734284
C16 H17 N6 O3 P3	C16 H17 N6 O3 P3	[C16 H17 N6 O3 P3, tgt=98.47, overall=98.47]	(469.0274, 58.1)(470.0288, 31.91)(471.0267, 31.22)(479.051	C16 H17 N6 O3 P3	FindByFormula	8 -	434.0575	15.696836
C16 H18 N16	C16 H18 N16	[C16 H18 N16, tgt=89.07, overall=89.07]	(469.1585, 146.403)(470.14664, 78.597496)(471.1482, 398.5	C16 H18 N16	FindByFormula	23 -	434.191	22.688652
C16 H18 N4 O4	C16 H18 N4 O4	[C16 H18 N4 O4, tgt=96.74, overall=96.74]	(375.1201, 53.44)(329.1248, 2884.015)(330.127, 534.545)(3	C16 H18 N4 O4	FindByFormula	28 -	330.132	7.8869977
C16 H19 N P2	C16 H19 N P2	[C16 H19 N P2, tgt=98.58, overall=98.58]	(332.09818, 1969.8564)(333.09866, 332.84427)(334.10306,	C16 H19 N P2	FindByFormula	28 -	287.0999	3.8773487
C16 H20 N4	C16 H20 N4	[C16 H20 N4, tgt=93.54, overall=93.54]	(303.13617, 67.665)(313.16278, 65.42786)(267.1602, 8075.1	C16 H20 N4	FindByFormula	28 -	268.1676	16.162428
C16 H21 N6 O7 P5	C16 H21 N6 O7 P5	[C16 H21 N6 O7 P5, tgt=62.99, overall=62.99]	(598.9804, 98.222)(599.9717, 29.549997)(563.00757, 2373.1	C16 H21 N6 O7 P5	FindByFormula	9 -	564.0146	15.7017145
C16 H22 N2 O15	C16 H22 N2 O15	[C16 H22 N2 O15, tgt=99.39, overall=99.39]	(517.0684, 90.935005)(518.0834, 55.225)(527.10364, 73.406	C16 H22 N2 O15	FindByFormula	6 -	482.101	1.0131658
C16 H22 N6 O3	C16 H22 N6 O3	[C16 H22 N6 O3, tgt=93.71, overall=93.71]	(391.174, 70.30091)(345.1691, 3714.1382)(346.1726, 788.92	C16 H22 N6 O3	FindByFormula	28 -	346.1765	19.783634
C16 H23 N2 O11 P S	C16 H23 N2 O11 P S	[C16 H23 N2 O11 P S, tgt=96.47, overall=96.47]	(517.0377, 139.03679)(518.04144, 49.661667)(519.03625, 5	C16 H23 N2 O11 P S	FindByFormula	28 -	482.0752	13.101373
C16 H23 N5 O4	C16 H23 N5 O4	[C16 H23 N5 O4, tgt=90.00, overall=90.00]	(348.16763, 2435.5667)(349.16736, 614.245)(350.1682, 82.9	C16 H23 N5 O4	FindByFormula	6 -	349.1741	4.309987
C16 H25 N6 O7 P3	C16 H25 N6 O7 P3	[C16 H25 N6 O7 P3, tgt=96.37, overall=96.37]	(541.0662, 289.11)(542.0711, 291.77)(551.0968, 206.13602)	C16 H25 N6 O7 P3	FindByFormula	7 -	506.0993	0.795428
C16 H25 O3 P3	C16 H25 O3 P3	[C16 H25 O3 P3, tgt=98.61, overall=98.61]	(393.0641, 60.96)(357.09406, 2888.8472)(358.09674, 581.04	C16 H25 O3 P3	FindByFormula	10 -	358.1015	18.633692
C16 H26 N6 O2	C16 H26 N6 O2	[C16 H26 N6 O2, tgt=89.42, overall=89.42]	(369.1907, 51.7)(379.2123, 160.48251)(380.21725, 61.41)(3	C16 H26 N6 O2	FindByFormula	7 -	334.2124	21.59905
C16 H26 O2	C16 H26 O2	[C16 H26 O2, tgt=50.99, overall=50.99]	(285.1588, 195.13275)(286.16168, 46.302498)(287.15628, 8	C16 H26 O2	FindByFormula	28 -	250.1915	22.302292
C16 H28 N13 O2 P5	C16 H28 N13 O2 P5	[C16 H28 N13 O2 P5, tgt=92.77, overall=92.77]	(588.1102, 3245.5234)(589.11285, 829.47046)(590.1144, 22	C16 H28 N13 O2 P5	FindByFormula	22 -	589.1176	3.0481794
C16 H28 O2	C16 H28 O2	[C16 H28 O2, tgt=90.07, overall=90.07]	(251.20187, 2350.4832)(252.20593, 449.6796)(253.20683, 1	C16 H28 O2	FindByFormula	25 -	252.2089	22.320297
C16 H30 N6 O2	C16 H30 N6 O2	[C16 H30 N6 O2, tgt=96.03, overall=96.03]	(373.2116, 86.43626)(383.24884, 230.27245)(384.25104, 71.	C16 H30 N6 O2	FindByFormula	28 -	338.2441	22.971354
C16 H30 O2	C16 H30 O2	[C16 H30 O2, tgt=90.29, overall=90.29]	(289.19714, 78.64667)(290.2013, 29.55)(291.1962, 52.38)(2	C16 H30 O2	FindByFormula	28 -	254.2249	22.586546
C16 H30 O3	C16 H30 O3	[C16 H30 O3, tgt=89.52, overall=89.52]	(305.1873, 65.138885)(269.21255, 4209.206)(270.2158, 776.	C16 H30 O3	FindByFormula	28 -	270.2198	21.989428
C16 H32 O2	C16 H32 O2	[C16 H32 O2, tgt=72.63, overall=72.63]	(291.20316, 190.48637)(292.20477, 42.56428)(301.23917, 2	C16 H32 O2	FindByFormula	28 -	256.2409	22.84576
C16 H32 O3	C16 H32 O3	[C16 H32 O3, tgt=98.86, overall=98.86]	(307.2041, 119.93429)(308.20004, 28.800001)(317.2363, 69.	C16 H32 O3	FindByFormula	28 -	272.2355	22.27943
C16 H34 N14 O6 P6	C16 H34 N14 O6 P6	[C16 H34 N14 O6 P6, tgt=81.59, overall=81.59]	(739.0849, 205.08643)(740.0865, 68.351425)(741.08716, 18	C16 H34 N14 O6 P6	FindByFormula	28 -	704.1225	22.458952
C16 H34 O8 S	C16 H34 O8 S	[C16 H34 O8 S, tgt=94.11, overall=94.11]	(421.1559, 120.78)(422.149, 42.28)(423.1476, 851.3)(431.19	C16 H34 O8 S	FindByFormula	27 -	386.1967	22.879452
C16 H4 N2 O3 P2 S3	C16 H4 N2 O3 P2 S3	[C16 H4 N2 O3 P2 S3, tgt=72.38, overall=72.38]	(464.86136, 1562.5043)(465.866, 260.92426)(466.85345, 12	C16 H4 N2 O3 P2 S3	FindByFormula	7 -	429.8835	18.923565
C16 H9 N7 S	C16 H9 N7 S	[C16 H9 N7 S, tgt=98.80, overall=98.80]	(366.026, 70.24)(330.05624, 8410.676)(331.05905, 1717.298	C16 H9 N7 S	FindByFormula	6 -	331.0637	13.109875
C17 H14 Cl3 N2 O P3 S2	C17 H14 Cl3 N2 O P3 S2	[C17 H14 Cl3 N2 O P3 S2, tgt=78.75, overall=78.75]	(559.24994, 827.5721)(560.24774, 152.574)(561.2547, 602.3	C17 H14 Cl3 N2 O P3 S2	FindByFormula	5 -	523.8796	20.916378
C17 H15 Cl O4	C17 H15 Cl O4	[C17 H15 Cl O4, tgt=97.63, overall=97.63]	(317.05817, 4946.7466)(318.0621, 923.5283)(319.05698, 15	C17 H15 Cl O4	FindByFormula	6 -	318.0661	18.476583
C17 H17 N2 O8 P	C17 H17 N2 O8 P	[C17 H17 N2 O8 P, tgt=98.12, overall=98.12]	(443.04193, 64.109)(444.0451, 26.26)(453.0691, 103.17786)	C17 H17 N2 O8 P	FindByFormula	28 -	408.0724	13.099336
C17 H18 N10 O	C17 H18 N10 O	[C17 H18 N10 O, tgt=77.35, overall=77.35]	(413.13885, 53.190002)(423.1549, 52.405)(377.15945, 2107.	C17 H18 N10 O	FindByFormula	28 -	378.1662	17.262041
C17 H18 N2 O4	C17 H18 N2 O4	[C17 H18 N2 O4, tgt=37.65, overall=37.65]	(349.09848, 87.064285)(350.10635, 43.74)(351.09595, 41.59	C17 H18 N2 O4	FindByFormula	13 -	314.1271	14.322931
C17 H18 N4	C17 H18 N4	[C17 H18 N4, tgt=96.06, overall=96.06]	(313.1159, 53.67)(277.14673, 7369.5986)(278.14996, 1341.5	C17 H18 N4	FindByFormula	7 -	278.1536	20.033464
C17 H18 N4 O S	C17 H18 N4 O S	[C17 H18 N4 O S, tgt=57.65, overall=57.65]	(371.12003, 66.18667)(325.11276, 1510.0304)(326.11542, 5	C17 H18 N4 O S	FindByFormula	24 -	326.1206	22.062195
C17 H20 N10 O12 P4	C17 H20 N10 O12 P4	[C17 H20 N10 O12 P4, tgt=93.59, overall=93.59]	(714.98083, 208.2989)(715.98364, 45.001926)(716.98, 45.72	C17 H20 N10 O12 P4	FindByFormula	28 -	680.02	13.105909
C17 H21 N O3	C17 H21 N O3	[C17 H21 N O3, tgt=96.80, overall=96.80]	(286.14514, 3361.4636)(287.14868, 722.6983)(288.1482, 91.	C17 H21 N O3	FindByFormula	6 -	287.1527	18.096092
C17 H21 O3 P3	C17 H21 O3 P3	[C17 H21 O3 P3, tgt=97.26, overall=97.26]	(411.05942, 221.2825)(412.05884, 76.36)(365.0628, 4327.62	C17 H21 O3 P3	FindByFormula	8 -	366.0694	15.705086
C17 H22 N12 O P4	C17 H22 N12 O P4	[C17 H22 N12 O P4, tgt=93.30, overall=93.30]	(569.0777, 57.81)(579.099, 95.670586)(580.0988, 54.660004	C17 H22 N12 O P4	FindByFormula	28 -	534.0998	21.745378
C17 H22 N16 O2 P2	C17 H22 N16 O2 P2	[C17 H22 N16 O2 P2, tgt=56.81, overall=56.81]	(579.1287, 388.7591)(580.13116, 121.35429)(581.1263, 276.	C17 H22 N16 O2 P2	FindByFormula	28 -	544.1558	22.742998
C17 H24 N2 O6 P4	C17 H24 N2 O6 P4	[C17 H24 N2 O6 P4, tgt=97.08, overall=97.08]	(511.02203, 69.593575)(512.03156, 30.413998)(513.0115, 2	C17 H24 N2 O6 P4	FindByFormula	28 -	476.0588	13.1038
C17 H24 N4 O3	C17 H24 N4 O3	[C17 H24 N4 O3, tgt=77.26, overall=77.26]	(367.15833, 3283.1665)(368.15994, 911.64996)(369.14978,	C17 H24 N4 O3	FindByFormula	10 -	332.1881	16.427824
C17 H25 Cl N10 O4 S	C17 H25 Cl N10 O4 S	[C17 H25 Cl N10 O4 S, tgt=94.84, overall=94.84]	(545.1364, 57.97333)(546.1322, 28.09)(547.144, 23.78)(499.	C17 H25 Cl N10 O4 S	FindByFormula	28 -	500.1471	3.877098
C17 H25 N2 O2 P3	C17 H25 N2 O2 P3	[C17 H25 N2 O2 P3, tgt=86.73, overall=86.73]	(417.0782, 579.9)(418.08017, 84.15)(419.08078, 95.841675)	C17 H25 N2 O2 P3	FindByFormula	16 -	382.1116	4.4224157
C17 H26 O3	C17 H26 O3	[C17 H26 O3, tgt=99.18, overall=99.18]	(313.15836, 62.424)(314.1492, 30.66)(323.18475, 167.41264	C17 H26 O3	FindByFormula	28 -	278.1886	19.78042
C17 H26 O4	C17 H26 O4	[C17 H26 O4, tgt=99.10, overall=99.10]	(329.1481, 254.84265)(330.15146, 70.48928)(331.1485, 275.	C17 H26 O4	FindByFormula	28 -	294.1833	17.457403
C17 H26 O5	C17 H26 O5	[C17 H26 O5, tgt=85.49, overall=85.49]	(345.1485, 124.7763)(346.1561, 34.357338)(347.14484, 60.9	C17 H26 O5	FindByFormula	28 -	310.1791	17.260578
C17 H28 O3 S	C17 H28 O3 S	[C17 H28 O3 S, tgt=96.95, overall=96.95]	(347.15308, 224.33928)(348.1541, 56.734)(349.14484, 40.03	C17 H28 O3 S	FindByFormula	28 -	312.1768	22.865927
C17 H28 O5	C17 H28 O5	[C17 H28 O5, tgt=98.76, overall=98.76]	(347.16492, 119.23161)(348.16916, 36.834545)(349.1639, 7	C17 H28 O5	FindByFormula	28 -	312.1929	16.43712
C17 H30 N6 O3	C17 H30 N6 O3	[C17 H30 N6 O3, tgt=89.86, overall=89.86]	(401.20544, 454.2625)(402.20377, 110.64001)(403.20926, 9	C17 H30 N6 O3	FindByFormula	25 -	366.2387	22.408228
C17 H31 N4 O3 P	C17 H31 N4 O3 P	[C17 H31 N4 O3 P, tgt=87.11, overall=87.11]	(405.1763, 388.5475)(406.1768, 716.54)(415.20493, 5403.23	C17 H31 N4 O3 P	FindByFormula	27 -	370.213	22.539927
C17 H32 N2 O8	C17 H32 N2 O8	[C17 H32 N2 O8, tgt=88.82, overall=88.82]	(427.1801, 249.09)(437.20728, 487.44244)(438.20462, 234.5	C17 H32 N2 O8	FindByFormula	28 -	392.2156	22.84751
C17 H32 N6 O4 P2	C17 H32 N6 O4 P2	[C17 H32 N6 O4 P2, tgt=93.14, overall=93.14]	(481.1581, 676.8918)(482.15604, 234.92502)(483.15332, 26	C17 H32 N6 O4 P2	FindByFormula	20 -	446.194	1.6202005
C17 H32 O2	C17 H32 O2	[C17 H32 O2, tgt=90.61, overall=90.61]	(313.23297, 1221.2834)(314.23285, 210.17366)(315.2358, 8	C17 H32 O2	FindByFormula	27 -	268.24	22.767624
C17 H32 O2 S	C17 H32 O2 S	[C17 H32 O2 S, tgt=89.38, overall=89.38]	(335.1811, 69.81714)(299.20392, 6898.244)(300.2076, 1516.	C17 H32 O2 S	FindByFormula	22 -	300.2108	22.273499
C17 H33 N4 O3 P	C17 H33 N4 O3 P	[C17 H33 N4 O3 P, tgt=98.64, overall=98.64]	(407.19006, 181.52249)(417.21725, 6925.7065)(418.21558,	C17 H33 N4 O3 P	FindByFormula	28 -	372.2289	22.70835
C17 H33 N4 O4 P	C17 H33 N4 O4 P	[C17 H33 N4 O4 P, tgt=84.06, overall=84.06]	(423.1909, 110.34)(424.18948, 32.983334)(425.18365, 501.8	C17 H33 N4 O4 P	FindByFormula	22 -	388.2229	21.741972
C17 H33 N8 O P	C17 H33 N8 O P	[C17 H33 N8 O P, tgt=51.87, overall=51.87]	(441.24777, 351.61362)(442.24768, 167.6)(443.2352, 702.92	C17 H33 N8 O P	FindByFormula	26 -	396.2509	22.52082
C17 H34 O2	C17 H34 O2	[C17 H34 O2, tgt=96.69, overall=96.69]	(315.2528, 188.68)(316.25748, 46.198574)(269.24893, 1494	C17 H34 O2	FindByFormula	28 -	270.2562	22.989054
C17 H35 O2 P3	C17 H35 O2 P3	[C17 H35 O2 P3, tgt=90.68, overall=90.68]	(399.15225, 266.81787)(400.15317, 485.02335)(401.1475, 3	C17 H35 O2 P3	FindByFormula	28 -	364.1844	22.448605
C17 H36 N2 O12 P2	C17 H36 N2 O12 P2	[C17 H36 N2 O12 P2, tgt=96.17, overall=96.17]	(557.1438, 106.771996)(558.14557, 48.15)(559.133, 145.32)	C17 H36 N2 O12 P2	FindByFormula	28 -	522.1741	22.852045
C17 H38 N2 P2 S	C17 H38 N2 P2 S	[C17 H38 N2 P2 S, tgt=92.47, overall=92.47]	(399.18378, 119.39601)(400.1792, 43.690002)(401.1929, 35.	C17 H38 N2 P2 S	FindByFormula	27 -	364.2235	21.475937
C17 H38 N6	C17 H38 N6	[C17 H38 N6, tgt=94.06, overall=94.06]	(361.281, 51.54)(371.31183, 55.425)(325.3086, 2865.3003)(	C17 H38 N6	FindByFormula	26 -	326.3165	23.189945
C17 H38 N6 P4	C17 H38 N6 P4	[C17 H38 N6 P4, tgt=94.54, overall=94.54]	(485.1805, 136.98889)(486.18668, 52.076252)(487.18643, 4	C17 H38 N6 P4	FindByFormula	11 -	450.2106	12.223334
C17 H44 Cl N9 O7 S	C17 H44 Cl N9 O7 S	[C17 H44 Cl N9 O7 S, tgt=70.99, overall=70.99]	(588.2356, 59.5875)(589.24036, 31.25)(590.2294, 44.84)(59	C17 H44 Cl N9 O7 S	FindByFormula	19 -	553.2768	24.567352
C17 H6 Cl N7 O4 S	C17 H6 Cl N7 O4 S	[C17 H6 Cl N7 O4 S, tgt=92.14, overall=92.14]	(473.9691, 65.920006)(437.98135, 2246.8037)(438.98392, 5	C17 H6 Cl N7 O4 S	FindByFormula	22 -	438.9885	8.7214575
C17 H9 N6 O2 P	C17 H9 N6 O2 P	[C17 H9 N6 O2 P, tgt=93.36, overall=93.36]	(395.02405, 65.6325)(359.0458, 2710.5288)(360.0489, 582.9	C17 H9 N6 O2 P	FindByFormula	8 -	360.0528	15.700711
C18 H13 Cl N10	C18 H13 Cl N10	[C18 H13 Cl N10, tgt=97.82, overall=97.82]	(449.0924, 57.53)(403.09396, 3034.6208)(404.0978, 700.14	C18 H13 Cl N10	FindByFormula	28 -	404.1011	8.459828
C18 H13 N P4	C18 H13 N P4	[C18 H13 N P4, tgt=68.45, overall=68.45]	(365.99548, 1551.5726)(366.99026, 552.45245)(367.993, 22	C18 H13 N P4	FindByFormula	8 -	367.0005	22.71834
C18 H14 N10 O	C18 H14 N10 O	[C18 H14 N10 O, tgt=95.22, overall=95.22]	(421.10895, 263.31)(422.09674, 80.96)(423.10358, 36.92500	C18 H14 N10 O	FindByFormula	28 -	386.1345	3.8794556
C18 H14 N6	C18 H14 N6	[C18 H14 N6, tgt=70.30, overall=70.30]	(349.10135, 138.23001)(350.10535, 42.745)(351.1059, 76.68	C18 H14 N6	FindByFormula	22 -	314.1272	13.963053
C18 H15 N O3	C18 H15 N O3	[C18 H15 N O3, tgt=95.98, overall=95.98]	(292.09906, 1999.886)(293.10132, 388.107)(294.10147, 87.2	C18 H15 N O3	FindByFormula	10 -	293.1072	17.949505
C18 H16 N12 O P4	C18 H16 N12 O P4	[C18 H16 N12 O P4, tgt=94.93, overall=94.93]	(575.0327, 65.93)(539.0439, 2800.9514)(540.0476, 650.0816	C18 H16 N12 O P4	FindByFormula	6 -	540.0511	18.844406
C18 H17 N5 O4 P2	C18 H17 N5 O4 P2	[C18 H17 N5 O4 P2, tgt=68.75, overall=68.75]	(464.0431, 58.0075)(465.0249, 28.22)(474.07678, 892.8542)	C18 H17 N5 O4 P2	FindByFormula	26 -	429.0756	2.5137293
C18 H19 N14 O2 P5	C18 H19 N14 O2 P5	[C18 H19 N14 O2 P5, tgt=86.17, overall=86.17]	(653.01056, 241.01537)(654.01044, 54.682594)(655.00635,	C18 H19 N14 O2 P5	FindByFormula	28 -	618.0496	13.100194
C18 H21 N16 O4 P5	C18 H21 N16 O4 P5	[C18 H21 N16 O4 P5, tgt=95.63, overall=95.63]	(715.021, 113.17917)(716.0168, 40.241177)(717.01135, 133.	C18 H21 N16 O4 P5	FindByFormula	28 -	680.0613	8.461291
C18 H21 N2 O2 P	C18 H21 N2 O2 P	[C18 H21 N2 O2 P, tgt=85.05, overall=85.05]	(373.13046, 712.213)(374.13297, 202.89037)(375.1373, 155	C18 H21 N2 O2 P	FindByFormula	28 -	328.1348	22.448282
C18 H22 N2 O5	C18 H22 N2 O5	[C18 H22 N2 O5, tgt=98.48, overall=98.48]	(381.12088, 383.73)(382.1213, 93.421425)(383.1224, 45.84)	C18 H22 N2 O5	FindByFormula	10 -	346.1534	13.907926
C18 H22 N4 O4	C18 H22 N4 O4	[C18 H22 N4 O4, tgt=97.52, overall=97.52]	(403.1604, 1896.2162)(404.16052, 1533.1768)(405.1674, 11	C18 H22 N4 O4	FindByFormula	28 -	358.163	22.490175
C18 H22 O2 P2	C18 H22 O2 P2	[C18 H22 O2 P2, tgt=95.01, overall=95.01]	(377.1143, 66.26)(331.1032, 8113.062)(332.10446, 1371.232	C18 H22 O2 P2	FindByFormula	7 -	332.1098	4.4106946
C18 H23 N3 O9	C18 H23 N3 O9	[C18 H23 N3 O9, tgt=97.97, overall=97.97]	(460.11276, 92.215)(461.1006, 55.766666)(470.14435, 122.2	C18 H23 N3 O9	FindByFormula	24 -	425.1436	1.3540002
C18 H23 N9 O11 S	C18 H23 N9 O11 S	[C18 H23 N9 O11 S, tgt=94.74, overall=94.74]	(608.0829, 52.92)(572.11554, 10097.48)(573.1181, 2487.174	C18 H23 N9 O11 S	FindByFormula	22 -	573.123	3.0135431
C18 H24 N4 O12 P4	C18 H24 N4 O12 P4	[C18 H24 N4 O12 P4, tgt=94.34, overall=94.34]	(646.9954, 181.14786)(647.99475, 36.6232)(648.9981, 43.71	C18 H24 N4 O12 P4	FindByFormula	28 -	612.0329	13.107336
C18 H26 N10 O2	C18 H26 N10 O2	[C18 H26 N10 O2, tgt=89.21, overall=89.21]	(449.19885, 76.99777)(450.19348, 40.199997)(459.2245, 50	C18 H26 N10 O2	FindByFormula	28 -	414.2244	23.186361
C18 H26 N18 P4 S	C18 H26 N18 P4 S	[C18 H26 N18 P4 S, tgt=96.28, overall=96.28]	(685.10236, 64.72)(686.0985, 60.555)(695.1268, 86.21)(649.	C18 H26 N18 P4 S	FindByFormula	7 -	650.1267	0.70557106
C18 H27 N3 O2 P2	C18 H27 N3 O2 P2	[C18 H27 N3 O2 P2, tgt=86.53, overall=86.53]	(414.133, 52.29)(424.1499, 111.369995)(425.15015, 60.3660	C18 H27 N3 O2 P2	FindByFormula	23 -	379.1587	15.762031
C18 H28 O2	C18 H28 O2	[C18 H28 O2, tgt=85.01, overall=85.01]	(311.1703, 4630.027)(312.1735, 957.94336)(313.16928, 431.	C18 H28 O2	FindByFormula	6 -	276.2064	22.52778
C18 H28 O3 P2	C18 H28 O3 P2	[C18 H28 O3 P2, tgt=81.11, overall=81.11]	(399.1493, 700.92883)(400.15475, 371.24146)(353.14413, 2	C18 H28 O3 P2	FindByFormula	28 -	354.1505	22.581976
C18 H28 P6	C18 H28 P6	[C18 H28 P6, tgt=84.79, overall=84.79]	(465.0311, 127.763336)(466.02856, 30.83)(467.02783, 42.16	C18 H28 P6	FindByFormula	6 -	430.0615	15.442491
C18 H29 N18 O6 P5	C18 H29 N18 O6 P5	[C18 H29 N18 O6 P5, tgt=54.00, overall=54.00]	(783.0827, 308.18237)(784.08496, 105.186874)(785.0864, 2	C18 H29 N18 O6 P5	FindByFormula	27 -	748.1169	22.650492
C18 H30 Cl2 N4 O2	C18 H30 Cl2 N4 O2	[C18 H30 Cl2 N4 O2, tgt=84.32, overall=84.32]	(439.1405, 71.455)(440.1432, 29.19)(449.16638, 1081.8254)	C18 H30 Cl2 N4 O2	FindByFormula	28 -	404.1732	22.864075
C18 H30 N2 O2 P2 S2	C18 H30 N2 O2 P2 S2	[C18 H30 N2 O2 P2 S2, tgt=83.76, overall=83.76]	(431.11475, 2372.4912)(432.11707, 602.5834)(433.1143, 24	C18 H30 N2 O2 P2 S2	FindByFormula	18 -	432.1224	3.8939302
C18 H30 O2	C18 H30 O2	[C18 H30 O2, tgt=97.17, overall=97.17]	(323.21893, 4130.821)(324.21765, 920.15857)(277.21738, 4	C18 H30 O2	FindByFormula	27 -	278.2241	22.53068
C18 H32 N4 O14	C18 H32 N4 O14	[C18 H32 N4 O14, tgt=97.58, overall=97.58]	(563.15796, 199.02806)(564.1591, 125.14637)(565.15533, 1	C18 H32 N4 O14	FindByFormula	28 -	528.1897	22.846333
C18 H32 O2	C18 H32 O2	[C18 H32 O2, tgt=98.01, overall=98.01]	(315.20865, 119.07833)(316.20486, 42.17143)(317.2083, 20	C18 H32 O2	FindByFormula	28 -	280.241	22.730165
C18 H32 O3	C18 H32 O3	[C18 H32 O3, tgt=98.24, overall=98.24]	(331.20425, 154.75313)(332.20673, 63.03625)(341.23572, 8	C18 H32 O3	FindByFormula	28 -	296.2354	21.581867
C18 H32 O4	C18 H32 O4	[C18 H32 O4, tgt=76.23, overall=76.23]	(357.23135, 67.2525)(358.2356, 21.8)(311.22195, 4749.838)	C18 H32 O4	FindByFormula	16 -	312.2308	21.585463
C18 H33 Cl O16	C18 H33 Cl O16	[C18 H33 Cl O16, tgt=99.76, overall=99.76]	(575.12805, 274.87)(576.1333, 94.38)(577.1357, 81.08)(585.	C18 H33 Cl O16	FindByFormula	24 -	540.1463	0.7138336
C18 H34 N3 O P S4	C18 H34 N3 O P S4	[C18 H34 N3 O P S4, tgt=77.03, overall=77.03]	(502.1024, 81.58571)(503.0868, 24.400002)(504.0864, 21.53	C18 H34 N3 O P S4	FindByFormula	24 -	467.1324	0.7067085
C18 H34 O2	C18 H34 O2	[C18 H34 O2, tgt=96.83, overall=96.83]	(317.22433, 310.79813)(318.2281, 61.60251)(319.21927, 10	C18 H34 O2	FindByFormula	28 -	282.2567	22.9269
C18 H34 O3	C18 H34 O3	[C18 H34 O3, tgt=88.18, overall=88.18]	(333.21887, 238.83531)(334.22028, 62.941536)(335.2198, 1	C18 H34 O3	FindByFormula	27 -	298.2499	22.175673
C18 H34 O5	C18 H34 O5	[C18 H34 O5, tgt=96.20, overall=96.20]	(365.205, 107.61786)(366.20975, 35.592857)(367.2025, 80.2	C18 H34 O5	FindByFormula	28 -	330.2402	16.740955
C18 H34 S4	C18 H34 S4	[C18 H34 S4, tgt=67.15, overall=67.15]	(423.14844, 598.86816)(424.14447, 310.7794)(425.1543, 27	C18 H34 S4	FindByFormula	26 -	378.1517	22.579264
C18 H36 O2	C18 H36 O2	[C18 H36 O2, tgt=97.44, overall=97.44]	(319.2416, 78.661674)(320.2397, 46.65)(329.2697, 1364.085	C18 H36 O2	FindByFormula	28 -	284.2725	23.18279
C18 H36 O3	C18 H36 O3	[C18 H36 O3, tgt=97.67, overall=97.67]	(335.2325, 124.284)(336.2365, 38.556667)(337.2338, 87.693	C18 H36 O3	FindByFormula	28 -	300.2664	22.09995
C18 H36 O4	C18 H36 O4	[C18 H36 O4, tgt=96.02, overall=96.02]	(351.22754, 148.58722)(352.23013, 38.380833)(353.22528,	C18 H36 O4	FindByFormula	28 -	316.2616	21.123468
C18 H37 N10 O3 P5 S	C18 H37 N10 O3 P5 S	[C18 H37 N10 O3 P5 S, tgt=98.49, overall=98.49]	(663.1144, 61.62)(664.1244, 22.68)(627.13824, 54653.094)(	C18 H37 N10 O3 P5 S	FindByFormula	6 -	628.1455	0.7754994
C18 H37 N2 O14 P3 S	C18 H37 N2 O14 P3 S	[C18 H37 N2 O14 P3 S, tgt=76.05, overall=76.05]	(665.08435, 115.93608)(666.08124, 45.3453)(667.07776, 77.	C18 H37 N2 O14 P3 S	FindByFormula	28 -	630.117	22.448927
C18 H39 Cl N2 O S3	C18 H39 Cl N2 O S3	[C18 H39 Cl N2 O S3, tgt=79.39, overall=79.39]	(465.16776, 104.49)(475.18948, 486.20166)(476.18915, 167.	C18 H39 Cl N2 O S3	FindByFormula	26 -	430.1922	22.928074
C18 H41 O P3	C18 H41 O P3	[C18 H41 O P3, tgt=92.17, overall=92.17]	(401.2027, 95.399994)(402.20642, 25.515)(403.2033, 36.315	C18 H41 O P3	FindByFormula	27 -	366.2362	21.760674
C19 H14 N10 O2	C19 H14 N10 O2	[C19 H14 N10 O2, tgt=98.34, overall=98.34]	(449.0924, 66.62)(459.12003, 146.94637)(460.11636, 68.571	C19 H14 N10 O2	FindByFormula	28 -	414.1303	8.459543
C19 H16 N10 O8 S	C19 H16 N10 O8 S	[C19 H16 N10 O8 S, tgt=87.88, overall=87.88]	(579.05164, 66.32399)(589.0737, 83.423996)(590.0832, 25.9	C19 H16 N10 O8 S	FindByFormula	27 -	544.0863	8.460637
C19 H18 N6 O	C19 H18 N6 O	[C19 H18 N6 O, tgt=58.83, overall=58.83]	(381.1242, 317.1614)(382.1246, 68.671425)(391.1526, 71.78	C19 H18 N6 O	FindByFormula	9 -	346.1535	13.469648
C19 H18 N8 O12	C19 H18 N8 O12	[C19 H18 N8 O12, tgt=98.07, overall=98.07]	(585.06635, 57.543335)(595.0889, 243.49)(596.08936, 106.4	C19 H18 N8 O12	FindByFormula	28 -	550.1042	8.4619
C19 H21 Cl N2 O10	C19 H21 Cl N2 O10	[C19 H21 Cl N2 O10, tgt=96.89, overall=96.89]	(517.0768, 59.828003)(471.08127, 2258.6746)(472.08432, 5	C19 H21 Cl N2 O10	FindByFormula	28 -	472.089	8.4618635
C19 H22 N14 O3 S2	C19 H22 N14 O3 S2	[C19 H22 N14 O3 S2, tgt=73.20, overall=73.20]	(593.1126, 147.55165)(594.12006, 59.16)(595.11127, 74.896	C19 H22 N14 O3 S2	FindByFormula	21 -	558.1444	1.8286673
C19 H22 N2 O2 P2	C19 H22 N2 O2 P2	[C19 H22 N2 O2 P2, tgt=82.67, overall=82.67]	(371.10803, 3093.4016)(372.11157, 788.3416)(373.1082, 31	C19 H22 N2 O2 P2	FindByFormula	6 -	372.1149	9.041775
C19 H23 N2 O2 P	C19 H23 N2 O2 P	[C19 H23 N2 O2 P, tgt=77.54, overall=77.54]	(387.1521, 407.85416)(388.148, 120.41144)(341.1435, 8450.	C19 H23 N2 O2 P	FindByFormula	28 -	342.1509	22.66537
C19 H23 N8 O2 P5	C19 H23 N8 O2 P5	[C19 H23 N8 O2 P5, tgt=92.41, overall=92.41]	(585.0243, 232.65465)(586.0256, 53.059277)(587.0253, 40.5	C19 H23 N8 O2 P5	FindByFormula	28 -	550.0627	13.105979
C19 H25 N10 O4 P5	C19 H25 N10 O4 P5	[C19 H25 N10 O4 P5, tgt=95.34, overall=95.34]	(647.03394, 64.422226)(648.0261, 28.810001)(649.0246, 29	C19 H25 N10 O4 P5	FindByFormula	28 -	612.0747	8.462186
C19 H26 N3 P S2	C19 H26 N3 P S2	[C19 H26 N3 P S2, tgt=82.97, overall=82.97]	(426.10693, 83.708)(427.102, 26.68)(428.0982, 130.02)(436.	C19 H26 N3 P S2	FindByFormula	14 -	391.1314	3.7930586
C19 H30 N4	C19 H30 N4	[C19 H30 N4, tgt=42.40, overall=42.40]	(349.2181, 66.96)(359.24768, 122.44667)(360.25293, 193.76	C19 H30 N4	FindByFormula	14 -	314.2459	22.355295
C19 H30 N6 O2	C19 H30 N6 O2	[C19 H30 N6 O2, tgt=87.88, overall=87.88]	(409.20752, 411.464)(410.2085, 153.30833)(411.2061, 228.0	C19 H30 N6 O2	FindByFormula	28 -	374.2419	22.959578
C19 H32 N2 O7 S	C19 H32 N2 O7 S	[C19 H32 N2 O7 S, tgt=93.78, overall=93.78]	(467.1554, 73.98923)(468.15234, 27.973999)(469.14633, 62.	C19 H32 N2 O7 S	FindByFormula	28 -	432.1925	18.959705
C19 H32 N2 O8	C19 H32 N2 O8	[C19 H32 N2 O8, tgt=99.50, overall=99.50]	(451.1959, 95.79)(461.2111, 1252.0428)(462.20688, 646.268	C19 H32 N2 O8	FindByFormula	26 -	416.2153	22.727194
C19 H32 N3 O2 P	C19 H32 N3 O2 P	[C19 H32 N3 O2 P, tgt=82.75, overall=82.75]	(410.2186, 182.75998)(411.21036, 200.14626)(364.21545, 5	C19 H32 N3 O2 P	FindByFormula	27 -	365.2232	22.814787
C19 H32 N6 O2	C19 H32 N6 O2	[C19 H32 N6 O2, tgt=82.32, overall=82.32]	(411.2211, 215.8525)(421.24915, 136.565)(375.25232, 1334.	C19 H32 N6 O2	FindByFormula	26 -	376.2595	23.026487
C19 H33 N4 O3 P	C19 H33 N4 O3 P	[C19 H33 N4 O3 P, tgt=77.22, overall=77.22]	(431.19208, 1677.317)(432.19403, 423.57428)(433.1949, 14	C19 H33 N4 O3 P	FindByFormula	26 -	396.2285	22.689474

C19 H34 N2 O8	C19 H34 N2 O8	[C19 H34 N2 O8, tgt=99.11, overall=99.11]	(463.2227, 1078.9211)(464.21667, 443.38403)(465.2158, 42	C19 H34 N2 O8	FindByFormula	28 -	418.2316	22.92569
C19 H34 N8 O7 P2 S3	C19 H34 N8 O7 P2 S3	[C19 H34 N8 O7 P2 S3, tgt=97.89, overall=97.89]	(679.0821, 86.9725)(680.1016, 111.66)(689.1041, 114.4)(64	C19 H34 N8 O7 P2 S3	FindByFormula	8 -	644.1188	0.7877499
C19 H36 O2	C19 H36 O2	[C19 H36 O2, tgt=86.74, overall=86.74]	(341.2691, 631.2753)(342.2727, 170.40561)(343.2681, 69.88	C19 H36 O2	FindByFormula	28 -	296.2715	23.097258
C19 H37 O2 P3	C19 H37 O2 P3	[C19 H37 O2 P3, tgt=88.14, overall=88.14]	(425.16605, 255.03648)(435.19394, 308.24625)(436.18845,	C19 H37 O2 P3	FindByFormula	28 -	390.2	22.598688
C19 H38 N2 O12 P2	C19 H38 N2 O12 P2	[C19 H38 N2 O12 P2, tgt=96.23, overall=96.23]	(583.17017, 71.72)(584.1803, 31.1)(585.1842, 65.22)(593.17	C19 H38 N2 O12 P2	FindByFormula	28 -	548.1897	22.93051
C19 H38 O2	C19 H38 O2	[C19 H38 O2, tgt=89.09, overall=89.09]	(343.2814, 80.69582)(344.2859, 37.95)(297.27917, 2934.447	C19 H38 O2	FindByFormula	27 -	298.2866	22.99725
C19 H38 S2	C19 H38 S2	[C19 H38 S2, tgt=90.48, overall=90.48]	(365.2064, 145.93333)(366.206, 40.97222)(367.20114, 185.6	C19 H38 S2	FindByFormula	28 -	330.2412	16.898905
C19 H39 Cl S4	C19 H39 Cl S4	[C19 H39 Cl S4, tgt=71.61, overall=71.61]	(465.13126, 108.912)(466.1315, 47.796665)(467.1058, 89.43	C19 H39 Cl S4	FindByFormula	25 -	430.1624	3.6000726
C19 H39 Cl2 N4 O3 P3 S2	C19 H39 Cl2 N4 O3 P3 S2	[C19 H39 Cl2 N4 O3 P3 S2, tgt=98.16, overall=98.16]	(635.0604, 55.85)(597.09735, 3773.025)(598.1011, 863.9332	C19 H39 Cl2 N4 O3 P3 S2	FindByFormula	21 -	598.1045	0.7121432
C20 H15 O2 P	C20 H15 O2 P	[C20 H15 O2 P, tgt=87.66, overall=87.66]	(353.0495, 708.6545)(354.0514, 113.781876)(363.0795, 203	C20 H15 O2 P	FindByFormula	21 -	318.0806	4.1368904
C20 H18 N4 O2	C20 H18 N4 O2	[C20 H18 N4 O2, tgt=98.23, overall=98.23]	(381.11172, 3588.2305)(382.11505, 843.9982)(383.1099, 12	C20 H18 N4 O2	FindByFormula	28 -	346.1426	8.457685
C20 H20 N10 O2	C20 H20 N10 O2	[C20 H20 N10 O2, tgt=73.37, overall=73.37]	(467.145, 99.060005)(477.17313, 299.4031)(478.173, 92.087	C20 H20 N10 O2	FindByFormula	18 -	432.1791	22.448643
C20 H20 N4 O2	C20 H20 N4 O2	[C20 H20 N4 O2, tgt=95.59, overall=95.59]	(383.12778, 225.28035)(384.1283, 52.9756)(385.1183, 166.9	C20 H20 N4 O2	FindByFormula	28 -	348.1577	8.875769
C20 H22 N10	C20 H22 N10	[C20 H22 N10, tgt=97.12, overall=97.12]	(437.17975, 80.35)(447.1987, 135.85501)(448.19092, 60.696	C20 H22 N10	FindByFormula	9 -	402.2029	15.248652
C20 H22 N2 O12	C20 H22 N2 O12	[C20 H22 N2 O12, tgt=99.42, overall=99.42]	(517.0768, 60.988)(527.1028, 905.5104)(528.10504, 374.278	C20 H22 N2 O12	FindByFormula	28 -	482.1164	8.4618635
C20 H24 N18 O P4	C20 H24 N18 O P4	[C20 H24 N18 O P4, tgt=82.72, overall=82.72]	(691.0887, 175.20433)(692.08923, 60.738506)(693.07825, 6	C20 H24 N18 O P4	FindByFormula	28 -	656.1326	22.592512
C20 H24 N4 O4	C20 H24 N4 O4	[C20 H24 N4 O4, tgt=88.31, overall=88.31]	(419.1526, 106.705)(420.1498, 55.51)(429.17114, 593.5933)	C20 H24 N4 O4	FindByFormula	27 -	384.1795	22.584185
C20 H25 N2 O2 P	C20 H25 N2 O2 P	[C20 H25 N2 O2 P, tgt=83.62, overall=83.62]	(401.16183, 1027.5864)(402.16296, 322.7463)(355.15878, 3	C20 H25 N2 O2 P	FindByFormula	28 -	356.1661	22.852829
C20 H25 N6 P5	C20 H25 N6 P5	[C20 H25 N6 P5, tgt=38.42, overall=38.42]	(539.04663, 81.5675)(540.0546, 32.958)(541.0291, 196.1299	C20 H25 N6 P5	FindByFormula	15 -	504.0829	1.0028666
C20 H26 N6 O4	C20 H26 N6 O4	[C20 H26 N6 O4, tgt=52.47, overall=52.47]	(449.1671, 845.96155)(450.1649, 454.245)(451.1672, 188.65	C20 H26 N6 O4	FindByFormula	27 -	414.1991	22.703127
C20 H27 N12 O7 P3 S	C20 H27 N12 O7 P3 S	[C20 H27 N12 O7 P3 S, tgt=75.22, overall=75.22]	(707.071, 62.03)(671.09717, 7960.652)(672.0974, 2349.135)	C20 H27 N12 O7 P3 S	FindByFormula	6 -	672.1037	0.6938328
C20 H28 O P2	C20 H28 O P2	[C20 H28 O P2, tgt=26.90, overall=26.90]	(381.13364, 61.066)(382.1355, 20.1)(391.1621, 52.665)(345.	C20 H28 O P2	FindByFormula	9 -	346.1625	11.390941
C20 H28 O4	C20 H28 O4	[C20 H28 O4, tgt=96.10, overall=96.10]	(367.17346, 68.12333)(377.19473, 73.854)(331.1905, 2005.7	C20 H28 O4	FindByFormula	10 -	332.198	13.764387
C20 H29 N14 O P5	C20 H29 N14 O P5	[C20 H29 N14 O P5, tgt=78.86, overall=78.86]	(671.1005, 175.58)(672.09894, 68.33297)(673.10114, 146.39	C20 H29 N14 O P5	FindByFormula	28 -	636.1358	22.448244
C20 H30 N6 O P4	C20 H30 N6 O P4	[C20 H30 N6 O P4, tgt=90.42, overall=90.42]	(529.11945, 80.86083)(530.1298, 41.97)(531.12146, 73.002)	C20 H30 N6 O P4	FindByFormula	28 -	494.1436	22.448605
C20 H30 O2	C20 H30 O2	[C20 H30 O2, tgt=97.89, overall=97.89]	(337.1922, 142.69751)(338.19058, 38.666004)(347.21704, 6	C20 H30 O2	FindByFormula	28 -	302.225	22.522825
C20 H30 O4	C20 H30 O4	[C20 H30 O4, tgt=97.90, overall=97.90]	(369.18256, 143.58)(370.1791, 41.02)(379.2113, 104.575)(3	C20 H30 O4	FindByFormula	9 -	334.2147	15.25118
C20 H31 N2 O5 P	C20 H31 N2 O5 P	[C20 H31 N2 O5 P, tgt=95.95, overall=95.95]	(445.1534, 53.1)(455.19345, 260.0637)(456.1815, 637.0325)	C20 H31 N2 O5 P	FindByFormula	27 -	410.1973	22.730091
C20 H31 N6 O17 P	C20 H31 N6 O17 P	[C20 H31 N6 O17 P, tgt=97.10, overall=97.10]	(693.1141, 150.14336)(694.11163, 71.39526)(695.1097, 124.	C20 H31 N6 O17 P	FindByFormula	28 -	658.1482	22.867931
C20 H32 N4	C20 H32 N4	[C20 H32 N4, tgt=91.39, overall=91.39]	(363.23135, 82.18)(364.22186, 30.54)(373.26367, 144.38573	C20 H32 N4	FindByFormula	28 -	328.262	22.510511
C20 H32 N4 O14	C20 H32 N4 O14	[C20 H32 N4 O14, tgt=98.71, overall=98.71]	(587.1495, 319.29846)(588.1494, 181.18777)(589.1404, 529.	C20 H32 N4 O14	FindByFormula	27 -	552.1896	22.723497
C20 H32 O2	C20 H32 O2	[C20 H32 O2, tgt=97.54, overall=97.54]	(339.2075, 658.7252)(340.2095, 151.70332)(341.20273, 155.	C20 H32 O2	FindByFormula	28 -	304.2413	22.700317
C20 H32 O3	C20 H32 O3	[C20 H32 O3, tgt=98.02, overall=98.02]	(355.20044, 508.61212)(356.19788, 147.82454)(357.19577,	C20 H32 O3	FindByFormula	28 -	320.2349	21.745169
C20 H34 N4 O14	C20 H34 N4 O14	[C20 H34 N4 O14, tgt=99.06, overall=99.06]	(599.19336, 958.0421)(600.19446, 437.88428)(601.187, 293.	C20 H34 N4 O14	FindByFormula	28 -	554.2056	22.928116
C20 H34 O2	C20 H34 O2	[C20 H34 O2, tgt=98.78, overall=98.78]	(351.2492, 2665.792)(352.25052, 408.75)(353.25198, 42.679	C20 H34 O2	FindByFormula	28 -	306.2561	22.849045
C20 H34 O3	C20 H34 O3	[C20 H34 O3, tgt=97.32, overall=97.32]	(357.21832, 105.10285)(358.22046, 42.593334)(359.2181, 1	C20 H34 O3	FindByFormula	24 -	322.2509	21.94564
C20 H35 N5 O7 P2 S	C20 H35 N5 O7 P2 S	[C20 H35 N5 O7 P2 S, tgt=96.54, overall=96.54]	(586.1422, 826.6794)(587.14453, 366.72668)(588.1311, 380.	C20 H35 N5 O7 P2 S	FindByFormula	21 -	551.1724	1.8298576
C20 H35 N6 O2 P3	C20 H35 N6 O2 P3	[C20 H35 N6 O2 P3, tgt=95.27, overall=95.27]	(519.17, 198.01498)(520.1679, 180.46333)(521.16473, 479.6	C20 H35 N6 O2 P3	FindByFormula	27 -	484.2039	22.72331
C20 H36 N12 O2 P6	C20 H36 N12 O2 P6	[C20 H36 N12 O2 P6, tgt=73.31, overall=73.31]	(697.1026, 627.5108)(698.1046, 207.79121)(699.1069, 133.2	C20 H36 N12 O2 P6	FindByFormula	28 -	662.1485	22.592688
C20 H36 N2 O14 P2 S	C20 H36 N2 O14 P2 S	[C20 H36 N2 O14 P2 S, tgt=98.18, overall=98.18]	(657.1076, 663.38574)(658.11755, 163.008)(659.1207, 91.09	C20 H36 N2 O14 P2 S	FindByFormula	13 -	622.1368	0.6976922
C20 H36 N4 O14	C20 H36 N4 O14	[C20 H36 N4 O14, tgt=96.91, overall=96.91]	(591.18604, 176.09999)(592.18744, 146.48)(593.1832, 91.12	C20 H36 N4 O14	FindByFormula	28 -	556.221	23.183077
C20 H36 O2	C20 H36 O2	[C20 H36 O2, tgt=98.26, overall=98.26]	(353.2705, 311.8896)(354.27298, 78.021774)(355.27997, 36	C20 H36 O2	FindByFormula	27 -	308.2721	23.03084
C20 H37 N6 O2 P3	C20 H37 N6 O2 P3	[C20 H37 N6 O2 P3, tgt=97.49, overall=97.49]	(531.2073, 730.15436)(532.20953, 416.8656)(533.202, 199.1	C20 H37 N6 O2 P3	FindByFormula	28 -	486.2192	22.926617
C20 H38 O2	C20 H38 O2	[C20 H38 O2, tgt=70.62, overall=70.62]	(355.28482, 561.0196)(356.28732, 147.60501)(357.2904, 51.	C20 H38 O2	FindByFormula	27 -	310.2875	23.252811
C20 H39 N19 P2	C20 H39 N19 P2	[C20 H39 N19 P2, tgt=65.06, overall=65.06]	(642.2739, 71.23)(643.2733, 42.1475)(644.2579, 52.33)(652.	C20 H39 N19 P2	FindByFormula	24 -	607.3095	21.862474
C20 H40 N2 O3 S2	C20 H40 N2 O3 S2	[C20 H40 N2 O3 S2, tgt=88.82, overall=88.82]	(455.21866, 159.3119)(465.2336, 829.57996)(466.22653, 37	C20 H40 N2 O3 S2	FindByFormula	28 -	420.2468	23.182222
C20 H41 N3 O P2	C20 H41 N3 O P2	[C20 H41 N3 O P2, tgt=94.59, overall=94.59]	(436.23853, 120.99501)(437.23, 429.19)(446.2642, 62.86)(4	C20 H41 N3 O P2	FindByFormula	27 -	401.2713	22.82184
C20 H42 O4 S	C20 H42 O4 S	[C20 H42 O4 S, tgt=90.65, overall=90.65]	(413.2379, 60.97)(423.27686, 123.57715)(424.27393, 69.045	C20 H42 O4 S	FindByFormula	28 -	378.2802	22.815018
C21 H14 N O P S	C21 H14 N O P S	[C21 H14 N O P S, tgt=84.44, overall=84.44]	(394.01852, 695.3333)(395.00433, 2687.49)(396.00525, 522.	C21 H14 N O P S	FindByFormula	8 -	359.0528	0.8051246
C21 H18 N4 O	C21 H18 N4 O	[C21 H18 N4 O, tgt=60.83, overall=60.83]	(387.15237, 411.31183)(388.14865, 123.185265)(341.1434,	C21 H18 N4 O	FindByFormula	26 -	342.1509	22.665401
C21 H19 N18 O P	C21 H19 N18 O P	[C21 H19 N18 O P, tgt=87.49, overall=87.49]	(605.1379, 234.75543)(606.1358, 93.172005)(607.13446, 38	C21 H19 N18 O P	FindByFormula	28 -	570.1694	22.756601
C21 H20 N6 O2	C21 H20 N6 O2	[C21 H20 N6 O2, tgt=91.36, overall=91.36]	(423.13474, 107.70875)(424.14532, 31.595999)(425.14337,	C21 H20 N6 O2	FindByFormula	27 -	388.165	22.207664
C21 H20 O2 P4	C21 H20 O2 P4	[C21 H20 O2 P4, tgt=95.56, overall=95.56]	(463.00635, 75.6425)(463.9958, 23.759998)(473.0254, 55.37	C21 H20 O2 P4	FindByFormula	8 -	428.0406	15.698835
C21 H26 N4 O3	C21 H26 N4 O3	[C21 H26 N4 O3, tgt=80.26, overall=80.26]	(427.20383, 216.71965)(381.19318, 2869.336)(382.19693, 9	C21 H26 N4 O3	FindByFormula	28 -	382.2018	23.195326
C21 H28 N4 O S	C21 H28 N4 O S	[C21 H28 N4 O S, tgt=85.08, overall=85.08]	(429.19083, 1902.2686)(430.1922, 560.81647)(383.19046, 5	C21 H28 N4 O S	FindByFormula	28 -	384.1979	23.20232
C21 H29 N2 O4 P5	C21 H29 N2 O4 P5	[C21 H29 N2 O4 P5, tgt=93.77, overall=93.77]	(563.05237, 59.11)(527.07275, 6202.41)(528.077, 1389.9271	C21 H29 N2 O4 P5	FindByFormula	7 -	528.081	0.78999966
C21 H30 N6 O2	C21 H30 N6 O2	[C21 H30 N6 O2, tgt=76.56, overall=76.56]	(433.21603, 293.4717)(434.22324, 129.43288)(435.2186, 41	C21 H30 N6 O2	FindByFormula	26 -	398.2409	22.842623
C21 H31 N2 O7 P	C21 H31 N2 O7 P	[C21 H31 N2 O7 P, tgt=89.71, overall=89.71]	(489.15067, 75.17834)(490.17575, 36.565002)(499.17926, 2	C21 H31 N2 O7 P	FindByFormula	28 -	454.1873	22.851725
C21 H32 N2 O8	C21 H32 N2 O8	[C21 H32 N2 O8, tgt=99.29, overall=99.29]	(475.17758, 326.15103)(476.1634, 262.86)(485.20352, 1102.	C21 H32 N2 O8	FindByFormula	28 -	440.2161	22.704462
C21 H32 N6 O2	C21 H32 N6 O2	[C21 H32 N6 O2, tgt=95.69, overall=95.69]	(435.22757, 187.4875)(436.23688, 73.145004)(437.22446, 2	C21 H32 N6 O2	FindByFormula	27 -	400.2589	22.94947
C21 H32 N6 O4 P6	C21 H32 N6 O4 P6	[C21 H32 N6 O4 P6, tgt=94.64, overall=94.64]	(653.05286, 76.372505)(654.0542, 32.971428)(655.05206, 2	C21 H32 N6 O4 P6	FindByFormula	28 -	618.0911	8.461505
C21 H33 N10 P S	C21 H33 N10 P S	[C21 H33 N10 P S, tgt=95.08, overall=95.08]	(523.20233, 81.56333)(533.221, 469.97382)(534.22235, 202.	C21 H33 N10 P S	FindByFormula	26 -	488.2345	23.181456
C21 H33 N3 O3	C21 H33 N3 O3	[C21 H33 N3 O3, tgt=98.06, overall=98.06]	(410.22208, 1024.6544)(411.22278, 319.51907)(412.21954,	C21 H33 N3 O3	FindByFormula	22 -	375.2529	17.268518
C21 H33 N8 O P5	C21 H33 N8 O P5	[C21 H33 N8 O P5, tgt=95.80, overall=95.80]	(603.11584, 157.91573)(604.1151, 57.6585)(605.1107, 212.8	C21 H33 N8 O P5	FindByFormula	28 -	568.148	22.450354
C21 H34 N2 O5 S2	C21 H34 N2 O5 S2	[C21 H34 N2 O5 S2, tgt=70.24, overall=70.24]	(493.1665, 132.105)(494.1451, 148.77)(495.1596, 93.96)(49	C21 H34 N2 O5 S2	FindByFormula	27 -	458.1883	22.602915
C21 H34 O P4	C21 H34 O P4	[C21 H34 O P4, tgt=88.06, overall=88.06]	(461.12128, 53.22)(471.15158, 128.29056)(472.1567, 66.598	C21 H34 O P4	FindByFormula	27 -	426.1567	22.446012
C21 H34 O20	C21 H34 O20	[C21 H34 O20, tgt=97.51, overall=97.51]	(641.13715, 93.274994)(642.144, 43.13)(643.138, 48.9)(605.	C21 H34 O20	FindByFormula	7 -	606.1639	0.77857083
C21 H35 O17 P	C21 H35 O17 P	[C21 H35 O17 P, tgt=97.70, overall=97.70]	(625.12506, 126.3432)(626.1245, 50.7575)(627.1179, 106.97	C21 H35 O17 P	FindByFormula	28 -	590.1608	22.863575
C21 H36 S2	C21 H36 S2	[C21 H36 S2, tgt=86.48, overall=86.48]	(387.1935, 269.05597)(388.1947, 67.93157)(389.18515, 123.	C21 H36 S2	FindByFormula	22 -	352.226	16.750896
C21 H37 Cl N2 O S2	C21 H37 Cl N2 O S2	[C21 H37 Cl N2 O S2, tgt=90.22, overall=90.22]	(477.20447, 186.47592)(478.2046, 101.4)(479.19992, 99.534	C21 H37 Cl N2 O S2	FindByFormula	27 -	432.2041	23.182585
C21 H37 N25 P2	C21 H37 N25 P2	[C21 H37 N25 P2, tgt=61.84, overall=61.84]	(736.27783, 72.33375)(746.31256, 103.09417)(747.32196, 1	C21 H37 N25 P2	FindByFormula	27 -	701.3147	22.02242
C21 H38 O10 S	C21 H38 O10 S	[C21 H38 O10 S, tgt=95.02, overall=95.02]	(517.194, 56.47)(518.1941, 32.92)(527.21967, 70.722)(528.2	C21 H38 O10 S	FindByFormula	28 -	482.2187	23.183685
C21 H40 N6 O2 P6	C21 H40 N6 O2 P6	[C21 H40 N6 O2 P6, tgt=78.19, overall=78.19]	(629.1165, 565.4016)(630.1177, 162.22368)(631.1137, 157.2	C21 H40 N6 O2 P6	FindByFormula	28 -	594.1607	22.598404
C21 H44 N4 O14 P4 S	C21 H44 N4 O14 P4 S	[C21 H44 N4 O14 P4 S, tgt=96.65, overall=96.65]	(767.11566, 374.13248)(768.1175, 155.77641)(769.1152, 30	C21 H44 N4 O14 P4 S	FindByFormula	28 -	732.1522	22.86529
C21 H44 O4 S	C21 H44 O4 S	[C21 H44 O4 S, tgt=76.83, overall=76.83]	(427.2665, 69.75428)(428.276, 31.49)(429.2813, 72.01)(437.	C21 H44 O4 S	FindByFormula	28 -	392.2962	22.87478
C22 H17 N6 O5 P	C22 H17 N6 O5 P	[C22 H17 N6 O5 P, tgt=95.60, overall=95.60]	(511.0665, 65.31)(521.10114, 71.40692)(522.1162, 21.64)(4	C22 H17 N6 O5 P	FindByFormula	28 -	476.1004	8.463471
C22 H19 P	C22 H19 P	[C22 H19 P, tgt=64.78, overall=64.78]	(349.0984, 61.54)(359.12067, 85.77555)(360.1135, 26.81499	C22 H19 P	FindByFormula	17 -	314.1194	22.158672
C22 H23 O3 P S2	C22 H23 O3 P S2	[C22 H23 O3 P S2, tgt=93.73, overall=93.73]	(465.06116, 102.011665)(466.05927, 33.651997)(467.05963,	C22 H23 O3 P S2	FindByFormula	26 -	430.0812	2.516614
C22 H24 N4 O4	C22 H24 N4 O4	[C22 H24 N4 O4, tgt=65.60, overall=65.60]	(443.14377, 144.2875)(444.14603, 75.13)(453.1794, 6135.19	C22 H24 N4 O4	FindByFormula	28 -	408.1806	22.705414
C22 H25 N2 O2 P	C22 H25 N2 O2 P	[C22 H25 N2 O2 P, tgt=88.26, overall=88.26]	(415.1395, 70.74)(416.1393, 30.45)(417.1225, 23.4)(425.162	C22 H25 N2 O2 P	FindByFormula	28 -	380.1652	22.744265
C22 H26 Cl N4 O5 P	C22 H26 Cl N4 O5 P	[C22 H26 Cl N4 O5 P, tgt=60.09, overall=60.09]	(527.1076, 108.252)(528.1031, 92.54667)(529.11426, 25.215	C22 H26 Cl N4 O5 P	FindByFormula	22 -	492.1329	3.6375818
C22 H26 N4 O22	C22 H26 N4 O22	[C22 H26 N4 O22, tgt=81.77, overall=81.77]	(743.0962, 156.81406)(744.0994, 62.984585)(745.1028, 202.	C22 H26 N4 O22	FindByFormula	28 -	698.1051	22.450603
C22 H27 Cl N4 O	C22 H27 Cl N4 O	[C22 H27 Cl N4 O, tgt=56.90, overall=56.90]	(433.1608, 51.8)(443.18994, 86.37858)(444.19662, 40.40666	C22 H27 Cl N4 O	FindByFormula	15 -	398.1869	13.765737
C22 H27 N O2 P2	C22 H27 N O2 P2	[C22 H27 N O2 P2, tgt=64.61, overall=64.61]	(434.12668, 114.61941)(435.12695, 39.938335)(444.1416, 9	C22 H27 N O2 P2	FindByFormula	26 -	399.1502	22.581371
C22 H27 N2 O2 P	C22 H27 N2 O2 P	[C22 H27 N2 O2 P, tgt=82.54, overall=82.54]	(427.17822, 884.05005)(428.1875, 931.11)(381.17456, 3512	C22 H27 N2 O2 P	FindByFormula	28 -	382.1821	22.926401
C22 H27 N5 O4	C22 H27 N5 O4	[C22 H27 N5 O4, tgt=93.67, overall=93.67]	(460.1704, 61.84)(424.19827, 1665.568)(425.2009, 462.4991	C22 H27 N5 O4	FindByFormula	11 -	425.2051	13.767395
C22 H28 O3 P2	C22 H28 O3 P2	[C22 H28 O3 P2, tgt=47.54, overall=47.54]	(437.11322, 66.10126)(438.1119, 29.906668)(439.1173, 49.9	C22 H28 O3 P2	FindByFormula	26 -	402.1483	22.562458
C22 H30 N10 O4 P2 S4	C22 H30 N10 O4 P2 S4	[C22 H30 N10 O4 P2 S4, tgt=85.43, overall=85.43]	(723.0497, 176.6325)(724.0519, 103.735)(725.06116, 139.25	C22 H30 N10 O4 P2 S4	FindByFormula	9 -	688.0805	0.6749999
C22 H30 N12 O2 P4 S	C22 H30 N12 O2 P4 S	[C22 H30 N12 O2 P4 S, tgt=42.58, overall=42.58]	(685.09564, 53.995003)(686.1016, 61.333332)(687.11035, 3	C22 H30 N12 O2 P4 S	FindByFormula	12 -	650.123	1.0638328
C22 H31 N7 O2 S	C22 H31 N7 O2 S	[C22 H31 N7 O2 S, tgt=85.27, overall=85.27]	(492.19254, 58.936665)(493.2029, 32.37)(502.23138, 100.76	C22 H31 N7 O2 S	FindByFormula	27 -	457.2268	23.184732
C22 H32 N2 O9 P2 S	C22 H32 N2 O9 P2 S	[C22 H32 N2 O9 P2 S, tgt=79.23, overall=79.23]	(597.10254, 81.56286)(598.0967, 28.900002)(599.1083, 88.2	C22 H32 N2 O9 P2 S	FindByFormula	28 -	562.1301	22.44864
C22 H32 N4 O	C22 H32 N4 O	[C22 H32 N4 O, tgt=57.24, overall=57.24]	(367.2503, 2215.33)(368.25214, 506.1028)(369.2478, 170.22	C22 H32 N4 O	FindByFormula	25 -	368.2569	22.724808
C22 H32 O2	C22 H32 O2	[C22 H32 O2, tgt=94.86, overall=94.86]	(363.21005, 337.606)(364.1944, 83.75)(365.2144, 328.73)(3	C22 H32 O2	FindByFormula	27 -	328.2415	22.69932
C22 H33 N6 O17 P	C22 H33 N6 O17 P	[C22 H33 N6 O17 P, tgt=92.11, overall=92.11]	(719.1128, 386.57)(720.1172, 102.32)(721.1041, 38.165)(72	C22 H33 N6 O17 P	FindByFormula	27 -	684.1639	22.938404
C22 H34 O2	C22 H34 O2	[C22 H34 O2, tgt=92.97, overall=92.97]	(365.22134, 2102.6072)(366.2201, 570.8261)(367.2261, 23.1	C22 H34 O2	FindByFormula	27 -	330.257	22.816116
C22 H35 N5	C22 H35 N5	[C22 H35 N5, tgt=90.30, overall=90.30]	(404.255, 89.99)(414.2916, 80.90333)(368.28015, 4246.6284	C22 H35 N5	FindByFormula	20 -	369.2885	22.329403
C22 H35 N6 O17 P	C22 H35 N6 O17 P	[C22 H35 N6 O17 P, tgt=96.93, overall=96.93]	(721.13824, 187.875)(722.1387, 79.42556)(723.13525, 62.57	C22 H35 N6 O17 P	FindByFormula	28 -	686.1801	23.182505
C22 H36 N12 O2 P6	C22 H36 N12 O2 P6	[C22 H36 N12 O2 P6, tgt=40.81, overall=40.81]	(721.1128, 471.51596)(722.1186, 160.0658)(723.11584, 205.	C22 H36 N12 O2 P6	FindByFormula	27 -	686.1481	22.702896
C22 H36 O2	C22 H36 O2	[C22 H36 O2, tgt=97.34, overall=97.34]	(367.2414, 254.90715)(368.24512, 56.962776)(369.24033, 8	C22 H36 O2	FindByFormula	28 -	332.2722	22.949749
C22 H36 S4	C22 H36 S4	[C22 H36 S4, tgt=61.47, overall=61.47]	(463.1305, 70.56)(473.16983, 410.07635)(474.17856, 74.373	C22 H36 S4	FindByFormula	24 -	428.173	22.692339
C22 H37 N2 O P5	C22 H37 N2 O P5	[C22 H37 N2 O P5, tgt=83.79, overall=83.79]	(535.1297, 136.57333)(536.1284, 46.51118)(537.12506, 130.	C22 H37 N2 O P5	FindByFormula	27 -	500.16	22.4479
C22 H37 O12 P S2	C22 H37 O12 P S2	[C22 H37 O12 P S2, tgt=94.22, overall=94.22]	(623.10364, 143.45421)(624.1043, 51.06643)(625.1008, 51.4	C22 H37 O12 P S2	FindByFormula	28 -	588.1445	22.581259
C22 H38 O P2 S	C22 H38 O P2 S	[C22 H38 O P2 S, tgt=90.19, overall=90.19]	(447.17947, 181.38223)(448.18854, 98.53999)(457.215, 436.	C22 H38 O P2 S	FindByFormula	28 -	412.2123	22.930826
C22 H38 O4	C22 H38 O4	[C22 H38 O4, tgt=85.68, overall=85.68]	(401.23853, 84.244995)(411.28104, 288.87003)(412.28546,	C22 H38 O4	FindByFormula	6 -	366.2763	22.321795
C22 H38 S2	C22 H38 S2	[C22 H38 S2, tgt=29.33, overall=29.33]	(401.2153, 132.12334)(402.2153, 53.96857)(403.2112, 103.4	C22 H38 S2	FindByFormula	21 -	366.2386	22.308073
C22 H4 N O P	C22 H4 N O P	[C22 H4 N O P, tgt=66.97, overall=66.97]	(363.97195, 471.51083)(364.97733, 228.25334)(365.97174,	C22 H4 N O P	FindByFormula	19 -	329.0019	5.3312974
C22 H40 N4 S	C22 H40 N4 S	[C22 H40 N4 S, tgt=82.56, overall=82.56]	(427.26727, 61.43)(437.29245, 126.93555)(438.29865, 53.34	C22 H40 N4 S	FindByFormula	28 -	392.2963	22.912336
C22 H40 N5 O3 P	C22 H40 N5 O3 P	[C22 H40 N5 O3 P, tgt=84.32, overall=84.32]	(488.25488, 78.94714)(489.2775, 53.16)(498.28473, 78.0111	C22 H40 N5 O3 P	FindByFormula	26 -	453.2843	22.276152
C22 H41 N4 O4 P3 S	C22 H41 N4 O4 P3 S	[C22 H41 N4 O4 P3 S, tgt=95.60, overall=95.60]	(585.1751, 63.08667)(595.1936, 60.66)(549.19806, 6972.966	C22 H41 N4 O4 P3 S	FindByFormula	28 -	550.2059	23.182829
C22 H41 N8 O4 P	C22 H41 N8 O4 P	[C22 H41 N8 O4 P, tgt=90.28, overall=90.28]	(547.27094, 59.789997)(548.2875, 27.35)(549.2714, 67.77)(	C22 H41 N8 O4 P	FindByFormula	13 -	512.2972	18.988228
C22 H43 N3 O6 S	C22 H43 N3 O6 S	[C22 H43 N3 O6 S, tgt=95.21, overall=95.21]	(512.2644, 457.36728)(513.2698, 207.11716)(514.26434, 86.	C22 H43 N3 O6 S	FindByFormula	27 -	477.2869	21.981947
C22 H44 N2 O5	C22 H44 N2 O5	[C22 H44 N2 O5, tgt=79.26, overall=79.26]	(451.294, 210.72299)(452.29462, 69.14)(453.29428, 133.174	C22 H44 N2 O5	FindByFormula	16 -	416.3281	22.622879
C22 H44 O2	C22 H44 O2	[C22 H44 O2, tgt=93.36, overall=93.36]	(339.3263, 3708.9263)(340.32962, 924.9403)(341.33154, 16	C22 H44 O2	FindByFormula	25 -	340.3342	24.087296
C22 H44 O2 P6	C22 H44 O2 P6	[C22 H44 O2 P6, tgt=76.31, overall=76.31]	(561.1345, 435.83502)(562.1347, 190.48141)(563.12946, 13	C22 H44 O2 P6	FindByFormula	27 -	526.1743	22.585405
C22 H45 N19 P2	C22 H45 N19 P2	[C22 H45 N19 P2, tgt=54.15, overall=54.15]	(672.3239, 123.43001)(673.32904, 115.14667)(674.3276, 15	C22 H45 N19 P2	FindByFormula	22 -	637.358	22.618938
C22 H52 N15 O4 P5	C22 H52 N15 O4 P5	[C22 H52 N15 O4 P5, tgt=59.64, overall=59.64]	(780.2869, 59.47)(790.2976, 104.85999)(791.30493, 59.465)	C22 H52 N15 O4 P5	FindByFormula	27 -	745.3012	22.249878
C23 H23 Cl N4 O2	C23 H23 Cl N4 O2	[C23 H23 Cl N4 O2, tgt=99.63, overall=99.63]	(457.1209, 109.48)(467.1495, 138.798)(468.14926, 47.42000	C23 H23 Cl N4 O2	FindByFormula	23 -	422.1508	16.421474
C23 H24 N4 O S	C23 H24 N4 O S	[C23 H24 N4 O S, tgt=77.64, overall=77.64]	(449.159, 765.9145)(450.16055, 184.3)(403.15952, 12920.66	C23 H24 N4 O S	FindByFormula	27 -	404.167	22.690506
C23 H26 N10	C23 H26 N10	[C23 H26 N10, tgt=98.34, overall=98.34]	(477.20398, 117.16)(478.20953, 43.714)(479.2242, 201.27)(	C23 H26 N10	FindByFormula	28 -	442.234	14.180948
C23 H26 N8 P2	C23 H26 N8 P2	[C23 H26 N8 P2, tgt=82.68, overall=82.68]	(511.14526, 65.845)(521.1701, 309.47998)(475.16745, 3316.	C23 H26 N8 P2	FindByFormula	8 -	476.1773	22.527054
C23 H27 Cl O8 S	C23 H27 Cl O8 S	[C23 H27 Cl O8 S, tgt=91.03, overall=91.03]	(497.10416, 17653.89)(498.10608, 4833.204)(499.10022, 85	C23 H27 Cl O8 S	FindByFormula	18 -	498.1113	8.654968
C23 H28 N12 O P4	C23 H28 N12 O P4	[C23 H28 N12 O P4, tgt=55.71, overall=55.71]	(647.1127, 348.4615)(648.1128, 114.064995)(649.10834, 28	C23 H28 N12 O P4	FindByFormula	28 -	612.1435	22.732285
C23 H30 N14 O5 P4	C23 H30 N14 O5 P4	[C23 H30 N14 O5 P4, tgt=78.63, overall=78.63]	(741.1082, 166.19997)(742.1079, 69.6395)(743.1035, 400.02	C23 H30 N14 O5 P4	FindByFormula	28 -	706.1445	22.713957
C23 H30 N4 O2 S2	C23 H30 N4 O2 S2	[C23 H30 N4 O2 S2, tgt=78.14, overall=78.14]	(493.1475, 244.20076)(494.14954, 85.20635)(495.14713, 39	C23 H30 N4 O2 S2	FindByFormula	26 -	458.1786	22.707817
C23 H31 N2 O7 P	C23 H31 N2 O7 P	[C23 H31 N2 O7 P, tgt=91.41, overall=91.41]	(513.1642, 625.22284)(514.1678, 197.353)(515.17, 55.48)(5	C23 H31 N2 O7 P	FindByFormula	20 -	478.1853	22.726023
C23 H32 O2	C23 H32 O2	[C23 H32 O2, tgt=97.73, overall=97.73]	(375.2204, 73.38)(385.23688, 74.4475)(339.2336, 11727.257	C23 H32 O2	FindByFormula	8 -	340.241	22.520807
C23 H33 N2 O7 P	C23 H33 N2 O7 P	[C23 H33 N2 O7 P, tgt=97.07, overall=97.07]	(525.1985, 133.4161)(526.2065, 135.66)(479.195, 8791.795)	C23 H33 N2 O7 P	FindByFormula	28 -	480.2021	22.928404
C23 H34 N4	C23 H34 N4	[C23 H34 N4, tgt=87.45, overall=87.45]	(401.24612, 107.26667)(402.2541, 31.34)(403.24023, 84.39)	C23 H34 N4	FindByFormula	6 -	366.277	22.248632
C23 H34 N6 O13 P2	C23 H34 N6 O13 P2	[C23 H34 N6 O13 P2, tgt=97.93, overall=97.93]	(699.1284, 372.85214)(700.13, 166.11858)(701.1278, 342.10	C23 H34 N6 O13 P2	FindByFormula	28 -	664.1655	22.859114
C23 H35 O17 P	C23 H35 O17 P	[C23 H35 O17 P, tgt=98.19, overall=98.19]	(649.1372, 535.8888)(650.1425, 187.17807)(651.1542, 73.02	C23 H35 O17 P	FindByFormula	27 -	614.1617	22.73059
C23 H36 O P4	C23 H36 O P4	[C23 H36 O P4, tgt=84.10, overall=84.10]	(487.1404, 78.57533)(488.14258, 26.55)(489.12296, 77.375)	C23 H36 O P4	FindByFormula	27 -	452.1719	22.583517
C23 H36 O2 S2	C23 H36 O2 S2	[C23 H36 O2 S2, tgt=68.80, overall=68.80]	(443.1913, 77.87909)(444.19818, 33.71)(445.1961, 94.00500	C23 H36 O2 S2	FindByFormula	25 -	408.2162	13.760431
C23 H37 O17 P	C23 H37 O17 P	[C23 H37 O17 P, tgt=99.06, overall=99.06]	(661.16266, 209.18932)(662.16144, 116.141815)(615.1696,	C23 H37 O17 P	FindByFormula	28 -	616.1766	22.935827
C23 H37 O2 P3	C23 H37 O2 P3	[C23 H37 O2 P3, tgt=93.97, overall=93.97]	(473.1734, 263.29224)(483.1932, 5921.9717)(484.19724, 16	C23 H37 O2 P3	FindByFormula	27 -	438.1985	22.57781
C23 H39 N8 O7 P5 S	C23 H39 N8 O7 P5 S	[C23 H39 N8 O7 P5 S, tgt=97.95, overall=97.95]	(761.102, 191.39964)(762.1032, 62.909176)(763.0987, 137.7	C23 H39 N8 O7 P5 S	FindByFormula	28 -	726.1349	22.869108
C23 H39 O17 P	C23 H39 O17 P	[C23 H39 O17 P, tgt=99.70, overall=99.70]	(653.159, 125.184006)(654.16284, 62.574444)(655.16003, 6	C23 H39 O17 P	FindByFormula	28 -	618.1924	23.183077
C23 H40 N6 O2 P6	C23 H40 N6 O2 P6	[C23 H40 N6 O2 P6, tgt=49.64, overall=49.64]	(653.1254, 559.07495)(654.12787, 187.3068)(655.12665, 28	C23 H40 N6 O2 P6	FindByFormula	28 -	618.1603	22.730253
C23 H42 S4	C23 H42 S4	[C23 H42 S4, tgt=81.01, overall=81.01]	(481.19183, 219.79399)(482.1908, 65.4825)(483.1702, 35.91	C23 H42 S4	FindByFormula	28 -	446.2164	22.994154
C23 H43 N O4 P2 S	C23 H43 N O4 P2 S	[C23 H43 N O4 P2 S, tgt=94.60, overall=94.60]	(526.20844, 3340.176)(527.2115, 968.6828)(528.20856, 126	C23 H43 N O4 P2 S	FindByFormula	22 -	491.2391	7.7875156
C23 H43 N13 P2	C23 H43 N13 P2	[C23 H43 N13 P2, tgt=50.08, overall=50.08]	(598.2946, 57.1575)(608.314, 222.46)(609.30774, 107.24801	C23 H43 N13 P2	FindByFormula	14 -	563.322	21.766644
C23 H44 N6 O4 P4 S	C23 H44 N6 O4 P4 S	[C23 H44 N6 O4 P4 S, tgt=99.27, overall=99.27]	(659.17084, 250.51958)(660.179, 140.07933)(661.1678, 98.8	C23 H44 N6 O4 P4 S	FindByFormula	28 -	624.2095	23.18279
C23 H45 N7 P2	C23 H45 N7 P2	[C23 H45 N7 P2, tgt=60.09, overall=60.09]	(516.29913, 70.846)(517.2941, 56.9525)(526.31635, 758.116	C23 H45 N7 P2	FindByFormula	13 -	481.3172	22.232811
C23 H47 Cl N3 O3 P	C23 H47 Cl N3 O3 P	[C23 H47 Cl N3 O3 P, tgt=59.07, overall=59.07]	(524.29456, 230.11496)(525.2926, 225.894)(478.29474, 371	C23 H47 Cl N3 O3 P	FindByFormula	28 -	479.3045	22.304302
C23 H48 N O9 P	C23 H48 N O9 P	[C23 H48 N O9 P, tgt=88.96, overall=88.96]	(548.2654, 54.64)(558.3118, 65.21)(512.29913, 3606.4294)(	C23 H48 N O9 P	FindByFormula	27 -	513.3055	21.574226
C23 H48 N5 P3	C23 H48 N5 P3	[C23 H48 N5 P3, tgt=97.19, overall=97.19]	(522.28186, 299.175)(523.27936, 82.21999)(524.279, 112.91	C23 H48 N5 P3	FindByFormula	6 -	487.3126	5.3178124
C23 H9 Cl N6 O	C23 H9 Cl N6 O	[C23 H9 Cl N6 O, tgt=80.35, overall=80.35]	(455.0192, 83.38334)(456.02713, 36.9175)(457.01984, 78.49	C23 H9 Cl N6 O	FindByFormula	26 -	420.0543	2.51246
C24 H17 N8 O2 P	C24 H17 N8 O2 P	[C24 H17 N8 O2 P, tgt=87.25, overall=87.25]	(515.0931, 79.444496)(516.0972, 28.228)(517.0819, 41.735)	C24 H17 N8 O2 P	FindByFormula	28 -	480.1225	8.464005
C24 H19 N3 O9 P2	C24 H19 N3 O9 P2	[C24 H19 N3 O9 P2, tgt=98.15, overall=98.15]	(600.0738, 104.121994)(601.07404, 41.018574)(554.0526, 1	C24 H19 N3 O9 P2	FindByFormula	22 -	555.0599	8.658918
C24 H21 N12 O P	C24 H21 N12 O P	[C24 H21 N12 O P, tgt=87.45, overall=87.45]	(523.1633, 3825.5947)(524.1666, 1193.2483)(525.16345, 42	C24 H21 N12 O P	FindByFormula	6 -	524.1706	5.703644
C24 H24 N4 O4	C24 H24 N4 O4	[C24 H24 N4 O4, tgt=98.84, overall=98.84]	(467.15277, 251.72134)(468.15646, 80.12)(469.1605, 44.977	C24 H24 N4 O4	FindByFormula	28 -	432.1796	16.422014
C24 H27 N23 O	C24 H27 N23 O	[C24 H27 N23 O, tgt=91.47, overall=91.47]	(688.23206, 100.58)(689.2323, 30.32)(690.2261, 28.005001)	C24 H27 N23 O	FindByFormula	10 -	653.2772	20.231833
C24 H28 N12 O12 S	C24 H28 N12 O12 S	[C24 H28 N12 O12 S, tgt=96.26, overall=96.26]	(743.1269, 124.337395)(744.1275, 45.670715)(745.12964, 4	C24 H28 N12 O12 S	FindByFormula	28 -	708.1668	13.099122
C24 H32 N10	C24 H32 N10	[C24 H32 N10, tgt=73.91, overall=73.91]	(495.25757, 81.9675)(496.2501, 22.12)(497.2474, 22.91)(50	C24 H32 N10	FindByFormula	15 -	460.2799	21.67234
C24 H32 N2 O5	C24 H32 N2 O5	[C24 H32 N2 O5, tgt=61.21, overall=61.21]	(463.1995, 466.03278)(464.19824, 137.47096)(465.1987, 56.	C24 H32 N2 O5	FindByFormula	24 -	428.233	16.441856
C24 H32 O P2	C24 H32 O P2	[C24 H32 O P2, tgt=90.81, overall=90.81]	(443.19543, 88.9025)(444.2019, 20.27)(397.1852, 3168.9119	C24 H32 O P2	FindByFormula	6 -	398.1919	8.531446
C24 H32 P4	C24 H32 P4	[C24 H32 P4, tgt=73.14, overall=73.14]	(479.127, 53.3)(489.14587, 75.57333)(490.1445, 30.98)(443.	C24 H32 P4	FindByFormula	23 -	444.146	2.516954
C24 H33 N3 O2	C24 H33 N3 O2	[C24 H33 N3 O2, tgt=99.27, overall=99.27]	(430.2264, 1126.8281)(431.2273, 395.48154)(432.22482, 44	C24 H33 N3 O2	FindByFormula	22 -	395.2582	13.134186
C24 H34 N2 O10	C24 H34 N2 O10	[C24 H34 N2 O10, tgt=99.75, overall=99.75]	(545.18805, 85.30501)(546.18756, 31.425001)(547.1803, 54.	C24 H34 N2 O10	FindByFormula	28 -	510.2191	13.096982
C24 H35 N10 O7 P5	C24 H35 N10 O7 P5	[C24 H35 N10 O7 P5, tgt=78.16, overall=78.16]	(765.09143, 486.6823)(766.09467, 171.86398)(767.089, 151.	C24 H35 N10 O7 P5	FindByFormula	28 -	730.1362	22.605001
C24 H35 N6 O2 P3	C24 H35 N6 O2 P3	[C24 H35 N6 O2 P3, tgt=68.50, overall=68.50]	(567.1706, 190.96426)(568.1664, 260.725)(577.19305, 482.3	C24 H35 N6 O2 P3	FindByFormula	27 -	532.2062	22.702095
C24 H36 N12 O5	C24 H36 N12 O5	[C24 H36 N12 O5, tgt=55.23, overall=55.23]	(607.27234, 91.94666)(608.27545, 89.06)(609.2584, 23.09)(	C24 H36 N12 O5	FindByFormula	17 -	572.2927	3.5785193
C24 H36 N2 O3 S2	C24 H36 N2 O3 S2	[C24 H36 N2 O3 S2, tgt=85.82, overall=85.82]	(499.18756, 119.5)(500.17563, 287.36002)(509.20743, 751.8	C24 H36 N2 O3 S2	FindByFormula	27 -	464.2153	22.702532
C24 H36 O10 P6	C24 H36 O10 P6	[C24 H36 O10 P6, tgt=78.51, overall=78.51]	(705.043, 103.255005)(706.0345, 38.062)(707.0488, 43.9925	C24 H36 O10 P6	FindByFormula	28 -	670.0737	21.74595
C24 H37 N2 O10 P S	C24 H37 N2 O10 P S	[C24 H37 N2 O10 P S, tgt=98.19, overall=98.19]	(611.1473, 344.35052)(612.1498, 158.39001)(621.17584, 79	C24 H37 N2 O10 P S	FindByFormula	27 -	576.1888	22.709242
C24 H37 O4 P3	C24 H37 O4 P3	[C24 H37 O4 P3, tgt=61.50, overall=61.50]	(517.15564, 87.805)(518.1503, 59.53)(527.18634, 250.47156	C24 H37 O4 P3	FindByFormula	19 -	482.1888	22.558834
C24 H38 N2 O17 P2	C24 H38 N2 O17 P2	[C24 H38 N2 O17 P2, tgt=98.74, overall=98.74]	(723.1208, 481.1465)(724.12244, 206.12346)(725.12115, 45	C24 H38 N2 O17 P2	FindByFormula	27 -	688.1642	22.72905
C24 H38 O13 P2	C24 H38 O13 P2	[C24 H38 O13 P2, tgt=97.82, overall=97.82]	(631.1422, 430.89325)(632.1446, 187.64928)(633.1419, 648.	C24 H38 O13 P2	FindByFormula	28 -	596.1779	22.849903
C24 H38 O19 P2 S	C24 H38 O19 P2 S	[C24 H38 O19 P2 S, tgt=76.34, overall=76.34]	(759.0776, 183.38615)(760.0769, 67.82084)(761.0762, 109.5	C24 H38 O19 P2 S	FindByFormula	27 -	724.1202	22.581223
C24 H40 N12 O2 P6	C24 H40 N12 O2 P6	[C24 H40 N12 O2 P6, tgt=93.11, overall=93.11]	(749.13947, 150.53917)(750.1407, 58.583633)(751.1413, 41.	C24 H40 N12 O2 P6	FindByFormula	28 -	714.1818	13.099983
C24 H40 N2 O17 P2	C24 H40 N2 O17 P2	[C24 H40 N2 O17 P2, tgt=24.57, overall=24.57]	(725.1294, 2646.874)(726.1346, 804.12445)(727.1315, 353.4	C24 H40 N2 O17 P2	FindByFormula	24 -	690.1765	23.070251
C24 H40 O4	C24 H40 O4	[C24 H40 O4, tgt=68.45, overall=68.45]	(427.2608, 167.43399)(428.25906, 69.024284)(429.2592, 14	C24 H40 O4	FindByFormula	12 -	392.2928	21.463768
C24 H42 N2 O17 P2	C24 H42 N2 O17 P2	[C24 H42 N2 O17 P2, tgt=98.71, overall=98.71]	(727.15247, 403.44955)(728.1549, 161.352)(729.15717, 92.5	C24 H42 N2 O17 P2	FindByFormula	28 -	692.1957	23.18222
C24 H42 N6 O3	C24 H42 N6 O3	[C24 H42 N6 O3, tgt=31.56, overall=31.56]	(497.2983, 259.33453)(498.30008, 87.9111)(499.299, 95.658	C24 H42 N6 O3	FindByFormula	23 -	462.3302	22.707926
C24 H43 Cl O21	C24 H43 Cl O21	[C24 H43 Cl O21, tgt=99.28, overall=99.28]	(737.1605, 124.815)(747.2026, 93.705)(748.1892, 34.345)(7	C24 H43 Cl O21	FindByFormula	25 -	702.1995	0.71636015
C24 H43 N19 P2	C24 H43 N19 P2	[C24 H43 N19 P2, tgt=42.74, overall=42.74]	(694.30835, 140.88501)(695.3122, 82.365)(704.3328, 147.87	C24 H43 N19 P2	FindByFormula	18 -	659.341	22.335274
C24 H43 N9 O S3	C24 H43 N9 O S3	[C24 H43 N9 O S3, tgt=86.63, overall=86.63]	(604.2448, 75.046)(605.2369, 31.663332)(614.26746, 120.06	C24 H43 N9 O S3	FindByFormula	28 -	569.2744	21.995213
C24 H44 N6 P4	C24 H44 N6 P4	[C24 H44 N6 P4, tgt=80.42, overall=80.42]	(585.2559, 59.015)(539.25085, 1861.0017)(540.2521, 601.27	C24 H44 N6 P4	FindByFormula	13 -	540.2589	14.338486
C24 H44 O2 P6	C24 H44 O2 P6	[C24 H44 O2 P6, tgt=48.88, overall=48.88]	(585.14124, 629.49005)(586.1395, 210.778)(587.14355, 338.	C24 H44 O2 P6	FindByFormula	28 -	550.1726	22.67714
C24 H45 O18 P S3	C24 H45 O18 P S3	[C24 H45 O18 P S3, tgt=92.04, overall=92.04]	(783.11774, 72.67273)(784.1259, 32.143333)(785.09955, 59.	C24 H45 O18 P S3	FindByFormula	28 -	748.1517	23.184576
C24 H46 N6 P4	C24 H46 N6 P4	[C24 H46 N6 P4, tgt=88.10, overall=88.10]	(577.2416, 87.86714)(578.2411, 37.796)(579.2291, 31.3325)	C24 H46 N6 P4	FindByFormula	12 -	542.274	13.88564
C24 H46 O2	C24 H46 O2	[C24 H46 O2, tgt=83.42, overall=83.42]	(365.34317, 1457.9319)(366.3463, 404.0064)(367.352, 206.6	C24 H46 O2	FindByFormula	25 -	366.3512	24.14249
C24 H47 N5 O P4	C24 H47 N5 O P4	[C24 H47 N5 O P4, tgt=90.81, overall=90.81]	(580.23456, 71.015)(581.23724, 24.42)(582.23083, 40.1525)	C24 H47 N5 O P4	FindByFormula	28 -	545.2737	21.98036
C24 H47 N7 O2 S2	C24 H47 N7 O2 S2	[C24 H47 N7 O2 S2, tgt=87.00, overall=87.00]	(564.2972, 55.61)(574.3129, 272.93146)(575.30884, 77.822)	C24 H47 N7 O2 S2	FindByFormula	16 -	529.3234	3.6116161
C24 H48 N O2 P S2	C24 H48 N O2 P S2	[C24 H48 N O2 P S2, tgt=85.87, overall=85.87]	(512.2613, 445.64297)(513.273, 244.45143)(514.26166, 93.3	C24 H48 N O2 P S2	FindByFormula	28 -	477.2876	22.097704
C24 H48 N6 O3	C24 H48 N6 O3	[C24 H48 N6 O3, tgt=49.03, overall=49.03]	(503.35074, 278.0172)(504.3535, 128.22166)(505.35318, 58	C24 H48 N6 O3	FindByFormula	24 -	468.3797	22.905754
C24 H48 O2	C24 H48 O2	[C24 H48 O2, tgt=98.37, overall=98.37]	(403.3242, 80.74)(404.3302, 25.5)(367.35876, 13623.031)(3	C24 H48 O2	FindByFormula	26 -	368.3658	24.716787
C24 H49 Cl N8	C24 H49 Cl N8	[C24 H49 Cl N8, tgt=42.31, overall=42.31]	(519.35016, 145.845)(520.35114, 64.73857)(521.34796, 115.	C24 H49 Cl N8	FindByFormula	16 -	484.3756	22.547932
C24 H51 N3 O8 S	C24 H51 N3 O8 S	[C24 H51 N3 O8 S, tgt=94.95, overall=94.95]	(586.338, 87.544)(587.319, 38.875)(540.33185, 81356.516)(	C24 H51 N3 O8 S	FindByFormula	28 -	541.3391	22.304445
C24 H52 N O2 P S2	C24 H52 N O2 P S2	[C24 H52 N O2 P S2, tgt=60.86, overall=60.86]	(516.2895, 85.52857)(517.2863, 75.71334)(518.292, 31.73)(	C24 H52 N O2 P S2	FindByFormula	28 -	481.3181	22.68258
C24 H53 Cl N4 O3	C24 H53 Cl N4 O3	[C24 H53 Cl N4 O3, tgt=68.12, overall=68.12]	(515.35175, 242.09526)(516.3513, 91.44601)(517.3477, 97.4	C24 H53 Cl N4 O3	FindByFormula	25 -	480.3759	22.88441
C25 H15 N O2	C25 H15 N O2	[C25 H15 N O2, tgt=18.06, overall=18.06]	(396.0911, 80.97)(406.1048, 60.99)(360.1038, 2927.4514)(3	C25 H15 N O2	FindByFormula	7 -	361.1094	12.269094
C25 H21 P	C25 H21 P	[C25 H21 P, tgt=77.08, overall=77.08]	(387.10684, 97.395996)(388.10556, 33.09833)(389.1074, 83.	C25 H21 P	FindByFormula	26 -	352.1391	2.5165753
C25 H25 Cl N O P5	C25 H25 Cl N O P5	[C25 H25 Cl N O P5, tgt=97.38, overall=97.38]	(580.015, 182.92181)(590.0307, 53.19)(544.0236, 6341.0996	C25 H25 Cl N O P5	FindByFormula	24 -	545.0312	8.710628
C25 H27 Cl N4 O2	C25 H27 Cl N4 O2	[C25 H27 Cl N4 O2, tgt=95.14, overall=95.14]	(485.1525, 78.895004)(486.1561, 30.16)(487.1456, 98.79)(4	C25 H27 Cl N4 O2	FindByFormula	22 -	450.1823	18.38285
C25 H30 N O2 P5	C25 H30 N O2 P5	[C25 H30 N O2 P5, tgt=94.86, overall=94.86]	(530.0895, 3433.897)(531.09247, 1078.3875)(532.0948, 290.	C25 H30 N O2 P5	FindByFormula	28 -	531.0967	16.42462
C25 H30 N10 O3	C25 H30 N10 O3	[C25 H30 N10 O3, tgt=94.36, overall=94.36]	(563.2356, 78.36)(517.24194, 1469.8899)(518.2476, 634.388	C25 H30 N10 O3	FindByFormula	8 -	518.2505	21.764479

C25 H31 N17 O	C25 H31 N17 O	[C25 H31 N17 O, tgt=59.15, overall=59.15]	(620.2473, 66.21)(621.2578, 23.62)(630.2837, 73.23)(584.28	C25 H31 N17 O	FindByFormula	11 -	585.2895	20.234009
C25 H32 N6 O12 S	C25 H32 N6 O12 S	[C25 H32 N6 O12 S, tgt=96.96, overall=96.96]	(675.1432, 78.10728)(676.1339, 32.316666)(677.1357, 55.31	C25 H32 N6 O12 S	FindByFormula	28 -	640.1793	13.102336
C25 H32 N8 O7 P4	C25 H32 N8 O7 P4	[C25 H32 N8 O7 P4, tgt=48.14, overall=48.14]	(715.0958, 327.1421)(716.09576, 103.13501)(717.0943, 199.	C25 H32 N8 O7 P4	FindByFormula	25 -	680.1298	22.672966
C25 H32 N8 O9 P2 S	C25 H32 N8 O9 P2 S	[C25 H32 N8 O9 P2 S, tgt=93.82, overall=93.82]	(717.1214, 685.0208)(718.12354, 206.14418)(719.10187, 10	C25 H32 N8 O9 P2 S	FindByFormula	24 -	682.1428	22.727526
C25 H36 N11 O3 P	C25 H36 N11 O3 P	[C25 H36 N11 O3 P, tgt=88.31, overall=88.31]	(604.2531, 62.882)(605.251, 41.975)(614.26245, 119.59749)	C25 H36 N11 O3 P	FindByFormula	28 -	569.2725	22.107738
C25 H36 N4	C25 H36 N4	[C25 H36 N4, tgt=41.05, overall=41.05]	(427.26038, 92.74)(428.2648, 41.65333)(429.26398, 84.5050	C25 H36 N4	FindByFormula	12 -	392.292	21.612139
C25 H36 N4 O	C25 H36 N4 O	[C25 H36 N4 O, tgt=78.83, overall=78.83]	(443.25604, 106.89)(444.25952, 37.583332)(445.25067, 46.5	C25 H36 N4 O	FindByFormula	9 -	408.2878	20.302706
C25 H36 N5 O2 P	C25 H36 N5 O2 P	[C25 H36 N5 O2 P, tgt=87.79, overall=87.79]	(504.22943, 115.192856)(505.22156, 53.16)(514.2525, 97.66	C25 H36 N5 O2 P	FindByFormula	21 -	469.2602	22.8251
C25 H37 N10 O5 P5	C25 H37 N10 O5 P5	[C25 H37 N10 O5 P5, tgt=79.23, overall=79.23]	(747.11975, 352.84113)(748.1213, 112.942406)(757.15027,	C25 H37 N10 O5 P5	FindByFormula	28 -	712.1578	22.72495
C25 H38 N6 O6 P2 S2	C25 H38 N6 O6 P2 S2	[C25 H38 N6 O6 P2 S2, tgt=91.26, overall=91.26]	(679.1332, 323.24268)(680.13226, 128.0096)(681.1288, 120.	C25 H38 N6 O6 P2 S2	FindByFormula	28 -	644.1745	22.7217
C25 H40 N2 O10 S4	C25 H40 N2 O10 S4	[C25 H40 N2 O10 S4, tgt=79.85, overall=79.85]	(691.13525, 52.225)(655.1486, 2762.035)(656.1528, 826.083	C25 H40 N2 O10 S4	FindByFormula	23 -	656.1572	18.707329
C25 H41 Cl N8	C25 H41 Cl N8	[C25 H41 Cl N8, tgt=96.64, overall=96.64]	(523.2703, 150.84799)(524.26794, 176.294)(533.30164, 144.	C25 H41 Cl N8	FindByFormula	28 -	488.3125	10.694066
C25 H42 N4	C25 H42 N4	[C25 H42 N4, tgt=45.71, overall=45.71]	(433.31613, 228.69858)(434.3169, 174.73)(435.3112, 240.63	C25 H42 N4	FindByFormula	19 -	398.3405	23.21778
C25 H43 N12 P	C25 H43 N12 P	[C25 H43 N12 P, tgt=96.12, overall=96.12]	(577.3151, 74.89916)(578.3221, 29.292002)(579.315, 49.578	C25 H43 N12 P	FindByFormula	28 -	542.3463	17.418253
C25 H43 N13 P2	C25 H43 N13 P2	[C25 H43 N13 P2, tgt=54.13, overall=54.13]	(622.28864, 122.47809)(623.29297, 82.19307)(624.2895, 76.	C25 H43 N13 P2	FindByFormula	27 -	587.3205	21.98393
C25 H44 N O7 P	C25 H44 N O7 P	[C25 H44 N O7 P, tgt=95.20, overall=95.20]	(536.25287, 77.72727)(537.2538, 39.185)(538.2639, 33.37)(	C25 H44 N O7 P	FindByFormula	28 -	501.2862	22.108274
C25 H44 N11 O5 P	C25 H44 N11 O5 P	[C25 H44 N11 O5 P, tgt=91.65, overall=91.65]	(644.2979, 68.81571)(645.2831, 64.08)(646.2988, 114.17)(6	C25 H44 N11 O5 P	FindByFormula	27 -	609.3264	22.192942
C25 H44 N6 O2 P6	C25 H44 N6 O2 P6	[C25 H44 N6 O2 P6, tgt=92.43, overall=92.43]	(681.1567, 92.35591)(682.1552, 47.4975)(683.15784, 46.834	C25 H44 N6 O2 P6	FindByFormula	28 -	646.1949	13.100339
C25 H46 N5 P3	C25 H46 N5 P3	[C25 H46 N5 P3, tgt=99.03, overall=99.03]	(544.25745, 89.14)(545.2553, 46.3)(546.245, 45.54)(554.305	C25 H46 N5 P3	FindByFormula	9 -	509.2966	6.457956
C25 H48 O4	C25 H48 O4	[C25 H48 O4, tgt=49.53, overall=49.53]	(447.33142, 355.09186)(448.33548, 132.05922)(449.31866,	C25 H48 O4	FindByFormula	26 -	412.3563	22.889397
C25 H48 P2 S3	C25 H48 P2 S3	[C25 H48 P2 S3, tgt=92.74, overall=92.74]	(541.20844, 869.65424)(542.2091, 269.70773)(543.2069, 34	C25 H48 P2 S3	FindByFormula	22 -	506.239	10.771051
C25 H49 N2 O2 P	C25 H49 N2 O2 P	[C25 H49 N2 O2 P, tgt=34.78, overall=34.78]	(475.32513, 172.47499)(476.3287, 96.438)(477.32172, 226.1	C25 H49 N2 O2 P	FindByFormula	21 -	440.3545	22.706789
C25 H50 N2 S3	C25 H50 N2 S3	[C25 H50 N2 S3, tgt=82.28, overall=82.28]	(509.28488, 114.594444)(510.30066, 66.4)(511.2772, 47.59)	C25 H50 N2 S3	FindByFormula	23 -	474.313	22.757008
C25 H50 O2	C25 H50 O2	[C25 H50 O2, tgt=96.46, overall=96.46]	(381.37393, 4002.529)(382.37772, 1158.0494)(383.379, 253.	C25 H50 O2	FindByFormula	22 -	382.3814	25.1289
C25 H50 O3	C25 H50 O3	[C25 H50 O3, tgt=0.25, overall=0.25]	(433.34763, 446.475)(434.34595, 136.56834)(435.35455, 11	C25 H50 O3	FindByFormula	14 -	398.3786	22.958715
C25 H52 N O2 P S3	C25 H52 N O2 P S3	[C25 H52 N O2 P S3, tgt=74.03, overall=74.03]	(560.26184, 103.20799)(561.2289, 105.99)(562.2421, 67.69)	C25 H52 N O2 P S3	FindByFormula	26 -	525.2864	22.08062
C25 H52 O4 S	C25 H52 O4 S	[C25 H52 O4 S, tgt=66.70, overall=66.70]	(483.3207, 62.895)(493.35834, 420.60608)(494.35623, 111.1	C25 H52 O4 S	FindByFormula	25 -	448.3602	22.96514
C25 H53 N8 P	C25 H53 N8 P	[C25 H53 N8 P, tgt=94.94, overall=94.94]	(531.3768, 101.296364)(532.4071, 61.09)(541.4207, 233.85)	C25 H53 N8 P	FindByFormula	15 -	496.4116	23.09955
C25 H54 N O3 P	C25 H54 N O3 P	[C25 H54 N O3 P, tgt=77.96, overall=77.96]	(446.3774, 2751.771)(447.38037, 983.16473)(448.38336, 10	C25 H54 N O3 P	FindByFormula	26 -	447.385	23.814976
C25 H54 N O4 P S2	C25 H54 N O4 P S2	[C25 H54 N O4 P S2, tgt=64.54, overall=64.54]	(562.3024, 111.16501)(563.319, 66.729996)(572.3165, 84.21	C25 H54 N O4 P S2	FindByFormula	23 -	527.321	22.001795
C25 H55 N3 O3 S3	C25 H55 N3 O3 S3	[C25 H55 N3 O3 S3, tgt=84.47, overall=84.47]	(576.29816, 83.94333)(586.33734, 70.14749)(587.318, 78.89	C25 H55 N3 O3 S3	FindByFormula	28 -	541.3395	22.164608
C25 H55 N5 O7 S3	C25 H55 N5 O7 S3	[C25 H55 N5 O7 S3, tgt=82.83, overall=82.83]	(668.29193, 92.4)(669.2827, 213.46)(678.31555, 351.84073)	C25 H55 N5 O7 S3	FindByFormula	27 -	633.3265	22.116934
C26 H14 N2	C26 H14 N2	[C26 H14 N2, tgt=90.23, overall=90.23]	(399.11505, 1725.2262)(400.11682, 432.8781)(401.11746, 6	C26 H14 N2	FindByFormula	21 -	354.1144	2.4849515
C26 H19 N5	C26 H19 N5	[C26 H19 N5, tgt=80.97, overall=80.97]	(400.158, 2005.1587)(401.1623, 843.1219)(402.16098, 246.4	C26 H19 N5	FindByFormula	27 -	401.1651	22.878231
C26 H22 N14	C26 H22 N14	[C26 H22 N14, tgt=93.94, overall=93.94]	(575.2123, 69.29)(576.1914, 28.79)(529.2079, 2426.2563)(	C26 H22 N14	FindByFormula	8 -	530.2132	20.066025
C26 H25 P	C26 H25 P	[C26 H25 P, tgt=68.13, overall=68.13]	(413.169, 236.10397)(414.17456, 210.65332)(367.15958, 47	C26 H25 P	FindByFormula	27 -	368.1678	22.769178
C26 H26 O11 P6	C26 H26 O11 P6	[C26 H26 O11 P6, tgt=55.64, overall=55.64]	(734.9475, 92.118)(735.94995, 24.77)(744.98016, 61.385002	C26 H26 O11 P6	FindByFormula	9 -	699.9886	15.701604
C26 H27 N8 O5 P5	C26 H27 N8 O5 P5	[C26 H27 N8 O5 P5, tgt=93.61, overall=93.61]	(721.03937, 136.57924)(722.0452, 40.684586)(723.043, 34.6	C26 H27 N8 O5 P5	FindByFormula	28 -	686.0777	8.464079
C26 H28 N4 O4	C26 H28 N4 O4	[C26 H28 N4 O4, tgt=99.05, overall=99.05]	(495.1915, 87.795)(505.208, 346.836)(506.2123, 466.36)(50	C26 H28 N4 O4	FindByFormula	28 -	460.2106	18.393686
C26 H28 N6 O P2	C26 H28 N6 O P2	[C26 H28 N6 O P2, tgt=84.52, overall=84.52]	(537.1462, 91.98)(538.13165, 54.9)(539.1371, 347.35)(547.1	C26 H28 N6 O P2	FindByFormula	28 -	502.1799	22.71428
C26 H29 N6 O3 P	C26 H29 N6 O3 P	[C26 H29 N6 O3 P, tgt=96.31, overall=96.31]	(539.17175, 70.45929)(540.1559, 236.215)(541.1453, 99.96)	C26 H29 N6 O3 P	FindByFormula	28 -	504.2046	13.102552
C26 H30 N4 O S	C26 H30 N4 O S	[C26 H30 N4 O S, tgt=69.55, overall=69.55]	(481.17886, 976.1688)(482.18066, 337.98904)(483.17383, 8	C26 H30 N4 O S	FindByFormula	28 -	446.2159	22.701239
C26 H31 N17	C26 H31 N17	[C26 H31 N17, tgt=47.47, overall=47.47]	(616.268, 79.98)(626.2877, 52.93)(580.28955, 959.8656)(58	C26 H31 N17	FindByFormula	21 -	581.2941	21.577372
C26 H32 O7 S2	C26 H32 O7 S2	[C26 H32 O7 S2, tgt=81.78, overall=81.78]	(555.1226, 90.56182)(556.123, 39.67625)(557.12634, 48.396	C26 H32 O7 S2	FindByFormula	28 -	520.1613	22.593653
C26 H34 N4 O3	C26 H34 N4 O3	[C26 H34 N4 O3, tgt=63.48, overall=63.48]	(485.24063, 60.125)(486.2366, 23.23)(487.2548, 30.69)(495.	C26 H34 N4 O3	FindByFormula	11 -	450.2635	21.781687
C26 H34 N6 O P2	C26 H34 N6 O P2	[C26 H34 N6 O P2, tgt=84.46, overall=84.46]	(543.19586, 91.594284)(544.20184, 57.848)(545.181, 53.71)	C26 H34 N6 O P2	FindByFormula	28 -	508.226	13.100553
C26 H35 N11 O	C26 H35 N11 O	[C26 H35 N11 O, tgt=79.56, overall=79.56]	(552.2577, 57.38)(516.2938, 4269.82)(517.2958, 1393.6127)	C26 H35 N11 O	FindByFormula	18 -	517.3029	20.246887
C26 H37 N15	C26 H37 N15	[C26 H37 N15, tgt=78.06, overall=78.06]	(604.3174, 50.51)(558.32904, 2208.7883)(559.32404, 982.69	C26 H37 N15	FindByFormula	28 -	559.3332	18.829487
C26 H38 O13 P2	C26 H38 O13 P2	[C26 H38 O13 P2, tgt=94.57, overall=94.57]	(655.1317, 552.5335)(656.1332, 250.07346)(657.13074, 511.	C26 H38 O13 P2	FindByFormula	27 -	620.1752	22.723902
C26 H39 O2 P	C26 H39 O2 P	[C26 H39 O2 P, tgt=73.29, overall=73.29]	(449.23447, 377.69998)(450.24, 100.34)(451.25, 90.74)(459.	C26 H39 O2 P	FindByFormula	8 -	414.2722	22.530045
C26 H40 N5 O3 P	C26 H40 N5 O3 P	[C26 H40 N5 O3 P, tgt=98.04, overall=98.04]	(536.24786, 105.611664)(537.25, 40.002502)(546.2757, 164.	C26 H40 N5 O3 P	FindByFormula	28 -	501.286	21.989462
C26 H40 N6 O3	C26 H40 N6 O3	[C26 H40 N6 O3, tgt=30.60, overall=30.60]	(519.28906, 101.043335)(529.3148, 559.45154)(530.3116, 1	C26 H40 N6 O3	FindByFormula	19 -	484.3123	22.493967
C26 H40 N6 O3 S2	C26 H40 N6 O3 S2	[C26 H40 N6 O3 S2, tgt=88.13, overall=88.13]	(583.22974, 2374.5583)(584.2321, 768.5899)(585.2289, 905.	C26 H40 N6 O3 S2	FindByFormula	22 -	548.2602	7.705655
C26 H40 O13 P2	C26 H40 O13 P2	[C26 H40 O13 P2, tgt=96.20, overall=96.20]	(667.18634, 291.1096)(668.1834, 143.49051)(669.17084, 93.	C26 H40 O13 P2	FindByFormula	28 -	622.1936	22.92344
C26 H40 O19 P2 S	C26 H40 O19 P2 S	[C26 H40 O19 P2 S, tgt=92.41, overall=92.41]	(785.10626, 553.2361)(786.1069, 202.54332)(787.091, 1234.	C26 H40 O19 P2 S	FindByFormula	23 -	750.1406	22.73489
C26 H41 N2 P	C26 H41 N2 P	[C26 H41 N2 P, tgt=80.68, overall=80.68]	(447.2822, 61.02)(448.282, 30.86)(457.29468, 456.2825)(45	C26 H41 N2 P	FindByFormula	5 -	412.3003	22.622713
C26 H43 N O5	C26 H43 N O5	[C26 H43 N O5, tgt=89.63, overall=89.63]	(484.28247, 73.39)(485.2814, 24.17)(448.30667, 10097.218)	C26 H43 N O5	FindByFormula	26 -	449.3151	20.229258
C26 H43 N4 P3	C26 H43 N4 P3	[C26 H43 N4 P3, tgt=97.43, overall=97.43]	(539.2485, 181.0)(549.2666, 172.13)(503.26273, 3799.5117)	C26 H43 N4 P3	FindByFormula	7 -	504.2694	4.281562
C26 H44 N6 O3	C26 H44 N6 O3	[C26 H44 N6 O3, tgt=38.58, overall=38.58]	(523.3173, 211.86636)(524.31445, 131.666)(525.31744, 166.	C26 H44 N6 O3	FindByFormula	13 -	488.3475	22.755463
C26 H44 N8 O8	C26 H44 N8 O8	[C26 H44 N8 O8, tgt=98.67, overall=98.67]	(631.2886, 75.67)(641.3174, 140.69)(595.32227, 7848.5503)	C26 H44 N8 O8	FindByFormula	7 -	596.3289	6.5146866
C26 H46 N8 O	C26 H46 N8 O	[C26 H46 N8 O, tgt=46.69, overall=46.69]	(521.3487, 218.93001)(522.3503, 84.600006)(523.35706, 29	C26 H46 N8 O	FindByFormula	13 -	486.3755	22.649902
C26 H47 N O6 P2 S	C26 H47 N O6 P2 S	[C26 H47 N O6 P2 S, tgt=96.47, overall=96.47]	(598.2295, 2176.1482)(599.2332, 718.48456)(600.2283, 870.	C26 H47 N O6 P2 S	FindByFormula	22 -	563.2605	9.516397
C26 H48 N6 O3	C26 H48 N6 O3	[C26 H48 N6 O3, tgt=80.80, overall=80.80]	(527.3432, 206.455)(528.34, 91.36666)(529.33295, 201.8016	C26 H48 N6 O3	FindByFormula	7 -	492.3786	22.913588
C26 H50 N6 O2	C26 H50 N6 O2	[C26 H50 N6 O2, tgt=84.86, overall=84.86]	(513.3589, 581.7717)(514.35425, 266.5925)(515.36176, 515.	C26 H50 N6 O2	FindByFormula	27 -	478.3985	22.453026
C26 H52 N3 O15 P	C26 H52 N3 O15 P	[C26 H52 N3 O15 P, tgt=78.92, overall=78.92]	(712.27765, 106.762856)(713.26196, 44.785)(714.26807, 99.	C26 H52 N3 O15 P	FindByFormula	28 -	677.3132	22.231833
C26 H52 O2	C26 H52 O2	[C26 H52 O2, tgt=97.74, overall=97.74]	(395.39005, 2870.4932)(396.39307, 861.5759)(397.3963, 16	C26 H52 O2	FindByFormula	22 -	396.3974	25.600056
C26 H52 O3	C26 H52 O3	[C26 H52 O3, tgt=35.33, overall=35.33]	(447.35303, 1063.115)(448.35376, 433.17398)(449.36343, 4	C26 H52 O3	FindByFormula	9 -	412.3921	23.164566
C26 H54 N O4 P S2	C26 H54 N O4 P S2	[C26 H54 N O4 P S2, tgt=76.68, overall=76.68]	(574.2977, 50.99)(584.3267, 89.440765)(585.3098, 50.04)(	C26 H54 N O4 P S2	FindByFormula	28 -	539.3241	21.864866
C26 H55 N9 O P6	C26 H55 N9 O P6	[C26 H55 N9 O P6, tgt=92.40, overall=92.40]	(730.2576, 200.73958)(731.2597, 105.77529)(732.26044, 72.	C26 H55 N9 O P6	FindByFormula	23 -	695.2917	22.121344
C26 H9 Cl N9 O2 P	C26 H9 Cl N9 O2 P	[C26 H9 Cl N9 O2 P, tgt=81.50, overall=81.50]	(580.01337, 157.91374)(590.0307, 53.19)(544.0238, 6124.56	C26 H9 Cl N9 O2 P	FindByFormula	26 -	545.0312	8.639957
C27 H19 N9 O5	C27 H19 N9 O5	[C27 H19 N9 O5, tgt=83.50, overall=83.50]	(584.12274, 1331.8379)(585.1151, 1534.4586)(586.1192, 62	C27 H19 N9 O5	FindByFormula	26 -	549.1509	2.5140758
C27 H22 N4 O3	C27 H22 N4 O3	[C27 H22 N4 O3, tgt=79.04, overall=79.04]	(495.16388, 163.66878)(496.16748, 117.496666)(449.16293,	C27 H22 N4 O3	FindByFormula	27 -	450.1701	22.918892
C27 H24 N4 O2	C27 H24 N4 O2	[C27 H24 N4 O2, tgt=81.56, overall=81.56]	(471.15594, 341.04355)(472.15933, 129.61682)(473.15424,	C27 H24 N4 O2	FindByFormula	27 -	436.1925	22.927626
C27 H26 N11 P5	C27 H26 N11 P5	[C27 H26 N11 P5, tgt=84.05, overall=84.05]	(704.1041, 228.336)(705.10297, 84.15066)(658.0991, 15055.	C27 H26 N11 P5	FindByFormula	19 -	659.1063	8.659221
C27 H26 N4 O	C27 H26 N4 O	[C27 H26 N4 O, tgt=95.67, overall=95.67]	(457.18417, 1250.538)(458.18793, 369.6425)(459.182, 63.45	C27 H26 N4 O	FindByFormula	28 -	422.2105	22.408907
C27 H26 N4 O2	C27 H26 N4 O2	[C27 H26 N4 O2, tgt=80.27, overall=80.27]	(473.1769, 78.55858)(474.186, 32.78)(475.1881, 55.2)(483.2	C27 H26 N4 O2	FindByFormula	22 -	438.2079	23.170458
C27 H30 O12	C27 H30 O12	[C27 H30 O12, tgt=95.14, overall=95.14]	(581.1514, 693.8874)(582.15674, 219.57738)(583.1361, 448.	C27 H30 O12	FindByFormula	27 -	546.1757	22.727234
C27 H31 N5 O2 P2	C27 H31 N5 O2 P2	[C27 H31 N5 O2 P2, tgt=94.97, overall=94.97]	(554.1659, 546.15643)(555.1626, 218.84395)(556.15454, 38	C27 H31 N5 O2 P2	FindByFormula	26 -	519.1954	2.515037
C27 H32 N4 O6	C27 H32 N4 O6	[C27 H32 N4 O6, tgt=70.71, overall=70.71]	(543.2105, 87.88)(544.1976, 43.4)(545.2092, 79.05)(507.224	C27 H32 N4 O6	FindByFormula	13 -	508.2321	20.123314
C27 H36 N2 O P2	C27 H36 N2 O P2	[C27 H36 N2 O P2, tgt=68.09, overall=68.09]	(501.20157, 223.21286)(502.20703, 114.62858)(503.19547,	C27 H36 N2 O P2	FindByFormula	24 -	466.2305	22.769835
C27 H36 N4 O2	C27 H36 N4 O2	[C27 H36 N4 O2, tgt=73.72, overall=73.72]	(447.27502, 2494.545)(448.27957, 790.16327)(449.26938, 3	C27 H36 N4 O2	FindByFormula	6 -	448.2815	21.52799
C27 H37 N5 O	C27 H37 N5 O	[C27 H37 N5 O, tgt=71.33, overall=71.33]	(482.26556, 57.004997)(483.2609, 34.67)(492.2951, 51.96)(	C27 H37 N5 O	FindByFormula	8 -	447.2996	18.623123
C27 H38 N4 O4	C27 H38 N4 O4	[C27 H38 N4 O4, tgt=90.10, overall=90.10]	(517.2606, 64.195)(518.2748, 43.91)(519.2642, 28.94)(527.2	C27 H38 N4 O4	FindByFormula	9 -	482.2886	20.383915
C27 H39 N5 O	C27 H39 N5 O	[C27 H39 N5 O, tgt=52.65, overall=52.65]	(484.2921, 54.04)(448.30692, 5238.8853)(449.30795, 1577.3	C27 H39 N5 O	FindByFormula	21 -	449.3152	19.111563
C27 H39 N5 O2	C27 H39 N5 O2	[C27 H39 N5 O2, tgt=63.22, overall=63.22]	(500.29013, 99.32201)(501.29892, 80.0575)(510.3105, 59.44	C27 H39 N5 O2	FindByFormula	11 -	465.3096	18.826044
C27 H42 N4	C27 H42 N4	[C27 H42 N4, tgt=55.75, overall=55.75]	(457.31396, 526.00446)(458.31924, 226.10187)(459.3128, 1	C27 H42 N4	FindByFormula	23 -	422.3371	22.7469
C27 H42 N4 O2	C27 H42 N4 O2	[C27 H42 N4 O2, tgt=46.91, overall=46.91]	(489.30334, 226.11444)(490.30475, 98.53715)(491.30222, 7	C27 H42 N4 O2	FindByFormula	16 -	454.329	21.895805
C27 H44 N4	C27 H44 N4	[C27 H44 N4, tgt=24.77, overall=24.77]	(459.32208, 458.89276)(460.3222, 185.37125)(461.33234, 1	C27 H44 N4	FindByFormula	17 -	424.3551	22.956656
C27 H44 O3	C27 H44 O3	[C27 H44 O3, tgt=63.89, overall=63.89]	(451.29385, 177.40666)(452.30066, 43.653336)(453.2988, 2	C27 H44 O3	FindByFormula	13 -	416.3255	22.730467
C27 H44 O4	C27 H44 O4	[C27 H44 O4, tgt=4.03, overall=4.03]	(467.29987, 256.97202)(468.3061, 134.76001)(469.3178, 86.	C27 H44 O4	FindByFormula	22 -	432.3233	22.462122
C27 H46 N4	C27 H46 N4	[C27 H46 N4, tgt=65.30, overall=65.30]	(461.34195, 148.48917)(462.34473, 58.03143)(463.3395, 29	C27 H46 N4	FindByFormula	21 -	426.3723	23.01787
C27 H48 N11 O5 P	C27 H48 N11 O5 P	[C27 H48 N11 O5 P, tgt=72.52, overall=72.52]	(672.319, 133.79126)(673.3108, 78.905)(674.3072, 44.73)(6	C27 H48 N11 O5 P	FindByFormula	25 -	637.3595	22.685093
C27 H50 O3	C27 H50 O3	[C27 H50 O3, tgt=37.19, overall=37.19]	(457.3416, 101.932495)(458.3548, 23.22)(459.3386, 76.62)(	C27 H50 O3	FindByFormula	17 -	422.3738	22.974588
C27 H50 O5	C27 H50 O5	[C27 H50 O5, tgt=76.04, overall=76.04]	(489.33633, 205.23734)(490.3378, 88.991005)(491.3177, 22.	C27 H50 O5	FindByFormula	27 -	454.3653	22.843132
C27 H50 S2	C27 H50 S2	[C27 H50 S2, tgt=38.44, overall=38.44]	(473.30518, 4940.2964)(474.30627, 1828.548)(475.30566, 5	C27 H50 S2	FindByFormula	27 -	438.3356	22.701338
C27 H51 Cl N2 S	C27 H51 Cl N2 S	[C27 H51 Cl N2 S, tgt=57.45, overall=57.45]	(505.32205, 184.67668)(506.31775, 76.35999)(507.31497, 1	C27 H51 Cl N2 S	FindByFormula	17 -	470.3493	22.900284
C27 H51 N8 P	C27 H51 N8 P	[C27 H51 N8 P, tgt=33.19, overall=33.19]	(553.36566, 170.11)(554.37665, 139.36333)(563.3959, 92.59	C27 H51 N8 P	FindByFormula	13 -	518.3964	22.909832
C27 H52 N O9 P	C27 H52 N O9 P	[C27 H52 N O9 P, tgt=98.11, overall=98.11]	(600.3085, 67.61625)(601.3094, 52.11)(610.32825, 362.5793	C27 H52 N O9 P	FindByFormula	28 -	565.3386	22.117163
C27 H52 N2 P2	C27 H52 N2 P2	[C27 H52 N2 P2, tgt=57.16, overall=57.16]	(501.32535, 251.59)(502.3221, 127.121994)(503.3257, 205.6	C27 H52 N2 P2	FindByFormula	15 -	466.3622	22.859188
C27 H52 N4 S2	C27 H52 N4 S2	[C27 H52 N4 S2, tgt=61.39, overall=61.39]	(531.332, 148.63188)(532.33496, 85.79666)(533.33484, 101.	C27 H52 N4 S2	FindByFormula	19 -	496.3656	22.902222
C27 H53 N2 P3	C27 H53 N2 P3	[C27 H53 N2 P3, tgt=98.49, overall=98.49]	(533.3008, 144.32)(534.2983, 79.47666)(535.312, 23.49)(49	C27 H53 N2 P3	FindByFormula	28 -	498.3425	10.697101
C27 H54 Cl2 O	C27 H54 Cl2 O	[C27 H54 Cl2 O, tgt=65.57, overall=65.57]	(500.9582, 482.37082)(501.94583, 174.34521)(502.8745, 16	C27 H54 Cl2 O	FindByFormula	27 -	464.3507	22.780764
C27 H54 N7 O2 P3 S	C27 H54 N7 O2 P3 S	[C27 H54 N7 O2 P3 S, tgt=85.45, overall=85.45]	(668.29517, 66.533)(678.3297, 72.30875)(679.3387, 51.7450	C27 H54 N7 O2 P3 S	FindByFormula	27 -	633.3264	21.982433
C27 H54 O4	C27 H54 O4	[C27 H54 O4, tgt=29.83, overall=29.83]	(477.3702, 323.75897)(478.36948, 156.54332)(479.36966, 5	C27 H54 O4	FindByFormula	17 -	442.3991	22.995964
C27 H55 N3 O3 S3	C27 H55 N3 O3 S3	[C27 H55 N3 O3 S3, tgt=77.95, overall=77.95]	(600.3088, 66.13286)(601.303, 44.345)(610.3296, 65.995)(5	C27 H55 N3 O3 S3	FindByFormula	28 -	565.3399	21.98143
C27 H55 O2 P	C27 H55 O2 P	[C27 H55 O2 P, tgt=34.30, overall=34.30]	(477.3637, 400.7378)(478.35562, 319.93253)(479.3694, 136	C27 H55 O2 P	FindByFormula	11 -	442.3896	22.845219
C27 H56 N14 O2	C27 H56 N14 O2	[C27 H56 N14 O2, tgt=62.14, overall=62.14]	(643.4434, 334.05182)(644.42926, 248.455)(645.4332, 86.53	C27 H56 N14 O2	FindByFormula	27 -	608.476	22.923851
C27 H56 N3 O10 P S2	C27 H56 N3 O10 P S2	[C27 H56 N3 O10 P S2, tgt=92.95, overall=92.95]	(712.2846, 79.15)(713.2996, 38.06)(714.2644, 121.73)(722.3	C27 H56 N3 O10 P S2	FindByFormula	28 -	677.3141	22.306194
C28 H14 N2	C28 H14 N2	[C28 H14 N2, tgt=63.13, overall=63.13]	(423.1118, 88.476364)(424.1071, 39.254)(377.1086, 1684.08	C28 H14 N2	FindByFormula	15 -	378.1123	19.789999
C28 H18 N9 O3 P	C28 H18 N9 O3 P	[C28 H18 N9 O3 P, tgt=85.92, overall=85.92]	(604.12634, 55.676003)(605.1172, 38.23)(558.1208, 2081.71	C28 H18 N9 O3 P	FindByFormula	27 -	559.1264	18.377602
C28 H19 N4 P3	C28 H19 N4 P3	[C28 H19 N4 P3, tgt=57.76, overall=57.76]	(539.05145, 79.41)(540.0602, 24.55)(541.0456, 91.95)(549.0	C28 H19 N4 P3	FindByFormula	15 -	504.0836	0.83986664
C28 H19 N5	C28 H19 N5	[C28 H19 N5, tgt=77.96, overall=77.96]	(470.16025, 106.78761)(471.15164, 468.69)(424.15778, 178	C28 H19 N5	FindByFormula	26 -	425.1654	22.749992
C28 H23 N10 O5 P3	C28 H23 N10 O5 P3	[C28 H23 N10 O5 P3, tgt=70.59, overall=70.59]	(707.0805, 74.196)(708.0891, 36.86)(709.0943, 38.03)(717.0	C28 H23 N10 O5 P3	FindByFormula	10 -	672.1032	0.9949996
C28 H23 N5	C28 H23 N5	[C28 H23 N5, tgt=88.28, overall=88.28]	(464.16278, 73.463745)(465.1439, 47.92)(474.19943, 98.340	C28 H23 N5	FindByFormula	28 -	429.1956	23.199642
C28 H25 N3 O P6	C28 H25 N3 O P6	[C28 H25 N3 O P6, tgt=79.92, overall=79.92]	(640.0203, 76.15)(641.0245, 31.61)(650.0237, 57.8)(604.035	C28 H25 N3 O P6	FindByFormula	20 -	605.0414	8.696033
C28 H26 N3 O2 P	C28 H26 N3 O2 P	[C28 H26 N3 O2 P, tgt=71.73, overall=71.73]	(502.1434, 80.38)(503.15775, 114.18)(512.17975, 102.27308	C28 H26 N3 O2 P	FindByFormula	24 -	467.1787	22.720484
C28 H28 N2 O15	C28 H28 N2 O15	[C28 H28 N2 O15, tgt=98.25, overall=98.25]	(667.1198, 117.95)(677.1581, 71.294)(678.152, 42.015)(631.	C28 H28 N2 O15	FindByFormula	19 -	632.1491	8.650168
C28 H33 N2 O9 P	C28 H33 N2 O9 P	[C28 H33 N2 O9 P, tgt=91.87, overall=91.87]	(607.158, 65.585556)(608.1599, 34.101997)(609.1536, 45.74	C28 H33 N2 O9 P	FindByFormula	28 -	572.1919	13.100837
C28 H34 N2 O3 P2	C28 H34 N2 O3 P2	[C28 H34 N2 O3 P2, tgt=88.18, overall=88.18]	(543.16486, 163.24501)(544.17004, 107.04)(545.16113, 131.	C28 H34 N2 O3 P2	FindByFormula	28 -	508.203	22.731134
C28 H38 N4	C28 H38 N4	[C28 H38 N4, tgt=74.04, overall=74.04]	(475.304, 659.96277)(476.30356, 261.802)(477.31116, 138.6	C28 H38 N4	FindByFormula	19 -	430.3083	21.87019
C28 H40 N5 O3 P	C28 H40 N5 O3 P	[C28 H40 N5 O3 P, tgt=84.21, overall=84.21]	(560.2512, 89.229996)(561.2567, 55.6075)(562.2499, 40.326	C28 H40 N5 O3 P	FindByFormula	27 -	525.2846	22.005205
C28 H40 O13 S3	C28 H40 O13 S3	[C28 H40 O13 S3, tgt=93.37, overall=93.37]	(715.12823, 73.89333)(716.1359, 35.676666)(717.13336, 20.	C28 H40 O13 S3	FindByFormula	28 -	680.1647	23.186718
C28 H43 N8 P3	C28 H43 N8 P3	[C28 H43 N8 P3, tgt=90.20, overall=90.20]	(583.2742, 1836.4751)(584.27686, 597.9067)(585.2766, 144.	C28 H43 N8 P3	FindByFormula	6 -	584.2812	7.71279
C28 H44 Cl N10 P S3	C28 H44 Cl N10 P S3	[C28 H44 Cl N10 P S3, tgt=71.02, overall=71.02]	(717.19305, 1091.5188)(718.1973, 484.69232)(719.19226, 6	C28 H44 Cl N10 P S3	FindByFormula	19 -	682.2286	3.599675
C28 H44 O4	C28 H44 O4	[C28 H44 O4, tgt=50.14, overall=50.14]	(479.29285, 171.38333)(489.32257, 92.54)(490.32495, 35.51	C28 H44 O4	FindByFormula	19 -	444.3232	22.735178
C28 H45 Cl N2	C28 H45 Cl N2	[C28 H45 Cl N2, tgt=33.62, overall=33.62]	(479.29572, 481.85068)(480.29477, 175.7057)(481.3026, 81.	C28 H45 Cl N2	FindByFormula	22 -	444.3235	22.60594
C28 H46 N O2 P3	C28 H46 N O2 P3	[C28 H46 N O2 P3, tgt=75.05, overall=75.05]	(556.2296, 54.4665)(520.266, 1374.1448)(521.26715, 501.444	C28 H46 N O2 P3	FindByFormula	27 -	521.274	22.307741
C28 H48 N6 O3	C28 H48 N6 O3	[C28 H48 N6 O3, tgt=21.56, overall=21.56]	(551.3481, 142.565)(552.355, 85.47)(553.3474, 106.987495)	C28 H48 N6 O3	FindByFormula	21 -	516.3788	22.917233
C28 H50 O4	C28 H50 O4	[C28 H50 O4, tgt=18.63, overall=18.63]	(485.34326, 194.65167)(486.3495, 119.34)(487.34064, 224.8	C28 H50 O4	FindByFormula	12 -	450.3707	23.030016
C28 H51 N3 O8 S	C28 H51 N3 O8 S	[C28 H51 N3 O8 S, tgt=87.85, overall=87.85]	(624.3124, 70.48799)(625.3181, 27.28)(634.325, 295.79843)	C28 H51 N3 O8 S	FindByFormula	27 -	589.3389	21.99748
C28 H52 N5 O4 P	C28 H52 N5 O4 P	[C28 H52 N5 O4 P, tgt=72.35, overall=72.35]	(588.35236, 92.106)(589.3594, 130.175)(598.3729, 241.8291	C28 H52 N5 O4 P	FindByFormula	18 -	553.3753	22.686821
C28 H52 N5 O5 P	C28 H52 N5 O5 P	[C28 H52 N5 O5 P, tgt=55.49, overall=55.49]	(604.34814, 81.565)(605.348, 75.51)(606.3546, 644.23)(614.	C28 H52 N5 O5 P	FindByFormula	24 -	569.3662	22.654709
C28 H52 O4	C28 H52 O4	[C28 H52 O4, tgt=22.93, overall=22.93]	(487.35678, 181.69443)(488.36426, 108.80599)(489.3546, 4	C28 H52 O4	FindByFormula	15 -	452.3854	23.00652
C28 H52 S2	C28 H52 S2	[C28 H52 S2, tgt=35.22, overall=35.22]	(487.32004, 170.58693)(488.31827, 67.520004)(489.31024,	C28 H52 S2	FindByFormula	23 -	452.35	22.676235
C28 H54 N8 P4	C28 H54 N8 P4	[C28 H54 N8 P4, tgt=26.69, overall=26.69]	(661.3153, 132.11401)(662.3041, 45.245003)(663.2985, 62.0	C28 H54 N8 P4	FindByFormula	12 -	626.341	22.891848
C28 H55 Cl N8	C28 H55 Cl N8	[C28 H55 Cl N8, tgt=45.86, overall=45.86]	(573.39374, 92.32334)(574.39624, 44.18)(575.3884, 119.703	C28 H55 Cl N8	FindByFormula	16 -	538.4244	23.006098
C28 H55 N3 P2 S	C28 H55 N3 P2 S	[C28 H55 N3 P2 S, tgt=70.50, overall=70.50]	(562.326, 85.21917)(563.3326, 126.61001)(572.3621, 137.36	C28 H55 N3 P2 S	FindByFormula	19 -	527.3587	22.57455
C28 H58 N O4 P S2	C28 H58 N O4 P S2	[C28 H58 N O4 P S2, tgt=90.83, overall=90.83]	(602.3226, 68.08)(603.3225, 115.705)(604.3771, 50.61)(612.	C28 H58 N O4 P S2	FindByFormula	28 -	567.3545	22.437998
C28 H60 N O4 P S2	C28 H60 N O4 P S2	[C28 H60 N O4 P S2, tgt=68.53, overall=68.53]	(604.34393, 116.916664)(605.3521, 59.074997)(606.324, 69.	C28 H60 N O4 P S2	FindByFormula	26 -	569.3708	22.720936
C29 H18 N P5	C29 H18 N P5	[C29 H18 N P5, tgt=55.40, overall=55.40]	(569.9836, 68.07834)(570.9729, 43.225)(580.0096, 87.63999	C29 H18 N P5	FindByFormula	12 -	535.013	1.1269996
C29 H18 N8	C29 H18 N8	[C29 H18 N8, tgt=62.95, overall=62.95]	(513.1353, 123.30063)(514.1335, 56.612503)(515.1322, 319.	C29 H18 N8	FindByFormula	22 -	478.1617	22.810951
C29 H22 N2	C29 H22 N2	[C29 H22 N2, tgt=78.04, overall=78.04]	(443.18018, 158.104)(444.17676, 70.90571)(397.16962, 114	C29 H22 N2	FindByFormula	23 -	398.178	22.214655
C29 H22 O P4	C29 H22 O P4	[C29 H22 O P4, tgt=97.40, overall=97.40]	(545.0273, 2685.5867)(546.0227, 3045.9766)(547.02313, 95	C29 H22 O P4	FindByFormula	3 -	510.0573	8.652762
C29 H24 N9 P	C29 H24 N9 P	[C29 H24 N9 P, tgt=62.47, overall=62.47]	(574.1834, 54.91)(528.1795, 1328.2838)(529.1853, 587.8915	C29 H24 N9 P	FindByFormula	18 -	529.1871	20.291264
C29 H26 N2 P4	C29 H26 N2 P4	[C29 H26 N2 P4, tgt=80.76, overall=80.76]	(561.0705, 52.07)(571.1085, 77.7725)(572.11835, 37.695)(5	C29 H26 N2 P4	FindByFormula	15 -	526.103	8.677662
C29 H27 N O4	C29 H27 N O4	[C29 H27 N O4, tgt=39.19, overall=39.19]	(488.15317, 82.87667)(489.1566, 40.84)(498.1879, 153.1189	C29 H27 N O4	FindByFormula	13 -	453.1918	22.80415
C29 H27 N19 O4	C29 H27 N19 O4	[C29 H27 N19 O4, tgt=77.35, overall=77.35]	(740.20917, 60.726665)(741.1933, 28.91)(750.2389, 89.9166	C29 H27 N19 O4	FindByFormula	28 -	705.252	22.093245
C29 H27 N2 O P S2	C29 H27 N2 O P S2	[C29 H27 N2 O P S2, tgt=92.34, overall=92.34]	(549.0937, 346.71695)(550.0907, 361.07907)(551.08875, 88.	C29 H27 N2 O P S2	FindByFormula	25 -	514.128	18.386002
C29 H29 P	C29 H29 P	[C29 H29 P, tgt=60.79, overall=60.79]	(443.17453, 331.0265)(444.1665, 159.81999)(407.1911, 1683.	C29 H29 P	FindByFormula	24 -	408.1974	23.014387
C29 H31 N5 P4	C29 H31 N5 P4	[C29 H31 N5 P4, tgt=71.11, overall=71.11]	(608.12115, 419.14536)(609.12067, 102.21636)(610.1186, 2	C29 H31 N5 P4	FindByFormula	19 -	573.1491	1.8272635
C29 H35 N23	C29 H35 N23	[C29 H35 N23, tgt=45.14, overall=45.14]	(740.32043, 112.62125)(741.3184, 91.35333)(742.3035, 40.3	C29 H35 N23	FindByFormula	19 -	705.3465	22.556713
C29 H37 N11	C29 H37 N11	[C29 H37 N11, tgt=68.30, overall=68.30]	(574.289, 61.76)(575.3078, 24.38)(576.2854, 30.64)(584.325	C29 H37 N11	FindByFormula	28 -	539.3242	21.743622
C29 H37 N7 S	C29 H37 N7 S	[C29 H37 N7 S, tgt=75.76, overall=75.76]	(550.2618, 70.755005)(560.2917, 130.69286)(561.2991, 109.	C29 H37 N7 S	FindByFormula	18 -	515.284	24.548492
C29 H39 N8 O P3	C29 H39 N8 O P3	[C29 H39 N8 O P3, tgt=81.76, overall=81.76]	(607.2402, 1015.54)(608.2405, 351.54672)(609.24994, 283.7	C29 H39 N8 O P3	FindByFormula	12 -	608.2463	14.337079
C29 H42 N4	C29 H42 N4	[C29 H42 N4, tgt=52.42, overall=52.42]	(481.31226, 401.2544)(482.31747, 120.46071)(483.31912, 3	C29 H42 N4	FindByFormula	25 -	446.3407	22.806433
C29 H43 N3 O3 S2	C29 H43 N3 O3 S2	[C29 H43 N3 O3 S2, tgt=95.02, overall=95.02]	(580.2398, 55.96)(544.266, 2567.6152)(545.2694, 811.0856)	C29 H43 N3 O3 S2	FindByFormula	28 -	545.2749	22.095205
C29 H44 N4 O3	C29 H44 N4 O3	[C29 H44 N4 O3, tgt=99.17, overall=99.17]	(531.3102, 3349.1677)(532.3124, 1186.9509)(533.3077, 142	C29 H44 N4 O3	FindByFormula	28 -	496.3412	18.827915
C29 H45 Cl N4 O2	C29 H45 Cl N4 O2	[C29 H45 Cl N4 O2, tgt=99.68, overall=99.68]	(551.2988, 143.145)(552.3009, 68.60333)(553.3073, 107.25)	C29 H45 Cl N4 O2	FindByFormula	28 -	516.3229	19.772352
C29 H45 N5 O5	C29 H45 N5 O5	[C29 H45 N5 O5, tgt=91.72, overall=91.72]	(578.31464, 76.6875)(588.3404, 67.39)(589.3327, 78.39667)	C29 H45 N5 O5	FindByFormula	28 -	543.3412	19.776707
C29 H46 N10	C29 H46 N10	[C29 H46 N10, tgt=69.40, overall=69.40]	(569.3628, 2696.5776)(570.36, 653.9228)(571.364, 314.2537	C29 H46 N10	FindByFormula	23 -	534.3958	22.702372
C29 H48 N10	C29 H48 N10	[C29 H48 N10, tgt=46.43, overall=46.43]	(571.37427, 263.7623)(572.3735, 124.66125)(573.36554, 14	C29 H48 N10	FindByFormula	15 -	536.4058	22.771605
C29 H48 N4 O3	C29 H48 N4 O3	[C29 H48 N4 O3, tgt=82.69, overall=82.69]	(535.34, 125.238)(536.34503, 47.732002)(537.3387, 165.153	C29 H48 N4 O3	FindByFormula	22 -	500.3715	22.86949
C29 H48 N8 O	C29 H48 N8 O	[C29 H48 N8 O, tgt=81.62, overall=81.62]	(559.36707, 74.322)(560.3572, 38.005)(561.3437, 39.66)(56	C29 H48 N8 O	FindByFormula	13 -	524.3975	23.126377
C29 H50 N10	C29 H50 N10	[C29 H50 N10, tgt=38.38, overall=38.38]	(573.397, 96.691826)(574.3949, 43.7875)(575.3903, 116.842	C29 H50 N10	FindByFormula	20 -	538.4217	22.863163
C29 H50 N11 O2 P5	C29 H50 N11 O2 P5	[C29 H50 N11 O2 P5, tgt=76.23, overall=76.23]	(774.24536, 127.60737)(775.25214, 78.22571)(776.2555, 72.	C29 H50 N11 O2 P5	FindByFormula	24 -	739.2826	22.31463
C29 H54 N2 P2	C29 H54 N2 P2	[C29 H54 N2 P2, tgt=79.03, overall=79.03]	(527.34064, 225.23833)(528.33844, 82.57666)(529.3304, 22	C29 H54 N2 P2	FindByFormula	6 -	492.378	22.928772
C29 H56 N O6 P S2	C29 H56 N O6 P S2	[C29 H56 N O6 P S2, tgt=91.56, overall=91.56]	(644.30347, 108.90626)(645.3004, 110.35667)(646.3121, 67.	C29 H56 N O6 P S2	FindByFormula	28 -	609.3271	22.29909
C29 H64 N6 O2 P2	C29 H64 N6 O2 P2	[C29 H64 N6 O2 P2, tgt=50.91, overall=50.91]	(625.42926, 224.81834)(626.43304, 123.20857)(627.4321, 1	C29 H64 N6 O2 P2	FindByFormula	13 -	590.4539	22.934074
C3 H10 N8	C3 H10 N8	[C3 H10 N8, tgt=71.41, overall=71.41]	(193.07, 76.59)(203.10062, 4722.651)(204.10156, 657.015)(	C3 H10 N8	FindByFormula	14 -	158.1028	0.7142143
C3 H4 O3	C3 H4 O3	[C3 H4 O3, tgt=60.51, overall=60.51]	(133.01443, 7453.088)(134.01595, 397.02618)(87.00866, 36	C3 H4 O3	FindByFormula	24 -	88.0158	0.88100046
C3 H8 N O3 P	C3 H8 N O3 P	[C3 H8 N O3 P, tgt=94.18, overall=94.18]	(136.01674, 38438.496)(137.02081, 3153.829)(138.02135, 5	C3 H8 N O3 P	FindByFormula	22 -	137.024	8.653962
C30 H20 N2 O	C30 H20 N2 O	[C30 H20 N2 O, tgt=76.38, overall=76.38]	(469.14993, 211.73822)(470.14966, 81.13687)(471.1515, 56	C30 H20 N2 O	FindByFormula	23 -	424.1558	22.83422
C30 H22 N2	C30 H22 N2	[C30 H22 N2, tgt=41.16, overall=41.16]	(445.1532, 86.9)(446.1449, 29.89)(455.18256, 405.4305)(45	C30 H22 N2	FindByFormula	20 -	410.18	22.788195
C30 H24 N4 O4	C30 H24 N4 O4	[C30 H24 N4 O4, tgt=56.81, overall=56.81]	(539.1404, 548.3388)(540.1412, 250.6341)(541.1431, 277.99	C30 H24 N4 O4	FindByFormula	25 -	504.1797	22.924353
C30 H25 N5	C30 H25 N5	[C30 H25 N5, tgt=79.85, overall=79.85]	(490.1835, 130.11)(491.179, 97.67)(492.174, 72.01)(500.211	C30 H25 N5	FindByFormula	27 -	455.2087	22.94014
C30 H25 N5 O	C30 H25 N5 O	[C30 H25 N5 O, tgt=91.74, overall=91.74]	(506.18582, 279.97614)(507.19107, 90.38666)(516.20593, 7	C30 H25 N5 O	FindByFormula	28 -	471.2068	23.184647
C30 H37 N11 P2	C30 H37 N11 P2	[C30 H37 N11 P2, tgt=69.90, overall=69.90]	(648.23175, 58.016)(658.258, 133.75667)(659.2433, 103.805	C30 H37 N11 P2	FindByFormula	17 -	613.2721	22.298548
C30 H39 N4 P	C30 H39 N4 P	[C30 H39 N4 P, tgt=98.74, overall=98.74]	(521.2619, 122.59889)(522.2659, 33.236664)(523.2771, 208.	C30 H39 N4 P	FindByFormula	9 -	486.2911	25.190346
C30 H41 N O4	C30 H41 N O4	[C30 H41 N O4, tgt=84.67, overall=84.67]	(514.2731, 60.4775)(515.2701, 27.3)(524.29144, 69.6675)(5	C30 H41 N O4	FindByFormula	28 -	479.3025	22.39623
C30 H41 N2 O P5	C30 H41 N2 O P5	[C30 H41 N2 O P5, tgt=66.47, overall=66.47]	(635.15094, 394.80252)(636.1528, 285.43002)(637.1557, 32	C30 H41 N2 O P5	FindByFormula	27 -	600.1891	22.704908
C30 H41 N7 O2 S	C30 H41 N7 O2 S	[C30 H41 N7 O2 S, tgt=86.37, overall=86.37]	(598.28613, 77.525)(608.3194, 103.32)(609.3269, 183.405)(	C30 H41 N7 O2 S	FindByFormula	26 -	563.3045	24.56895
C30 H41 O5 P3 S2	C30 H41 O5 P3 S2	[C30 H41 O5 P3 S2, tgt=88.88, overall=88.88]	(673.1246, 176.88863)(674.1241, 82.66687)(675.13745, 163.	C30 H41 O5 P3 S2	FindByFormula	28 -	638.1592	22.708956
C30 H42 N10 O	C30 H42 N10 O	[C30 H42 N10 O, tgt=35.18, overall=35.18]	(593.319, 183.14641)(594.31415, 100.731995)(595.3049, 17	C30 H42 N10 O	FindByFormula	17 -	558.3555	22.875406
C30 H44 N4 O4	C30 H44 N4 O4	[C30 H44 N4 O4, tgt=84.07, overall=84.07]	(559.2945, 261.0452)(560.2938, 87.25616)(561.29254, 63.79	C30 H44 N4 O4	FindByFormula	28 -	524.3353	19.566273
C30 H45 N12 P3	C30 H45 N12 P3	[C30 H45 N12 P3, tgt=94.84, overall=94.84]	(701.29474, 90.746666)(711.3146, 101.42857)(712.31104, 9	C30 H45 N12 P3	FindByFormula	7 -	666.3113	15.165276
C30 H46 N4 O4	C30 H46 N4 O4	[C30 H46 N4 O4, tgt=99.17, overall=99.17]	(561.31213, 100.173996)(562.3374, 40.32)(571.34906, 72.14	C30 H46 N4 O4	FindByFormula	28 -	526.3522	19.773243
C30 H46 N4 O5	C30 H46 N4 O5	[C30 H46 N4 O5, tgt=99.25, overall=99.25]	(577.31384, 78.23)(578.31256, 36.663334)(579.31177, 73.46	C30 H46 N4 O5	FindByFormula	28 -	542.3464	17.770739
C30 H48 N O2 P3	C30 H48 N O2 P3	[C30 H48 N O2 P3, tgt=81.90, overall=81.90]	(582.2522, 61.795)(583.2552, 23.19)(592.2882, 65.854996)(	C30 H48 N O2 P3	FindByFormula	27 -	547.2908	22.386679
C30 H49 N5 P2 S3	C30 H49 N5 P2 S3	[C30 H49 N5 P2 S3, tgt=86.09, overall=86.09]	(672.2246, 69.63)(673.23096, 37.52)(674.2283, 171.83)(682.	C30 H49 N5 P2 S3	FindByFormula	28 -	637.2608	21.994822
C30 H50 N O2 P3	C30 H50 N O2 P3	[C30 H50 N O2 P3, tgt=76.86, overall=76.86]	(584.2766, 103.67438)(585.27527, 55.231426)(586.2638, 11	C30 H50 N O2 P3	FindByFormula	25 -	549.3054	22.677786
C30 H50 N5 O5 P	C30 H50 N5 O5 P	[C30 H50 N5 O5 P, tgt=86.57, overall=86.57]	(626.3186, 107.86167)(627.3207, 47.379997)(636.351, 378.5	C30 H50 N5 O5 P	FindByFormula	23 -	591.3523	22.331352
C30 H50 O17	C30 H50 O17	[C30 H50 O17, tgt=97.64, overall=97.64]	(717.2747, 70.6)(727.30963, 89.468)(681.2974, 13637.466)(	C30 H50 O17	FindByFormula	28 -	682.3042	22.525606
C30 H50 O4	C30 H50 O4	[C30 H50 O4, tgt=50.80, overall=50.80]	(509.34274, 178.11665)(510.34464, 67.145996)(511.3389, 7	C30 H50 O4	FindByFormula	17 -	474.372	22.93096
C30 H51 N O20	C30 H51 N O20	[C30 H51 N O20, tgt=90.58, overall=90.58]	(780.28424, 68.70333)(790.2963, 107.104004)(791.31287, 7	C30 H51 N O20	FindByFormula	25 -	745.3007	22.305037
C30 H54 N5 O2 P5	C30 H54 N5 O2 P5	[C30 H54 N5 O2 P5, tgt=53.70, overall=53.70]	(706.2597, 202.12682)(707.2585, 108.361115)(708.25494, 1	C30 H54 N5 O2 P5	FindByFormula	24 -	671.2967	22.303152
C30 H54 O3 S2	C30 H54 O3 S2	[C30 H54 O3 S2, tgt=92.05, overall=92.05]	(561.31244, 64.176)(562.2945, 37.22)(563.28766, 89.82)(57	C30 H54 O3 S2	FindByFormula	28 -	526.3517	17.893064

C30 H54 O4	C30 H54 O4	[C30 H54 O4, tgt=25.73, overall=25.73]	(513.3719, 309.1178)(514.3758, 109.447495)(515.3721, 106	C30 H54 O4	FindByFormula	10 -	478.3977	23.04781
C30 H55 N3 O P2 S	C30 H55 N3 O P2 S	[C30 H55 N3 O P2 S, tgt=73.42, overall=73.42]	(602.3226, 86.18334)(603.3045, 84.40667)(604.3161, 22.14)	C30 H55 N3 O P2 S	FindByFormula	28 -	567.3537	22.339325
C30 H55 N5 O3 P4	C30 H55 N5 O3 P4	[C30 H55 N5 O3 P4, tgt=90.01, overall=90.01]	(692.30005, 63.823997)(693.30493, 38.876667)(702.3139, 2	C30 H55 N5 O3 P4	FindByFormula	28 -	657.322	22.010132
C30 H56 N O4 P S2	C30 H56 N O4 P S2	[C30 H56 N O4 P S2, tgt=88.14, overall=88.14]	(624.3088, 78.57667)(625.30975, 53.5)(626.2954, 28.42)(63	C30 H56 N O4 P S2	FindByFormula	28 -	589.3386	22.119736
C30 H56 S2	C30 H56 S2	[C30 H56 S2, tgt=35.36, overall=35.36]	(515.3526, 290.92725)(516.35614, 137.28833)(517.349, 113.	C30 H56 S2	FindByFormula	24 -	480.3807	22.98395
C30 H57 N O11 P2 S	C30 H57 N O11 P2 S	[C30 H57 N O11 P2 S, tgt=85.27, overall=85.27]	(736.27673, 85.58999)(737.3027, 34.275)(738.2929, 91.63)(	C30 H57 N O11 P2 S	FindByFormula	27 -	701.3135	22.119081
C30 H58 N6 O2	C30 H58 N6 O2	[C30 H58 N6 O2, tgt=96.94, overall=96.94]	(569.4306, 203.32213)(570.42316, 192.49666)(571.4113, 43	C30 H58 N6 O2	FindByFormula	28 -	534.4627	22.84751
C30 H62 N2 O S2	C30 H62 N2 O S2	[C30 H62 N2 O S2, tgt=84.06, overall=84.06]	(565.3931, 67.11714)(566.4018, 21.07)(567.3854, 105.86)(5	C30 H62 N2 O S2	FindByFormula	24 -	530.431	22.586632
C30 H63 N O9 P4	C30 H63 N O9 P4	[C30 H63 N O9 P4, tgt=61.94, overall=61.94]	(740.30774, 138.5325)(741.2779, 36.43)(750.34454, 425.945	C30 H63 N O9 P4	FindByFormula	19 -	705.3461	22.638971
C30 H64 N10 S	C30 H64 N10 S	[C30 H64 N10 S, tgt=72.62, overall=72.62]	(631.47864, 148.33167)(632.4783, 103.952)(633.47894, 120.	C30 H64 N10 S	FindByFormula	21 -	596.5018	23.138685
C30 H65 Cl N4 O S3	C30 H65 Cl N4 O S3	[C30 H65 Cl N4 O S3, tgt=57.85, overall=57.85]	(663.3639, 95.45429)(664.3651, 35.673336)(665.3576, 43.53	C30 H65 Cl N4 O S3	FindByFormula	14 -	628.404	22.782274
C31 H27 N17	C31 H27 N17	[C31 H27 N17, tgt=79.84, overall=79.84]	(672.2368, 59.1)(673.2568, 44.14)(674.2307, 239.49)(682.25	C31 H27 N17	FindByFormula	28 -	637.2594	22.101778
C31 H27 P	C31 H27 P	[C31 H27 P, tgt=58.59, overall=58.59]	(475.18427, 295.28143)(476.18912, 187.52)(477.18887, 187.	C31 H27 P	FindByFormula	23 -	430.1879	22.850174
C31 H34 N2 O7 S	C31 H34 N2 O7 S	[C31 H34 N2 O7 S, tgt=93.83, overall=93.83]	(613.17426, 77.95167)(614.1869, 38.515)(615.1876, 81.955)(	C31 H34 N2 O7 S	FindByFormula	28 -	578.2073	13.10048
C31 H35 N9	C31 H35 N9	[C31 H35 N9, tgt=82.39, overall=82.39]	(568.2632, 65.92)(532.29376, 3372.4753)(533.2984, 1684.76	C31 H35 N9	FindByFormula	6 -	533.3017	18.826073
C31 H37 N14 O P S	C31 H37 N14 O P S	[C31 H37 N14 O P S, tgt=96.18, overall=96.18]	(719.2391, 154.7187)(720.23145, 85.28333)(721.23413, 66.3	C31 H37 N14 O P S	FindByFormula	26 -	684.2729	2.5150373
C31 H45 N9 O10	C31 H45 N9 O10	[C31 H45 N9 O10, tgt=60.37, overall=60.37]	(738.3039, 190.99715)(739.2959, 113.22191)(740.28235, 70.	C31 H45 N9 O10	FindByFormula	26 -	703.3291	22.439537
C31 H46 N4 O	C31 H46 N4 O	[C31 H46 N4 O, tgt=26.94, overall=26.94]	(525.3374, 295.76498)(526.34106, 207.66713)(527.3527, 16	C31 H46 N4 O	FindByFormula	18 -	490.3643	22.461153
C31 H47 N O13 S2	C31 H47 N O13 S2	[C31 H47 N O13 S2, tgt=72.70, overall=72.70]	(740.2131, 80.079994)(750.2358, 66.74375)(751.2396, 61.39	C31 H47 N O13 S2	FindByFormula	27 -	705.2485	21.998722
C31 H50 N4 O	C31 H50 N4 O	[C31 H50 N4 O, tgt=77.49, overall=77.49]	(529.36914, 255.5809)(530.3676, 120.05556)(531.3706, 96.5	C31 H50 N4 O	FindByFormula	11 -	494.3965	23.101303
C31 H50 N7 P3	C31 H50 N7 P3	[C31 H50 N7 P3, tgt=64.08, overall=64.08]	(648.30225, 217.87222)(649.30304, 211.878)(658.33057, 40	C31 H50 N7 P3	FindByFormula	21 -	613.3324	22.136515
C31 H52 N8 O P2	C31 H52 N8 O P2	[C31 H52 N8 O P2, tgt=78.80, overall=78.80]	(649.34174, 161.56909)(650.35693, 226.92001)(651.3408, 3	C31 H52 N8 O P2	FindByFormula	28 -	614.3747	22.456892
C31 H54 S2	C31 H54 S2	[C31 H54 S2, tgt=7.06, overall=7.06]	(525.33777, 183.18846)(526.34436, 94.642)(527.33, 86.3)(5	C31 H54 S2	FindByFormula	17 -	490.3678	22.78158
C31 H56 N7 O3 P3	C31 H56 N7 O3 P3	[C31 H56 N7 O3 P3, tgt=99.02, overall=99.02]	(666.3587, 22937.318)(667.3614, 8278.941)(668.3641, 1953.	C31 H56 N7 O3 P3	FindByFormula	6 -	667.3657	6.636968
C31 H58 N O6 P S2	C31 H58 N O6 P S2	[C31 H58 N O6 P S2, tgt=63.36, overall=63.36]	(670.3171, 138.84544)(671.31433, 106.935)(672.30756, 87.7	C31 H58 N O6 P S2	FindByFormula	28 -	635.3425	22.435001
C31 H59 Cl2 N2 O3 P	C31 H59 Cl2 N2 O3 P	[C31 H59 Cl2 N2 O3 P, tgt=26.00, overall=26.00]	(643.9653, 512.445)(644.7521, 246.76997)(645.6647, 374.75	C31 H59 Cl2 N2 O3 P	FindByFormula	23 -	608.3583	22.463879
C31 H60 O S2	C31 H60 O S2	[C31 H60 O S2, tgt=47.33, overall=47.33]	(547.38324, 203.30785)(548.38416, 85.261)(549.38074, 122.	C31 H60 O S2	FindByFormula	19 -	512.408	22.831854
C31 H67 N5 O5 P2	C31 H67 N5 O5 P2	[C31 H67 N5 O5 P2, tgt=9.29, overall=9.29]	(686.4294, 712.91895)(687.4279, 380.1232)(688.4228, 184.4	C31 H67 N5 O5 P2	FindByFormula	21 -	651.4682	23.104664
C32 H21 N7 O6 P2	C32 H21 N7 O6 P2	[C32 H21 N7 O6 P2, tgt=99.08, overall=99.08]	(706.1078, 65.57)(707.0884, 21.64)(660.09515, 228382.81)(	C32 H21 N7 O6 P2	FindByFormula	22 -	661.1024	8.653916
C32 H23 N O11 P2	C32 H23 N O11 P2	[C32 H23 N O11 P2, tgt=37.03, overall=37.03]	(694.03577, 128.38875)(695.03784, 398.96335)(704.0632, 1	C32 H23 N O11 P2	FindByFormula	9 -	659.0755	0.8298887
C32 H33 N6 O2 P S3	C32 H33 N6 O2 P S3	[C32 H33 N6 O2 P S3, tgt=66.25, overall=66.25]	(695.12317, 166.20874)(696.12415, 59.305)(697.12933, 169.	C32 H33 N6 O2 P S3	FindByFormula	22 -	660.1621	21.616524
C32 H35 N23	C32 H35 N23	[C32 H35 N23, tgt=96.12, overall=96.12]	(776.3079, 89.68333)(777.3145, 84.52)(778.2998, 25.3)(786.	C32 H35 N23	FindByFormula	8 -	741.3446	6.662695
C32 H41 N7 P2	C32 H41 N7 P2	[C32 H41 N7 P2, tgt=95.86, overall=95.86]	(584.28235, 1522.9225)(585.2817, 538.56006)(586.2849, 20	C32 H41 N7 P2	FindByFormula	8 -	585.2889	20.603844
C32 H43 N O4	C32 H43 N O4	[C32 H43 N O4, tgt=86.69, overall=86.69]	(550.31555, 76.225716)(551.3208, 42.69)(504.31024, 2657.9	C32 H43 N O4	FindByFormula	20 -	505.3196	22.116638
C32 H45 N18 O P	C32 H45 N18 O P	[C32 H45 N18 O P, tgt=66.72, overall=66.72]	(763.3402, 136.59941)(764.3424, 91.93286)(765.3407, 128.2	C32 H45 N18 O P	FindByFormula	22 -	728.3785	22.594877
C32 H47 N O5	C32 H47 N O5	[C32 H47 N O5, tgt=79.75, overall=79.75]	(560.3182, 65.263336)(570.34515, 146.02667)(571.3562, 19	C32 H47 N O5	FindByFormula	17 -	525.3442	22.510788
C32 H54 N8 P4	C32 H54 N8 P4	[C32 H54 N8 P4, tgt=90.24, overall=90.24]	(709.3126, 89.263756)(710.29865, 45.993336)(719.3277, 81	C32 H54 N8 P4	FindByFormula	26 -	674.337	13.098744
C32 H56 N O3 P3	C32 H56 N O3 P3	[C32 H56 N O3 P3, tgt=58.62, overall=58.62]	(630.3138, 75.244995)(640.3422, 108.29667)(641.3416, 237.	C32 H56 N O3 P3	FindByFormula	12 -	595.3472	22.599123
C32 H56 N2 O P2	C32 H56 N2 O P2	[C32 H56 N2 O P2, tgt=76.39, overall=76.39]	(581.3545, 177.44135)(582.35657, 816.39)(591.37897, 221.7	C32 H56 N2 O P2	FindByFormula	27 -	546.3857	22.448685
C32 H58 N8 O3 S2	C32 H58 N8 O3 S2	[C32 H58 N8 O3 S2, tgt=33.64, overall=33.64]	(701.3733, 175.07501)(702.3732, 61.2325)(703.3662, 127.89	C32 H58 N8 O3 S2	FindByFormula	23 -	666.4133	22.633821
C32 H59 Cl N2 O	C32 H59 Cl N2 O	[C32 H59 Cl N2 O, tgt=52.89, overall=52.89]	(557.4016, 82.753006)(558.41565, 51.449997)(559.4016, 29	C32 H59 Cl N2 O	FindByFormula	19 -	522.4288	22.981674
C32 H60 O6	C32 H60 O6	[C32 H60 O6, tgt=85.19, overall=85.19]	(575.40106, 226.54642)(576.41266, 129.60571)(577.39795,	C32 H60 O6	FindByFormula	20 -	540.4375	22.862726
C32 H61 N4 O2 P S	C32 H61 N4 O2 P S	[C32 H61 N4 O2 P S, tgt=91.95, overall=91.95]	(631.3967, 126.447495)(632.40454, 79.076004)(633.3947, 1	C32 H61 N4 O2 P S	FindByFormula	24 -	596.4218	22.849295
C32 H66 N6 O P2	C32 H66 N6 O P2	[C32 H66 N6 O P2, tgt=63.06, overall=63.06]	(647.4472, 3649.8518)(648.4514, 1494.7682)(649.44995, 61	C32 H66 N6 O P2	FindByFormula	27 -	612.477	22.908228
C32 H67 O2 P S2	C32 H67 O2 P S2	[C32 H67 O2 P S2, tgt=61.47, overall=61.47]	(613.40076, 2502.4385)(614.4037, 1157.7104)(615.399, 174	C32 H67 O2 P S2	FindByFormula	28 -	578.4312	22.720219
C33 H36 N20 O2	C33 H36 N20 O2	[C33 H36 N20 O2, tgt=85.48, overall=85.48]	(779.30554, 138.25801)(780.3053, 67.03223)(781.3069, 205.	C33 H36 N20 O2	FindByFormula	28 -	744.3341	22.456068
C33 H37 N5	C33 H37 N5	[C33 H37 N5, tgt=71.27, overall=71.27]	(538.27594, 94.81)(539.2529, 34.99)(548.30054, 311.53278)	C33 H37 N5	FindByFormula	13 -	503.3017	22.267803
C33 H37 N6 O2 P	C33 H37 N6 O2 P	[C33 H37 N6 O2 P, tgt=91.36, overall=91.36]	(615.2371, 277.93106)(616.23083, 258.8869)(617.23267, 77.	C33 H37 N6 O2 P	FindByFormula	28 -	580.2692	19.43256
C33 H41 N11	C33 H41 N11	[C33 H41 N11, tgt=65.47, overall=65.47]	(626.3214, 88.02599)(627.3275, 42.425)(628.3197, 31.065)(	C33 H41 N11	FindByFormula	24 -	591.3539	22.314621
C33 H43 N11 P2	C33 H43 N11 P2	[C33 H43 N11 P2, tgt=63.89, overall=63.89]	(690.2875, 91.585)(691.2819, 66.52)(700.30853, 96.98399)(	C33 H43 N11 P2	FindByFormula	10 -	655.3172	22.659292
C33 H45 N P2	C33 H45 N P2	[C33 H45 N P2, tgt=69.11, overall=69.11]	(552.27686, 83.02)(553.291, 154.92)(562.2889, 74.78)(516.2	C33 H45 N P2	FindByFormula	12 -	517.3018	17.700064
C33 H46 Cl N O4	C33 H46 Cl N O4	[C33 H46 Cl N O4, tgt=59.87, overall=59.87]	(600.31793, 88.666245)(601.3384, 26.89)(554.30225, 788.01	C33 H46 Cl N O4	FindByFormula	23 -	555.3127	22.106976
C33 H48 O P4	C33 H48 O P4	[C33 H48 O P4, tgt=89.02, overall=89.02]	(629.2812, 50.4)(583.2572, 1877.5414)(584.26404, 744.1642	C33 H48 O P4	FindByFormula	7 -	584.2656	23.22742
C33 H50 N4 O	C33 H50 N4 O	[C33 H50 N4 O, tgt=62.56, overall=62.56]	(553.3679, 119.345825)(554.37494, 34.82)(555.3661, 110.12	C33 H50 N4 O	FindByFormula	14 -	518.3969	22.568758
C33 H51 N O2 P2	C33 H51 N O2 P2	[C33 H51 N O2 P2, tgt=73.13, overall=73.13]	(590.3113, 96.608)(591.31146, 34.545002)(592.31665, 123.4	C33 H51 N O2 P2	FindByFormula	24 -	555.3369	22.474577
C33 H52 N4 O	C33 H52 N4 O	[C33 H52 N4 O, tgt=44.46, overall=44.46]	(555.3828, 139.6875)(556.3826, 69.97)(557.3779, 192.08)(5	C33 H52 N4 O	FindByFormula	13 -	520.4112	23.086548
C33 H54 N4 O2	C33 H54 N4 O2	[C33 H54 N4 O2, tgt=72.56, overall=72.56]	(573.3968, 106.54785)(574.398, 46.59714)(575.3956, 86.0)(	C33 H54 N4 O2	FindByFormula	21 -	538.4208	22.830858
C33 H59 Cl N2 O6	C33 H59 Cl N2 O6	[C33 H59 Cl N2 O6, tgt=64.38, overall=64.38]	(649.3782, 256.34)(659.4034, 271.91998)(660.4063, 301.737	C33 H59 Cl N2 O6	FindByFormula	24 -	614.4075	22.862474
C33 H62 N4 O14	C33 H62 N4 O14	[C33 H62 N4 O14, tgt=96.52, overall=96.52]	(773.3932, 203.12129)(774.37775, 83.97)(775.3843, 165.195	C33 H62 N4 O14	FindByFormula	28 -	738.4245	22.846369
C33 H66 Cl2 O P4	C33 H66 Cl2 O P4	[C33 H66 Cl2 O P4, tgt=78.69, overall=78.69]	(708.9343, 85.945)(709.2996, 87.00666)(709.80286, 54.14)(	C33 H66 Cl2 O P4	FindByFormula	28 -	672.3454	13.102267
C33 H66 N2 O P2	C33 H66 N2 O P2	[C33 H66 N2 O P2, tgt=19.88, overall=19.88]	(603.4413, 259.505)(604.44745, 122.45333)(613.4513, 5754.	C33 H66 N2 O P2	FindByFormula	12 -	568.4597	22.941317
C33 H66 N2 O3 S2	C33 H66 N2 O3 S2	[C33 H66 N2 O3 S2, tgt=89.30, overall=89.30]	(637.42096, 160.86287)(647.45764, 1271.7012)(648.459, 67	C33 H66 N2 O3 S2	FindByFormula	28 -	602.4517	22.848082
C33 H69 N O4	C33 H69 N O4	[C33 H69 N O4, tgt=31.14, overall=31.14]	(578.492, 934.83563)(579.4938, 1311.176)(588.522, 77.79)(	C33 H69 N O4	FindByFormula	7 -	543.521	23.100496
C33 H69 N4 P S2	C33 H69 N4 P S2	[C33 H69 N4 P S2, tgt=58.27, overall=58.27]	(651.4432, 579.38995)(652.44495, 236.5736)(653.4329, 45.4	C33 H69 N4 P S2	FindByFormula	20 -	616.4735	22.900173
C34 H10 Cl N3 O3	C34 H10 Cl N3 O3	[C34 H10 Cl N3 O3, tgt=64.67, overall=64.67]	(542.037, 1872.64)(543.03766, 880.15106)(544.0288, 2256.7	C34 H10 Cl N3 O3	FindByFormula	10 -	543.0416	2.5226967
C34 H25 N5 O3	C34 H25 N5 O3	[C34 H25 N5 O3, tgt=88.47, overall=88.47]	(586.17426, 270.88773)(596.1875, 67.990005)(597.1987, 42.	C34 H25 N5 O3	FindByFormula	28 -	551.1978	13.102622
C34 H28 N2 O4	C34 H28 N2 O4	[C34 H28 N2 O4, tgt=23.19, overall=23.19]	(563.1733, 426.06833)(564.1748, 137.69)(565.16504, 113.43	C34 H28 N2 O4	FindByFormula	18 -	528.2029	21.67345
C34 H29 Cl N6	C34 H29 Cl N6	[C34 H29 Cl N6, tgt=81.14, overall=81.14]	(591.17303, 100.2025)(592.1729, 61.97333)(601.2097, 72.74	C34 H29 Cl N6	FindByFormula	28 -	556.2129	13.104087
C34 H32 N8 O2	C34 H32 N8 O2	[C34 H32 N8 O2, tgt=97.51, overall=97.51]	(619.2289, 65.98)(629.2746, 59.433334)(630.2646, 22.11)(5	C34 H32 N8 O2	FindByFormula	6 -	584.265	15.298995
C34 H47 N3 O10	C34 H47 N3 O10	[C34 H47 N3 O10, tgt=81.08, overall=81.08]	(692.2896, 119.48667)(693.2827, 65.825714)(694.2884, 290.	C34 H47 N3 O10	FindByFormula	28 -	657.3224	22.112055
C34 H48 Cl N2 O5 P3 S	C34 H48 Cl N2 O5 P3 S	[C34 H48 Cl N2 O5 P3 S, tgt=51.89, overall=51.89]	(759.1845, 52.64)(769.21814, 57.53)(723.2109, 1351.5668)(	C34 H48 Cl N2 O5 P3 S	FindByFormula	19 -	724.2137	3.5990965
C34 H52 N3 O4 P5	C34 H52 N3 O4 P5	[C34 H52 N3 O4 P5, tgt=95.46, overall=95.46]	(756.2323, 66.8)(757.2451, 20.94)(766.27795, 118.145004)(	C34 H52 N3 O4 P5	FindByFormula	8 -	721.2645	20.235798
C34 H54 N2 O2 P2	C34 H54 N2 O2 P2	[C34 H54 N2 O2 P2, tgt=54.39, overall=54.39]	(619.3366, 120.36714)(620.3146, 43.21)(629.35767, 60.265)(	C34 H54 N2 O2 P2	FindByFormula	14 -	584.3616	22.920046
C34 H55 N4 O4 P	C34 H55 N4 O4 P	[C34 H55 N4 O4 P, tgt=81.27, overall=81.27]	(649.37537, 65.93199)(659.39453, 784.61523)(660.3962, 33	C34 H55 N4 O4 P	FindByFormula	26 -	614.3944	22.728153
C34 H57 Cl N2 O	C34 H57 Cl N2 O	[C34 H57 Cl N2 O, tgt=34.93, overall=34.93]	(579.39, 223.1)(580.387, 186.92)(581.3934, 48.32)(589.4242	C34 H57 Cl N2 O	FindByFormula	6 -	544.4184	23.034342
C34 H57 Cl N2 O2	C34 H57 Cl N2 O2	[C34 H57 Cl N2 O2, tgt=68.75, overall=68.75]	(595.37805, 128.59125)(596.3771, 55.475002)(597.3862, 32.	C34 H57 Cl N2 O2	FindByFormula	14 -	560.4087	22.83742
C34 H57 N4 O4 P	C34 H57 N4 O4 P	[C34 H57 N4 O4 P, tgt=78.55, overall=78.55]	(651.3834, 124.53143)(652.3941, 113.81666)(661.4129, 217.	C34 H57 N4 O4 P	FindByFormula	22 -	616.4095	22.931444
C34 H58 N6 O2	C34 H58 N6 O2	[C34 H58 N6 O2, tgt=98.25, overall=98.25]	(617.4301, 149.74367)(618.4339, 66.825005)(619.4556, 130.	C34 H58 N6 O2	FindByFormula	27 -	582.463	22.73334
C34 H60 N6 O2	C34 H60 N6 O2	[C34 H60 N6 O2, tgt=73.04, overall=73.04]	(619.4471, 588.38525)(620.4499, 280.25003)(621.4428, 392.	C34 H60 N6 O2	FindByFormula	24 -	584.4734	22.846397
C34 H62 N6 O2	C34 H62 N6 O2	[C34 H62 N6 O2, tgt=95.15, overall=95.15]	(621.47107, 169.88333)(622.4754, 136.035)(623.479, 472.21	C34 H62 N6 O2	FindByFormula	27 -	586.4948	22.928846
C34 H62 N6 O4	C34 H62 N6 O4	[C34 H62 N6 O4, tgt=78.53, overall=78.53]	(653.4625, 244.39832)(654.4677, 97.420006)(655.4547, 88.7	C34 H62 N6 O4	FindByFormula	12 -	618.4837	23.166672
C34 H63 Cl N2 O2	C34 H63 Cl N2 O2	[C34 H63 Cl N2 O2, tgt=6.66, overall=6.66]	(601.4266, 1045.788)(602.43085, 495.41498)(603.4295, 333.	C34 H63 Cl N2 O2	FindByFormula	11 -	566.4615	22.94851
C34 H64 N2 O2 S4	C34 H64 N2 O2 S4	[C34 H64 N2 O2 S4, tgt=54.48, overall=54.48]	(695.36084, 168.11)(696.3632, 71.91166)(697.35925, 141.81	C34 H64 N2 O2 S4	FindByFormula	25 -	660.3853	22.5996
C34 H65 O2 P3	C34 H65 O2 P3	[C34 H65 O2 P3, tgt=55.03, overall=55.03]	(633.3892, 134.45268)(634.38544, 1068.0801)(635.3873, 66	C34 H65 O2 P3	FindByFormula	28 -	598.4186	22.638382
C34 H66 N6 O2	C34 H66 N6 O2	[C34 H66 N6 O2, tgt=96.84, overall=96.84]	(625.49365, 164.04053)(626.50037, 73.56727)(627.4873, 52.	C34 H66 N6 O2	FindByFormula	28 -	590.5255	23.182005
C34 H70 S3	C34 H70 S3	[C34 H70 S3, tgt=55.35, overall=55.35]	(609.42773, 83.29399)(610.42316, 34.996666)(611.4043, 59	C34 H70 S3	FindByFormula	14 -	574.4696	23.127234
C35 H34 N6 O	C35 H34 N6 O	[C35 H34 N6 O, tgt=91.42, overall=91.42]	(589.26, 54.905)(590.2666, 28.189999)(591.25574, 27.325)(	C35 H34 N6 O	FindByFormula	6 -	554.2793	25.153524
C35 H37 N O	C35 H37 N O	[C35 H37 N O, tgt=97.35, overall=97.35]	(522.2516, 96.49454)(523.27026, 222.89333)(524.26526, 62.	C35 H37 N O	FindByFormula	25 -	487.286	24.569592
C35 H40 N14	C35 H40 N14	[C35 H40 N14, tgt=34.37, overall=34.37]	(691.3244, 173.76714)(692.3252, 94.48)(693.3236, 146.21)(	C35 H40 N14	FindByFormula	26 -	656.3526	22.304874
C35 H44 N8 O P2	C35 H44 N8 O P2	[C35 H44 N8 O P2, tgt=41.72, overall=41.72]	(689.2884, 128.13545)(690.2871, 59.929996)(699.3145, 199.	C35 H44 N8 O P2	FindByFormula	12 -	654.3116	22.639685
C35 H45 Cl N2 O2 S3	C35 H45 Cl N2 O2 S3	[C35 H45 Cl N2 O2 S3, tgt=69.42, overall=69.42]	(691.2102, 73.9)(701.2275, 69.82833)(702.2335, 37.52)(703.	C35 H45 Cl N2 O2 S3	FindByFormula	22 -	656.2333	3.5980353
C35 H49 N7 O5 S2	C35 H49 N7 O5 S2	[C35 H49 N7 O5 S2, tgt=92.10, overall=92.10]	(746.29596, 595.9238)(747.3023, 279.03384)(748.297, 287.9	C35 H49 N7 O5 S2	FindByFormula	21 -	711.3249	9.295551
C35 H56 N O2 P3	C35 H56 N O2 P3	[C35 H56 N O2 P3, tgt=70.29, overall=70.29]	(650.3207, 191.26201)(651.33405, 164.44)(652.3154, 527.66	C35 H56 N O2 P3	FindByFormula	12 -	615.3478	22.296694
C35 H57 N7 O2 S	C35 H57 N7 O2 S	[C35 H57 N7 O2 S, tgt=77.56, overall=77.56]	(674.39417, 181.49335)(675.4021, 133.69)(676.4003, 588.10	C35 H57 N7 O2 S	FindByFormula	27 -	639.4339	22.909895
C35 H58 N10	C35 H58 N10	[C35 H58 N10, tgt=42.59, overall=42.59]	(653.4609, 274.3925)(654.4624, 113.10834)(655.456, 83.67)(	C35 H58 N10	FindByFormula	11 -	618.4822	23.256815
C35 H62 N8 O8	C35 H62 N8 O8	[C35 H62 N8 O8, tgt=94.53, overall=94.53]	(757.4383, 123.81333)(767.4558, 522.12946)(768.46027, 60	C35 H62 N8 O8	FindByFormula	28 -	722.4682	22.923367
C35 H63 N5	C35 H63 N5	[C35 H63 N5, tgt=92.80, overall=92.80]	(588.47876, 685.072)(589.4787, 356.21213)(590.47723, 361.	C35 H63 N5	FindByFormula	20 -	553.5078	24.040457
C35 H65 Cl O7 S2	C35 H65 Cl O7 S2	[C35 H65 Cl O7 S2, tgt=7.92, overall=7.92]	(731.36224, 101.53111)(732.3511, 32.343334)(733.3553, 76.	C35 H65 Cl O7 S2	FindByFormula	19 -	696.3848	22.579508
C35 H65 O6 P S	C35 H65 O6 P S	[C35 H65 O6 P S, tgt=85.29, overall=85.29]	(679.39874, 197.72774)(680.3969, 155.7954)(681.3974, 702.	C35 H65 O6 P S	FindByFormula	25 -	644.4195	22.74299
C35 H67 Cl2 O3 P	C35 H67 Cl2 O3 P	[C35 H67 Cl2 O3 P, tgt=75.89, overall=75.89]	(673.2976, 150.825)(674.0566, 198.45332)(675.39014, 199.6	C35 H67 Cl2 O3 P	FindByFormula	24 -	636.4196	23.273552
C35 H68 Cl2	C35 H68 Cl2	[C35 H68 Cl2, tgt=54.77, overall=54.77]	(557.4595, 2019.0701)(558.45966, 803.86005)(559.4715, 14	C35 H68 Cl2	FindByFormula	2 -	558.4751	24.124601
C35 H69 O6 P S	C35 H69 O6 P S	[C35 H69 O6 P S, tgt=89.56, overall=89.56]	(683.434, 658.17426)(684.44666, 1225.88)(685.4466, 952.73	C35 H69 O6 P S	FindByFormula	26 -	648.4551	22.918781
C35 H70 Cl2 O2	C35 H70 Cl2 O2	[C35 H70 Cl2 O2, tgt=57.84, overall=57.84]	(629.0143, 232.97429)(629.8405, 79.824)(630.45105, 73.17)(	C35 H70 Cl2 O2	FindByFormula	16 -	592.4774	22.90221
C35 H70 N2 O P2	C35 H70 N2 O P2	[C35 H70 N2 O P2, tgt=53.53, overall=53.53]	(631.46497, 129.562)(632.478, 55.225002)(633.46796, 93.02	C35 H70 N2 O P2	FindByFormula	23 -	596.5008	23.202087
C35 H71 N S2	C35 H71 N S2	[C35 H71 N S2, tgt=91.28, overall=91.28]	(604.4729, 210.42877)(605.47205, 173.9955)(606.4709, 116.	C35 H71 N S2	FindByFormula	24 -	569.5032	23.354485
C35 H72 O4 S	C35 H72 O4 S	[C35 H72 O4 S, tgt=81.91, overall=81.91]	(623.49243, 107.21001)(624.5002, 55.94222)(625.50165, 16	C35 H72 O4 S	FindByFormula	28 -	588.5126	22.840796
C35 H73 P S5	C35 H73 P S5	[C35 H73 P S5, tgt=64.03, overall=64.03]	(719.37665, 129.74144)(720.3674, 62.37)(729.40265, 175.67	C35 H73 P S5	FindByFormula	23 -	684.4062	22.890827
C35 H74 N2 O S2	C35 H74 N2 O S2	[C35 H74 N2 O S2, tgt=89.32, overall=89.32]	(637.49805, 306.82852)(638.5104, 106.515)(639.5208, 61.24	C35 H74 N2 O S2	FindByFormula	28 -	602.5261	22.850756
C35 H74 N9 O4 P	C35 H74 N9 O4 P	[C35 H74 N9 O4 P, tgt=90.73, overall=90.73]	(750.5368, 326.85806)(751.5371, 151.45476)(752.5277, 125.	C35 H74 N9 O4 P	FindByFormula	22 -	715.5598	23.701288
C36 H25 N2 P S	C36 H25 N2 P S	[C36 H25 N2 P S, tgt=87.92, overall=87.92]	(583.11755, 3726.6392)(584.12213, 1311.3911)(585.1152, 1	C36 H25 N2 P S	FindByFormula	26 -	548.1493	2.5144985
C36 H27 N2 O12 P S	C36 H27 N2 O12 P S	[C36 H27 N2 O12 P S, tgt=99.26, overall=99.26]	(777.074, 67.666664)(778.1057, 21.84)(779.0733, 41.45)(78	C36 H27 N2 O12 P S	FindByFormula	25 -	742.1015	18.711058
C36 H36 N8 O3	C36 H36 N8 O3	[C36 H36 N8 O3, tgt=92.05, overall=92.05]	(663.2474, 50.86)(664.2655, 36.88)(665.2484, 26.95)(673.30	C36 H36 N8 O3	FindByFormula	28 -	628.2918	18.522573
C36 H37 N O3	C36 H37 N O3	[C36 H37 N O3, tgt=83.77, overall=83.77]	(566.2483, 1326.6624)(567.25323, 488.89786)(568.24927, 5	C36 H37 N O3	FindByFormula	24 -	531.2791	24.566437
C36 H41 N7 O P4	C36 H41 N7 O P4	[C36 H41 N7 O P4, tgt=80.31, overall=80.31]	(746.20483, 61.87375)(747.22516, 36.533337)(748.2139, 31.	C36 H41 N7 O P4	FindByFormula	25 -	711.2317	2.5165184
C36 H52 N4 O7 P2	C36 H52 N4 O7 P2	[C36 H52 N4 O7 P2, tgt=56.78, overall=56.78]	(749.2975, 111.935715)(750.3104, 42.524998)(751.267, 98.5	C36 H52 N4 O7 P2	FindByFormula	16 -	714.3296	22.545933
C36 H54 N6 O2	C36 H54 N6 O2	[C36 H54 N6 O2, tgt=81.90, overall=81.90]	(637.3988, 281.12125)(638.39124, 277.41498)(639.3949, 18	C36 H54 N6 O2	FindByFormula	12 -	602.4259	22.528381
C36 H58 N6 O2	C36 H58 N6 O2	[C36 H58 N6 O2, tgt=97.76, overall=97.76]	(641.4304, 161.94998)(642.4168, 1566.3374)(651.44794, 14	C36 H58 N6 O2	FindByFormula	26 -	606.4622	22.713238
C36 H61 N O2 P6	C36 H61 N O2 P6	[C36 H61 N O2 P6, tgt=76.94, overall=76.94]	(760.27435, 137.06142)(761.2707, 97.057144)(762.2768, 36	C36 H61 N O2 P6	FindByFormula	27 -	725.3086	22.127161
C36 H62 N11 P	C36 H62 N11 P	[C36 H62 N11 P, tgt=85.01, overall=85.01]	(714.4581, 197.55666)(715.4563, 223.15001)(716.4579, 177.	C36 H62 N11 P	FindByFormula	24 -	679.4915	22.833511
C36 H65 N5 O	C36 H65 N5 O	[C36 H65 N5 O, tgt=98.43, overall=98.43]	(582.5113, 11140.464)(583.5138, 4554.717)(584.51526, 109	C36 H65 N5 O	FindByFormula	26 -	583.5188	24.320732
C36 H66 N2 O10	C36 H66 N2 O10	[C36 H66 N2 O10, tgt=45.64, overall=45.64]	(721.44965, 256.566)(722.4491, 107.90501)(723.4532, 95.54	C36 H66 N2 O10	FindByFormula	15 -	686.4692	23.139042
C36 H66 N2 O6 S	C36 H66 N2 O6 S	[C36 H66 N2 O6 S, tgt=93.33, overall=93.33]	(689.4338, 234.754)(690.4032, 1162.31)(699.4469, 1237.948	C36 H66 N2 O6 S	FindByFormula	17 -	654.4621	22.68025
C36 H66 N2 O8	C36 H66 N2 O8	[C36 H66 N2 O8, tgt=97.73, overall=97.73]	(689.46826, 87.38)(699.4656, 839.5833)(700.4637, 520.7052	C36 H66 N2 O8	FindByFormula	27 -	654.4807	22.927551
C36 H67 Cl N2 O	C36 H67 Cl N2 O	[C36 H67 Cl N2 O, tgt=52.10, overall=52.10]	(613.4483, 155.97)(614.4505, 54.27)(615.4627, 558.04)(616.	C36 H67 Cl N2 O	FindByFormula	17 -	578.4941	23.159172
C36 H67 N2 O P	C36 H67 N2 O P	[C36 H67 N2 O P, tgt=92.04, overall=92.04]	(609.47626, 378.63953)(610.4787, 173.00179)(611.4725, 12	C36 H67 N2 O P	FindByFormula	28 -	574.4999	22.447708
C36 H70 N2 O8	C36 H70 N2 O8	[C36 H70 N2 O8, tgt=98.38, overall=98.38]	(693.483, 269.9527)(703.4966, 373.75098)(704.50104, 214.6	C36 H70 N2 O8	FindByFormula	28 -	658.5129	23.183111
C36 H72 Cl N3	C36 H72 Cl N3	[C36 H72 Cl N3, tgt=78.01, overall=78.01]	(616.5135, 309.1322)(617.5122, 146.77823)(618.5131, 182.2	C36 H72 Cl N3	FindByFormula	20 -	581.5416	24.576973
C36 H72 O4 S	C36 H72 O4 S	[C36 H72 O4 S, tgt=84.68, overall=84.68]	(635.4879, 125.085)(636.48865, 79.522)(637.4878, 123.6366	C36 H72 O4 S	FindByFormula	25 -	600.5148	22.59314
C36 H73 Cl P4	C36 H73 Cl P4	[C36 H73 Cl P4, tgt=54.97, overall=54.97]	(699.40497, 196.98)(700.4062, 142.605)(701.40265, 126.915	C36 H73 Cl P4	FindByFormula	23 -	664.4341	23.005058
C36 H75 N S2	C36 H75 N S2	[C36 H75 N S2, tgt=81.32, overall=81.32]	(620.51953, 117.46)(621.5269, 58.77)(622.5401, 44.63)(630.	C36 H75 N S2	FindByFormula	25 -	585.5342	24.531174
C36 H75 N9 O2 P2	C36 H75 N9 O2 P2	[C36 H75 N9 O2 P2, tgt=79.05, overall=79.05]	(762.5357, 190.0925)(763.54034, 125.762)(764.5337, 178.73	C36 H75 N9 O2 P2	FindByFormula	22 -	727.5468	25.259407
C37 H33 N S4	C37 H33 N S4	[C37 H33 N S4, tgt=85.08, overall=85.08]	(654.1198, 112.02)(655.1216, 56.31143)(656.1107, 63.97400	C37 H33 N S4	FindByFormula	21 -	619.15	2.5218077
C37 H34 N15 P	C37 H34 N15 P	[C37 H34 N15 P, tgt=71.58, overall=71.58]	(754.2521, 126.387146)(755.2459, 52.969997)(756.2495, 13	C37 H34 N15 P	FindByFormula	18 -	719.2835	22.130297
C37 H39 N10 P	C37 H39 N10 P	[C37 H39 N10 P, tgt=55.22, overall=55.22]	(653.3028, 1319.8569)(654.30493, 516.1099)(655.3087, 190.	C37 H39 N10 P	FindByFormula	24 -	654.312	24.483658
C37 H42 N5 O2 P3 S	C37 H42 N5 O2 P3 S	[C37 H42 N5 O2 P3 S, tgt=95.40, overall=95.40]	(748.2054, 95.503334)(749.21124, 55.216663)(712.2203, 31	C37 H42 N5 O2 P3 S	FindByFormula	26 -	713.2275	2.5159986
C37 H43 Cl O S4	C37 H43 Cl O S4	[C37 H43 Cl O S4, tgt=77.39, overall=77.39]	(701.1506, 653.6966)(702.14734, 1244.0925)(703.151, 544.9	C37 H43 Cl O S4	FindByFormula	11 -	666.1835	3.5976288
C37 H49 N O S	C37 H49 N O S	[C37 H49 N O S, tgt=63.99, overall=63.99]	(590.3065, 83.71)(591.3042, 49.23)(592.3135, 48.86)(600.35	C37 H49 N O S	FindByFormula	8 -	555.3504	22.54721
C37 H58 N4	C37 H58 N4	[C37 H58 N4, tgt=64.11, overall=64.11]	(603.4689, 66.985)(604.46985, 26.794998)(557.45953, 3005.	C37 H58 N4	FindByFormula	11 -	558.4666	23.655512
C37 H61 N7 O2 S	C37 H61 N7 O2 S	[C37 H61 N7 O2 S, tgt=88.09, overall=88.09]	(702.4307, 102.151665)(703.4292, 36.3)(712.464, 280.96738	C37 H61 N7 O2 S	FindByFormula	24 -	667.4608	23.183619
C37 H62 N4	C37 H62 N4	[C37 H62 N4, tgt=93.38, overall=93.38]	(607.4931, 59.949997)(561.4885, 1449.8617)(562.4937, 601.	C37 H62 N4	FindByFormula	6 -	562.4962	24.345888
C37 H64 O3 P6	C37 H64 O3 P6	[C37 H64 O3 P6, tgt=89.50, overall=89.50]	(777.2953, 73.770004)(778.3013, 71.95)(787.3192, 365.8827	C37 H64 O3 P6	FindByFormula	25 -	742.326	13.099955
C37 H66 Cl N11	C37 H66 Cl N11	[C37 H66 Cl N11, tgt=76.43, overall=76.43]	(744.51086, 611.1414)(745.5113, 351.07193)(746.51324, 76	C37 H66 Cl N11	FindByFormula	25 -	699.5201	24.550312
C37 H66 N5 P	C37 H66 N5 P	[C37 H66 N5 P, tgt=85.83, overall=85.83]	(646.4742, 135.907)(647.4751, 93.84)(656.50586, 180.86421	C37 H66 N5 P	FindByFormula	24 -	611.5062	22.852442
C37 H66 S2	C37 H66 S2	[C37 H66 S2, tgt=37.49, overall=37.49]	(609.43134, 92.855995)(610.42865, 40.03)(619.46344, 306.4	C37 H66 S2	FindByFormula	12 -	574.4662	23.007729
C37 H68 N2 O5 S2	C37 H68 N2 O5 S2	[C37 H68 N2 O5 S2, tgt=60.62, overall=60.62]	(719.42865, 401.38705)(720.42773, 237.65266)(721.4311, 1	C37 H68 N2 O5 S2	FindByFormula	23 -	684.4634	22.957212
C37 H70 O S2	C37 H70 O S2	[C37 H70 O S2, tgt=70.33, overall=70.33]	(629.4574, 10411.77)(630.45953, 4715.6025)(631.46045, 12	C37 H70 O S2	FindByFormula	27 -	594.4845	22.91826
C37 H75 N S2	C37 H75 N S2	[C37 H75 N S2, tgt=88.83, overall=88.83]	(642.545, 71.05)(643.5367, 55.67)(596.52686, 1883.4564)(5	C37 H75 N S2	FindByFormula	24 -	597.5344	24.60489
C37 H77 N3 O S	C37 H77 N3 O S	[C37 H77 N3 O S, tgt=85.33, overall=85.33]	(646.53894, 95.40625)(647.5473, 39.075)(648.5269, 55.75)(	C37 H77 N3 O S	FindByFormula	28 -	611.581	22.819912
C37 H80 N9 O P	C37 H80 N9 O P	[C37 H80 N9 O P, tgt=80.27, overall=80.27]	(732.6088, 85.76)(733.6308, 46.95)(734.6159, 63.6)(742.611	C37 H80 N9 O P	FindByFormula	20 -	697.621	25.772919
C38 H35 N5 O4	C38 H35 N5 O4	[C38 H35 N5 O4, tgt=93.22, overall=93.22]	(670.2705, 70.39917)(671.2615, 49.434998)(624.26154, 229	C38 H35 N5 O4	FindByFormula	28 -	625.2686	19.78178
C38 H41 N10 P	C38 H41 N10 P	[C38 H41 N10 P, tgt=85.22, overall=85.22]	(703.2995, 81.038895)(704.29736, 64.520004)(705.301, 22.6	C38 H41 N10 P	FindByFormula	27 -	668.3247	13.102587
C38 H41 N2 O2 P5	C38 H41 N2 O2 P5	[C38 H41 N2 O2 P5, tgt=45.13, overall=45.13]	(747.15466, 1335.675)(748.149, 813.96)(749.148, 498.68)(7	C38 H41 N2 O2 P5	FindByFormula	2 -	712.1796	23.061363
C38 H47 N O P2 S	C38 H47 N O P2 S	[C38 H47 N O P2 S, tgt=74.68, overall=74.68]	(662.2697, 283.72498)(663.26166, 146.47112)(664.26587, 1	C38 H47 N O P2 S	FindByFormula	19 -	627.2861	22.294012
C38 H48 N5 O P	C38 H48 N5 O P	[C38 H48 N5 O P, tgt=79.07, overall=79.07]	(656.31866, 272.436)(657.3108, 173.905)(658.3001, 34.0)(6	C38 H48 N5 O P	FindByFormula	9 -	621.354	22.671728
C38 H55 O P5 S	C38 H55 O P5 S	[C38 H55 O P5 S, tgt=94.96, overall=94.96]	(759.25305, 75.07124)(760.26794, 52.554005)(713.2585, 49	C38 H55 O P5 S	FindByFormula	28 -	714.267	8.460364
C38 H58 N6 O2	C38 H58 N6 O2	[C38 H58 N6 O2, tgt=97.33, overall=97.33]	(665.42633, 145.424)(666.4138, 1656.3451)(667.4415, 117.5	C38 H58 N6 O2	FindByFormula	27 -	630.4618	22.70391
C38 H60 N9 P	C38 H60 N9 P	[C38 H60 N9 P, tgt=95.05, overall=95.05]	(708.44116, 228.88867)(709.4263, 161.07857)(710.4418, 18	C38 H60 N9 P	FindByFormula	24 -	673.4666	22.896193
C38 H63 Cl N2 O S2	C38 H63 Cl N2 O S2	[C38 H63 Cl N2 O S2, tgt=75.40, overall=75.40]	(697.3874, 148.192)(698.3847, 65.36666)(707.397, 345.5599	C38 H63 Cl N2 O S2	FindByFormula	27 -	662.4064	22.727644
C38 H64 O10 S	C38 H64 O10 S	[C38 H64 O10 S, tgt=90.94, overall=90.94]	(747.3888, 159.58786)(748.37695, 59.879997)(757.42865, 3	C38 H64 O10 S	FindByFormula	28 -	712.4207	22.724346
C38 H65 O2 P3	C38 H65 O2 P3	[C38 H65 O2 P3, tgt=28.25, overall=28.25]	(681.3877, 1003.8269)(682.39185, 993.97455)(683.3969, 75	C38 H65 O2 P3	FindByFormula	27 -	646.4174	22.6704
C38 H66 O3 P2 S	C38 H66 O3 P2 S	[C38 H66 O3 P2 S, tgt=48.32, overall=48.32]	(699.39417, 102.585)(700.38324, 118.87333)(701.4061, 152.	C38 H66 O3 P2 S	FindByFormula	20 -	664.423	22.776058
C38 H67 Cl N2	C38 H67 Cl N2	[C38 H67 Cl N2, tgt=56.20, overall=56.20]	(621.4642, 98.641)(622.4709, 82.375)(623.46106, 114.48)(6	C38 H67 Cl N2	FindByFormula	25 -	586.4955	22.687035
C38 H67 Cl N2 O S2	C38 H67 Cl N2 O S2	[C38 H67 Cl N2 O S2, tgt=82.07, overall=82.07]	(701.4133, 127.51889)(702.4155, 171.196)(703.41547, 140.0	C38 H67 Cl N2 O S2	FindByFormula	26 -	666.4383	22.930998
C38 H71 N O3 S3	C38 H71 N O3 S3	[C38 H71 N O3 S3, tgt=88.87, overall=88.87]	(720.4191, 57.92)(730.4793, 109.58)(731.4737, 55.79)(684.4	C38 H71 N O3 S3	FindByFormula	20 -	685.4594	24.043705
C38 H74 O4 S	C38 H74 O4 S	[C38 H74 O4 S, tgt=92.70, overall=92.70]	(661.5033, 154.19844)(662.5115, 79.01)(663.50507, 78.2411	C38 H74 O4 S	FindByFormula	27 -	626.5299	22.744894
C38 H75 N S2	C38 H75 N S2	[C38 H75 N S2, tgt=77.08, overall=77.08]	(654.53345, 86.40333)(655.53265, 47.543335)(656.5185, 54.	C38 H75 N S2	FindByFormula	25 -	609.536	24.487717
C38 H76 O4 S	C38 H76 O4 S	[C38 H76 O4 S, tgt=97.41, overall=97.41]	(663.5184, 70.341995)(664.5322, 39.405)(673.5457, 75.6406	C38 H76 O4 S	FindByFormula	28 -	628.5459	22.929579
C38 H77 N S2	C38 H77 N S2	[C38 H77 N S2, tgt=90.45, overall=90.45]	(646.5261, 84.36)(647.5243, 20.07)(610.54254, 3374.1982)(	C38 H77 N S2	FindByFormula	26 -	611.55	24.950762
C38 H78 N2 P2 S3	C38 H78 N2 P2 S3	[C38 H78 N2 P2 S3, tgt=92.21, overall=92.21]	(755.4536, 321.655)(756.4605, 130.11)(765.47626, 158.8425	C38 H78 N2 P2 S3	FindByFormula	28 -	720.4809	23.181684
C38 H78 N3 O P5	C38 H78 N3 O P5	[C38 H78 N3 O P5, tgt=61.38, overall=61.38]	(782.45624, 183.83)(783.46387, 138.2825)(792.474, 293.945	C38 H78 N3 O P5	FindByFormula	27 -	747.4814	22.866405
C39 H33 N9	C39 H33 N9	[C39 H33 N9, tgt=39.52, overall=39.52]	(662.2677, 266.7794)(663.2625, 131.575)(664.2614, 137.878	C39 H33 N9	FindByFormula	18 -	627.2863	22.246395
C39 H40 N9 O4 P	C39 H40 N9 O4 P	[C39 H40 N9 O4 P, tgt=93.33, overall=93.33]	(774.2972, 72.158005)(775.2983, 38.5925)(728.28735, 1577.	C39 H40 N9 O4 P	FindByFormula	24 -	729.2944	13.102704
C39 H58 N4 O	C39 H58 N4 O	[C39 H58 N4 O, tgt=60.92, overall=60.92]	(633.4263, 136.64667)(634.4377, 61.563335)(635.3997, 179.	C39 H58 N4 O	FindByFormula	14 -	598.4612	22.928951
C39 H60 N P3	C39 H60 N P3	[C39 H60 N P3, tgt=61.81, overall=61.81]	(670.3647, 124.255005)(671.37335, 94.636665)(672.381, 16	C39 H60 N P3	FindByFormula	22 -	635.3974	22.682573
C39 H61 N7 O2 S	C39 H61 N7 O2 S	[C39 H61 N7 O2 S, tgt=90.47, overall=90.47]	(726.4326, 225.14705)(727.42847, 175.38498)(728.44653, 1	C39 H61 N7 O2 S	FindByFormula	26 -	691.4606	22.937756
C39 H62 N2 O3 P2	C39 H62 N2 O3 P2	[C39 H62 N2 O3 P2, tgt=86.19, overall=86.19]	(703.39594, 225.69391)(704.4023, 148.00166)(705.4259, 12	C39 H62 N2 O3 P2	FindByFormula	26 -	668.4219	22.719269
C39 H62 N2 O5 S	C39 H62 N2 O5 S	[C39 H62 N2 O5 S, tgt=97.86, overall=97.86]	(705.4098, 152.452)(706.42004, 506.252)(707.4104, 350.675	C39 H62 N2 O5 S	FindByFormula	28 -	670.4375	22.84726
C39 H63 N4 P S	C39 H63 N4 P S	[C39 H63 N4 P S, tgt=98.17, overall=98.17]	(685.41797, 185.03)(686.4162, 90.27)(687.416, 95.79)(695.4	C39 H63 N4 P S	FindByFormula	27 -	650.4494	22.734266
C39 H65 N7 O2 S	C39 H65 N7 O2 S	[C39 H65 N7 O2 S, tgt=92.68, overall=92.68]	(730.4538, 105.66901)(731.4412, 76.45167)(732.43933, 64.1	C39 H65 N7 O2 S	FindByFormula	28 -	695.4929	23.18133
C39 H67 N2 O P5	C39 H67 N2 O P5	[C39 H67 N2 O P5, tgt=59.73, overall=59.73]	(769.3644, 151.04347)(770.3639, 120.05798)(771.36536, 29	C39 H67 N2 O P5	FindByFormula	25 -	734.3993	22.650967
C39 H72 Cl O2 P S	C39 H72 Cl O2 P S	[C39 H72 Cl O2 P S, tgt=79.31, overall=79.31]	(705.45135, 101.278)(706.44763, 45.005)(707.454, 92.81)(7	C39 H72 Cl O2 P S	FindByFormula	28 -	670.4685	23.177473
C39 H72 O3 S2	C39 H72 O3 S2	[C39 H72 O3 S2, tgt=91.97, overall=91.97]	(697.4843, 50.61)(651.48456, 3754.5562)(652.4881, 1648.86	C39 H72 O3 S2	FindByFormula	28 -	652.4923	19.786917
C39 H81 N2 O3 P S2	C39 H81 N2 O3 P S2	[C39 H81 N2 O3 P S2, tgt=71.96, overall=71.96]	(755.50305, 65.035)(765.5485, 72.93)(766.5679, 23.6)(719.5	C39 H81 N2 O3 P S2	FindByFormula	24 -	720.5424	23.697378
C39 H84 N9 P	C39 H84 N9 P	[C39 H84 N9 P, tgt=94.10, overall=94.10]	(744.6256, 423.6535)(745.6255, 315.59)(746.62634, 245.471	C39 H84 N9 P	FindByFormula	21 -	709.6578	26.700663
C4 H11 O3 P	C4 H11 O3 P	[C4 H11 O3 P, tgt=96.53, overall=96.53]	(137.03757, 57998.082)(138.04092, 4550.784)(139.04172, 3	C4 H11 O3 P	FindByFormula	28 -	138.045	5.330579
C4 H13 N2 O13 P3 S3	C4 H13 N2 O13 P3 S3	[C4 H13 N2 O13 P3 S3, tgt=95.15, overall=95.15]	(520.84155, 262.32748)(521.8443, 169.95)(522.8375, 374.22	C4 H13 N2 O13 P3 S3	FindByFormula	25 -	485.8785	0.5940001
C4 H13 N4 P S	C4 H13 N4 P S	[C4 H13 N4 P S, tgt=92.24, overall=92.24]	(215.02875, 741386.8)(216.0323, 51111.27)(217.02715, 252	C4 H13 N4 P S	FindByFormula	6 -	180.0609	0.66616625
C4 H14 O2 P2 S4	C4 H14 O2 P2 S4	[C4 H14 O2 P2 S4, tgt=93.30, overall=93.30]	(318.90607, 4862.84)(319.90805, 363.78143)(320.90106, 26	C4 H14 O2 P2 S4	FindByFormula	7 -	283.9358	18.922422
C4 H15 N3 P2 S2	C4 H15 N3 P2 S2	[C4 H15 N3 P2 S2, tgt=73.72, overall=73.72]	(265.9909, 74.43)(276.00977, 52.84)(230.01224, 14707.197)(	C4 H15 N3 P2 S2	FindByFormula	19 -	231.0202	2.529944
C4 H4 N3 P	C4 H4 N3 P	[C4 H4 N3 P, tgt=88.54, overall=88.54]	(159.98302, 495.97998)(160.9824, 98.81333)(124.00704, 97	C4 H4 N3 P	FindByFormula	26 -	125.0142	0.63615406
C4 H5 N O4 S	C4 H5 N O4 S	[C4 H5 N O4 S, tgt=87.49, overall=87.49]	(161.98703, 8613.469)(162.99171, 1072.27)(163.98529, 497.	C4 H5 N O4 S	FindByFormula	9 -	162.9945	1.6585549
C4 H5 N2 P S2	C4 H5 N2 P S2	[C4 H5 N2 P S2, tgt=83.84, overall=83.84]	(174.95615, 25837.33)(175.96098, 959.8946)(176.95946, 48	C4 H5 N2 P S2	FindByFormula	28 -	175.9637	0.54625005
C4 H6 N6 O3	C4 H6 N6 O3	[C4 H6 N6 O3, tgt=77.10, overall=77.10]	(221.02036, 61.935)(231.0508, 65.15)(185.0433, 3328.9136)(	C4 H6 N6 O3	FindByFormula	26 -	186.0505	3.5428784
C4 H6 O4	C4 H6 O4	[C4 H6 O4, tgt=96.47, overall=96.47]	(163.02557, 94.22667)(117.01954, 17936.416)(118.02494, 9	C4 H6 O4	FindByFormula	25 -	118.0269	1.32736
C4 H6 O5 P2 S	C4 H6 O5 P2 S	[C4 H6 O5 P2 S, tgt=79.30, overall=79.30]	(262.912, 858.7367)(263.90646, 555.9)(264.91156, 1009.12)(	C4 H6 O5 P2 S	FindByFormula	28 -	227.9412	5.3283997
C4 H7 N O4	C4 H7 N O4	[C4 H7 N O4, tgt=85.78, overall=85.78]	(178.03542, 191.06003)(132.02979, 10484.143)(133.02989,	C4 H7 N O4	FindByFormula	20 -	133.0367	0.64190036

C4 H8 O7	C4 H8 O7	[C4 H8 O7, tgt=56.64, overall=56.64]		(213.02426, 130.624)(167.02022, 40738.36)(168.02606, 300	C4 H8 O7		FindByFormula	27 -	168.0281	0.81274086
C4 H9 Cl N2 O	C4 H9 Cl N2 O	[C4 H9 Cl N2 O, tgt=85.14, overall=85.14]		(171.00826, 907.2261)(172.01091, 45.11111)(173.00836, 69	C4 H9 Cl N2 O		FindByFormula	11 -	136.0405	1.0928187
C4 H9 N2 O4 P3 S2	C4 H9 N2 O4 P3 S2	[C4 H9 N2 O4 P3 S2, tgt=65.22, overall=65.22]		(350.91626, 53.120003)(304.91193, 17749.098)(305.9123, 1	C4 H9 N2 O4 P3 S2		FindByFormula	27 -	305.9221	0.54311115
C40 H46 O2	C40 H46 O2	[C40 H46 O2, tgt=43.86, overall=43.86]		(593.32574, 238.48929)(594.33356, 133.685)(603.3464, 77.5	C40 H46 O2		FindByFormula	15 -	558.3453	22.462828
C40 H50 N3 O2 P3	C40 H50 N3 O2 P3	[C40 H50 N3 O2 P3, tgt=59.75, overall=59.75]		(732.27277, 270.83188)(733.2762, 180.78453)(734.27234, 1	C40 H50 N3 O2 P3		FindByFormula	19 -	697.3058	22.471838
C40 H53 N3 O P4	C40 H53 N3 O P4	[C40 H53 N3 O P4, tgt=89.41, overall=89.41]		(750.2947, 245.14667)(751.2712, 127.62)(760.31573, 58.024	C40 H53 N3 O P4		FindByFormula	26 -	715.3162	13.0992985
C40 H60 O12	C40 H60 O12	[C40 H60 O12, tgt=78.62, overall=78.62]		(767.37463, 126.70211)(768.3732, 67.15401)(769.3594, 79.7	C40 H60 O12		FindByFormula	28 -	732.4126	22.847012
C40 H67 O4 P S	C40 H67 O4 P S	[C40 H67 O4 P S, tgt=99.09, overall=99.09]		(709.42883, 218.305)(710.4195, 540.975)(719.4356, 1370.17	C40 H67 O4 P S		FindByFormula	26 -	674.4482	22.72032
C40 H68 N3 O P S2	C40 H68 N3 O P S2	[C40 H68 N3 O P S2, tgt=95.75, overall=95.75]		(736.43854, 69.86)(737.4518, 271.13)(738.4426, 156.62)(74	C40 H68 N3 O P S2		FindByFormula	21 -	701.4548	23.382563
C40 H69 Cl N2	C40 H69 Cl N2	[C40 H69 Cl N2, tgt=89.59, overall=89.59]		(647.483, 141.69556)(648.4837, 80.856)(649.4946, 174.2999	C40 H69 Cl N2		FindByFormula	24 -	612.5152	22.728958
C40 H70 N3 O P S2	C40 H70 N3 O P S2	[C40 H70 N3 O P S2, tgt=90.30, overall=90.30]		(748.47876, 51.72667)(749.507, 24.34)(702.4625, 2100.8281	C40 H70 N3 O P S2		FindByFormula	20 -	703.4698	23.790009
C40 H73 N3 O6 S	C40 H73 N3 O6 S	[C40 H73 N3 O6 S, tgt=92.54, overall=92.54]		(758.503, 71.89)(759.50275, 42.46)(760.5061, 37.443333)(7	C40 H73 N3 O6 S		FindByFormula	27 -	723.5214	24.529976
C40 H75 N3 O6 S	C40 H75 N3 O6 S	[C40 H75 N3 O6 S, tgt=58.68, overall=58.68]		(760.5247, 227.45625)(761.5279, 103.68125)(762.5203, 103.	C40 H75 N3 O6 S		FindByFormula	25 -	725.5338	24.755344
C40 H76 N2 O S3	C40 H76 N2 O S3	[C40 H76 N2 O S3, tgt=90.55, overall=90.55]		(741.5143, 55.88)(742.5248, 358.9)(695.5047, 1525.0304)(6	C40 H76 N2 O S3		FindByFormula	24 -	696.5119	25.81109
C40 H81 N O S2	C40 H81 N O S2	[C40 H81 N O S2, tgt=93.69, overall=93.69]		(700.58905, 74.835)(701.60834, 37.146664)(654.5684, 1971.	C40 H81 N O S2		FindByFormula	22 -	655.5754	24.529213
C40 H81 N2 O8 P	C40 H81 N2 O8 P	[C40 H81 N2 O8 P, tgt=99.05, overall=99.05]		(783.5261, 78.56)(793.57477, 61.59)(794.576, 37.79)(747.56	C40 H81 N2 O8 P		FindByFormula	27 -	748.5734	24.132805
C41 H35 N9	C41 H35 N9	[C41 H35 N9, tgt=85.02, overall=85.02]		(688.26666, 125.70142)(689.26855, 91.715)(690.26965, 88.6	C41 H35 N9		FindByFormula	9 -	653.3007	22.398434
C41 H49 N5	C41 H49 N5	[C41 H49 N5, tgt=88.53, overall=88.53]		(646.3772, 139.835)(647.3771, 100.45)(648.3672, 70.81)(65	C41 H49 N5		FindByFormula	25 -	611.4001	22.851501
C41 H54 O6 P2 S	C41 H54 O6 P2 S	[C41 H54 O6 P2 S, tgt=97.04, overall=97.04]		(771.2851, 68.92286)(772.2769, 36.923332)(773.3111, 49.14	C41 H54 O6 P2 S		FindByFormula	28 -	736.3119	13.098481
C41 H62 N4	C41 H62 N4	[C41 H62 N4, tgt=40.62, overall=40.62]		(645.4767, 93.2943)(646.4806, 47.168)(647.479, 99.51667)(	C41 H62 N4		FindByFormula	17 -	610.4933	22.60766
C41 H79 N3 O2 S3	C41 H79 N3 O2 S3	[C41 H79 N3 O2 S3, tgt=64.69, overall=64.69]		(786.54114, 124.272934)(787.537, 102.142006)(788.5488, 1	C41 H79 N3 O2 S3		FindByFormula	24 -	741.5314	24.51594
C41 H81 N3 O2 S3	C41 H81 N3 O2 S3	[C41 H81 N3 O2 S3, tgt=92.51, overall=92.51]		(778.5176, 53.864998)(779.5202, 61.11)(788.54895, 103.196	C41 H81 N3 O2 S3		FindByFormula	27 -	743.5482	24.929874
C41 H85 N2 O P3 S	C41 H85 N2 O P3 S	[C41 H85 N2 O P3 S, tgt=88.64, overall=88.64]		(781.5268, 95.17799)(782.52734, 60.909996)(783.52014, 44.	C41 H85 N2 O P3 S		FindByFormula	25 -	746.5589	23.819336
C41 H86 O2 P4	C41 H86 O2 P4	[C41 H86 O2 P4, tgt=86.74, overall=86.74]		(769.5151, 66.98)(770.506, 54.01)(771.5226, 117.32)(779.55	C41 H86 O2 P4		FindByFormula	25 -	734.5564	23.910227
C42 H42 N3 P S	C42 H42 N3 P S	[C42 H42 N3 P S, tgt=57.60, overall=57.60]		(686.26025, 93.4425)(687.2479, 51.197998)(688.2464, 114.1	C42 H42 N3 P S		FindByFormula	20 -	651.2843	22.11527
C42 H45 O P S	C42 H45 O P S	[C42 H45 O P S, tgt=97.78, overall=97.78]		(663.2471, 121.12154)(664.2443, 54.65)(665.2411, 54.71555	C42 H45 O P S		FindByFormula	28 -	628.292	18.833344
C42 H64 N4	C42 H64 N4	[C42 H64 N4, tgt=19.47, overall=19.47]		(659.4829, 128.56334)(660.49756, 223.53)(661.5002, 44.77)	C42 H64 N4		FindByFormula	12 -	624.5114	22.567398
C42 H65 N2 P S2	C42 H65 N2 P S2	[C42 H65 N2 P S2, tgt=94.68, overall=94.68]		(727.389, 74.36)(728.3701, 62.47)(729.3654, 82.91)(691.425	C42 H65 N2 P S2		FindByFormula	27 -	692.4331	25.629759
C42 H67 N2 P S2	C42 H67 N2 P S2	[C42 H67 N2 P S2, tgt=93.29, overall=93.29]		(693.441, 3535.7402)(694.44446, 1922.1719)(695.44495, 69	C42 H67 N2 P S2		FindByFormula	27 -	694.4482	26.344532
C42 H67 O4 P S	C42 H67 O4 P S	[C42 H67 O4 P S, tgt=97.75, overall=97.75]		(733.4229, 400.56638)(734.4241, 675.85876)(743.43835, 10	C42 H67 O4 P S		FindByFormula	27 -	698.4476	22.709871
C42 H70 O3 P2 S	C42 H70 O3 P2 S	[C42 H70 O3 P2 S, tgt=79.54, overall=79.54]		(751.423, 734.77893)(752.4248, 667.356)(753.4181, 542.712	C42 H70 O3 P2 S		FindByFormula	25 -	716.4511	22.924053
C42 H70 O3 S3	C42 H70 O3 S3	[C42 H70 O3 S3, tgt=81.07, overall=81.07]		(717.4403, 2204.45)(718.444, 1256.0781)(719.4399, 522.699	C42 H70 O3 S3		FindByFormula	28 -	718.448	25.861515
C42 H72 N3 O P S2	C42 H72 N3 O P S2	[C42 H72 N3 O P S2, tgt=92.70, overall=92.70]		(774.50433, 104.53)(775.50165, 71.85333)(776.4815, 27.45)	C42 H72 N3 O P S2		FindByFormula	20 -	729.4854	23.739487
C42 H72 N3 P S2	C42 H72 N3 P S2	[C42 H72 N3 P S2, tgt=87.10, overall=87.10]		(758.5071, 101.254)(759.525, 78.44)(712.4839, 1296.3408)(	C42 H72 N3 P S2		FindByFormula	20 -	713.4926	23.998533
C42 H73 N3 O6 S	C42 H73 N3 O6 S	[C42 H73 N3 O6 S, tgt=87.60, overall=87.60]		(782.4986, 382.78595)(783.50214, 226.02777)(784.50256, 1	C42 H73 N3 O6 S		FindByFormula	23 -	747.5228	24.490894
C42 H79 N5 O	C42 H79 N5 O	[C42 H79 N5 O, tgt=86.42, overall=86.42]		(704.59656, 180.57555)(705.59607, 98.285)(706.5931, 103.4	C42 H79 N5 O		FindByFormula	20 -	669.6266	26.24183
C42 H83 N O5	C42 H83 N O5	[C42 H83 N O5, tgt=98.30, overall=98.30]		(716.5965, 542.17053)(717.5996, 366.83664)(718.5978, 286.	C42 H83 N O5		FindByFormula	20 -	681.6275	25.594742
C42 H85 N O S2	C42 H85 N O S2	[C42 H85 N O S2, tgt=94.62, overall=94.62]		(728.61646, 83.333336)(682.5997, 1483.427)(683.6027, 716.	C42 H85 N O S2		FindByFormula	20 -	683.6076	25.251926
C42 H85 N S2	C42 H85 N S2	[C42 H85 N S2, tgt=93.11, overall=93.11]		(702.5791, 454.8925)(703.5807, 242.80736)(704.58026, 215.	C42 H85 N S2		FindByFormula	24 -	667.6118	25.20257
C43 H58 S2	C43 H58 S2	[C43 H58 S2, tgt=81.91, overall=81.91]		(673.3663, 206.52)(674.3663, 86.486664)(675.35333, 194.93	C43 H58 S2		FindByFormula	26 -	638.4003	22.693733
C43 H62 N2 O5 S	C43 H62 N2 O5 S	[C43 H62 N2 O5 S, tgt=94.24, overall=94.24]		(753.4018, 285.538)(754.3967, 205.41)(755.394, 599.06)(76	C43 H62 N2 O5 S		FindByFormula	26 -	718.4372	22.72304
C43 H65 N2 O2 P S2	C43 H65 N2 O2 P S2	[C43 H65 N2 O2 P S2, tgt=91.27, overall=91.27]		(771.39124, 224.39311)(772.3932, 156.03145)(773.401, 138.	C43 H65 N2 O2 P S2		FindByFormula	27 -	736.4185	22.720503
C43 H67 O6 P S	C43 H67 O6 P S	[C43 H67 O6 P S, tgt=88.26, overall=88.26]		(777.4012, 230.25002)(778.3956, 221.102)(787.42554, 1002.	C43 H67 O6 P S		FindByFormula	26 -	742.438	22.715506
C43 H70 N2 O5 S	C43 H70 N2 O5 S	[C43 H70 N2 O5 S, tgt=94.76, overall=94.76]		(761.4719, 165.7675)(762.4717, 490.34335)(763.4666, 181.0	C43 H70 N2 O5 S		FindByFormula	28 -	726.4994	23.18222
C43 H76 N O7 P	C43 H76 N O7 P	[C43 H76 N O7 P, tgt=86.73, overall=86.73]		(784.5124, 347.6971)(785.51575, 285.02426)(786.51, 23.33)	C43 H76 N O7 P		FindByFormula	27 -	749.537	24.681934
C43 H85 N O6	C43 H85 N O6	[C43 H85 N O6, tgt=96.69, overall=96.69]		(746.6231, 77.022)(747.6204, 32.42)(756.65393, 57.629997)	C43 H85 N O6		FindByFormula	20 -	711.6384	26.245829
C43 H89 N S2	C43 H89 N S2	[C43 H89 N S2, tgt=91.53, overall=91.53]		(718.61115, 256.847)(719.60657, 184.0847)(720.604, 184.29	C43 H89 N S2		FindByFormula	20 -	683.6424	26.81455
C44 H69 N2 P S2	C44 H69 N2 P S2	[C44 H69 N2 P S2, tgt=91.86, overall=91.86]		(719.45593, 3280.7993)(720.45905, 1851.3218)(721.46027,	C44 H69 N2 P S2		FindByFormula	26 -	720.4637	26.728788
C44 H81 N S	C44 H81 N S	[C44 H81 N S, tgt=92.91, overall=92.91]		(690.5826, 168.62003)(691.5782, 78.1311)(692.57556, 88.06	C44 H81 N S		FindByFormula	20 -	655.6106	25.74438
C44 H82 N O3 P S2	C44 H82 N O3 P S2	[C44 H82 N O3 P S2, tgt=62.69, overall=62.69]		(802.5319, 70.4)(803.542, 98.865005)(804.5054, 76.65)(812.	C44 H82 N O3 P S2		FindByFormula	27 -	767.5469	24.890793
C44 H89 N S2	C44 H89 N S2	[C44 H89 N S2, tgt=88.02, overall=88.02]		(694.6359, 1672.2787)(695.63916, 836.9734)(696.63983, 24	C44 H89 N S2		FindByFormula	27 -	695.6438	28.702568
C45 H49 N5	C45 H49 N5	[C45 H49 N5, tgt=86.88, overall=86.88]		(694.3746, 142.35)(704.4031, 151.50616)(705.4281, 201.762	C45 H49 N5		FindByFormula	24 -	659.399	22.709291
C46 H52 N8	C46 H52 N8	[C46 H52 N8, tgt=72.62, overall=72.62]		(715.42444, 820.2001)(716.42365, 557.04)(717.42487, 210.8	C46 H52 N8		FindByFormula	28 -	716.4299	25.243956
C46 H56 N4 O2	C46 H56 N4 O2	[C46 H56 N4 O2, tgt=61.50, overall=61.50]		(731.4019, 1511.3699)(732.40765, 752.2093)(733.4176, 585.	C46 H56 N4 O2		FindByFormula	28 -	696.4343	22.731491
C46 H93 N O S2	C46 H93 N O S2	[C46 H93 N O S2, tgt=89.50, overall=89.50]		(774.657, 71.81)(775.6489, 33.23)(784.68915, 70.744995)(7	C46 H93 N O S2		FindByFormula	20 -	739.6705	27.626709
C47 H59 N5 O	C47 H59 N5 O	[C47 H59 N5 O, tgt=86.01, overall=86.01]		(744.45264, 226.03499)(745.45166, 198.112)(746.4646, 145.	C47 H59 N5 O		FindByFormula	24 -	709.4725	23.159708
C5 H11 N O3 S2	C5 H11 N O3 S2	[C5 H11 N O3 S2, tgt=97.37, overall=97.37]		(242.01323, 808.2866)(243.01364, 121.705)(244.005, 68.62)	C5 H11 N O3 S2		FindByFormula	8 -	197.018	4.8680882
C5 H12 N2 O2	C5 H12 N2 O2	[C5 H12 N2 O2, tgt=93.41, overall=93.41]		(177.08835, 174.14252)(178.0947, 40.6)(131.08177, 32910.3	C5 H12 N2 O2		FindByFormula	16 -	132.0886	0.6538127
C5 H4 N4 O3	C5 H4 N4 O3	[C5 H4 N4 O3, tgt=98.05, overall=98.05]		(213.025, 85.024994)(167.02092, 82793.82)(168.02477, 571	C5 H4 N4 O3		FindByFormula	27 -	168.0282	1.030741
C5 H4 O3	C5 H4 O3	[C5 H4 O3, tgt=96.98, overall=96.98]		(146.98297, 2228.8923)(147.98535, 64.96)(148.98167, 635.2	C5 H4 O3		FindByFormula	9 -	112.0158	0.9878886
C5 H5 Cl N2 S	C5 H5 Cl N2 S	[C5 H5 Cl N2 S, tgt=71.44, overall=71.44]		(158.97867, 23679.83)(159.98003, 3852.1309)(160.97647, 3	C5 H5 Cl N2 S		FindByFormula	28 -	159.9859	0.5532858
C5 H5 N5	C5 H5 N5	[C5 H5 N5, tgt=89.95, overall=89.95]		(134.0469, 9229.118)(135.04773, 719.2504)(136.04663, 39.6	C5 H5 N5		FindByFormula	26 -	135.0542	3.8755674
C5 H7 N O3	C5 H7 N O3	[C5 H7 N O3, tgt=70.13, overall=70.13]		(164.0133, 362.16287)(165.01689, 56.999996)(174.03943, 7	C5 H7 N O3		FindByFormula	21 -	129.0429	1.1939529
C5 H9 N O4	C5 H9 N O4	[C5 H9 N O4, tgt=89.83, overall=89.83]		(182.0279, 83.04)(192.04947, 266.42715)(146.04552, 49687.	C5 H9 N O4		FindByFormula	21 -	147.0528	0.65919065
C5 H9 N2 O8 P3	C5 H9 N2 O8 P3	[C5 H9 N2 O8 P3, tgt=96.30, overall=96.30]		(316.94858, 55716.27)(317.952, 3545.0542)(318.95306, 134	C5 H9 N2 O8 P3		FindByFormula	28 -	317.956	0.5854287
C6 H10 Cl3 O4 P	C6 H10 Cl3 O4 P	[C6 H10 Cl3 O4 P, tgt=98.92, overall=98.92]		(318.1103, 19959.826)(319.1132, 1488.4039)(320.1031, 203	C6 H10 Cl3 O4 P		FindByFormula	5 -	281.941	19.30634
C6 H10 N6 O4	C6 H10 N6 O4	[C6 H10 N6 O4, tgt=97.24, overall=97.24]		(265.04623, 181.42499)(266.04913, 40.465)(267.04993, 39.9	C6 H10 N6 O4		FindByFormula	13 -	230.0766	3.525762
C6 H10 N8 O4	C6 H10 N8 O4	[C6 H10 N8 O4, tgt=80.88, overall=80.88]		(293.0541, 1500.5132)(294.05405, 41.630627)(295.04813, 7	C6 H10 N8 O4		FindByFormula	26 -	258.0809	2.4614217
C6 H10 O3	C6 H10 O3	[C6 H10 O3, tgt=61.22, overall=61.22]		(165.03134, 276.605)(175.0611, 124.35223)(129.05592, 281	C6 H10 O3		FindByFormula	27 -	130.0632	5.058264
C6 H10 O4	C6 H10 O4	[C6 H10 O4, tgt=65.30, overall=65.30]		(181.0313, 54.49)(191.05539, 75.065)(145.05116, 12946.268	C6 H10 O4		FindByFormula	7 -	146.0576	1.9178551
C6 H13 Cl N6	C6 H13 Cl N6	[C6 H13 Cl N6, tgt=78.73, overall=78.73]		(239.05904, 684.1272)(240.05869, 97.58002)(241.05652, 37	C6 H13 Cl N6		FindByFormula	27 -	204.09	3.5994
C6 H13 Cl O6	C6 H13 Cl O6	[C6 H13 Cl O6, tgt=98.78, overall=98.78]		(251.01117, 92.57616)(252.00806, 41.205)(261.0395, 137.72	C6 H13 Cl O6		FindByFormula	23 -	216.0387	0.6597829
C6 H13 N3 O3	C6 H13 N3 O3	[C6 H13 N3 O3, tgt=89.20, overall=89.20]		(210.06372, 10107.05)(211.06761, 1082.3518)(212.06024, 3	C6 H13 N3 O3		FindByFormula	13 -	175.0944	0.6608465
C6 H6 N2 O2	C6 H6 N2 O2	[C6 H6 N2 O2, tgt=99.24, overall=99.24]		(173.01152, 1415.234)(174.0116, 51.90333)(175.00487, 39.0	C6 H6 N2 O2		FindByFormula	19 -	138.0429	0.90826344
C6 H9 N3 O2	C6 H9 N3 O2	[C6 H9 N3 O2, tgt=99.30, overall=99.30]		(190.03519, 156.896)(200.06807, 618.836)(201.06647, 162.0	C6 H9 N3 O2		FindByFormula	27 -	155.0697	0.63644457
C7 H13 N O3 S	C7 H13 N O3 S	[C7 H13 N O3 S, tgt=94.04, overall=94.04]		(226.0307, 64.12)(227.0327, 22.97)(228.0218, 26.66)(236.06	C7 H13 N O3 S		FindByFormula	27 -	191.0615	4.061396
C7 H13 N2 O16 P3 S2	C7 H13 N2 O16 P3 S2	[C7 H13 N2 O16 P3 S2, tgt=98.31, overall=98.31]		(572.856, 1197.6849)(573.85876, 479.08627)(574.8545, 738.	C7 H13 N2 O16 P3 S2		FindByFormula	28 -	537.8917	0.5874644
C7 H13 O P3	C7 H13 O P3	[C7 H13 O P3, tgt=59.91, overall=59.91]		(240.9856, 50.78)(251.0098, 70.06)(205.01248, 5636.488)(2	C7 H13 O P3		FindByFormula	13 -	206.0191	8.180555
C7 H17 N2 O P S4	C7 H17 N2 O P S4	[C7 H17 N2 O P S4, tgt=81.34, overall=81.34]		(338.97498, 59.53)(348.9958, 711.7037)(349.9945, 140.1333	C7 H17 N2 O P S4		FindByFormula	26 -	303.9967	5.3283944
C7 H17 N6 P S	C7 H17 N6 P S	[C7 H17 N6 P S, tgt=78.89, overall=78.89]		(283.06238, 221.51)(284.0616, 74.67)(285.0542, 551.68)(29	C7 H17 N6 P S		FindByFormula	23 -	248.0987	0.72039145
C7 H18 N2 O15 P4 S4	C7 H18 N2 O15 P4 S4	[C7 H18 N2 O15 P4 S4, tgt=97.69, overall=97.69]		(656.82666, 486.87857)(657.8205, 267.52832)(658.8218, 40	C7 H18 N2 O15 P4 S4		FindByFormula	28 -	621.8532	0.5815358
C7 H19 N2 P S2	C7 H19 N2 P S2	[C7 H19 N2 P S2, tgt=80.05, overall=80.05]		(261.0415, 4747.9272)(262.04398, 726.8999)(263.03775, 35	C7 H19 N2 P S2		FindByFormula	28 -	226.0717	3.601279
C7 H2 Cl N O3	C7 H2 Cl N O3	[C7 H2 Cl N O3, tgt=94.72, overall=94.72]		(217.9437, 55.9175)(227.9716, 573.06)(228.97742, 37.31666	C7 H2 Cl N O3		FindByFormula	26 -	182.9723	0.6458079
C7 H22 N6 O2 S2	C7 H22 N6 O2 S2	[C7 H22 N6 O2 S2, tgt=85.26, overall=85.26]		(331.1245, 55.123333)(285.1173, 9441.753)(286.11807, 199	C7 H22 N6 O2 S2		FindByFormula	12 -	286.1248	19.774061
C7 H6 O2	C7 H6 O2	[C7 H6 O2, tgt=81.65, overall=81.65]		(157.0092, 218.90059)(158.01791, 23.626)(159.01385, 74.53	C7 H6 O2		FindByFormula	20 -	122.0364	4.928725
C7 H6 O3	C7 H6 O3	[C7 H6 O3, tgt=99.78, overall=99.78]		(173.0009, 119.29399)(137.02461, 54988.855)(138.02737, 4	C7 H6 O3		FindByFormula	28 -	138.0319	4.94141
C7 H8 N2 O17 P2	C7 H8 N2 O17 P2	[C7 H8 N2 O17 P2, tgt=96.29, overall=96.29]		(488.89197, 670.74756)(489.89606, 416.76288)(490.88715,	C7 H8 N2 O17 P2		FindByFormula	25 -	453.9305	0.58340013
C7 H8 N4 O2	C7 H8 N4 O2	[C7 H8 N4 O2, tgt=97.53, overall=97.53]		(215.03334, 111.76333)(216.0359, 63.989998)(217.0266, 60.	C7 H8 N4 O2		FindByFormula	25 -	180.0647	4.410623
C7 H8 N4 O3	C7 H8 N4 O3	[C7 H8 N4 O3, tgt=83.11, overall=83.11]		(231.03157, 59.34834)(241.059, 79.361435)(195.05222, 332	C7 H8 N4 O3		FindByFormula	18 -	196.0592	4.033095
C7 H8 O4 S	C7 H8 O4 S	[C7 H8 O4 S, tgt=99.58, overall=99.58]		(222.98451, 397.09424)(223.98232, 61.056664)(224.98283,	C7 H8 O4 S		FindByFormula	28 -	188.0144	5.697034
C7 H9 N4 O6 P3 S2	C7 H9 N4 O6 P3 S2	[C7 H9 N4 O6 P3 S2, tgt=93.79, overall=93.79]		(436.87738, 1007.455)(437.87817, 155.40001)(438.87143, 6	C7 H9 N4 O6 P3 S2		FindByFormula	24 -	401.9158	0.5897502
C8 H10 N4 O3	C8 H10 N4 O3	[C8 H10 N4 O3, tgt=73.19, overall=73.19]		(245.04987, 261.38333)(246.0623, 21.34)(255.07803, 114.07	C8 H10 N4 O3		FindByFormula	10 -	210.0746	4.945266
C8 H11 O5 P	C8 H11 O5 P	[C8 H11 O5 P, tgt=92.88, overall=92.88]		(253.00488, 164.852)(263.02826, 219.015)(264.0326, 63.36)	C8 H11 O5 P		FindByFormula	11 -	218.034	0.6877273
C8 H12 N2 O4	C8 H12 N2 O4	[C8 H12 N2 O4, tgt=92.83, overall=92.83]		(235.051, 824.22107)(236.05415, 149.09645)(237.04279, 17	C8 H12 N2 O4		FindByFormula	28 -	200.0798	1.6390715
C8 H12 N2 O5	C8 H12 N2 O5	[C8 H12 N2 O5, tgt=89.06, overall=89.06]		(251.04433, 163.47636)(252.04395, 49.556667)(253.03452,	C8 H12 N2 O5		FindByFormula	24 -	216.0741	0.9824588
C8 H12 N6 O4	C8 H12 N6 O4	[C8 H12 N6 O4, tgt=96.71, overall=96.71]		(301.0874, 52.515)(255.08539, 17002.412)(256.08853, 1991.	C8 H12 N6 O4		FindByFormula	6 -	256.0928	8.538447
C8 H12 O18 P2 S3	C8 H12 O18 P2 S3	[C8 H12 O18 P2 S3, tgt=95.35, overall=95.35]		(588.83997, 448.11893)(589.83734, 179.47571)(590.83527,	C8 H12 O18 P2 S3		FindByFormula	28 -	553.8633	0.5862144
C8 H12 O3 S	C8 H12 O3 S	[C8 H12 O3 S, tgt=75.94, overall=75.94]		(223.0213, 145.78125)(233.05084, 149.60092)(234.0653, 47.	C8 H12 O3 S		FindByFormula	25 -	188.05	0.9866402
C8 H14 Cl N2 P	C8 H14 Cl N2 P	[C8 H14 Cl N2 P, tgt=64.96, overall=64.96]		(239.02681, 391.66003)(240.03232, 87.197)(241.02382, 298.	C8 H14 Cl N2 P		FindByFormula	22 -	204.0576	1.5109998
C8 H14 N6 O4	C8 H14 N6 O4	[C8 H14 N6 O4, tgt=41.03, overall=41.03]		(293.08, 224.00713)(294.08817, 58.735)(303.1067, 106.7575	C8 H14 N6 O4		FindByFormula	16 -	258.108	3.5483663
C8 H15 N O4	C8 H15 N O4	[C8 H15 N O4, tgt=97.21, overall=97.21]		(224.06805, 150.48)(225.06538, 36.239998)(226.06546, 64.4	C8 H15 N O4		FindByFormula	20 -	189.1	5.7608523
C8 H15 N3 P2 S	C8 H15 N3 P2 S	[C8 H15 N3 P2 S, tgt=73.45, overall=73.45]		(282.01782, 70.86666)(283.0268, 33.11)(292.0496, 52.35)(2	C8 H15 N3 P2 S		FindByFormula	24 -	247.0466	4.806685
C8 H18 O20 P4 S	C8 H18 O20 P4 S	[C8 H18 O20 P4 S, tgt=94.59, overall=94.59]		(624.86316, 214.448)(625.85846, 37.83)(626.8545, 70.5)(63	C8 H18 O20 P4 S		FindByFormula	22 -	589.906	0.58031845
C8 H19 N6 P3	C8 H19 N6 P3	[C8 H19 N6 P3, tgt=58.09, overall=58.09]		(327.0553, 368.0911)(328.05054, 121.27334)(329.04327, 80.	C8 H19 N6 P3		FindByFormula	13 -	292.0911	0.75030744
C8 H3 N2 O9 P S	C8 H3 N2 O9 P S	[C8 H3 N2 O9 P S, tgt=91.50, overall=91.50]		(368.8929, 96.35571)(369.90384, 29.04)(370.8841, 52.59)(3	C8 H3 N2 O9 P S		FindByFormula	22 -	333.9293	0.5905003
C8 H6 N2 O4	C8 H6 N2 O4	[C8 H6 N2 O4, tgt=63.45, overall=63.45]		(229.00008, 1103.6631)(230.00562, 97.15)(239.0339, 123.70	C8 H6 N2 O4		FindByFormula	14 -	194.0309	0.7405001
C8 H7 Cl2 N5 O4 P2	C8 H7 Cl2 N5 O4 P2	[C8 H7 Cl2 N5 O4 P2, tgt=91.86, overall=91.86]		(403.90488, 4636.34)(404.90887, 668.6855)(405.90216, 436	C8 H7 Cl2 N5 O4 P2		FindByFormula	22 -	368.9361	1.387728
C8 H7 N O4 S	C8 H7 N O4 S	[C8 H7 N O4 S, tgt=81.27, overall=81.27]		(247.9812, 204.86714)(248.97993, 29.159998)(249.9703, 15	C8 H7 N O4 S		FindByFormula	25 -	213.0099	3.6164322
C8 H7 O13 P3 S	C8 H7 O13 P3 S	[C8 H7 O13 P3 S, tgt=91.74, overall=91.74]		(480.87112, 124.94167)(434.87265, 32927.12)(435.8754, 31	C8 H7 O13 P3 S		FindByFormula	6 -	435.88	0.543333
C8 H8 O3	C8 H8 O3	[C8 H8 O3, tgt=99.88, overall=99.88]		(187.01476, 81.57)(188.01309, 22.935)(189.01834, 156.165)	C8 H8 O3		FindByFormula	28 -	152.0475	8.629852
C8 H9 N O4	C8 H9 N O4	[C8 H9 N O4, tgt=68.46, overall=68.46]		(218.02173, 154.525)(228.0527, 202.45624)(229.05411, 75.9	C8 H9 N O4		FindByFormula	14 -	183.0523	1.88707
C9 H10 O3	C9 H10 O3	[C9 H10 O3, tgt=89.31, overall=89.31]		(165.05553, 18940.076)(166.05518, 2263.2913)(167.05934,	C9 H10 O3		FindByFormula	8 -	166.0622	11.358495
C9 H10 O4	C9 H10 O4	[C9 H10 O4, tgt=84.44, overall=84.44]		(217.0259, 137.87091)(218.02611, 33.2)(219.0289, 45.67)(2	C9 H10 O4		FindByFormula	23 -	182.0576	3.7849457
C9 H10 S	C9 H10 S	[C9 H10 S, tgt=93.06, overall=93.06]		(185.0204, 706.0294)(186.02254, 114.607994)(187.02335, 7	C9 H10 S		FindByFormula	21 -	150.0509	0.7040476
C9 H11 N O2	C9 H11 N O2	[C9 H11 N O2, tgt=98.47, overall=98.47]		(200.04811, 164.99928)(201.04276, 58.54)(202.0326, 34.0)(	C9 H11 N O2		FindByFormula	20 -	165.0785	2.5164003
C9 H11 N O3	C9 H11 N O3	[C9 H11 N O3, tgt=99.77, overall=99.77]		(216.04279, 209.25684)(217.04167, 96.38285)(218.03633, 8	C9 H11 N O3		FindByFormula	26 -	181.0738	1.3450774
C9 H13 O12 P3 S2	C9 H13 O12 P3 S2	[C9 H13 O12 P3 S2, tgt=96.58, overall=96.58]		(504.8739, 2607.5088)(505.88043, 1011.06287)(506.87314,	C9 H13 O12 P3 S2		FindByFormula	28 -	469.9045	0.58750015
C9 H14 N2 O23 P4 S	C9 H14 N2 O23 P4 S	[C9 H14 N2 O23 P4 S, tgt=95.17, overall=95.17]		(708.82007, 546.00195)(709.82184, 233.68)(710.8225, 353.9	C9 H14 N2 O23 P4 S		FindByFormula	25 -	673.8658	0.58560014
C9 H14 N2 O5	C9 H14 N2 O5	[C9 H14 N2 O5, tgt=96.32, overall=96.32]		(265.05823, 100.385)(266.0574, 731.3)(275.0819, 108.85363	C9 H14 N2 O5		FindByFormula	16 -	230.0901	1.5468127
C9 H16 O3	C9 H16 O3	[C9 H16 O3, tgt=91.02, overall=91.02]		(207.0762, 50.31)(171.10228, 4160.9385)(172.10501, 409.86	C9 H16 O3		FindByFormula	26 -	172.1098	12.232596
C9 H16 O4	C9 H16 O4	[C9 H16 O4, tgt=99.80, overall=99.80]		(223.07108, 75.182495)(187.09763, 18373.35)(188.10103, 1	C9 H16 O4		FindByFormula	28 -	188.1051	10.220396
C9 H17 N O4	C9 H17 N O4	[C9 H17 N O4, tgt=97.41, overall=97.41]		(238.07996, 76.855)(248.11763, 85.504005)(202.1083, 4968.	C9 H17 N O4		FindByFormula	26 -	203.1158	8.252947
C9 H17 N O5	C9 H17 N O5	[C9 H17 N O5, tgt=95.15, overall=95.15]		(254.07887, 225.1752)(255.08037, 52.254993)(256.07092, 1	C9 H17 N O5		FindByFormula	27 -	219.1106	3.2593288
C9 H18 N P3	C9 H18 N P3	[C9 H18 N P3, tgt=93.21, overall=93.21]		(268.0317, 51.75)(278.05872, 595.87286)(279.05685, 180.58	C9 H18 N P3		FindByFormula	28 -	233.0658	2.5155702
C9 H19 N4 O4 P	C9 H19 N4 O4 P	[C9 H19 N4 O4 P, tgt=96.47, overall=96.47]		(313.085, 95.03876)(314.07935, 31.4525)(277.1064, 79313.9	C9 H19 N4 O4 P		FindByFormula	28 -	278.1137	13.097588
C9 H2 N2 O5 S	C9 H2 N2 O5 S	[C9 H2 N2 O5 S, tgt=88.86, overall=88.86]		(284.9318, 81.744995)(248.96085, 55984.355)(249.96422, 2	C9 H2 N2 O5 S		FindByFormula	28 -	249.9682	0.58628577
C9 H20 N8 P2 S	C9 H20 N8 P2 S	[C9 H20 N8 P2 S, tgt=89.84, overall=89.84]		(369.06818, 1492.811)(370.06778, 441.6832)(371.06042, 25	C9 H20 N8 P2 S		FindByFormula	26 -	334.1017	1.0453464
C9 H6 N2 O4	C9 H6 N2 O4	[C9 H6 N2 O4, tgt=97.57, overall=97.57]		(240.9995, 72.095)(251.02956, 86.838326)(205.02493, 2708	C9 H6 N2 O4		FindByFormula	28 -	206.0322	5.329006
C9 H7 N O	C9 H7 N O	[C9 H7 N O, tgt=92.76, overall=92.76]		(180.02312, 92.75085)(181.0336, 30.67)(182.0179, 29.76)(1	C9 H7 N O		FindByFormula	27 -	145.0526	7.624532
C9 H8 O13 P2	C9 H8 O13 P2	[C9 H8 O13 P2, tgt=97.56, overall=97.56]		(420.90393, 138.31667)(421.91376, 42.645)(422.9057, 23.25	C9 H8 O13 P2		FindByFormula	27 -	385.9426	0.5840002
C9 H9 N O3	C9 H9 N O3	[C9 H9 N O3, tgt=80.59, overall=80.59]		(214.0278, 1027.6864)(215.03165, 90.06364)(216.03088, 75.	C9 H9 N O3		FindByFormula	27 -	179.0575	4.8047934
CAPRYLIC ACID (CAS# 124-07-2); (M-H)-	CAPRYLIC ACID (CAS# 124-07-2); (M-H)-	CAPRYLIC ACID (CAS# 124-07-2); (M-H)- [, tgt=68.24, ove	124-07-2	(143.1083, 325.97)(144.1037, 20.45)	CAPRYLIC ACID (CAS# 124-07-2); (M-H)-	C06423	FindByFormula	1 -	144.1151	10.009617
CARNOSINE (CAS# 305-84-0); (M-H)-	CARNOSINE (CAS# 305-84-0); (M-H)-	CARNOSINE (CAS# 305-84-0); (M-H)- [, tgt=84.88, overall	305-84-0	(225.09802, 3508.1743)(226.099, 549.67444)(227.10141, 86.	CARNOSINE (CAS# 305-84-0); (M-H)-		FindByFormula	9 -	226.1057	0.63255596
CATECHOL (CAS# 120-80-9); (M-H)-	CATECHOL (CAS# 120-80-9); (M-H)-	CATECHOL (CAS# 120-80-9); (M-H)- [, tgt=55.54, overall=	120-80-9	(109.02986, 748.244)(110.02999, 38.477997)	CATECHOL (CAS# 120-80-9); (M-H)-		FindByFormula	5 -	110.0368	2.873396
CELLOBIOSE (CAS# 528-50-7); (M+Cl)-	CELLOBIOSE (CAS# 528-50-7); (M+Cl)-	CELLOBIOSE (CAS# 528-50-7); (M+Cl)- [, tgt=97.21, overa	528-50-7	(377.08475, 25323.936)(378.08945, 4187.432)(379.08237, 1	CELLOBIOSE (CAS# 528-50-7); (M+Cl)-	C06422	FindByFormula	24 -	342.116	0.7031669
CHOLATE (CAS# 81-25-4); (M-H)-	CHOLATE (CAS# 81-25-4); (M-H)-	CHOLATE (CAS# 81-25-4); (M-H)- [, tgt=69.96, overall=69	81-25-4	(407.27997, 3199.7307)(408.2817, 798.15356)(409.28134, 1	CHOLATE (CAS# 81-25-4); (M-H)-		FindByFormula	11 -	408.288	20.301538
CHOLESTEROL HYDROGEN SULFATE (CAS# 12	CHOLESTEROL HYDROGEN SULFATE (CAS# 12	CHOLESTEROL HYDROGEN SULFATE (CAS# 1256-86-6); (M	1256-86-6	(465.30725, 795.6625)(466.30615, 252.49501)(467.30145, 1	CHOLESTEROL HYDROGEN SULFATE (CAS# 1256-86-6); (M-H)-	C18043	FindByFormula	4 -	466.3158	23.800903
CHOLINE PHOSPHATE (CAS# 107-73-3); (M+H	CHOLINE PHOSPHATE (CAS# 107-73-3); (M+H	CHOLINE PHOSPHATE (CAS# 107-73-3); (M+HCOO)- [, tgt	107-73-3	(228.06453, 874.3587)(229.06444, 96.27874)(230.0591, 82.5	CHOLINE PHOSPHATE (CAS# 107-73-3); (M+HCOO)-	C00588	FindByFormula	8 -	183.0658	0.88287556
CIS-11-EICOSENOIC ACID (CAS# 5561-99-9); (	CIS-11-EICOSENOIC ACID (CAS# 5561-99-9); (	CIS-11-EICOSENOIC ACID (CAS# 5561-99-9); (M-H)- [, tgt	5561-99-9	(309.2803, 7625.6743)(310.28354, 1747.0411)(311.2894, 25	CIS-11-EICOSENOIC ACID (CAS# 5561-99-9); (M-H)-		FindByFormula	27 -	310.2877	23.253443
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (C	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (C	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-5	28874-58-0	(367.2408, 696.56)(368.2373, 94.22)(369.2479, 45.86)	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0); (M+Cl)-		FindByFormula	1 -	332.2711	22.917269
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (C	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (C	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-5	28874-58-0	(377.26907, 978.1873)(378.2709, 251.71388)(379.27502, 64	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0); (M+HCOO)-		FindByFormula	23 -	332.2706	23.252993
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (C	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (C	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-5	28874-58-0	(331.26492, 29855.125)(332.26843, 7284.844)(333.27078, 1	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0); (M-H)-		FindByFormula	27 -	332.2723	22.964758
CIS-ACONITATE (CAS# 585-84-2); (M-H)-	CIS-ACONITATE (CAS# 585-84-2); (M-H)-	CIS-ACONITATE (CAS# 585-84-2); (M-H)- [, tgt=51.44, ove	585-84-2	(173.00923, 12987.938)(174.0166, 976.2754)(175.0113, 21.7	CIS-ACONITATE (CAS# 585-84-2); (M-H)-		FindByFormula	11 -	174.0165	1.2276362
CIS-VACCENIC ACID (CAS# 506-17-2); (M-H)-	CIS-VACCENIC ACID (CAS# 506-17-2); (M-H)-	CIS-VACCENIC ACID (CAS# 506-17-2); (M-H)- [, tgt=92.65,	506-17-2	(281.24942, 474812.47)(282.25266, 93290.77)(283.25778, 1	CIS-VACCENIC ACID (CAS# 506-17-2); (M-H)-		FindByFormula	28 -	282.2568	22.9269
CIS-ZEATIN (CAS# 1637-39-4); (M+Cl)-	CIS-ZEATIN (CAS# 1637-39-4); (M+Cl)-	CIS-ZEATIN (CAS# 1637-39-4); (M+Cl)- [, tgt=89.32, overa	1637-39-4	(254.08186, 80646.96)(255.08424, 10402.217)(256.07898, 2	CIS-ZEATIN (CAS# 1637-39-4); (M+Cl)-	C00371	FindByFormula	28 -	219.1123	3.8765266
CIS-ZEATIN (CAS# 1637-39-4); (M-H)-	CIS-ZEATIN (CAS# 1637-39-4); (M-H)-	CIS-ZEATIN (CAS# 1637-39-4); (M-H)- [, tgt=89.22, overal	1637-39-4	(218.10513, 473471.16)(219.10771, 59817.344)(220.10983,	CIS-ZEATIN (CAS# 1637-39-4); (M-H)-	C00371	FindByFormula	28 -	219.1125	3.8769913
CITRAMALATE (CAS# 2306-22-1); (M-H)-	CITRAMALATE (CAS# 2306-22-1); (M-H)-	CITRAMALATE (CAS# 2306-22-1); (M-H)- [, tgt=96.91, ove	2306-22-1	(147.02931, 4090.854)(148.03178, 169.43999)(149.031, 97.3	CITRAMALATE (CAS# 2306-22-1); (M-H)-	C00815	FindByFormula	7 -	148.0365	1.4311427
CITRATE (CAS# 77-92-9); (M-H)-	CITRATE (CAS# 77-92-9); (M-H)-	CITRATE (CAS# 77-92-9); (M-H)- [, tgt=80.02, overall=80.	77-92-9	(191.02022, 62122.7)(192.02023, 4261.5835)(193.018, 1589.	CITRATE (CAS# 77-92-9); (M-H)-		FindByFormula	25 -	192.0272	0.97984004
CITRULLINE (CAS# 372-75-8); (M-H)-	CITRULLINE (CAS# 372-75-8); (M-H)-	CITRULLINE (CAS# 372-75-8); (M-H)- [, tgt=86.16, overall	372-75-8	(174.08754, 118458.37)(175.08887, 11428.832)(176.08873,	CITRULLINE (CAS# 372-75-8); (M-H)-		FindByFormula	15 -	175.0944	0.65966684
CMP (CAS# 63-37-6); (M-H)-	CMP (CAS# 63-37-6); (M-H)-	CMP (CAS# 63-37-6); (M-H)- [, tgt=44.97, overall=44.97]	63-37-6	(322.0459, 1783.2037)(323.04294, 336.4931)(324.0391, 122.	CMP (CAS# 63-37-6); (M-H)-	C00055	FindByFormula	16 -	323.0518	0.8752504
CORTICOSTERONE (CAS# 50-22-6); (M+HCO	CORTICOSTERONE (CAS# 50-22-6); (M+HCO	CORTICOSTERONE (CAS# 50-22-6); (M+HCOO)- [, tgt=57.	50-22-6	(391.2114, 677.9683)(392.2117, 187.82166)(393.20694, 79.1	CORTICOSTERONE (CAS# 50-22-6); (M+HCOO)-		FindByFormula	6 -	346.2121	15.369161
CORTISOL (CAS# 50-23-7); (M+Cl)-	CORTISOL (CAS# 50-23-7); (M+Cl)-	CORTISOL (CAS# 50-23-7); (M+Cl)- [, tgt=93.42, overall=9	50-23-7	(397.17877, 2608.881)(398.17905, 641.96454)(399.17752, 9	CORTISOL (CAS# 50-23-7); (M+Cl)-	C00735	FindByFormula	13 -	362.2103	13.767254
CORTISOL (CAS# 50-23-7); (M+HCOO)-	CORTISOL (CAS# 50-23-7); (M+HCOO)-	CORTISOL (CAS# 50-23-7); (M+HCOO)- [, tgt=69.35, over	50-23-7	(407.2077, 14819.3955)(408.2099, 3618.32)(409.2119, 1044.	CORTISOL (CAS# 50-23-7); (M+HCOO)-	C00735	FindByFormula	26 -	362.2102	13.762661
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+C	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+C	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+Cl)- [, tgt=58.	50-03-3	(439.1918, 518.37)(440.1941, 112.07)	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+Cl)-	C02821	FindByFormula	1 -	404.2222	15.802427
CORTISONE (CAS# 53-06-5); (M+Cl)-	CORTISONE (CAS# 53-06-5); (M+Cl)-	CORTISONE (CAS# 53-06-5); (M+Cl)- [, tgt=68.24, overall	53-06-5	(395.16455, 936.36896)(396.16464, 240.34372)(397.16302,	CORTISONE (CAS# 53-06-5); (M+Cl)-	C00762	FindByFormula	19 -	360.1947	13.349795
CORTISONE (CAS# 53-06-5); (M+HCOO)-	CORTISONE (CAS# 53-06-5); (M+HCOO)-	CORTISONE (CAS# 53-06-5); (M+HCOO)- [, tgt=77.82, ove	53-06-5	(405.193, 4162.886)(406.19604, 1085.1388)(407.19443, 302.	CORTISONE (CAS# 53-06-5); (M+HCOO)-	C00762	FindByFormula	27 -	360.1941	13.34283
CREATINE (CAS# 57-00-1); (M-H)-	CREATINE (CAS# 57-00-1); (M-H)-	CREATINE (CAS# 57-00-1); (M-H)- [, tgt=91.82, overall=9	57-00-1	(130.0611, 8661.3)(131.066, 538.51)(132.0636, 83.69)	CREATINE (CAS# 57-00-1); (M-H)-		FindByFormula	1 -	131.0685	0.68900037
CREATININE-(GUANIDINO-13C) [ISTD] (CAS#	CREATININE-(GUANIDINO-13C) [ISTD] (CAS#)	CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (M-H)- [, tgt=77.85, overall=77.85]		(113.0551, 554.19)(114.0507, 43.62)	CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (M-H)-		FindByFormula	1 -	114.0619	0.6570006
CYCLOHEPTANECARBOXYLIC ACID (CAS# 146	CYCLOHEPTANECARBOXYLIC ACID (CAS# 146	CYCLOHEPTANECARBOXYLIC ACID (CAS# 1460-16-8); (M	1460-16-8	(187.09763, 14757.177)(188.10095, 1535.3376)(189.10541,	CYCLOHEPTANECARBOXYLIC ACID (CAS# 1460-16-8); (M+HCOO)-	C12104	FindByFormula	28 -	142.0993	10.678747
CYSTATHIONINE (CAS# 56-88-2); (M-H)-	CYSTATHIONINE (CAS# 56-88-2); (M-H)-	CYSTATHIONINE (CAS# 56-88-2); (M-H)- [, tgt=45.37, ove	56-88-2	(221.05896, 943.9801)(222.06201, 175.78201)(223.06308, 6	CYSTATHIONINE (CAS# 56-88-2); (M-H)-		FindByFormula	5 -	222.0693	0.70959955
CYTIDINE (CAS# 65-46-3); (M+Cl)-	CYTIDINE (CAS# 65-46-3); (M+Cl)-	CYTIDINE (CAS# 65-46-3); (M+Cl)- [, tgt=51.68, overall=5	65-46-3	(278.05545, 1402.1525)(279.05658, 321.95)(280.0521, 714.3	CYTIDINE (CAS# 65-46-3); (M+Cl)-		FindByFormula	4 -	243.0859	0.71100044
CYTIDINE (CAS# 65-46-3); (M-H)-	CYTIDINE (CAS# 65-46-3); (M-H)-	CYTIDINE (CAS# 65-46-3); (M-H)- [, tgt=31.44, overall=31	65-46-3	(242.07854, 2604.858)(243.07915, 247.43198)(244.07455, 1	CYTIDINE (CAS# 65-46-3); (M-H)-		FindByFormula	5 -	243.0846	0.66379994
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+C	987-78-0	(523.0801, 913.2262)(524.07904, 238.98375)(525.07477, 39	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+Cl)-	C00307	FindByFormula	8 -	488.1073	0.69225025
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+H	987-78-0	(533.1057, 511.9)(534.1004, 89.79)(535.1186, 52.6)	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+HCOO)-	C00307	FindByFormula	3 -	488.108	0.8083342
D-(-)-ARABINOSE (CAS# 10323-20-3); (M+HC	D-(-)-ARABINOSE (CAS# 10323-20-3); (M+HC	D-(-)-ARABINOSE (CAS# 10323-20-3); (M+HCOO)- [, tgt=	10323-20-3	(195.05046, 4235.6133)(196.0577, 223.71333)(197.05534, 1	D-(-)-ARABINOSE (CAS# 10323-20-3); (M+HCOO)-		FindByFormula	3 -	150.0522	0.6620002
DECANOATE (CAS# 334-48-5); (M-H)-	DECANOATE (CAS# 334-48-5); (M-H)-	DECANOATE (CAS# 334-48-5); (M-H)- [, tgt=88.85, overal	334-48-5	(171.13895, 2105.2114)(172.14223, 245.14714)(173.1413, 3	DECANOATE (CAS# 334-48-5); (M-H)-	C01571	FindByFormula	28 -	172.1462	19.800201
DEHYDROASCORBATE (CAS# 490-83-5); (M+	DEHYDROASCORBATE (CAS# 490-83-5); (M+	DEHYDROASCORBATE (CAS# 490-83-5); (M+Cl)- [, tgt=53	490-83-5	(208.98485, 4353.1562)(209.98341, 215.80875)(210.98312,	DEHYDROASCORBATE (CAS# 490-83-5); (M+Cl)-		FindByFormula	8 -	174.0148	0.65975034
DEHYDROASCORBATE (CAS# 490-83-5); (M+	DEHYDROASCORBATE (CAS# 490-83-5); (M+	DEHYDROASCORBATE (CAS# 490-83-5); (M+HCOO)- [, tg	490-83-5	(219.01471, 1132.49)(220.02435, 312.75)(221.0128, 75.8549	DEHYDROASCORBATE (CAS# 490-83-5); (M+HCOO)-		FindByFormula	2 -	174.0169	0.85200083
DEHYDROASCORBATE (CAS# 490-83-5); (M-	DEHYDROASCORBATE (CAS# 490-83-5); (M-H	DEHYDROASCORBATE (CAS# 490-83-5); (M-H)- [, tgt=90.	490-83-5	(173.00903, 11349.945)(174.0114, 171.54411)(175.00842, 8	DEHYDROASCORBATE (CAS# 490-83-5); (M-H)-		FindByFormula	17 -	174.016	0.7424707
DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Cl)-	DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Cl)-	DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Cl)- [, tgt=47.70,	83-44-3	(427.26263, 431.14502)(428.2621, 73.305)(429.25735, 288.0	DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Cl)-	C04483	FindByFormula	2 -	392.2924	21.690178
DEOXYCHOLIC ACID (CAS# 83-44-3); (M-H)-	DEOXYCHOLIC ACID (CAS# 83-44-3); (M-H)-	DEOXYCHOLIC ACID (CAS# 83-44-3); (M-H)- [, tgt=67.55,	83-44-3	(391.28604, 10356.1875)(392.28882, 2849.5466)(393.28082,	DEOXYCHOLIC ACID (CAS# 83-44-3); (M-H)-	C04483	FindByFormula	9 -	392.2928	21.684036
DEOXYCYTIDINE (CAS# 951-77-9); (M+HCOO	DEOXYCYTIDINE (CAS# 951-77-9); (M+HCOO)	DEOXYCYTIDINE (CAS# 951-77-9); (M+HCOO)- [, tgt=67.4	951-77-9	(272.0891, 5747.797)(273.09036, 709.4412)(274.09952, 350.	DEOXYCYTIDINE (CAS# 951-77-9); (M+HCOO)-		FindByFormula	17 -	227.0899	0.8335297
DEOXYCYTIDINE (CAS# 951-77-9); (M-H)-	DEOXYCYTIDINE (CAS# 951-77-9); (M-H)-	DEOXYCYTIDINE (CAS# 951-77-9); (M-H)- [, tgt=38.14, ov	951-77-9	(226.08206, 2775.6892)(227.08853, 563.0446)(228.08571, 8	DEOXYCYTIDINE (CAS# 951-77-9); (M-H)-		FindByFormula	13 -	227.0899	0.7083077
DEOXYURIDINE (CAS# 951-78-0); (M+Cl)-	DEOXYURIDINE (CAS# 951-78-0); (M+Cl)-	DEOXYURIDINE (CAS# 951-78-0); (M+Cl)- [, tgt=85.51, ov	951-78-0	(263.04434, 1403.96)(264.0458, 181.64355)(265.04092, 480.	DEOXYURIDINE (CAS# 951-78-0); (M+Cl)-		FindByFormula	14 -	228.0752	1.6105716
DEOXYURIDINE (CAS# 951-78-0); (M+HCOO)-	DEOXYURIDINE (CAS# 951-78-0); (M+HCOO)-	DEOXYURIDINE (CAS# 951-78-0); (M+HCOO)- [, tgt=84.9	951-78-0	(273.07208, 1277.595)(274.07825, 121.62)(275.0721, 42.05)	DEOXYURIDINE (CAS# 951-78-0); (M+HCOO)-		FindByFormula	2 -	228.0735	1.6680017
DEOXYURIDINE (CAS# 951-78-0); (M-H)-	DEOXYURIDINE (CAS# 951-78-0); (M-H)-	DEOXYURIDINE (CAS# 951-78-0); (M-H)- [, tgt=67.14, ove	951-78-0	(227.06668, 804.13257)(228.06842, 150.72)	DEOXYURIDINE (CAS# 951-78-0); (M-H)-		FindByFormula	4 -	228.0736	1.6417515
D-GALACTOSAMINE (CAS# 7535-00-4); (M+C	D-GALACTOSAMINE (CAS# 7535-00-4); (M+Cl	D-GALACTOSAMINE (CAS# 7535-00-4); (M+Cl)- [, tgt=60.	7535-00-4	(214.04855, 3263.423)(215.05301, 289.68)(216.0594, 53.34)	D-GALACTOSAMINE (CAS# 7535-00-4); (M+Cl)-	C02262	FindByFormula	7 -	179.0792	0.64028597
D-GALACTOSAMINE (CAS# 7535-00-4); (M-H)	D-GALACTOSAMINE (CAS# 7535-00-4); (M-H)	D-GALACTOSAMINE (CAS# 7535-00-4); (M-H)-[-H2O] [, t	7535-00-4	(160.0605, 1846.315)(161.06435, 56.260002)(162.0548, 55.1	D-GALACTOSAMINE (CAS# 7535-00-4); (M-H)-[-H2O]	C02262	FindByFormula	2 -	179.078	0.7015003
D-GLUCOSAMINE (CAS# 3416-24-8); (M+Cl)-	D-GLUCOSAMINE (CAS# 3416-24-8); (M+Cl)-	D-GLUCOSAMINE (CAS# 3416-24-8); (M+Cl)- [, tgt=56.45,	3416-24-8	(214.04855, 3263.423)(215.05301, 289.68)(216.0594, 53.34)	D-GLUCOSAMINE (CAS# 3416-24-8); (M+Cl)-	C00329	FindByFormula	7 -	179.0792	0.64028597
D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (	D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (	D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (M-H)- [, tgt=	56-73-5	(259.0233, 3746.5427)(260.02527, 663.85583)(261.02234, 6	D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (M-H)-	C00092	FindByFormula	12 -	260.0289	0.7489169
DGMP (CAS# 902-04-5); (M-H)-	DGMP (CAS# 902-04-5); (M-H)-	DGMP (CAS# 902-04-5); (M-H)- [, tgt=38.17, overall=38.1	902-04-5	(346.05466, 1719.4668)(347.0613, 244.83667)(348.06012, 1	DGMP (CAS# 902-04-5); (M-H)-		FindByFormula	3 -	347.0636	1.3406681
DIACETYL (CAS# 431-03-8); (M+HCOO)-	DIACETYL (CAS# 431-03-8); (M+HCOO)-	DIACETYL (CAS# 431-03-8); (M+HCOO)- [, tgt=96.63, ove	431-03-8	(131.03494, 1460.3936)(132.03487, 83.628395)(133.03816,	DIACETYL (CAS# 431-03-8); (M+HCOO)-	C00741	FindByFormula	25 -	86.0363	2.0453193
DIETHYLSTILBESTROL (CAS# 56-53-1); (M-H)-	DIETHYLSTILBESTROL (CAS# 56-53-1); (M-H)-	DIETHYLSTILBESTROL (CAS# 56-53-1); (M-H)- [, tgt=37.06	56-53-1	(267.13983, 2567.2349)(268.14105, 278.4025)(269.1317, 19	DIETHYLSTILBESTROL (CAS# 56-53-1); (M-H)-		FindByFormula	4 -	268.146	18.666403
DIHYDROXYMANDELIC ACID (CAS# 775-01-9)	DIHYDROXYMANDELIC ACID (CAS# 775-01-9);	DIHYDROXYMANDELIC ACID (CAS# 775-01-9); (M-H)- [, t	775-01-9	(183.03108, 682.395)(184.03352, 54.204998)	DIHYDROXYMANDELIC ACID (CAS# 775-01-9); (M-H)-	C05580	FindByFormula	4 -	184.0385	0.8327507
D-LYXOSE (CAS# 1114-34-7); (M+Cl)-	D-LYXOSE (CAS# 1114-34-7); (M+Cl)-	D-LYXOSE (CAS# 1114-34-7); (M+Cl)- [, tgt=64.27, overall	1114-34-7	(185.02158, 4432.47)(186.02509, 415.6259)(187.0234, 145.6	D-LYXOSE (CAS# 1114-34-7); (M+Cl)-	C00476	FindByFormula	17 -	150.0525	0.70423555
D-LYXOSE (CAS# 1114-34-7); (M+HCOO)-	D-LYXOSE (CAS# 1114-34-7); (M+HCOO)-	D-LYXOSE (CAS# 1114-34-7); (M+HCOO)- [, tgt=86.53, ov	1114-34-7	(195.05046, 4235.6133)(196.0577, 223.71333)(197.05534, 1	D-LYXOSE (CAS# 1114-34-7); (M+HCOO)-	C00476	FindByFormula	3 -	150.0522	0.6620002
D-LYXOSE (CAS# 1114-34-7); (M-H)-	D-LYXOSE (CAS# 1114-34-7); (M-H)-	D-LYXOSE (CAS# 1114-34-7); (M-H)- [, tgt=82.38, overall=	1114-34-7	(149.04419, 4519.0996)(150.0481, 302.285)(151.0461, 303.9	D-LYXOSE (CAS# 1114-34-7); (M-H)-	C00476	FindByFormula	2 -	150.0514	0.68650043
D-MANNOSAMINE (CAS# 14307-02-9); (M-H)	D-MANNOSAMINE (CAS# 14307-02-9); (M-H)	D-MANNOSAMINE (CAS# 14307-02-9); (M-H)-[-H2O] [, t	14307-02-9	(160.0605, 1846.315)(161.06435, 56.260002)(162.0548, 55.1	D-MANNOSAMINE (CAS# 14307-02-9); (M-H)-[-H2O]	C03570	FindByFormula	2 -	179.078	0.7015003
DOCOSAHEXAENOIC ACID (CAS# 6217-54-5);	DOCOSAHEXAENOIC ACID (CAS# 6217-54-5);	DOCOSAHEXAENOIC ACID (CAS# 6217-54-5); (M-H)- [, t	6217-54-5	(327.23438, 102130.41)(328.23746, 24592.979)(329.24042,	DOCOSAHEXAENOIC ACID (CAS# 6217-54-5); (M-H)-		FindByFormula	26 -	328.2416	22.69186
D-ORNITHINE (CAS# 348-66-3); (M-H)-	D-ORNITHINE (CAS# 348-66-3); (M-H)-	D-ORNITHINE (CAS# 348-66-3); (M-H)- [, tgt=69.86, over	348-66-3	(131.08171, 39899.71)(132.08327, 2849.1602)(133.08354, 3	D-ORNITHINE (CAS# 348-66-3); (M-H)-	C00515	FindByFormula	15 -	132.0886	0.657867
D-PSICOSE (CAS# 551-68-8); (M+Cl)-	D-PSICOSE (CAS# 551-68-8); (M+Cl)-	D-PSICOSE (CAS# 551-68-8); (M+Cl)- [, tgt=98.40, overall	551-68-8	(215.03189, 305403.94)(216.03542, 21093.553)(217.02994,	D-PSICOSE (CAS# 551-68-8); (M+Cl)-	C06468	FindByFormula	23 -	180.062	0.6597829
D-TAGATOSE (CAS# 87-81-0); (M+Cl)-	D-TAGATOSE (CAS# 87-81-0); (M+Cl)-	D-TAGATOSE (CAS# 87-81-0); (M+Cl)- [, tgt=98.29, overa	87-81-0	(215.03189, 305403.94)(216.03542, 21093.553)(217.02994,	D-TAGATOSE (CAS# 87-81-0); (M+Cl)-	C00795	FindByFormula	23 -	180.062	0.6597829
DUMP (CAS# 964-26-1); (M-H)-	DUMP (CAS# 964-26-1); (M-H)-	DUMP (CAS# 964-26-1); (M-H)- [, tgt=71.17, overall=71.1	964-26-1	(307.03363, 1052.8048)(308.0391, 230.32166)(309.03302, 1	DUMP (CAS# 964-26-1); (M-H)-	C00365	FindByFormula	6 -	308.04	1.002833
EDTA (CAS# 60-00-4); (M-2H)-2	EDTA (CAS# 60-00-4); (M-2H)-2	EDTA (CAS# 60-00-4); (M-2H)-2 [, tgt=44.53, overall=44.5	60-00-4	(145.0375, 1283.37)(145.532, 64.01)	EDTA (CAS# 60-00-4); (M-2H)-2	C00284	FindByFormula	1 -	292.0889	0.96000195
EDTA (CAS# 60-00-4); (M-H)-	EDTA (CAS# 60-00-4); (M-H)-	EDTA (CAS# 60-00-4); (M-H)- [, tgt=33.37, overall=33.37	60-00-4	(291.08368, 584832.06)(292.08585, 69425.9)(293.08795, 15	EDTA (CAS# 60-00-4); (M-H)-	C00284	FindByFormula	7 -	292.0912	0.8428567
ELAIDIC ACID (CAS# 112-79-8); (M-H)-	ELAIDIC ACID (CAS# 112-79-8); (M-H)-	ELAIDIC ACID (CAS# 112-79-8); (M-H)- [, tgt=93.52, overa	112-79-8	(281.24942, 474812.47)(282.25266, 93290.77)(283.25778, 1	ELAIDIC ACID (CAS# 112-79-8); (M-H)-		FindByFormula	28 -	282.2568	22.9269

EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9);	EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (	EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (M+Cl)- [, tg	78821-43-9	(515.31573, 70691.414)(516.3189, 21985.654)(517.31433, 2	EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (M+Cl)-	C11049	FindByFormula	28 -	480.3461	19.772638
EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9);	EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (	EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (M+HCOO)-	78821-43-9	(525.3448, 727041.6)(526.3486, 239078.08)(527.35065, 491	EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (M+HCOO)-	C11049	FindByFormula	28 -	480.3466	19.773243
ERUCIC ACID (CAS# 112-86-7); (M-H)-	ERUCIC ACID (CAS# 112-86-7); (M-H)-	ERUCIC ACID (CAS# 112-86-7); (M-H)- [, tgt=76.14, overa	112-86-7	(337.31125, 1052.8237)(338.31488, 272.85443)(339.319, 17	ERUCIC ACID (CAS# 112-86-7); (M-H)-		FindByFormula	27 -	338.3185	23.653072
ETHANOLAMINE PHOSPHATE (CAS# 1071-23-	ETHANOLAMINE PHOSPHATE (CAS# 1071-23-	ETHANOLAMINE PHOSPHATE (CAS# 1071-23-4); (M-H)- [	1071-23-4	(140.0119, 2435.3442)(141.01279, 70.04401)(142.01299, 13	ETHANOLAMINE PHOSPHATE (CAS# 1071-23-4); (M-H)-		FindByFormula	20 -	141.0191	0.78910035
ETHYLMALONIC ACID (CAS# 601-75-2); (M-H	ETHYLMALONIC ACID (CAS# 601-75-2); (M-H)	ETHYLMALONIC ACID (CAS# 601-75-2); (M-H)- [, tgt=55.	601-75-2	(131.0346, 1021.05133)(132.03741, 71.35133)	ETHYLMALONIC ACID (CAS# 601-75-2); (M-H)-		FindByFormula	15 -	132.0425	2.5844653
FRUCTOSE (CAS# 57-48-7); (M+Cl)-	FRUCTOSE (CAS# 57-48-7); (M+Cl)-	FRUCTOSE (CAS# 57-48-7); (M+Cl)- [, tgt=98.64, overall=	57-48-7	(215.03189, 305403.94)(216.03542, 21093.553)(217.02994, 1	FRUCTOSE (CAS# 57-48-7); (M+Cl)-	C00095	FindByFormula	23 -	180.062	0.6597829
FRUCTOSE (CAS# 57-48-7); (M+HCOO)-	FRUCTOSE (CAS# 57-48-7); (M+HCOO)-	FRUCTOSE (CAS# 57-48-7); (M+HCOO)- [, tgt=89.47, over	57-48-7	(225.06142, 7458.561)(226.06499, 673.5037)(227.06584, 36	FRUCTOSE (CAS# 57-48-7); (M+HCOO)-	C00095	FindByFormula	19 -	180.062	0.7177895
FUMARATE (CAS# 110-17-8); (M-H)-	FUMARATE (CAS# 110-17-8); (M-H)-	FUMARATE (CAS# 110-17-8); (M-H)- [, tgt=56.12, overall	110-17-8	(115.00441, 2265.7986)(116.00452, 60.868572)	FUMARATE (CAS# 110-17-8); (M-H)-	C00122	FindByFormula	14 -	116.0119	1.1677147
GALACTARATE (CAS# 526-99-8); (M-H)-	GALACTARATE (CAS# 526-99-8); (M-H)-	GALACTARATE (CAS# 526-99-8); (M-H)- [, tgt=27.91, over	526-99-8	(209.03, 838.67)(210.0435, 223.97)	GALACTARATE (CAS# 526-99-8); (M-H)-	C00879	FindByFormula	1 -	210.0394	0.9149985
GALACTURONIC ACID (CAS# 91510-62-2); (M	GALACTURONIC ACID (CAS# 91510-62-2); (M	GALACTURONIC ACID (CAS# 91510-62-2); (M-H)- [, tgt=8	91510-62-2	(193.03423, 788.27)(194.04053, 51.47333)	GALACTURONIC ACID (CAS# 91510-62-2); (M-H)-		FindByFormula	3 -	194.0412	0.6530003
GAMMA-BUTYROLACTONE (CAS# 96-48-0); (	GAMMA-BUTYROLACTONE (CAS# 96-48-0); (	GAMMA-BUTYROLACTONE (CAS# 96-48-0); (M+HCOO)- [	96-48-0	(131.03494, 1446.4476)(132.03485, 82.8496)(133.03815, 52.	GAMMA-BUTYROLACTONE (CAS# 96-48-0); (M+HCOO)-		FindByFormula	25 -	86.0367	2.0453193
GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686	GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-	GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M-H	686-58-8	(249.0563, 400.4)(250.0557, 64.835)	GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M-H)-	C03320	FindByFormula	2 -	250.0625	1.3115017
GAMMA-LINOLENIC ACID (CAS# 506-26-3); (	GAMMA-LINOLENIC ACID (CAS# 506-26-3); (	GAMMA-LINOLENIC ACID (CAS# 506-26-3); (M+HCOO)- [	506-26-3	(323.2211, 78457.055)(324.22437, 14621.172)(325.22064, 1	GAMMA-LINOLENIC ACID (CAS# 506-26-3); (M+HCOO)-		FindByFormula	28 -	278.2229	22.851686
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M-H)- [, tgt=	77-06-5	(691.27637, 4305.9497)(692.2801, 1909.9968)(693.28314, 5	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M-H)-	C01699	FindByFormula	28 -	346.1425	8.459148
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Cl)- [, tgt=8	77-06-5	(381.11172, 3485.8792)(382.11508, 815.84686)(383.10986, 1	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Cl)-	C01699	FindByFormula	28 -	346.1419	8.461257
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M-	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M-H)- [, tgt=8	77-06-5	(345.13525, 109841.89)(346.1384, 23055.178)(347.13995, 3	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M-H)-	C01699	FindByFormula	28 -	346.1425	8.458006
GLUCARIC ACID (CAS# 87-73-0); (M-H)-	GLUCARIC ACID (CAS# 87-73-0); (M-H)-	GLUCARIC ACID (CAS# 87-73-0); (M-H)- [, tgt=29.30, over	87-73-0	(209.03072, 815.87335)(210.03426, 190.92665)	GLUCARIC ACID (CAS# 87-73-0); (M-H)-		FindByFormula	3 -	210.0394	0.93733215
GLUCARIC ACID (CAS# 87-73-0); (M-H)+[-H2	GLUCARIC ACID (CAS# 87-73-0); (M-H)+[-H2	GLUCARIC ACID (CAS# 87-73-0); (M-H)+[-H2O] [, tgt=78.	87-73-0	(191.01959, 126384.62)(192.01973, 8762.211)(193.01912, 2	GLUCARIC ACID (CAS# 87-73-0); (M-H)+[-H2O]		FindByFormula	25 -	210.0382	0.73828006
GLUCONIC ACID (CAS# 526-95-4); (M-H)-	GLUCONIC ACID (CAS# 526-95-4); (M-H)-	GLUCONIC ACID (CAS# 526-95-4); (M-H)- [, tgt=76.15, ov	526-95-4	(195.0501, 4414.5474)(196.05713, 233.19499)(197.05534, 1	GLUCONIC ACID (CAS# 526-95-4); (M-H)-		FindByFormula	4 -	196.0576	0.6692499
GLUCOSE (CAS# 50-99-7); (2M+Cl)-[-H2O]	GLUCOSE (CAS# 50-99-7); (2M+Cl)-[-H2O]	GLUCOSE (CAS# 50-99-7); (2M+Cl)-[-H2O] [, tgt=91.35, o	50-99-7	(377.0849, 25632.664)(378.09003, 4016.057)(379.0828, 979	GLUCOSE (CAS# 50-99-7); (2M+Cl)-[-H2O]		FindByFormula	21 -	180.0632	0.70161927
GLUCOSE (CAS# 50-99-7); (2M+HCOO)-[-H2	GLUCOSE (CAS# 50-99-7); (2M+HCOO)-[-H2O	GLUCOSE (CAS# 50-99-7); (2M+HCOO)-[-H2O] [, tgt=65.2	50-99-7	(387.11404, 1092.23)(388.11487, 259.5125)(389.12103, 83.2	GLUCOSE (CAS# 50-99-7); (2M+HCOO)-[-H2O]		FindByFormula	4 -	180.0624	0.7135006
GLUCOSE (CAS# 50-99-7); (M+Cl)-	GLUCOSE (CAS# 50-99-7); (M+Cl)-	GLUCOSE (CAS# 50-99-7); (M+Cl)- [, tgt=98.43, overall=9	50-99-7	(215.03189, 305403.94)(216.03542, 21093.553)(217.02994, 1	GLUCOSE (CAS# 50-99-7); (M+Cl)-		FindByFormula	23 -	180.062	0.6597829
GLUCOSE 1-PHOSPHATE (CAS# 59-56-3); (M-	GLUCOSE 1-PHOSPHATE (CAS# 59-56-3); (M-	GLUCOSE 1-PHOSPHATE (CAS# 59-56-3); (M-H)- [, tgt=71	59-56-3	(259.0233, 3648.1812)(260.02444, 614.36)(261.0225, 608.64	GLUCOSE 1-PHOSPHATE (CAS# 59-56-3); (M-H)-		FindByFormula	13 -	260.0289	0.74800026
GLUCURONIC ACID (CAS# 6556-12-3); (M+Cl)	GLUCURONIC ACID (CAS# 6556-12-3); (M+Cl)	GLUCURONIC ACID (CAS# 6556-12-3); (M+Cl)- [, tgt=38.2	12/3/6556	(229.0112, 690.7)(230.0217, 40.97)	GLUCURONIC ACID (CAS# 6556-12-3); (M+Cl)-	C16245	FindByFormula	1 -	194.0422	0.7900003
GLUCURONIC ACID (CAS# 6556-12-3); (M-H)-	GLUCURONIC ACID (CAS# 6556-12-3); (M-H)-	GLUCURONIC ACID (CAS# 6556-12-3); (M-H)- [, tgt=88.62	12/3/6556	(193.03503, 701.325)(194.03839, 61.7225)	GLUCURONIC ACID (CAS# 6556-12-3); (M-H)-	C16245	FindByFormula	4 -	194.0412	0.65625024
GLUTAMATE (CAS# 56-86-0); (M-H)-	GLUTAMATE (CAS# 56-86-0); (M-H)-	GLUTAMATE (CAS# 56-86-0); (M-H)- [, tgt=88.64, overall	56-86-0	(146.04552, 50460.11)(147.04558, 3180.6726)(148.04509, 4	GLUTAMATE (CAS# 56-86-0); (M-H)-		FindByFormula	20 -	147.0528	0.65335023
GLUTAMINE (CAS# 56-85-9); (M-H)-	GLUTAMINE (CAS# 56-85-9); (M-H)-	GLUTAMINE (CAS# 56-85-9); (M-H)- [, tgt=81.08, overall=	56-85-9	(145.06181, 41264.38)(146.06108, 1677.9513)(147.06245, 2	GLUTAMINE (CAS# 56-85-9); (M-H)-		FindByFormula	7 -	146.0686	0.64842826
GLUTARATE (CAS# 110-94-1); (M-H)-	GLUTARATE (CAS# 110-94-1); (M-H)-	GLUTARATE (CAS# 110-94-1); (M-H)- [, tgt=97.50, overall	110-94-1	(131.03494, 1446.4476)(132.03485, 82.8496)(133.03815, 52.	GLUTARATE (CAS# 110-94-1); (M-H)-	C00489	FindByFormula	25 -	132.0422	2.0453193
GLUTATHIONE (CAS# 27025-41-8); (M-H)-	GLUTATHIONE (CAS# 27025-41-8); (M-H)-	GLUTATHIONE (CAS# 27025-41-8); (M-H)- [, tgt=78.18, o	27025-41-8	(611.14417, 711.6018)(612.14606, 223.01471)(613.138, 129.	GLUTATHIONE (CAS# 27025-41-8); (M-H)-	C00127	FindByFormula	17 -	612.1506	1.3853538
GLYCERALDEHYDE (CAS# 367-47-5); (2M-H)-[	GLYCERALDEHYDE (CAS# 367-47-5); (2M-H)-[	GLYCERALDEHYDE (CAS# 367-47-5); (2M-H)-[-H2O] [, tgt	367-47-5	(161.04494, 3745.9172)(162.04668, 92.85876)(163.04419, 8	GLYCERALDEHYDE (CAS# 367-47-5); (2M-H)-[-H2O]	C02154	FindByFormula	8 -	90.0311	1.6247497
GLYCEROL 2-PHOSPHATE (CAS#); (M-H)-	GLYCEROL 2-PHOSPHATE (CAS#); (M-H)-	GLYCEROL 2-PHOSPHATE (CAS#); (M-H)- [, tgt=53.55, overall=53.55]		(171.0071, 1465.22)(172.0089, 91.796364)(173.00586, 823.4	GLYCEROL 2-PHOSPHATE (CAS#); (M-H)-		FindByFormula	11 -	172.0136	0.88709104
GLYCINE (CAS# 56-40-6); (M-H)-	GLYCINE (CAS# 56-40-6); (M-H)-	GLYCINE (CAS# 56-40-6); (M-H)- [, tgt=84.72, overall=84.	56-40-6	(74.02489, 1417.442)(75.026634, 35.489002)	GLYCINE (CAS# 56-40-6); (M-H)-		FindByFormula	10 -	75.0319	0.65150034
GLYCOCHOLATE (CAS# 475-31-0); (M-H)-	GLYCOCHOLATE (CAS# 475-31-0); (M-H)-	GLYCOCHOLATE (CAS# 475-31-0); (M-H)- [, tgt=64.77, ov	475-31-0	(464.30243, 6007.9883)(465.30145, 2062.6338)(466.3043, 5	GLYCOCHOLATE (CAS# 475-31-0); (M-H)-	C01921	FindByFormula	10 -	465.3094	18.82955
GLYCOLITHOCHOLATE (CAS# 474-74-8); (M-	GLYCOLITHOCHOLATE (CAS# 474-74-8); (M-	GLYCOLITHOCHOLATE (CAS# 474-74-8); (M-H)- [, tgt=79	474-74-8	(432.3126, 1155.6433)(433.31616, 470.76)(434.31436, 79.16	GLYCOLITHOCHOLATE (CAS# 474-74-8); (M-H)-	C15557	FindByFormula	6 -	433.3193	21.543154
GUANINE (CAS# 73-40-5); (M-H)-	GUANINE (CAS# 73-40-5); (M-H)-	GUANINE (CAS# 73-40-5); (M-H)- [, tgt=80.18, overall=80	73-40-5	(150.04173, 1839.0991)(151.0396, 114.57684)	GUANINE (CAS# 73-40-5); (M-H)-		FindByFormula	19 -	151.0487	0.8657373
GUANOSINE (CAS# 118-00-3); (M+Cl)-	GUANOSINE (CAS# 118-00-3); (M+Cl)-	GUANOSINE (CAS# 118-00-3); (M+Cl)- [, tgt=73.23, overa	118-00-3	(318.06134, 2867.9182)(319.06345, 437.35724)(320.05954, 1	GUANOSINE (CAS# 118-00-3); (M+Cl)-	C00387	FindByFormula	22 -	283.0924	1.8078644
GUANOSINE (CAS# 118-00-3); (M-H)-	GUANOSINE (CAS# 118-00-3); (M-H)-	GUANOSINE (CAS# 118-00-3); (M-H)- [, tgt=90.76, overal	118-00-3	(282.08444, 13363.771)(283.08594, 1926.2386)(284.08405, 1	GUANOSINE (CAS# 118-00-3); (M-H)-	C00387	FindByFormula	22 -	283.0915	1.8300458
GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (	GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (	GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (2M-H)+ [, t	85-32-5	(725.1087, 2514.7866)(726.11066, 676.9767)(727.0993, 305.	GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (2M-H)+		FindByFormula	6 -	363.058	0.7876661
GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (	GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (	GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (M-H)- [, tgt	85-32-5	(362.04987, 870.09)(363.04898, 79.53999)(364.0365, 99.98)	GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (M-H)-		FindByFormula	5 -	363.055	1.0171999
GULONO-1,4-LACTONE (CAS# 1128-23-0); (M	GULONO-1,4-LACTONE (CAS# 1128-23-0); (M	GULONO-1,4-LACTONE (CAS# 1128-23-0); (M-H)- [, tgt=5	1128-23-0	(177.0401, 476.54)(178.053, 128.05)	GULONO-1,4-LACTONE (CAS# 1128-23-0); (M-H)-	C05410	FindByFormula	1 -	178.0494	0.7110003
HEPTADECANOATE (CAS# 506-12-7); (M-H)-	HEPTADECANOATE (CAS# 506-12-7); (M-H)-	HEPTADECANOATE (CAS# 506-12-7); (M-H)- [, tgt=91.71,	506-12-7	(269.24893, 14721.725)(270.25238, 2821.1946)(271.2514, 3	HEPTADECANOATE (CAS# 506-12-7); (M-H)-		FindByFormula	28 -	270.2562	22.990265
HEXACOSANOIC ACID (CAS# 506-46-7); (M-H	HEXACOSANOIC ACID (CAS# 506-46-7); (M-H)	HEXACOSANOIC ACID (CAS# 506-46-7); (M-H)- [, tgt=82.	506-46-7	(395.39, 2902.86)(396.3931, 871.9664)(397.3963, 167.44835	HEXACOSANOIC ACID (CAS# 506-46-7); (M-H)-		FindByFormula	22 -	396.3974	25.599693
HIPPURATE (CAS# 495-69-2); (M-H)-	HIPPURATE (CAS# 495-69-2); (M-H)-	HIPPURATE (CAS# 495-69-2); (M-H)- [, tgt=78.81, overall	495-69-2	(178.05109, 19676.477)(179.05043, 2365.2034)(180.0529, 3	HIPPURATE (CAS# 495-69-2); (M-H)-	C01586	FindByFormula	26 -	179.0574	4.8059034
HOMOCYSTINE (CAS# 462-10-2); (M-H)-	HOMOCYSTINE (CAS# 462-10-2); (M-H)-	HOMOCYSTINE (CAS# 462-10-2); (M-H)- [, tgt=45.60, ove	462-10-2	(267.0459, 1305.97)(268.0419, 181.79)(269.0445, 123.76)	HOMOCYSTINE (CAS# 462-10-2); (M-H)-	C01817	FindByFormula	1 -	268.0526	0.9870011
HOMOGENTISATE (CAS# 451-13-8); (M-H)-	HOMOGENTISATE (CAS# 451-13-8); (M-H)-	HOMOGENTISATE (CAS# 451-13-8); (M-H)- [, tgt=51.04,	451-13-8	(167.03369, 1526.2749)(168.0388, 115.08)	HOMOGENTISATE (CAS# 451-13-8); (M-H)-		FindByFormula	2 -	168.0414	2.5264912
HOMOSERINE (CAS# 672-15-1); (M-H)-	HOMOSERINE (CAS# 672-15-1); (M-H)-	HOMOSERINE (CAS# 672-15-1); (M-H)- [, tgt=85.48, over	672-15-1	(118.05052, 13900.508)(119.04657, 762.22296)(120.04493, 9	HOMOSERINE (CAS# 672-15-1); (M-H)-	C00263	FindByFormula	10 -	119.0571	0.64800036
HOMOVANILLATE (CAS# 306-08-1); (M-H)-	HOMOVANILLATE (CAS# 306-08-1); (M-H)-	HOMOVANILLATE (CAS# 306-08-1); (M-H)- [, tgt=53.70,	306-08-1	(181.04956, 555.21)(182.05133, 40.103333)	HOMOVANILLATE (CAS# 306-08-1); (M-H)-		FindByFormula	3 -	182.0564	5.6583056
HYODEOXYCHOLATE (CAS# 83-49-8); (M-H)-	HYODEOXYCHOLATE (CAS# 83-49-8); (M-H)-	HYODEOXYCHOLATE (CAS# 83-49-8); (M-H)- [, tgt=80.02,	83-49-8	(391.2889, 72641.23)(392.29178, 19384.63)(393.29044, 588	HYODEOXYCHOLATE (CAS# 83-49-8); (M-H)-		FindByFormula	28 -	392.2958	22.88042
HYPOXANTHINE (CAS# 68-94-0); (M-H)-	HYPOXANTHINE (CAS# 68-94-0); (M-H)-	HYPOXANTHINE (CAS# 68-94-0); (M-H)- [, tgt=80.33, ove	68-94-0	(135.03096, 31095.531)(136.03328, 2061.1755)(137.03441, 1	HYPOXANTHINE (CAS# 68-94-0); (M-H)-		FindByFormula	26 -	136.0387	1.0976539
IBUPROFEN (CAS# 15687-27-1); (M-H)-	IBUPROFEN (CAS# 15687-27-1); (M-H)-	IBUPROFEN (CAS# 15687-27-1); (M-H)- [, tgt=89.60, over	15687-27-1	(205.12347, 2847.7402)(206.12688, 450.45667)	IBUPROFEN (CAS# 15687-27-1); (M-H)-	C01588	FindByFormula	6 -	206.131	18.84157
IBUPROFEN CARBOXYLIC ACID (CAS# 15935-5	IBUPROFEN CARBOXYLIC ACID (CAS# 15935-5	IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M-H)	15935-54-3	(235.09752, 3417.8)(236.10016, 583.51)(237.09862, 91.2033	IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M-H)-		FindByFormula	6 -	236.1047	12.951045
INDICAN (CAS# 487-60-5); (2M+Cl)-[-H2O]	INDICAN (CAS# 487-60-5); (2M+Cl)-[-H2O]	INDICAN (CAS# 487-60-5); (2M+Cl)-[-H2O] [, tgt=57.87, o	487-60-5	(607.1663, 235.63)(608.178, 41.32)	INDICAN (CAS# 487-60-5); (2M+Cl)-[-H2O]	C08481	FindByFormula	1 -	295.1031	0.74700063
INDOLE-3-ACETATE (CAS# 87-51-4); (M-H)-	INDOLE-3-ACETATE (CAS# 87-51-4); (M-H)-	INDOLE-3-ACETATE (CAS# 87-51-4); (M-H)- [, tgt=84.98,	87-51-4	(174.05577, 824.8567)(175.05293, 65.96)	INDOLE-3-ACETATE (CAS# 87-51-4); (M-H)-	C00954	FindByFormula	3 -	175.0625	8.382953
INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M	INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M	INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M-H)- [, tgt=	392-12-1	(202.05124, 567.45746)(203.04846, 131.4775)(204.0491, 69.	INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M-H)-	C00331	FindByFormula	8 -	203.0581	10.482648
INOSINE (CAS# 58-63-9); (M+Cl)-	INOSINE (CAS# 58-63-9); (M+Cl)-	INOSINE (CAS# 58-63-9); (M+Cl)- [, tgt=93.17, overall=93	58-63-9	(303.05084, 14589.606)(304.05374, 2159.729)(305.04794, 5	INOSINE (CAS# 58-63-9); (M+Cl)-		FindByFormula	25 -	268.0816	1.81556
INOSINE (CAS# 58-63-9); (M-H)-	INOSINE (CAS# 58-63-9); (M-H)-	INOSINE (CAS# 58-63-9); (M-H)- [, tgt=96.46, overall=96.	58-63-9	(267.074, 115438.25)(268.07565, 14363.893)(269.07727, 22	INOSINE (CAS# 58-63-9); (M-H)-		FindByFormula	28 -	268.0812	1.8236428
INOSINE 5'-DIPHOSPHATE (CAS# 86-04-4); (M	INOSINE 5'-DIPHOSPHATE (CAS# 86-04-4); (M	INOSINE 5'-DIPHOSPHATE (CAS# 86-04-4); (M-H)- [, tgt=	86-04-4	(427.0069, 1080.3931)(428.0069, 94.151)(429.00674, 151.74	INOSINE 5'-DIPHOSPHATE (CAS# 86-04-4); (M-H)-	C00104	FindByFormula	10 -	428.016	0.6715998
INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M	INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M-	INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M-H)- [, tgt=4	131-99-7	(347.04175, 1750.1544)(348.0402, 219.94183)(349.04266, 9	INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M-H)-		FindByFormula	11 -	348.0492	1.1312736
ISOCITRATE (CAS# 320-77-4); (M-H)-	ISOCITRATE (CAS# 320-77-4); (M-H)-	ISOCITRATE (CAS# 320-77-4); (M-H)- [, tgt=74.67, overall	320-77-4	(191.0197, 121515.01)(192.02043, 8425.642)(193.01888, 32	ISOCITRATE (CAS# 320-77-4); (M-H)-	C00311	FindByFormula	26 -	192.0265	0.7537692
ISOLEUCINE (CAS# 73-32-5); (M-H)-	ISOLEUCINE (CAS# 73-32-5); (M-H)-	ISOLEUCINE (CAS# 73-32-5); (M-H)- [, tgt=74.86, overall=	73-32-5	(130.08688, 25122.994)(131.08922, 1918.8585)(132.08742, 8	ISOLEUCINE (CAS# 73-32-5); (M-H)-		FindByFormula	24 -	131.0941	1.6091666
ITACONATE (CAS# 97-65-4); (M-H)-	ITACONATE (CAS# 97-65-4); (M-H)-	ITACONATE (CAS# 97-65-4); (M-H)- [, tgt=87.84, overall=	97-65-4	(129.01999, 805.16626)(130.0195, 42.295)	ITACONATE (CAS# 97-65-4); (M-H)-	C00490	FindByFormula	8 -	130.0273	1.8394997
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (2	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (2	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (2M-H)- [, tgt	77026-92-7	(419.24448, 10023.5205)(420.24786, 2745.0857)(421.2469, 5	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (2M-H)-		FindByFormula	28 -	210.126	13.099159
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M-H)- [, tgt=	77026-92-7	(209.11877, 310429.66)(210.12192, 41206.48)(211.12395, 4	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M-H)-		FindByFormula	28 -	210.1261	13.099695
KYNURENINE (CAS# 343-65-7); (M-H)-	KYNURENINE (CAS# 343-65-7); (M-H)-	KYNURENINE (CAS# 343-65-7); (M-H)- [, tgt=64.90, overa	343-65-7	(207.07664, 733.7431)(208.07635, 77.34)	KYNURENINE (CAS# 343-65-7); (M-H)-	C00328	FindByFormula	16 -	208.0842	2.2110608
L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (	L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M	L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M-H)- [, tgt=90.81, overall=90.81]		(137.03757, 57847.863)(138.04094, 4539.907)(139.0418, 38	L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M-H)-		FindByFormula	28 -	138.0449	5.330579
LACTOSE (CAS# 63-42-3); (M+Cl)-	LACTOSE (CAS# 63-42-3); (M+Cl)-	LACTOSE (CAS# 63-42-3); (M+Cl)- [, tgt=90.04, overall=90	63-42-3	(377.08475, 25323.936)(378.08945, 4187.432)(379.08237, 1	LACTOSE (CAS# 63-42-3); (M+Cl)-		FindByFormula	24 -	342.116	0.7031669
LACTOSE (CAS# 63-42-3); (M-H)-	LACTOSE (CAS# 63-42-3); (M-H)-	LACTOSE (CAS# 63-42-3); (M-H)- [, tgt=69.08, overall=69.	63-42-3	(341.10934, 669.135)(342.10712, 138.40001)(343.10754, 86.	LACTOSE (CAS# 63-42-3); (M-H)-		FindByFormula	4 -	342.1159	0.7170005
L-ALLOTHREONINE (CAS# 28954-12-3); (M-H)	L-ALLOTHREONINE (CAS# 28954-12-3); (M-H)	L-ALLOTHREONINE (CAS# 28954-12-3); (M-H)- [, tgt=84.2	28954-12-3	(118.05054, 14212.939)(119.04679, 790.74994)(120.04591, 9	L-ALLOTHREONINE (CAS# 28954-12-3); (M-H)-	C05519	FindByFormula	9 -	119.0571	0.6473338
L-ARGININE (CAS# 74-79-3); (M-H)-	L-ARGININE (CAS# 74-79-3); (M-H)-	L-ARGININE (CAS# 74-79-3); (M-H)- [, tgt=73.01, overall=	74-79-3	(173.10349, 3315.088)(174.10353, 118.36221)(175.0984, 19	L-ARGININE (CAS# 74-79-3); (M-H)-	C02385	FindByFormula	18 -	174.1104	0.62894464
L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD]	L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD]	L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (CAS#); (M-H)- [, tgt=75.80, overall=7		(175.09798, 2833.1687)(176.09871, 226.278)(177.10056, 44.	L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (CAS#); (M-H)-		FindByFormula	10 -	176.1049	0.6254004
LAURIC ACID (CAS# 143-07-7); (M-H)-	LAURIC ACID (CAS# 143-07-7); (M-H)-	LAURIC ACID (CAS# 143-07-7); (M-H)- [, tgt=97.76, overa	143-07-7	(199.17046, 6761.0356)(200.17395, 928.2221)(201.17508, 1	LAURIC ACID (CAS# 143-07-7); (M-H)-	C02679	FindByFormula	28 -	200.1778	21.743986
L-CARNITINE (CAS# 541-15-1); (M+Cl)-	L-CARNITINE (CAS# 541-15-1); (M+Cl)-	L-CARNITINE (CAS# 541-15-1); (M+Cl)- [, tgt=60.21, overa	541-15-1	(196.07367, 3182.2874)(197.07187, 247.1175)(198.0689, 49	L-CARNITINE (CAS# 541-15-1); (M+Cl)-		FindByFormula	4 -	161.104	0.66350013
LEUCINE (CAS# 328-39-2); (M-H)-	LEUCINE (CAS# 328-39-2); (M-H)-	LEUCINE (CAS# 328-39-2); (M-H)- [, tgt=95.87, overall=95	328-39-2	(130.08688, 25122.994)(131.08922, 1918.8585)(132.08742, 8	LEUCINE (CAS# 328-39-2); (M-H)-	C16439	FindByFormula	24 -	131.0941	1.6091666
LEUKOTRIENE B4 (CAS# 71160-24-2); (M-H)-	LEUKOTRIENE B4 (CAS# 71160-24-2); (M-H)-	LEUKOTRIENE B4 (CAS# 71160-24-2); (M-H)- [, tgt=18.87,	71160-24-2	(335.22183, 848.97003)(336.2229, 194.31645)(337.2204, 13	LEUKOTRIENE B4 (CAS# 71160-24-2); (M-H)-		FindByFormula	17 -	336.2284	20.777426
L-GULONATE (CAS# 6322-07-2); (M-H)-	L-GULONATE (CAS# 6322-07-2); (M-H)-	L-GULONATE (CAS# 6322-07-2); (M-H)- [, tgt=76.79, over	7/2/6322	(195.0501, 4414.5474)(196.05713, 233.19499)(197.05534, 1	L-GULONATE (CAS# 6322-07-2); (M-H)-		FindByFormula	4 -	196.0576	0.6692499
L-GULONATE (CAS# 6322-07-2); (M-H)+[-H2	L-GULONATE (CAS# 6322-07-2); (M-H)+[-H2O	L-GULONATE (CAS# 6322-07-2); (M-H)+[-H2O] [, tgt=67.7	7/2/6322	(177.03825, 645.92004)(178.04324, 98.365005)	L-GULONATE (CAS# 6322-07-2); (M-H)+[-H2O]		FindByFormula	2 -	196.057	0.7095003
L-HISTIDINE (CAS# 71-00-1); (M-H)-	L-HISTIDINE (CAS# 71-00-1); (M-H)-	L-HISTIDINE (CAS# 71-00-1); (M-H)- [, tgt=95.73, overall=	71-00-1	(154.062, 44628.684)(155.06445, 3456.2207)(156.06584, 37	L-HISTIDINE (CAS# 71-00-1); (M-H)-		FindByFormula	28 -	155.0693	0.6365715
LIGNOCERIC ACID (CAS# 557-59-5); (M-H)-	LIGNOCERIC ACID (CAS# 557-59-5); (M-H)-	LIGNOCERIC ACID (CAS# 557-59-5); (M-H)- [, tgt=94.98,	557-59-5	(367.35876, 13640.365)(368.3626, 3644.732)(369.365, 579.4	LIGNOCERIC ACID (CAS# 557-59-5); (M-H)-		FindByFormula	26 -	368.3659	24.715824
LINOLEATE (CAS# 60-33-3); (M-H)-	LINOLEATE (CAS# 60-33-3); (M-H)-	LINOLEATE (CAS# 60-33-3); (M-H)- [, tgt=97.08, overall=	60-33-3	(279.2338, 296856.8)(280.2369, 58168.19)(281.24048, 7446.	LINOLEATE (CAS# 60-33-3); (M-H)-		FindByFormula	28 -	280.241	22.72988
LITHOCHOLIC ACID (CAS# 434-13-9); (M+HC	LITHOCHOLIC ACID (CAS# 434-13-9); (M+HC	LITHOCHOLIC ACID (CAS# 434-13-9); (M+HCOO)- [, tgt=4	434-13-9	(421.29507, 736.05994)(422.29565, 260.768)(423.30005, 17	LITHOCHOLIC ACID (CAS# 434-13-9); (M+HCOO)-		FindByFormula	5 -	376.2979	22.50918
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M-H)	583-93-7	(189.08653, 1966.1367)(190.08537, 93.69)	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M-H)-	C00666	FindByFormula	3 -	190.0938	0.7766664
L-ORNITHINE (CAS# 70-26-8); (M-H)-	L-ORNITHINE (CAS# 70-26-8); (M-H)-	L-ORNITHINE (CAS# 70-26-8); (M-H)- [, tgt=71.70, overall	70-26-8	(131.08171, 39899.71)(132.08327, 2849.1602)(133.08354, 3	L-ORNITHINE (CAS# 70-26-8); (M-H)-	C00077	FindByFormula	15 -	132.0886	0.657867
L-RHAMNOSE (CAS# 10030-85-0); (M+Cl)-	L-RHAMNOSE (CAS# 10030-85-0); (M+Cl)-	L-RHAMNOSE (CAS# 10030-85-0); (M+Cl)- [, tgt=46.09, o	10030-85-0	(199.03676, 21567.576)(200.04205, 1505.14)(201.03456, 83	L-RHAMNOSE (CAS# 10030-85-0); (M+Cl)-		FindByFormula	12 -	164.0673	0.7944166
L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M-H)-	L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M-H)-	L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M-H)- [, tgt=99.47, overall=99.47]		(205.07729, 25486.346)(206.08028, 3279.5344)(207.07933, 1	L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M-H)-		FindByFormula	28 -	206.0841	3.5985644
LUMICHROME (CAS# 1086-80-2); (M-H)-	LUMICHROME (CAS# 1086-80-2); (M-H)-	LUMICHROME (CAS# 1086-80-2); (M-H)- [, tgt=65.23, ov	1086-80-2	(241.071, 410.8)(242.0783, 104.69)	LUMICHROME (CAS# 1086-80-2); (M-H)-	C01727	FindByFormula	1 -	242.0792	10.872496
LYSINE (CAS# 56-87-1); (M-H)-	LYSINE (CAS# 56-87-1); (M-H)-	LYSINE (CAS# 56-87-1); (M-H)- [, tgt=87.03, overall=87.0	56-87-1	(145.09787, 2479.82)(146.09935, 158.05421)(147.10239, 27.	LYSINE (CAS# 56-87-1); (M-H)-	C00047	FindByFormula	26 -	146.1048	0.5993847
MALATE (CAS# 97-67-6); (M-H)-	MALATE (CAS# 97-67-6); (M-H)-	MALATE (CAS# 97-67-6); (M-H)- [, tgt=67.86, overall=67.	97-67-6	(133.01448, 7481.5)(134.016, 363.66687)	MALATE (CAS# 97-67-6); (M-H)-	C00149	FindByFormula	25 -	134.022	0.89236015
MALATE (CAS# 97-67-6); (M-H)+[-H2O]	MALATE (CAS# 97-67-6); (M-H)+[-H2O]	MALATE (CAS# 97-67-6); (M-H)+[-H2O] [, tgt=57.01, over	97-67-6	(115.003456, 2545.6292)(116.00393, 55.154163)	MALATE (CAS# 97-67-6); (M-H)+[-H2O]	C00149	FindByFormula	12 -	134.0223	0.7919168
MALEAMATE (CAS# 557-24-4); (M-H)-	MALEAMATE (CAS# 557-24-4); (M-H)-	MALEAMATE (CAS# 557-24-4); (M-H)- [, tgt=77.25, overa	557-24-4	(114.02, 1051.1267)(115.01974, 53.846664)	MALEAMATE (CAS# 557-24-4); (M-H)-	C01596	FindByFormula	3 -	115.0274	0.7670007
MALEIC ACID (CAS# 110-16-7); (M-H)-	MALEIC ACID (CAS# 110-16-7); (M-H)-	MALEIC ACID (CAS# 110-16-7); (M-H)- [, tgt=84.30, overa	110-16-7	(115.00429, 2592.486)(116.00466, 49.447144)	MALEIC ACID (CAS# 110-16-7); (M-H)-		FindByFormula	21 -	116.012	1.0034287
MALTOSE (CAS# 69-79-4); (M+Cl)-	MALTOSE (CAS# 69-79-4); (M+Cl)-	MALTOSE (CAS# 69-79-4); (M+Cl)- [, tgt=89.81, overall=8	69-79-4	(377.08475, 25323.936)(378.08945, 4187.432)(379.08237, 1	MALTOSE (CAS# 69-79-4); (M+Cl)-	C00208	FindByFormula	24 -	342.116	0.7031669
MALTOSE (CAS# 69-79-4); (M+HCOO)-	MALTOSE (CAS# 69-79-4); (M+HCOO)-	MALTOSE (CAS# 69-79-4); (M+HCOO)- [, tgt=63.59, overa	69-79-4	(387.11395, 959.8128)(388.11154, 277.31714)(389.1217, 11	MALTOSE (CAS# 69-79-4); (M+HCOO)-	C00208	FindByFormula	7 -	342.1152	0.7178578
MANDELIC ACID (CAS# 611-71-2); (M-H)-	MANDELIC ACID (CAS# 611-71-2); (M-H)-	MANDELIC ACID (CAS# 611-71-2); (M-H)- [, tgt=99.95, ov	611-71-2	(151.04016, 624920.8)(152.04326, 54833.457)(153.0454, 74	MANDELIC ACID (CAS# 611-71-2); (M-H)-	C01983	FindByFormula	27 -	152.0475	8.084817
MANNITOL (CAS# 69-65-8); (M-H)-	MANNITOL (CAS# 69-65-8); (M-H)-	MANNITOL (CAS# 69-65-8); (M-H)- [, tgt=96.91, overall=	69-65-8	(181.07101, 2150.875)(182.07434, 200.15)(183.0754, 40.68)	MANNITOL (CAS# 69-65-8); (M-H)-	C00392	FindByFormula	2 -	182.0784	0.64399976
MANNOSE-6-PHOSPHATE (CAS# 3672-15-9);	MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (	MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (M-H)- [, tgt	3672-15-9	(259.0233, 3648.1812)(260.02444, 614.36)(261.0225, 608.64	MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (M-H)-	C00275	FindByFormula	13 -	260.0289	0.74800026
MELIBIOSE (CAS# 585-99-9); (M+Cl)-	MELIBIOSE (CAS# 585-99-9); (M+Cl)-	MELIBIOSE (CAS# 585-99-9); (M+Cl)- [, tgt=94.09, overall	585-99-9	(377.08475, 25323.936)(378.08945, 4187.432)(379.08237, 1	MELIBIOSE (CAS# 585-99-9); (M+Cl)-	C05402	FindByFormula	24 -	342.116	0.7031669
MELIBIOSE (CAS# 585-99-9); (M+HCOO)-	MELIBIOSE (CAS# 585-99-9); (M+HCOO)-	MELIBIOSE (CAS# 585-99-9); (M+HCOO)- [, tgt=68.29, ov	585-99-9	(387.11395, 959.8128)(388.11154, 277.31714)(389.1217, 11	MELIBIOSE (CAS# 585-99-9); (M+HCOO)-	C05402	FindByFormula	7 -	342.1152	0.7178578
METHIONINE (CAS# 63-68-3); (M-H)-	METHIONINE (CAS# 63-68-3); (M-H)-	METHIONINE (CAS# 63-68-3); (M-H)- [, tgt=67.21, overal	63-68-3	(148.04369, 2078.3962)(149.04276, 306.29318)(150.04123, 1	METHIONINE (CAS# 63-68-3); (M-H)-		FindByFormula	22 -	149.0515	0.89077324
METHYL VANILLATE (CAS# 3943-74-6); (M-H)	METHYL VANILLATE (CAS# 3943-74-6); (M-H)	METHYL VANILLATE (CAS# 3943-74-6); (M-H)- [, tgt=49.3	3943-74-6	(181.0515, 502.19)(182.0578, 31.43)	METHYL VANILLATE (CAS# 3943-74-6); (M-H)-		FindByFormula	1 -	182.0589	9.295519
METHYLMALONATE (CAS# 516-05-2); (M-H)-	METHYLMALONATE (CAS# 516-05-2); (M-H)-	METHYLMALONATE (CAS# 516-05-2); (M-H)- [, tgt=67.82	516-05-2	(117.019554, 17337.795)(118.02498, 887.87604)(119.02759	METHYLMALONATE (CAS# 516-05-2); (M-H)-	C02170	FindByFormula	25 -	118.0268	1.3372802
MEVALONIC ACID (CAS# 674-26-0); (M-H)-	MEVALONIC ACID (CAS# 674-26-0); (M-H)-	MEVALONIC ACID (CAS# 674-26-0); (M-H)- [, tgt=55.32,	674-26-0	(147.0653, 1457.92)(148.0668, 84.71)	MEVALONIC ACID (CAS# 674-26-0); (M-H)-		FindByFormula	1 -	148.0724	1.7549973
MONO-METHYL GLUTARATE (CAS# 1501-27-5	MONO-METHYL GLUTARATE (CAS# 1501-27-5	MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M-H)- [,	1501-27-5	(145.05101, 4445.3584)(146.04971, 233.67116)(147.05116, 6	MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M-H)-		FindByFormula	26 -	146.0582	3.5393395
MYRISTIC ACID (CAS# 544-63-8); (M-H)-	MYRISTIC ACID (CAS# 544-63-8); (M-H)-	MYRISTIC ACID (CAS# 544-63-8); (M-H)- [, tgt=99.74, ove	544-63-8	(227.20193, 53595.977)(228.20528, 8360.702)(229.2075, 88	MYRISTIC ACID (CAS# 544-63-8); (M-H)-		FindByFormula	28 -	228.2092	22.448605
MYRISTOLEIC ACID (CAS# 544-64-9); (M-H)-	MYRISTOLEIC ACID (CAS# 544-64-9); (M-H)-	MYRISTOLEIC ACID (CAS# 544-64-9); (M-H)- [, tgt=86.71,	544-64-9	(225.18639, 1773.7521)(226.18898, 301.1615)(227.1913, 56.	MYRISTOLEIC ACID (CAS# 544-64-9); (M-H)-		FindByFormula	26 -	226.1939	22.07019
N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6	N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6)	N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6); (M+Cl)- [,	7512-17-6	(256.05856, 13167.926)(257.05972, 1551.6116)(258.05743, 5	N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6); (M+Cl)-		FindByFormula	25 -	221.0887	0.69056016
N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6	N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6)	N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6); (M+HCOO	7512-17-6	(266.08652, 1013.76337)(267.09375, 301.46664)(268.1009, 7	N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6); (M+HCOO)-		FindByFormula	3 -	221.0881	0.71433395
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5)	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5);	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M-H)- [, t	1115-47-5	(190.0543, 7123.114)(191.05417, 687.3852)(192.05121, 396.	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M-H)-		FindByFormula	27 -	191.0615	4.060766
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M-H)-	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M-H)-	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M-H)- [, tgt=59.08	97-14-3	(146.04558, 38528.605)(147.045, 2369.9568)(148.04453, 31	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M-H)-		FindByFormula	20 -	147.0528	0.68865025
N-ACETYL-D-MANNOSAMINE (CAS# 3615-17-	N-ACETYL-D-MANNOSAMINE (CAS# 3615-17-	N-ACETYL-D-MANNOSAMINE (CAS# 3615-17-6); (M+Cl)-	3615-17-6	(256.05856, 13167.926)(257.05972, 1551.6116)(258.05743, 5	N-ACETYL-D-MANNOSAMINE (CAS# 3615-17-6); (M+Cl)-	C00645	FindByFormula	25 -	221.0887	0.69056016
N-ACETYL-D-TRYPTOPHAN (CAS# 2280-01-5);	N-ACETYL-D-TRYPTOPHAN (CAS# 2280-01-5);	N-ACETYL-D-TRYPTOPHAN (CAS# 2280-01-5); (M-H)- [, t	1/5/2280	(245.09236, 798.53406)(246.08801, 80.354)	N-ACETYL-D-TRYPTOPHAN (CAS# 2280-01-5); (M-H)-	C03137	FindByFormula	5 -	246.0992	7.917754
N-ACETYLGALACTOSAMINE (CAS# 1811-31-0)	N-ACETYLGALACTOSAMINE (CAS# 1811-31-0);	N-ACETYLGALACTOSAMINE (CAS# 1811-31-0); (M+Cl)- [,	1811-31-0	(256.05856, 13167.926)(257.05972, 1551.6116)(258.05743, 5	N-ACETYLGALACTOSAMINE (CAS# 1811-31-0); (M+Cl)-		FindByFormula	25 -	221.0887	0.69056016
N-ACETYLGLYCINE (CAS# 543-24-8); (M-H)-	N-ACETYLGLYCINE (CAS# 543-24-8); (M-H)-	N-ACETYLGLYCINE (CAS# 543-24-8); (M-H)- [, tgt=81.79,	543-24-8	(116.03486, 1052.2555)(117.03336, 28.12889)	N-ACETYLGLYCINE (CAS# 543-24-8); (M-H)-		FindByFormula	9 -	117.0417	0.8557778
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M-H)-	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M-H)-	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M-H)- [, tgt=95.85	97-69-8	(130.05083, 8586.265)(131.05049, 459.76212)(132.05038, 6	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M-H)-		FindByFormula	23 -	131.0581	1.5098696
N-ACETYL-L-ASPARTIC ACID (CAS# 997-55-7);	N-ACETYL-L-ASPARTIC ACID (CAS# 997-55-7);	N-ACETYL-L-ASPARTIC ACID (CAS# 997-55-7); (M-H)- [, t	997-55-7	(174.0404, 2674.8623)(175.03767, 181.05109)(176.04051, 7	N-ACETYL-L-ASPARTIC ACID (CAS# 997-55-7); (M-H)-		FindByFormula	18 -	175.0474	1.0065007
N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M-H	N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M-H	N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M-H)- [, tgt=90.	1188-21-2	(172.09714, 593.84454)(173.09724, 49.02091)	N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M-H)-		FindByFormula	11 -	173.104	7.1582813
N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-	N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-3	N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-3); (M-H)- [	2018-61-3	(206.08203, 531.315)(207.08249, 86.086)	N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-3); (M-H)-	C03519	FindByFormula	10 -	207.0891	7.6781287
N-ACETYLNEURAMINATE (CAS# 131-48-6); (	N-ACETYLNEURAMINATE (CAS# 131-48-6); (	N-ACETYLNEURAMINATE (CAS# 131-48-6); (M-H)- [, tgt=	131-48-6	(308.0984, 1989.8804)(309.09763, 391.06528)(310.09674, 1	N-ACETYLNEURAMINATE (CAS# 131-48-6); (M-H)-		FindByFormula	21 -	309.1041	0.70842886
NAD (CAS# 53-84-9); (M-H)-	NAD (CAS# 53-84-9); (M-H)-	NAD (CAS# 53-84-9); (M-H)- [, tgt=57.01, overall=57.01]	53-84-9	(662.10187, 524.69556)(663.1016, 171.37224)(664.1017, 73.	NAD (CAS# 53-84-9); (M-H)-		FindByFormula	18 -	663.1086	1.0270004
N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3);	N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3);	N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3); (M-H)- [, t	1946-82-3	(187.108, 713.42)(188.1056, 103.46)	N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3); (M-H)-		FindByFormula	1 -	188.1146	0.9350009
N-AMIDINO-L-ASPARTATE (CAS# 6133-30-8);	N-AMIDINO-L-ASPARTATE (CAS# 6133-30-8);	N-AMIDINO-L-ASPARTATE (CAS# 6133-30-8); (M+Cl)+[-H	6133-30-8	(192.0223, 162.76)(193.0122, 206.08)	N-AMIDINO-L-ASPARTATE (CAS# 6133-30-8); (M+Cl)+[-H2O]	C03139	FindByFormula	1 -	175.0576	0.97399956
NAPROXEN (CAS# 22204-53-1); (M-H)-	NAPROXEN (CAS# 22204-53-1); (M-H)-	NAPROXEN (CAS# 22204-53-1); (M-H)- [, tgt=86.81, overa	22204-53-1	(229.08653, 723.0717)(230.08447, 85.695)	NAPROXEN (CAS# 22204-53-1); (M-H)-	C01517	FindByFormula	6 -	230.094	15.702487
N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8);	N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8);	N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8); (M+HCOO)-	75251-80-8	(324.13037, 607.11005)(325.13766, 150.21666)(326.1276, 4	N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8); (M+HCOO)-		FindByFormula	3 -	279.1326	3.607331
NERVONIC ACID (CAS# 506-37-6); (M-H)-	NERVONIC ACID (CAS# 506-37-6); (M-H)-	NERVONIC ACID (CAS# 506-37-6); (M-H)- [, tgt=77.17, ov	506-37-6	(365.34314, 1437.414)(366.3463, 396.86438)(367.35156, 19	NERVONIC ACID (CAS# 506-37-6); (M-H)-	C08323	FindByFormula	25 -	366.3501	24.14249
N-ETHYLMALEIMIDE (CAS# 128-53-0); (M-H)-	N-ETHYLMALEIMIDE (CAS# 128-53-0); (M-H)-	N-ETHYLMALEIMIDE (CAS# 128-53-0); (M-H)- [, tgt=79.2	128-53-0	(124.03987, 782.04126)(125.041626, 39.30875)	N-ETHYLMALEIMIDE (CAS# 128-53-0); (M-H)-	C02441	FindByFormula	8 -	125.047	3.4024932
NICOTINAMIDE HYPOXANTHINE DINUCLEOTI	NICOTINAMIDE HYPOXANTHINE DINUCLEOTI	NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE (CAS# 22	22052-73-9	(663.0901, 263.89)(664.0782, 233.9)	NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE (CAS# 22052-73-9); (M-H)-		FindByFormula	1 -	664.0905	1.0649995
NICOTINATE (CAS# 59-67-6); (M-H)-	NICOTINATE (CAS# 59-67-6); (M-H)-	NICOTINATE (CAS# 59-67-6); (M-H)- [, tgt=74.81, overall	59-67-6	(122.02472, 4330.347)(123.02565, 346.28687)(124.03013, 1	NICOTINATE (CAS# 59-67-6); (M-H)-	C00253	FindByFormula	16 -	123.0321	1.07475
N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-	N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5	N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M-H)- [	6384-92-5	(146.04552, 50460.11)(147.04558, 3180.6726)(148.04509, 4	N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M-H)-	C12269	FindByFormula	20 -	147.0528	0.65335023
N-METHYL-L-GLUTAMATE (CAS# 6753-62-4);	N-METHYL-L-GLUTAMATE (CAS# 6753-62-4);	N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M-H)- [, tg	6753-62-4	(160.06055, 1960.115)(161.06439, 60.79)(162.055, 61.22)	N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M-H)-	C01046	FindByFormula	2 -	161.0675	0.7015003
N-NITROSODIETHANOLAMINE (CAS# 1116-54	N-NITROSODIETHANOLAMINE (CAS# 1116-54	N-NITROSODIETHANOLAMINE (CAS# 1116-54-7); (M+Cl)-	1116-54-7	(169.0413, 357.65)(170.0389, 162.58)	N-NITROSODIETHANOLAMINE (CAS# 1116-54-7); (M+Cl)-		FindByFormula	1 -	134.0704	0.71200067
N-OLEOYLGLYCINE (CAS# 2601-90-3); (M-H)-	N-OLEOYLGLYCINE (CAS# 2601-90-3); (M-H)-	N-OLEOYLGLYCINE (CAS# 2601-90-3); (M-H)- [, tgt=65.84	2601-90-3	(338.27075, 1055.1338)(339.27145, 356.18124)(340.27316, 1	N-OLEOYLGLYCINE (CAS# 2601-90-3); (M-H)-		FindByFormula	8 -	339.2782	22.53124
NONANOATE (CAS# 112-05-0); (M-H)-	NONANOATE (CAS# 112-05-0); (M-H)-	NONANOATE (CAS# 112-05-0); (M-H)- [, tgt=90.91, overa	112-05-0	(157.12337, 2710.0376)(158.12685, 284.51566)(159.12764, 4	NONANOATE (CAS# 112-05-0); (M-H)-		FindByFormula	23 -	158.1307	18.330784
NORLEUCINE (CAS# 327-57-1); (M-H)-	NORLEUCINE (CAS# 327-57-1); (M-H)-	NORLEUCINE (CAS# 327-57-1); (M-H)- [, tgt=86.21, overa	327-57-1	(130.08688, 25122.994)(131.08922, 1918.8585)(132.08742, 8	NORLEUCINE (CAS# 327-57-1); (M-H)-	C01933	FindByFormula	24 -	131.0941	1.6091666
OLEIC ACID (CAS# 112-80-1); (M-H)-	OLEIC ACID (CAS# 112-80-1); (M-H)-	OLEIC ACID (CAS# 112-80-1); (M-H)- [, tgt=96.79, overall	112-80-1	(281.24942, 474812.47)(282.25266, 93290.77)(283.25778, 1	OLEIC ACID (CAS# 112-80-1); (M-H)-		FindByFormula	28 -	282.2568	22.9269
OMEGA-HYDROXYDODECANOIC ACID (CAS#	OMEGA-HYDROXYDODECANOIC ACID (CAS# 5	OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (	505-95-3	(215.16513, 780.2933)(216.16826, 108.90251)(217.1693, 25.	OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M-H)-		FindByFormula	28 -	216.1724	16.980358
OMEPRAZOLE (CAS# 73590-58-6); (M-H)-	OMEPRAZOLE (CAS# 73590-58-6); (M-H)-	OMEPRAZOLE (CAS# 73590-58-6); (M-H)- [, tgt=71.77, ov	73590-58-6	(344.1062, 651.59)(345.1024, 65.75)(346.1155, 45.62)	OMEPRAZOLE (CAS# 73590-58-6); (M-H)-	C07324	FindByFormula	1 -	345.1135	11.124
OMEPRAZOLE SULFONE (CAS# 88546-55-8); (	OMEPRAZOLE SULFONE (CAS# 88546-55-8); (	OMEPRAZOLE SULFONE (CAS# 88546-55-8); (M-H)- [, tgt	88546-55-8	(360.1028, 3851.135)(361.10596, 900.4417)(362.1028, 389.2	OMEPRAZOLE SULFONE (CAS# 88546-55-8); (M-H)-		FindByFormula	6 -	361.1099	12.295391
O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-	O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5	O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5); (M-H)- [,	1492-23-5	(218.0676, 861.04504)(219.0684, 78.14)	O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5); (M-H)-	C01118	FindByFormula	2 -	219.0756	1.0250008
OXALOACETATE (CAS# 328-42-7); (M-H)-[-H2	OXALOACETATE (CAS# 328-42-7); (M-H)-[-H2	OXALOACETATE (CAS# 328-42-7); (M-H)-[-H2O] [, tgt=56	328-42-7	(112.9869, 2114.09)(113.9884, 76.15)	OXALOACETATE (CAS# 328-42-7); (M-H)-[-H2O]		FindByFormula	1 -	132.0047	0.7270003
OXIDIZED GLUTATHIONE (CAS# 27025-41-8);	OXIDIZED GLUTATHIONE (CAS# 27025-41-8);	OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M-H)- [, tg	27025-41-8	(611.14417, 711.6018)(612.14606, 223.01471)(613.138, 129.	OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M-H)-	C00127	FindByFormula	17 -	612.1506	1.3853538
P-ACETAMIDOPHENYL BETA-D-GLUCURONID	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120	120595-80-4	(653.1825, 733.4)(654.1865, 227.272)(655.188, 291.37)(656.	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (2M-H)-		FindByFormula	5 -	327.0954	2.2537968
P-ACETAMIDOPHENYL BETA-D-GLUCURONID	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120	120595-80-4	(326.08868, 11988.383)(327.09116, 2022.7794)(328.09262, 1	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (M-H)-		FindByFormula	17 -	327.0959	2.2619395
PALATINOSE (CAS# 343336-76-5); (M+Cl)-	PALATINOSE (CAS# 343336-76-5); (M+Cl)-	PALATINOSE (CAS# 343336-76-5); (M+Cl)- [, tgt=97.29, o	343336-76-5	(377.08475, 25323.936)(378.08945, 4187.432)(379.08237, 1	PALATINOSE (CAS# 343336-76-5); (M+Cl)-		FindByFormula	24 -	342.116	0.7031669
PALATINOSE (CAS# 343336-76-5); (M+HCOO	PALATINOSE (CAS# 343336-76-5); (M+HCOO)	PALATINOSE (CAS# 343336-76-5); (M+HCOO)- [, tgt=72.4	343336-76-5	(387.11395, 959.8128)(388.11154, 277.31714)(389.1217, 11	PALATINOSE (CAS# 343336-76-5); (M+HCOO)-		FindByFormula	7 -	342.1152	0.7178578
PALMITATE (CAS# 57-10-3); (M-H)-	PALMITATE (CAS# 57-10-3); (M-H)-	PALMITATE (CAS# 57-10-3); (M-H)- [, tgt=98.02, overall=	57-10-3	(255.23369, 256823.33)(256.2368, 44381.24)(257.23944, 48	PALMITATE (CAS# 57-10-3); (M-H)-		FindByFormula	28 -	256.241	22.84576
PALMITIC ACID-13,13,14,14,15,15,16,16,16-D	PALMITIC ACID-13,13,14,14,15,15,16,16,16-D9	PALMITIC ACID-13,13,14,14,15,15,16,16,16-D9 [ISTD] (CAS	1173022-49-5	(264.2898, 28247.504)(265.29303, 4972.081)(266.2962, 602.	PALMITIC ACID-13,13,14,14,15,15,16,16,16-D9 [ISTD] (CAS# 1173022-49-5); (M-H)-		FindByFormula	28 -	265.297	22.820448
PALMITOLEIC ACID (CAS# 373-49-9); (M-H)-	PALMITOLEIC ACID (CAS# 373-49-9); (M-H)-	PALMITOLEIC ACID (CAS# 373-49-9); (M-H)- [, tgt=90.52,	373-49-9	(253.21773, 80275.695)(254.221, 14064.781)(255.22649, 39	PALMITOLEIC ACID (CAS# 373-49-9); (M-H)-		FindByFormula	28 -	254.2249	22.58626
PANTOTHENATE (CAS# 79-83-4); (M+Cl)-	PANTOTHENATE (CAS# 79-83-4); (M+Cl)-	PANTOTHENATE (CAS# 79-83-4); (M+Cl)- [, tgt=70.68, ov	79-83-4	(254.07922, 385.53998)(255.08226, 77.479996)(256.07312, 1	PANTOTHENATE (CAS# 79-83-4); (M+Cl)-	C02349	FindByFormula	8 -	219.1087	3.260495
PANTOTHENATE (CAS# 79-83-4); (M-H)-	PANTOTHENATE (CAS# 79-83-4); (M-H)-	PANTOTHENATE (CAS# 79-83-4); (M-H)- [, tgt=95.14, ove	79-83-4	(218.10344, 6997.086)(219.10509, 821.4415)(220.1046, 130.	PANTOTHENATE (CAS# 79-83-4); (M-H)-	C02349	FindByFormula	28 -	219.1106	3.2714958
PARAXANTHINE (CAS# 611-59-6); (M-H)-	PARAXANTHINE (CAS# 611-59-6); (M-H)-	PARAXANTHINE (CAS# 611-59-6); (M-H)- [, tgt=97.64, ov	611-59-6	(179.05705, 21513.652)(180.05917, 1987.6523)(181.05615, 2	PARAXANTHINE (CAS# 611-59-6); (M-H)-	C13747	FindByFormula	25 -	180.0647	4.4103026
PENTANOATE (CAS# 109-52-4); (M+HCOO)-	PENTANOATE (CAS# 109-52-4); (M+HCOO)-	PENTANOATE (CAS# 109-52-4); (M+HCOO)- [, tgt=64.11,	109-52-4	(147.0666, 461.41)(148.0688, 22.62)	PENTANOATE (CAS# 109-52-4); (M+HCOO)-		FindByFormula	1 -	102.0683	1.9799938
PHENOL (CAS# 108-95-2); (M-H)-	PHENOL (CAS# 108-95-2); (M-H)-	PHENOL (CAS# 108-95-2); (M-H)- [, tgt=88.38, overall=88	108-95-2	(93.03532, 2277.5684)(94.03815, 139.1906)	PHENOL (CAS# 108-95-2); (M-H)-	C00146	FindByFormula	17 -	94.0427	4.058928
PHENYL ACETATE (CAS# 122-79-2); (M+HCO	PHENYL ACETATE (CAS# 122-79-2); (M+HCO	PHENYL ACETATE (CAS# 122-79-2); (M+HCOO)- [, tgt=84.	122-79-2	(181.05063, 3403.1184)(182.05168, 370.546)(183.05458, 13	PHENYL ACETATE (CAS# 122-79-2); (M+HCOO)-	C00548	FindByFormula	25 -	136.0521	3.7870307
PHENYL ACETATE (CAS# 122-79-2); (M-H)-	PHENYL ACETATE (CAS# 122-79-2); (M-H)-	PHENYL ACETATE (CAS# 122-79-2); (M-H)- [, tgt=59.19, o	122-79-2	(135.04602, 1052.6533)(136.04297, 62.716663)	PHENYL ACETATE (CAS# 122-79-2); (M-H)-	C00548	FindByFormula	6 -	136.0537	3.8521595
PHENYLACETIC ACID (CAS# 103-82-2); (M+H	PHENYLACETIC ACID (CAS# 103-82-2); (M+HC	PHENYLACETIC ACID (CAS# 103-82-2); (M+HCOO)- [, tgt=	103-82-2	(181.04974, 465.52502)(182.0511, 29.169998)	PHENYLACETIC ACID (CAS# 103-82-2); (M+HCOO)-	C07086	FindByFormula	2 -	136.0517	5.6539884
PHENYLALANINE (CAS# 63-91-2); (M-H)-	PHENYLALANINE (CAS# 63-91-2); (M-H)-	PHENYLALANINE (CAS# 63-91-2); (M-H)- [, tgt=98.01, ove	63-91-2	(164.07146, 90555.67)(165.07332, 9628.031)(166.07288, 10	PHENYLALANINE (CAS# 63-91-2); (M-H)-	C00079	FindByFormula	20 -	165.0785	2.5164003
PHENYLPYRUVATE (CAS# 156-06-9); (M-H)-	PHENYLPYRUVATE (CAS# 156-06-9); (M-H)-	PHENYLPYRUVATE (CAS# 156-06-9); (M-H)- [, tgt=48.97,	156-06-9	(163.0396, 723.8)(164.0387, 97.48)	PHENYLPYRUVATE (CAS# 156-06-9); (M-H)-	C00166	FindByFormula	1 -	164.0464	5.625941
PHYTANATE (CAS# 14721-66-5); (M-H)-	PHYTANATE (CAS# 14721-66-5); (M-H)-	PHYTANATE (CAS# 14721-66-5); (M-H)- [, tgt=50.60, over	14721-66-5	(311.29388, 2916.9985)(312.29675, 639.5481)(313.2987, 94.	PHYTANATE (CAS# 14721-66-5); (M-H)-	C01607	FindByFormula	26 -	312.3017	23.378174
PICOLINIC ACID (CAS# 98-98-6); (M-H)-	PICOLINIC ACID (CAS# 98-98-6); (M-H)-	PICOLINIC ACID (CAS# 98-98-6); (M-H)- [, tgt=78.28, over	98-98-6	(122.02465, 4033.3428)(123.02432, 274.235)(124.0207, 37.7	PICOLINIC ACID (CAS# 98-98-6); (M-H)-		FindByFormula	16 -	123.0311	0.9675001
PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1	PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 11	PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (	1190-94-9	(161.0913, 478.78)(162.1013, 51.93)	PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M-H)-	C01211	FindByFormula	1 -	162.0993	0.5679996
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)- [, tgt=28.7	363-24-6	(387.19272, 511.37875)(388.19965, 114.659996)(389.18927,	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)-		FindByFormula	8 -	352.2263	16.814354
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)-[-H2O] [, t	363-24-6	(369.1819, 506.32)(370.1956, 53.93)(371.1853, 204.05)	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)-[-H2O]		FindByFormula	1 -	352.2253	16.413092
PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-	PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-	PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)- [, tgt=91.2	363-24-6	(351.21796, 5734.8726)(352.22122, 1324.3142)(353.22116, 2	PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-		FindByFormula	21 -	352.2251	16.733694
PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-	PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-	PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-[-H2O] [, tg	363-24-6	(333.20648, 953.09503)(334.2092, 220.09927)(335.206, 102.	PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-[-H2O]		FindByFormula	14 -	352.224	16.742407
PROTOPORPHYRIN (CAS# 553-12-8); (M-H)-	PROTOPORPHYRIN (CAS# 553-12-8); (M-H)-	PROTOPORPHYRIN (CAS# 553-12-8); (M-H)- [, tgt=20.21,	553-12-8	(561.2539, 380.69)(562.2517, 219.28)(563.268, 285.48)	PROTOPORPHYRIN (CAS# 553-12-8); (M-H)-	C02191	FindByFormula	1 -	562.2624	22.684462
PTERIN (CAS# 2236-60-4); (M-H)-	PTERIN (CAS# 2236-60-4); (M-H)-	PTERIN (CAS# 2236-60-4); (M-H)- [, tgt=67.64, overall=67	2236-60-4	(162.0406, 1204.2)(163.0507, 264.84)	PTERIN (CAS# 2236-60-4); (M-H)-	C00715	FindByFormula	1 -	163.0493	1.508
PURINE (CAS# 120-73-0); (M-H)-	PURINE (CAS# 120-73-0); (M-H)-	PURINE (CAS# 120-73-0); (M-H)- [, tgt=65.31, overall=65.	120-73-0	(119.0352, 701.05)(120.0379, 55.23)	PURINE (CAS# 120-73-0); (M-H)-	C00465	FindByFormula	1 -	120.0425	1.3069988
PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9	PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9)	PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M-H)- [,	89-00-9	(166.01459, 8518.224)(167.02187, 757.7933)(168.0361, 79.6	PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M-H)-		FindByFormula	3 -	167.0224	1.0743335
PYRUVATE (CAS# 127-17-3); (M-H)-	PYRUVATE (CAS# 127-17-3); (M-H)-	PYRUVATE (CAS# 127-17-3); (M-H)- [, tgt=72.27, overall=	127-17-3	(87.00874, 13411.96)(88.01095, 507.4272)(89.02014, 277.69	PYRUVATE (CAS# 127-17-3); (M-H)-		FindByFormula	7 -	88.0154	0.7251426
RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84	RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84	RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-6); (M+HC	75685-84-6	(347.2532, 670.35)(348.2682, 123.82)(349.2358, 785.68)	RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-6); (M+HCOO)-		FindByFormula	1 -	302.2443	22.122347
RAFFINOSE (CAS# 512-69-6); (M+Cl)-	RAFFINOSE (CAS# 512-69-6); (M+Cl)-	RAFFINOSE (CAS# 512-69-6); (M+Cl)- [, tgt=91.21, overall	512-69-6	(539.1383, 26812.88)(540.1419, 5683.4507)(541.13574, 101	RAFFINOSE (CAS# 512-69-6); (M+Cl)-	C00492	FindByFormula	24 -	504.1696	0.713542
RAFFINOSE (CAS# 512-69-6); (M+HCOO)-	RAFFINOSE (CAS# 512-69-6); (M+HCOO)-	RAFFINOSE (CAS# 512-69-6); (M+HCOO)- [, tgt=46.25, ov	512-69-6	(549.1673, 545.66)(550.1749, 208.45)(551.1687, 98.90749)	RAFFINOSE (CAS# 512-69-6); (M+HCOO)-	C00492	FindByFormula	10 -	504.1688	0.73020047
RETINOATE (CAS# 302-79-4); (M-H)-	RETINOATE (CAS# 302-79-4); (M-H)-	RETINOATE (CAS# 302-79-4); (M-H)- [, tgt=88.06, overall	302-79-4	(299.20255, 6179.6562)(300.20587, 1334.1323)(301.2076, 2	RETINOATE (CAS# 302-79-4); (M-H)-		FindByFormula	23 -	300.211	22.273697
RIBITOL (CAS# 488-81-3); (M+Cl)-	RIBITOL (CAS# 488-81-3); (M+Cl)-	RIBITOL (CAS# 488-81-3); (M+Cl)- [, tgt=69.17, overall=6	488-81-3	(187.0381, 789.37396)(188.04286, 80.229)(189.03424, 685.5	RIBITOL (CAS# 488-81-3); (M+Cl)-	C00474	FindByFormula	10 -	152.0684	0.68880033
RIBOFLAVIN (CAS# 83-88-5); (M+Cl)-	RIBOFLAVIN (CAS# 83-88-5); (M+Cl)-	RIBOFLAVIN (CAS# 83-88-5); (M+Cl)- [, tgt=79.97, overall	83-88-5	(411.1046, 423.85)(412.119, 66.08)(413.109, 141.51)	RIBOFLAVIN (CAS# 83-88-5); (M+Cl)-		FindByFormula	1 -	376.1379	7.5868506
RIBOFLAVIN (CAS# 83-88-5); (M+HCOO)-	RIBOFLAVIN (CAS# 83-88-5); (M+HCOO)-	RIBOFLAVIN (CAS# 83-88-5); (M+HCOO)- [, tgt=82.41, ov	83-88-5	(421.13788, 490.50504)(422.13824, 106.01214)(423.14444, 1	RIBOFLAVIN (CAS# 83-88-5); (M+HCOO)-		FindByFormula	14 -	376.1406	7.5752797
RIBOFLAVIN (CAS# 83-88-5); (M-H)-	RIBOFLAVIN (CAS# 83-88-5); (M-H)-	RIBOFLAVIN (CAS# 83-88-5); (M-H)- [, tgt=74.96, overall=	83-88-5	(375.13156, 540.84216)(376.1336, 126.32)(377.1321, 85.35)	RIBOFLAVIN (CAS# 83-88-5); (M-H)-		FindByFormula	14 -	376.1383	7.577216
RIBOSE (CAS# 50-69-1); (M+Cl)-	RIBOSE (CAS# 50-69-1); (M+Cl)-	RIBOSE (CAS# 50-69-1); (M+Cl)- [, tgt=69.33, overall=69.	50-69-1	(185.02158, 4432.47)(186.02509, 415.6259)(187.0234, 145.6	RIBOSE (CAS# 50-69-1); (M+Cl)-	C00121	FindByFormula	17 -	150.0525	0.70423555
RIBOSE 5-PHOSPHATE (CAS# 4300-28-1); (M-	RIBOSE 5-PHOSPHATE (CAS# 4300-28-1); (M-	RIBOSE 5-PHOSPHATE (CAS# 4300-28-1); (M-H)- [, tgt=3	4300-28-1	(229.01059, 742.43)(230.01764, 86.235)	RIBOSE 5-PHOSPHATE (CAS# 4300-28-1); (M-H)-	C00117	FindByFormula	2 -	230.0189	0.9055005
S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92	S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92	S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-0); (M-H)-	979-92-0	(383.11435, 2881.1194)(384.11172, 608.08264)(385.11368, 1	S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-0); (M-H)-	C00021	FindByFormula	19 -	384.1182	1.4600528
SALICYLATE (CAS# 69-72-7); (M-H)-	SALICYLATE (CAS# 69-72-7); (M-H)-	SALICYLATE (CAS# 69-72-7); (M-H)- [, tgt=67.60, overall=	69-72-7	(137.02461, 55225.105)(138.02739, 4405.768)(139.02837, 5	SALICYLATE (CAS# 69-72-7); (M-H)-	C00805	FindByFormula	28 -	138.0319	4.94141
SALICYLURIC ACID (CAS# 487-54-7); (M-H)-	SALICYLURIC ACID (CAS# 487-54-7); (M-H)-	SALICYLURIC ACID (CAS# 487-54-7); (M-H)- [, tgt=86.35,	487-54-7	(194.0473, 4536.7944)(195.05121, 430.55334)(196.05145, 8	SALICYLURIC ACID (CAS# 487-54-7); (M-H)-	C07588	FindByFormula	6 -	195.0545	6.1931396
S-CARBOXYMETHYL-L-CYSTEINE (CAS# 638-2	S-CARBOXYMETHYL-L-CYSTEINE (CAS# 638-23	S-CARBOXYMETHYL-L-CYSTEINE (CAS# 638-23-3); (M-H)-	638-23-3	(178.0184, 702.99)(179.0119, 55.54)	S-CARBOXYMETHYL-L-CYSTEINE (CAS# 638-23-3); (M-H)-	C03727	FindByFormula	1 -	179.025	0.71800035
SEBACIC ACID (CAS# 111-20-6); (M-H)-	SEBACIC ACID (CAS# 111-20-6); (M-H)-	SEBACIC ACID (CAS# 111-20-6); (M-H)- [, tgt=91.01, over	111-20-6	(201.11348, 1853.9978)(202.11597, 212.03821)(203.11848, 1	SEBACIC ACID (CAS# 111-20-6); (M-H)-	C08277	FindByFormula	28 -	202.1205	12.897008
SERINE (CAS# 56-45-1); (M-H)-	SERINE (CAS# 56-45-1); (M-H)-	SERINE (CAS# 56-45-1); (M-H)- [, tgt=97.41, overall=97.4	56-45-1	(104.03567, 6585.9756)(105.037796, 251.84573)(106.03967,	SERINE (CAS# 56-45-1); (M-H)-	C00065	FindByFormula	21 -	105.0431	0.6302859
SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 283	SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 283	SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (	28319-77-9	(292.07208, 6594.7095)(293.06958, 785.005)(294.06845, 19	SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (M+Cl)-	C00670	FindByFormula	20 -	257.1029	0.66250026
SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 283	SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 283	SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (	28319-77-9	(302.0976, 774.95)(303.1126, 111.82)	SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (M+HCOO)-	C00670	FindByFormula	1 -	257.1009	0.8590005
SPHINGANINE (CAS# 764-22-7); (M+HCOO)-[	SPHINGANINE (CAS# 764-22-7); (M+HCOO)-[-	SPHINGANINE (CAS# 764-22-7); (M+HCOO)-[-H2O] [, tgt=	764-22-7	(328.2882, 492.62)(329.2914, 35.17)	SPHINGANINE (CAS# 764-22-7); (M+HCOO)-[-H2O]	C00836	FindByFormula	1 -	301.3006	22.455553
STACHYOSE (CAS# 54261-98-2); (M+Cl)-	STACHYOSE (CAS# 54261-98-2); (M+Cl)-	STACHYOSE (CAS# 54261-98-2); (M+Cl)- [, tgt=98.48, ove	54261-98-2	(701.19147, 10831.811)(702.195, 3127.9875)(703.19006, 43	STACHYOSE (CAS# 54261-98-2); (M+Cl)-		FindByFormula	22 -	666.2218	0.7156367
STACHYOSE (CAS# 54261-98-2); (M+HCOO)-	STACHYOSE (CAS# 54261-98-2); (M+HCOO)-	STACHYOSE (CAS# 54261-98-2); (M+HCOO)- [, tgt=71.21,	54261-98-2	(711.2185, 299.47)(712.2155, 123.57)(713.2307, 25.0)	STACHYOSE (CAS# 54261-98-2); (M+HCOO)-		FindByFormula	1 -	666.2189	0.7150007
STACHYOSE (CAS# 54261-98-2); (M-H)-	STACHYOSE (CAS# 54261-98-2); (M-H)-	STACHYOSE (CAS# 54261-98-2); (M-H)- [, tgt=68.38, over	54261-98-2	(665.2145, 415.6042)(666.2166, 125.616844)(667.2114, 53.8	STACHYOSE (CAS# 54261-98-2); (M-H)-		FindByFormula	19 -	666.2205	0.8014216
STEARATE (CAS# 57-11-4); (M-H)-	STEARATE (CAS# 57-11-4); (M-H)-	STEARATE (CAS# 57-11-4); (M-H)- [, tgt=97.43, overall=9	57-11-4	(283.2653, 266807.4)(284.26828, 52189.59)(285.2711, 6171.	STEARATE (CAS# 57-11-4); (M-H)-		FindByFormula	28 -	284.2725	23.18279
SUBERIC ACID (CAS# 505-48-6); (M-H)-	SUBERIC ACID (CAS# 505-48-6); (M-H)-	SUBERIC ACID (CAS# 505-48-6); (M-H)- [, tgt=71.25, over	505-48-6	(173.08185, 5482.7417)(174.08395, 500.47845)(175.07655, 7	SUBERIC ACID (CAS# 505-48-6); (M-H)-	C08278	FindByFormula	19 -	174.0883	8.203414
SUCCINATE (CAS# 110-15-6); (M-H)-	SUCCINATE (CAS# 110-15-6); (M-H)-	SUCCINATE (CAS# 110-15-6); (M-H)- [, tgt=94.17, overall	110-15-6	(117.01954, 18082.283)(118.024925, 926.7444)(119.02761, 1	SUCCINATE (CAS# 110-15-6); (M-H)-	C00042	FindByFormula	25 -	118.0268	1.3276801
SUCROSE (CAS# 57-50-1); (M+Cl)-	SUCROSE (CAS# 57-50-1); (M+Cl)-	SUCROSE (CAS# 57-50-1); (M+Cl)- [, tgt=96.37, overall=9	57-50-1	(377.08475, 25323.936)(378.08945, 4187.432)(379.08237, 1	SUCROSE (CAS# 57-50-1); (M+Cl)-	C00089	FindByFormula	24 -	342.116	0.7031669
SUCROSE (CAS# 57-50-1); (M+HCOO)-	SUCROSE (CAS# 57-50-1); (M+HCOO)-	SUCROSE (CAS# 57-50-1); (M+HCOO)- [, tgt=73.50, overa	57-50-1	(387.11395, 959.8128)(388.11154, 277.31714)(389.1217, 11	SUCROSE (CAS# 57-50-1); (M+HCOO)-	C00089	FindByFormula	7 -	342.1152	0.7178578
SULFADIMETHOXINE (CAS# 122-11-2); (M-H)	SULFADIMETHOXINE (CAS# 122-11-2); (M-H)	SULFADIMETHOXINE (CAS# 122-11-2); (M-H)- [, tgt=91.2	122-11-2	(309.0675, 1801.49)(310.0704, 350.59)(311.0669, 149.56)	SULFADIMETHOXINE (CAS# 122-11-2); (M-H)-		FindByFormula	1 -	310.0749	9.309787

TAURINE (CAS# 107-35-7); (M-H)-	TAURINE (CAS# 107-35-7); (M-H)-	TAURINE (CAS# 107-35-7); (M-H)- [, tgt=95.96, overall=9	107-35-7	(124.00702, 103095.24)(125.008156, 3793.3652)(126.00447,	TAURINE (CAS# 107-35-7); (M-H)-		FindByFormula	25	-	125.0145	0.6439602
THEOPHYLLINE (CAS# 58-55-9); (M-H)-	THEOPHYLLINE (CAS# 58-55-9); (M-H)-	THEOPHYLLINE (CAS# 58-55-9); (M-H)- [, tgt=96.23, over	58-55-9	(179.05705, 21523.885)(180.05888, 1979.4075)(181.05612,	THEOPHYLLINE (CAS# 58-55-9); (M-H)-	C07130	FindByFormula	25	-	180.0647	4.4103026
THREONINE (CAS# 72-19-5); (M+HCOO)-[-H2	THREONINE (CAS# 72-19-5); (M+HCOO)-[-H2	THREONINE (CAS# 72-19-5); (M+HCOO)-[-H2O] [, tgt=59.	72-19-5	(146.04578, 30461.088)(147.04471, 1815.8488)(148.04332,	THREONINE (CAS# 72-19-5); (M+HCOO)-[-H2O]	C00188	FindByFormula	17	-	119.0579	0.69370615
THROMBOXANE B2 (CAS# 54397-85-2); (M-H	THROMBOXANE B2 (CAS# 54397-85-2); (M-H	THROMBOXANE B2 (CAS# 54397-85-2); (M-H)-[-H2O] [, t	54397-85-2	(351.21796, 5736.2153)(352.22122, 1324.3314)(353.22116,	THROMBOXANE B2 (CAS# 54397-85-2); (M-H)-[-H2O]	C05963	FindByFormula	21	-	370.2357	16.733694
THYMIDINE (CAS# 50-89-5); (M+Cl)-	THYMIDINE (CAS# 50-89-5); (M+Cl)-	THYMIDINE (CAS# 50-89-5); (M+Cl)- [, tgt=64.33, overall	50-89-5	(277.06055, 651.3729)(278.0616, 72.255714)(279.05344, 28	THYMIDINE (CAS# 50-89-5); (M+Cl)-	C00214	FindByFormula	7	-	242.0893	2.6792862
THYMIDINE (CAS# 50-89-5); (M+HCOO)-	THYMIDINE (CAS# 50-89-5); (M+HCOO)-	THYMIDINE (CAS# 50-89-5); (M+HCOO)- [, tgt=74.64, ov	50-89-5	(287.08832, 600.225)(288.09088, 100.15101)(289.094, 74.30	THYMIDINE (CAS# 50-89-5); (M+HCOO)-	C00214	FindByFormula	10	-	242.0895	2.5594974
THYMIDINE (CAS# 50-89-5); (M-H)-	THYMIDINE (CAS# 50-89-5); (M-H)-	THYMIDINE (CAS# 50-89-5); (M-H)- [, tgt=87.83, overall=	50-89-5	(241.08212, 608.8375)(242.07901, 71.1375)	THYMIDINE (CAS# 50-89-5); (M-H)-	C00214	FindByFormula	4	-	242.0886	2.7365015
THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-	THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-	THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-07-1); (M-H	365-07-1	(321.0501, 546.975)(322.04858, 365.5875)	THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-07-1); (M-H)-	C00364	FindByFormula	4	-	322.0548	1.5852507
THYMINE (CAS# 65-71-4); (M-H)-	THYMINE (CAS# 65-71-4); (M-H)-	THYMINE (CAS# 65-71-4); (M-H)- [, tgt=86.47, overall=86	65-71-4	(125.0354, 1106.2554)(126.03504, 59.565456)	THYMINE (CAS# 65-71-4); (M-H)-		FindByFormula	11	-	126.0419	1.7209107
THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#	THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#	THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#); (M-H)- [, tgt=90.36, overall=90.36]		(129.06088, 41481.46)(130.06883, 1227.6729)(131.06749, 1	THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#); (M-H)-		FindByFormula	7	-	130.0683	1.7010012
THYROXINE (CAS# 51-48-9); (M-H)-	THYROXINE (CAS# 51-48-9); (M-H)-	THYROXINE (CAS# 51-48-9); (M-H)- [, tgt=98.16, overall=	51-48-9	(775.6804, 1759.5111)(776.6852, 312.76498)(777.67377, 54.	THYROXINE (CAS# 51-48-9); (M-H)-	C01829	FindByFormula	8	-	776.6864	16.161041
TRANS-ACONITATE (CAS# 4023-65-8); (M-H)-	TRANS-ACONITATE (CAS# 4023-65-8); (M-H)-	TRANS-ACONITATE (CAS# 4023-65-8); (M-H)- [, tgt=76.3	4023-65-8	(173.00903, 10563.931)(174.0162, 766.6757)(175.0144, 55.4	TRANS-ACONITATE (CAS# 4023-65-8); (M-H)-	C02341	FindByFormula	14	-	174.0165	1.1733572
TRANS-VACCENIC ACID (CAS# 693-72-1); (M-	TRANS-VACCENIC ACID (CAS# 693-72-1); (M-	TRANS-VACCENIC ACID (CAS# 693-72-1); (M-H)- [, tgt=96	693-72-1	(281.24942, 474812.47)(282.25266, 93290.77)(283.25778, 1	TRANS-VACCENIC ACID (CAS# 693-72-1); (M-H)-	C08367	FindByFormula	28	-	282.2568	22.9269
TRIACONTANOIC ACID (CAS# 506-50-3); (M-	TRIACONTANOIC ACID (CAS# 506-50-3); (M-	TRIACONTANOIC ACID (CAS# 506-50-3); (M-H)- [, tgt=40.	506-50-3	(451.45212, 255.72002)(452.4543, 71.30167)	TRIACONTANOIC ACID (CAS# 506-50-3); (M-H)-		FindByFormula	6	-	452.4593	28.595987
TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)	TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)-	TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)- [, tgt=89.7	99-14-9	(175.02493, 7621.221)(176.02663, 576.0175)(177.0291, 384.	TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)-		FindByFormula	8	-	176.0322	1.2839994
TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)	TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)-	TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)-[-H2O] [, tg	99-14-9	(157.01324, 2124.54)(158.01321, 70.848)(159.01933, 86.533	TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)-[-H2O]		FindByFormula	10	-	176.0315	1.2156998
TRICOSANOIC ACID (CAS# 2433-96-7); (M-H)	TRICOSANOIC ACID (CAS# 2433-96-7); (M-H)-	TRICOSANOIC ACID (CAS# 2433-96-7); (M-H)- [, tgt=92.9	2433-96-7	(353.34283, 1861.1282)(354.34598, 505.54803)(355.346, 12	TRICOSANOIC ACID (CAS# 2433-96-7); (M-H)-		FindByFormula	26	-	354.35	24.37251
TRIDECANOIC ACID (CAS# 638-53-9); (M-H)-	TRIDECANOIC ACID (CAS# 638-53-9); (M-H)-	TRIDECANOIC ACID (CAS# 638-53-9); (M-H)- [, tgt=86.43,	638-53-9	(213.18607, 1049.6925)(214.18855, 157.49258)(215.18658,	TRIDECANOIC ACID (CAS# 638-53-9); (M-H)-		FindByFormula	27	-	214.1931	22.160337
TRYPTOPHAN (CAS# 73-22-3); (2M-H)-	TRYPTOPHAN (CAS# 73-22-3); (2M-H)-	TRYPTOPHAN (CAS# 73-22-3); (2M-H)- [, tgt=71.45, over	73-22-3	(407.17258, 7499.9463)(408.1751, 2065.9465)(409.16965, 2	TRYPTOPHAN (CAS# 73-22-3); (2M-H)-		FindByFormula	9	-	204.0883	3.5992177
TRYPTOPHAN (CAS# 73-22-3); (M-H)-	TRYPTOPHAN (CAS# 73-22-3); (M-H)-	TRYPTOPHAN (CAS# 73-22-3); (M-H)- [, tgt=79.01, overal	73-22-3	(203.08286, 136922.19)(204.08514, 17779.248)(205.07806,	TRYPTOPHAN (CAS# 73-22-3); (M-H)-		FindByFormula	11	-	204.0893	3.598719
TYROSINE (CAS# 60-18-4); (M-H)-	TYROSINE (CAS# 60-18-4); (M-H)-	TYROSINE (CAS# 60-18-4); (M-H)- [, tgt=94.96, overall=9	60-18-4	(180.06654, 21716.54)(181.06943, 2336.4119)(182.06744, 2	TYROSINE (CAS# 60-18-4); (M-H)-		FindByFormula	27	-	181.0738	1.3452226
UDP-GALACTOSE (CAS# 2956-16-3); (M-H)-	UDP-GALACTOSE (CAS# 2956-16-3); (M-H)-	UDP-GALACTOSE (CAS# 2956-16-3); (M-H)- [, tgt=31.64,	2956-16-3	(565.0498, 662.6475)(566.0499, 114.145004)(567.0559, 43.2	UDP-GALACTOSE (CAS# 2956-16-3); (M-H)-	C00052	FindByFormula	4	-	566.0541	1.6315026
UDP-GLUCOSE (CAS# 133-89-1); (M-H)-	UDP-GLUCOSE (CAS# 133-89-1); (M-H)-	UDP-GLUCOSE (CAS# 133-89-1); (M-H)- [, tgt=31.55, over	133-89-1	(565.0501, 661.99664)(566.0562, 144.09999)(567.0691, 59.6	UDP-GLUCOSE (CAS# 133-89-1); (M-H)-	C00029	FindByFormula	3	-	566.0599	1.6110026
UDP-N-ACETYL-D-GALACTOSAMINE (CAS#);	UDP-N-ACETYL-D-GALACTOSAMINE (CAS#);	UDP-N-ACETYL-D-GALACTOSAMINE (CAS#); (M-H)- [, tgt=30.31, overall=30.31]		(606.07837, 404.7)(607.0714, 160.515)(608.0608, 124.18)	UDP-N-ACETYL-D-GALACTOSAMINE (CAS#); (M-H)-		FindByFormula	2	-	607.0789	1.2479998
UDP-N-ACETYL-D-GLUCOSAMINE (CAS# 528-	UDP-N-ACETYL-D-GLUCOSAMINE (CAS# 528-0	UDP-N-ACETYL-D-GLUCOSAMINE (CAS# 528-04-1); (M-H)	528-04-1	(606.077, 548.052)(607.0758, 162.728)(608.07245, 70.62749	UDP-N-ACETYL-D-GLUCOSAMINE (CAS# 528-04-1); (M-H)-	C00043	FindByFormula	5	-	607.0836	1.3654001
URACIL (CAS# 66-22-8); (M-H)-	URACIL (CAS# 66-22-8); (M-H)-	URACIL (CAS# 66-22-8); (M-H)- [, tgt=84.44, overall=84.4	66-22-8	(111.01948, 4086.7827)(112.01888, 211.83412)(113.020164,	URACIL (CAS# 66-22-8); (M-H)-		FindByFormula	17	-	112.0267	0.96076494
URATE (CAS# 69-93-2); (M-H)-	URATE (CAS# 69-93-2); (M-H)-	URATE (CAS# 69-93-2); (M-H)- [, tgt=92.23, overall=92.2	69-93-2	(167.02092, 82761.05)(168.02473, 5714.6543)(169.02174, 8	URATE (CAS# 69-93-2); (M-H)-		FindByFormula	27	-	168.0282	1.030741
URIDINE (CAS# 58-96-8); (M+Cl)-	URIDINE (CAS# 58-96-8); (M+Cl)-	URIDINE (CAS# 58-96-8); (M+Cl)- [, tgt=96.09, overall=96	58-96-8	(279.03998, 160541.1)(280.04343, 17646.764)(281.03677, 5	URIDINE (CAS# 58-96-8); (M+Cl)-		FindByFormula	27	-	244.0705	1.3595186
URIDINE (CAS# 58-96-8); (M+HCOO)-	URIDINE (CAS# 58-96-8); (M+HCOO)-	URIDINE (CAS# 58-96-8); (M+HCOO)- [, tgt=91.73, overal	58-96-8	(289.06772, 20915.973)(290.07178, 2824.9512)(291.07196,	URIDINE (CAS# 58-96-8); (M+HCOO)-		FindByFormula	27	-	244.0701	1.3691114
URIDINE (CAS# 58-96-8); (M-H)-	URIDINE (CAS# 58-96-8); (M-H)-	URIDINE (CAS# 58-96-8); (M-H)- [, tgt=96.54, overall=96.	58-96-8	(243.06258, 77735.414)(244.06436, 8517.014)(245.06505, 1	URIDINE (CAS# 58-96-8); (M-H)-		FindByFormula	28	-	244.07	1.3696432
URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9	URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9)	URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (M-H)- [,	58-97-9	(323.0288, 1266.5648)(324.02756, 203.5678)(325.0233, 322.	URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (M-H)-		FindByFormula	18	-	324.035	1.0441116
UROCANATE (CAS# 104-98-3); (M-H)-	UROCANATE (CAS# 104-98-3); (M-H)-	UROCANATE (CAS# 104-98-3); (M-H)- [, tgt=95.72, overa	104-98-3	(137.03535, 30811.092)(138.03662, 2394.9229)(139.03648,	UROCANATE (CAS# 104-98-3); (M-H)-	C00785	FindByFormula	21	-	138.0429	0.92214346
URSODIOL (CAS# 128-13-2); (M+HCOO)-	URSODIOL (CAS# 128-13-2); (M+HCOO)-	URSODIOL (CAS# 128-13-2); (M+HCOO)- [, tgt=74.13, ov	128-13-2	(437.29025, 2400.5334)(438.2942, 712.6084)(439.29596, 20	URSODIOL (CAS# 128-13-2); (M+HCOO)-		FindByFormula	18	-	392.2932	21.573147
URSODIOL (CAS# 128-13-2); (M-H)-	URSODIOL (CAS# 128-13-2); (M-H)-	URSODIOL (CAS# 128-13-2); (M-H)- [, tgt=83.00, overall=	128-13-2	(391.286, 11166.975)(392.28894, 3071.2961)(393.28168, 87	URSODIOL (CAS# 128-13-2); (M-H)-		FindByFormula	8	-	392.2928	21.683474
VALINE (CAS# 72-18-4); (M-H)-	VALINE (CAS# 72-18-4); (M-H)-	VALINE (CAS# 72-18-4); (M-H)- [, tgt=86.61, overall=86.6	72-18-4	(116.07103, 1693.4573)(117.0716, 88.30191)	VALINE (CAS# 72-18-4); (M-H)-		FindByFormula	21	-	117.0783	0.8793337
XANTHINE (CAS# 69-89-6); (M-H)-	XANTHINE (CAS# 69-89-6); (M-H)-	XANTHINE (CAS# 69-89-6); (M-H)- [, tgt=75.51, overall=7	69-89-6	(151.02612, 28418.771)(152.02945, 2280.396)(153.02898, 3	XANTHINE (CAS# 69-89-6); (M-H)-		FindByFormula	28	-	152.0336	1.2346431
XANTHOSINE (CAS# 146-80-5); (M-H)-	XANTHOSINE (CAS# 146-80-5); (M-H)-	XANTHOSINE (CAS# 146-80-5); (M-H)- [, tgt=94.73, overa	146-80-5	(283.06952, 2564.6318)(284.07065, 339.33078)(285.0692, 7	XANTHOSINE (CAS# 146-80-5); (M-H)-	C01762	FindByFormula	25	-	284.076	2.2859988
XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8)	XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8);	XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8); (M-H)- [, t	523-98-8	(363.0345, 584.96)(364.0295, 46.02)	XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8); (M-H)-	C00655	FindByFormula	1	-	364.0412	1.130002
XANTHURENIC ACID (CAS# 59-00-7); (M-H)-	XANTHURENIC ACID (CAS# 59-00-7); (M-H)-	XANTHURENIC ACID (CAS# 59-00-7); (M-H)- [, tgt=61.38,	59-00-7	(204.02911, 452.53336)(205.03076, 65.55)	XANTHURENIC ACID (CAS# 59-00-7); (M-H)-	C02470	FindByFormula	3	-	205.0362	4.610952
XYLOSE (CAS# 58-86-6); (M+HCOO)-	XYLOSE (CAS# 58-86-6); (M+HCOO)-	XYLOSE (CAS# 58-86-6); (M+HCOO)- [, tgt=56.41, overall	58-86-6	(195.05046, 4235.6133)(196.0577, 223.71333)(197.05534, 1	XYLOSE (CAS# 58-86-6); (M+HCOO)-	C00181	FindByFormula	3	-	150.0522	0.6620002
ZEATIN [ISTD] (CAS# 13114-27-7); (M+Cl)-	ZEATIN [ISTD] (CAS# 13114-27-7); (M+Cl)-	ZEATIN [ISTD] (CAS# 13114-27-7); (M+Cl)- [, tgt=97.41, o	13114-27-7	(254.08186, 80646.96)(255.08424, 10402.217)(256.07898, 2	ZEATIN [ISTD] (CAS# 13114-27-7); (M+Cl)-		FindByFormula	28	-	219.1123	3.8765266
ZEATIN [ISTD] (CAS# 13114-27-7); (M-H)-	ZEATIN [ISTD] (CAS# 13114-27-7); (M-H)-	ZEATIN [ISTD] (CAS# 13114-27-7); (M-H)- [, tgt=97.31, ov	13114-27-7	(218.10513, 473471.16)(219.10771, 59817.344)(220.10983,	ZEATIN [ISTD] (CAS# 13114-27-7); (M-H)-		FindByFormula	28	-	219.1125	3.8769913

Compound	Neg Pool QC 1	Neg Pool QC 2	Neg Pool QC 3	Neg Pool QC 4	Neg_Human Plasma Extraction_1	Neg_Human Plasma Extraction_2	Neg_Human Plasma Extraction_3	Neg_Human Plasma Extraction_4	Neg_Human Plasma Extraction_5	Neg_Human Plasma Extraction_6	Neg_S00015447_1	Neg_S00015448_2	Neg_S00015449_3	Neg_S00015450_4	Neg_S00015451_5	Neg_S00015452_6	Neg_S00015453_7	Neg_S00015454_8	Neg_S00015455_9	Neg_S00015456_10	Neg_S00015457_11	Neg_S00015458_12	Neg_S00015459_13	Neg_S00015460_14	Neg_S00015461_15	Neg_S00015462_16	Neg_S00015463_17	Neg_S00015464_18
(S)-3-METHYL-2-OXOPENTANOATE (CAS# 1460-34-0); (M-H)-	23718	25047	19576	24388	1867888	1867747	1822256	1837820	1821625	1738295		28134			8896			7972	38479	12757	6312	5049	37361	37892		49762	8539	9775
(S)-DIHYDROOROTATE (CAS# 5988-19-2); (M-H)-																												1659
1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 3436-44-0); (M+HCOO)-																							2529			2206		
1,3,7-TRIMETHYLURIC ACID (CAS# 5415-44-1); (M-H)-		1463		2010	64466	64285	62742	60255	64666	64261											5076		3739	3817				
1,3-DIMETHYLURIC ACID (CAS# 944-73-0); (M-H)-					17473	15827	19792	15629	15223	14726																		1796
1,7-DIMETHYL URIC ACID (CAS# 33868-03-0); (M-H)-	2619		2102	2570	93717	90629	86258	85171	86332	86991	3447						3898	16794			7783		11580	6263				16155
1051.555@4.949982					28951	28381	27233	25323	26242	26692																		
1054.5459@11.908065					40645	40205	40511	39137	34910	35528																		
1097.5635@8.565948					146933	144119	149435	145403	146793	140086																		
10-HYDROXYDECANOATE (CAS# 1679-53-4); (M-H)-	9100	7305	5760	5928					3975			8102	4465	3529	6995		8421	8896	11718	6307	8938	1918	12665	7557		10512	3825	4396
11-DEOXYCORTISOL (CAS# 152-58-9); (M+HCOO)-					4344	4379	4968	3938	4056																			
1210.6486@10.216925					402426	380883	384587	367399	374056	368815																		
1232.6279@10.218259					62411	60721	62279	60399	58366	57632																		
1395.5635@11.9522295					49113	44994	47166	46131	47754	45515																		
1435.7188@12.801547					38755	35732	38513	35248	36380	37163																		
1535.6862@9.177106					47543	47865	49932	46884	45617	45384																		
1557.6674@9.176914					18712	20515	19557		18804																			
16:0 LYSO PC (CAS# 17364-16-8); (M+Cl)-	2182		1736	1254			11568	9612		8077	2297					1702	1226	2956	3488	7134	5316		2481	1737				6436
16:0 LYSO PC (CAS# 17364-16-8); (M+HCOO)-	127984	118679	112512	110276	3210624	3106695	3186391	2970551	2903015	2705662	96041	69801	23174	30033	39803	66482	87313	151603	129066	279613	275004	51392	135532	104585	8221	75533	57752	212627
16:0-18:0 PC (CAS# 59403-51-9); (M+Cl)-				54679							16566	26916		9730	42516	98035			151828									156618
16:0-18:0 PC (CAS# 59403-51-9); (M+HCOO)-	8242	9273	11265	6364	5205						13349					4916	8727	16757	17349	16259	27143		13862	8382		8525	5315	22333
18:0 LYSO-PE (CAS# 69747-55-3); (M-H)-	12706	13468	10475	11275	43545	39194	42569	34419	36041	40424	62511	10539	1343	4583	11732	47010	5908	16052	9165	19762	16352	14156	9270	10096		8221	5866	18435
196.8179@0.71062976	3793687	3560021	3522029	3366354	11623	10756	8647	11711		9994	3033940	3617748	2811705	3266512	3041040	2975478	5379001	2260866	1823671	2559972	2627589	3977539	3848974	4442906	2804021	4025268	2782336	2048880
1-HYDROXY-2-NAPHTHOATE (CAS# 86-48-6); (M-H)-					3670	2992	6882	2839	5287	2731																		
1-METHYLADENOSINE (CAS# 15763-06-1); (M+Cl)-						2263				2220								1219	1522									
1-METHYLADENOSINE (CAS# 15763-06-1); (M+HCOO)-					3154		1973		2236										2011		2415							
1-METHYLURIC ACID (CAS# 708-79-2); (2M-H)-					6366	4638	6403	2272	1189	2747																		
1-METHYLURIC ACID (CAS# 708-79-2); (M-H)-				2331							7115						6570	24070			2160							16131
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+HCOO)-															2121		1614											
2',3'-CYCLIC CMP (CAS# 15718-51-1); (M-H)-											3890	6532	2722			6311						1299			1068			
2,3-DIHYDROXY-2-PHOSPHONOPROPANOIC ACID (CAS# 2553-59-5); (M-H)-								4548																				
2,3-DIHYDROXYBENZOATE (CAS# 303-38-8); (M-H)-					245977	235563	230061	130348	229980	222056									14791	24239	19107					11313		15315
2',4'-DIHYDROXYACETOPHENONE (CAS# 89-84-9); (M-H)-					18006		18758	15884	16578	18336															7742			
2,5-DIOXOPIPERAZINE (CAS# 106-57-0); (M-H)-						12219																						
20:0 LYSO PC (CAS# 108341-80-6); (M+Cl)-												1201		1207	1301													
24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M+HCOO)-	11681	3900	7203	4707		1024			1472		12677	1408		4087	1659	2094	6476	13997	21302	29345	75532		12898	6347		3416	3911	45719
265.2973@22.820448	133980	143012	152802	149276	130644	128062	131922	138962	153657	148225	232475	139796	119979	167832	308199	154437	93986	121537	77921	106432	117785	175560	151483	135543	150764	124629	175397	115453
2-AMINOETHYL DIHYDROGEN PHOSPHATE (CAS# 1071-23-4);	52158	63410	65741	41292							231482	52783	7582	40035	226571	78447	20821	7860		23307	34821	33400	25458		24421	50819	140051	
2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Cl)-	88876	84527			297986	291385		283657	274879	265511			6316						103172	235508			108304				32930	
2'-DEOXYINOSINE (CAS# 890-38-0); (M-H)-	2475	5810		1198								67208			2192					7851	13841		3961			5157		
2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 4026-18-0); (M-H	68586	69755	66587	63777	1015303	989421	963325	939521	972149	14930	82574	9860			52780	35288	114628	78825	152004	215829	20251	16654	78764	53539		53905	33768	144297
2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-5); (M-H)-					6420					6385																		
2-HYDROXYBUTYRATE (CAS#); (M-H)-						16037		16806	16631	13941																		
2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M-H)-		51084		49639	40634	42882	39955	42003	51632	42989	27823	19022		11889	47481	24381	21181	52243	114523	35070	52289		32784	20894	12493	119858	28193	113897
2-METHYLMALEATE (CAS# 498-23-7); (M-H)-						16746								5876	6942	2126				1435	4834		1986			7268		7840
2-OXOADIPATE (CAS# 3184-35-8); (M-H)-										4862																		
3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M-H)-	11208	13453	14046	11205	190356	176878	177583	174819	176890	165662	20952	8435		7416	25722	12343	10398	23771	15511	18581	49441		17262	9400		14528	8658	35774
3,3'-DITHIODIVALINE (PENICILLAMINE SS DIMER) (CAS# 20902-45-8); (M-H)-																												3251
3,4-DIHYDROXYBENZOATE (CAS# 99-50-3); (M-H)-					245977	235563	230061	130348	229980	222056									14791	24239	19107					11313		15315
3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-92-7); (M-H)-							7350		10029																			
3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+Cl)-																										1845		
3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CAS# 28822-73-3); (M-H)-[-H2O]					2884																					1051		
3',5'-CYCLIC AMP (CAS# 60-92-4); (M-H)-																		5740	7190							6893		1924
3,5-DIBROMO-4-HYDROXYBENZONITRILE (CAS# 1689-84-5); (M-H)-						3241																						
317.9225@19.306116	771878	759939	743869	707369											70877				238333				327236					
370.1825@23.004324	47254	51628	54735	48912	55498	50729	57508	56503	56714	57926	52616	78013		47711	47406		53157	54663	66057	63966	70431		80561	60608		80707	83875	53124
3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (CAS# 516-55-2); (M+Cl)-[-H2O]				11006						2298									10878					2193				2446
3BETA-HYDROXYANDROST-5-EN-17-ONE 3-SULFATE (CAS#);	53048	60686	55392	59478	3770151	3721986	3839175	3764027	3845527	3733257	21280			4269	17062	11367	72126	93832	493907	131516	222313	14759	80267	37123		23209	3665	135059
3'-CMP (CAS# 63-37-6); (M-H)-			52457								16063	14888		4293		11824	15302	32767	70524	32154	1923	26543	72904	59318	16854	41250	19914	36771
3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M-H)-					17563	10915	8982	9811										1042										
3-HYDROXY-3-METHYLGLUTARATE (CAS# 503-49-1); (M-H)-	18481	14180	15250	15421	109168	93057	93644	111678	97825	98078		2569			21988			19279	24776	16628				9536				26501
3-HYDROXYBENZALDEHYDE (CAS# 100-83-4); (M-H)-	480136	497482	466426	482966								585369	233664	319481		293874	1102241	881735	2063094	569448	874466	342073	683926	680486	355646	939556	501581	922125
3-HYDROXYKYNURENINE (CAS# 2147-61-7); (M-H)-	2880	3802		2280							1752	12117		1429	4729	3182		11968			6224		10322	9260		20597	8068	10085
3-HYDROXYPHENYLACETATE (CAS# 621-37-4); (M-H)-					18076		18758	15884	16578	18371															7742			
3-METHOXY-4-HYDROXYMANDELATE (CAS# 55-10-7); (M-H)-															3031													
3-METHOXYTYROSINE (CAS# 4214-13-5); (M-H)-																					1467							
3-METHYGLUTARIC ACID (CAS# 626-51-7); (M-H)-	54425	51084	49545	49639	40621	42611	40134	41618	42522	38773	27882	19022		11889	47481	24472	21091	50304	113097	35070	52289		32667	21198	12504	119858	28179	112163
3-METHYLADIPIC ACID (CAS# 3058-01-3); (M-H)-	18965	18364	15993	15663	5792	5044	5474	6024	6450	6126	8082	6612			12589	8494	7861	16543	23651	12538	19798	2775	11101	6958		17792		21911
3-NITRO-L-TYROSINE (CAS# 621-44-3); (M-H)-		1050																	4604									
3-OXALOMALATE (CAS# 89304-26-7); (M-H)-[-H2O]																		2340										
3-PHOSPHOGLYCERATE (CAS#); (M-H)-								4548																				
3-SULFINO-L-ALANINE (CAS# 1115-65-7); (M-H)-				14049											19772												33820	13396
3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (M-H)-													5584						14219									
410.2124@23.249462				6612																								
427.8849@19.306257	3165938	3066428	3059636	2904810											397183				1221443				1512830					
468.2923@24.718874	20286	19735	18515	17224							14389			9304	3612	17364	30204	34944	63985	60447	69637	13034	42092	26569		49952	26180	80185
486.3341@22.79494					49358	44099	45653	42595	49372	46303											56116		15968					
498.3864@23.170763					61585	73598	79462	76692	78227	69541																		
4-ACETAMIDOBUTANOATE (CAS# 3025-96-5); (M-H)-			6478																									
4-ACETAMINOPHEN SULFATE (CAS# 32113-41-0); (M-H)-	245796	233329	234417	229084	331232	322746	331507	304590	261920	287362	311563	6107	58194		10713	7667							125553	79798				
4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-KRYNURENIC ACID (CAS# 492-27-3); (M-H)-															4326													
4-HYDROXYBENZALDEHYDE (CAS# 123-08-0); (M-H)-	480136	497787	472336	482966								583821	233569	320599		293655	1102865	880534	2088562	569448	874131	342319	683926	676830	354913	955832	500688	922125
4-HYDROXYBENZOATE (CAS# 99-96-7); (M-H)-	506722	503298	485691	488479	6758		5879	5546	7566	5458	167201	382189	19733	103447	592251	507833	336554	786768	944009	329309	972507	183123	1399770	827414	17416	718747	491487	1361283
4-HYDROXYPHENYLACETATE (CAS# 156-38-7); (M-H)-						1500																						
4-METHYL-2-OXOPENTANOATE (CAS# 816-66-0); (M-H)-	63695	59472	51886	60632	3132882	3037252	2977361	2935520	2921537	2843260	20228	44501		9661	33454	15209	101696	65109	176258	12993	221149	24541	73562	44960		57994	21921	180656
4-METHYL-2-OXOVALERIC ACID (CAS# 816-66-0); (M-H)-	63699	65536	51886	60509	3126682	3037046	2976566	2934004	2919289	2842069	20142	43300		7547	33398	15209	101632	65137	175962	12993	7911	24541	73416	46035		49142	20113	180672
4-NITROBENZOIC ACID (CAS# 62-23-7); (M-H)-		26346	8156	63860		32181		9833	8532	27979	78568	11007	10789	57680	139446		2097	3182	23587		20814	35478		44365		21622		26860
4-NITROPHENOL (CAS# 100-02-7); (M-H)-	86292	80625	76602	74408	18516	20789	20110	19686	20418	17571	28546	41124	28952	29868	112992	38679	37330	52275	82886	46850	41735	19108	70887	43931	21079	65177	37945	55441
4-PYRIDOXATE (CAS# 82-82-6); (M-H)-	12961	15381	14652	12809	230901	207895	205279	162312	174855	167524										193591								2373
518.3953@22.578754																			2304	2729	5800		2850					
518.3984@22.878284	2703	2169			164176	152891	164548	153293	153722	149886																		
520.4115@23.179062							457572												6585									
520.4118@22.931578		1466			156564	111783		199933	202131	152461																		
520.4139@22.747055																				2547						1999		
539.3401@22.711172														4975														
539.3414@22.447004		12472	12900	12746		38622	36591	41407	37023	36544	7125	16358	3415		5081		16762	21674	28430	19176	24876		23311	20491				
546.4274@22.924608					81811	62852	107072	79175	74128	71246																		
548.4426@23.1736					71120	51126	61205	64650	70591	50537																		
548.4469@22.920895																					4555		1459					
564.4392@22.893457				1544													6079							1488				
592.4735@23.019382											5315					1834		18711	15963									
592.4751@23.119793	11452	9588	11537	11090	122912	116777	113509	120517	117726	120662		1144		1438	5949		1653			53827	63264		31171	2531		2353	2844	15818
5ALPHA-ANDROSTANE-3ALPHA,17BETA-DIOL (CAS# 1852-53-5); (M+Cl)-[-H2O]																							4512				4091	
5-AMINOPENTANOATE (CAS# 660-88-8); (M-H)-	19589	22515	24805	21186				2250	15114	8129	6902			11312		25957	19468	53157	52056	20080	23149	12891	25523	41176		46972	23973	32514
5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+HCOO)-	21667	20267	17766	23371							19950	43171	1768	35861	36200	16492					27718						1531	2587
5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M-H)-					39829	39636	40930	38967	40700	38268																		
5-HYDROXYINDOLEACETATE (CAS# 54-16-0); (M-H)-					19347																				2291			
5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (M-H)-	6186	4697	7022	6685			11119		8421	12799	5776	3374			3446	5040	4966	18780	31487	5211	10015	4579	8986	10520		13029		15709
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+Cl)-	1847	2117				7055					4213	3528		4085	1813				2009		6394					2689		2514
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+HCOO)-	2677	2777	2592	2738							6170	3416		6466	3821	2630	3405	2278			7560		1291	2492		4028	1387	4080
5-OXOPROLINE (CAS# 4042-36-8); (M-H)-	1.67E+07	1.12E+07	1.14E+07	1.08E+07							1696173	9991478	382652	3013128	2574199	1.05E+07	1.00E+07	1.90E+07	2.99E+07	1.18E+07	5500963	7569625	1.65E+07	2.02E+07	1101161	2.00E+07	1.31E+07	2.03E+07
5-VALEROLACTONE (CAS# 542-28-9); (M+HCOO)-								652247		631854																		
663.4302@22.925947	17582	18039	18099	16468							16253	25232		13772	19671		18068	26181	24635	29877	28806	4810	27282	24145		26657	20074	32173
6-CARBOXYHEXANOATE (CAS# 111-16-0); (M-H)-	18986	18364	15993	15663	5792	5044	5474	6024	6450	6126	8082	6612			12589	8494	7861	16543	23651	12538	19798	2775	11101	6958		17792		21911
706.3872@22.69812	13439	10828	11390	11364							18437	11731		3341	10266		7118	17452	19618	12122	20843	1231	19402	14968		11443	8948	24766
743.8369@21.5465																				2174								
743.84@22.061306																		21490			1956							
743.8414@21.734903	118187	104054	101963	116288											21537				50786				73168					
745.5704@23.833296											35418	21364		14560	13789	11543					88442	5435					17107	
751.5512@25.219986	30717	28463	31366	32055	257785	255675	274794	266911	297291	264405	38819	17863	2530	22633	36840	24073	61552	60108	160223	152009	329733	10478	36964	29911		49562	32549	252511
752.1517@22.943537	91148	89098	87668	86795	55025	56375	57787	55462	57808	53458	85859	98755	31911	80344	80544	62176	93007	102403	96961	96701	95788	39790	98408	96329	11386	97540	91007	95334
752.4377@23.038685					68446	67140	69812	62779	64945	59943										3993	4197							
752.445@22.738989																											1468	
754.1354@22.516384		2951			15830	14707	16838	15269	18342	14363								5558	4088	2706	4819		2803	3117		2402	2124	4036
754.167@23.181934	97810	96298	95912	95652	83126	83751	83475	83979	87100	82509	104198	107600	83742	95708	88648	98668	91918	86013	87189	102763	106681	76137	107668	93988	63246	100957	121609	97527
754.4549@23.16386					61402	53251	56201	56326	57915	48805								1564		2858	1856							
756.1528@22.731094	47981	47285	47147	46851	45118	43969	44698	30768	32614	46055	42462	56239	7954	27726	34594	23616	41287	61346	53035	57359	54981	15042	57070	52163	2123	56559	54648	53608
756.3416@15.243095	24155	22290	21856	22435															9968				8240					
756.3914@6.6580634					97906	96581	100594	92424	91440	93751									1804		2900							1332
757.5168@24.177675	17632	16108	15276	16665							26808	33457		17923	17574	37825	17235	26692	48486	14232	31209	6560	10954	15796		16361	12443	36714
757.8295@0.5829288	25067	22873	20160	21488	13608	14257	13517	13529	13416	10928	46959	38959	50443	53994	51981	39435	11672	14785	14533	8812	13238	24054	15658	13200	29889	17183	56063	9508
758.1685@22.93772	60926	62470	61685	59261	62675	59576	43278	61071	65716	40995	56274	74135	18055	52907	56338	37694	62875	78214	70013	71707	73198	21313	75338	69009	6340	73905	66893	71737
760.1843@23.183365	52893	53231	53789	51522	49795	47752	48637	46851	49253	50336	57583	61457	43232	52792	46029	55099	51684	49591	50830	59732	61644	38273	64631	52227	30272	55381	71447	54690
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765.5312@24.455208			14296	12220	221504	219213	222777	216517	235213	215196	27494	19307		21480	11884	3042	18136	38786	57666	46403	101670	1681	18266	12858		13499	5036	
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789.5848@25.24628						11998					1260																	
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968.4186@13.099865	20199	19164	17692	15573		3603	3018	3571	2818		14075	16002	8903	21792	13827	10001	8119	14949	30091	7197	16266	16670	32176	22107	49050	42767	33591	21577
969.5907@25.74866	11835	11238	12435	11826	52981	48632	56219	45986	49203	43880	13421			4191	5251	2528	12453	20280	22632	28126	31349		10922	13223		17453	3639	36062
970.0489@22.452425	19065	16916	13379	15672	16342	18244	13710	13438	17263	18544	12325	12482	10306	13894	13839	12623	17338	15566	17522	13810	13817	11011	16750	23620	13347	18566	15732	23964
970.6544@22.714334	6200	5456	6637	6199	15502	16869	14492	13715	15121	17312	7113	7550			5579		4927	14269	9993	11019	15805		12753	6393		5920	5901	15314
973.1458@0.8071661					310144	303595	298513	344946	340538	341035																		
973.2642@22.120821	4483	4638	4771	5339	41689	40107	40076	38341	37492	35887	5189	9436		3448	3461		4630	9751	7607	11231	9642		5714	4344		4981	3282	7075
975.2786@22.430065	1738				45998	38820	41734	43314	38448	39214	4119	4106		1700	2251	2181	2084	4075	1487	4064	4584		2315	5353		2762	4799	2670
976.6711@22.716951	10529	8811	9641	10819	16732	15690	15221	16616	17212	15931	8657	10577		1350	6012		6594	20715	12054	16198	21857		18529	9293		12486	10800	20919
980.1707@0.77266604					252770	249327	248712	197451	195782	199295																		
981.5181@24.339703					50478	46076	48189	47177		44184																		
984.3693@22.730658	19104	20352	19768	19035	30829	28676	28108	30231	30325	29778	15959	26807		8249	10693		13691	33589	29249	34735	28639		32105	24963		26762	24447	31441
986.4176@23.184006	9783	10248	9064	8977	8728	8135	8784	8185	9226	7738	11201	12030	6285	9027	8728	9090	9466	8875	7600	11049	11947	5897	12831	9078	3593	10180	15068	9903
987.536@24.185728					20145	20862	23250	23254	21951	21362																		
987.5417@24.357668		1150			96979	92942	91953	90168	91504	90633																		
988.4018@22.932953	36248	39021	37798	35092	50440	50808	52040	49782	51928	49048	35688	53610		26144	31976	16132	37432	55174	49058	51975	53895	6474	57472	47164		51743	40773	58183
989.5563@24.561628		1523		1022	80361	81274	78543	80617	79840	77020		1185			1079						5866		2307					
990.3873@22.72658	12853	13590	13222	13146	25627	23750	25328	24160	25845	25797	10500	19486			6354	4073	9094	26485	19253	26672	23401		23909	15586		19582	17455	24453
991.5681@25.086418	12647	15012	13751	14764	176849	164047	169247	165373	169005	165835	19875	4778		6839	7210		25996	23484	32346	29824	54005	1152	14028	12450		14943	4819	44283
992.4333@23.181005	28018	28647	28896	27126	25192	24159	23516	24792	24606	25674	35577	37100	17986	26068	21738	27855	23499	22904	23786	37948	38027	14974	38161	27207	10686	30177	47601	29338
993.5878@25.416513					88859	82932	86228	80483	85301	81509																		
994.4194@22.931183	22455	22784	22001	20103	40649	39539	41746	42050	39956	40094	18592	34745		14124	18831	7492	21288	35241	30611	32850	36521	4056	37828	30873		35183	23021	40641
995.1276@0.79599935					242296	239792	236084	251729	244800	255151																		
996.054@22.584139					13703	14669	14065	14222	13835	13911		14793						14795		12864	13793	1707	10207					20155
996.6188@22.10788					23187	22910	21662	18445	18550	19318										3058	1542							
998.4517@23.18197	14520	14376	13696	13644	12273	11293	12528	11608	11952	11341	17071	19384	7899	12217	10684	13698	13186	11920	10781	17184	18927	7302	19044	16396	5877	14403	29664	13410
ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M-H)-	7387	6975	6654	7449	7667	7324	7506	7357	7298	7249	13526						24088						3038	34165				
ADENOSINE (CAS# 58-61-7); (M+HCOO)-	12497	15589	14124	15971							16073	31064	6496	4308	21184	19727	22172	17424	24855	20792	22518	8224	12692	8647		17520	7228	19303
ADENOSINE 2',3'-CYCLIC MONOPHOSPHATE (CAS# 634-01-5); (M-H)-																								2534				
ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-73-2); (M-H)-												3728		2202			1955				1553			2651		3142		
ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-19-8); (M-H)-					9512							18070		1776							76183							
ADENOSINE 5'-PHOSPHOSULFATE (CAS# 485-84-7); (M-H)-	2481		2936	2853								5207				9948	2053	1363	2549					4737		3470	2058	
ADIPIC ACID (CAS# 124-04-9); (M-H)-	54425	51084	49545	49639	40621	42611	40134	41618	42522	38773	27882	19022		11889	47481	24472	21091	50304	113097	35070	52289		32667	21198	12504	119858	28151	112163
ALLANTOIN (CAS# 97-59-6); (M-H)-		18551		11204							2205		8379	8022				3141	7163	14223		22216		9359	13903	4634	30589	3587
ALLOSE (CAS# 2595-97-3); (M-H)+[-H2O]	22633	14180	11769	18949	100059	100208	102499	101112	97560	99302	22822	2569			18862	4950		15698	24995	11939			6698	13102				32774
ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 2255-14-3); (M-H)-				103041							415118	8431	21578	162668	213795	128177	59175	54905					24836		20896		90898	47525
ALPHA-HYDROXYISOBUTYRIC ACID (CAS# 594-61-6); (M-H)-						16037		16806	16631	13941																		
ALPHA-KETO-GLUTARATE (CAS# 328-50-7); (M-H)-						160927		153565	144798	157208																		
ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+HCOO)-	451623	482919	501454	501700	482857	454368	480951	497333	522874	517633	461453	475874	442607	492269	451928	457300	482894	515080	470038	518566	509761	394454	506524	465949	371705	504296	525901	461853
ARABITOL (CAS# 7643-75-6); (M+Cl)-	9649	4320						1617			8014							9385	19567					13351			4503	13091
ARABITOL (CAS# 7643-75-6); (M+HCOO)-					3866		1459																					
ARACHIDIC ACID (CAS# 506-30-9); (M-H)-	9712	14523	14892	14065	5240	6087	6036	7001	6867	7648	22073	21701		15172	8314	16500	14733	18057	23378	15315	47432	7457	16682	11566	2810	16414	24276	18352
ARACHIDONATE (CAS# 506-32-1); (M-H)-	2162546	2190849	2191096	2119308	1486898	1408050	1498791	1542453	1612528	1501489	2634697	2342652	94454	613608	2350139	1323434	1859516	4128884	3229199	3063736	4751292	375342	3854319	2259185	14161	2046862	1884319	4493087
ASPARAGINE (CAS# 70-47-3); (M-H)-													5584						14219									
ASPARTATE (CAS# 56-84-8); (M-H)-	43697	43573	46272	42124							62755	99173	6116	24701		257774	15252	60121	31959	25842	13055	62168	16290	38002	23340	50932	65795	28674
AZELAIC ACID (CAS# 123-99-9); (M-H)-	174392	178773	171492	168453	71492	65903	69260	65390	68396	64953	119405	128512	42022	67161	354033	201294	137045	286131	344754	216641	287246	67967	172183	139690	55469	236467	105026	390046
BEHENIC ACID (CAS# 112-85-6); (M-H)-	19207	21057	22606	19802	5648	5209	5042	6555	6595	6799	32359	21655		19874	5449	23823	43795		89898	43053	112139	9479	28405	28470		59878	28917	70440
BENZALDEHYDE (CAS# 100-52-7); (M+HCOO)-						1500																						
BENZOATE (CAS# 65-85-0); (M-H)-	480136	497787	465724	482966								586103	233569	320431		293655	1102902	879618	2088652	569448	874131	342319	683926	676830	354913	949539	500688	922125
BETA-ALANINE (CAS# 107-95-9); (M-H)-				49396							56746	25703	29637	58089			56687	67170	39520			34054		47527				
BETA-MALTOSE (CAS# 69-79-4); (2M+Cl)-[-H2O]	95488	95184	95265	99060							31804	47008	23707	155812	56770	117091	40692	110832	150398	69915	69571	99261	104023	147816	162788	210894	91915	64238
BETA-MALTOSE (CAS# 69-79-4); (2M-H)-[-H2O]	6860	1482	4885	7614							1386	3908	1679	13781		4190	1268	5006	7476	3046	2744	5886		8451	21245	10834	9485	
BETA-MALTOSE (CAS# 69-79-4); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	230558	153754	175605	376002	252819	235981	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
BETA-MALTOSE (CAS# 69-79-4); (M+HCOO)-											3431	7760	10207	6248	10228										13195		6609	
BIOTIN (CAS# 58-85-5); (M-H)-	1025												4277				4746			2319			3520					
C10 H10 Cl3 N8 O3 P3 S	193433	163908	166250	160125															67503				85198					
C10 H10 N6 O3		4398	3071	3807	183033	178788	189517	181438	183043	175381								4953	6395	17143				28228		1618		
C10 H11 N5	65051	65978	68008	73467	47606	47624	48078	47937	52150	51615	68200	66338	64845	78651	61842	67922	51961	68697	83499	60526	60029	73680	69874	64740	97124	88180	80906	62408
C10 H11 N5 O4	169495	190982	210229	178192						2038	31927	259823			84111	197684	113901	256927		166186	138837	50799	226250	224866	1701	277383	125359	
C10 H12 N4 O5	2467944	2256734	2211471	2225479		104982	93677	51485	44663	116175	2108080	1760310	727431	2947692	1595546	680640	4282341	5043282	5775255	3645856	3596081	1672235	3552232	2341151	229044	3283676	1940363	4082467
C10 H12 N6 O4					95216	94163	98212	93241	99139	103304																		
C10 H13 Cl N6 O	74008	74094	68477	68600	42090	40728		39815	45977	40309	64876	65532	56145	72062	69389	55493	57206	68763	84733	55478	67678	67171	85004	74682	103492	87113	85148	77372
C10 H13 N5 O	6503857	6253075	6135540	6148021	4808928	4683166	4601809	4588622	4647948	4476127	5962684	6299962	5706067	6635641	5657756	5743718	5113892	5928865	7153534	5222759	5868800	6523082	7038624	6323196	8683839	7594913	7456046	6217109
C10 H13 N5 O5	468452	464579	455753	448109			2816				360790	238098	84299	373556	368184	251567	701982	929877	920818	515636	850679	307551	467221	563279	86641	794161	647636	727788
C10 H16 N2 O4	607705	596801	585552	594879	4898			5650	4652		66069	417637	9666	84587	74367	463490	726725	1771002	2969453	630089	398422	299924	1066960	1082222	29521	2119106	257845	1526971
C10 H16 N2 O8		14058	2528	9447	6.21E+07	6.29E+07	5.52E+07	5.68E+07	5.73E+07	5.54E+07					8726	15680	9212		21463	5699				5490			8220	10588
C10 H18 Cl3 N4 O7 P3 S2	136847	114979	116208	111894								2307							45836				58515					
C10 H19 N4 O4 P					119285	122377	125742	120593	117781	114993									3455	4517	10453							
C10 H20 N2 O P2 S					58859		51409	60170	65772	56649									1386	3230				2265				
C10 H20 O6 P2 S					185977	369955	397350	258679	401920	344993					1801	2070				1752								
C10 H5 N5					60217	56636	56338	54798	55669	55118																		
C10 H6 S2					2174716	2066635	2040246	2041448	2061446	1979863																		
C10 H8 N2 O19 P2	152912	153439	150572	155898							119659	36364	124380	84212	84519	82340	168787	146470	102465	185985	168746	199756	153148	135985	142814	122350	94488	163155
C10 H8 N3 O9 P	113209	48672	59083	15015	540830	517603	142787	315075	717290	656016	44523	2133	18402	1282	74487	27456	1579					27963			83122		26288	
C10 H9 N O2					45635	42050	46047	43047	40252	38785									3456									
C10 H9 N3					54023	55006	57777	58936	62803	61300											14489							27031
C11 H10 N10					223261	218243	226718	218160	213719	219003									40966		18617							35543
C11 H10 N6 O2					57604	57264	54773	59282	55880	56952									5238	1883				2272				7429
C11 H11 N O3				1575	127597	128195	128723	133178	132915	125690								11166	40363	4080	13427		2716	10131				8147
C11 H13 N3 O5		116321	29723						1157					37066			2050	201270	402202	68583	34057	10952	166515	29634		176053	79319	280279
C11 H13 N7 O3 P2					64630	63288	61792	60496	62339	57020														4037		9622		
C11 H13 N8 O2 P3				1991	51028	51592	54671	46654	47383	47966				4277														
C11 H14 N6 O S3	168367	165199	164833	160121								105266	7002	47087		90269	204070	191537	491717	190548		52626	132186	192456	3735		131166	292919
C11 H14 O19 P4 S	89317	85861	84929	82614	44659	42932	45182				103395	59179	108488	100853	97283	80663	65057	67625	58857	58600	70089	99195	77216	64008	92774	66894	100827	58829
C11 H14 O3	89963	85359	87966	84455	93867	77499	82225	81325	81824	72540	86900	80059	82472	85294	96127	87325	89484	70074	87435	80036	79102	88284	97974	82860	87107	62845	98668	75294
C11 H16 O3	6619	7212	6796	11470	55990	73306	69701	64872	65419	69018		7410		2621			6755	11916	26686	18161			16630	11058			3263	8875
C11 H17 O20 P3 S4	34037	33398	33167	34647	42656	38340	37523	38050	39128	36060	56683	59498	61569	69342	67527	52622	22073	1176	28893	18320	19813	33524	27082	25061	36383	34213	67108	17193
C11 H18 N2 O S2	39988	39296	35224	37894	51435		52012	25538			21767	19562		8954	21856	22248	34622	112552	156067	39606	49476	231865	44619	46130	2117	100592	26630	174195
C11 H18 N2 O4	98044	95249	92307	89940	19520	19121	20268	19020	20126	19463	64079	117255	9710	62651	46283	73417	77526	426638	362872	79156	87690	46221	139711	132847	4639	228678	60303	285530
C11 H19 N3 O3	29621	30061	28836	28811								12447	18137	12654	5100	8609	49695	37641	79366	25334	31598	14987	53314	32690	20450	23449	33885	36678
C11 H19 N7 O	133911	127791	125804	122456	12245	11939	13168	11092	12577	11933	44753	147293	53702	69996	129708	45239	99202	149547	261720	159220	214451	35027	249735	215458	19542	107311	85280	151807
C11 H19 P3	5640788	5281369	5253698	5200677	516713	518771	589264	719192	760041	707674	3865677	4625709	694504	2183698	3480231	3550886	7280330	9796574	1.29E+07	6618084	1.13E+07	2072377	8889675	7354435	255198	1.05E+07	4490552	1.07E+07
C11 H20 Cl P3	3559613	3272213	3247891	3209617	345363	333135	346674	584381	518050	486650	4161716	2485768	239713	1068094	2207586	2241027	4162701	6542356	9015740	4289623	7810354	1118469	5368182	4665757	52284	6879081	2523080	7627634
C11 H22 N2 O3	5676	5499	5865	4791	159920	151569	155116	153451	155479	152520	16038	8780			4326	6089	4314	28622	29225	3763	10368	2367	2450	5329		12299		25793
C11 H22 O2 S4					78684	74751	76245	57480	83146	77586																		
C11 H9 Cl N8 O	664911	283850	225974	270753	34379	28625	3898	1985	43275	34324	286119	130162	86469	170020	230228	106097	541340	644912	840963	640174	656664	257488	358200	341847	22038	501105	283746	588214
C12 H12 N8 O4	64046	61280	59757	59434	102855	106309	109494	107465	105162	107518	9239	4910			5772	2322	78328	165737		150845	97838		75714	98290		88081	5111	204281
C12 H14 Cl O12 P					100685	84503	99495	78172	92945	90215		1280						1094				32993		3771		1903		117087
C12 H14 N6 O2					71368	64534	66090	68036	68507	68336																		
C12 H14 N8 O9	213371	201541	203219	194434	128144	120401	121416	119375	119848	121016	198206	202251	176798	230735	192973	185709	164629	203115	225615	169641	197048	216460	231577	206155	285551	256692	243097	206415
C12 H14 O4	58974	55507	55768	53495	1927	4045		3593	3684	2729	15956	36208	33825	48495	10125	39089	38765	39085	46427	30304	67448	33920	60148	61920	43975	118924	138243	132659
C12 H15 N O4	23154	22016	23655	23266	33404	34499	35168		34341	17005	3380	11084			3556	2848	55430	79368	183657	66953	133290	9672	36512	5961		9274	8931	49351
C12 H15 N3 O2 P2					53560	51122	53552	48618	50101	48769																		
C12 H16					46098	40525	45696	43114	43343	41266																		
C12 H16 Cl N O S	96318				71937	65887	64594	67128	67331	68570	60048	74936	5321	23168	47743	65469	139611	288562	268359	152411	276492	44444	4487			83514	54201	251157
C12 H16 O2					131672	127817	131184	129976	127574	129056															1945	1252		
C12 H16 O5	21805	17485	13453	18242	671126	667527	684655	648201	684961	650584								25685	53126	60330	35089			100875		4648		11669
C12 H16 O6	3649	1829	3070	2363	213355	209379	210774	216436	219745	208746		1328							5335	19133	6466			14414			1501	3288
C12 H18 O3	4321629	4090117	4048407	3854742	2179416	2115376	2158440	2105200	2101366	2071605	3597771	3822252	2981649	4064610	3705276	3285813	3176987	3919915	5300993	3257931	4245171	3894552	5007911	4314052	5796654	5773911	5139562	4559723
C12 H20 O3	40957	44254	40001	37733	23847	24292	22639	21197	23049	22771	32243	37827	29335	41503	45197	31676	32574	36780	59339	29678	110631	37675	45185	42692	61965	59937	47130	48362
C12 H23 Cl O11	266928	260671	243125	240328		54476	46649				314978	245746	154756	183186	404051	265118	235808	263899	292500	168991	187401	212907	263658	187321	164357	734277	235026	208480
C12 H23 N O3	76444	73840	71264	69606	8163		4499	9452	8770		20650	72268	31305	22146	58896	21671	54717	86763	182484	103385	147695	17679	164696	158507	7334	53048	37857	64964
C12 H24 O2	35209	35682	35716	34560	39040	33707	37925	40427	43598	41215	15287	28859	11562	17152	20987	11739	46697	81025	107999	47744	69572	9966	74611	67582	8700	97065	28866	60857
C12 H27 N4 O P3 S	474278	472743	472017	464153	371238	376067	407619	398204	416707	431919	194302	81030	36290	82728	339808	290021	333117	508492	301187	588989	808236	636779	1036137	403839	142266	291909	692492	498779
C12 H3 Cl N3 P	321016	312370	320116	305490	300585	317835	321028	341831	342007	312793	338636	309295	38149	202743	332310	338925	288292	357053	361653	369331	365587	227506	297581	298077	10840	390716	285427	365829
C12 H3 Cl O4		2349		2299	42609	42895	40175	42979	40672	41450									8928					1890	4245			
C12 H6 N6 O4					456919	459965	467344	452064	446026	441947																		1343
C12 H8 N5 P					44724	43999	42985	43646	46645	44212																		
C13 H11 N2 O2 P	76249	77738	74953	77413				2374	3949	3931	17885	90597	25395	69546	22346	18798	87150	109410	140130	95400	148587	13659	136250	115189	9926	113553	96336	107829
C13 H12 N10	66827	66283	66351		25066	20199	21326	17767	20122	18818	22405	49495	55919	56978	21440	22789	49603	46554	73896	55103	52883	20954	62505	52761	28372	152758	115942	117919
C13 H13 N7 O4	2439	1339		1770	173315	175861	171909	163545	167939	166254	3742	3424			1440				3513							4184		
C13 H13 O28 P3 S	52530	52588	52441	52311							58338	21790	63914	50881	47805	38682	41932	43213	35977	39971	48041	66060	47796	40675	56700	41704	49882	39121
C13 H14 O					37925	40456	41856	38528	40581	37224											11079							18788
C13 H14 O P2	18500	14907	16817	17648	83641	86050	77997	79589	81589	73965	5013	20199			6686	5250	9010	73070	2006	9667	46045	5122	76967	26238		2878		55624
C13 H16 N2 O4	33397	28917	31755	32044	537653	526572	526816	530249	529516	536862	39989	21496	7895	1493	25021	9941	45960	45061	16168	24921	68763	6689	148430	59909		51354	23487	181104
C13 H16 N4 O5 S	159374	150060	149986	150309	91100	88871	90069	88246	89817	94425	140494	145072	130354	154150	141045	133893	124048	143867	179489	130272	156905	152032	175674	160542	195095	193748	181588	159433
C13 H16 O4					49397	49044	52536	51446	48570	47431										1358								
C13 H18 N2 O9	312706	297648	297894	285999	184505	182989	186700	183787	182553	177417	280863	292967	247641	311301	282052	259224	249284	289594	342748	251083	295595	309066	343018	305594	391651	381476	354703	314121
C13 H19 N2 P S	54299	55721	59049	57497							5598				10418	27921	42210	94881	147105	53894		71159	64169	130214	10094	134076	80907	99731
C13 H19 N5 O4	19386	15588	17865	14463	139278	136001	125306	123325	128609	126093	11534	10983			32955	9410	6017	15960	29929	11498	29050	4473	13410	9497		10533	7338	32461
C13 H20 N2 P2 S		2173	1013	2222	176358	174945	183065	169499	174373	171333					1862						43484							77565
C13 H20 O2	1093271	1155785	1171007	1013907	1142193	1148224	1209008	1086065	1205536	1171075	1056524	1156603	1110190	1110562	1157617	1161655	1146332	1063630	1093591	1166315	1208574	1150666	1145244	1164751	1041205	1142075	1067044	1201875
C13 H20 O4	98348	102037	94621	93874	29215	27149	29849	27654	27094	27608	31912	71145	69781	75011	36738	29657	67885	72139	116088	77743	78906	33754	90204	75995	32676	211560	158592	174675
C13 H21 Cl3 N12 O S	13502	15531	12304	14108	41158	44624	41551	36580	43248	43463		1450			11551	18444	15559	32789	25955	29546	17171		19475	22827		34399	6919	26011
C13 H22 O3	175961	170735	169485	161791	171967	175687	169248	160064	174263	170436	168878	174079	165250	165160	165676	170349	169229	174633	176498	169380	180660	174467	161654	167305	169351	168529	169169	170283
C13 H23 Cl N O5 P	69967	66270	69477	65805	24048	23925	25417	22130	24017	23582									7250								13000	2001288
C13 H23 N2 O P S	117466	155664	150124	112206				3234				9002		5047	1713	20059	104692	327319	511381	141884	158893	84484	223067	162023	15459	292946	124014	504087
C13 H24 N6 O2	87361	90480	91660	90127	195857	185929	194137	196211	210004	201877	49160	100563	37823	62415	48979	33007	118892	151678	178457	125316	166505	33474	146175	123091	30574	232866	100018	196675
C13 H25 N O3	583804	570166	553078	538660	48668	51022	53301	51972	51527	51484	186598	661382	228488	293862	581927	192872	425920	665999	1238633	706718	980622	153687	1155013	979429	77689	464532	362192	691224
C13 H28 O6 S2	8981	8379	7203	7780		34896	24301	21939	23150	24037	9295	6341		1284	4416	6465	9471	1057		12783	13699	2595	8548	8859			3563	10429
C13 H3 Cl O5	29403	30292	28702	29156	542993	522934	521488	523431	514653	503236	48886	10555	56847	11522	10184		67945	39449	86040	16451	15353	9837	6287	25244	39699	30038	5583	23935
C13 H3 N2 O5 P	25732	25519	27529	22674							21121						93417	103905	121694	56796	90320	16067		39866		75332		86201
C13 H31 N4 O3 P	65154	62971	68113	68139	263971	259220	271612	275852	299727	282509	74628	221810	8978	37138	115091	34812		143985	194216	114437	141862	11948	103369	81027	4224	168564	53488	300571
C13 H32 N10				2093	30319	28985	32436	27722		26077	1560	5111		1373	1926			2826	4127	1787			2145	1120		2544		4393
C13 H33 N4 O3 P	460813	487027	498407	500903	487208	459521	482141	502903	546856	520806	467246	483493	447007	494385	451409	460099	489092	517982	471694	518792	517421	399764	508994	474925	373188	508792	526983	464700
C13 H33 N4 O4 P	27067	26862	23958	27303	37560	35090	35768	35662	35617	39725	59245	47443	7340	43479	65211	28244	26050	43601	33709	30261	44383	6110	34737	26138	4214	41657	20371	45095
C13 H7 P S3	20805	23306	19524	19309	655493	629698	631929	638565	638841	616108	32521	10789	31345	9321	9325	5192	17444	11916	15284	10678	5932	8654		11154	45155	12164	5957	8694
C13 H9 Cl O2					87383	87138	88465	86898	91699	88005																		
C14 H13 N2 O2 P	36790	36465	38441	39725	44576	42442	39437	40537	42397	38069	20819	47984	23682	30441	24572	20198	53885	54989	66083	57473	56504	19626	54216	51546	11047	45964	33365	41853
C14 H13 N3 O4 S2					437228	436759	449460	423168	425310	411789																		
C14 H14 O22 P4	75566	75037	76418	73387							51193	14384	55012	35163	34622	33997	92836	74781	48716	108558	93325	99986	84099	69501	69289	58846	41258	90896
C14 H16 N12 O P4	42291	40248	40817	40219	3941		4026	2760	2993	3434	11850	51545	16173	41659	14994	10897	46221	56970	59987	46880	57179	7902	66783	59900	6508	54668	49124	51911

C14 H16 N2 O4	44343	43729	42853	44275			7090	2827		2734	15937	23736	3215	13963	10736	21496	39572	272375	210295	46944		29321	69398	79588		115198	38940	147916
C14 H16 N2 O5	40883	39918	38169	38351				1130			11660	15653	1364	10106	7983	15139	39724	161701	181900	42074	42453	26712	65587	70394	3511	109459	37590	136587
C14 H17 N O8	134668	143275	138047	139485	283809	286006	280920	273843	417614	271962	95986	26727	12407				82475	9534		1012			71159	1460564				
C14 H18 O4	57848	42337	48096	45655	72637	62117	56390	42081	45342	46466	48186	53261	47446	43938	43751	40458	48538	46771	42379	45499	26502	46478	49100	58496	50123	46043	43784	45557
C14 H20 O P2 S	295817	287119	280687	278740	88647	80755	87291	84956	85599	82738	288053	347327	190484	436508	378185	297323	173481	292413	417639	212379	310630	263837	410514	356940	362488	536136	450129	379158
C14 H21 N O3	68084	65481	64193	66901	147864	146066	186014	174463	169828	163465	53452	74758	57537	56024	77441	59770	64416	55918	87462	60315	64089	52684	79671	59422		82619	89209	76514
C14 H21 O3 P3					70562	68555	70791	68629	71012	67402														10342				
C14 H22 N2 O5 S	450506	458847	444403	444716							461996	17829	98754	94149	59757	67151	1237984	1271081	2160846	479730	598104	126457	212901	1178307	58131	461524	18979	486800
C14 H22 O4 S	157600	149800	148267	141516									157558	135767												414839	118125	446678
C14 H23 N6 O8 P S2		1702			85024	78584	90461	80998	80004	78212		1680					11936											
C14 H23 N6 O9 P3 S	129777	122531	126073	116358	81220	78697	77226	75884	77470	76076	123044	134597	111598	138964	115877	114110	107538	121220	132031	101844	117081	128025	142301	126739	161925	146867	149763	122029
C14 H23 O5 P S	206650	198553	197647	192983	88527	97405	73856	87206	85763	94236	174081	336604		179258	315622	209538	125578	261752	391097	244562	418311	98087	304363			178680	208598	327021
C14 H24 N2 S4		7411		12808	26773	29914	28798	31819	30698	27831		37317	3922	11798			7630	8118	20279	6505	7914	4723	7573					12494
C14 H26 N6 O2	27969	17987	29492	31101	23622	21477	22217	23782	14892	23064	15701		8130	20669				26298	31894	25141	33123	9463	47814	18442	7889	38909	18453	25634
C14 H26 O2	7231	9645	9193	10074	36885	33737	36332	38543	41627	36754	2556	13382		4673	3454	2491	5509	23589	33558	18297	16984	1743	10849	10848		23792	6256	33686
C14 H28 O2	243241	240315	261855	255355	416520	409432	422724	431162	475278	441157	176395	289097	128810	186099	144892	123190	305207	370082	424314	317387	386131	98708	372158	330462	84384	491566	274268	413358
C14 H28 O3	22952	21639	21695	20157	10284	9627	11013	10699	13435	11072	7707	17974	5094	7564	6890	4239	28653	36333	53843	38641	32433	5048	40761	33554	3985	56570	12678	32747
C14 H30 N6 O	116106	130902	112080	117427	124101	119533	132182	116711	121520	108671	91997	158031	150354	85441	65375	78134	144120	192530	353380	162034	186262	58458	216636	207829	91129	241669	131268	199253
C14 H33 N6 O9 P	139486	142483	141284	135789	176061	164099	174429	169043	183713	175990	129033	156027	96947	133858	119309	115452	142188	150367	144415	169953	179657	89869	185527	152854	72814	166980	173091	168386
C14 H5 N4 O2 P S4	6741		6024	5077	316898	311319	307718	305098	313090	304718											1208				13957			
C14 H6 Cl2 N O5 P	171593	208341	212467	197808								466647	81675	340912	26873	196187	356624	147690	107715	226553	408859	240442	241200	239257		242427	210803	89721
C14 H9 Cl2 N2 P3 S2	71258	67219	68197	64835											9883				30816				35297					
C15 H12 N2 O6 S					250665	247810	251509	247410	246357	248488																		
C15 H14 O3	9549	15933	11001	15533	92890	93689	95920	99556	98150	97679							6901				23243			124952				18839
C15 H15 N7 O5	4393642	4363504	4345424	4198811	31984	33517	33525	31082	31913	31107	406789	2536794	39897	473361	602866	2251814	3921067	1.03E+07	1.04E+07	4086773	2451420	1002173	9148655	9359058	36030	1.01E+07	3609234	8320599
C15 H15 N9 O	49623	45489	47756	43195	30481	29505	29593	27649	28265	27221	39856	39710	32973	43586	42677	34998	35643	45428	63695	37612	50285	45115	57971	47881	62621	66746	55602	52649
C15 H16 N10	37184	34343	34883	35267	44988	45369	43018	42824	43642	43914	32095	32821	21793	32699	32080	26473	28483	37285	58558	32166	38443	32423	29868	34988	45158	51283	37010	37191
C15 H16 N4 O					416099	421104	427842	428704	435107	413353				1129				12691		5321							2802	
C15 H16 N4 O S	77335	73759	75827	71120	78632	80832	85084	82575	82064	76365	26841	62951	17892	35173	37286	24212	98555	135614	190830	101273	144253	20534	149980	135624	12787	175885	57874	128009
C15 H17 N12 O7 P5					29861	32655	31349	29810	31299	28602											9123							18235
C15 H18 N6 P2	60892	63066	57334	58547	39750	39082	40999	43063	42021	45162	62779	62438	53799	64288	59322	55281	55739	60895	75855	59714	69597	62579	71165	69965	72233	74640	71350	73553
C15 H20 N6 O11					408773	395212	387355	426986	430846	429665																1168		
C15 H20 O5					57478	55453	57771	67647	65116	54590																		
C15 H21 N10 O3 P3					198789	200327	168811	174641	179315	183937																		
C15 H22 O2	317922	333396	328479	324229	340788	332789	345496	339811	356532	336945	335387	327984	330063	332065	333666	322614	333617	335342	354504	343716	316898	337918	336240	327325	330856	342299	353439	330262
C15 H22 O6	226101	219336	217431	215407	12409	9966	10986	10393	16960	17670	197372	177996	225885	174953	301797	160972	167452	210764	299329	234564	256850	177341	248708	242243	173714	197232	221805	262128
C15 H24 N3 O6 P S	55410	56017	59376	58029	1461			3104			71049	104177	43560	44808	83385	85728	30092	26356	46426	20684	16432	31369	49420	47394	31284	127177	73392	21918
C15 H24 N5 O3 P3	29247	28279	25386	27071	46488	41594	41695	35432	32495	34155	39914	63800	50447	58476	64608	52630	4182	6454	17655	6815	11896	48098	34705	15466	77096	11081	69192	13629
C15 H24 O4 S3		4557			110896	116185	117061	115829	121736	121507	15771				24619													
C15 H25 O4 P3	43181	43828	44427	39848	10831		15953	8820	8991	9142	47859	23794		16969		36483	23742	62716	63654	42172	92362	10528	33415	35418		54388	17284	64142
C15 H26 N3 O4 P S3				1693	73884	74286	70773	66772	68615	65283									1332		1616		3297	1901				
C15 H28 N4 S2	133832	132897	129431	136929							25053	52720	95075	74771	25886	39970	189799	127297	461883	88199	105580	69686	230002	128649	68099	118149	153475	130760
C15 H30 O2	63609	104681	67437	68900	77208	74766	44241	81682	86153	76705	87052	133822	24659	54093	65323	59448	75723	90525	116185	84670	113877	38400	103956	76192	33053	130262	61509	79634
C15 H31 N4 O3 P	26931	32029	24618	24593	227732	212599	225320	227445	244378	231061	26578	45530		23604	28017	165361	23012	53210	55644	39884	51565	149489	35447	32355	127552	43747	22810	67986
C15 H31 N4 P S2	53570	55990	50897	47766	3169	2878	3982	3676	7780	3722	9716	47147	44694	40972	16725	13410	43220	43191	65451	38051	45418	10015	59417	46900	15103	178466	140756	158731
C15 H33 Cl N4 O2	26500	24357	17181	5333	23563	22623	24316	22861	25069	22826	19116	62359	4711		21126		20577	40116	49680	26431	36613		33398	28426	1519	50311	17932	40063
C15 H33 N4 O3 P	354095	359596	371935	365232	869705	808132	852360	864456	936754	889983	318818	421278	21876	152639	242225	125182	296779	604578	437512	524187	454159	46356	438726	382787	8459	452246	402595	523484
C15 H35 N4 O3 P	550991	554183	580574	573343	777663	749216	793714	806651	883663	830426	534168	651754	86352	475795	382483	333413	556004	704157	635391	718656	676947	113630	661430	611297	13701	682000	566802	698726
C15 H37 N4 O3 P	303730	324236	336138	326606	253502	237061	251963	266680	287090	273791	368814	375589	220972	316913	268816	332447	304570	283507	286879	374891	378337	158224	372924	311130	93661	338065	428872	321397
C15 H9 N8 P	5501	4630	5847	4665	65436	64362	60978	63839	61700	61905	1706	4090		1652		3224		14073		13906	16607		10088			14627	4614	21961
C16 H11 Cl N6 O4				1152	70754	67493	70306	66539	67876	61714																		
C16 H12 N8 O4					74561	73880	65485	70184	74311	67545																		
C16 H16 N2 O3					103426	106339	115415	102585	101747	92719																		
C16 H16 O3 S3	5690		6395		68515	150166	149445	126353	133009	64699		9784						5694				4888	3042				5993	7561
C16 H17 N6 O3 P3					44177	43446	45537	43102	46254	43330											12668							23294
C16 H18 N16	31260	32144	33117	31355		2337					34603	34331	2788	15976	32610	25921	28082	46466	41988	42148	52393	1413	42284	35561	12085	32029	30594	49379
C16 H18 N4 O4	115246	108650	124514	109600	12207	19132	12040	11141	13152	12083	86646	92701	112552	111335	109219	73298	93217	126227	143664	112131	132370	104941	119102	106045	103111	109174	140631	139958
C16 H19 N P2	68252	63029	66743	64204	46509	42608	44019	44538	41344	39781	62276	66473	65243	76516	58034	61263	51164	62310	68909	51315	55836	73088	77490	65069	101398	75194	84832	58484
C16 H20 N4	217590	214299	190261	208856	217377	216986	220856	225626	223036	213159	216891	213509	220102	231222	222832	223236	225616	211870	200786	150121	124779	225294	217413	194182	215318	226576	210818	182560
C16 H21 N6 O7 P5			1256		37628	38040	38197	37761	38748	34921											12354							22062
C16 H22 N2 O15					559394	548958	570189	516899	521800	517524																		
C16 H22 N6 O3	35194	34776	34236	34814	23033	21140	21047	22191	23474	22253	32291	35175	26324	35784	31456	25615	30978	34029	41195	29752	32320	30266	45012	38353	43658	42399	39773	32863
C16 H23 N2 O11 P S	138198	128202	133390	128606	81557	77712	81221	77644	77926	80485	133847	137548	114628	148936	124248	123110	107409	126361	139856	107508	123812	136015	149816	131164	182705	163432	157831	134611
C16 H23 N5 O4					49709	47372	48031	46235	48496	46233																		
C16 H25 N6 O7 P3					98790	99221	100789	95072	91656	89737								2243										
C16 H25 O3 P3					46790	49354	50329	49656	47487	45277					1981				1091		1729							2721
C16 H26 N6 O2					24669	28993	33126	29421	26421	28578											2214							
C16 H26 O2	88668	90474	90339	89299	37188	37801	39382	37711	36619	36466	1230	99991	37849	60393	47486	35439	121519	2353	1944	2324	3979	33498	143766	125592	29427	230497	103938	3112
C16 H28 N13 O2 P5	31293	30528	31300	29247							20710	26632	1981	6456	41671	65984	51868	32206	55860	7770	67070	8551	26482	64074	11747	88906	28141	47813
C16 H28 O2	9676	8411	10204	8425	30448	28548	29058	33008	35167	33162	7440	12725		1216	3122	3539	6851	31261	21925	23561	29417		22206	16194		16284	7213	31439
C16 H30 N6 O2	28248	31594	31225	28947	29017	28957	28809	33637	35150	32801	23845	38656	12489	24935	25832	23815	30761	58807	33673	37994	41131	13064	43136	31381	8239	43604	37412	32239
C16 H30 O2	286818	292252	299127	294898	867407	819390	868592	872183	977462	914901	346334	810999	44810	190407	497005	98944	224632	589913	748912	491112	590147	45865	435394	361736	12188	675801	214811	948814
C16 H30 O3	30243	29584	26861	29608	11867	7522	11141	9807	8526	8436	12388	37292	13025	16346	16125	8436	39179	48956	66372	36822	45637	10192	59376	43163	9035	69201	22947	38896
C16 H32 O2	1363267	1433127	1497431	1504134	1831874	1676340	1800697	1865379	2067870	1961895	1394011	1480000	1292521	1477539	1259556	1342706	1480766	1528749	1465755	1605061	1746917	1125517	1739865	1490099	992906	1677649	1752000	1508412
C16 H32 O3	95921	93601	92491	91283	112424	105670	113252	111401	115292	122859	232722	179792	59593	137261	243673	102354	77057	138287	115607	116564	161920	43190	119757	85379	32614	146768	62781	150784
C16 H34 N14 O6 P6	28243	27941	21775	26484	36865	37236	37863	37497	39174	36037	20983	22158	13347	25822	21552	16978	27991	36619	36569	29513	36941	17457	32252	35472	20500	40374	28368	43979
C16 H34 O8 S	84227	99148	65052	82548	76341	70362	67749	72346	83354	76744	78125		88250	76710	57703	88293	86447	55561	79929	80256	86317	71816	77820	86560	64812	87396	90590	81715
C16 H4 N2 O3 P2 S3	75960	74602	73765	68429											13630				34824				36446					
C16 H9 N7 S					99108	98562	98751	96357	99147	96929																		
C17 H14 Cl3 N2 O P3 S2	170444	145984	145906	142521								1089																
C17 H15 Cl O4					97899	88136	87853	81979	120862	92839																		
C17 H17 N2 O8 P	154455	149511	151724	144048	91937	89397	89920	90032	91886	89821	143466	147285	126869	157388	142666	130796	123472	143818	160717	125259	142599	153033	162236	152386	188622	180639	173182	149349
C17 H18 N10 O	54299	39132	37141	49929	36607	40119	47828	48424	38126	32692	35321	46333	39312	38863	40886	47289	34819	35742	38093	46847	81573	46935	36359	34698	38115	43000	52776	57452
C17 H18 N2 O4		1790	3301		43327	39228	45792	43300	49665	52089							1901			4223						6001	1491	5560
C17 H18 N4					74804	74494	79045	74692	77515	70595		41699																
C17 H18 N4 O S	4428	7257	7435	5997	29033	27744	33677	28205	28730	26804	2242	6704		3785		3159	6475	15996	24195	15567	14579		9342	10080		16552	5990	28992
C17 H20 N10 O12 P4	60697	59123	60834	58231	39778	37651	42455	36386	38716	36914	55554	58078	53927	62363	53960	55947	50828	58635	59220	49947	55806	61782	67015	58456	72605	66159	70835	61276
C17 H21 N O3					38633	37725	37832	36529	35178	34129																		
C17 H21 O3 P3					62567	61741	64538	56787	61351	60482											17136							32554
C17 H22 N12 O P4	23570	20722	22715	21384	24200	23547	23155	24691	25858	25308	10902	17721	9365	16204	17014	12446	29592	30207	40571	27545	27699	8753	33028	33637	7344	37998	17023	26889
C17 H22 N16 O2 P2	1761	116080	116325	109542	28896	28411	34577	33640	33601	28566	113989	117622	119856	117819	102514	114600	119958	114063	112638	8836	10793	109609	114301	10971	103026	117371	119944	107859
C17 H24 N2 O6 P4	117432	109986	111599	103687	71285	70796	70756	69096	70402	71033	106380	115915	98634	121605	105327	101957	94680	102672	116425	91433	105714	117438	125573	117422	138193	130339	128039	115253
C17 H24 N4 O3	11503							11191	14999		11661	8278	1101			2445	11081	23211		31136								
C17 H25 Cl N10 O4 S	89842	83326	81225	86384	62485	61016	59720	53696	51493	57363	83536	93795	88606	94457	70153	84624	68988	76955	62460	66140	57575	85240	89683	84947	110764	85537	95811	64841
C17 H25 N2 O2 P3	3179	3902	3309	2954	134531	131166	132092	126219	127443	126108		3890						60408			29755		94184	9818				35068
C17 H26 O3	283555	285234	284807	276591	173586	166446	171514	172974	174161	170393	273118	268429	237983	291275	250146	222479	254635	277102	316505	237539	253337	285674	339720	297142	368259	338694	324060	264270
C17 H26 O4	177662	169102	167022	162706	83745	80132	79748	78860	78128	69065	100750	137503	139802	134699	83363	83312	132947	142611	219707	125511	154747	82107	181133	153201	81156	611576	449955	543442
C17 H26 O5	122452	129099	126180	123612	153813	126101	117671	143201	120787	135266	118748	128245	139995	120725	120109	121987	121054	126263	130187	121681	125566	142975	124516	118802	117157	137153	136290	129139
C17 H28 O3 S	832854	788382	754692	2190338	88769	194725	80401	123191	95136	73386	1109110	930867	6047584	2416504	532297	2568202	506912	644597	1270676	717283	1213320	1383327	1544558	1349873	1927928	1054477	901212	1352409
C17 H28 O5	24735	23592	20751	26758	13112	12765	13459	17551	14155	11550	18584	18562	20734	24840	19572	15180	22394	25433	33317	24959	23567	18919	24947	23734	22398	24959	27376	31606
C17 H30 N6 O3	35069	30312	30953	31059	13314	8871		13216	12957		11901	35521	4502	14378	17791	22576	44009	62785	75106	47702	65264	8152	72669	57407		103273	27783	58854
C17 H31 N4 O3 P	11173	12165	10537	13766	103896	103119	110603	104257	108621	101224	5327	18344	7214	5168	9613	2988	5318	17362	32623	18822	31213		15796	60431	7558	14371	159866	26799
C17 H32 N2 O8	258804	256050	252055	247119	268613	243277	259325	253836	269167	263323	236019	279751	184243	236089	220475	208905	271012	271296	268386	291648	304264	173907	318348	276121	129139	286803	286317	286115
C17 H32 N6 O4 P2	52222	62203	59585	55963							31268	194362		37953	28909	103876	54645	154921	83403	61384	68581	42442	116014	114827		123588	70353	86911
C17 H32 O2	82301	91281	88920	81340	89044	87517	86671	88909	96120	77563	75471	242872	12027	72830	96288	28562	87700	146404	173177	114076	145389	18607	136495	101267		176645	54866	134753
C17 H32 O2 S	22911	23682	23286	21355	16186	15403	15492	15325	14334	15169		62057			12013		15127	30863	136307	19145	23151	13991	10712			19805	64726	67413
C17 H33 N4 O3 P	528899	531517	533401	514260	407059	387653	402094	414464	416508	402694	619848	536000	23241	151322	566944	280656	460599	876655	713332	669886	944122	73626	794962	531725	3863	489173	467603	916707
C17 H33 N4 O4 P	72394	69686	68581	67662	25729	31571	24673			1079	56380			36200	55715	37278		203175	133989	84979	269616	16810	163256	92745		104325	71627	193346
C17 H33 N8 O P		1323		24524	37500	37109	39680	30170	37224	31076	14620	115035	23005	21633	5465	5579	12425	26824	29780	42551	17672	14101	45735	43134	17237	17930	30783	30810
C17 H34 O2	108573	113742	59980	121769	118188	113894	116554	119497	132871	125239	55284	103315	62164	109246	115568	43555	123810	127070	151232	157993	106595	57406	92145	67118	36436	174945	76675	141132
C17 H35 O2 P3	41911	47018	47877	37863	101149	97096	119093	109982	113049	108735	21319	39704	14923	24557	35363	19890	50280	62626	86468	57217	83263	14214	68560	48779	11730	109754	44839	110473
C17 H36 N2 O12 P2	70270	66765	69272	68716	77600	74271	62277	73634	69817	70121	67451	64927	67469	65811	66006	68118	73380	63278	71606	66216	78899	59263	82451	73214	56892	76227	77001	77498
C17 H38 N2 P2 S	39826	41186	37523	38553	17226	24150	13610	22948	22717	14014	40476	109294	11819	16367	30708	13001	11566	127806	80648	139746	104565	8885	28581	30614		35325	37451	70659
C17 H38 N6	35620	31241	31479	37649	2640	1188			2011	2061	37334	64939	25422	36817	10511	31101	46240	21146	58795	49889	30061	13705	92262	42087	12068	52787	73807	39879
C17 H38 N6 P4	52881	50753	50214	50263		17616	15165		1192	10573					14074				21676				18625					
C17 H44 Cl N9 O7 S	4740	4406	4209	4686			38793	37487	42501	46261	5338			2479			7915	7772	11158	12486	17773		4858	3933		7707		15152
C17 H6 Cl N7 O4 S	44258	45158	43910	43799							73742	8982	34079	46817	41068	38534	50672	49082	60600	51138	59206	68623	71552	52536	10721	53559	16151	48716
C17 H9 N6 O2 P					38095	38366	40946	37328	39449	37892											9935							19430
C18 H13 Cl N10	52687	47759	44438	47769	28022	26340	26407	26655	26755	25698	42848	45633	33192	47818	42922	36477	38486	45845	57707	38336	50236	42889	58990	51189	65303	64626	55802	53641
C18 H13 N P4					15389	14321	16336	13927	17836	15491										1162								1412
C18 H14 N10 O	87990	81699	78733	77030	87093	76706	70941	64877	65471	65785	76633	77222	67251	80242	67800	73645	65591	76411	103621	67067	82267	79613	92776	87205	102757	96389	88792	89884
C18 H14 N6	4245	2349	3566	2874	35323	36436	40067	40995	42507	50151					3020	2474		8413	24700	7705	29420	2623	13317	6576		6370	1911	22048
C18 H15 N O3					24957	25479	25645	25443	26492	28200				3240												14147	9267	22938
C18 H16 N12 O P4					32879	32053	32511	32571	31831	29660																		
C18 H17 N5 O4 P2	53650	55516	51704	51131	6432	6571	8302	7603	6334	6899	51505	62614		21733	48512	64471	56879	85794	72072	73497	70619	28910	63709	70392		90336	49376	78705
C18 H19 N14 O2 P5	53343	52271	54877	51954	31522	31541	34441	31376	32925	32386	51185	51891	45694	56332	49374	49262	44982	49378	55513	45008	51981	53542	58498	53799	72366	66189	61587	51407
C18 H21 N16 O4 P5	44299	41971	40275	39400	21304	22980	21479	22672	22104	22441	37960	41846	34687	44192	39526	34863	33794	40479	45870	34460	40218	39400	47465	42874	60698	52471	47283	38789
C18 H21 N2 O2 P	202211	196779	200435	186617	223512	226928	224784	231302	235412	215134	152675	201865	117675	168747	151098	118724	216073	225460	254820	217480	232548	115179	227234	228423	90148	252161	205076	236551
C18 H22 N2 O5					46028	50033	51829	48181	52228	61242										2660	2149		2753					7070
C18 H22 N4 O4	28974	27170	30787	33017	46514	40899	44173	45125	47186	42393	19831	36018	19034	29563	29532	17574	38717	41639	51366	41446	47088	23485	42320	40119	20904	56684	31010	47218
C18 H22 O2 P2					101281	97855	97994	95512	101152	94367													4784					
C18 H23 N3 O9	97106	139860	143059	99416			8469	9653		8485	47788	54683	1900	21771	45802	83879	132052	413948	371719	121998	190373	39407	209035	189244		357553	72752	373594
C18 H23 N9 O11 S	134086	131654	129861	127335							91721	95307	12996	54054	128072	125334	227753	148005	289214	19220	270968	44401	144639	231356	14819	274955	57374	165587
C18 H24 N4 O12 P4	79361	75694	78482	72508	48817	53486	52097	48509	48750	49830	75376	78284	69130	84406	71509	71726	66442	72733	84159	66896	72521	80748	86125	78375	95073	95560	89349	75260
C18 H26 N10 O2	102589	183876	192199	186826	69628	92175	70238	85283	80277	84930	202841	73687	210423	185801	201930	194010	102773	103010	102721	95221	127173	201933	94653	90328	250403	178310	201949	149307
C18 H26 N18 P4 S					343627	351472	320875	261523	244689	263926										1073								
C18 H27 N3 O2 P2	32288	32264	32275	27609		1023	1106				10485	35318	14480	15881	33622	12336	23903	36369	62529	39230	51436	8919	60652	52057		27280	20308	37524
C18 H28 O2					36344	300949	365252	345724	369637	333559																		
C18 H28 O3 P2	110489	113107	114132	106731	220508	216429	228235	232309	239990	222384	134370	198707	14777	80941	96708	44369	89793	190710	207258	143125	188540	21546	158304	148764	4187	165462	80992	224810
C18 H28 P6					54912	58501	57612	55242	54491	53584																		
C18 H29 N18 O6 P5	70377	14466	13092		38788	39066	37288	38065	45045	43344	26003	67279	72936	12462	16646	73761	75724	25378	10286	23078	24328	75430	17590	19936	73410	13369	13674	27088
C18 H30 Cl2 N4 O2	69606	72944	70834	57506	71958	67906	69831	73984	77540	72150	67260	75379	54273	63778	66641	56744	64315	87453	77183	74690	77847	52997	89856	72569	29228	71704	58976	84299
C18 H30 N2 O2 P2 S2	5023		4170	4630	110751	100720	103720	102562	103690	94531	5861				2284		5205	3269		6689	1046		6882			17745		3505
C18 H30 O2	46381	44404	45487	42943	981684	940029	995154	993046	1062061	1003511	38605	82107	444467	27269	41676		42220	138967	162069	114821	162768	5632	75349	88332	2608	101477	35720	169816
C18 H32 N4 O14	130954	128933	130511	127931	157628	147164	154929	138872	153613	150866	124785	137191	95759	124000	110960	112930	134243	131721	129460	147157	157528	91748	156739	137102	71988	152793	152050	151255
C18 H32 O2	1518802	1545486	1579617	1555834	3128356	2951955	3140717	3172929	3466053	3268745	1389537	1928816	114401	749135	1032706	622513	1275749	2477458	2020820	2429405	2289501	244405	2191282	1719389	29932	1969880	1776561	2213251
C18 H32 O3	210841	214735	208715	205479	59825	60935	63471	53882	58551	54681	216039	592199	52995	109717	160263	74740	191993	731056	467572	800492	504149	42655	272180	198747	24112	408774	228766	388367
C18 H32 O4	6452			4475	99349	105282	108816	104027	109032	99412	1093							3169		11154	25648			11550		13300	6611	14829
C18 H33 Cl O16	222175	234029	226784	234954		7895	5616				82265	128305	49269	324990	149369	254264	104218	296812	545179	198423	196606	234114	252527	357655	201583	488139	195482	165343
C18 H34 N3 O P S4	14525	15599	18642	18412	12877	14834				15969	36997	42521	8498	36279	40794	47500	15412	16038	9385	9341	10920	13771	17822		12038	53417	37767	7747
C18 H34 O2	2217312	2266761	2402050	2351713	4593173	4391799	4683733	4737040	5126743	4877430	2240499	2964048	483893	1891806	1859198	1335957	2334902	3067294	2820214	3073539	3229902	588876	3046605	2690546	89259	3050384	2426446	3456136
C18 H34 O3	246565	244473	126276	120375	120565	114543	131655	117537	119909	109660	38253	331454	19014	100171	46726	25891	294404	347695	567796	170339	370655	36387	248769	200172		320841	141800	210202
C18 H34 O5	36594	34186	39530	39297	23231	24649	24181	17268	17653	24145	49309	103333	13047	30693	32536	20697	15631	40567	60601	164896	32985	22698	26364	28508	7804	29279	21637	35090
C18 H34 S4	19297	23339	20066	18556	244203	233392	243949	242314	249165	232378	19108		14330	9154	18706	14258	12769	51384	52579	40870	62504		29176	15916	12145	36154	17290	57168

C18 H36 O2	1255364	1359781	1408617	1379580	1618546	1514902	1593440	1682963	1860051	1720386	1573158	1676190	1015760	1342603	1136381	1393385	1272971	1238228	1294581	1677665	1692644	777089	1644744	1338997	521587	1465930	1980648	1332630
C18 H36 O3	114994	105688	115643	106082	148709	135630	140236	137571	135004	135746	63466	126616	94856	69688	99420	63400	102341	136572	210321	115158	166082	62054	199586	158772	66216	238337	125052	137188
C18 H36 O4	56816	52717	52408	49551	43992	41128	41584	40833	42711	40364	18852	45751	8906	14460	16371	13813	72489	117106	160244	76975	99623	12848	117308	91409	5664	157526	29450	128334
C18 H37 N10 O3 P5 S					2442138	2408374	2325744	2038710	2058086	2063245																		
C18 H37 N2 O14 P3 S	48305	43337	43334	41508	46708	47788	44161	46987	49229	46229	36911	43047	34112	38791	37436	30675	51203	53008	59925	45354	52446	33538	55520	49178	30020	69051	43386	59481
C18 H39 Cl N2 O S3	57506	54567	58633	56878	26429	73614	75454	47882	81321	47260	71486	50477	23375	48546	51646	40763	58046	73304	78053	70967	75282		87579	63586		70245	58634	81271
C18 H41 O P3	47905	43599	48274	41768	17386	20023	24615	26361	24956	17934	19433	66515	12405	20756	22936	12911	54423	69488	107956	55348	68795	16578	81673	73987		41289	26933	70289
C19 H14 N10 O2	428089	417297	407657	406243	233702	232806	240268	230177	226827	222556	388361	407635	312384	434905	393358	334927	321781	389693	512570	337601	419802	385930	503851	457744	600464	568949	500473	457605
C19 H16 N10 O8 S	92224	89037	89959	85903	50730	47028	48259		48676	45341	86508	92918	74370	99710	85379	75878	77320	86908	104887	78969	88428	89743	107927	98180	136429	120880	109318	94866
C19 H18 N6 O	1022				33780	35750	39120	37329	39103	42924											2671							7390
C19 H18 N8 O12	93184	90396	90103	85587	50335	51215	49215	49904	50209	47080	87492	92978	78771	100670	85491	77754	73515	84099	100290	73150	84275	89768	103925	95987	137953	118938	108101	88732
C19 H21 Cl N2 O10	36628	35425	35144	32766	19518	19606	19429	17897	18891	18447	33932	34385	27355	37087	32035	29290	28523	34627	39148	26329	35098	33059	42087	36515	50731	44468	42159	37275
C19 H22 N14 O3 S2	71151	56825	61207	69643							54205	18778	3204	59511	23678	7193	205435	262268	276084	145622	144850	19957	137590	76592		128437	60977	167535
C19 H22 N2 O2 P2					26708	25767	25783	25745	25553	26452																		
C19 H23 N2 O2 P	62310	62199	64825	64317	43071	42645	45548	43947	43870	41115	61918	90089	31530	40569	46632	43669	55951	83150	110478	70181	93242	31237	97295	81257	19109	109008	69732	72862
C19 H23 N8 O2 P5	86714	80881	83287	78440	50491	49951	49310	49262	53212	51443	80995	84912	74151	91430	77723	74374	68486	80057	89990	71481	80172	86449	91549	82524	111677	99918	100526	80792
C19 H25 N10 O4 P5	46105	42993	43278	42840	25975	23051	24975	22621	23078	22290	38658	46711	37540	48073	41656	35797	35734	40566	47133	34769	40667	42595	49214	45925	65658	56866	49100	44164
C19 H26 N3 P S2	143682	137571	133251	130507		1669	1005	1164		1002		9208			1254775			30598					2003		12422			40331
C19 H30 N4			16678		25455	26315	28459	25823	25120	21942				11430						6805		4564	40412	22102		42064		4552
C19 H30 N6 O2	102579	36408	114067	36131	130988	125069	101592	129155	106076	121965	102146	46480	69630	107362	89265	32347	91270	61803	133633	142583	156576	19545	73779	107803	32358	135306	37320	166007
C19 H32 N2 O7 S	42183	41439	38474	36122	179045	172309	173968	166366	164749	156613	45704	32192	23096	32362	108138	49940	37939	48973	73369	56097	40904	30240	30186	42160	35829	30285	31280	46287
C19 H32 N2 O8	146171	139355	147471	144086	317556	306886	324544	321986	335688	307495	127348	175279		53137	94192	51095	115394	221041	175370	223412	197468	26315	205882	154415		185455	170196	207500
C19 H32 N3 O2 P	29566	33861	32952	29292	26737	22509	25763	25500		24311	48960	31741	28546	35427	57111	35817	22023	25182	19160	22603	24275	43577	30193	30225	38350	26753	36504	26618
C19 H32 N6 O2	7330	7843	9207	6628	17586	17370	17596	18127	18693	18873	7358	16397	1262	4290	7464		3485	7871	8835	8467	12582	1888	12350	5619		6886	9769	7926
C19 H33 N4 O3 P	112888	106330	97379	105560	215262	213118	220416	216932	217965	200321	111680		45814	45249	111413	21309	98789	115811	119430	101209	149075		133760	190047	11850	128767	52412	131382
C19 H34 N2 O8	208471	206241	206135	200855	357575	347152	366075	357194	369801	359816	185432	266054	32812	159496	120018	108674	205934	263594	237299	258630	286309	43264	277170	239608	16073	265186	218091	308415
C19 H34 N8 O7 P2 S3					661699	657001	645986	545138	573090	570398									2892		1197							
C19 H36 O2	12331	17411	19193	18659	46293	45117	48430	48066	51484	48823	21134	60882	8673	18893	22753	6620	16767	17420	23312	23733	16683	8877	24655	18601	3952	23731	13236	23557
C19 H37 O2 P3	27041	31107	27661	25282	103105	102235	103560	102987	113997	101770	37592	82459	14529	18883	42057	19455	18576	51594	59660	48409	47687	6901	37798	30300	4953	52240	25269	160749
C19 H38 N2 O12 P2	53972	59086	58000	54301	82306	80773	84514	83853	84502	77037	53012	74513	15629	43794	44079	32773	56861	74935	67907	73045	77877	20886	76584	67785	5204	75021	56354	81776
C19 H38 O2	57419	60432	60210	61120	5062	5103	6600	6198		8371	53056	64930	42908	71581	18466	52287	62515	51733	88152	46429	47275	35074	59271	40469	31480	53216	85104	46277
C19 H38 S2	120659	128292	126634	111184	26401	29183	27213	4674	27309	25160	143887	248899	26877	63715	90450	59494	69466	221932	132708	532710	128583	27564	159851	128055	5535	137609	83528	89820
C19 H39 Cl S4	64373	66787	70184	67440	274119	267922	273379	257442	269172	259898	31735	22834		12702		80155	75838	281267	278311	131745	134582	46609	74161	104787		216576	27990	223117
C19 H39 Cl2 N4 O3 P3 S2	52338	46887	45747	47705							11091	14900	3897	30412	18127		28257	74850	142436	54059	59401	34697	70853	82767	19726	107215	27727	55381
C20 H15 O2 P	35318	32424	31521	30503					1521			23503	1685	6216	3515	28156	38875	83972	105850	31183	23150	18030	54289	56330		94125	14816	69237
C20 H18 N4 O2	1272492	1220266	1187805	1179928	659120	651897	656909	641138	643502	622260	1088183	1159566	878838	1245539	1114114	947347	941021	1141980	1561314	973843	1251878	1102416	1498807	1339689	1790963	1774376	1459592	1357397
C20 H20 N10 O2	19867				55212	47618	52638	48765	55155	52395				19594			33808	38281	52007	30979	43419		36134	41081		58152	29352	54637
C20 H20 N4 O2	67174	62569	63518	61360	36056	34613	37437	34288	34786	34900	56291	62531	47924	66319	58346	51915	47928	60811	79341	50466	64258	58618	80415	69074	98147	96455	78270	70083
C20 H22 N10					29795	34137	35972	49727	48379	51152								2155			16498							3100
C20 H22 N2 O12	290479	284086	281456	274505	157137	150166	155114	151974	154330	148608	268227	286851	236061	310769	271934	243233	228264	268588	324332	228955	267028	280125	333656	296881	424333	370630	343374	289034
C20 H24 N18 O P4	20149	21243	21795	20673	40059	43728	41636	42746	42461	40525	26214	35704	5880	18015	25227	7275	19651	40475	43640	27766	29130	10563	25072	22604	4558	38078	17072	48998
C20 H24 N4 O4	19251	17427	16723	36326	37931	34942	33135	43386	43227	35868	21245	47286	2691	13927	18536	8678	15291	33346	46740	24060	41220	5665	23035	20071		32317	14721	42284
C20 H25 N2 O2 P	261365	279298	286009	245052	262916	244528	258488	298668	278278	258667	264288	265797	284060	271547	245198	281386	274836	280953	279888	290856	311530	285293	282435	294027	242733	318785	323937	285877
C20 H25 N6 P5			6850	5253	62259	55386	53999	49977	53491	56075	12694	8080								2267	1627		4780	3565				6841
C20 H26 N6 O4	22540	143971	150399	23921	59703	58885	58807	55696	55248	52148		155491	105332	139354	129808	120532	152059	40463	43362	30324	180164	94350	190060	156185	68774	37110	176489	50975
C20 H27 N12 O7 P3 S					121117	131394	124233	96662	99379	101135																		
C20 H28 O P2			7399		55617	42135	63362	38459	53147	53970					1604				6685									
C20 H28 O4					34022	32458	34946	32188	36395	33337								3242	1576		3043							1698
C20 H29 N14 O P5	30939	32607	30472	31699	40795	40182	41174	40546	40910	39225	20959	24087	15412	24521	21890	21384	33839	36747	45287	36771	44417	18037	37498	45998	16460	52142	28043	47396
C20 H30 N6 O P4	27352	25997	27067	29377	29625	27579	27881	30255	27955	27580	23271	26803	18163	24655	22190	17864	33167	35016	37917	26298	35199	19599	30956	29908	20526	42710	25675	39257
C20 H30 O2	54991	52787	53601	48705	418064	401824	421487	411033	423647	398035	32915	81608	25597	16903	51304	12521	28902	61895	116074	82812	154930	8930	68422	392082	6618	53701	31993	125321
C20 H30 O4					54021	55031	50799	57288	50130	50886											18526			1833				2512
C20 H31 N2 O5 P	44279	33667	42481	43569	69000	67811	74712	74881		73727	46527	59790	23482	26576	40193	23309	38759	63130	59043	67692	63366	12802	60264	57827	6722	60840	42525	68902
C20 H31 N6 O17 P	78971	78738	81294	75275	56062	51341	52539	59283	55054	50731	81324	66243	79396	79232	69937	77579	85174	83276	79551	70625	74278	63903	55002	77509	70240	77626	70349	72573
C20 H32 N4	154087	138670	127541	134394	175353	173645	171802	173825	162427	169565	109684	160129	105668	103797	120721	87525	153341	186682	139024	164579	194813	87007	205243	122046	83821	244742	118963	201550
C20 H32 N4 O14	65784	63405	60548	61447	140550	137110	143927	141724	141110	137974	55654	81929		31499	41535	27564	52540	109003	87832	109360	102948	17679	110701	76418	3920	81436	73057	108397
C20 H32 O2	2175312	2202192	2201370	2128574	1509471	1423866	1513240	1563203	1634785	1525070	2646620	2351439	94301	616887	2357438	1328836	1859182	4138656	3228068	3081379	4758252	372870	3859253	2241915	12039	2056344	1895910	4493614
C20 H32 O3	221869	222361	224689	205368	44816	45998	42786	85270	46005	87106	215697	359788	26932	77671	245913	134939	109570	760759	446327	288650	1061429	45141	614713	287884	7769	308418	215295	738670
C20 H34 N4 O14	91764	89211	91833	86322	179810	173452	179441	174555	189992	167171	81810	123254	22334	74120	63535	46714	96355	125760	113142	128115	145147	24992	138679	119162	26621	128261	98724	159989
C20 H34 O2	203221	206015	210284	211882	251276	252036	264793	265727	282127	260395	210396	298087	32907	114195	173719	180124	151471	400969	309558	357220	416462	79938	507452	186324	19220	278148	249750	423034
C20 H34 O3	47302	45093	44109	41659	34178	33350	26005	30906		9360	79125	107639		17958	64638	27352	19608	108449	72691	85344	103882		74671	30180		44221	34564	88075
C20 H35 N5 O7 P2 S	90027	80424	83655	84235							50987	16398	1842	62678	45824	9795	228104	326018	379186	130905	206261	21754	171647	109436		212393	108561	236824
C20 H35 N6 O2 P3	73599	68587	71195	69611	203521	190141	206332	203763	204239	196873	62411	89171	8568	28914	45826	24972	60645	127314	100169	129312	121901	14556	116508	81080		95365	82496	123735
C20 H36 N12 O2 P6	21853	22775	22076	26025	40583	34276	34611	38315	35499	35147	24643	36064	10160	15534	21461	14022	21687	29289	30432	23104	28958	7239	25491	22509	5055	33771	16752	40132
C20 H36 N2 O14 P2 S					708272	689619	673684	654525	641843	640198			2541	2839			1110		1315		1731	2913					1713	
C20 H36 N4 O14	61064	59760	59751	59118	56827	54440	54301	54718	59627	58315	69490	73112	46052	57406	50194	59561	55592	49899	52815	71128	72627	39722	75698	58294	32787	61725	95694	58717
C20 H36 O2	29394	36412	34645	34430	115066	108060	117045	115417	127344	128436	54576	119153	5331	24096	45124	18922	23316	48761	49851	77839	87981	7387	61074	34066		41679	53584	70728
C20 H37 N6 O2 P3	94672	94767	95853	91566	214446	208502	214945	214484	230713	212842	88064	140218	16175	71928	64635	45235	99615	137759	133213	138604	157535	20311	152418	120626	2609	143122	102644	175793
C20 H38 O2	26188	30562	31052	26486	57654	53974	59682	59673	64989	63416	47113	146530	5645	30431	52272	22794	36349	27793	42918	55499	71893	5190	54937	32791		31622	46618	42144
C20 H39 N19 P2	7349	8433	6676	10104	61996	60209	59415	53921	52626	46140	15688	19092	2759	8439	10276	2264	1899	8796	3726		6249		5383	3075		1452		5776
C20 H40 N2 O3 S2	150426	143972	146974	139434	125507	117440	127420	124006	121476	120220	153992	171999	97573	133606	118578	141556	136664	116730	122445	167186	172925	69178	170017	135649	47202	148518	202938	142726
C20 H41 N3 O P2	22876	28940	28995	20941	17440		19037	18867	19973	19599	35863	22242	17585	26452	60055	24627	17270	18337	12459	19920	19063	26946	23953	22859	22937	20028	25915	19265
C20 H42 O4 S	1058397	1019656	222882	933343	543507	495197	514822	1225374	498546	468267	950729	1147267	806034	893360	173281	609651	753501	211388	1152433	1121183	243695	658357	776731	705383	752392	1160223	1024844	1195467
C21 H14 N O P S					100637	98572	101384	89058	86150	83953						1814				2483								
C21 H18 N4 O		62146	64601	62995	43208	42645	45018	42211	43800	42733	55959	88762	30302	56538	46632		78608	82956	109212	69858	91661	31012	97059	81007	19109	109103	69732	72862
C21 H19 N18 O P	29466	32053	30141	30585	156166	148695	153005	152084	157521	15142	35157	33313	4871	19077	29772	22400	27309	46797	36607	39942	51029	15130	47500	30678	13073	33551	29560	51018
C21 H20 N6 O2	28942	25741	27127	24715	34858	31751	33608	32089	26349	26553	25553		25567	27322	29057	31439	31998	29304	29680	26529	30156	29767	31726	28667	28152	29096	29890	31657
C21 H20 O2 P4					36480	33936	36491	33870	34683	34275											9918							16857
C21 H26 N4 O3	20570	18008	20464	18145	14860	12777	13148	14727	14384	14637	19996	21167	16690	21257	18327	20945	18382	19363	17864	19364	18596	20457	19689	19953	12098	21002	23410	18953
C21 H28 N4 O S	475125	486147	493377	476143	350740	322427	344284	333274	340064	345105	505194	474854	470676	488379	468561	495465	457340	452293	474924	467914	452649	473996	481639	476672	350837	481900	561902	462485
C21 H29 N2 O4 P5					50294	51632	50546	39900	42644	38403														1870				
C21 H30 N6 O2	28994	29814	30164	29749	42994	40144	44995	42999	42349	41960	21444		5096	7883	45218	38797	29005	52395	41658	23305	36179	14628	30096	50524		30597	14076	35134
C21 H31 N2 O7 P	67833	67554	71963	71844	79090	77554	79676	71938	76521	70583	65250	77764	61598	67750	58376	64135	77603	69006	69814	78365	77220	55276	74974	72533	51207	74211	78445	80010
C21 H32 N2 O8	156301	147035	149888	147474	172298	166412	174976	170454	173463	161131	162255	158630	10415	46947	142226	72504	135225	259109	210909	213951	300288	27550	253810	161880	2516	148632	141676	286723
C21 H32 N6 O2	14571	16027	14375	15169	21299	25534	21410	21509	22423	21657	26730	27034	2135	7811	23862	9734	18930	23065	25226	22301	44798	8107	37592	9824		15856	18083	39889
C21 H32 N6 O4 P6	44533	45155	42472	41663	25419	23660	24085	25304	23537	23272	41256	45768	37021	52163	41368	37117	35039	40674	48527	36000	40244	43738	48272	45868	67027	56691	51861	43348
C21 H33 N10 P S	83360	83460	84967	80002	78337	73975	74771	73807	82106	71705	94799	95461	63853	74971	68966	80522	76499	74502	67319	95700	96437		100259	80868		83156	125596	85658
C21 H33 N3 O3	222174	212827	204311	192978							166343	210161	151127	200173	151471	290596	272650	322458	466172	329579	256602	154178	248604	179840	159755	198504	159460	209405
C21 H33 N8 O P5	36218	34785	29804	30921	43024	37689	30255	43691	41901	40370	18014	24161	15734	25470	21872	19588	34376	32262	48814	30302	47223	18243	41824	36370	15211	55173	28918	40308
C21 H34 N2 O5 S2	23102	21904	25095	25689	62820	59819	63224	63608	64627	61667	27555	55248	1732	17864	24540	9343	16812	37950	45227	31865	41083	4603	31512	26104		36425	20717	72914
C21 H34 O P4	25565		25222	26214	37400	36554	38778	37131	42815	40595	23309	24914	19369	21929	22986	19354	26432	33652	41595	30026	33867	16352	31709	28255	19106	41931	26092	40126
C21 H34 O20					4333727	4746145	4686129	4349605	3931429	4339058						1888												
C21 H35 O17 P	113298	104347	113679	110684	99233	80963	84448	87710	85019	88319	109458	116576	108247	114200	101005	116098	122171	117871	116436	107696	109533	102695	108518	112459	97782	112374	115214	110862
C21 H36 S2	63470	59077	61439	63668	3262						72084	98074	22343	28249	111111	45238	16161	357551	78470	189774	435733	16496	32687	54936		54238	150278	106219
C21 H37 Cl N2 O S2	36954	40275	36586	34045	36622	33519	39211	35709	34090	34723	42682		24905	36751	28694	37503	37532	33233	34889	44994	46146	20656	46971	36151	15968	40065	56817	38828
C21 H37 N25 P2	16885	3605	13632	16507	164992	42373	45375	40477	38528	34670	3211	5036	1359	2997	11517	3939	3456	5635	4933	10567	7592	6129	3945	13403		6974	14028	8140
C21 H38 O10 S	57865	58945	58675	51240	52255	46257	49812	46829	54190	46170	59858	65097	48877	49301	53334	58083	51903	56210	51930	64893	65423	36730	68492	57020	35600	55262	80178	56700
C21 H40 N6 O2 P6	18728	20948	17903	23283	42592	35154	39222	36109	41110	58922	24640	43597	6458	15288	21525	12825	9720	29001	29440	28324	29231	16982	26113	22534	12539	30843	17820	44332
C21 H44 N4 O14 P4 S	85589	80801	92858	85883	67637	44487	67232	61371	37758	59859	80560	83388	79384	87507	81643	81094	86842	91517	89574	79550	83257	78540	82802	87056	68866	83800	81545	78883
C21 H44 O4 S	2028441	2028527	2000110	1371496	720116	695178	2163483	2109696	691039	2031478	2578099	2629957	1403845	2306304	2140597	2073705	2403725	2344445	611978	689350	1919599	1896122	880868	2038785	1576041	891943	2063348	1806307
C22 H17 N6 O5 P	39002	38824	37616	38472	20559	19510	19104	19477	21409	19621	34210	38012	29244	40583	34290	29718	32197	37402	46177	32081	37655	37288	44907	40125	54270	53526	48492	40595
C22 H19 P	7355	6308		6351	3508	2828				3152	1844	9068					11913	13413	20483	8990	16348		15723	12046		18120		11689
C22 H23 O3 P S2	73234	70529	71730	71392	35041	39101	38839	34990	38014	35533	63966	77404		26285	63216	88323	60593	131912	95076	95254	81926	34027	92671	81799		122245	60496	115446
C22 H24 N4 O4	4877	68932	77842	78527	30703	28073	30094	28301	35404	30693	67688	83332	63498	77207	62012	64334	78018	79945	24286	7135	20702	57850	82953	12263	58250	15717	86026	85253
C22 H25 N2 O2 P	529585	411589	703278	568249	301085	286339	299057	312265	322041	300208	1062246	564958	685692	346835	405163	253168	419396	396078	730583	508955	647407	172435	521603	894020	322942	550386	541386	441581
C22 H26 Cl N4 O5 P		12904	13336	12656	34902	32272	32060	31487	32184	30442		1367			2212	12567	11921	35093	33935	17536	18620		16749	15854		27365	2483	30256
C22 H26 N4 O22	49058	48732	48651	52652	47222	45550	49928	51859	50646	50872	37852	49866	34486	45679	40002	32986	55908	58037	68184	51977	61598	36979	55009	57286	32590	70147	51097	63550
C22 H27 Cl N4 O	1748	2312			76514	69205	75777	70061	68435	72685							4723	4137	7626		3906		3037			1369		5917
C22 H27 N O2 P2	12029	12354	9341	11231	16881	16370	17460	18932	16942	17030	14125	19856		7966	10551	5896	8371	15748	18688	15467	16785	2235	15713	14265		15724	8274	18650
C22 H27 N2 O2 P	222847	228547	220354	213000	408780	385430	402006	397525	416566	397499	236333	306126	102617	210986	302723	184271	233223	287889	286122	303548	300705	143032	300966	286653	26682	301748	256027	322878
C22 H27 N5 O4					30794	31480	34479	31354	33941	32179							1964		1861	1645	1836							3488
C22 H28 O3 P2	213337	163806	155352	89073	37468	26795	38448	37145	40545	36454	214128	149660	245507	107479		106590	93445	104437	221793	166055	156219	13066	197346	247166		296122	135286	154233
C22 H30 N10 O4 P2 S4					63365	79572	63668	49602	51474	50551									1321		1661			1495				
C22 H30 N12 O2 P4 S	1751				265912	241366	266793	243671	263198	247819								15641	4854	2763			2314					1363
C22 H31 N7 O2 S	43264	42764	44617	38242	39427	40858	43708	46245	46576	35984	43935	54606	34444	29887	35209	44619	45531	38132	38896	43845	41910	26854	54377	45681		48392	49399	43101
C22 H32 N2 O9 P2 S	54895	56129	54000	51821	60748	57343	55853	56761	62473	57337	45165	52917	38112	50530	42902	37758	63133	66408	66246	56822	68608	38663	67677	64069	39177	86311	56802	72274
C22 H32 N4 O	8541	16501	15732	16951	9766	8838	11067			28933	14304	23934	9185	8183	9784	7045	21498	19139	20497	27674	17382	16511	26925	21462		25896	19492	19283
C22 H32 O2	261027	259684	257021	243923	868429	824290	866387	864849	886110	812597	343205	406588		92953	228981	164967	209516	320662	361021	314410	447327	38744	426708	724179	3331	439164	138995	429536
C22 H33 N6 O17 P	97423	89213	93673	91074	95222	58409	64031	67934	64149	60003	87219	112592	39928	88683	89432	72527	99334	114664	107352	103251	105908	41935	116759	99920	11320	119576	92619	
C22 H34 O2	71602	73067	78869	75444	244528	228781	259087	246959	255342	238924	75091	93175	21997	36156	73883	69621	57496	110741	124745	115321	164858	25545	158620	279144		83749	122841	173874
C22 H35 N5	14484	15226	13046	12625			2596	1498			10442	24964			9959			33918	10684	51412	54287	2116	44877	21097	5058	10795	34999	38250
C22 H35 N6 O17 P	89233	86466	84269	84861	80969	74676	76190	79403	81862	75446	93916	98030	71234	83627	79887	86943	82858	78058	78016	89467	97568	63247	96830	81460	57564	87354	108662	84160
C22 H36 N12 O2 P6	94420	34674	98913	91969	23557	23229	22602	21728	23463	68961	31583	95320	91936	93611	84641	87598	25227	98781	46809	41640	45774	81368	37963	95493	73257		87015	64069
C22 H36 O2	100702	111078	100974	96426	150198	146476	161791	151410	164447	154078	177143	169836	577674	57434	158728	75646	130918	144632	149462	137145	287989	719076	229723	69785	708345	95761	109836	249036
C22 H36 S4	38664	38862	36215	37893	90265	55684	89043	91260	93629	86043	38844	47860			29422	25802	28675	50533	44572	44518	49754		55057	64589		52378	29677	46649
C22 H37 N2 O P5	26876	33353	26083	34046	44766	45569	46480	46741	45700	45124	19334		18257	25340	20909	17211	39757	35684	45133	36919	46595	22157	37220	46138	15176	58135	31893	55341
C22 H37 O12 P S2	32008	33583	42859	32332	69106	64548	68797	65043	63466	65532	37888	56222	12972	27947	37931	17223	27517	66066	52808	40691	59875	9407	52214	36739	6645	50239	25708	78681
C22 H38 O P2 S	82928	90719	87461	81199	121714	114791	118844	122819	126481	120712	80525	103545	29445	74404	81494	58253	83537	102538	97230	112402	114410	44611	106216	95730	17332	101487	91334	104400
C22 H38 O4					16868	15613	16490	43677	15792	14393																		
C22 H38 S2	39527	36454	35967	11496	16529	14103		11647	12434	15708		21999		10026			66332	46275	68281	38661	46152		89087	67142		67745	26684	41882
C22 H4 N O P					3824	5453	2285	5085	3766	3970	30457	30157	9772	39687	32967	20457	22055		61518	26925	41637	13696			29395		44562	
C22 H40 N4 S	1993358	1998998	1895555	517177	857995	711121	2127480	2095643	758228	1998256	2577670	2477076	572196	1487783	473620	2061543	2350379	527826	586091	596494	1880440	1794444	608737	2092053	1288675	568544	2027473	1781581
C22 H40 N5 O3 P	11630	9237	10349	9915	101236	99137	106168	89732	86103	82589	39023	8816		3731	8035	24970	5811	10628	7270	16401	14269	11086	8154	6936		6256	5916	15310
C22 H41 N4 O4 P3 S	59468	62727	58775	60484	53532	52242	57267	57327	56088	55739	68576	66894	50973	56576	54751	59151	58390	53336	52576	62600	73262	42868	73928	60741	37717	60174	81083	65310
C22 H41 N8 O4 P					33664	34937	35021	37528	33281	31731								2525	5202	1871	5775		1292	3026				10054
C22 H43 N3 O6 S	38720	36172	35951	32723	277129	263498	38483	38166	46539	34795	25484		4764	26365	18580	11341	94817	61755	80667	103988	125687	8465	52638	24438	7125	63559	29901	152377
C22 H44 N2 O5					44739	63620	63987	46984	47296	90391		3139		1070				4396	11675	1356			6863	1587		3778	1406	1616
C22 H44 O2	20143	21294	23067	20014	5005	4908	4391	5992	5957	6186	33777	21927		19930	5314	23980	44461		90192	43239	112379	9650	29944	28573		60257	29045	70767
C22 H44 O2 P6	23334	20789	19125	21905	46514	42926	46454	64772	45802	45603	20360	46155	6457	18139	21211	10170	18667	36559	36715	27396	33493	7789	29456	22393		31543	17863	51438
C22 H45 N19 P2	7387	8212	6518	6767	41423	38718	38375	35119	36022	32872	2663	7508		2532	2096			5703	6733	6330	9689		2899			2336	4875	12655
C22 H52 N15 O4 P5	12688	14002		14180	41673	43332	37827	42709	39147	34717	9801	7641	2860	2916	4470	7586	1192	15736	12526	5769	4359	8573	3249	10642	1691	9119	6399	3319
C23 H23 Cl N4 O2	286312	287475	275150	261816					18306		179483	202972	235904	227514	203864	187167	249262	279798	378584	291404	273716	232856	316616	259379	261060	275310	304708	299985
C23 H24 N4 O S	119228	123722	124413	116048	66533	58535	62005	63989	69030	61443	151707	104697	87039	81793	150474	154984	118221	146600	124870	120225	161974	78049	139250	114256		98575	102179	163619
C23 H26 N10	192253	180739	178888	171004	52217	52581	68974	74148	55261	72699	150342	160837	100656	191945	155819	120071	101511	165481	298672	110865	182748	167323	272880	210934	373472	368709	281872	218623
C23 H26 N8 P2					28593	24056	28993	25147	27879	26701				3497														3181
C23 H27 Cl O8 S	241152	232048	226515	218756							139670			8271	5713	3964	507367	557080	678553	396114	551196	69003	88672	349180		440591		564744
C23 H28 N12 O P4	106445	105454	103873	3692	51530	53668	51956	55491	55775	50794	102966	99562	105681	104671	92846	101980	9969	104890	24655	106734	28638	101992	103306	15138	94260	105143	99201	83242
C23 H30 N14 O5 P4	41327	40595	43820	41162	13183	10510	13362	13460	12522	11727	42717	43371	35387	24756	39901	29144	38229	54489	48602	46135	53464	18609	50799	44458	22443	40841	39808	51066
C23 H30 N4 O2 S2	27590	29030	25010	28363	34742	35596	33780	30636	36168	33483	37601	37877		10761	26664	20033	23371	50370	34430	37739	53941	4765	45760	35084		27399	22217	52466
C23 H31 N2 O7 P		42040	46218	48299	100225	92102	99214	101099	94847	88137	44648			27300		23457	48057		81508	77358	74276		69897	47176			46915	77170
C23 H32 O2					80347	76130	79858	75471	79097	69891			2429												2213			
C23 H33 N2 O7 P	54502	52284	60226	52123	86659	88508	86465	85446	88779	85327	52059	72668	13859	45620	48517	36249	59362	79932	66794	72505	80881	18170	78647	64165	9218	80573	60007	81577
C23 H34 N4					41397	39526	41548	45587	43848	40029																		
C23 H34 N6 O13 P2	112618	107173	111027	106841	95971	92096	105435	91028	97916	39495	104682	107842	91436	110258	97387	106877	116406	113848	106123	103544	122243	90205	110686	116241	74299	114945	111852	112120

C23 H35 O17 P	62604	76808	89115	87191	125530	124521	121007	104019	127848	119105	68671	135266	6667	74635	86486	46503	78745	124214	154659	143996		39406	130473	78533	7520	142365	94287	80051
C23 H36 O P4	15265	14636	17530	14698	30922	36572	32003	31065	30482	38386	16925	30288	2658	13062	15978	7700	13637	26491	26762	22325	22267	3725	18670	17579		22918	11651	34893
C23 H36 O2 S2	16824	15345	15096	14631	784010	767711	797249	736248	747740	738258	14766	6792	1909			8586	42723	37974	56797	24119	44805	9270	27039	16088		17024	3583	57935
C23 H37 O17 P	115404	123309	124524	118243	152123	144057	146653	145444	147775	137956	112663	150917	37657	99184	100357	74310	131412	151855	136708	142948	149161	46326	149928	140924	12359	148439	128101	153864
C23 H37 O2 P3	3501	2183	3351	4333	42573	40300	44373	39738	42284	41113	61460	3161	5338	29008	2720	23188	54993	4796	7876	5362	11041	11522	126657	16363		96719	83681	8958
C23 H39 N8 O7 P5 S	99005	100474	101344	96762	45961	63775	41211	20291	38759	35956	94396	81128	105979	106320	90006	102217	103940	99849	102763	61154	60574	102990	84761	95804	96091	91711	85683	89409
C23 H39 O17 P	112379	112073	112668	106826	104097	93282	99298	103833	105174	101305	124408	126799	92114	111338	100871	107584	110923	104954	98770	120885	132552	80946	134693	110282	69510	118652	146524	115707
C23 H40 N6 O2 P6	118583	118360	115227	24937	19717	16662	22599	20236	111089	69673	106907	114565	103218	114371	101894	111181	28410	124116	115673	114090	36185	17976	25880	123805	7666	44824	118018	121630
C23 H42 S4	70995	93527	102012	99714	76317	70241	59092	76719	90404	75843	99355	94382	116897	112111	79786	100608	91381	108269	98905	82329	87070	340902	86927	94979	143337	109704	91373	79397
C23 H43 N O4 P2 S	147636	144467	142354	135350							26389	55372	128736	91586	26757	41658	355831	204258	417356	121915	125703	76953	220696	141158	93831	114833	169763	156592
C23 H43 N13 P2		2939			58857	48468	53292	50171	43943	43716				1418			1769	5280	2945					4679		3568		2814
C23 H44 N6 O4 P4 S	70446	68953	67746	68166	66331	60279	64971	63183	63749	64512	77238	79867	54277	62846	60473	68279	65037	62297	59446	73762	79217	47282	80357	67427	37583	68428	101019	71682
C23 H45 N7 P2		9544	5720		121942	118112	121220	120728	118053	112705	10630		1813		4671			15415					6743					
C23 H47 Cl N3 O3 P	26029	24468	24950	25105	139299	130123	132670	138993	128706	133148	32324	17864	20305	22355	19286	19989	37475	51801	43690	74455	96816	11558	39881	27376	4838	34309	19816	88072
C23 H48 N O9 P	6601	7656	6025	6304	119867	115783	116098	103496	103494	94056	9059	12554	1834	4951	7457	3094	4627	7269	7941	9245	13957	1653	12104	4409		5003	2859	12088
C23 H48 N5 P3					30898	27058	34834	34655	35149	36380																		
C23 H9 Cl N6 O	154497	156036	155264	154206	92699	102428	102905	107983	108378	103077	145255	149566		49535	142580	168708	137759	228364	176881	203126	189565	63488	170612	158725		219670	122522	213100
C24 H17 N8 O2 P	28720	29388	27944	25566	16808	15680	17831	16193	16617	15239	25913	27137	20149	27891	28269	24147	22868	26601	40381	25457	30351	23943	35491	34508	36012	39599	33277	37680
C24 H19 N3 O9 P2	329908	344098	338542	328067							290887	4605	43459	74514	54762	50808	663947	675810	857268	544843	719929	220295	235016	480683	7064	587774	12067	658747
C24 H21 N12 O P					42526	40515	38984	36750	34736	38093																		
C24 H24 N4 O4	702837	709620	711722	691189	45487	40734	42246	40960	43134	41710	530687	554476	649630	643907	557690	537782	642255	738422	939504	747124	683293	615913	766326	668777	709130	708752	760351	725058
C24 H27 N23 O					37660	39028	38724	40493	41845	38252									8711	2468	3862							1658
C24 H28 N12 O12 S	73760	70768	71288	65033	25119	24610	25203	24531	26252	24291	61664	71602	47175	78743	63224	55965	46143	60085	81806	44234	59310	75659	93414	75388	128456	110396	98217	73762
C24 H32 N10		6324	3681	3054	32828	29426	33537	33057	34238	32072		2534			34788			1688	2925		3925		22003					
C24 H32 N2 O5	12355	10546	14954	8580			69165	45181			11366	6321	9147	17472	2964	14818	6896	14594	23845	11067	17572	9055	15660	8461	10617	15667	11772	11921
C24 H32 O P2					30504	29643	30130	27362	27031	28261																		
C24 H32 P4	6571	7032	6640	6466	27706	28343	28271	30211	30959	28782	4478	5671		1892	8566	5811	3733	12333	14815	9086	17464		8565				2743	14081
C24 H33 N3 O2	287188	281812	282783	265252							187829	5788	36910	60098	66157	71019	699124	680273	1150933	897706	1164202	238759	317645	377421	15397	479040	20004	811885
C24 H34 N2 O10	132312	123703	122859	117059	38853	38504	39011	37987	40218	37883	107037	117331	78206	140826	104841	88200	74032	112820	181467	77863	121822	122612	178664	138300	245551	230013	186305	138803
C24 H35 N10 O7 P5	22510	23180	20918	22078	39526	35852	37499	37606	39047	37980	24608	39807	6947	18118	27738	11320	19234	35686	48329	30371	31595	10753	29462	25568	8816	30989	20856	46727
C24 H35 N6 O2 P3	25378	25584	28358	29561	43128	37570	40694	39408	36715	39570	39901	29494	2676	12907	28799	3481	22238	52467	34753	33480	46712	8200	37711	40184		31948	22582	44819
C24 H36 N12 O5	2602	2608		1773	433509	430813	431114	403688	413611	409674						1490		3302	10854	5593	13643			6603			1054	21655
C24 H36 N2 O3 S2	41824	41535	40649	41110	80000	71316	78501	72935	77693	70634	48595		4886	19714	42685	29607	37608	60556	73076	49731	87191	15311	64343	68764	4703	50880	28838	69539
C24 H36 O10 P6	18548	20652	19356	17404	19780	19347	20578	22094	21849	22006	8748	15876	8059	13964	13776	9618	26603	27697	32518	26555	26377	8623	30382	29004	7423	30197	15029	21689
C24 H37 N2 O10 P S	105653	105085	100289	103385	118798	107873	115032	110820	115113	107623	102109	114080	14698	54802	92132	57330	92157	163238	137585	142757	176974	32841	155752	114485		119375	109411	175435
C24 H37 O4 P3	20459	19793			34683	30945	24218	30503	29659	28931			10561		19206		19376	41816		27782	33027	8300		22762	3646		17936	43926
C24 H38 N2 O17 P2	62524	60997	61855	58569	74878	47165	71836	70713	77564	69348	53310	74202	9527	36716	43857	28524	50247	84353	76463	84965	76304	18563	76997	67536		75226	66281	80378
C24 H38 O13 P2	129672	129282	134889	129135	137366	119636	126846	134780	136680	122927	131013	134681	101043	128823	109309	117351	133940	144950	129281	140493	145329	92594	152330	139541	81047	144583	141616	142659
C24 H38 O19 P2 S	39540	41887	30980	42823	53885	52957	52462	56297	58126	55342	33248	48215	6037	27101	46684	15820	26664	49366	59760	48889	51419	9936	50376	46511		51559	24449	69628
C24 H40 N12 O2 P6	35230	33542	33398	30475	11707	10759	11741	12637	11135	12667	29528	33198	24182	39739	30333	27342	21436	31042	40723	22430	29478	35327	46871	34427	63176	55097	47545	35076
C24 H40 N2 O17 P2	4407	7252	91623		141368	128934	139081	140869	62751	5709	4727	9724		77155	85416	63311	94024	11568	5977	5997	5389	117100		4772		8305	7441	5848
C24 H40 O4	8730		11318		92072	91250	96447	90306	93915	89566					103387				7845				85634					7922
C24 H42 N2 O17 P2	66597	66231	64613	64490	61980	59916	64519	63618	63059	62224	72772	76319	52641	63122	60661	68336	60244	60370	58344	78542	80476	45536	84141	63963	40189	68155	97138	64709
C24 H42 N6 O3		2005		4708	92850	106576	124339	84854	75190	83142	5359	5506		1983	5240	3075		3562	19592	15116	16064	1477	15051	13124		13234	6055	6238
C24 H43 Cl O21	96278	95943	96345	99318	2413	5522	4904				31442	48732	23764	157185	60406	116904	40824	108153	152612	71278	69232	99811	105018	146743	163317	208881	92703	63136
C24 H43 N19 P2	1430	1895	1804	1268	24529	26145	23964	23380	23261	20834	1495	3392						2268	2684	3783	3702		3978	4442				
C24 H43 N9 O S3	31829	30290	27075	26626	16131	16081	17318	16619	17559	15285	33671	17444	7153	31464	25445	16184	58665	55813	60739	79866	133702	10626	41592	20718	8034	41183	18210	133190
C24 H44 N6 P4					42914	42377	45615	38888	47684	44165								1528	2953	3901	7611		3337			3433		6372
C24 H44 O2 P6	102626	101717	102167	30009	26952	23826	22178	26820	83264	26038	99504	108099	9926	27863	32952	90196	105779	105719	58825	45416	44976	77308	45391	112491	69434	114217	25406	1989
C24 H45 O18 P S3	29470	21679	28589	25549	25837	24687	26614	25324	24307	24100	29839	30075	25730	29809	25321	29250	25323	24447	26151	29833	31546	24082	29682	25578	21340	27919	30893	31649
C24 H46 N6 P4					41890	46388	43327	43014	38581	39214							4924		2962	2418	2486		2107					3997
C24 H46 O2	3504	5063	5173	3656	19478	19188	20415	20648	19694	22469	19812	17019		6687	7571	3577	7051	6954	15381	7997	16450		3001	3344		6090	4044	13968
C24 H47 N5 O P4	10059	10887	11195	9291	9639	11003	9350	12938	12489	6561	7541	5084	2138	9244	6957	3979	25321	15995	18178	27557	31490	13531	16273	7629	2380	15565	8879	35730
C24 H47 N7 O2 S2	54501	51712	52309	52621							44906			67501	11416	6990		338273	1109273	80875	161801	24720	8453	27738				34837
C24 H48 N O2 P S2	56058	50489	54436	46031	277556	267800	276300	242063	226347	213062	61660	20260	7000	28903	28543	29312	83248	57229	64857	99938	75170	23481	79775	49175	6918	73371	63269	63607
C24 H48 N6 O3	1264	21534	16217	9405	510758	496402	494133	497936	541409	487325	5055	9466	2787	1316			5727	16408	22477		60275	1258	1935	3733		19556	3034	6765
C24 H48 O2	66338	73938	73247	69959	14170	11926	11975	24152	25184	19031		37854	2015	33081	13696	55375	122806	148430	390039	369222	481913	37781	147645	104414		206794	98969	502589
C24 H49 Cl N8	2709			1517	83461	70751	110197	97539	84799	99941								5705	7386	12520			9700	7610		8518	2914	3478
C24 H51 N3 O8 S	130817	117889	111396	106950	3209998	3105810	3187914	2973024	2902432	2711524	96847	66792	23191	28039	39200	66042	86687	148728	129420	279727	276400	50382	134646	103513	8142	74643	61594	220561
C24 H52 N O2 P S2	26094	20905	18552	17753	56318	52068	55622	52116	48069	50322	84196	21813	7703	10568	19124	63265	13865	29898	10819	32297	27919	21128	13043	23198	1057	16710	12423	31296
C24 H53 Cl N4 O3	16598	4517	12598	9603		19875	20045	20167	21090	17658	6986	12446	6776		3354	13204	18537	5302	31190	32489	28982		13260	24559	2399	38589	13143	36094
C25 H15 N O2		1781			39471	40108	40498	38730	40573	40978																		
C25 H21 P	41477	40440	41964	40987	55219	53461	53289	50673	53923	53214	35549	37648		15395	31870	40955	47406	121394	115339	65065	80289	15933	58265	55950		80671	28065	104371
C25 H25 Cl N O P5	144997	145949	190588	112889			30450	2019			180226	6128	24517	42457	52408	30860	184617	114273	215884	182208	145893	144316	128205	113552	1781	115849	7004	137554
C25 H27 Cl N4 O2	42983	40385	43167	35117							29955	28001	34326	36189	43954	26141	38491	45127	69104	44735	41869	29638	52710	44570	39058	37043	46628	52579
C25 H30 N O2 P5	51604	54091	54656	48817	4630	5658	3059	4101	4895	4455	41063	47464	50181	52228	46676	40848	51520	55532	69084	57504	53876	48736	57568	50675	50485	51996	53471	55248
C25 H30 N10 O3					35744	26358	31218	29325	27384	27644		4923							1889									
C25 H31 N17 O		3999			67274	62663	65774	62660	66155	61443									13618	5050	4105							4819
C25 H32 N6 O12 S	69684	67742	66360	63377	24184	23551	24566	22984	23333	23173	58511	68393	47123	80515	59619	53536	41888	59614	81453	42330	60540	66816	88762	71900	120540	106579	98259	71232
C25 H32 N8 O7 P4	105765	19249	17778	18156	45705	44797	49879	46833	44975	47686	17043	99053	111858	110518	17476	99320	15744	33279		29959	25498	108685		8043	102251		19116	96080
C25 H32 N8 O9 P2 S	63881		71434	64682	68107	66349	71537	65858	70281	44759	64906		43693	49509		52273	77438	152075		100650	109506	35368	121958	149478	5675	111696	101248	101736
C25 H36 N11 O3 P	31500	29228	29435	29448	51358	43779	45679	43736	46059	40318	30744	36776	11283	24858	21097	23122	49275	35386	53251	53012	56508	22215	53520	40991	9414	50086	28291	42768
C25 H36 N4	8619		10038		51336	51010	51012	51726	55259	54052					129525					8388	13715		85079					
C25 H36 N4 O				7032	57148	57033	59775	57246	62363	58870									12133				60527					
C25 H36 N5 O2 P	15636	18671	18358	16939							26204	15188	14670	17712	34585	15126	11070	14963	18649		11895	19852	16855	18063	15795	13176	23620	15771
C25 H37 N10 O5 P5	76493	79804	73955	75821	21318	21167	22432	25781	21053	19384	76354	81329	20603	47617	69317	51852	70801	96189	88969	85797	93307	29554	89213	78747	6280	79993	78013	97937
C25 H38 N6 O6 P2 S2	83543	80024	78477	80873	72614	69387	31820	30915	74655	67119	79863	89118	22378	45302	73343	50050	71948	120572	97669	98440	115519	31900	110958	87113	8481	88592	81098	117597
C25 H40 N2 O10 S4	38462	35135	34301	30315	1170						24939	26716	21566	29806	189566	22805	36177	45457	49129	37466	22235	31136	10215	28000	31988	7497	10234	27516
C25 H41 Cl N8	44294	42991	41402	42256	3221	2925	3539	2545	2595	2386	64513	20658	22413	17227	74723	30404	26779	20901	57517	22851	61912	30365	37682	21971	139126	23727	38768	64630
C25 H42 N4	1644	1125		2219	27416	26824	27541	27968	28258	25553		1994		9987	2910	2917	1915		4434	1163				4108			2183	4228
C25 H43 N12 P	62587	62978	60103	57678	32678	33817	31605	28473	29697	28607	54645	63392	43704	62439	52432	44628	43213	56748	71070	45636	58213	55575	75339	60830	89697	87230	71233	60534
C25 H43 N13 P2	29224	29676	5214	1782	54034	49766	51966	50197	43402	42815	30816	39965	7659	1645	18480	9693	24853	46374	44704	69323	3237	7774	41215	23082		38967	4661	19385
C25 H44 N O7 P	81010	77634	78100	74739	175065	168110	170657	160468	149186	132290	81661	108659	22149	67683	53834	58092	142469	107202	151053	146793	167133	50858	149055	97968	13121	138301	77120	121473
C25 H44 N11 O5 P	6349	6822	4958	6457	163630	152848	153810	145454	137399	133295	6620	3172	8657	1949	2019	21441	5926	7895	6990	13745	13861	19440	6657	34560		4767	19001	13330
C25 H44 N6 O2 P6	55527	53333	50794	48649	17399	17363	17022	17248	17141	17415	47759	51116	35571	63273	45028	40502	31438	47467	64632	32698	44694	53993	69019	54702	101649	87410	78483	54399
C25 H46 N5 P3					90306	91650	88477	88025	89367	85460									1121		8159							5268
C25 H48 O4	17230	20456	6884		37297	36858	36998	36258	39691	35881	6810	25949	17736	19177	2073	3698	21903		31499	20679	17632	15357	22772	27220	6794	31154	27579	5379
C25 H48 P2 S3	54959	53305	49424	50288							11628	20285	41985	31861	9012	15764	131175	78388	198828	47782	56483	28162	96965	52367	29767	43774	58358	54875
C25 H49 N2 O2 P	14688	4097	7179		42146	86139	86684	41192	63405	14717				6988			4837	8050	31449	10046	25618		4234	18964	3294	1482	20119	6808
C25 H50 N2 S3	27317	32731	31826	27679				7694	4056		342907		13176	22044	24570	60114	44125	14422	34803	20392	33801	6269	61662	36982	6851	26097	43695	77521
C25 H50 O2	20418	17952	16490	16319				2892	3065		9993	6925		4784	1442	10855	27368	40759	102740	125295	145844	10626	38149	22200		46043	24607	159210
C25 H50 O3	6941		2984		38602	38949	30567	36055	39919	37884	1134	1436							16405				1275				2036	1458
C25 H52 N O2 P S3	18046	15724	16436	14474	69386	69896	71191	63362	61022	52344	17261	10787		14330	10719	12488	29633	17688	27053	49660	39088	9714	31595	27783		34801	11549	63472
C25 H52 O4 S	21243	2926		5375	483938	467089	485547	469673	461607	446639	10414	13782	1255	4252	5843	12166	2367	2279		48823		5799	2568	4984	2656	22397	2834	2333
C25 H53 N8 P					130507	123854	124033	126832	132639	128456								3080	2326	7953	11627		5602	1993		1438	2537	4460
C25 H54 N O3 P	8660	8985	8866	9326	27945	31985	32434	40977	46348	44315	10446	4854		4659	6987	10016	8534	20785	24731	45483	36287	4309	7942	20105		15031	5301	23515
C25 H54 N O4 P S2	5550	6144	6393	7314	67106	70790	68723	59301	59917	49492	9123	9090	2340	5487	8549	6015		11993	7765	10403	12699		6599			6286	3360	
C25 H55 N3 O3 S3	23456	23109	23401	20046	677421	633454	651329	600635	577525	534443	18425	11410	5775	8294	7166	12181	20231	29449	27944	51425	52681	8840	24620	18332	1492	15434	13706	45893
C25 H55 N5 O7 S3	29240	27658	26342	26224	409237	330767	340987	321514	312113	294121	27989	36786	7012	20441	16357	6756	32713	50367	46511	67901	60065	7872	37021	28464		35147	20584	40154
C26 H14 N2	41447	42232	41952	41861	3582		1766				32610	35752		9136		40724	42706	89076	77823	61155	67779	15490	48625	52059		76708	27489	79233
C26 H19 N5	30550	26081	30827	27880	21314	24260	20677	22597	22533	19531	27074		29612	27027	23338	35921	29899	30024	31473	32122	33771	33937	25849	23675	30955	27902	31081	31254
C26 H22 N14					63381	64391	61664	53825	54606	57982											1060		1150					
C26 H25 P	23390	25432	25151	23529	14156	13187	15182	16951	16223	14416	23957	55533	3300	23063	30978	11599	20399	33691	43926	24675	30075	4733	29896	31392		44673	18975	28178
C26 H26 O11 P6			1515		38665	38036	36514	37269	38730	38636											12232							22549
C26 H27 N8 O5 P5	35806	34542	34238	32888	18876	19243	19464	20562	18857	19259	32077	34947	30234	35853	31922	29461	28635	33045	38399	29004	31160	34013	39502	35301	49587	43664	40554	33768
C26 H28 N4 O4	203520	194318	196652	192126	10119	5540	6037	5872	25926	6293	137976	141846	171426	184987	212165	135052	190663	224487	300399	215117	198603	159584	227994	198367	191735	197941	216496	224470
C26 H28 N6 O P2	34279	32514	30470	33537	36833	33026	35213	35575	40931	34646	31793	35743	21538	15513	34437	23238	28674	56847	43204	46278	58062	12059	51640	34443	1516	37244	30891	54339
C26 H29 N6 O3 P	57905	58972	53965	53129	18825	15950	16389	16049	17325	17204	51586	50681	34221	62032	50118	40679	33182	55264	89892	38964	59148	54763	79045	67711	98024	92408	81784	67266
C26 H30 N4 O S	303007	247073	310557	315000	64914	68670	59721	71715	71198	62959	290772	198907	337475	306680	132264	339337	222785	160156	246282	212252	193839	366329	246157	124370	352432	188711	262756	199305
C26 H31 N17	4340	4908	2406	3442	34432	34381	35834	29484	31371	27366	8366	7705			3260	1414		2202	1861		3110		3174	2372			1246	2851
C26 H32 O7 S2	18239	19228	19169	24978	33175	37916	44351	36404	41245	42106	23424	35312	6088	16911	21749	8780	15710	29847	31396	24290	28600	1796	24004	21740	1737	31966	16319	41878
C26 H34 N4 O3		1842			87664	85952	89136	91974	93417	85609									5201				5126			2798	4461	
C26 H34 N6 O P2	39918	39734	36284	35438	11061	12151	13790	10805	11528	11495	33110	33078	21936	36085	33931	25761	25604	36359	67171	30899	47966	34865	52952	45753	53415	62905	50438	53425
C26 H35 N11 O	4467	5217	6695	3932	160716	154315	164557	157427	160777	155836								6564	34977	14141	8955		15089	2982		4814		9883
C26 H37 N15	38127	30671	32191	28294	22221	23824	20900	21810	20511	18795	23247	29056	22925	31929	26031	28710	25335	29804	39181	26622	31276	28662	37509	32854	46341	41584	37117	33633
C26 H38 O13 P2	65969	68257	66135	65894	106786	98955	105428	101900	106694	95914	56653	84535	15834	37284	44298	27916	57275	107058	81660	101737	96450	21058	101066	81018		83446	78419	97087
C26 H39 O2 P					20616		20052	44655	30826	24040											4111					1187	1280	
C26 H40 N5 O3 P	90602	81655	76971	72873	48252	44165	45658	48191	62792	46440	104215	53915	18241	83089	69127	41182	173537	181946	188520	257623	434618	25690	116680	59446	10472	118436	41618	418183
C26 H40 N6 O3		1679			19200	21842	21749	18105	18440	25887	6097	9411		2932	8491		8821	10707		15812	18321	1851		3307		1233	17228	
C26 H40 N6 O3 S2	118150	114813	114027	110917							18606	45123	119476	78202	20723	28952	303478	141844	295796	79096	70636	53523	157978	94947	87298	85498	147416	98288
C26 H40 O13 P2	94572	113792	109250	90733	177664	155716	145690	179600	149326	181679	95146	134257	52643	79544	75770	79136	101688	182874	163486	129182	142266	36340	124556	116352	36612	137854	111973	180060
C26 H40 O19 P2 S	98468	85582	86551	132159	40629	41811	44218	18148	41386	43016	107827	124787	54213		98800	49829		134986		108765	89061	43747	108826	125550		122329	133021	
C26 H41 N2 P					22887	19101	26206		16599								1051											
C26 H43 N O5	15844	17933	14901	15560	544815	527585	549478	528096	547724	522097	2919	4607		3166	2851	2950	9070	21503	117355	35182	23532	3448	48307	9158		9373	9704	22977
C26 H43 N4 P3					40414	40323	38466	34700	37686	37432									2799									
C26 H44 N6 O3	1980			1280	17871	19660	19551	93549	20047	20945	1162									2638	13379					5518		3185
C26 H44 N8 O8					124027	123403	123528	119443	118429	118530									1342									
C26 H46 N8 O				2564		11645	62297	64016	58795	50940							3018		1470	4655	4700		2347			3330		2007
C26 H47 N O6 P2 S	125943	117485	118858	115839							18036	50782	105659	82382	18216	36590	307432	152783	397048	97803	97997	62648	179884	115739	77286	101281	159788	119918
C26 H48 N6 O3					203563	186500	195419	197531	198809	186078		8184																
C26 H50 N6 O2	14771	13272	14131	13551	41182	30773	27688	36754	40169	36666	4910	15123	2142	6011	5258	2785	21338	27738	32402	22392	32114	2753	28912	22366		46175	16314	36862
C26 H52 N3 O15 P	5717	3736	22788	2919	83163	78472	76124	74316	70543	66073	14914	13813	3547	6373	6421	1211	13418	4628	21774	7890	8045	8331	4472	22051	1111	12883	10712	6071
C26 H52 O2	33817	31746	27847	31606				2646	4709		11551	7428		6190	4928	19200	24471	46269	74697	109265	125049	24832	60783	39747		51349	55783	142344
C26 H52 O3			2240		94617	93091	96266	97216	96486	93381							1761		4353									
C26 H54 N O4 P S2	29921	31209	32199	21370	239781	233029	230680	220174	209441	184236	54045	70200	12335	34902	43323	22218	10531	27891	22645	41649	65700	7174	28220	17913	1465	26514	16264	74273
C26 H55 N9 O P6	5119	4708	4032	8684	41832	36959	37193	39295	38325	34485	5169	4644		5321	1132		3983	7350		13462	9847	1398	6222	5184		6898	2924	
C26 H9 Cl N9 O2 P	144349	144427	180889	66852		1269		2034	4673	1523	164953	6133	25182	42127	30939	30937	182895	77835	213823	181843	43763	144633	128439	67900	1808	59836	28911	66032
C27 H19 N9 O5	102282	98143	96915	101153	31771	37813	40136	38070	41745	36304	82067	81345		15312	62935	93776	110156	267368	213603	184674	202646	24088	142129	152438		232355	57518	241042
C27 H22 N4 O3	25889	24381	27119	26665	27809	26788	29336	24868	32366	27814	21096	31389		18663	28461	9649	21478	23916	25496	32223	30766	4948	30062	24741	4435	28815	24123	29494
C27 H24 N4 O2	32085	31080	35293	32360	59793	52232	47386	56193	54764	50716	31125	34364	7682	29828	24692	17747	34355	43266	45178	45830	38526	11288	32472	35227		32628	27366	43874
C27 H26 N11 P5	140749	142129	143797	137731							97227		4002	2244	4673	3979	452713	494682	653149	327686	500266	50332	60495	252465		362115		461432
C27 H26 N4 O	51319	48097	50595	48086	95680	85735	87131	84529	89508	83646	58553	52201	57588	60932	54393	65357	54844	56534	42673	53333	47945	60439	36688	45243	54726	38853	48103	48003
C27 H26 N4 O2	16329	17165	17438	17740	17858				8877		20735		13228	18170		18384	18139	15124	11885	21846	16687	9508	20909	13119	6148	14885	23704	15624
C27 H30 O12	56512	54550	60969	52600	98015	101773	104187	107766	105115	81679	52609	77873	19634	41611	45099	29055	50741	106864	74284	77517	112917	26358	78277	54664		79340	60560	76417
C27 H31 N5 O2 P2	281615	273040	267694	266070	163674	169207	172323	162868	162567	160190	207440	219431		65841	162589	252567	277890	635040	494485	413276	484639	97696	337438	354689		532007	166534	593379
C27 H32 N4 O6	4657	4452	4147	3698	223507	221031	230433	214272	231278	216345								1261			7225							2807
C27 H36 N2 O P2	15047	17153	6765	10788	22521	25790	15477	15471	11421	14474	4831			3551	9577		5818	25250	7156	12754	9782		10060	19867	1958	10757	9457	14491
C27 H36 N4 O2					17996	17331	18704	19339	18034	17977																		
C27 H37 N5 O					33967	29039	28215	28377	30144	26143											1142							4137
C27 H38 N4 O4					47153	45456	46852	46121	53804	49239										1955	23882							20489
C27 H39 N5 O	8894	8597	7995	4284	233550	222094	231966	224512	232818	220233		3057			2211			11980	26606	25131	9651	1286	18612	10542			7302	20598
C27 H39 N5 O2	3669	4355	4422		139164	141029	150929	138390	141383	135054	2051							4755										
C27 H42 N4	2116	4888	10868	5780	96741	152773	168619	141069	146424	77140	5754	8318			6279		3022		7110	18264	5751	3594	15637	12535		11810	1623	18163
C27 H42 N4 O2	1612	2316			29076	24947	31957	32645	32138	31609					1801		1154		4116	8474	7637		3342			1897		4140

C27 H44 N4	4171				194314	169167	201292	169009	165862	98372	7439			6883	1195	2258	3219	2016				1676		2195		3595		3276
C27 H44 O3	1378				69652	26354		52991	61352					1165	4852		6453		8158				9819	2037		6015	2172	
C27 H44 O4	1422		5038		38514	35132	37935	35252	43480	32481	1281	33876		7409		11060	22443	12555	13855	3559	25257	2865	11691			33100	1374	2744
C27 H46 N4	1992	2221	4822	1285	105010	92416	99365	93016	99330	97087	1512	4139		1447		3022	1695		4861		40257			9851		3623	1946	8222
C27 H48 N11 O5 P	7207	6570	3907	6895	211287	206082	208109	194383	194569	181915	2620	10769		2457		4102	4341	5976	6884	5952	9874	2932	2883	4389		4281	9964	9705
C27 H50 O3	1026	10248	9516		586133	562211	529607	572799	591795	40771	3895	2861					1218			3243	3711		3096				5183	1726
C27 H50 O5	23635	28553	25120	29593	38449	40451		43806	42023	61915	13476	35766	16870	20730	27397	36108	20996	27251	31745	29605	41896	14028	33215	26171	4555	66922	56744	62730
C27 H50 S2	31197	43390	43494	28803	78350	20016	23926	35366	66666	61806	365647		16264	25655	26642	65620	40012	17910	36442	17741	43372	14889	73281	40804	7885	7230	44048	3565
C27 H51 Cl N2 S	9524	3670	3744	14082							3560	11268	7871	3702	1660	13001	3366			31865	16084			6754	1704	2182	9640	
C27 H51 N8 P			1982		48490	251794	49565	242229	55125	134159						2840			1565		29826		8809			5597	1227	
C27 H52 N O9 P	99580	99247	86582	91210	1533227	1453531	1488275	1401439	1349750	1267990	98047	133444	20531	70564	54836	30344	94886	160615	160977	251309	211805	25569	132490	79960	4054	123009	76511	134055
C27 H52 N2 P2		2912		2921	137585	39732	193198	159760	31291	140694									1549	8352	5406		7059	2418		6210		10260
C27 H52 N4 S2		7927	2289	3709	43131	38882	43298	39057	43254	38901		11564		8187	6178		6873	1395	12834	13319		2599		6348			2044	
C27 H53 N2 P3	41571	40847	42560	39219	1828	2477	3479	2938	2634	2951	62339	20515	22042	18384	71182	28479	23867	18801	46780	19977	49633	29441	33271	21579	138559	23001	36450	53473
C27 H54 Cl2 O	13401		11137	10736	90626	113822	89037	88468	96452	82337	7955	11180	2868	8334	2542	8643	12100	21304	5409	20401	26413	3925	9815	15290	1532	19594	20040	22676
C27 H54 N7 O2 P3 S	8920	6547	6948	7295	86211	84481	87151	78184	70257	68116	7360	7218	5737	6493	3153	8006	9175	11482	10509	19548	17218	7256	9491	7837		9929	4677	16025
C27 H54 O4	2030	1509				56982	64353	60992	1844	57185	1172	1769		4654	1961		1755	15541	2175	26988			7146			3770		
C27 H55 N3 O3 S3	25689	21059	22965	20065	332180	320097	323045	300011	286611	265558	26389	23852	8348	23576	10019	25248	33648	37521	36700	71254	61291	5196	28979	17663	5194	31444	16821	58504
C27 H55 O2 P			4212			59599	49731	47212	48303		2364				1952		1382	19205					27900					26131
C27 H56 N14 O2	93173	97754	102343	103866	213461	198241	199347	22609	22812	214075	96209	130863	6049	79615	46127	47948	7887	141130	120607	141148	142686	2798	134720	9747		140109	106855	161775
C27 H56 N3 O10 P S2	21750	19038	18728	17744	290927	273695	279000	281969	266177	250233	14723	13845	3657	4613	6365	13076	13425	22493	22776	39814	40988	8197	22133	17686	1455	13037	10832	34709
C28 H14 N2	23948	22688		23775	21512	22261			22704	21056							24981	22249	23512				24410		19641	20966	21774	19599
C28 H18 N9 O3 P	35958	39588	36205	36328	1319	2139	2176	2115		1085	28812	31985	32337	36622	36862	28076	37409	42736	56053	41439	40942	32967	46787	40496	31454	39888	40744	40585
C28 H19 N4 P3			1441	7854	77856	76363	74639	68797	66614	69419	13390					5306	4698				13347		6521	1296				9193
C28 H19 N5	24862	24661	25365	21490	30823	28351	44913	40708	45840	40961	22157	26682		23645	22286	19847	23524	27245	26287	33608	36805	12892	26035	25703		24414	22411	27717
C28 H23 N10 O5 P3		4126			53733	61158	64392	97114	96259	101468							6761	24057	2262									
C28 H23 N5	44643	44680	42815	40794	37570	35124	38370	38048	39543	36866	42440	45949	41461	45275	41373	43708	43229	41269	43032	43809	43820	40217	44178	43048	32324	44384	47198	44374
C28 H25 N3 O P6	51723	57517	56844	54915							57978	5505		17070	13179		34577	38262	42693	45321	46470	47803	51457	44721	1780	23136	3271	35292
C28 H26 N3 O2 P	25219	24934	11640	20612	27208	28333	28323	24589	22557	22989		2048			15440	13314	25363	12180	1113	27215	32761	11993	10664	10324		32362	21460	13642
C28 H28 N2 O15	532490	492261	477407	454951							173338		2656	4253	4539	3974	2883166	3268288	4414846	1672435	3144048	53398	66067	1083692		2097774		3043775
C28 H33 N2 O9 P	99608	90554	92747	89530	31827	32795	33190	32045	31619	31002	86973	92628	61684	109858	79880	72600	58094	82861	117819	61721	86392	97406	125640	102736	170766	154938	138728	97311
C28 H34 N2 O3 P2	106974	100460	101842	101808	121294	120137	122044	124724	125749	115392	103365	116990	20871	41628	94143	61950	84773	176697	134173	151957	198787	27216	174694	104602	9690	110481	96876	198233
C28 H38 N4	5323		6640	4910	62037	57103	56100	58851	56851	56816						1596	6611	12258	8949		11193		18515	7441		4139	1989	17907
C28 H40 N5 O3 P	18468	16240	15370	15976	18747	18211	18038	18700	18073	14780	17534	12023	8417	14213	13961	9457	30700	34302	32512	48673	74754	15911	25633	17148		32880	8901	64029
C28 H40 O13 S3	24921	23091	25451	22852	23063	21707	23911	20456	21629	22776	24153	28038	22501	21918	21160	23048	27202	21740	20234	21702	25377	18438	23989	22238	16749	25504	27663	23900
C28 H43 N8 P3					24101	22303	22789	23904	23209	23074																		
C28 H44 Cl N10 P S3	17393		15006		51795	53941	54490	47381	48430	49901						22559	19242	56640	61019	27301	28169	10803		26790		42005	8925	53935
C28 H44 O4		5942	7636	3855	63146	66677	69030	59072	66663	57561		2098			2038		1455	3256		6086	21903		8544	2916			2475	30773
C28 H45 Cl N2	18102	26143	20565	9640	294964	268705	113429	62875	233792	281157	38378	16893	5683	6192	20352		11225	21394		40349	25158	18329	3893	19850				
C28 H46 N O2 P3	23745	23053	18125	25978	32351	32223	36904	29128	26257	32988	25999	167401	2347	17812	12196	18250	31415	20101	15218	42175	35931	7456	26860	21782		29172	13452	22454
C28 H48 N6 O3	7699	7121	1250	2124	98845	102149	102642	104947	96804	89663		11421			10739	4857		3007	2376		8155		25722	1451		3450	6559	11570
C28 H50 O4			1635		31185	30519	32268	29130	28420	30848						3033				18393			27470	14904				16091
C28 H51 N3 O8 S	17944	14591	13988	13833	110163	101907	104917	98109	101080	86025	18791	10047	5156	10555	8256	5678	38803	30329	32681	39177	66020		23984	10898	1440	21476	8626	66348
C28 H52 N5 O4 P	7454	8484	6227	6067	53799	50488	46666	43440		45098	7342			2326		1043		10953	10901		7486		20870	12086				6454
C28 H52 N5 O5 P	30087	34159	32199	26786	117863	110214	113869	109654	104113	103483	19722	4575	4248	6682		2304		24663	32734	9973	46069	6923	9547	24773			6837	14565
C28 H52 O4			8366		91771	99526	85861	220074	222359	92950		2506								16212		1233	18971	2053		8312	2939	12660
C28 H52 S2	3083	13266	3984	9534	44266	42668	45366	56120	43977	60298	1174					2613	1237	5138	7806	20478	7588	2145	6897	10851		3025	3196	14540
C28 H54 N8 P4			1806		43409	42159	35183	34170	40106	27809		1220			3761		1027				4018							1935
C28 H55 Cl N8			12310	8200	20185	19340	18652	21412	21474	22518	1026		1849		6134				2046		79854	1462	33948		1669			
C28 H55 N3 P2 S	6782		4851	5441	83663	87858	83105	76936	79669	72372	5243							11172	20742	11471		5997	6058	5528		4862	1229	10475
C28 H58 N O4 P S2	49063	46577	44560	46369	819525	787783	816985	770417	746310	697063	71735	80925	15869	40403	42935	32954	39553	63381	54355	87676	88681	17863	59772	51431	3789	52143	36067	79870
C28 H60 N O4 P S2	40853	35303	32254	26483	649427	614149	639065	606293	605899	556539	19928	11128	4216		6035	2304	21792	22853	31887	48848	44990	6865	22313	24199		24391	3435	32103
C29 H18 N P5	1449				50691	53738	49713	59320	54020	61500		1677			1269		2981	2648						2868				
C29 H18 N8	71967		151858	144868	8732	9112				38262	101004	59364	86040	125489	43626	67539	66992		224466		73482	59073	191447	98129	105901	91141	119337	89167
C29 H22 N2	17733	39420	22873	18405	18185				4458			18867	16197	5347	11951	19923	16258	48763	46087	24113	32659	4754	60344	52412	7921	34762	16995	44702
C29 H22 O P4																	308838	317865	397659									
C29 H24 N9 P	3440	4131	2861	3928	37811	35027	32513	38168	43797	49198					9579			6593	1841	7069	11527		8966			5601		24477
C29 H26 N2 P4	211078	206363	202286	197781	1099						117181					4889	367526	381036	445609	307723	387998			281168		330306		394584
C29 H27 N O4			68994	14761	29923	29558	29776	36838	26905	89452						59381			65872	70838	80895			68102				
C29 H27 N19 O4	13694	13116	12712	14079	27384	13469	26908	26019	27810	26570	12496	13986	5217	11017	7661	7809	19233	16812	20849	32713	24745	14278	21765	7762	1681	21394	11220	50318
C29 H27 N2 O P S2	82313	89021	89240	84893	6001		4995	4619			80039	77223	87679	89076	97461	75441	86845	91453	106933	91185	85850	88121	90699	85507	93364	87843	93300	86446
C29 H29 P	7137	11171	12825	10703	79137	74894	40600	81965	78794	75193	15612	36024	14837	34352	13598		5298	14627	16691	20420			18636		3249	14818	17863	22123
C29 H31 N5 P4	26906	23160	25638	33411							17655			24235	16890	4854	83751	113271	87104	40619	87521	9559	69312	45898		71193	39559	73070
C29 H35 N23		1830	3097		108246	21486	22124	20561	22013	19432		2257	1272	1581			1311			2094	3709	1536	2517	1645			1883	4133
C29 H37 N11	5792	11459	11227	5507	32713	24184	36638	23489	29705	22582	13171	12268	5202	8660	6763	22324	17246	29192	22001	40303	7878	7202	28235	17987	1465	26514	16102	10959
C29 H37 N7 S	25226		17559	18336	202726	202048	212199	216399	202290	186785		3531		15218			41401	36342	76564	61129	133957					38396		100915
C29 H39 N8 O P3					33968	32851	31807	31815	31637	35137							1098		3127	2017	4419		1829					2285
C29 H42 N4	15121	13760	2310	10144	780449	741486	777054	747631	759425	737337	34419	5364		5776	8639	19577	11098	24172	16333	41157	93557	8892	19919			11447	7071	13907
C29 H43 N3 O3 S2	21060	16222	17254	19407	71933	65937	66485	62867	58616	54538	24854	17551	2419	10883	11804	9264	28727	15911	20109	29346	40607	10490	22288	16214	2100	24415	16719	23877
C29 H44 N4 O3	905195	847116	832916	802631	527182	504487	510777	477226	486456	451485	723352	783498	656335	879795	730532	685231	671506	824002	1039176	653173	860720	844262	1076350	905161	1386951	1226513	1023418	942847
C29 H45 Cl N4 O2	1212092	1103707	1077396	1056782	550186	519222	536779	507496	505710	484539	978670	1027184	838308	1175927	999709	860981	868338	1063458	1356198	842840	1161574	1141643	1454205	1206107	1898644	1615913	1363483	1265675
C29 H45 N5 O5	40606	41702	40129	43935	33622	32353	33246	29355	31901	30052	34416	37820	34201	45153	35600	37422	31726	40745	45938	39199	48423	39237	48938	43173	54255	51137	43691	52407
C29 H46 N10	10388	16450	10259	15504	73834	71618	283094	262813	266338	256918	5639	2655		1119	1449	3538		5919	15139	16269	35730	2866	17810	4672		5067		
C29 H48 N10	2616			4440	136119	153642	98247	168269	156981	135584								3200	4784	2042	3134			1055		1848		5030
C29 H48 N4 O3	20643	18625	22170	20013	5881		10006					28599	15962	15790	22995	34220	15811	23659	21508		19991	13487	14574	22014	4968	69323	57980	58232
C29 H48 N8 O					47090	39142	43384	48062	45644	46932					1038	1828	1228				4533			1333		1435		2615
C29 H50 N10	7409	10459	8494		52736	50633	53053	48822	51146	47801	6355				4121		3902	11559	24720	25018	39344		22668	3141	1825			6011
C29 H50 N11 O2 P5	4055	3167	3124	2856	44831	39916	40068	41898	44748	40459	2437	3085			1381	1784	2474	4392	6248	8343	8284		4425	3546		3175	1009	5904
C29 H54 N2 P2					197863	183929	232708	200668	197155	180020																		
C29 H56 N O6 P S2	39415	38492	38945	35155	650726	618776	650435	620788	610643	563155	30587	28604	9447	10018	13710	23494	28221	46556	37621	80630	81411	20194	43712	34891	4807	6364	19550	64902
C29 H64 N6 O2 P2	1546		2054	5282			63866	76523	77302							6043		11047		8391	4419		2694	1624			7303	
C3 H10 N8	6456		7299		45471	45069		46023	39993	42084	16600	27364	1489	6193		15574		26302										1295
C3 H4 O3	73873	80690	71365	88064	493126	477871	457497	401266	430601	380427	225243	77166		35056	261147			8069	147904	48251	90436	23066	39258	47592		100270	176942	119605
C3 H8 N O3 P	591985	633306	654043	653130							564235	43536	147700	220619	178861	171288	1144550	1343655	1624508	977624	1217542	440739	418812	777396	57863	1022885	76951	1139393
C30 H20 N2 O	14465	13334	14977	13930	14351	15974	15471	7191		17938		14345	12281		13211	12409	14060	16169	16245	17016	14906	12729	17439	15622	10292		16196	
C30 H22 N2			111211	110050	101465	13924	23230	21128	27055	24973	297832	72423	361087	31793		19684				87774	41053	22749	138447			156172	64636	135402
C30 H24 N4 O4	28583	30810	28873	28421	45617	43462	44222	40559	41432	43948	26517	24333		22992	15757	18463	26750	34008	22495	36535	24516		35719	32449		37690	31096	36538
C30 H25 N5	34634	37160	36733	33774	42900	38463	47334	38019	39567	35375	27939	7918	10471	30947	5154	30380	38690	39276	13294	41732	43171	16042	41118	38422		34547	36641	39830
C30 H25 N5 O	24826	21217	21596	19596	25746	22300	24296	21810	20690	20008	20839	24735	15114	19911	18755	18705	21123	15174	19926	25572	23840	15780	27685	25095	7807	22561	29496	24639
C30 H37 N11 P2		3001			43603	42252	46482	44698	39721	43139	3426				1371	1793		1831	3492	5102	8407		2502			1037		3810
C30 H39 N4 P					3403928	3483021	3358497	3343125	3442992	3227902									1191	2283								12965
C30 H41 N O4	34801	31565	30218	31748	86517	85750	90358	75710	76255	76810	131892	42664	10807	24743	32353	77144	30155	38677	27770	58833	52478	31134	27880	35172	4204	29471	19794	39083
C30 H41 N2 O P5	30380	28434	19526	30757	32462	31156	36116	32774	34683	31932	33474	35257	3303	15504	32930	24401	24052	41917	38020	37645	50766	14945	46763	37643		31542	24504	49600
C30 H41 N7 O2 S	8815	11828	10755	9732	138667	139676	140662	151201	165286	157093	15396	8092		5547	6473	2278	17342	18991	33053	31821	52298	1049	13406	8182		17458	5968	38473
C30 H41 O5 P3 S2	44721	44596	43363	50110	36931	34359	33283	34277	36680	17550	54767	47226	32801	25866	45368	33744	40849	67582	59970	53038	70751	22417	60009	49265	3740	44827	44116	63737
C30 H42 N10 O			1409		56586	60347	63594	61332		48821	3455	1214			1385	1081			5044	7580	10324	2197	8655	1678			1614	
C30 H44 N4 O4	49337	44400	49720	51701	25227	25164	22640	24528	26270	24632	43350	50492	42266	50200	46114	43254	36706	48256	58920	49809	52338	53919	64863	52778	93426	67256	69418	53055
C30 H45 N12 P3	39567	36186	36687	37030											2536				16074				12657					
C30 H46 N4 O4	1.43E+07	1.36E+07	1.33E+07	1.30E+07	7055679	6837070	7045593	6710031	6843479	6483283	1.19E+07	1.26E+07	1.07E+07	1.42E+07	1.22E+07	1.09E+07	1.08E+07	1.32E+07	1.64E+07	1.06E+07	1.40E+07	1.38E+07	1.71E+07	1.46E+07	2.17E+07	1.91E+07	1.63E+07	1.47E+07
C30 H46 N4 O5	394254	369608	357472	343784	202286	199582	200291	185995	188258	179307	309177	336400	272279	370247	322565	286515	279309	344052	448699	272168	362222	360421	461856	378116	599954	525490	442041	391237
C30 H48 N O2 P3	11092	10590	11073	12779	26040	24744	27518	29568	25479	21624	48162	20781	3541	8564	15344	32378	11615	14440	11014	23200	20036	13210	14099	13023		9049	7583	29518
C30 H49 N5 P2 S3	19092	14740	17556	14146	13662	17352	16525	14851	18940	12911	18328	12536	3741	14457	13118	8678	34290	31833	31173	46952	67996	5705	23120	13826	2590	24286	10118	67368
C30 H50 N O2 P3	7753	4984	8532	6211	19169	25588	27893	18892	28942	18849	36345	5267		3896	6655	25885	7867	10779		10306	10536	6792	8247	6097		4717	5474	11349
C30 H50 N5 O5 P	4618	7394	5949	11745	116891	86655	85403	83082	110460	78186	4658	3232		7401	2414			5664	17888	16753	9948		13265	2680		6937	3415	5899
C30 H50 O17	49327	51515	47448	44609	99293	97067	98851	90466	96146	86860	124614	300685	154091	205236	354475	64366	222868	65420	220444	54106	28749	50403	21605	62609	60361	14157	30027	38490
C30 H50 O4	6188		3451	1920	172786	160779	163632	167759	173352	153947					1906	1674		3619	7558		22037			1843			1026	5179
C30 H51 N O20	12737	11638	13150	10713	157333	151946	162406	153651	141708	134076	12644	6785		2965	4524	7282	8968	16073	13455	25521	26569	5767	15731	11141			6512	21934
C30 H54 N5 O2 P5	5011	5174	4566	3436	62430	61015	70523	64331	61940	58132	4101			1276		2631	3135	4881	4967	11358	8800	2324	8249	4240		2964	5658	8811
C30 H54 O3 S2	70952	67895	64089	60864	36359	36276	39582	36428	38168	36103	54842	59610	49118	67465	56836	50461	53575	64321	76605	48011	63127	65093	83362	71394	100745	90893	83781	69655
C30 H54 O4			5880				111349		70723	15987					4992		8795	7348			29068			1196				2543
C30 H55 N3 O P2 S	49063	9139	8958	10197	73288	74838	73843	68837	63578	61523	16356	12936	5914	12230	9109	32954	10936	14338	10696	20151	22491	17765	12573	8887	3466	7226	33070	21458
C30 H55 N5 O3 P4	7121	6599	7831	5876	40846	40871	42936	39944	35431	33457	5993	12797	2837	4756	2149	4825	12422	11053	9455	12518	20664	3189	7362	12679	1912	7824	2983	19376
C30 H56 N O4 P S2	35339	36664	32773	30191	377295	361862	370181	342726	335795	325870	41843	36012	9187	22422	27841	15309	52765	37620	62665	51191	74672	12671	67649	28637	1436	38707	21124	51166
C30 H56 S2	15469	18444	15314	10151	17918	16403	14738	18573	19046	25545	7883	2336		6958	5733		15870	29788	34976	46366	44383		22631	21308		30278	12010	39569
C30 H57 N O11 P2 S	17688	14049	15252	14887	211485	155455	155076	197686	149633	144487	15718	19066	3592	10261	6438	5714	14986	29789	23372	35709	30315	5375	27280	14154		19808	13006	20734
C30 H58 N6 O2	99589	105858	108741	114967	135802	127139	131418	169584	155023	161055	96836	113588	95728	110756	90087	98156	112486	113445	106160	123726	131635	76251	118875	110088	72510	119670	121724	109710
C30 H62 N2 O S2	6757	6022	6757	5141	52040	49369	51461	53883	54035	59543	7541	38755		3214	13406		4599	17642	24485	15501	20691		12161	7524		21127	4209	54812
C30 H63 N O9 P4		4886	1894	4300	103932	105096	104704	97703	98867	96243		2272	1307	1713			1274		1006	9633		1575	3427				2014	4129
C30 H64 N10 S	13847	9759	14544	10111	982744	951042	977899	968491	989843	874301					3003		2600	38482		40431	45431		56253	5770	1421	5210	2664	19266
C30 H65 Cl N4 O S3					81684	65919	75239	76562	80060	74798		2618		1372			7747		1502		2776	1254	2381					4901
C31 H27 N17	16772	18795	16423	14057	41701	45975	41074	38370	41186	37041	17847	22376	3636	15530	11086	11426	30776	22552	31092	30118	31043	9854	29187	20295	2550	27249	16724	24745
C31 H27 P	7992	6724	40844	7706	70448	63919	53951	60940	25939	63792	8650		3542	35094	18230		33770	13608	16044	52608	21298			33221		52613	44116	58236
C31 H34 N2 O7 S	82250	79491	75235	72564	23876	22981	25124	22538	24060	25934	69086	74523	50340	88281	63667	55130	45101	68397	101892	46398	71598	77351	106097	83392	150923	136400	115476	81517
C31 H35 N9					51511	52658	53175	49046	52622	51310																		
C31 H37 N14 O P S	454214	439431	437892	428355	233084	250679	248758	265617	264203	244849	281640	339487		47368	218812	392586	473929	1288435	804055	787290	963451	85866	665239	586931		936059	206282	1132795
C31 H45 N9 O10	13293	11816	13886	12167	126333	125601	131069	122583	113171	115402	15029	16943	4024	10450	11361	8144	10652	17516	14901	21214	25962	4862	17460	12441			14051	21568
C31 H46 N4 O			7195	7144	27586	23242	26623	21375	29563	31552	1967							11600	4898	24306	25131		10280	3112		1023	5308	14140
C31 H47 N O13 S2	13128	11564	10877	12013	11670	6604	14702	11374	8987	10947	13833	8166	5393	11555	9376	5774	25359	24537	24437	32718	50907	6914	15616	7867		15645	7303	50433
C31 H50 N4 O					39285	37677	35543	39291	35856	36434	3051	1544				1400							1366				3272	
C31 H50 N7 P3	2911	1270	2933	1271	66098	64957	61478	58975	57815	58681		1827	1459	10407	5562					9109	1835	2544	5367	3580		4741	3340	
C31 H52 N8 O P2	6190	6888	6425	6846	25876	23398	22574	21919	22134	19806	2914	12434	4397	5918	5376	1993	9365	11986	17291	9324	15711	1701	12845	11486	1766	28028	8787	21823
C31 H54 S2		3524	7195	5409								1735			2059		2256	12400	9911	19043	29026	1061	9360	5878	1557	14061	9097	17980
C31 H56 N7 O3 P3					306673	303407	310650	294447	296052	291352																		
C31 H58 N O6 P S2	19935	17987	21075	20191	238532	233468	236330	221087	217866	208077	25683	31217	6315	15673	17494	10161	15624	27103	5749	32770	32616	9542	23506	22096	5015	26942	18207	37183
C31 H59 Cl2 N2 O3 P	12018	20762		1456	43011	14266	38576				19016	20262		18892	22976	14855	26946	12591	35852	14918	22832	6790	30595	21667	12176	15030	20095	24226
C31 H60 O S2		1773		4869	79271	59980	83870	63043	93144	62423		6300		2911				4049	6277	2008	12233		10213	4646		4726	3368	1648
C31 H67 N5 O5 P2			25514	49068		16408	21775			1183	59224	64714	33001	15137	39220	49119	45753	48118	53302			25240	46941	53598	7057	7899	6306	1148
C32 H21 N7 O6 P2	2405417	2418168	2408499	2311808							1601443	5519	50725	89609	61338	60582	7880589	8642764	1.14E+07	5662843	8766276	812668	979426	4318428	4237	6276230	16053	8088684
C32 H23 N O11 P2				1873	972970	988044	972233	1146495	1181690	1166493							6921									10168		
C32 H33 N6 O2 P S3	8208	9964	8354	9765	32244	39189	37874	42646	44418	50668	23408	20291		19121	10357	5463	3444			29371	22158		9621	24425			29714	31395
C32 H35 N23					24752	24730	29107	23665	28769	24982						1480				1061								
C32 H41 N7 P2					29855	33892	29977	30876	28348	27519													5011					5212
C32 H43 N O4		3726	4341	4300	65608	62680	66004	61364	60847	62066	4633	5736					6683	7092	9985	17061	11274		6171	3517		5795		7864
C32 H45 N18 O P	3163	2578		3891		13083	17675	15508	12526	11617	3228	9761		2243	3108		2608	6431	7090	8717	6006		4503	2863		2695	1095	14680
C32 H47 N O5	4851	5102	5219	6937	67594	64196	60002	64944	58269			3777					5496	16588	4574	26161	18155		11394					15702
C32 H54 N8 P4	29352	25036	25588	23704	3972	4058	4221		4518	4599	20090	23699		32947	20551	14658	11234	21616	49113	12252	25907	24428	47070	30571	69153	67051	48496	33200
C32 H56 N O3 P3			5038	2310	37571	31090	28533	22621	31694	27006						1316		3268		5224	1242							
C32 H56 N2 O P2	15320	13156	15113	13250	45517	43671	45911	43808	44004	41165	7992	19033		9072	7120	2708	20657	27491	35482	22179	34585	3440	33217	24383	1718	53756	17721	45567
C32 H58 N8 O3 S2		33760	35196	5998	20678	20089	22947	23724	22938	20124	7032	20504	3615		5403		29216	63460	44767	56741	11421	6853	12822	3866	2835			35071
C32 H59 Cl N2 O	5714	3671			168405	155528	174333	170205	237480	176564						4819	5275		12006	15656	27963		14809	6427	2874	10588	2302	2151
C32 H60 O6		4423	10278		451559	435128	467701	433041	436528	425492	2627	2965		1483	4515		5300	18185	10498	23051	57941		22960				2257	14213
C32 H61 N4 O2 P S	44561	44547	45967	43165				43428		51064	40797	49025	31379	41612	35440	39915	44878	45431	48487	55238	56069	28683	53910	47417	19574	57429	54946	56305
C32 H66 N6 O P2	26937	29584	29730	29737	82107	33766	35321	84279	89451	32347	28038	43342	3789	23318	21888	16200	28926	42436	40944	11181	65918	5334	14621	37135		47713	35893	15271
C32 H67 O2 P S2	36820	37502	38568	1111	33821	30082	29571	31499	34572	34770	32595	3495	28858	35451	1817	33438	49156	40527	60790	40806	2182	26312	41116	41522	16999	66800	58005	4578

C33 H36 N20 O2	10778	10462	10570	19047	2791	13267	28301	15246	14124	24460	6475	10367	8765	7484	5494	4570	13656	17673	16329	14337	15672	4599	21333	15056	3337	29708	10914	24209
C33 H37 N5			6505		34889		27006	29619	31923	23604	9480	6637						2741	9262	13056	10057							24278
C33 H37 N6 O2 P	41872	43086	42007	39484	28637	26498	29799	26308	27168	23979	42470	44447	41762	50803	43548	44234	41252	44271	46406	39184	40125	48615	48065	46297	65367	59695	49450	43910
C33 H41 N11	4237	4626	11406	8466	24155	22681	85403	22239	21972	76622		7331		4182	4924	3045	1563	5590	18114	17075	9793		8902	2680		7548	3400	5865
C33 H43 N11 P2				1282	25217	22232	28365	20442	23540	23181		1488									4900						1056	
C33 H45 N P2			1157		32417	31665	33173	33640	33710	29245									5440	6849	2566		3759	1039				
C33 H46 Cl N O4	5638	5711	3980	5162	44459	38358	41737	39486	37367	38288	5577	6769		3919			6101	7724	7167	10898	10478		9766	8589		7864	3058	6503
C33 H48 O P4					25255	22720	28486	20221	22751	20651											1133							
C33 H50 N4 O				2254	71506	79376	74231	78470	72454	59825								4017	7298	4782	8762		4105			1522		1408
C33 H51 N O2 P2	8457	9057	8010	7172					21774	14178	3991	7703	2973	4073	6075	2276	8485	9778	19502	20768	17361	2224	14810	13999	1273	15513	12662	14225
C33 H52 N4 O	2168		2099	3048	7691	278167	79184	4925	45212	46259	2704	1635											1708			3920		
C33 H54 N4 O2	7200	10772	8485	4129	446392	421759	437340	48327	424537	411202			1595		4024		3983	10144	11655	24431	39209		18411		1902	6950		6438
C33 H59 Cl N2 O6	57447	56456	38483	39082		10634			25004		36003	59513	31505	47688	38076	35237	50347	42882	40740	53340	57716	27015	61071	58397	16831	66709	58376	61374
C33 H62 N4 O14	62323	63240	67233	64988	94219	88240	90607	91153	95033	93086	55694	75473	39789	56543	47743	51416	69109	65069	62939	82622	92213	38011	97792	74540	23174	85383	86207	81582
C33 H66 Cl2 O P4	34332	29323	31085	27524	4283	6127	5781	4750	5356	5880	23591	25478	12892	33873	24922	16793	13770	27622	62108	17978	36550	27920	52623	37873	71140	73864	51964	43125
C33 H66 N2 O P2				2623	23171	25190	282834	220877		20864	9438		6549				2397	7616	7642		20090							
C33 H66 N2 O3 S2	114413	108267	112835	116286	133304	117105	117806	130070	128870	136464	103376	118064	98649	102802	88677	97473	120815	115706	112260	132636	132251	77871	134985	108676	61998	126610	120702	129640
C33 H69 N O4					113480		107380	4476	103028	113033									43323			22515						
C33 H69 N4 P S2	3059	17933	13551	3932	346482	369819	394641	329885	332465	325501		24946		3467		6962		34845	28206	25674	18821		30330			24258		3961
C34 H10 Cl N3 O3		5050	27659		57817	51001	52530	74392	79879	80058							1739							1476				
C34 H25 N5 O3	30793	31783	31287	31233	7455	6724	6467	7987	7943	6506	28420	30006	19655	37127	27748	22550	21165	31288	55124	24960	36188	30154	43242	36550	55952	57080	47390	39388
C34 H28 N2 O4	12091	5253		2091	18312	16299	20937	22149	22295	28154		10367		1696			15838		1188	7709			15983			9487	11845	15082
C34 H29 Cl N6	20216	19014	18976	17708	7312	6315	6554	6989	6227	6466	19230	17999	13108	21223	17332	14881	12581	16814	25630	13021	18581	18994	25686	21990	33274	29643	27898	21076
C34 H32 N8 O2					26766	25291	31792	27714	26283	25459																		
C34 H47 N3 O10	14598	14675	11804	12713	115940	115429	114878	115143	108981	108367	16888	12747	3014	9602	9604	4907	20909	14872	22801	21848	26342	3049	22289	12379	1882	23579	8751	20538
C34 H48 Cl N2 O5 P3 S		8004	8028	7312	35501	35318	34069	32788	32993	33431		2496				8705	8908	32945	32000	14749	14666			13532		22351		30836
C34 H52 N3 O4 P5					27243	27213	25688	26577	25944	25191									6349				4683					
C34 H54 N2 O2 P2	1177		7333		21539	22120	21399	33673	21989	51070		2414				1245			3031	1458				2044		1553		
C34 H55 N4 O4 P	19399	19537	19495	18642	15885	14163	13136	17199	16664	15119	21205	42620		8243	11237	10325	13265	23778	31073	23795	24887	1538	28933	26321		25683	20431	32061
C34 H57 Cl N2 O								65130		13727	4248	4281							7344				13674					
C34 H57 Cl N2 O2	3489		2108	3616	260377				271288		2760			3025		2859	3327		10429	12859						20120	1226	4422
C34 H57 N4 O4 P	29941	30273	32048	28685	12711	24605					35652	36560	28357	22967	22773	17861	26340	34404	41764	43542	55460		58911	41681		57316	29680	59575
C34 H58 N6 O2	64289	66418	65582	67770	216152	201427	204218	198694	232797	209019	53873	81624	3014	24118	39069	18483	53819	113744	82372	104599	93892	2535	91986	72621		85388	77271	97822
C34 H60 N6 O2		16219	20696	19696		37651		43985	43332	63931	22304	26316	1241	13945	20981	18503	53276	31543	25944	25172	29043	10642	33993	20480	6683	27466		29140
C34 H62 N6 O2	127457	131816	138847	138584	234239	220428	232694	232911	257625	252390	128122	160126	10254	112223	69662	73872	127356	187401	157349	198606	171574	18692	162002	150392		174278	125707	188032
C34 H62 N6 O4		13489	12166		290442	308716	314506	308171	316476	303028								19246	12218	22900			24457					
C34 H63 Cl N2 O2			1565	1669	21428	350187	24243	382511	18457	23467		2760							1542							5710		
C34 H64 N2 O2 S4	2425	15301	2915	5083	18962	22121	17445	21494	16609	15334	4379	13501	5813	1867	3601		9623	8492	7432	6548	7402			6102	1503	6325	2085	16112
C34 H65 O2 P3	6130	6468	6349	4763	55560	50863	50153	51361	54847	49701	9381	41323	5918	1862	10991	12717	14112	17712	25244	12537	21035	1072	14170	20383	3925	20045	20470	60416
C34 H66 N6 O2	69203	68643	72409	73040	69984	63887	67371	71472	77877	73375	80596	79279	49579	70444	58520	74295	64813	63791	62922	80892	82560	31918	79534	69201	13230	73857	94606	68456
C34 H70 S3	4011			3221	241602	164904	167631	241956	254078	254923								2766	7408	22244	24601		5053					3795
C35 H34 N6 O					197382	222224	192023	180784	186845	204934																		
C35 H37 N O	21068	21442	19683	21920	78087	98265	97250	99887	99171	80943	31382	19150		14360	15104	10380	40085	44110	86082	66061	134063		34572	21628		45345	18180	100912
C35 H40 N14	12458	12047	6807	3204	22531	20405	19449	17281	12119	18469	4997	8059	3454	3719	2432	3588		5020	7133	8819		3510	4327	2835	2568	3547	4337	3937
C35 H44 N8 O P2			1323		10231	10042	14507	13124	14591	13117					1208		1302									1708	1099	2000
C35 H45 Cl N2 O2 S3	8272	7341	7943	7725	45860	46710	45170	43165	46365	44128		2197				9525	9174	46822	48515	16786	18222	3607	10758	16136		30382		40191
C35 H49 N7 O5 S2	36104	34684	35316	31899							2416	21468	53370	22235	4728		89377	29442	60104	19938	20375	13499	52882	31097	37562	27753	66114	22259
C35 H56 N O2 P3					34085	33682	20774	7693	19834	15599			3605				1866			10194	1892		4880					2204
C35 H57 N7 O2 S	51596	49607	48361	41561	47166	23610	50144	37977	54286	46975	46156		5096	43667	35347	47948	55597	50099	56126	61011	46259	36676	56222	44588	1183	7508	49104	46894
C35 H58 N10		11986	11967		12755	13039	14448	14984	15962	14470								18788	7118	22354								
C35 H62 N8 O8	62917	59532	61174	55882	164500	157996	159482	162142	166052	162053	54208	88469	4928	42858	33705	28269	65098	89199	85034	95273	108955	8626	101136	73948	2457	99502	64843	127836
C35 H63 N5	97581	100853	97934	92476							326467	322925		128732	88023	190450	120619	95949	211595	90261	219839	18767	47166	64277		117993	64269	150130
C35 H65 Cl O7 S2	2907	3427	3912	1518					6553	8352		19068	1489			2459	2113	4450	2966	2112	2691	2291		2091	3262	3059	2251	
C35 H65 O6 P S	31010	33297		10281	61006	57118	56136	61700	68965	61411	28836			13299	17514	7612	24981	61106	5854	24080	3667	8645	50013	46327	5275	45688	34639	57605
C35 H67 Cl2 O3 P	13119	12287	12461	13504	14929		12744	13248		16421	304226	13608		10143	9267	41640	11619	2912	7819	5205	8516	2216	24460	14901		9475	10307	33729
C35 H68 Cl2							102485														30834							
C35 H69 O6 P S	33606	36226	59694	37681	110172		128886	139819	115890	124270	41199	73562	21660	28723	29767	24935	36146	72219	79703	62110	68029	21620	84280	69041		67512	60091	73636
C35 H70 Cl2 O2	6700				412486	394029	418911	388303	405675	382003				2975		13285	1252	13014		22630	36440		23945	9907				25764
C35 H70 N2 O P2	12528	14173	14618	11468	976146	953722	26024	29273	29582	25694	3732	4390			2817		2121	33370	21391	40297	57112		48061	4202		8171	2681	19770
C35 H71 N S2	33445	29607	30391	31679		7490	10322		8887	8606	71507	108396		38947	27919	57210	34384	50775	64463	30200	52170	7945	19175	38589		62977	21453	43800
C35 H72 O4 S	40443	59038	57468	58219	74916	62258	62662	65312	67064	75108	38706	45145	36034	43922	45993	35789	56736	62056	57128	72838	67729	33519	69120	58612	25891	69530	68199	46377
C35 H73 P S5	55026	16410	53008	17565	18678	51587					22274	59024	34487	11362	32395	8480	51660	19475	64040	19629		1742	70927	28017	18403	65055	58235	25893
C35 H74 N2 O S2	141368	137978	144449	154395	155402	148997	145462	151263	161270	162167	130218	135647	136072	155668	123323	135898	154284	141309	135269	149503	163503	124002	144833	144590	108988	150984	154023	138215
C35 H74 N9 O4 P	34509	33702	31321	31549		2671				2428	59692	42494		46254	26298	24559	60072	40676	56196	39752	78045	5738	35899	23152		36364	30640	87069
C36 H25 N2 P S	234883	235932	231577	231287	60624	69006	70323	71704	74579	70243	193328	204411		36561	146457	236554	259524	641874	508600	427531	495565	60157	325688	372266		562975	137212	566335
C36 H27 N2 O12 P S	87844	87311	85887	89727	2091		2840			2200	72959	65439	61738	82719	428866	64316	102622	116707	121515	103683	52547	90998	22765	72752	97330	18834	25305	65651
C36 H36 N8 O3	25581	22698	22260	22431	12612	12609	14763	13391	14343	15952	25606	21294	20176	25865	19337	22246	17239	22284	25521	16365	26784	25262	25971	23529	40743	32513	26159	24014
C36 H37 N O3	14006	14561	14161	11843	143648	141711	142006	148578	151465	148308	21034	9805		8322	7884	4263	25212	26918	47660	40467	79240		18205	12483		23523		56645
C36 H41 N7 O P4	19382	19286	17834	19522	4942	5381	5634	4826	5129	4921	13893	12682			8422	15749	22809	70811	52968	38880	52247	1943	29691	34031		59003	7324	60446
C36 H52 N4 O7 P2	1649			2911	36688	40001	40180	38298	38940	37243	2785	3115			4256		1909	2379	6217					1651				2086
C36 H54 N6 O2					20366	22152	25954	23181	21263	21283				5838					1676				2034	4158		28762	1365	
C36 H58 N6 O2	89282	92009	100601	97263	128420	151153	125599	126790	137353	130748	97875	99575		24894	86869	37724	80846	160423	120165	136216	152167	5308	134690	95469		99024	92461	140685
C36 H61 N O2 P6	8127	6617	7067	6550	67236	61540	67413	59553	62120	58108	8387	8154	1890	6139	5782	2600	10786	9176	13304	7442	15667	3294	11270	11406		8100	5048	9971
C36 H62 N11 P	15561	16836	16653	18587	17390	14866	14547	15015	17410			17266	13499		28429	16710	10969	13304	9938	14148	14643	13978	22328	15914	11084	13550	21138	
C36 H65 N5 O	91905	90022	87863	83553	52813	53039	52963	56321	53214	50907	357666	180905		84055	62813	64239	136662	103207	230219	235291	492364	10760	72714	54230		93019	51689	340190
C36 H66 N2 O10	4935		6056	7248	106610	101287	103245	100211	102059	101273	5097							13121		9250	3711	2186						17007
C36 H66 N2 O6 S			29079	27372	49324		44741	45431	48173	45500	37131				28323		24615	52581	45589	2037	65750			55517		41627		59668
C36 H66 N2 O8	130522	136809	133373	131972	242279	229899	239668	248743	258363	240944	126825	171499	10492	103618	60757	66443	136893	188509	155805	177038	182074	15318	175320	157480		180259	138782	206959
C36 H67 Cl N2 O		8572			124178	113182	122879	131103	93806	89763			1409		1666		2379	2382	2535	19818		1189	9285	2722				1838
C36 H67 N2 O P	18184	16686	19577	18295	80027	36211	75322	73240	74237	4562	13410	23267	7770	13834	11077	7827	22439	26563	37090	31777	30873	4621	26003	23243	3642	31365	18698	28792
C36 H70 N2 O8	86180	82948	83297	79913	104618	97927	100594	96434	97496	95422	91443	101656	48061	77898	64356	82339	80572	70998	79515	100070	103908	33979	107607	86067	11993	94048	117596	92383
C36 H72 Cl N3	39696	40110	36887	36491							78272	46688		24192	27535	30549	67333	87994	154277	65636	151586	6376	34765	34582		92270	28226	162587
C36 H72 O4 S	15919	16941	15957	16262	51461	55760	49956	47885	58776	49280	18457	46682		7341	24751	2759	12565	30687	37938	30536	32774		22619	20453		35011	11513	52555
C36 H73 Cl P4	2688	35490		32503	63848	69212	70900	45303	72976	62639	32416	53565		25287	27602		32029	49414	42941	51546	53069		51643	42553		46928	34445	58327
C36 H75 N S2	26408	26202	26465	24052	7648	7862	9329	7831	7540	7499	111528	38023		27815	15815	11159	32236	20557	132414	37822	65381		10748	7580		14825	9288	62398
C36 H75 N9 O2 P2	29799	27991	32858	28469	36410	29521	27024	33437	43531	36827	25150	31396		21665			50552	63850	90577	80248	136307		35776	29990		49349		126149
C37 H33 N S4	12072	12132	12319	11629		2432		2164	2128			8641		2301	4258	7051	18198	77193	98365	23062	26048	2041	17647	23906		58029		45108
C37 H34 N15 P	2667	1067	1318	1382	20930	22158	5282	18850	18316	19336				1456			2480		2928	3990	6168		3051			2519	1115	
C37 H39 N10 P	5782	5838	7856	5668	175458	66538	62832	196419	60794	66057	6223	3116		2376	8894		3666	11447	6974	23033	20465		3725	3415		29852	2838	26246
C37 H42 N5 O2 P3 S	272574	273730	269114	267715	57179	69827	71137	81087	82711	74411	188721	180890		11322	124128	224211	313571	1069826	731308	606687	754246	26239	441657	497183		842741	98908	892122
C37 H43 Cl O S4					56898	61074	61510	59967	63512	59897								87949	99084			12472					8162	85917
C37 H49 N O S					109526	123064	120692	125368	116199	108819								8088									13029	
C37 H58 N4					146517	145097	146946	141418	148070	141226		6113						1673		15206	16253							4585
C37 H61 N7 O2 S	23021	21134	22226	22063	26747					31349	26018	28398	17306	21610	20532	20601	20700	20445	18756	26271	25455	14383	28514	24644	8319	26627	34779	25807
C37 H62 N4					21934	22565	22992	32752	35137	32215																		
C37 H64 O3 P6	18051	17293	15820	14079		1574	1874	1025			11933	14193	7297	19725	11487	8277	5813	14121	29873	6040	14548	15591	30547	20592	49918	44628	31581	19902
C37 H66 Cl N11	39818	36761	36818	38793		337363	349684	360003	382409	327510	32281	23945		25617	17585	18963	99240	85468	184617	97038	143401	12633	51128	40703		88180	40106	157087
C37 H66 N5 P	27520	27496	28473	29207	34492	41103		35055			41473	27466	21486	28302	48937	30164	22325	21958	22612		27594	28701	29358	31552	25462	26711	30232	23499
C37 H66 S2	3925	3261		4652	178675		173851	164599	158996		1932						3817	2669			26707		5186					
C37 H68 N2 O5 S2	7082	3498		3051	114942	125918	106276	137010	95564	101749	16653	18203		13340	10371	5131	13294	15453	12595	13097	20503	13409	27305			24164	3814	
C37 H70 O S2	9560	78177	10133	10193	172537	172407	167658	155275	160418	168063	5758	73248		13405	9972	2989	3510	173981	16834	54605	62033	4487	31071	5493	1941	64917	55649	12267
C37 H75 N S2	22347	23466	20652	20018		2102	4777		2031	4035	54435	35001		22344	14865	20909	49972	32166	72204	49162	94748	1895	19763	12193		31012	11680	60255
C37 H77 N3 O S	17777	20366	19306	19463	10521	16590	18098	15419	9936	15344	28764	12013	16619	21867	34229	20294	6508	14150	13073	9242	16721	22989	17263	20326	19300	18854	25242	13903
C37 H80 N9 O P	43193	43460	39387	35660							47781	53867		37259	33878	66756	43180	66946	99355	59640	104352	16273	44134	47344		73051	37599	103683
C38 H35 N5 O4	48267	54333	47929	52627	36330	38607	40141	34095	37409	36127	47511	46847	45052	51322	47078	48397	45621	49850	53678	45740	51240	48365	52080	50536	63393	58354	53231	49858
C38 H41 N10 P	16692	15681	17614	13273	2631	2894	1810	2438		1971	13122	13711	7352	16517	14217	7616	7929	15089	31374	9292	20069	16022	26765	21197	35533	35667	26886	23440
C38 H41 N2 O2 P5												44949													4248			
C38 H47 N O P2 S	2609	4089	3115		114038	114381	104089	105894	106702	101160		4527					3312	7914	4125		8181	1688	8251	4041			1648	6596
C38 H48 N5 O P					18216	16158	19472	17181	15176	13831										3201	4361			2100				
C38 H55 O P5 S	54729	48066	48430	46401	14077	13060	13123	12841	12631	13474	40929	45125	24654	55454	40745	30126	25878	44344	87970	29737	50391	40727	82728	62813	120303	119141	75052	66953
C38 H58 N6 O2	83401	86211	86610	87330	67643	65358	69627	70251	71280	69499	115806	83782		16966	110263	46083	69446	183014	125202	120123	210062	5624	156907	89684	5599	74237	63326	200522
C38 H60 N9 P	13896		16097	29788		6237	23043	16128		22357	32145	17526	9141	14266	27278	17985	9737	18002	28960	1713		9920	28589	21338	10131	16782	14438	16426
C38 H63 Cl N2 O S2	25429	23697	24622	22871	66546	58491	59902	59706	69010	64985	26866	30798	26082	10138	16350	11157	20715	37835	40555	40661	37740	7672	45038	35449		31606	25965	43678
C38 H64 O10 S	31333	30027	28992	29032	93834	91257	89110	89581	90469	87448	28659	45387	3432	10243	21432	14868	25053	47900	54668	48672	51431	6494	53797	38173	2846	47698	27173	55809
C38 H65 O2 P3	31657	33815	34056	32239	35148	25552	33056	30719	35489	26252	3800	45253	6786		26475	16550	24972	46204	50755	43211	3281	4155	53723	48954	5183	38339	8921	7644
C38 H66 O3 P2 S	59526	56736	58930	57137			3880				53145	8878	36206	51840	46588	44526	57643		15446	74228	9099	30146	10881		22172	72829	67469	
C38 H67 Cl N2	23773	22560		152972	48513	45779	45648	45380	45714	47457	15420	32662	12724	12911	75124	81376		199752	43535	216227	26946	21847	22043	24891		44954	19114	44668
C38 H67 Cl N2 O S2	38404	42081	36898	34629	82335	88660	95110	97195	97072	90178	49259	79995		37703		13951	50991	54725	72196	52374	87716	6310	61326	64431	4466	81488	40704	87710
C38 H71 N O3 S3	37428	36953	35872	36224							101731	102893		44635	34987	76413	37293	35336	58970	25405	54729	6822	15020	23708		37051	22325	37198
C38 H74 O4 S	40516	41096	41802	41532	65074	60360	61339	61251	68594	67987	34565	50247	2199	23854	32476	21032	40439	60573	47668	54562	48880	5958	50217	45702		49485	43459	51420
C38 H75 N S2	9461	10126	10059	9279	41845	38872	40722	38559	38221	40022	27893	12576		2634	3821	2080	26594	35976	62331	105945	126421		11605	8745		18715	3344	97906
C38 H76 O4 S	92146	95447	101641	99602	167150	147313	166653	159463	172336	170751	99033	110034	27973	93215	21161	72256	100408	124920	111648	106995	113359	35385	109949	103723	3163	117910	103235	116744
C38 H77 N S2	31356	29709	28310	25427	23023	19921	23715	22061	20797	22745	116093	47868		29494	26301	37893	39418	39394	132353	103376	280299	3303	17406	13507		33627	14472	186816
C38 H78 N2 P2 S3	18553	19135	17848	18731	13812	20376	17802	16184	19455	20483	20785	23564	10497	17929	15038	17236	19512	16050	18081	22912	25782	8687	26987	19405	5136	21241	32932	22958
C38 H78 N3 O P5	9642	13365	31561	11793	17595	16831	14297	20945	21796	20331	21606	12815	22655	15200	25467	17695	9419	12886	45148	8784	11471		17530	12690	14998	9985	27856	11018
C39 H33 N9	3519	4036	3230		22027	26335	20124	23315	21712	20815							3291	3616	9146	8438	7950	1657	6370				1648	6491
C39 H40 N9 O4 P	13154	13201	13511	12915	1309				2276		10079	10674	5398	13627	11845	6795	7961	13914	32183	9971	19513	13150	21423	18309	24955	31629	20827	21870
C39 H58 N4 O	5269				47283	43062	52308	37403	52531	37779				1116						11074	11295		9959	2240		6344		2048
C39 H60 N P3	12388	12943	10725	12960	15182	15244	18195	15920	17945	15378	7688	15509		3900		3909		10508	7005				4294	10053	2551	10637	4144	19614
C39 H61 N7 O2 S	39565	36179	35983	35100	55835	54841	58487	60287	56076	50231	33470	51487		32329	17217	21198	37070	44581	43036	39740	46776	7325	50055	41792		48606	38478	46551
C39 H62 N2 O3 P2	25733	24589	26037	25954	24136	23790	27272	27198	26345	23993			4203	9351	22601	15985	19694	44111	42374	35859	47841	2365	45123	9699	1814	28915	23646	49047
C39 H62 N2 O5 S	73313	73954	75609	74139	104772	95556	100966	100229	107092	104537	66559	83572	57299	69239	55693	78361	76208	77549	77446	90081	100747	50107	99543	83059	35139	97653	93898	90289
C39 H63 N4 P S	81935	81329	82159	77800	216948	202164	218473	212894	221707	220820	67808	102913	7423	21427	43944	18118	63691	137063	104834	137461	123089	2967	125294	93150		117278	97988	130738
C39 H65 N7 O2 S	33494	34841	30393	27055	62613	55908	57177	51952	53313	49707	31768	39674	18507	28530	23522	30984	30684	25196	30347	38298	41222	14139	47077	35283	5080	38972	44228	36106
C39 H67 N2 O P5	6146	4891	5374	4180	12720	14377	13663	12926	16360	14760	4717	14027	2220	6062	5462			12032	13665		11915	2896	6732	4552	1328	13031	4672	23413
C39 H72 Cl O2 P S	19627	16718	18053	16250	21165	21508	23130	22672	20176	18114	25273	24963	10920	19847	11800	16931	16116	18298	16646	25514	28810	6315	29787	22640	3050	26636	41424	33210
C39 H72 O3 S2	42995	40979	41312	41859	17379	16203	17965	16503	18462	19165	21591	42341	20277	41262	22148	17825	39550	61015	83824	40235	61600	20231	76727	63483	29020	71048	44580	52137
C39 H81 N2 O3 P S2	19427	15518	16014	15879	61563	64925	60544	59989	61043	53784	15096	15460		8945	8108	7239	26771	31335	44006	34226	45175		30481	22264		32330		52398
C39 H84 N9 P	128131	118074	110019	119383							234754	256854	1758	78651	141706	232375	114508	235017	253355	218336	537581	100340	79359	80863		142129	154697	310903
C4 H11 O3 P	1094454	1100325	1061623	1069208	169784	172647	166526	171630	175594	176779	959147	425819	272238	493777	460661	370082	834013	1142101	1422197	953836	1122017	593249	1311936	1236951	424146	1625510	520084	1296531
C4 H13 N2 O13 P3 S3	19776	22164	19940	19457	17621	1450			17988	15575	42794	73927	41543	56758	58176	42159	11075	12925	14911	7760	10963	21329	12779	13012	24756	17152	55962	
C4 H13 N4 P S					4111735	3948953	3868057	3915510	3851534	3714196																		
C4 H14 O2 P2 S4	112561	111590	106539	101823											17626				50159				55207					
C4 H15 N3 P2 S2	247475	231501	234663	229941	447934	416495	410768	373590	419774	381819	308954		59504		11378	5347	269662			2515	2644		121843	1704851				
C4 H4 N3 P	609758	594568	580437	575806	31002	88251	30324	27458	29904	89260	815596	856403	559587	850663	859889		567796	545859	369404	426699	434731	488671		391594	537284	696586	1082844	407291
C4 H5 N O4 S					344013	333317	318974	337192	330877	317877		3049								10658				5186				
C4 H5 N2 P S2	52015	50333	50331	48135	571988	541798	527980	558721	571066	550918	50361	34019	42794	35334	41316	33101	26617	30506	22085	24327	21075	35280	24613	27359	80397	33202	33512	18349
C4 H6 N6 O3	24207	27496	24905	15058	111576	113179	106466	121244	112215	102853	29707	8832		1172	16024	12111	26196	14899	18149	43458	53420	9248	12956	12584		10203	13220	28179
C4 H6 O4	256701	239253	232371	227075	390053	373395	360847	349848	354194	339199	390026	101938		137488	281681	207975		395280	388848	205836	604751	72706	101640	151561		315602	51516	410936
C4 H6 O5 P2 S	129452	128144	124883	121574	16330	14628	16040	18453	15544	14536	113416	52453	31171	52528	50495	39633	110700	133884	157933	125146	146381	21229	167064	151726	48236	182845	53080	146768
C4 H7 N O4	43964	43998	47225	42396							63535	100387	3648	24961		257975		66198	32739	26083	14411	62634	33676	35515	23569	50932	66797	29828
C4 H8 O7	873934	850334	132146	832845	843280	790058	782927	809419	806750	800377	1650898	79697	8023	95835	438490	181653	217821	706293	226131	325762	299817	323600	119320		14877	164586	120857	245972
C4 H9 Cl N2 O	1025095	1060643	1056141	1018837													875004		2217655	1245128				521972	114269		980975	91411
C4 H9 N2 O4 P3 S2	13552	12835	14517	11360	337839	324557	322654	327685	327488	317385	16860	9196	17242	6803	7379	4638	13084	9667	13664	5978	3823	7007	4628	11313	23574	9752		6933

C40 H46 O2		3108	1847	3943				21944	23169	11698	3396						3453	7082	5747	4684	16869					15641	4627	9012
C40 H50 N3 O2 P3	12493	17705	12098	11829	30528	30570	28474	31526	32326	27288	1074	14509		3756	9262	6631		16420	18430	17129	27950							
C40 H53 N3 O P4	18968	16743	18010	15507			1409	2670	1179	1722	13027	14604	7026	18885	14715	9312	7894	15744	39901	10445	21805	16071	29596	21234	38889	40929	28381	25253
C40 H60 O12	49309	48113	48868	51705	75619	68728	75814	76855	76642	84117	39004	55187	31603	44364	39937	38905	51586	49603	49592	58243	65933	28132	66667	57494	21820	59581	61430	55011
C40 H67 O4 P S	98550	107820	108032	97638	144590	141445	154031	142369	150036	138495	101756	110437	6245	31676	84816	39095	83592	170882	129695	143552	175933		155155	115760		97257	96913	164952
C40 H68 N3 O P S2	48516	40717	41477	39492							89506	138855	4231	51481	40225	71657	48994	61798	77253	36202	57559	11611	28574	47394		66003	21905	50504
C40 H69 Cl N2	42661	44521	43415	47071	78948	78893		27527	31472		37669	58133		22913	31875	19265	37446	66981	58014	76766	75784	6453	59951	50905		71427	48212	61455
C40 H70 N3 O P S2	23204	19008	19141	19987							24465	28495		10337	9380	14158	33269	32620	49568	22854	39920	7385	25984	31012		32421	16559	47121
C40 H73 N3 O6 S	50399	55118	54679	48128	423877	420798	434913	432302	475074	412548	81573	23336	3634	36446	33266	14632	127019	110216	237441	264537	498985	13359	76994	35940		99577	29727	394332
C40 H75 N3 O6 S	11633	11370	14192	12863	84763	90098	92485	93004	115025	86408	12027	3174		6237	4523		35193	27606	50218	55143	96067	6803	21151	12686		26833	16248	95188
C40 H76 N2 O S3	38993	38882	41876	38314	12939	17634	19257	15049			91549	18353		35839	11521	91944	18537	17743	29855	34531	26545	42567	45308	41214		75652	65176	43525
C40 H81 N O S2	28049	32350	28431	25470				57380	59439		57830	44903		33695	17721	30182	40468	44110	105955	45241	127019	2728	17841	14719		45781	14680	104420
C40 H81 N2 O8 P	206469	177196	184319	171786	208525	202781	209774	200169	198894	185773	220012	99968	4285	85361	69900	51496	343547	263792	395252	415681	534147	33978	272004	178451		232059	114268	526933
C41 H35 N9					26892	25457	25736	25019	27410	28132										1553			1682	1013				
C41 H49 N5	28707	28856	26623	25533		26798		29380	31108		25733	28829	29662	23058	21264	26592	27726	25394	36755	32683	32037	17053	34301	34349	12775	33088	31185	14701
C41 H54 O6 P2 S	53953	49600	47170	46304	8719	8476	9652	7356	7012	7466	41148	46879	26414	60058	38879	32439	22041	40858	77948	22974	43699	49675	81697	58805	118574	103214	85817	59481
C41 H62 N4		1241		1325	34425		24843	34662	31956	28097	28161	1508			34258	22255	1885		14298	6803	1345				18996	3741		
C41 H79 N3 O2 S3	40944	41533	37784	41363	247094	243857	239597	249011	277362	246762	13792		1977	10060	27675		65255	69406	156387	111268	212951		30228	29785		57616	24581	161998
C41 H81 N3 O2 S3	42300	40931	42138	37723	153674	143219	146012	154111	180540	148515	57128	34859	7136	49741	36297	16644	83510	87808	155603	174437	306084	12527	42923	37083		63083	33807	237581
C41 H85 N2 O P3 S	20188	19272	18020	15188	120860	127682	126741	118606	121404	108205	37912	15726		10300		5902	30864	37245	31477	41243	64304	2730	26927	17630		19979	9097	65467
C41 H86 O2 P4	16498	12881	13981	12436	22076	18937	20863	19347	20296	18153	11967	5501		6143	3518		28059	19461	30833	23165	39077	1405	20140	13444		19253	5281	38508
C42 H42 N3 P S	1431	2244	2537	1778	45203	48187	45443	44420	40416	37608	3123	3361		1883			2253	3098		5786	9862		2633	1402		3448		
C42 H45 O P S	106589	110034	111404	115170	93763	93412	96588	97800	97843	101582	143162	121899	120396	147053	120286	118744	112771	129816	136893	111680	134937	142945	139961	134409	223562	177037	152587	133700
C42 H64 N4		2505			21992	22202	24235	23821	22627	21959								4633	2734		14291		1788					2883
C42 H65 N2 P S2	44220	44409	50276	43276	70614	76322	87379	83171	84052	84208	94432	44591	1827	34545	48420	39028	65511	80472	75433	53653	82072	12350	78640	61977		66058	60089	72752
C42 H67 N2 P S2	46958	46133	49386	43344	140491	150924	180039	147722	158385	140882	95485	42508	1727	41294	59992	49605	65663	81023	78222	70548	110384	16016	69036	58558		51417	46617	99178
C42 H67 O4 P S	59752	64918	60278	62341	64333	62234	64454	60976	64575	63079	75443	66031	19188	12751	72630	30870	50945	149070	90601	108112	152206	14366	118830	70620		64175	63105	148941
C42 H70 O3 P2 S	33491	35030	40192	30334	92705	143906	95984		102222		30379	57955	5281	30362	27229	17549	7763	15108	57353	63078	72182	7186	64795	7991		76858	36781	82928
C42 H70 O3 S3	27155	27618	34856	28173	118409	125357	145397	127323	126988	132027	60029	28170	6607	22395	27563	36688	51666	67279	58058	46581	62944	11587	39703	45797	6389	52392	29268	40401
C42 H72 N3 O P S2	25982	23211	22500	23869							18747	21200		17934	12840	30085	34870	44092	65827	28234	35380	12166	25510	37248		39860	18427	48652
C42 H72 N3 P S2	23393	14566	16420	14682							34417	36924		24698	17064	36614	26100	27097	47618	19892	31012	4549	14066	13246		11088	11646	40287
C42 H73 N3 O6 S	20595	32858	10725	27991	502827	504465	506236	492651	526469	491237	24372			17275	12975		41517	40675	90955	112270	211146		16329	31054		19194	8506	159054
C42 H79 N5 O	45080	44710	42940	41517							32517	47148		13427	28188	48134	54455	98929	101181	54177	144777	36636	66886	46629		78182	88777	118652
C42 H83 N O5	140712	130828	137139	122340							246423	235152		116520	147586	259158	126869	213447	259148	160283	396607	90070	115404	97229		181321	151680	276333
C42 H85 N O S2	34475	33949	30435	32832							51576	53724		33688	28771	52262	31386	41838	80213	49028	89091	7251	27869	27935		55566	24038	94157
C42 H85 N S2	63926	63445	61974	62962		1340		4526	1048	3334	63346	80866		39753	40952	84126	107900	162920	253691	154930	406808	31744	81227	66139		139800	58864	295855
C43 H58 S2	27040	23660	21438	22981		17863	17147	4493		10601	36729	27032	8798	8695	22190	17610	17431	28294	36398	25638	37856	3048	39483	29082	2187	23450	17947	41921
C43 H62 N2 O5 S	35879	37254	36505	33699	135519	129751	130672	133970	143065	158703	32704	52310		10748	20448	9693	28345	73296	56016	72325	69149	2022	66159	44499		52001	45068	68448
C43 H65 N2 O2 P S2	22568	26227	20634	21159	29773	28370	30963	30389	28520	27251	26979	27693		9176	18090	8914	19144	43216	36241	33702	49462	2650	43022	28142	2207	28180	19420	53312
C43 H67 O6 P S	43743	43327	43707	43143	91016	90029	91820	93323	95697	91827	43421	56188		12605	32023	14167	33440	95263	71660	80714	100607	3627	86429	51143		53353	46188	109660
C43 H70 N2 O5 S	26888	25712	27061	23044	25996	29035	27673	24273	28409	30175	29590	33367	14867	25559	19876	25897	24913	20518	19917	33430	35056	11404	36641	25360	6262	27583	47031	26677
C43 H76 N O7 P	40781	42641	38409	46282	291063	339203	345399	348297	363430	323581	75709	25833	2601	31464	27364	15270	97652	123069	164712	207000	300226	11167	55726	45845		71710	27201	314566
C43 H85 N O6	79624	82672	74748	74511							109153	78507		64869	86783	121806	62740	78663	161918	122033	191976	39515	69685	87534		110774	86461	196911
C43 H89 N S2	81485	77819	72594	77894							107422	114239		32534	64128	92762	94864	161673	198498	120499	388116	65513	90179	72287		114527	145276	254087
C44 H69 N2 P S2	80380	69204	83465	74688	162657	186425	210681	175878	192196	164304	119879	60293		58491	65223	73629	160452	128792	108583	86482	143018	14231	152151	111125		131147	113571	115612
C44 H81 N S	44223	41300	42385	40818							32691	38855		15729	23274	37677	62669	91958	114807	63567	145930	20010	61937	41202		75453	71144	139139
C44 H82 N O3 P S2	39234	31483	33010	28018	219298	215324	223835	228677	229763	219784	53608	24195	2535	37810	31559	14653	56645	70145	144301	127165	318204	6489	48362	30219		68394	18607	242350
C44 H89 N S2	59377	55873	59121	62648	6038	8413	8081	9030	7790	8749	260595	132223	1866	72148	123461	127798	29556	58577	86770	73861	228340	21951	22154	24690		32458	47658	82588
C45 H49 N5	18418	18124	16580	16804	23460	25893	27965	30844	27991	28528	20000	26958		6684		6802	12043	24850	6826	21031	37333		26559	21349		16476	17934	28632
C46 H52 N8	10924	11153	11943	12345	30916	35249	38590	34132	35064	38165	20131	16527	14369	12136	11405	13877	16299	22178	21099	16346	19853	13190	14246	16804	12694	17945	12310	10154
C46 H56 N4 O2	37194	38449	38926	70168	61368	60953	62760	63293	66095	64353	62025	43656	8768	9897	54005	13435	71264	80789	62285	69911	83993	39714	72632	43848	29778	46150	37139	18048
C46 H93 N O S2	60356	59448	59516	58469							64345	59894		26031	57272	75830	42845	102447	171113	161513	239223	51526	55115	72379		86681	81845	227606
C47 H59 N5 O	12720	11839	10563	9047	17098				18946	22950	13679	14933	7915	9743	7966		12020	6466	9603	11677	16569	4694	13809	10522	1271	12216	19204	12335
C5 H11 N O3 S2																	100268	119988	373664	127213	241492		30313			31037		129009
C5 H12 N2 O2			224486	220177	7973		3922	8808	8012	8375	36770		11139	45314				641647	358528		62883	271475			85029			380744
C5 H4 N4 O3	743696	864854	741897	840802	3479179	3334171	3380404	3394173	3366900	3380762	1664213	287620		304845	2029167	550199	1095241	697350	225055	1822389	1818908	336547	589566	128317	46801	1049382	463824	1430036
C5 H4 O3					1135020	544653	986235	1036253	998737	975779	12749				8225												20753	
C5 H5 Cl N2 S	75726	70013	73441	67635	452876	427994	416676	429539	429732	412879	101052	46751	113926	35847	24691	19200	123685	92342	152158	50321	57602	28974	21975	73188	92702	75636	20902	71079
C5 H5 N5	133242	130252	135417		80189	67974	71961	75565	83077	83651	107679	100154	94494	112729		103346	79273	106473	119943	93022	92595	105587	107191	104612	156668	132063	125579	99513
C5 H7 N O3	1.69E+07	1.14E+07	1.15E+07	1.57E+07							1364392	1.02E+07		3180410	2687358	1.07E+07	1.01E+07	1.91E+07	3.01E+07	1.18E+07	5573684	7718894	1.66E+07	2.03E+07	1100031	2.01E+07	1.33E+07	2.04E+07
C5 H9 N O4	339477	336388	362957	341802	54500			23008	3617			383188		385118		929139	203594	334136	194914	321041	449392		318902	314898	48738	297916	331811	425939
C5 H9 N2 O8 P3	261951	253994	255997	249330	90424	64272	58882	64394	63208	59582	256775	158874	246808	231786	237181	218482	241926	230537	190921	246237	250917	328275	246082	224424	256426	226343	247783	238143
C6 H10 Cl3 O4 P	898229	900782													92024				278055				340381					
C6 H10 N6 O4					103484	104147	106203	102871	103216	98250							8507	17848	8689	5456	4661					4957		15984
C6 H10 N8 O4	72084	72510	68654	75788	69015	76822	70001	81848	73663	74775	111360	304490	14512	66064	90622	93655		78133	145763	45956	86881	14330	66512	48730		79051	21413	91805
C6 H10 O3	63304	27021	54209	55790	3115061	3057860	2976797	2938029	2931730	2852873	20705	43621	2417	7682	32571	8857	240030	150133	441111	236688	544453	23025	64210	69047		241658	21321	369120
C6 H10 O4						746731		2876	703098	667539		2063				3175												3192
C6 H13 Cl N6	650977	632725	635237	634283	1757098	1705254	1696580	1652772	1722954	1661029	470786	391525	155735	382599	464919	675363	589178	1665235	1992621	856699	903787	550438	747915	814781		1324064	538428	1580812
C6 H13 Cl O6	2258750	2244743	2203978	2082172		1019750					625076	472280	205826	411844	1248410	1382512	1766954	2276636	2239766	3845585	4411072	1673398	3895458	2194873	458471	2042103	2129213	3250452
C6 H13 N3 O3	643589	630496	630258	616338							95423						806465	1763799				781653		576876	204306	1126103	907024	1060098
C6 H6 N2 O2	371547	260637	267663	254336								119569			1997	877037	292802	1.16E+07	1289306	228884	311257	913624	793127	113533	21439	815468	335468	1104144
C6 H9 N3 O2	229028	218458	214826	205984	48315	43370	48614	47410	37997	48903	79872	255549	6005	45094	97133	365497	189556	236043	347819	174854		206385	122121	466355	51857	378752	94087	217515
C7 H13 N O3 S	74023	72574	71776	70318	20853	20080	22262	21362	19474	21391	81358	126666	10191	45733	70647	67125	60842	138332	228804	66679	221718	18115	97442		1954	137748	44212	198148
C7 H13 N2 O16 P3 S2	90885	89292	88809	91193	65555	67714	64646	66061	63467	61002	117013	80279	120669	112538	114079	93405	66313	69784	63907	57907	67334	105435	75448	65589	96328	75801	119799	55671
C7 H13 O P3	1560				291440	341820	331641	343788	287775	314153		1153				1815	2479	3755								3555		9809
C7 H17 N2 O P S4	57857	59149	55898	54694	8312	10153		9245		8794	47685	24765	16111	25652	25183	22688	49190	59539	74499	53012	60261	11325	67993	66627	24517	80836	27985	69323
C7 H17 N6 P S	14991	5294	7717	7071	110973		172332	174798		197612	22120	59376		6145	1875	36270	2128	22723	18468		8837	4317	9057	8536	1338		6271	21359
C7 H18 N2 O15 P4 S4	37849	37925	36959	33910	58905	59295	56149	53521	55614	51715	67740	79866	68416	81039	82643	61252	25269	27442	33625	17612	21991	38780	33111	29831	42102	37649	82280	20604
C7 H19 N2 P S2	206699	207629	204107	208161	484665	480436	477725	471403	483481	469164	125068	123343	19342	70540	119555	242915	201019	405734	389210	273648	252737	166699	229714	251868	25638	329540	151202	371847
C7 H2 Cl N O3	117740	110433	105788	101958	7960			8518	9012	10336	138038	165473	114523	150911	143519	128211	107782	106705	87150	71616	82349	81798	129025	86811	86010	121988	195447	81042
C7 H22 N6 O2 S2	42144	39414	38827	35905								1408	46858	49297					4791						6926	183399	223564	179343
C7 H6 O2	481674	497963	465238	475422								585820	233741	322244		299689	1101971	879175	2086740	571645	873902	341591	682436	674789	358059	937525	506083	924574
C7 H6 O3	510579	508217	492440	494048	1793495	1755213	1757557	1824461	1811540	1732257	175997	391212	19847	104090	590556	507922	342492	786768	944009	330257	972873	183309	1401767	829205	17736	721533	491220	1361283
C7 H8 N2 O17 P2	180449	181523	178607	173517		68295	67408	66498			152956	58696	152696	116173	116382	109610	187256	167485	124773	205354	188995	233744	175426	161827	171388	142398	127321	177354
C7 H8 N4 O2	78452	78667	74218	75632	608270	587887	560739	570127	567448	555101	17811	85974			31000	26859	46621	328929	14711	49441	211064	26846	381686	131349		7526	14479	272881
C7 H8 N4 O3	2969	2829	2019	2136	94655	89704	90507	85874	91454	89324	3357						6271	17867		1562	7950		9749	9278				15287
C7 H8 O4 S	826013	792341	721164	727234	1.94E+07	1.93E+07	1.65E+07	2.08E+07	2.19E+07	1.87E+07	251936	18173	19427	10909	107350	90874	663335	616825	219788	27020	1461005	75807	3296746	1848876	19050	457022	139039	3721944
C7 H9 N4 O6 P3 S2	58431	55744	55231	53743	65260				65422		80539	84027	78036	90639	91959	76333	36912	38149	39621	29563	37284	60279	43979	41577	61310	46779	92491	29560
C8 H10 N4 O3					89107	63754	64540	61835	70982	99063								14001			15506		5428					18389
C8 H11 O5 P					1033078	1004587	972129	981908	990649	915273				1539					629147		1124936		1001137			555517		
C8 H12 N2 O4	304450	269942	262453	269859	154175	156539	157911	167649	166328	172561	71970	88808	5425	34141	43199	59882	281353	1116708	2147548	325137	264200	82470	439789	627010	6583	1109366	136899	1273762
C8 H12 N2 O5	205926	219522	225296	206779	22055	8054			28236		22157	65571		17498	17346	51951	167452	703806	1123030	185461	83539	121269	317850	502111	19981	728009	233299	532982
C8 H12 N6 O4					287981	281395	286934	280041	275687	271360																		
C8 H12 O18 P2 S3	33818	31793	32491	29760	46300	44855	6680	44301	44460	44246	54363	78919	53221	69799	69741	51852	23064	24717	29503	16147	17266	30500	27409	30697	33211	33662	67847	19647
C8 H12 O3 S	62330	62832	66899	60568	1324830	1297945	734961	1302975	820178	1301551	129441	1054		43917	321537		10548	115561	164848	95335	236817	11813	61955	25357		42426	36733	172542
C8 H14 Cl N2 P	15800	13324	17044	14913		232901	216969	207842	208257			12888		6369		8676	6433	14080	44895	8565	24517	7518	51641	15955		14628	8097	13087
C8 H14 N6 O4		2255	2310		272981	278056	271342	261129	261765	248056	3275						5797		7859	12610	27672		2928			4192		10778
C8 H15 N O4	86363	85135	79392	82523							6529	28514	1144	4460	7992	8712	246652	223812	782378	257047	252171	27094	135584			22552	24665	197090
C8 H15 N3 P2 S	17654	16779	18437	15435	207065	201719	191958	198690	201150	201942	39305	5848	6163		19122	3431	33877	19963	12522		53749		2483	67865	2540	12950		10675
C8 H18 O20 P4 S	128286	128187	129182	125141							92054	24658	99407	65430	62814	60380	142044	121277	85804	168914	148166	168116	134163	115829	117181	96477	71637	142861
C8 H19 N6 P3		14758	13562		5.80E+07	6.01E+07	5.92E+07	5.58E+07	5.61E+07	5.41E+07					9803	16981	8196									16821	7822	
C8 H3 N2 O9 P S	48134	46029	46063	42560							73370	99341	70259	86947	89395	70331	29970	31623	31774	24051	30300	47046	35554	31360	52494	40032	89101	26735
C8 H6 N2 O4	17827			11765	94426	105742	98466	99039	107026	93931		1989				12527	17640		29930			2901				18592		
C8 H7 Cl2 N5 O4 P2	310071	199157	289967	302451							242306	335026	87517	212462	168395	142068	430632	253469	339878	288549	393765	173349	279675	377054	74166	403020	132232	321873
C8 H7 N O4 S	34260	35042	34695	43102	1572779	1525572	1591941	1565117	1649945	1396057	65728	5436		14835	23369	21795	2285	8285		3202	32076	14353	54247	28755	3295	104519		18919
C8 H7 O13 P3 S					131951	130228	128819	131831	134810	128113																		
C8 H8 O3	3.38E+07	3.48E+07	3.46E+07	3.36E+07	10942	25777	29912	24948	28216	20133	2.97E+07	2561358	7986472	1.18E+07	9534250	9322922	6.42E+07	6.80E+07	8.37E+07	5.18E+07	6.66E+07	2.45E+07	2.39E+07	4.28E+07	3055046	5.47E+07	4084270	6.19E+07
C8 H9 N O4	14348	19471	14943	14314	221402	200594	198358	168587	169622	164508								1315	8724	203000								
C9 H10 O3	111861	258636	260836	255266								118596							93617	70249			46939					1264
C9 H10 O4	11775	19003	11384	12254	190630	180196	170680		183972	163885	19662			7989	24918	14701	11316	22685	19524	25408	50327		26066	9952		32991	8474	37113
C9 H10 S					146341	98740	94382	132843	142611	130925		57395	3701	23066	89374	33607	13466	19002	32126		55322	10183	42473	14540		28159	28527	45380
C9 H11 N O2		766738	742175	761300							679008	629986	77465	267126	562832	652416	730481	2311792	2235662	1168022	1595766	308834	924255	1128420	22842	1743681	472800	
C9 H11 N O3	412853	331788	345846	333056	326025	312066	308521	293288	305808		347791	300415	69314	225903		439045	327706	614587	619929	376929	522615	294193	385760	471067	43283	654434	294306	594154
C9 H13 O12 P3 S2	86483	81379	79131	80279	85475	85403	80752	85560	82329	80714	115283	95276	111925	119369	121109	98647	58668	60803	59284	47232	59397	92668	66838	60196	87460	67987	120933	47204
C9 H14 N2 O23 P4 S	65142	61400	64350	61941	31480	29281		27507			73377	35421	78476	66856	65364	55161	51856	51828	44002	46013	53305	77348	55534	48600	68572	52697	69283	44002
C9 H14 N2 O5	178091	108735	154265	155826												35299	139093	475113	803415	183719	95900	64185	216584	270953		434908	116872	577394
C9 H16 O3	75332	65713	65944	62877		2363	1124	3672	3569		14114	79892	21994	73434	12081	20475	64817	107046	105847	67826	90504	9256	108759	101051	8998	99085	64537	85443
C9 H16 O4	176228	183091	176158	169426	363948	368363	345600	359157	362831	347841	118885	131895	42695	66702	354104	202381	141006	283039	341317	216491	289549	66517	167030	141617	55350	238401	105429	389577
C9 H17 N O4	61180		61234	58100	12385	12262	14117	11975	13140	11720	7996	28796	2144	6150	14142	11110	167195	175997	488092	166433	207459	20869	87950	10962		17804	21517	131621
C9 H17 N O5	75277	66786	67734		80143	77976	79036	73039	78184	74937	39352	38023	5675	22648	50585	31372	52049	105551	215958	298127	148266	14615	77815	80571	2112	142710	31102	169639
C9 H18 N P3	148190	143627	145018	149122	207270	210129	204469	207881	208185	195135	139362	144831	24065	83226	127956	151337	134259	272557	222040	199605	225339	91460	173948	180778	6225	218812	114937	248015
C9 H19 N4 O4 P	1192637	1185538	1175258	1126909	697209	681292	696638	682400	700758	687588	1097670	1114567	909327	1180877	1120695	989743	898200	1118265	1449136	984237	1145564	1145762	1379346	1243458	1531754	1544759	1407959	1270341
C9 H2 N2 O5 S	269116	250492	250616	248397	74292	70531	67593	72242	67455	66310	282338	221058	273338	269930	274315	251195	231355	222545	180641	235549	233519	320888	236431	219123	256773	221238	285861	222264
C9 H20 N8 P2 S	291057	307087	316227	298504	86664	101837		37186	97137	36042	484178	460739	62398	256522	515851	274326	234671		637248	404677	812582	105260	330616	214065	30964	353852	281456	427190
C9 H6 N2 O4	388821	387468	376657	369800	172764	170111	166064	166049	168954	166505	376374	514417	370345	565266	534621	475294	289742	382809	486148	335589	404724	392207	458289	428760	517421	569714	603929	471490
C9 H7 N O	117517	111263	106225	111681	29685	26402	27468	28997	28438	30379	19102	163367	37809	74001		80672	122688	145059	352441	94224	146438	80232	226934	183524	62868	208109	106399	146882
C9 H8 O13 P2	189837	187172	188804	179813	60656		52023	59017	53060	56099	167020	78564	171973	142717	143023	133391	192587	177030	134884	204319	192076	239449	182537	166761	176704	155709	148686	184178
C9 H9 N O3	48360	45579	44208	44122	902820	895883	887029	850085	864860	863928		20321	12261	3080	46680	5764	142467	78209	54495	11296	237492	5397	13063	184841	6354	33475	2844	37632
CAPRYLIC ACID (CAS# 124-07-2); (M-H)-																				1785								
CARNOSINE (CAS# 305-84-0); (M-H)-			5433	3767							7553					1416	3352		8506			6474		5435		4927		
CATECHOL (CAS# 120-80-9); (M-H)-					37985															1130	13441			3975				8636
CELLOBIOSE (CAS# 528-50-7); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	230558	153754	175605	376002	252819	242875	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
CHOLATE (CAS# 81-25-4); (M-H)-	4518		6075	6146	44707	43401	44789	43149	43201	41957									8801				46633					
CHOLESTEROL HYDROGEN SULFATE (CAS# 1256-86-6); (M-H)-								5219		10323			2252															6422
CHOLINE PHOSPHATE (CAS# 107-73-3); (M+HCOO)-			5766	1504							17480	3032		9053		9816	1815					2231						
CIS-11-EICOSENOIC ACID (CAS# 5561-99-9); (M-H)-	27430	27962	30029	27177	49824	44261	49948	49662	55318	54581	43348	142246	4512	28290	51064	20983	34156	25573	41799	51689	69570	4729	56705	31194		30365	42515	40432
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0); (M+Cl)-																	1848											
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0);	5728		5007	4236	4921	4228	9620	9336	5943	4813	5498	15547		3585	6864	4457	5086	3070	5260	6830	7505		8145	3195		3491	4402	
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0);	88822	89392	91821	89370	139422	132002	139940	138834	146226	136912	168491	159501	8540	47311	165017	66060	108799	137198	137445	127060	272084	19460	216371	58378		81854	102804	239383
CIS-ACONITATE (CAS# 585-84-2); (M-H)-				14565	841007	794295	789491	763835	764002	731517									48357	29432	25692							47001
CIS-VACCENIC ACID (CAS# 506-17-2); (M-H)-	2200452	2246825	2383423	2333273	4578393	4377086	4675424	4722233	5114890	4866890	2222956	2932617	470396	1874049	1848271	1321191	2315616	3044264	2795376	3052671	3204952	580299	3022238	2667418	80120	3029775	2403120	3426477
CIS-ZEATIN (CAS# 1637-39-4); (M+Cl)-	1262394	1214463	1175325	1179909	1088759	1042235	1023905	1054016	1050914	1012686	1147535	1234596	1092031	1226566	1181863	1093038	1084816	1159462	1381980	1078927	1218485	1235920	1343159	1243819	1474228	1374567	1335296	1218619
CIS-ZEATIN (CAS# 1637-39-4); (M-H)-	5150839	4948356	4846205	4879881	3666881	3587482	3524702	3483908	3552764	3422781	4734372	4940454	4521397	5287717	4380612	4561982	3924479	4681290	5641733	4084019	4564538	5185517	5573641	4987998	7043392	6115498	6002832	4931434
CITRAMALATE (CAS# 2306-22-1); (M-H)-					253861		237336	247074	244495	231371		7611														18164		
CITRATE (CAS# 77-92-9); (M-H)-	30458	29217	35265	29485	6790375	6120787	6308846	7847343	8177476	8306729	288050	3934			111207	12626	39932	52843	142898	47641	66708	4590	17230	1164		46425	13161	125980
CITRULLINE (CAS# 372-75-8); (M-H)-	589652	579535	576891	563818				4212	1924		81583						736906	1626521				732092		524013	186101	1032255	824904	973049
CMP (CAS# 63-37-6); (M-H)-			52457								13982	14888		4293		11824	15302	32767		32154	1923	24513	72904	59318	16854	41250	19869	36771
CORTICOSTERONE (CAS# 50-22-6); (M+HCOO)-					4344	4413	5026	3943	4075	4103																		
CORTISOL (CAS# 50-23-7); (M+Cl)-					77245	70164	76429	73127	70256	72494							5280	4014	6683	2104	4683		2573				5993
CORTISOL (CAS# 50-23-7); (M+HCOO)-	13464	12616	13109	12715	636440	619539	647206	591125	599039	586129	12232	5316	1537		2736	6402	33642	31306	46752	17958	33350	7262	22192	12292		12793	3774	46907
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+Cl)-																												1571
CORTISONE (CAS# 53-06-5); (M+Cl)-	2189	1955	1320	1548	28785	29211	29253	29539	28005	27552	2157						3338	6226	9441	3590	6359		4854			1356		5691
CORTISONE (CAS# 53-06-5); (M+HCOO)-	10370	10332	10049	9526	142491	143219	145475	136149	137440	135684	10743	5631	2082	1932	5255	5287	15215	26789	41548	18160	28174	3664	22698	11580		8496	6173	25229
CREATINE (CAS# 57-00-1); (M-H)-													37345															

CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (M-H)-																									1380			
CYCLOHEPTANECARBOXYLIC ACID (CAS# 1460-16-8); (M+HCC	174392	178773	171492	168453	71492	65897	69205	65390	68396	64953	119519	128512	42022	67161	358076	201294	137045	286131	344754	222662	287032	67644	172183	139569	55469	236467	105026	390046
CYSTATHIONINE (CAS# 56-88-2); (M-H)-					4521	4669	5094		3252																2660			
CYTIDINE (CAS# 65-46-3); (M+Cl)-													4836	10048		15398										34494		
CYTIDINE (CAS# 65-46-3); (M-H)-						1565		16504	16320				19374	47280														
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+Cl)-	2786	1941		1154					6506		7468	33043		12222	20576													
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+HCOO)-												8208		2735	3011													
D-(-)-ARABINOSE (CAS# 10323-20-3); (M+HCOO)-								5587	4684		94207																	
DECANOATE (CAS# 334-48-5); (M-H)-	22430	23327	23495	23440	16222	14412	16717	16463	16031	18006	14633	22492	11411	23055	14491	10541	25745	34829	40686	27247	33086	11455	34453	32541	8682	28747	21006	26375
DEHYDROASCORBATE (CAS# 490-83-5); (M+Cl)-	47381		43200								58310						51391	39923	40754					4046				32746
DEHYDROASCORBATE (CAS# 490-83-5); (M+HCOO)-														10542	9162													
DEHYDROASCORBATE (CAS# 490-83-5); (M-H)-		7837	10917	9434	416074	421176	405174	393585	381501	362334	78572			57497	83110	1948	16476					1656				29285		28509
DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Cl)-						2123			1749																			
DEOXYCHOLIC ACID (CAS# 83-44-3); (M-H)-			9470		117795	110087	116607	118800	112440	112857					127300								79829					
DEOXYCYTIDINE (CAS# 951-77-9); (M+HCOO)-	11981	4660	7927	3989					1087		31320	2375		8558	38571	9465	5857	12975	13115			7627	12843		5635		15495	
DEOXYCYTIDINE (CAS# 951-77-9); (M-H)-	11174	9687	10166	8929		1572	3203			1638							18701	7359	47540		21596	2139						14551
DEOXYURIDINE (CAS# 951-78-0); (M+Cl)-	18216			17828				2901	2171	4148	36709	106059			27910			49413	50322	12288	62873		8192					32050
DEOXYURIDINE (CAS# 951-78-0); (M+HCOO)-												20208									4577							
DEOXYURIDINE (CAS# 951-78-0); (M-H)-												29964					5435		9353		13175							
D-GALACTOSAMINE (CAS# 7535-00-4); (M+Cl)-					6170							19463		29410		23975			21346			16354					9260	
D-GALACTOSAMINE (CAS# 7535-00-4); (M-H)-[-H2O]	7001										14649																	
D-GLUCOSAMINE (CAS# 3416-24-8); (M+Cl)-					6170							19463		29410		23975			21346			16354					9260	
D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (M-H)-											421535	8431	21578	162668	213795	128177	59175	54905					24836		20896		90898	47525
DGMP (CAS# 902-04-5); (M-H)-												18070		1776							76183							
DIACETYL (CAS# 431-03-8); (M+HCOO)-	21928	22746	21617	19158	22968	23323	19055	19561	21393	14266	11888	5238		7416	20524	15667	6934	14924	24452	15439	17872		9256	7603		21590	7794	24618
DIETHYLSTILBESTROL (CAS# 56-53-1); (M-H)-								5965										4387	9718	5236								
DIHYDROXYMANDELIC ACID (CAS# 775-01-9); (M-H)-													3079	3477	2925												4020	
D-LYXOSE (CAS# 1114-34-7); (M+Cl)-	41641	33261	38468	26916					2885		11884		7783	9812	11994	1443	4204		8054	291911	8212	2788	27223				14106	
D-LYXOSE (CAS# 1114-34-7); (M+HCOO)-								5587	4684		94207																	
D-LYXOSE (CAS# 1114-34-7); (M-H)-								53381						1681														
D-MANNOSAMINE (CAS# 14307-02-9); (M-H)-[-H2O]	7001										14649																	
DOCOSAHEXAENOIC ACID (CAS# 6217-54-5); (M-H)-	244406	244003	236700	230970	850529	807426	850359	847314	867928	801495	320796	385458		88513	208893	155399	190935	288925	334010	287271	417891	35182	395819	703047		426617	122945	400384
D-ORNITHINE (CAS# 348-66-3); (M-H)-			227239	222918				8667	7870	8324	36621		10131	47692				638413	357920		69068	273313			84676		255760	379035
D-PSICOSE (CAS# 551-68-8); (M+Cl)-	2300487	2239844	2202478	2056951		1291615					622547	471894	208198	415656	1246316	1394161	1763423	2270298	2238216	3849839	4405232	1671150	3891124	2191065	458044	2038278	2131468	3247491
D-TAGATOSE (CAS# 87-81-0); (M+Cl)-	2300487	2239844	2202478	2056951		1291615					622547	471894	208198	415656	1246316	1394161	1763423	2270298	2238216	3849839	4400844	1673138	3891124	2191065	458044	2038278	2131468	3247491
DUMP (CAS# 964-26-1); (M-H)-					10161	4454		12028	3365	9002				1799														
EDTA (CAS# 60-00-4); (M-2H)-2																			1277									
EDTA (CAS# 60-00-4); (M-H)-			1841		6.33E+07	5.98E+07	5.85E+07	5.95E+07	6.00E+07	5.80E+07																		
ELAIDIC ACID (CAS# 112-79-8); (M-H)-	2200452	2246825	2383423	2333273	4578411	4377086	4675479	4722233	5114890	4866890	2222956	2932617	470396	1874049	1848271	1321191	2315616	3044264	2795376	3052671	3204756	580299	3022238	2667418	80120	3029775	2403120	3426477
EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (M+Cl)-	980526	903121	878398	860421	452278	421144	436153	410093	410215	393581	791577	832595	680179	954759	815088	700400	703867	870252	1102978	679768	938716	930979	1188642	980801	1550329	1317646	1106258	1028462
EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (M+HCOO)-	1.43E+07	1.36E+07	1.33E+07	1.30E+07	7055591	6842051	7052532	6710630	6845103	6482337	1.19E+07	1.26E+07	1.07E+07	1.42E+07	1.22E+07	1.09E+07	1.08E+07	1.32E+07	1.64E+07	1.06E+07	1.40E+07	1.38E+07	1.71E+07	1.46E+07	2.17E+07	1.91E+07	1.63E+07	1.47E+07
ERUCIC ACID (CAS# 112-86-7); (M-H)-	6083	6266	6355	6188	3658	2900	3110	3544	3632	3538	10055	22973	1263	6443	7604	3385	12124	7469	9212	10948	13068	1030	9539	7638		6298	11131	6445
ETHANOLAMINE PHOSPHATE (CAS# 1071-23-4); (M-H)-	52158	63410	65741	41292							231482	52783	7582	40035	226571	78447	20821	7860	23898	23307	34821	33400	25458		24421	50819	140051	
ETHYLMALONIC ACID (CAS# 601-75-2); (M-H)-	13832	10893	10549	12481							4665				3861	1906	2891		20697	2574	13995		3134	4613		8434	2531	
FRUCTOSE (CAS# 57-48-7); (M+Cl)-	2300487	2239844	2202478	2056951		1291615					622547	471894	208198	415656	1246316	1394161	1763423	2270298	2238216	3849839	4400844	1673138	3891124	2191065	458044	2038278	2131468	3247491
FRUCTOSE (CAS# 57-48-7); (M+HCOO)-	10423	10083				11556	10897	10299	10790	10757			18912		15457	17109				12863	15720	12120	22118	11517	50851	10260	19842	3620
FUMARATE (CAS# 110-17-8); (M-H)-	38085										27260	11903			81712	41269	15608	43309	41322	14073	57334		22703	20673		73305		53664
GALACTARATE (CAS# 526-99-8); (M-H)-						1670																						
GALACTURONIC ACID (CAS# 91510-62-2); (M-H)-				1248																3406								1759
GAMMA-BUTYROLACTONE (CAS# 96-48-0); (M+HCOO)-	21928	22746	21617	20266	22968	23323	19055	19561	21393	17483	12633	5238		7416	20524	15667	6934	14924	24452	15439	17872		9256	7603		22543	7794	24364
GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M-H)-			4812											2543														
GAMMA-LINOLENIC ACID (CAS# 506-26-3); (M+HCOO)-	451623	482919	501454	501700	482857	454368	480951	497333	522874	517633	461453	475874	442607	492269	451928	457300	482894	515080	470038	518566	509761	394361	506524	465949	371705	504296	525901	461853
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M-H)-	50257	46252	43144	43518	13663	13346	13105	12674	13365	11963	37270	40887	23046	47284	35972	27258	26145	38573	77838	27843	46048	37279	74244	56681	102958	103514	66478	58220
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Cl)-	53351	50205	49445	49324	30036	28862	29118	30252	29117	26279	47304	47972	38324	52115	45362	39213	40780	46455	64469	41538	54225	46409	62959	54466	71650	70209	60577	55483
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M-H)-	1216842	1168727	1138361	1129403	631173	623779	625057	608096	613828	595315	1039164	1113919	842095	1193389	1067509	906067	899970	1099275	1490442	930183	1197252	1053610	1436971	1287576	1718317	1707111	1399081	1295088
GLUCARIC ACID (CAS# 87-73-0); (M-H)-						1670	1127		1277																			
GLUCARIC ACID (CAS# 87-73-0); (M-H)+[-H2O]	25081	36296	29013	13590	5419210	5646061	5220357	4833424	5218682	4766202	298050	3934		86416	172715	29137	22795	33313	142898	26323	46684	2582		1164		30353	13161	45710
GLUCONIC ACID (CAS# 526-95-4); (M-H)-						33538		5587	4684		94207																	
GLUCOSE (CAS# 50-99-7); (2M+Cl)-[-H2O]	256678	252588	246966	247141			41380					235508	153754	176066		259358	242875	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
GLUCOSE (CAS# 50-99-7); (2M+HCOO)-[-H2O]											3431		10207		10228										13195			
GLUCOSE (CAS# 50-99-7); (M+Cl)-	2300487	2239844	2202478	2056951		1291615					622547	471894	208198	415656	1246316	1394161	1763423	2270298	2238216	3849839	4400844	1673138	3891124	2191065	458044	2038278	2131468	3247491
GLUCOSE 1-PHOSPHATE (CAS# 59-56-3); (M-H)-				103041							423462	8431	21578	162668	213795	128177	59175	54905					24836		20896		90898	47525
GLUCURONIC ACID (CAS# 6556-12-3); (M+Cl)-																						4302						
GLUCURONIC ACID (CAS# 6556-12-3); (M-H)-				1248																3406		1097						1759
GLUTAMATE (CAS# 56-86-0); (M-H)-	336778	333946	361211	340056	53086			22870				405233		384608		928460	202688	561946	223847	320120	448328		316105	309753	45869	448472	326592	270804
GLUTAMINE (CAS# 56-85-9); (M-H)-			220820		73430	42922	79041	71708	70900	68185																		
GLUTARATE (CAS# 110-94-1); (M-H)-	21928	22746	21617	20266	22968	23323	19055	19561	21393	17483	12633	5238		7416	20524	15667	6934	14924	24452	15439	17872		9256	7603		22543	7794	24364
GLUTATHIONE (CAS# 27025-41-8); (M-H)-	13763	11912	12230	12172							33155	6089		6718	46450	23421	12545	15657	45408		4048	1799				18803	4450	5244
GLYCERALDEHYDE (CAS# 367-47-5); (2M-H)-[-H2O]					109168		93644	111678	97825	98078		2569								16628				9536				
GLYCEROL 2-PHOSPHATE (CAS#); (M-H)-	20650	23079		19996							35122	16227				11730		14453		1848			38985				93238	4076
GLYCINE (CAS# 56-40-6); (M-H)-				9024											3127	8488	8168	26125	8046		3272			8995		20705	6547	
GLYCOCHOLATE (CAS# 475-31-0); (M-H)-	3718	4139	4875		135453	132622	138820	137686	140221	136797	1991																	
GLYCOLITHOCHOLATE (CAS# 474-74-8); (M-H)-					12950	12859	13671	12101	11488	12598																		
GUANINE (CAS# 73-40-5); (M-H)-	16517	16786	17419	12696						2319					5626	11639	19792	18145	46734	21753	48217	20821	38006	29732	8039	40204	24125	24649
GUANOSINE (CAS# 118-00-3); (M+Cl)-	113266	47779	100130	42950							35076	21966	11738	71280	90683	69647	161707	113435	133901	132818	123553	64300	158273	61414	12373	91062	140703	94517
GUANOSINE (CAS# 118-00-3); (M-H)-	369400	342992	353630	355124							251801	172993	68743	296552	302300	178407	526800	693255	679217	367892	623262	241356	523233	425996	73479	623846	517447	552279
GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (2M-H)+					143928	136680	131638	118524	121253	124812																		
GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (M-H)-					1233		1372			1142	15440				16077													
GULONO-1,4-LACTONE (CAS# 1128-23-0); (M-H)-															3321													
HEPTADECANOATE (CAS# 506-12-7); (M-H)-	105535	55703	58803	119270	113920	110351	117576	117919	129206	122500	55486	102203	61158	107473	114893	42868	121333	123182	150767	153540	105553	56597	90186	67790	39465	171073	75610	138826
HEXACOSANOIC ACID (CAS# 506-46-7); (M-H)-	34533	31628	27792	31084				2584	4187		11468	7316		6074	4768	19933	24434	46380	69937	105231	121493	23739	60218	39477		48888	56983	141807
HIPPURATE (CAS# 495-69-2); (M-H)-	46653	45384	42326	43438	836513	826543	816475	789935	804273	795070		18772	10836	2131	46386	4203	141709	78404	53053	12428	232651	5379		182592	4673	34577	3213	32246
HOMOCYSTINE (CAS# 462-10-2); (M-H)-												7726																
HOMOGENTISATE (CAS# 451-13-8); (M-H)-						4441																						1228
HOMOSERINE (CAS# 672-15-1); (M-H)-			75485									56520	8914	32445				152247	89697			78918		104488	14406			106927
HOMOVANILLATE (CAS# 306-08-1); (M-H)-											2002				2651						4038							
HYODEOXYCHOLATE (CAS# 83-49-8); (M-H)-	1119229	1574395	1565026	1070009	483001	550786	1719110	1661579	461442	493665	1578147	2046096	1025541	1177915	501035	1642930	1882261	709131	485440	516259	1524181	1377572	730193	1595612	1190923	429850	1601550	717391
HYPOXANTHINE (CAS# 68-94-0); (M-H)-	919018	906817	930360	932067	242519	215596	133155	136256	141026	210793		1219359	266963	617543	1065649	786764	782367	1178830	1257054		2125673	459618	1001002	919283	87673	801364	787514	1179526
IBUPROFEN (CAS# 15687-27-1); (M-H)-					27825	23809	23709	28216	28826	27016																		
IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M-H)-					44462	44917	46753	42562	42826	40979																		
INDICAN (CAS# 487-60-5); (2M+Cl)-[-H2O]												1224																
INDOLE-3-ACETATE (CAS# 87-51-4); (M-H)-									11349	11939		3640																
INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M-H)-			1844	2174								2022						4667	15506	1680			3931	4824				
INOSINE (CAS# 58-63-9); (M+Cl)-	243122	236475	227254	237375		5979	12032			23775	226634	89800	72971	178946	164314	63173	487665	641976	630655	425572	469218	94977	348341	262733	20921	321773	209195	487698
INOSINE (CAS# 58-63-9); (M-H)-	3393489	3217383	1947154	3235410	82480	82249	75999	81971	84282	80073	1954422	1545078	648904	2630326	2326671	1041397	6173835	4409568	5039280	3341644	3264693	1479630	3130446	2174303	207342	3142147	2695749	3568358
INOSINE 5'-DIPHOSPHATE (CAS# 86-04-4); (M-H)-						86237	88734	66356	73141	68751	1161	1575			1253	2395						1812						
INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M-H)-			29509	6771	19129						53498	6062		5009	32898	4348						2787			1045		3449	
ISOCITRATE (CAS# 320-77-4); (M-H)-	34033	34011	32570	27083	5419210	5652530	5220367	4833424	5218682	4766202	298050	3934		87040	172715	29137	39932	52843	142898	26234	48412	4590	17230	1164		30353	13161	45710
ISOLEUCINE (CAS# 73-32-5); (M-H)-	363758	359884	360616	367643	457779	455575		398696	431700	428446	307793		64024		244810	337269	342808	969944	926650	401776	533689	162506	461876	549748	8648	757802		729804
ITACONATE (CAS# 97-65-4); (M-H)-														5876	6942	2116				1435	3773		1986			7268		7840
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (2M-H)-	85249	80992	76532	77952	19243	16902	19946	14723	15498	19539	61313	66943	40013	87048	66530	45758	43993	75076	147320	50501	86309	71806	129623	92880	174097	180998	127682	100091
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M-H)-	4311086	4080472	4034614	3849207	2167498	2105838	2157009	2086948	2091193	2064416	3585364	3807563	2970965	4049909	3691556	3274832	3162847	3901817	5290611	3245856	4229147	3882157	4992450	4297937	5779296	5787021	5125441	4540813
KYNURENINE (CAS# 343-65-7); (M-H)-	1090	1742			16546	13955	15312	13282	12455	12669					3427		2626		5485	3115	7100			1526		5520		3813
L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M-H)-	1098351	1099922	1059011	1074154	172092	172075	168708	167610	173657	175827	951362	418154	271808	482335	455817	369683	837766	1137133	1414191	959187	1120660	593249	1304413	1236346	423814	1635585	519471	1296133
LACTOSE (CAS# 63-42-3); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	235508	153754	176066	376002	259358	242875	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
LACTOSE (CAS# 63-42-3); (M-H)-													6522	9032			6054								11568			
L-ALLOTHREONINE (CAS# 28954-12-3); (M-H)-			75485									56520	8914	32445				152247	89697			77652		104488	14406			
L-ARGININE (CAS# 74-79-3); (M-H)-	22312	20981	19315	19715					1833				10568				19827	12560	22426	9660	12929	29477	12112	16384	29358	30048	20484	19016
L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (CAS#); (M-H)-			1776	2956							9525	2276	15331				1922			1900		6629		1158	71149			
LAURIC ACID (CAS# 143-07-7); (M-H)-	34476	34554	35435	34177	38397	35191	37501	40017	41171	38937	16220	28452	11313	16740	21135	13697	46317	77926	106732	47279	71058	9914	75894	66724	8389	95621	26803	62002
L-CARNITINE (CAS# 541-15-1); (M+Cl)-	8419		7022																	9125								10090
LEUCINE (CAS# 328-39-2); (M-H)-	363758	359884	361022	367643	460793	455575		398696	431700	428446	304477		64024		244810	337269	342808	969944	926650	401776	533689	162506	455496	549748	8648	757802		729804
LEUKOTRIENE B4 (CAS# 71160-24-2); (M-H)-	3812	2445	3548	3229							6257	5650	1067		6732	4447	2376	13301	8260	21829	13746		3993	3718				8377
L-GULONATE (CAS# 6322-07-2); (M-H)-						33538		5587	4684		94207																	
L-GULONATE (CAS# 6322-07-2); (M-H)+[-H2O]											1195																	3232
L-HISTIDINE (CAS# 71-00-1); (M-H)-	225350	213253	211377	208857	38345	33787	47908	46623	37480	48518	78198	258139	5600	46942	89195	358442	191021	231073	345434	167292	58565	203642	126785	459530	51340	374298	93140	226976
LIGNOCERIC ACID (CAS# 557-59-5); (M-H)-	66171	73782	73196	69778	13831	12677	11737	25008	26354	18820		37669	1961	31758	13595	55312	122409	149324	389330	368426	479999	37611	147218	102234		202682	98772	501410
LINOLEATE (CAS# 60-33-3); (M-H)-	1520080	1541883	1581867	1552777	3128056	2949590	3136249	3173944	3463166	3269032	1390101	1931445	114041	749488	1032336	621962	1269347	2479618	2017230	2431669	2285447	247479	2188905	1716912	30387	1965454	1774390	2208290
LITHOCHOLIC ACID (CAS# 434-13-9); (M+HCOO)-					1043	1170																		2247		5104		9566
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M-H)-							36802	47777					1458															
L-ORNITHINE (CAS# 70-26-8); (M-H)-			227239	222918				8667	7870	8324	33243		11073	47692				638413	357920		69068	273313			84676		255760	379035
L-RHAMNOSE (CAS# 10030-85-0); (M+Cl)-	88876	84527			297986	291385		283657	274879	265511			6316						103172	235508			108304				32930	
L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M-H)-	241027	228135	221015	224340	142699	140211	140453	135425	140522	131084	253738	168974	138122	269328	249311	211694	169739	260317	310942	208915	251365	272367	268544	238114	261564	358228	275903	285934
LUMICHROME (CAS# 1086-80-2); (M-H)-																				1022								
LYSINE (CAS# 56-87-1); (M-H)-	7758	8724	7317	8399	54779		9146	6500	8855		23291	6329	4239	12639	23146	25061	7466	17953	17855	5906	8754	13581	2707	8807	11718	11900	9972	16279
MALATE (CAS# 97-67-6); (M-H)-	58614	74004	60934	82666	303493	292253	289540	270605	257950	249462	330870	65263		26118	267645	50146	2549	24195	62952	35383	81067		25269	33475		60621	157028	110252
MALATE (CAS# 97-67-6); (M-H)+[-H2O]					35231	34449	33574		34109	31885	32790	3215			15014	9206	3219		2814								5055	
MALEAMATE (CAS# 557-24-4); (M-H)-												27011		2165	4254													
MALEIC ACID (CAS# 110-16-7); (M-H)-	38085	18145	20674		35231	35388	35257		34109	31885		32346			20725	41269	15608	43309	41322	8696	57334		22703	20673		73305	67089	53664
MALTOSE (CAS# 69-79-4); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	235508	153754	176066	376002	259358	242875	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
MALTOSE (CAS# 69-79-4); (M+HCOO)-											3431	7760	10207	6248	10228										13195		6609	
MANDELIC ACID (CAS# 611-71-2); (M-H)-	3.42E+07	3.52E+07	3.50E+07	3.40E+07	8295	9955	10431		10254	7715	3.00E+07	2575788	8033911	1.19E+07	9553794	9375880	6.42E+07	6.96E+07	8.38E+07	5.18E+07	6.81E+07	2.46E+07	2.42E+07	4.35E+07	3071887	5.47E+07	4105377	6.32E+07
MANNITOL (CAS# 69-65-8); (M-H)-					3368			3247																				
MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (M-H)-				103041							423971	8431	21578	162668	213795	128177	59175	54905					24836		20896		90898	47525
MELIBIOSE (CAS# 585-99-9); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	235508	153754	176066	376002	259358	242875	253677	280201	166009	187200	206808	269193	187103	163135	718741	233804	209281
MELIBIOSE (CAS# 585-99-9); (M+HCOO)-											3431	7760	10207	6248	10228										13195		6609	
METHIONINE (CAS# 63-68-3); (M-H)-	35981	35475	35211	36080							2192	47780	17867	31110	21644	49523	31791	46298	36125	33564	36706	26334	31057	54345	3671	65870	44317	41708
METHYL VANILLATE (CAS# 3943-74-6); (M-H)-																		1250										
METHYLMALONATE (CAS# 516-05-2); (M-H)-	253387	237950	229909	225392	379570	364663	356842	5743	343646	332279	385278	100823		132582	280653	208118		393118	385835	194742	603325	70960	100778	150324		312863	50525	407424
MEVALONIC ACID (CAS# 674-26-0); (M-H)-					11429																							
MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M-H)-	54425	51084	49512	49639	40686	42558	40186	41490	42579	38773	27882	19022		11889	47783	24482	21081	52243	113097	35070	52289		32667	21198	12504	119858	28193	112163
MYRISTIC ACID (CAS# 544-63-8); (M-H)-	236151	238017	258624	252928	414818	403791	416324	425443	464671	436630	171491	290563	126976	184118	148682	122928	300591	364924	420897	317751	384807	97277	364269	320506	83559	477686	273204	410629
MYRISTOLEIC ACID (CAS# 544-64-9); (M-H)-	6984	9820	10029	9265	16756	15992	17359	16374	19050	17825	2773	11388		5147	3835	2966	5338	25369	34465	18692	19738	1638	10603	11322		19255	7286	31509
N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6); (M+Cl)-	86746	82491	78160	78779	66089		48778	59023		60175	48982	65755	10564	19532	33301	56529	136349	276776	250903	144849	262451	47255	117286	77836		80450	50997	243024
N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6); (M+HCOO)-												3739									4581				1550			
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M-H)-	74584	73357	70725	71242	22063	20581	23246	22712	20123	21031	80988	127358	10035	44919	71825	67319	62025	137765	231893	67128	221007	18638	97764		1956	138170	44386	198337
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M-H)-	313474	333946	361211	340056	40497			11323				192962		384608		928460	202688	184922	225093	320120	448328		316105	309753	49249	466814	326592	425343
N-ACETYL-D-MANNOSAMINE (CAS# 3615-17-6); (M+Cl)-	86746	82491	78160	78779	66089		48778	59023		60175	48982	65755	10564	19532	33301	56529	136349	276776	250903	142867	262451	47255	117286	76274		80450	50997	243024
N-ACETYL-D-TRYPTOPHAN (CAS# 2280-01-5); (M-H)-					7497	4287		8077	7649	6874																		
N-ACETYLGALACTOSAMINE (CAS# 1811-31-0); (M+Cl)-	86746	82491	76173	78779	66089		48778	59023		60175	48982	65755	10564	19532	33301	56529	134242	276776	250903	144849	262451	47255	117286	75438		80450	50997	243024
N-ACETYLGLYCINE (CAS# 543-24-8); (M-H)-		14138			6583			9404				21944					7659	31430				6885					6225	15453
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M-H)-		99109	94160	92283	126896	123793	127768	120809	119993	115480	77940	142353	11745	46901	90435		85981	180791		100154	179971	26686	141228	156617		200590	75193	
N-ACETYL-L-ASPARTIC ACID (CAS# 997-55-7); (M-H)-	25922	26448	27021	25292							103711	22474		13714	60781	21008	14454		143682	21550		6553	13148	33955	1948	59568	26696	
N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M-H)-					6997	7359	7007	7906		6866		1233						2974	4968		2066		2104					3707

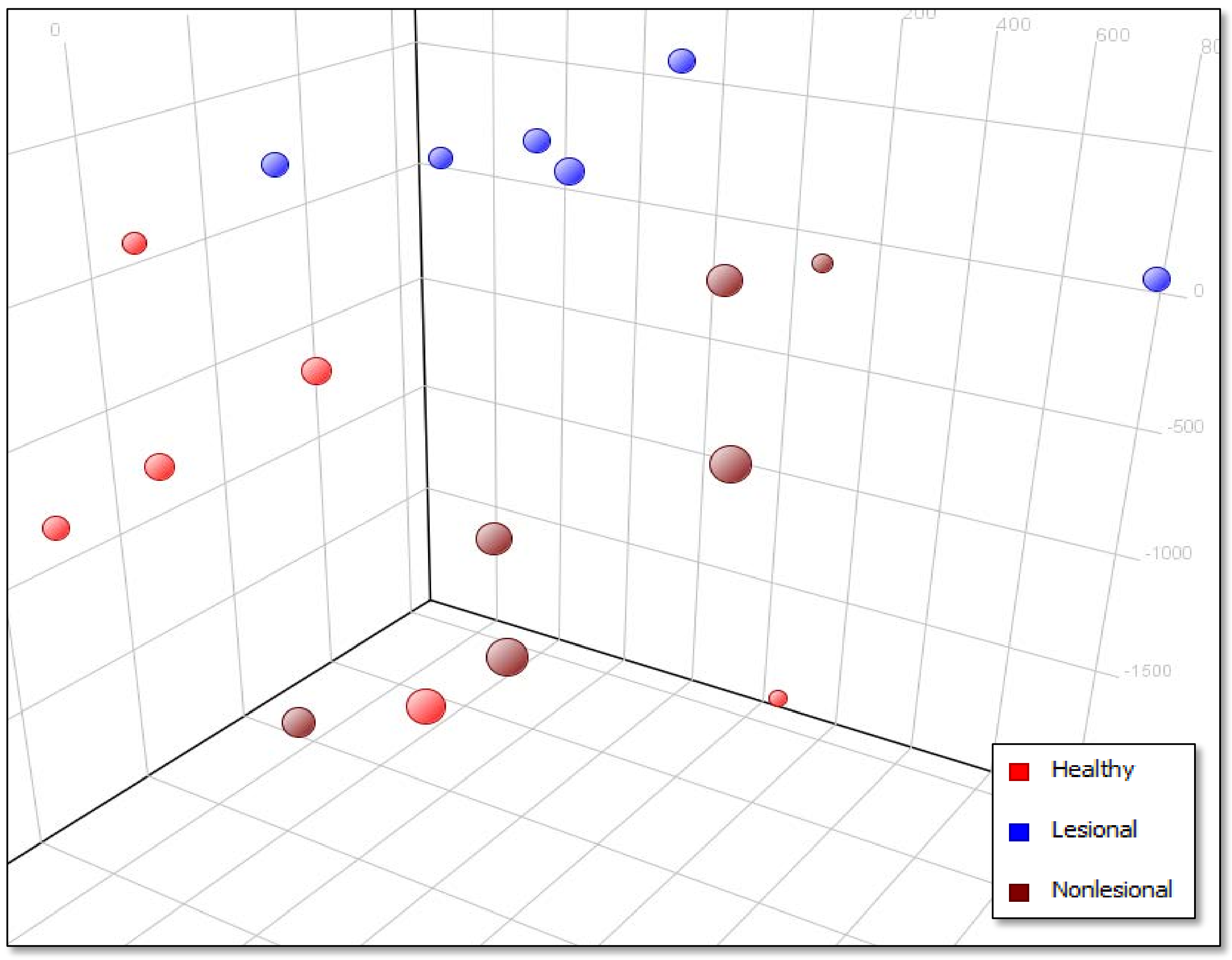
N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-3); (M-H)-					7703	7952	6741	6894	8209	6580		1149					1671									1729		1444
N-ACETYLNEURAMINATE (CAS# 131-48-6); (M-H)-	14583	45376	14197	19005					19471		47319	35342		34215	50607	35797	5567	24160	24482	4012	25772	6119	13954	22503		24131	22752	15404
NAD (CAS# 53-84-9); (M-H)-	8759	7793	10307	7554							22317	11269		7777	38700	15709	1838	4752	15253		3956	1154	1225	3384		3244		5419
N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3); (M-H)-																								6349				
N-AMIDINO-L-ASPARTATE (CAS# 6133-30-8); (M+Cl)+[-H2O]																		10985										
NAPROXEN (CAS# 22204-53-1); (M-H)-					5118	4853	6260	4559	4144	3976																		
N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8); (M+HCOO)-																			5263	1060	2604							
NERVONIC ACID (CAS# 506-37-6); (M-H)-	4722	4904	5045	4084	19744	19470	20256	21176	19817	22349	20182	18090		7244	7401	4871	6482	6593	15828	8808	17083		4083	3283		6740	3933	12824
N-ETHYLMALEIMIDE (CAS# 128-53-0); (M-H)-					8127	10957	9271	8428	8577	9368											1421			1036				
NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE (CAS# 22052-73-9); (M-H)-																		1707										
NICOTINATE (CAS# 59-67-6); (M-H)-		3652	7319		10931	12615	4520			17934				30114	11451	22690	1971				6019	23256	2737	2555		41472	23573	
N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M-H)-	336778	333946	361211	340056	53086			11343				405233		384608		928460	202688	561946	223847	320120	448328		316105	309753	46416	466814	326592	270804
N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M-H)-	7001										13505																	
N-NITROSODIETHANOLAMINE (CAS# 1116-54-7); (M+Cl)-				3956																								
N-OLEOYLGLYCINE (CAS# 2601-90-3); (M-H)-				3945								5357			10062		3204			6450	2629		5517	12760				
NONANOATE (CAS# 112-05-0); (M-H)-	28386	29158	28439	28990				1612			6732	35323	8680	27058	8704	5051	33548	47282	63972	36275	55253	3245	61106	50101	3966	43924	37831	43126
NORLEUCINE (CAS# 327-57-1); (M-H)-	363758	359884	361156	367643	460793	455575		398696	431700	428446	304504		64024		244810	337797	342808	969944	926650	401776	533689	162506	461876	549748	8648	757802		729804
OLEIC ACID (CAS# 112-80-1); (M-H)-	2200452	2246825	2383423	2333273	4581859	4379810	4675737	4726518	5114890	4872846	2222956	2932617	470396	1874049	1848271	1321191	2315616	3044264	2795376	3052671	3209138	580299	3022238	2667418	80120	3029775	2403120	3430366
OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M-H)	6785	10161	8299	6767	5416	4982	3222	3785	1872	3400	3792	5889	3842	4182	5171	2904	8004	6827	12951	8506	10345	6027	12289	12706	4293	12095	5066	5879
OMEPRAZOLE (CAS# 73590-58-6); (M-H)-								4866																				
OMEPRAZOLE SULFONE (CAS# 88546-55-8); (M-H)-					39014	39636	40930	38967	40700	39415																		
O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5); (M-H)-																		1452	5668									
OXALOACETATE (CAS# 328-42-7); (M-H)-[-H2O]															6444													
OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M-H)-	13763	11912	12230	12172							33155	6089		6718	46450	23421	12545	15657	45408		4048	1799				18803	4450	5244
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (2M-H)-					1981	1918	2594			1455														49502				
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-8	136658	133461	129904	131650	286346	280909	282704	268550	254112	257699	90560	23087	13818		1012		71511						63433	1451909				
PALATINOSE (CAS# 343336-76-5); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	230558	153754	175605	376002	252819	242875	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
PALATINOSE (CAS# 343336-76-5); (M+HCOO)-											3431	7760	10207	6248	10228										13195		6609	
PALMITATE (CAS# 57-10-3); (M-H)-	1348828	1419985	1481028	1488279	1808388	1655796	1780409	1833346	2046898	1939591	1380266	1526907	1280263	1462174	1246986	1326939	1466969	1514517	1444850	1587093	1728744	1113267	1722496	1473757	983631	1660844	1727663	1489531
PALMITIC ACID-13,13,14,14,15,15,16,16,16-D9 [ISTD] (CAS# 1	132660	141718	149397	146909	130123	125827	130466	136595	150882	146079	228866	136166	117944	161804	303744	153007	91770	119816	75667	104411	115517	173801	148398	133068	149573	122376	172700	112793
PALMITOLEIC ACID (CAS# 373-49-9); (M-H)-	286086	289941	300443	291959	864085	819150	867964	871226	977002	915423	346955	810339	45110	191930	497975	99788	224244	589536	747873	496427	589466	46644	434621	363988	12144	677462	211653	953765
PANTOTHENATE (CAS# 79-83-4); (M+Cl)-								2277		2944							2150	2797		8689				2274		5027		6340
PANTOTHENATE (CAS# 79-83-4); (M-H)-	71830	65091	66986	63092	76407	77313	77136	72546	75044	70885	37404	36390	5417	21537	49391	30076	49755	101314	207481	288031	142116	13959	76979	77736	1903	136104	29880	161305
PARAXANTHINE (CAS# 611-59-6); (M-H)-	78308	78756	74881	75356	594677	575289	552443	552981	568787	555372	17390	85689			31022	25833	47348	332512	13653	51140	215859	26207	380606	132782		7780	12809	275922
PENTANOATE (CAS# 109-52-4); (M+HCOO)-																							2986					
PHENOL (CAS# 108-95-2); (M-H)-	18772	16975	15953	15835							6713	13358			21396	16493		27519	31351	10412	33628		49570	28147		24196	16717	48941
PHENYL ACETATE (CAS# 122-79-2); (M+HCOO)-	11208	13453	14046	11205	190356	176878	177583	174819	176890	165662	20952	8435		7416	25722	12343	10398	23771	15511	18581	49441		17262	9400		14528	8658	35774
PHENYL ACETATE (CAS# 122-79-2); (M-H)-					8016		2985	5394		7184					5746						9054							
PHENYLACETIC ACID (CAS# 103-82-2); (M+HCOO)-											2002				2651													
PHENYLALANINE (CAS# 63-91-2); (M-H)-		766949	742630	759000							677636	630186	76991	266352	563615	653738	727861	2307476	2229555	1164463	1592083	308143	921044	1128005	22429	1735259	473160	
PHENYLPYRUVATE (CAS# 156-06-9); (M-H)-																					3964							
PHYTANATE (CAS# 14721-66-5); (M-H)-	11946	14523	14892	14065	15434	16627	17844	19495	19041	17623	24996	21701		14031	8314	53362	19765	9597	23378	80781	38379	7457	123437		5015	89194	99760	18352
PICOLINIC ACID (CAS# 98-98-6); (M-H)-	42396	38561			11780	12374		24690		17934			16815	9120	11451	23096					6120	25184	2726	2578		41472	36539	
PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M-H)-					1907																							
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)-		2094	1882								4330				1030			7967		8661	9416		2261					
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)-[-H2O]																				3075								
PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-	37565	38761	39740	35966							43766	52242	7050	6920	52088	17030	6225	235499	43976	119725	323374	7936	17940	37349		32662	100488	78089
PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-[-H2O]	3033	3889	4032								7262	4503			7277			29336	4180	12302	32914			4091		3777	11198	9570
PROTOPORPHYRIN (CAS# 553-12-8); (M-H)-							1448																					
PTERIN (CAS# 2236-60-4); (M-H)-								1199																				
PURINE (CAS# 120-73-0); (M-H)-									3490																			
PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M-H)-																							13316	78702		129429		
PYRUVATE (CAS# 127-17-3); (M-H)-					178594	177999	176179	1088	1066	158180	11055																	
RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-6); (M+HCOO)-									1335																			
RAFFINOSE (CAS# 512-69-6); (M+Cl)-	221220	233216	227829	233901				2687		2526	81050	124104	49148	323951	144073	252452	103998	293703	544123	196065	196262	232026	251909	356752	201481	485835	194086	167780
RAFFINOSE (CAS# 512-69-6); (M+HCOO)-					1948									8641					2175	1173		2913	1273	1735	7966	4709	5953	
RETINOATE (CAS# 302-79-4); (M-H)-	22028	24200	21220	20597				14759			2120	59480	3181	5728	12025	7380	14353	30105	137135	19022	23113	13758	13590	14042	2019	17648	62459	67425
RIBITOL (CAS# 488-81-3); (M+Cl)-	9649	2121						1617			8014							9385	19567					13351		29305	4503	13091
RIBOFLAVIN (CAS# 83-88-5); (M+Cl)-																				1652								
RIBOFLAVIN (CAS# 83-88-5); (M+HCOO)-	2695		2132	2310											1004	1686	2875	3615	6420	5931	4560		1157	1088		4519		5272
RIBOFLAVIN (CAS# 83-88-5); (M-H)-	2803	2972	1546	2028							1011						2929	4467	6882	6988	4521		1644	3085		4169		6096
RIBOSE (CAS# 50-69-1); (M+Cl)-	41641	31673	38468	26916					2292		11884		7783	8995	10925	1443	3559		8054	291911	8212	2788	27223				12689	
RIBOSE 5-PHOSPHATE (CAS# 4300-28-1); (M-H)-																					1186	4126						
S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-0); (M-H)-	15216	17412	16877	16702		3409	4716			5254	34687			8570	53491	25501	17374	54795	46348	32229	84398					48531	11651	101497
SALICYLATE (CAS# 69-72-7); (M-H)-	507010	504370	483071	488846	1792837	1755639	1756619	1823311	1810794	1731667	167919	384389	19597	103429	596445	508365	337344	786768	944009	329378	972507	183123	1399770	828157	17492	718747	491943	1361283
SALICYLURIC ACID (CAS# 487-54-7); (M-H)-					59438	57223	56952	55876	57529	55355																		
S-CARBOXYMETHYL-L-CYSTEINE (CAS# 638-23-3); (M-H)-			2450																									
SEBACIC ACID (CAS# 111-20-6); (M-H)-	28080	26692	26178	23756	17924	14252	14827	15448	14944	15319	16791	11722	7983	10756	26753	17732	15118	30343	42133	25912	35684	10043	21165	16998	8230	24476	10670	37805
SERINE (CAS# 56-45-1); (M-H)-	19828	17294		17955							6805	19307	4273	14942	12358	37901	13317	34027	29646	14473	8539	33136	15517	21268	13934	24627	25143	24419
SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (M+Cl	85068	79185	77915	77160							81589	105764	56155	111054	42244	78569	58113	102012	99789		85570		92436	41938	15424	94381	27377	95988
SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (M+HCOO)-			3858																									
SPHINGANINE (CAS# 764-22-7); (M+HCOO)-[-H2O]										1717																		
STACHYOSE (CAS# 54261-98-2); (M+Cl)-	95488	95184	95265	99060							31804	47008	23707	155812	59528	117091	40692	110832	150398	71399	69571	100740	104023	147816	162788	210894	91915	64238
STACHYOSE (CAS# 54261-98-2); (M+HCOO)-																									2738			
STACHYOSE (CAS# 54261-98-2); (M-H)-		1482	4885	7614							1386	3908	1679	13781		6920	1268	5006	7476	3046	2744	7688	6421	8451	21245	10834	9485	
STEARATE (CAS# 57-11-4); (M-H)-	1248190	1356301	1404064	1374009	1612867	1505152	1589883	1676032	1850681	1714883	1565062	1675774	1010872	1336953	1133358	1386597	1265848	1239842	1296738	1670751	1689189	773949	1642948	1340447	519404	1466799	1971321	1333296
SUBERIC ACID (CAS# 505-48-6); (M-H)-	63111	59746	56803	56777							34158		12672	17121	65912	51152	36126	82743	118383	61452	77085		53814	39767	12333	78698		93977
SUCCINATE (CAS# 110-15-6); (M-H)-	253387	237950	229909	225392	379570	364663	356842	341811	343646	332279	385278	100823		132582	280653	208118		393118	385835	194742	603325	70960	100778	150324		312863	50525	407424
SUCROSE (CAS# 57-50-1); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	230558	153754	175605	376002	252819	235981	253677	280201	166009	187200	206855	269193	187103	164529	711000	233804	209281
SUCROSE (CAS# 57-50-1); (M+HCOO)-											3431	7760	10207	6248	10228										13195		6609	
SULFADIMETHOXINE (CAS# 122-11-2); (M-H)-																										13856		
TAURINE (CAS# 107-35-7); (M-H)-	609286	594931	579961	575381	30774	25620	30931	27549	29662	7060	811250	856240	558916	850285	861271	800714	567316	547098	369255	426127		488390		393575		693871	1105175	406859
THEOPHYLLINE (CAS# 58-55-9); (M-H)-	79508	78756	74881	76620	594677	575505	552233	553092	568787	555372	17390	85098			31826	25694	47348	332512	13009	51140	215859	24312	380606	132782		7783	13821	275922
THREONINE (CAS# 72-19-5); (M+HCOO)-[-H2O]	313474	333946	361211	340056				22870				192962		384608			202688	184922	225093	320120			316105	309753	49249	466814	326592	425343
THROMBOXANE B2 (CAS# 54397-85-2); (M-H)-[-H2O]	37565	38761	39740	35966							43766	52242	5874	6920	52088	17030	6225	235499	43976	119725	323374	7916	17940	37349		32662	100488	78089
THYMIDINE (CAS# 50-89-5); (M+Cl)-		2431		4250					6081	7617	2020	16333			13435													
THYMIDINE (CAS# 50-89-5); (M+HCOO)-	1399	1123				6079	3190	3159	2026			14935			9203				2480		5593							
THYMIDINE (CAS# 50-89-5); (M-H)-												10692			7224				3209									1879
THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-07-1); (M-H)-			1161								1202							3300			2481							
THYMINE (CAS# 65-71-4); (M-H)-	7813		8570	6868							14953	81952		6438	5702	5360				1565					2510	2302		
THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#); (M-H)-	455127											508785		542425		417029						533326			891806		575767	
THYROXINE (CAS# 51-48-9); (M-H)-					24921	25198	23635	23087	21156	22609											1944							1120
TRANS-ACONITATE (CAS# 4023-65-8); (M-H)-				14565	841007	794295	789491	763835	764002	731517	185059			24325			3689	16641	48357	29432	30897							
TRANS-VACCENIC ACID (CAS# 693-72-1); (M-H)-	2200452	2246825	2383423	2333273	4581859	4377198	4675712	4726518	5114890	4872846	2222956	2932617	470396	1874049	1848271	1321191	2315616	3044264	2795376	3052671	3209138	580299	3022238	2667418	80120	3029775	2403120	3430366
TRIACONTANOIC ACID (CAS# 506-50-3); (M-H)-																		2899	3988	4240	5730						3735	5064
TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)-		1781			289836	294816		562060	253571	262594									3652									2198
TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)-[-H2O]		13950		11691		47437	41653	36989	35638	105372											24676			4124				12501
TRICOSANOIC ACID (CAS# 2433-96-7); (M-H)-	10400	11925	11989	10848	2305	1666	2129	3338	3855	2597	10383	8187		7771	2234	13472	20755	23371	53678	28018	57437	6300	18622	13756		29825	14805	47869
TRIDECANOIC ACID (CAS# 638-53-9); (M-H)-	7029	6423	10410	7345	6398	6899	8171	7378	6880	7189	3683	9538	2661	9013	3063	3015	8994	12623	17358	9591	12063		14628	11007	2306	15014	10453	16363
TRYPTOPHAN (CAS# 73-22-3); (2M-H)-					67310	66020	66175	60148	63660	61663	1481				2000				88818									
TRYPTOPHAN (CAS# 73-22-3); (M-H)-					1599399	1553255	1535893	1498712	1574653	1514970			17701	101071				1388305	1656120									1278435
TYROSINE (CAS# 60-18-4); (M-H)-	407544	324430	337281	328089	309082	302476	297472	287321	296563		331514	293543	67824	220917	315852	432896	317871	613251	592665	370396	499880	284051	381473	451344	41803	644888	288874	581644
UDP-GALACTOSE (CAS# 2956-16-3); (M-H)-											12291	23729		17724	52043													
UDP-GLUCOSE (CAS# 133-89-1); (M-H)-											11829			12326	19412													
UDP-N-ACETYL-D-GALACTOSAMINE (CAS#); (M-H)-																					5446							1818
UDP-N-ACETYL-D-GLUCOSAMINE (CAS# 528-04-1); (M-H)-	56225												2861					6982	58892									1378
URACIL (CAS# 66-22-8); (M-H)-	79628	65373	73526	68300								274856	54241	97932		76006	43722	63358			133578	28777	69246	74590		80726	53616	72449
URATE (CAS# 69-93-2); (M-H)-	728312	836301	736881	836407	3476872	3326810	3356511	3392986	3507728	3376438	1663664	278771		296466	2032550	562710	1095610	706709	261303	1817172	1827438	342322	591612	127045	42743	1038537	464974	1432354
URIDINE (CAS# 58-96-8); (M+Cl)-	3503462	3201514	3238420	3191118	361858	354900	350726	578707	527000	480866	4116900	2470510	233380	1056439	2123743	2232223	4147652	6533600	8978312	4271198	7797565	1115299	5359348	4638156		6833874	2503737	7604267
URIDINE (CAS# 58-96-8); (M+HCOO)-	633045	615021	645803	625630	36806	36367		33334	34964	32339	505293	665297	206024	385600	383655	404742	740365	741828	877308	683531	944606	334699	826698	623673	78490	869121	697055	857202
URIDINE (CAS# 58-96-8); (M-H)-	1672007	1498290	1556182	1564614	145046	137330	142287	155584	154350	151761	1798129	1586680	574437	1219049	1422068	1020277	2331936	2551078	3065925	1801528	2609351	992430	2660977	2076216	221528	2856582	1498048	2480974
URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (M-H)-	37067	23004	47931	37873	3390		8106		6674		128796	44000			58570	45466			1804		1259	10016		1568	12974	1619	65713	
UROCANATE (CAS# 104-98-3); (M-H)-	340814	231699	343783	241267							29807	115594		56613	41534	365015	266637	1274190	1227672	217869	524378	150512	778311	97763	29555	793776	327831	999000
URSODIOL (CAS# 128-13-2); (M+HCOO)-	5733	6249	4693	5297	44344	42293	45212	42253	46182	45027						1618			8229	7579	3741	2638	51817				1333	2311
URSODIOL (CAS# 128-13-2); (M-H)-					117795	110087	116607	118800	112440	112857					127300								79829					
VALINE (CAS# 72-18-4); (M-H)-	19589	22515	24805	21539				3677	15114	8671	6902			11312		25957	19468	53157	53128	20080	23149	16797	25854	37318		52193	23973	32514
XANTHINE (CAS# 69-89-6); (M-H)-	909394	878651	889764	877554	122281	112361	112221	136035	49676	119464	1493633	3214280	242298	581565	1581314	1383843	373016	718899	1642866	368892	519009	105881	221982	345972	4684	511931	473556	665742
XANTHOSINE (CAS# 146-80-5); (M-H)-	67342	63163	64102	66422		31630	26099		30620	23864	331082	132495	38165	82688	121334	94344	12493	25287	50978	6927	78461	2308	37055	36472		25190	69429	46076
XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8); (M-H)-											1456																	
XANTHURENIC ACID (CAS# 59-00-7); (M-H)-		1919																					4123					1739
XYLOSE (CAS# 58-86-6); (M+HCOO)-								5587	4684		94207																	
ZEATIN [ISTD] (CAS# 13114-27-7); (M+Cl)-	1262394	1214463	1175325	1179909	1088759	1042235	1023905	1054016	1050914	1012686	1147535	1234596	1092031	1226566	1181863	1093038	1084816	1159462	1381980	1078927	1218485	1235920	1343159	1243819	1474228	1374567	1335296	1218619
ZEATIN [ISTD] (CAS# 13114-27-7); (M-H)-	5150839	4948356	4846205	4879881	3666881	3587482	3524702	3483908	3552764	3422781	4734372	4940454	4521397	5287717	4380612	4561982	3924479	4681290	5641733	4084019	4564538	5185517	5573641	4987998	7043392	6115498	6002832	4931434

Compound	Neg Pool QC 1	Neg Pool QC 2	Neg Pool QC 3	Neg Pool QC 4	Neg_Human Plasma Extraction_1	Neg_Human Plasma Extraction_2	Neg_Human Plasma Extraction_3	Neg_Human Plasma Extraction_4	Neg_Human Plasma Extraction_5	Neg_Human Plasma Extraction_6	Neg_S00015447_1	Neg_S00015448_2	Neg_S00015449_3	Neg_S00015450_4	Neg_S00015451_5	Neg_S00015452_6	Neg_S00015453_7	Neg_S00015454_8	Neg_S00015455_9	Neg_S00015456_10	Neg_S00015457_11	Neg_S00015458_12	Neg_S00015459_13	Neg_S00015460_14	Neg_S00015461_15	Neg_S00015462_16	Neg_S00015463_17	Neg_S00015464_18
CHOLESTEROL HYDROGEN SULFATE (CAS# 1256-86-6); (M-H)-								5219		10323			2252															6422
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M-H)-	50257	46252	43144	43518	13663	13346	13105	12674	13365	11963	37270	40887	23046	47284	35972	27258	26145	38573	77838	27843	46048	37279	74244	56681	102958	103514	66478	58220
HIPPURATE (CAS# 495-69-2); (M-H)-	46653	45384	42326	43438	836513	826543	816475	789935	804273	795070		18772	10836	2131	46386	4203	141709	78404	53053	12428	232651	5379		182592	4673	34577	3213	32246
2,3-DIHYDROXY-2-PHOSPHONOPROPANOIC ACID (CAS# 2553-59-5); (M-H)-								4548																				
MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M-H)-	54425	51084	49512	49639	40686	42558	40186	41490	42579	38773	27882	19022		11889	47783	24482	21081	52243	113097	35070	52289		32667	21198	12504	119858	28193	112163
GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (2M-H)+					143928	136680	131638	118524	121253	124812																		
PTERIN (CAS# 2236-60-4); (M-H)-								1199																				
TRANS-ACONITATE (CAS# 4023-65-8); (M-H)-				14565	841007	794295	789491	763835	764002	731517	185059			24325			3689	16641	48357	29432	30897							
D-(-)-ARABINOSE (CAS# 10323-20-3); (M+HCOO)-								5587	4684		94207																	
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Cl)-	53351	50205	49445	49324	30036	28862	29118	30252	29117	26279	47304	47972	38324	52115	45362	39213	40780	46455	64469	41538	54225	46409	62959	54466	71650	70209	60577	55483
NONANOATE (CAS# 112-05-0); (M-H)-	28386	29158	28439	28990				1612			6732	35323	8680	27058	8704	5051	33548	47282	63972	36275	55253	3245	61106	50101	3966	43924	37831	43126
ARACHIDIC ACID (CAS# 506-30-9); (M-H)-	9712	14523	14892	14065	5240	6087	6036	7001	6867	7648	22073	21701		15172	8314	16500	14733	18057	23378	15315	47432	7457	16682	11566	2810	16414	24276	18352
ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+HCOO)-	451623	482919	501454	501700	482857	454368	480951	497333	522874	517633	461453	475874	442607	492269	451928	457300	482894	515080	470038	518566	509761	394454	506524	465949	371705	504296	525901	461853
N-ACETYLGLYCINE (CAS# 543-24-8); (M-H)-		14138			6583			9404				21944					7659	31430				6885					6225	15453
DEOXYCHOLIC ACID (CAS# 83-44-3); (M-H)-			9470		117795	110087	116607	118800	112440	112857					127300								79829					
XYLOSE (CAS# 58-86-6); (M+HCOO)-								5587	4684		94207																	
TYROSINE (CAS# 60-18-4); (M-H)-	407544	324430	337281	328089	309082	302476	297472	287321	296563		331514	293543	67824	220917	315852	432896	317871	613251	592665	370396	499880	284051	381473	451344	41803	644888	288874	581644
3-HYDROXY-3-METHYLGLUTARATE (CAS# 503-49-1); (M-H)	18481	14180	15250	15421	109168	93057	93644	111678	97825	98078		2569			21988			19279	24776	16628				9536				26501
N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M-H)-	336778	333946	361211	340056	53086			11343				405233		384608		928460	202688	561946	223847	320120	448328		316105	309753	46416	466814	326592	270804
ADIPIC ACID (CAS# 124-04-9); (M-H)-	54425	51084	49545	49639	40621	42611	40134	41618	42522	38773	27882	19022		11889	47481	24472	21091	50304	113097	35070	52289		32667	21198	12504	119858	28151	112163
TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)-		1781			289836	294816		562060	253571	262594									3652									2198
INOSINE (CAS# 58-63-9); (M-H)-	3393489	3217383	1947154	3235410	82480	82249	75999	81971	84282	80073	1954422	1545078	648904	2630326	2326671	1041397	6173835	4409568	5039280	3341644	3264693	1479630	3130446	2174303	207342	3142147	2695749	3568358
RAFFINOSE (CAS# 512-69-6); (M+Cl)-	221220	233216	227829	233901				2687		2526	81050	124104	49148	323951	144073	252452	103998	293703	544123	196065	196262	232026	251909	356752	201481	485835	194086	167780
TAURINE (CAS# 107-35-7); (M-H)-	609286	594931	579961	575381	30774	25620	30931	27549	29662	7060	811250	856240	558916	850285	861271	800714	567316	547098	369255	426127		488390		393575		693871	1105175	406859
DIETHYLSTILBESTROL (CAS# 56-53-1); (M-H)-								5965										4387	9718	5236								
(S)-3-METHYL-2-OXOPENTANOATE (CAS# 1460-34-0); (M-H	23718	25047	19576	24388	1867888	1867747	1822256	1837820	1821625	1738295		28134			8896			7972	38479	12757	6312	5049	37361	37892		49762	8539	9775
2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 4026-18-0); (M	68586	69755	66587	63777	1015303	989421	963325	939521	972149	14930	82574	9860			52780	35288	114628	78825	152004	215829	20251	16654	78764	53539		53905	33768	144297
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-	5728		5007	4236	4921	4228	9620	9336	5943	4813	5498	15547		3585	6864	4457	5086	3070	5260	6830	7505		8145	3195		3491	4402	
CORTISONE (CAS# 53-06-5); (M+Cl)-	2189	1955	1320	1548	28785	29211	29253	29539	28005	27552	2157						3338	6226	9441	3590	6359		4854			1356		5691
HEXACOSANOIC ACID (CAS# 506-46-7); (M-H)-	34533	31628	27792	31084				2584	4187		11468	7316		6074	4768	19933	24434	46380	69937	105231	121493	23739	60218	39477		48888	56983	141807
11-DEOXYCORTISOL (CAS# 152-58-9); (M+HCOO)-					4344	4379	4968	3938	4056																			
DECANOATE (CAS# 334-48-5); (M-H)-	22430	23327	23495	23440	16222	14412	16717	16463	16031	18006	14633	22492	11411	23055	14491	10541	25745	34829	40686	27247	33086	11455	34453	32541	8682	28747	21006	26375
STEARATE (CAS# 57-11-4); (M-H)-	1248190	1356301	1404064	1374009	1612867	1505152	1589883	1676032	1850681	1714883	1565062	1675774	1010872	1336953	1133358	1386597	1265848	1239842	1296738	1670751	1689189	773949	1642948	1340447	519404	1466799	1971321	1333296
CIS-VACCENIC ACID (CAS# 506-17-2); (M-H)-	2200452	2246825	2383423	2333273	4578393	4377086	4675424	4722233	5114890	4866890	2222956	2932617	470396	1874049	1848271	1321191	2315616	3044264	2795376	3052671	3204952	580299	3022238	2667418	80120	3029775	2403120	3426477
OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M-	6785	10161	8299	6767	5416	4982	3222	3785	1872	3400	3792	5889	3842	4182	5171	2904	8004	6827	12951	8506	10345	6027	12289	12706	4293	12095	5066	5879
SALICYLURIC ACID (CAS# 487-54-7); (M-H)-					59438	57223	56952	55876	57529	55355																		
CIS-ZEATIN (CAS# 1637-39-4); (M+Cl)-	1262394	1214463	1175325	1179909	1088759	1042235	1023905	1054016	1050914	1012686	1147535	1234596	1092031	1226566	1181863	1093038	1084816	1159462	1381980	1078927	1218485	1235920	1343159	1243819	1474228	1374567	1335296	1218619
THEOPHYLLINE (CAS# 58-55-9); (M-H)-	79508	78756	74881	76620	594677	575505	552233	553092	568787	555372	17390	85098			31826	25694	47348	332512	13009	51140	215859	24312	380606	132782		7783	13821	275922
TRICARBALLYLIC ACID (CAS# 99-14-9); (M-H)-[-H2O]		13950		11691		47437	41653	36989	35638	105372											24676			4124				12501
6-CARBOXYHEXANOATE (CAS# 111-16-0); (M-H)-	18986	18364	15993	15663	5792	5044	5474	6024	6450	6126	8082	6612			12589	8494	7861	16543	23651	12538	19798	2775	11101	6958		17792		21911
THREONINE (CAS# 72-19-5); (M+HCOO)-[-H2O]	313474	333946	361211	340056				22870				192962		384608			202688	184922	225093	320120			316105	309753	49249	466814	326592	425343
1,3,7-TRIMETHYLURIC ACID (CAS# 5415-44-1); (M-H)-		1463		2010	64466	64285	62742	60255	64666	64261											5076		3739	3817				
GLYCERALDEHYDE (CAS# 367-47-5); (2M-H)-[-H2O]					109168		93644	111678	97825	98078		2569								16628				9536				
N-ETHYLMALEIMIDE (CAS# 128-53-0); (M-H)-					8127	10957	9271	8428	8577	9368											1421			1036				
CIS-ACONITATE (CAS# 585-84-2); (M-H)-				14565	841007	794295	789491	763835	764002	731517									48357	29432	25692							47001
CIS-ZEATIN (CAS# 1637-39-4); (M-H)-	5150839	4948356	4846205	4879881	3666881	3587482	3524702	3483908	3552764	3422781	4734372	4940454	4521397	5287717	4380612	4561982	3924479	4681290	5641733	4084019	4564538	5185517	5573641	4987998	7043392	6115498	6002832	4931434
PALMITOLEIC ACID (CAS# 373-49-9); (M-H)-	286086	289941	300443	291959	864085	819150	867964	871226	977002	915423	346955	810339	45110	191930	497975	99788	224244	589536	747873	496427	589466	46644	434621	363988	12144	677462	211653	953765
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M-H)-							36802	47777					1458															
NORLEUCINE (CAS# 327-57-1); (M-H)-	363758	359884	361156	367643	460793	455575		398696	431700	428446	304504		64024		244810	337797	342808	969944	926650	401776	533689	162506	461876	549748	8648	757802		729804
ALPHA-HYDROXYISOBUTYRIC ACID (CAS# 594-61-6); (M-H)-						16037		16806	16631	13941																		
OMEPRAZOLE (CAS# 73590-58-6); (M-H)-								4866																				
2,3-DIHYDROXYBENZOATE (CAS# 303-38-8); (M-H)-					245977	235563	230061	130348	229980	222056									14791	24239	19107					11313		15315
IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M-H)-					44462	44917	46753	42562	42826	40979																		
4-METHYL-2-OXOVALERIC ACID (CAS# 816-66-0); (M-H)-	63699	65536	51886	60509	3126682	3037046	2976566	2934004	2919289	2842069	20142	43300		7547	33398	15209	101632	65137	175962	12993	7911	24541	73416	46035		49142	20113	180672
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M-H)-	4311086	4080472	4034614	3849207	2167498	2105838	2157009	2086948	2091193	2064416	3585364	3807563	2970965	4049909	3691556	3274832	3162847	3901817	5290611	3245856	4229147	3882157	4992450	4297937	5779296	5787021	5125441	4540813
ISOCITRATE (CAS# 320-77-4); (M-H)-	34033	34011	32570	27083	5419210	5652530	5220367	4833424	5218682	4766202	298050	3934		87040	172715	29137	39932	52843	142898	26234	48412	4590	17230	1164		30353	13161	45710
16:0 LYSO PC (CAS# 17364-16-8); (M+Cl)-	2182		1736	1254			11568	9612		8077	2297					1702	1226	2956	3488	7134	5316		2481	1737				6436
FRUCTOSE (CAS# 57-48-7); (M+HCOO)-	10423	10083				11556	10897	10299	10790	10757			18912		15457	17109				12863	15720	12120	22118	11517	50851	10260	19842	3620
CITRAMALATE (CAS# 2306-22-1); (M-H)-					253861		237336	247074	244495	231371		7611														18164		
18:0 LYSO-PE (CAS# 69747-55-3); (M-H)-	12706	13468	10475	11275	43545	39194	42569	34419	36041	40424	62511	10539	1343	4583	11732	47010	5908	16052	9165	19762	16352	14156	9270	10096		8221	5866	18435
D-ORNITHINE (CAS# 348-66-3); (M-H)-			227239	222918				8667	7870	8324	36621		10131	47692				638413	357920		69068	273313			84676		255760	379035
PALMITATE (CAS# 57-10-3); (M-H)-	1348828	1419985	1481028	1488279	1808388	1655796	1780409	1833346	2046898	1939591	1380266	1526907	1280263	1462174	1246986	1326939	1466969	1514517	1444850	1587093	1728744	1113267	1722496	1473757	983631	1660844	1727663	1489531
CYTIDINE (CAS# 65-46-3); (M-H)-						1565		16504	16320				19374	47280														
CITRATE (CAS# 77-92-9); (M-H)-	30458	29217	35265	29485	6790375	6120787	6308846	7847343	8177476	8306729	288050	3934			111207	12626	39932	52843	142898	47641	66708	4590	17230	1164		46425	13161	125980
4-PYRIDOXATE (CAS# 82-82-6); (M-H)-	12961	15381	14652	12809	230901	207895	205279	162312	174855	167524										193591								2373
N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6); (M+Cl)-	86746	82491	78160	78779	66089		48778	59023		60175	48982	65755	10564	19532	33301	56529	136349	276776	250903	144849	262451	47255	117286	77836		80450	50997	243024
GLYCOCHOLATE (CAS# 475-31-0); (M-H)-	3718	4139	4875		135453	132622	138820	137686	140221	136797	1991																	
3-PHOSPHOGLYCERATE (CAS#); (M-H)-								4548																				
LEUCINE (CAS# 328-39-2); (M-H)-	363758	359884	361022	367643	460793	455575		398696	431700	428446	304477		64024		244810	337269	342808	969944	926650	401776	533689	162506	455496	549748	8648	757802		729804
ALLOSE (CAS# 2595-97-3); (M-H)+[-H2O]	22633	14180	11769	18949	100059	100208	102499	101112	97560	99302	22822	2569			18862	4950		15698	24995	11939			6698	13102				32774
N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-3); (M-H)-					7703	7952	6741	6894	8209	6580		1149					1671									1729		1444
GAMMA-BUTYROLACTONE (CAS# 96-48-0); (M+HCOO)-	21928	22746	21617	20266	22968	23323	19055	19561	21393	17483	12633	5238		7416	20524	15667	6934	14924	24452	15439	17872		9256	7603		22543	7794	24364
PANTOTHENATE (CAS# 79-83-4); (M+Cl)-								2277		2944							2150	2797		8689				2274		5027		6340
5-VALEROLACTONE (CAS# 542-28-9); (M+HCOO)-								652247		631854																		
CHOLATE (CAS# 81-25-4); (M-H)-	4518		6075	6146	44707	43401	44789	43149	43201	41957									8801				46633					
L-HISTIDINE (CAS# 71-00-1); (M-H)-	225350	213253	211377	208857	38345	33787	47908	46623	37480	48518	78198	258139	5600	46942	89195	358442	191021	231073	345434	167292	58565	203642	126785	459530	51340	374298	93140	226976
SALICYLATE (CAS# 69-72-7); (M-H)-	507010	504370	483071	488846	1792837	1755639	1756619	1823311	1810794	1731667	167919	384389	19597	103429	596445	508365	337344	786768	944009	329378	972507	183123	1399770	828157	17492	718747	491943	1361283
OMEPRAZOLE SULFONE (CAS# 88546-55-8); (M-H)-					39014	39636	40930	38967	40700	39415																		
LINOLEATE (CAS# 60-33-3); (M-H)-	1520080	1541883	1581867	1552777	3128056	2949590	3136249	3173944	3463166	3269032	1390101	1931445	114041	749488	1032336	621962	1269347	2479618	2017230	2431669	2285447	247479	2188905	1716912	30387	1965454	1774390	2208290
GLUTAMINE (CAS# 56-85-9); (M-H)-			220820		73430	42922	79041	71708	70900	68185																		
SEBACIC ACID (CAS# 111-20-6); (M-H)-	28080	26692	26178	23756	17924	14252	14827	15448	14944	15319	16791	11722	7983	10756	26753	17732	15118	30343	42133	25912	35684	10043	21165	16998	8230	24476	10670	37805
CORTISOL (CAS# 50-23-7); (M+Cl)-					77245	70164	76429	73127	70256	72494							5280	4014	6683	2104	4683		2573					5993
PYRUVATE (CAS# 127-17-3); (M-H)-					178594	177999	176179	1088	1066	158180	11055																	
ERUCIC ACID (CAS# 112-86-7); (M-H)-	6083	6266	6355	6188	3658	2900	3110	3544	3632	3538	10055	22973	1263	6443	7604	3385	12124	7469	9212	10948	13068	1030	9539	7638		6298	11131	6445
IBUPROFEN (CAS# 15687-27-1); (M-H)-					27825	23809	23709	28216	28826	27016																		
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M-H)-		99109	94160	92283	126896	123793	127768	120809	119993	115480	77940	142353	11745	46901	90435		85981	180791		100154	179971	26686	141228	156617		200590	75193	
PHENYL ACETATE (CAS# 122-79-2); (M+HCOO)-	11208	13453	14046	11205	190356	176878	177583	174819	176890	165662	20952	8435		7416	25722	12343	10398	23771	15511	18581	49441		17262	9400		14528	8658	35774
3BETA-HYDROXYANDROST-5-EN-17-ONE 3-SULFATE (CAS#	53048	60686	55392	59478	3770151	3721986	3839175	3764027	3845527	3733257	21280			4269	17062	11367	72126	93832	493907	131516	222313	14759	80267	37123		23209	3665	135059
ZEATIN [ISTD] (CAS# 13114-27-7); (M+Cl)-	1262394	1214463	1175325	1179909	1088759	1042235	1023905	1054016	1050914	1012686	1147535	1234596	1092031	1226566	1181863	1093038	1084816	1159462	1381980	1078927	1218485	1235920	1343159	1243819	1474228	1374567	1335296	1218619
PARAXANTHINE (CAS# 611-59-6); (M-H)-	78308	78756	74881	75356	594677	575289	552443	552981	568787	555372	17390	85689			31022	25833	47348	332512	13653	51140	215859	26207	380606	132782		7780	12809	275922
TRIDECANOIC ACID (CAS# 638-53-9); (M-H)-	7029	6423	10410	7345	6398	6899	8171	7378	6880	7189	3683	9538	2661	9013	3063	3015	8994	12623	17358	9591	12063		14628	11007	2306	15014	10453	16363
MANNITOL (CAS# 69-65-8); (M-H)-					3368			3247																				
MYRISTIC ACID (CAS# 544-63-8); (M-H)-	236151	238017	258624	252928	414818	403791	416324	425443	464671	436630	171491	290563	126976	184118	148682	122928	300591	364924	420897	317751	384807	97277	364269	320506	83559	477686	273204	410629
CORTISONE (CAS# 53-06-5); (M+HCOO)-	10370	10332	10049	9526	142491	143219	145475	136149	137440	135684	10743	5631	2082	1932	5255	5287	15215	26789	41548	18160	28174	3664	22698	11580		8496	6173	25229
PALMITIC ACID-13,13,14,14,15,15,16,16,16-D9 [ISTD] (CAS#	132660	141718	149397	146909	130123	125827	130466	136595	150882	146079	228866	136166	117944	161804	303744	153007	91770	119816	75667	104411	115517	173801	148398	133068	149573	122376	172700	112793
URSODIOL (CAS# 128-13-2); (M-H)-					117795	110087	116607	118800	112440	112857					127300								79829					
5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M-H)-					39829	39636	40930	38967	40700	38268																		
3,4-DIHYDROXYBENZOATE (CAS# 99-50-3); (M-H)-					245977	235563	230061	130348	229980	222056									14791	24239	19107					11313		15315
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-	88822	89392	91821	89370	139422	132002	139940	138834	146226	136912	168491	159501	8540	47311	165017	66060	108799	137198	137445	127060	272084	19460	216371	58378		81854	102804	239383
ARABITOL (CAS# 7643-75-6); (M+Cl)-	9649	4320						1617			8014							9385	19567					13351			4503	13091
AZELAIC ACID (CAS# 123-99-9); (M-H)-	174392	178773	171492	168453	71492	65903	69260	65390	68396	64953	119405	128512	42022	67161	354033	201294	137045	286131	344754	216641	287246	67967	172183	139690	55469	236467	105026	390046
ISOLEUCINE (CAS# 73-32-5); (M-H)-	363758	359884	360616	367643	457779	455575		398696	431700	428446	307793		64024		244810	337269	342808	969944	926650	401776	533689	162506	461876	549748	8648	757802		729804
XANTHINE (CAS# 69-89-6); (M-H)-	909394	878651	889764	877554	122281	112361	112221	136035	49676	119464	1493633	3214280	242298	581565	1581314	1383843	373016	718899	1642866	368892	519009	105881	221982	345972	4684	511931	473556	665742
GLYCOLITHOCHOLATE (CAS# 474-74-8); (M-H)-					12950	12859	13671	12101	11488	12598																		
3-HYDROXYPHENYLACETATE (CAS# 621-37-4); (M-H)-					18076		18758	15884	16578	18371															7742			
2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Cl)-	88876	84527			297986	291385		283657	274879	265511			6316						103172	235508			108304				32930	
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 12059	136658	133461	129904	131650	286346	280909	282704	268550	254112	257699	90560	23087	13818		1012		71511						63433	1451909				
PHENYL ACETATE (CAS# 122-79-2); (M-H)-					8016		2985	5394		7184					5746						9054							
2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M-H)-		51084		49639	40634	42882	39955	42003	51632	42989	27823	19022		11889	47481	24381	21181	52243	114523	35070	52289		32784	20894	12493	119858	28193	113897
3-METHYLADIPIC ACID (CAS# 3058-01-3); (M-H)-	18965	18364	15993	15663	5792	5044	5474	6024	6450	6126	8082	6612			12589	8494	7861	16543	23651	12538	19798	2775	11101	6958		17792		21911
EDTA (CAS# 60-00-4); (M-H)-			1841		6.33E+07	5.98E+07	5.85E+07	5.95E+07	6.00E+07	5.80E+07																		
THYMIDINE (CAS# 50-89-5); (M+HCOO)-	1399	1123				6079	3190	3159	2026			14935			9203				2480		5593							
HYODEOXYCHOLATE (CAS# 83-49-8); (M-H)-	1119229	1574395	1565026	1070009	483001	550786	1719110	1661579	461442	493665	1578147	2046096	1025541	1177915	501035	1642930	1882261	709131	485440	516259	1524181	1377572	730193	1595612	1190923	429850	1601550	717391
THYROXINE (CAS# 51-48-9); (M-H)-					24921	25198	23635	23087	21156	22609											1944							1120
4-ACETAMINOPHEN SULFATE (CAS# 32113-41-0); (M-H)-	245796	233329	234417	229084	331232	322746	331507	304590	261920	287362	311563	6107	58194		10713	7667							125553	79798				
N-ACETYL-D-TRYPTOPHAN (CAS# 2280-01-5); (M-H)-					7497	4287		8077	7649	6874																		
URIDINE (CAS# 58-96-8); (M+HCOO)-	633045	615021	645803	625630	36806	36367		33334	34964	32339	505293	665297	206024	385600	383655	404742	740365	741828	877308	683531	944606	334699	826698	623673	78490	869121	697055	857202
TRICOSANOIC ACID (CAS# 2433-96-7); (M-H)-	10400	11925	11989	10848	2305	1666	2129	3338	3855	2597	10383	8187		7771	2234	13472	20755	23371	53678	28018	57437	6300	18622	13756		29825	14805	47869
N-ACETYL-D-MANNOSAMINE (CAS# 3615-17-6); (M+Cl)-	86746	82491	78160	78779	66089		48778	59023		60175	48982	65755	10564	19532	33301	56529	136349	276776	250903	142867	262451	47255	117286	76274		80450	50997	243024
DEHYDROASCORBATE (CAS# 490-83-5); (M-H)-		7837	10917	9434	416074	421176	405174	393585	381501	362334	78572			57497	83110	1948	16476					1656				29285		28509
L-ORNITHINE (CAS# 70-26-8); (M-H)-			227239	222918				8667	7870	8324	33243		11073	47692				638413	357920		69068	273313			84676		255760	379035
TRYPTOPHAN (CAS# 73-22-3); (M-H)-					1599399	1553255	1535893	1498712	1574653	1514970			17701	101071				1388305	1656120									1278435
DEOXYURIDINE (CAS# 951-78-0); (M+Cl)-	18216			17828				2901	2171	4148	36709	106059			27910			49413	50322	12288	62873		8192					32050
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (2M-H)-	85249	80992	76532	77952	19243	16902	19946	14723	15498	19539	61313	66943	40013	87048	66530	45758	43993	75076	147320	50501	86309	71806	129623	92880	174097	180998	127682	100091
2',4'-DIHYDROXYACETOPHENONE (CAS# 89-84-9); (M-H)-					18006		18758	15884	16578	18336															7742			
RIBITOL (CAS# 488-81-3); (M+Cl)-	9649	2121						1617			8014							9385	19567					13351		29305	4503	13091
HYPOXANTHINE (CAS# 68-94-0); (M-H)-	919018	906817	930360	932067	242519	215596	133155	136256	141026	210793		1219359	266963	617543	1065649	786764	782367	1178830	1257054		2125673	459618	1001002	919283	87673	801364	787514	1179526
3-METHYGLUTARIC ACID (CAS# 626-51-7); (M-H)-	54425	51084	49545	49639	40621	42611	40134	41618	42522	38773	27882	19022		11889	47481	24472	21091	50304	113097	35070	52289		32667	21198	12504	119858	28179	112163
5-AMINOPENTANOATE (CAS# 660-88-8); (M-H)-	19589	22515	24805	21186				2250	15114	8129	6902			11312		25957	19468	53157	52056	20080	23149	12891	25523	41176		46972	23973	32514
PHYTANATE (CAS# 14721-66-5); (M-H)-	11946	14523	14892	14065	15434	16627	17844	19495	19041	17623	24996	21701		14031	8314	53362	19765	9597	23378	80781	38379	7457	123437		5015	89194	99760	18352
GLUTARATE (CAS# 110-94-1); (M-H)-	21928	22746	21617	20266	22968	23323	19055	19561	21393	17483	12633	5238		7416	20524	15667	6934	14924	24452	15439	17872		9256	7603		22543	7794	24364
EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (M+HCOO)-	1.43E+07	1.36E+07	1.33E+07	1.30E+07	7055591	6842051	7052532	6710630	6845103	6482337	1.19E+07	1.26E+07	1.07E+07	1.42E+07	1.22E+07	1.09E+07	1.08E+07	1.32E+07	1.64E+07	1.06E+07	1.40E+07	1.38E+07	1.71E+07	1.46E+07	2.17E+07	1.91E+07	1.63E+07	1.47E+07
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M-H)-	1216842	1168727	1138361	1129403	631173	623779	625057	608096	613828	595315	1039164	1113919	842095	1193389	1067509	906067	899970	1099275	1490442	930183	1197252	1053610	1436971	1287576	1718317	1707111	1399081	1295088
N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M-H)-					6997	7359	7007	7906		6866		1233						2974	4968		2066		2104					3707
DOCOSAHEXAENOIC ACID (CAS# 6217-54-5); (M-H)-	244406	244003	236700	230970	850529	807426	850359	847314	867928	801495	320796	385458		88513	208893	155399	190935	288925	334010	287271	417891	35182	395819	703047		426617	122945	400384
HEPTADECANOATE (CAS# 506-12-7); (M-H)-	105535	55703	58803	119270	113920	110351	117576	117919	129206	122500	55486	102203	61158	107473	114893	42868	121333	123182	150767	153540	105553	56597	90186	67790	39465	171073	75610	138826
N-ACETYLGALACTOSAMINE (CAS# 1811-31-0); (M+Cl)-	86746	82491	76173	78779	66089		48778	59023		60175	48982	65755	10564	19532	33301	56529	134242	276776	250903	144849	262451	47255	117286	75438		80450	50997	243024
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M-H)-	313474	333946	361211	340056	40497			11323				192962		384608		928460	202688	184922	225093	320120	448328		316105	309753	49249	466814	326592	425343
DUMP (CAS# 964-26-1); (M-H)-					10161	4454		12028	3365	9002				1799														
ZEATIN [ISTD] (CAS# 13114-27-7); (M-H)-	5150839	4948356	4846205	4879881	3666881	3587482	3524702	3483908	3552764	3422781	4734372	4940454	4521397	5287717	4380612	4561982	3924479	4681290	5641733	4084019	4564538	5185517	5573641	4987998	7043392	6115498	6002832	4931434
TRANS-VACCENIC ACID (CAS# 693-72-1); (M-H)-	2200452	2246825	2383423	2333273	4581859	4377198	4675712	4726518	5114890	4872846	2222956	2932617	470396	1874049	1848271	1321191	2315616	3044264	2795376	3052671	3209138	580299	3022238	2667418	80120	3029775	2403120	3430366
NERVONIC ACID (CAS# 506-37-6); (M-H)-	4722	4904	5045	4084	19744	19470	20256	21176	19817	22349	20182	18090		7244	7401	4871	6482	6593	15828	8808	17083		4083	3283		6740	3933	12824

MALATE (CAS# 97-67-6); (M-H)-	58614	74004	60934	82666	303493	292253	289540	270605	257950	249462	330870	65263		26118	267645	50146	2549	24195	62952	35383	81067		25269	33475		60621	157028	110252
EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (M+Cl)-	980526	903121	878398	860421	452278	421144	436153	410093	410215	393581	791577	832595	680179	954759	815088	700400	703867	870252	1102978	679768	938716	930979	1188642	980801	1550329	1317646	1106258	1028462
L-GULONATE (CAS# 6322-07-2); (M-H)-						33538		5587	4684		94207																	
CITRULLINE (CAS# 372-75-8); (M-H)-	589652	579535	576891	563818				4212	1924		81583						736906	1626521				732092		524013	186101	1032255	824904	973049
BEHENIC ACID (CAS# 112-85-6); (M-H)-	19207	21057	22606	19802	5648	5209	5042	6555	6595	6799	32359	21655		19874	5449	23823	43795		89898	43053	112139	9479	28405	28470		59878	28917	70440
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M-H)-	74584	73357	70725	71242	22063	20581	23246	22712	20123	21031	80988	127358	10035	44919	71825	67319	62025	137765	231893	67128	221007	18638	97764		1956	138170	44386	198337
GLUTAMATE (CAS# 56-86-0); (M-H)-	336778	333946	361211	340056	53086			22870				405233		384608		928460	202688	561946	223847	320120	448328		316105	309753	45869	448472	326592	270804
ARACHIDONATE (CAS# 506-32-1); (M-H)-	2162546	2190849	2191096	2119308	1486898	1408050	1498791	1542453	1612528	1501489	2634697	2342652	94454	613608	2350139	1323434	1859516	4128884	3229199	3063736	4751292	375342	3854319	2259185	14161	2046862	1884319	4493087
GLUCARIC ACID (CAS# 87-73-0); (M-H)+[-H2O]	25081	36296	29013	13590	5419210	5646061	5220357	4833424	5218682	4766202	298050	3934		86416	172715	29137	22795	33313	142898	26323	46684	2582		1164		30353	13161	45710
CIS-11-EICOSENOIC ACID (CAS# 5561-99-9); (M-H)-	27430	27962	30029	27177	49824	44261	49948	49662	55318	54581	43348	142246	4512	28290	51064	20983	34156	25573	41799	51689	69570	4729	56705	31194		30365	42515	40432
URATE (CAS# 69-93-2); (M-H)-	728312	836301	736881	836407	3476872	3326810	3356511	3392986	3507728	3376438	1663664	278771		296466	2032550	562710	1095610	706709	261303	1817172	1827438	342322	591612	127045	42743	1038537	464974	1432354
KYNURENINE (CAS# 343-65-7); (M-H)-	1090	1742			16546	13955	15312	13282	12455	12669					3427		2626		5485	3115	7100			1526		5520		3813
LYSINE (CAS# 56-87-1); (M-H)-	7758	8724	7317	8399	54779		9146	6500	8855		23291	6329	4239	12639	23146	25061	7466	17953	17855	5906	8754	13581	2707	8807	11718	11900	9972	16279
4-HYDROXYBENZOATE (CAS# 99-96-7); (M-H)-	506722	503298	485691	488479	6758		5879	5546	7566	5458	167201	382189	19733	103447	592251	507833	336554	786768	944009	329309	972507	183123	1399770	827414	17416	718747	491487	1361283
2-HYDROXYBUTYRATE (CAS#); (M-H)-						16037		16806	16631	13941																		
3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M-H)-					17563	10915	8982	9811										1042										
4-NITROPHENOL (CAS# 100-02-7); (M-H)-	86292	80625	76602	74408	18516	20789	20110	19686	20418	17571	28546	41124	28952	29868	112992	38679	37330	52275	82886	46850	41735	19108	70887	43931	21079	65177	37945	55441
1-METHYLURIC ACID (CAS# 708-79-2); (2M-H)-					6366	4638	6403	2272	1189	2747																		
OLEIC ACID (CAS# 112-80-1); (M-H)-	2200452	2246825	2383423	2333273	4581859	4379810	4675737	4726518	5114890	4872846	2222956	2932617	470396	1874049	1848271	1321191	2315616	3044264	2795376	3052671	3209138	580299	3022238	2667418	80120	3029775	2403120	3430366
D-LYXOSE (CAS# 1114-34-7); (M+HCOO)-								5587	4684		94207																	
TRYPTOPHAN (CAS# 73-22-3); (2M-H)-					67310	66020	66175	60148	63660	61663	1481				2000				88818									
CORTISOL (CAS# 50-23-7); (M+HCOO)-	13464	12616	13109	12715	636440	619539	647206	591125	599039	586129	12232	5316	1537		2736	6402	33642	31306	46752	17958	33350	7262	22192	12292		12793	3774	46907
METHYLMALONATE (CAS# 516-05-2); (M-H)-	253387	237950	229909	225392	379570	364663	356842	5743	343646	332279	385278	100823		132582	280653	208118		393118	385835	194742	603325	70960	100778	150324		312863	50525	407424
4-METHYL-2-OXOPENTANOATE (CAS# 816-66-0); (M-H)-	63695	59472	51886	60632	3132882	3037252	2977361	2935520	2921537	2843260	20228	44501		9661	33454	15209	101696	65109	176258	12993	221149	24541	73562	44960		57994	21921	180656
16:0 LYSO PC (CAS# 17364-16-8); (M+HCOO)-	127984	118679	112512	110276	3210624	3106695	3186391	2970551	2903015	2705662	96041	69801	23174	30033	39803	66482	87313	151603	129066	279613	275004	51392	135532	104585	8221	75533	57752	212627
CORTICOSTERONE (CAS# 50-22-6); (M+HCOO)-					4344	4413	5026	3943	4075	4103																		
L-RHAMNOSE (CAS# 10030-85-0); (M+Cl)-	88876	84527			297986	291385		283657	274879	265511			6316						103172	235508			108304				32930	
1-HYDROXY-2-NAPHTHOATE (CAS# 86-48-6); (M-H)-					3670	2992	6882	2839	5287	2731																		
ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M-H)-	7387	6975	6654	7449	7667	7324	7506	7357	7298	7249	13526						24088						3038	34165				
CYCLOHEPTANECARBOXYLIC ACID (CAS# 1460-16-8); (M+H	174392	178773	171492	168453	71492	65897	69205	65390	68396	64953	119519	128512	42022	67161	358076	201294	137045	286131	344754	222662	287032	67644	172183	139569	55469	236467	105026	390046
3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M-H)-	11208	13453	14046	11205	190356	176878	177583	174819	176890	165662	20952	8435		7416	25722	12343	10398	23771	15511	18581	49441		17262	9400		14528	8658	35774
1,3-DIMETHYLURIC ACID (CAS# 944-73-0); (M-H)-					17473	15827	19792	15629	15223	14726																		1796
ELAIDIC ACID (CAS# 112-79-8); (M-H)-	2200452	2246825	2383423	2333273	4578411	4377086	4675479	4722233	5114890	4866890	2222956	2932617	470396	1874049	1848271	1321191	2315616	3044264	2795376	3052671	3204756	580299	3022238	2667418	80120	3029775	2403120	3426477
URIDINE (CAS# 58-96-8); (M+Cl)-	3503462	3201514	3238420	3191118	361858	354900	350726	578707	527000	480866	4116900	2470510	233380	1056439	2123743	2232223	4147652	6533600	8978312	4271198	7797565	1115299	5359348	4638156		6833874	2503737	7604267
MYRISTOLEIC ACID (CAS# 544-64-9); (M-H)-	6984	9820	10029	9265	16756	15992	17359	16374	19050	17825	2773	11388		5147	3835	2966	5338	25369	34465	18692	19738	1638	10603	11322		19255	7286	31509
NAPROXEN (CAS# 22204-53-1); (M-H)-					5118	4853	6260	4559	4144	3976																		
L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M-H)-	1098351	1099922	1059011	1074154	172092	172075	168708	167610	173657	175827	951362	418154	271808	482335	455817	369683	837766	1137133	1414191	959187	1120660	593249	1304413	1236346	423814	1635585	519471	1296133
GAMMA-LINOLENIC ACID (CAS# 506-26-3); (M+HCOO)-	451623	482919	501454	501700	482857	454368	480951	497333	522874	517633	461453	475874	442607	492269	451928	457300	482894	515080	470038	518566	509761	394361	506524	465949	371705	504296	525901	461853
LIGNOCERIC ACID (CAS# 557-59-5); (M-H)-	66171	73782	73196	69778	13831	12677	11737	25008	26354	18820		37669	1961	31758	13595	55312	122409	149324	389330	368426	479999	37611	147218	102234		202682	98772	501410
1,7-DIMETHYL URIC ACID (CAS# 33868-03-0); (M-H)-	2619		2102	2570	93717	90629	86258	85171	86332	86991	3447						3898	16794			7783		11580	6263				16155
ALPHA-KETO-GLUTARATE (CAS# 328-50-7); (M-H)-						160927		153565	144798	157208																		
VALINE (CAS# 72-18-4); (M-H)-	19589	22515	24805	21539				3677	15114	8671	6902			11312		25957	19468	53157	53128	20080	23149	16797	25854	37318		52193	23973	32514
DIACETYL (CAS# 431-03-8); (M+HCOO)-	21928	22746	21617	19158	22968	23323	19055	19561	21393	14266	11888	5238		7416	20524	15667	6934	14924	24452	15439	17872		9256	7603		21590	7794	24618
URSODIOL (CAS# 128-13-2); (M+HCOO)-	5733	6249	4693	5297	44344	42293	45212	42253	46182	45027						1618			8229	7579	3741	2638	51817				1333	2311
D-LYXOSE (CAS# 1114-34-7); (M-H)-								53381						1681														
URIDINE (CAS# 58-96-8); (M-H)-	1672007	1498290	1556182	1564614	145046	137330	142287	155584	154350	151761	1798129	1586680	574437	1219049	1422068	1020277	2331936	2551078	3065925	1801528	2609351	992430	2660977	2076216	221528	2856582	1498048	2480974
PANTOTHENATE (CAS# 79-83-4); (M-H)-	71830	65091	66986	63092	76407	77313	77136	72546	75044	70885	37404	36390	5417	21537	49391	30076	49755	101314	207481	288031	142116	13959	76979	77736	1903	136104	29880	161305
INOSINE 5'-DIPHOSPHATE (CAS# 86-04-4); (M-H)-						86237	88734	66356	73141	68751	1161	1575			1253	2395						1812						
L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M-H)-	241027	228135	221015	224340	142699	140211	140453	135425	140522	131084	253738	168974	138122	269328	249311	211694	169739	260317	310942	208915	251365	272367	268544	238114	261564	358228	275903	285934
SUCCINATE (CAS# 110-15-6); (M-H)-	253387	237950	229909	225392	379570	364663	356842	341811	343646	332279	385278	100823		132582	280653	208118		393118	385835	194742	603325	70960	100778	150324		312863	50525	407424
GLUCONIC ACID (CAS# 526-95-4); (M-H)-						33538		5587	4684		94207																	
4-NITROBENZOIC ACID (CAS# 62-23-7); (M-H)-		26346	8156	63860		32181		9833	8532	27979	78568	11007	10789	57680	139446		2097	3182	23587		20814	35478		44365		21622		26860
PICOLINIC ACID (CAS# 98-98-6); (M-H)-	42396	38561			11780	12374		24690		17934			16815	9120	11451	23096					6120	25184	2726	2578		41472	36539	
RETINOATE (CAS# 302-79-4); (M-H)-	22028	24200	21220	20597				14759			2120	59480	3181	5728	12025	7380	14353	30105	137135	19022	23113	13758	13590	14042	2019	17648	62459	67425
LAURIC ACID (CAS# 143-07-7); (M-H)-	34476	34554	35435	34177	38397	35191	37501	40017	41171	38937	16220	28452	11313	16740	21135	13697	46317	77926	106732	47279	71058	9914	75894	66724	8389	95621	26803	62002
ALLANTOIN (CAS# 97-59-6); (M-H)-		18551		11204							2205		8379	8022				3141	7163	14223		22216		9359	13903	4634	30589	3587
D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (M-H)-											421535	8431	21578	162668	213795	128177	59175	54905					24836		20896		90898	47525
BENZOATE (CAS# 65-85-0); (M-H)-	480136	497787	465724	482966								586103	233569	320431		293655	1102902	879618	2088652	569448	874131	342319	683926	676830	354913	949539	500688	922125
ITACONATE (CAS# 97-65-4); (M-H)-														5876	6942	2116				1435	3773		1986			7268		7840
HOMOGENTISATE (CAS# 451-13-8); (M-H)-						4441																						1228
16:0-18:0 PC (CAS# 59403-51-9); (M+Cl)-				54679							16566	26916		9730	42516	98035			151828									156618
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+HCOO)-	2677	2777	2592	2738							6170	3416		6466	3821	2630	3405	2278			7560		1291	2492		4028	1387	4080
OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M-H)-	13763	11912	12230	12172							33155	6089		6718	46450	23421	12545	15657	45408		4048	1799				18803	4450	5244
PALATINOSE (CAS# 343336-76-5); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	230558	153754	175605	376002	252819	242875	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
MALEIC ACID (CAS# 110-16-7); (M-H)-	38085	18145	20674		35231	35388	35257		34109	31885		32346			20725	41269	15608	43309	41322	8696	57334		22703	20673		73305	67089	53664
4-HYDROXYBENZALDEHYDE (CAS# 123-08-0); (M-H)-	480136	497787	472336	482966								583821	233569	320599		293655	1102865	880534	2088562	569448	874131	342319	683926	676830	354913	955832	500688	922125
L-ARGININE (CAS# 74-79-3); (M-H)-	22312	20981	19315	19715					1833				10568				19827	12560	22426	9660	12929	29477	12112	16384	29358	30048	20484	19016
MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (M-H)-				103041							423971	8431	21578	162668	213795	128177	59175	54905					24836		20896		90898	47525
2-METHYLMALEATE (CAS# 498-23-7); (M-H)-						16746								5876	6942	2126				1435	4834		1986			7268		7840
S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-0); (M-H)-	15216	17412	16877	16702		3409	4716			5254	34687			8570	53491	25501	17374	54795	46348	32229	84398					48531	11651	101497
3-HYDROXYKYNURENINE (CAS# 2147-61-7); (M-H)-	2880	3802		2280							1752	12117		1429	4729	3182		11968			6224		10322	9260		20597	8068	10085
GLUCOSE (CAS# 50-99-7); (M+Cl)-	2300487	2239844	2202478	2056951		1291615					622547	471894	208198	415656	1246316	1394161	1763423	2270298	2238216	3849839	4400844	1673138	3891124	2191065	458044	2038278	2131468	3247491
GUANOSINE (CAS# 118-00-3); (M-H)-	369400	342992	353630	355124							251801	172993	68743	296552	302300	178407	526800	693255	679217	367892	623262	241356	523233	425996	73479	623846	517447	552279
D-PSICOSE (CAS# 551-68-8); (M+Cl)-	2300487	2239844	2202478	2056951		1291615					622547	471894	208198	415656	1246316	1394161	1763423	2270298	2238216	3849839	4405232	1671150	3891124	2191065	458044	2038278	2131468	3247491
3-HYDROXYBENZALDEHYDE (CAS# 100-83-4); (M-H)-	480136	497482	466426	482966								585369	233664	319481		293874	1102241	881735	2063094	569448	874466	342073	683926	680486	355646	939556	501581	922125
XANTHOSINE (CAS# 146-80-5); (M-H)-	67342	63163	64102	66422		31630	26099		30620	23864	331082	132495	38165	82688	121334	94344	12493	25287	50978	6927	78461	2308	37055	36472		25190	69429	46076
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+Cl)-	1847	2117				7055					4213	3528		4085	1813				2009		6394					2689		2514
TRIACONTANOIC ACID (CAS# 506-50-3); (M-H)-																		2899	3988	4240	5730						3735	5064
SUBERIC ACID (CAS# 505-48-6); (M-H)-	63111	59746	56803	56777							34158		12672	17121	65912	51152	36126	82743	118383	61452	77085		53814	39767	12333	78698		93977
NAD (CAS# 53-84-9); (M-H)-	8759	7793	10307	7554							22317	11269		7777	38700	15709	1838	4752	15253		3956	1154	1225	3384		3244		5419
3-SULFINO-L-ALANINE (CAS# 1115-65-7); (M-H)-				14049											19772												33820	13396
PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-[-H2O]	3033	3889	4032								7262	4503			7277			29336	4180	12302	32914			4091		3777	11198	9570
DEOXYCYTIDINE (CAS# 951-77-9); (M-H)-	11174	9687	10166	8929		1572	3203			1638							18701	7359	47540		21596	2139						14551
L-CARNITINE (CAS# 541-15-1); (M+Cl)-	8419		7022																	9125								10090
GUANINE (CAS# 73-40-5); (M-H)-	16517	16786	17419	12696						2319					5626	11639	19792	18145	46734	21753	48217	20821	38006	29732	8039	40204	24125	24649
DEHYDROASCORBATE (CAS# 490-83-5); (M+Cl)-	47381		43200								58310						51391	39923	40754					4046				32746
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+Cl)-																												1571
3',5'-CYCLIC AMP (CAS# 60-92-4); (M-H)-																		5740	7190							6893		1924
16:0-18:0 PC (CAS# 59403-51-9); (M+HCOO)-	8242	9273	11265	6364	5205						13349					4916	8727	16757	17349	16259	27143		13862	8382		8525	5315	22333
STACHYOSE (CAS# 54261-98-2); (M+Cl)-	95488	95184	95265	99060							31804	47008	23707	155812	59528	117091	40692	110832	150398	71399	69571	100740	104023	147816	162788	210894	91915	64238
CMP (CAS# 63-37-6); (M-H)-			52457								13982	14888		4293		11824	15302	32767		32154	1923	24513	72904	59318	16854	41250	19869	36771
RIBOFLAVIN (CAS# 83-88-5); (M+HCOO)-	2695		2132	2310											1004	1686	2875	3615	6420	5931	4560		1157	1088		4519		5272
1-METHYLURIC ACID (CAS# 708-79-2); (M-H)-				2331							7115						6570	24070			2160							16131
MELIBIOSE (CAS# 585-99-9); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	235508	153754	176066	376002	259358	242875	253677	280201	166009	187200	206808	269193	187103	163135	718741	233804	209281
GLUCOSE 1-PHOSPHATE (CAS# 59-56-3); (M-H)-				103041							423462	8431	21578	162668	213795	128177	59175	54905					24836		20896		90898	47525
PROSTAGLANDIN E2 (CAS# 363-24-6); (M-H)-	37565	38761	39740	35966							43766	52242	7050	6920	52088	17030	6225	235499	43976	119725	323374	7936	17940	37349		32662	100488	78089
UROCANATE (CAS# 104-98-3); (M-H)-	340814	231699	343783	241267							29807	115594		56613	41534	365015	266637	1274190	1227672	217869	524378	150512	778311	97763	29555	793776	327831	999000
L-GULONATE (CAS# 6322-07-2); (M-H)+[-H2O]											1195																	3232
INOSINE (CAS# 58-63-9); (M+Cl)-	243122	236475	227254	237375		5979	12032			23775	226634	89800	72971	178946	164314	63173	487665	641976	630655	425572	469218	94977	348341	262733	20921	321773	209195	487698
THROMBOXANE B2 (CAS# 54397-85-2); (M-H)-[-H2O]	37565	38761	39740	35966							43766	52242	5874	6920	52088	17030	6225	235499	43976	119725	323374	7916	17940	37349		32662	100488	78089
GLYCEROL 2-PHOSPHATE (CAS#); (M-H)-	20650	23079		19996							35122	16227				11730		14453		1848			38985				93238	4076
3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (CAS# 516-55-2); (M+Cl)-[-H2O]				11006						2298									10878					2193				2446
GLUCURONIC ACID (CAS# 6556-12-3); (M-H)-				1248																3406		1097						1759
MANDELIC ACID (CAS# 611-71-2); (M-H)-	3.42E+07	3.52E+07	3.50E+07	3.40E+07	8295	9955	10431		10254	7715	3.00E+07	2575788	8033911	1.19E+07	9553794	9375880	6.42E+07	6.96E+07	8.38E+07	5.18E+07	6.81E+07	2.46E+07	2.42E+07	4.35E+07	3071887	5.47E+07	4105377	6.32E+07
D-TAGATOSE (CAS# 87-81-0); (M+Cl)-	2300487	2239844	2202478	2056951		1291615					622547	471894	208198	415656	1246316	1394161	1763423	2270298	2238216	3849839	4400844	1673138	3891124	2191065	458044	2038278	2131468	3247491
GALACTURONIC ACID (CAS# 91510-62-2); (M-H)-				1248																3406								1759
BETA-MALTOSE (CAS# 69-79-4); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	230558	153754	175605	376002	252819	235981	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+HCOO)-	21667	20267	17766	23371							19950	43171	1768	35861	36200	16492					27718						1531	2587
CELLOBIOSE (CAS# 528-50-7); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	230558	153754	175605	376002	252819	242875	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
10-HYDROXYDECANOATE (CAS# 1679-53-4); (M-H)-	9100	7305	5760	5928					3975			8102	4465	3529	6995		8421	8896	11718	6307	8938	1918	12665	7557		10512	3825	4396
N-ACETYLNEURAMINATE (CAS# 131-48-6); (M-H)-	14583	45376	14197	19005					19471		47319	35342		34215	50607	35797	5567	24160	24482	4012	25772	6119	13954	22503		24131	22752	15404
SERINE (CAS# 56-45-1); (M-H)-	19828	17294		17955							6805	19307	4273	14942	12358	37901	13317	34027	29646	14473	8539	33136	15517	21268	13934	24627	25143	24419
3'-CMP (CAS# 63-37-6); (M-H)-			52457								16063	14888		4293		11824	15302	32767	70524	32154	1923	26543	72904	59318	16854	41250	19914	36771
GUANOSINE (CAS# 118-00-3); (M+Cl)-	113266	47779	100130	42950							35076	21966	11738	71280	90683	69647	161707	113435	133901	132818	123553	64300	158273	61414	12373	91062	140703	94517
SUCROSE (CAS# 57-50-1); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	230558	153754	175605	376002	252819	235981	253677	280201	166009	187200	206855	269193	187103	164529	711000	233804	209281
SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (M+	85068	79185	77915	77160							81589	105764	56155	111054	42244	78569	58113	102012	99789		85570		92436	41938	15424	94381	27377	95988
ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 2255-14-3); (M-H)-				103041							415118	8431	21578	162668	213795	128177	59175	54905					24836		20896		90898	47525
BETA-MALTOSE (CAS# 69-79-4); (2M+Cl)-[-H2O]	95488	95184	95265	99060							31804	47008	23707	155812	56770	117091	40692	110832	150398	69915	69571	99261	104023	147816	162788	210894	91915	64238
UDP-N-ACETYL-D-GLUCOSAMINE (CAS# 528-04-1); (M-H)-	56225												2861					6982	58892									1378
FUMARATE (CAS# 110-17-8); (M-H)-	38085										27260	11903			81712	41269	15608	43309	41322	14073	57334		22703	20673		73305		53664
XANTHURENIC ACID (CAS# 59-00-7); (M-H)-		1919																					4123					1739
MALTOSE (CAS# 69-79-4); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	235508	153754	176066	376002	259358	242875	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M+HCOO)-	11681	3900	7203	4707		1024			1472		12677	1408		4087	1659	2094	6476	13997	21302	29345	75532		12898	6347		3416	3911	45719
3,3'-DITHIODIVALINE (PENICILLAMINE SS DIMER) (CAS# 20902-45-8); (M-H)-																												3251
ASPARTATE (CAS# 56-84-8); (M-H)-	43697	43573	46272	42124							62755	99173	6116	24701		257774	15252	60121	31959	25842	13055	62168	16290	38002	23340	50932	65795	28674
URACIL (CAS# 66-22-8); (M-H)-	79628	65373	73526	68300								274856	54241	97932		76006	43722	63358			133578	28777	69246	74590		80726	53616	72449
RIBOFLAVIN (CAS# 83-88-5); (M-H)-	2803	2972	1546	2028							1011						2929	4467	6882	6988	4521		1644	3085		4169		6096
LITHOCHOLIC ACID (CAS# 434-13-9); (M+HCOO)-					1043	1170																		2247		5104		9566
HOMOSERINE (CAS# 672-15-1); (M-H)-			75485									56520	8914	32445				152247	89697			78918		104488	14406			106927
PHENOL (CAS# 108-95-2); (M-H)-	18772	16975	15953	15835							6713	13358			21396	16493		27519	31351	10412	33628		49570	28147		24196	16717	48941
METHIONINE (CAS# 63-68-3); (M-H)-	35981	35475	35211	36080							2192	47780	17867	31110	21644	49523	31791	46298	36125	33564	36706	26334	31057	54345	3671	65870	44317	41708
GLUTATHIONE (CAS# 27025-41-8); (M-H)-	13763	11912	12230	12172							33155	6089		6718	46450	23421	12545	15657	45408		4048	1799				18803	4450	5244
LEUKOTRIENE B4 (CAS# 71160-24-2); (M-H)-	3812	2445	3548	3229							6257	5650	1067		6732	4447	2376	13301	8260	21829	13746		3993	3718				8377
UDP-N-ACETYL-D-GALACTOSAMINE (CAS#); (M-H)-																					5446							1818
5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (M-H)-	6186	4697	7022	6685			11119		8421	12799	5776	3374			3446	5040	4966	18780	31487	5211	10015	4579	8986	10520		13029		15709
GLUCOSE (CAS# 50-99-7); (2M+Cl)-[-H2O]	256678	252588	246966	247141			41380					235508	153754	176066		259358	242875	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
FRUCTOSE (CAS# 57-48-7); (M+Cl)-	2300487	2239844	2202478	2056951		1291615					622547	471894	208198	415656	1246316	1394161	1763423	2270298	2238216	3849839	4400844	1673138	3891124	2191065	458044	2038278	2131468	3247491
ADENOSINE (CAS# 58-61-7); (M+HCOO)-	12497	15589	14124	15971							16073	31064	6496	4308	21184	19727	22172	17424	24855	20792	22518	8224	12692	8647		17520	7228	19303
(S)-DIHYDROOROTATE (CAS# 5988-19-2); (M-H)-																												1659
CATECHOL (CAS# 120-80-9); (M-H)-					37985															1130	13441			3975				8636
LACTOSE (CAS# 63-42-3); (M+Cl)-	256678	252588	246966	247141		50234	41380				286987	235508	153754	176066	376002	259358	242875	253677	280201	166009	187200	206808	269193	187103	164529	718741	233804	209281
THYMIDINE (CAS# 50-89-5); (M-H)-												10692			7224				3209									1879
5-OXOPROLINE (CAS# 4042-36-8); (M-H)-	1.67E+07	1.12E+07	1.14E+07	1.08E+07							1696173	9991478	382652	3013128	2574199	1.05E+07	1.00E+07	1.90E+07	2.99E+07	1.18E+07	5500963	7569625	1.65E+07	2.02E+07	1101161	2.00E+07	1.31E+07	2.03E+07
1-METHYLADENOSINE (CAS# 15763-06-1); (M+HCOO)-					3154		1973		2236										2011		2415							
INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M-H)-			1844	2174								2022						4667	15506	1680			3931	4824				
URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (M-H)-	37067	23004	47931	37873	3390		8106		6674		128796	44000			58570	45466			1804		1259	10016		1568	12974	1619	65713	
3-NITRO-L-TYROSINE (CAS# 621-44-3); (M-H)-		1050																	4604									
ASPARAGINE (CAS# 70-47-3); (M-H)-													5584						14219									
PHENYLALANINE (CAS# 63-91-2); (M-H)-		766949	742630	759000							677636	630186	76991	266352	563615	653738	727861	2307476	2229555	1164463	1592083	308143	921044	1128005	22429	1735259	473160	
D-GLUCOSAMINE (CAS# 3416-24-8); (M+Cl)-					6170							19463		29410		23975			21346			16354					9260	
MALATE (CAS# 97-67-6); (M-H)+[-H2O]					35231	34449	33574		34109	31885	32790	3215			15014	9206	3219		2814								5055	
BETA-MALTOSE (CAS# 69-79-4); (2M-H)-[-H2O]	6860	1482	4885	7614							1386	3908	1679	13781		4190	1268	5006	7476	3046	2744	5886		8451	21245	10834	9485	
ETHANOLAMINE PHOSPHATE (CAS# 1071-23-4); (M-H)-	52158	63410	65741	41292							231482	52783	7582	40035	226571	78447	20821	7860	23898	23307	34821	33400	25458		24421	50819	140051	
BETA-ALANINE (CAS# 107-95-9); (M-H)-				49396							56746	25703	29637	58089			56687	67170	39520			34054		47527				

D-GALACTOSAMINE (CAS# 7535-00-4); (M+Cl)-					6170							19463		29410		23975			21346			16354					9260
3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (M-H)-													5584						14219								
N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8); (M+HCOO)-																			5263	1060	2604						
CARNOSINE (CAS# 305-84-0); (M-H)-			5433	3767							7553					1416	3352		8506			6474		5435		4927	
DEOXYURIDINE (CAS# 951-78-0); (M-H)-												29964					5435		9353		13175						
EDTA (CAS# 60-00-4); (M-2H)-2																			1277								
GLYCINE (CAS# 56-40-6); (M-H)-				9024											3127	8488	8168	26125	8046		3272			8995		20705	6547
N-ACETYL-L-ASPARTIC ACID (CAS# 997-55-7); (M-H)-	25922	26448	27021	25292							103711	22474		13714	60781	21008	14454		143682	21550		6553	13148	33955	1948	59568	26696
ETHYLMALONIC ACID (CAS# 601-75-2); (M-H)-	13832	10893	10549	12481							4665				3861	1906	2891		20697	2574	13995		3134	4613		8434	2531
RAFFINOSE (CAS# 512-69-6); (M+HCOO)-					1948									8641					2175	1173		2913	1273	1735	7966	4709	5953
RIBOSE (CAS# 50-69-1); (M+Cl)-	41641	31673	38468	26916					2292		11884		7783	8995	10925	1443	3559		8054	291911	8212	2788	27223				12689
D-LYXOSE (CAS# 1114-34-7); (M+Cl)-	41641	33261	38468	26916					2885		11884		7783	9812	11994	1443	4204		8054	291911	8212	2788	27223				14106
1-METHYLADENOSINE (CAS# 15763-06-1); (M+Cl)-						2263				2220								1219	1522								
L-ALLOTHREONINE (CAS# 28954-12-3); (M-H)-			75485									56520	8914	32445				152247	89697			77652		104488	14406		
STACHYOSE (CAS# 54261-98-2); (M-H)-		1482	4885	7614							1386	3908	1679	13781		6920	1268	5006	7476	3046	2744	7688	6421	8451	21245	10834	9485
O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5); (M-H)-																		1452	5668								
DEOXYCYTIDINE (CAS# 951-77-9); (M+HCOO)-	11981	4660	7927	3989					1087		31320	2375		8558	38571	9465	5857	12975	13115			7627	12843		5635		15495
ADENOSINE 5'-PHOSPHOSULFATE (CAS# 485-84-7); (M-H)-	2481		2936	2853								5207				9948	2053	1363	2549					4737		3470	2058
GLUCARIC ACID (CAS# 87-73-0); (M-H)-						1670	1127		1277																		
3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-92-7); (M-H)-							7350		10029																		
THYMIDINE (CAS# 50-89-5); (M+Cl)-		2431		4250					6081	7617	2020	16333			13435												
RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-6); (M+HCOO)-									1335																		
PURINE (CAS# 120-73-0); (M-H)-									3490																		
DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Cl)-						2123			1749																		
INDOLE-3-ACETATE (CAS# 87-51-4); (M-H)-									11349	11939		3640															
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+Cl)-	2786	1941		1154					6506		7468	33043		12222	20576												
CYSTATHIONINE (CAS# 56-88-2); (M-H)-					4521	4669	5094		3252																2660		
DGMP (CAS# 902-04-5); (M-H)-												18070		1776							76183						
PHENYLPYRUVATE (CAS# 156-06-9); (M-H)-																					3964						
HOMOVANILLATE (CAS# 306-08-1); (M-H)-											2002				2651						4038						
ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-73-2); (M-H)-												3728		2202			1955				1553			2651		3142	
N-OLEOYLGLYCINE (CAS# 2601-90-3); (M-H)-				3945								5357			10062		3204			6450	2629		5517	12760			
ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-19-8); (M-H)-					9512							18070		1776							76183						
2-AMINOETHYL DIHYDROGEN PHOSPHATE (CAS# 1071-23-4	52158	63410	65741	41292							231482	52783	7582	40035	226571	78447	20821	7860		23307	34821	33400	25458		24421	50819	140051
3-METHOXYTYROSINE (CAS# 4214-13-5); (M-H)-																					1467						
NICOTINATE (CAS# 59-67-6); (M-H)-		3652	7319		10931	12615	4520			17934				30114	11451	22690	1971				6019	23256	2737	2555		41472	23573
DEOXYURIDINE (CAS# 951-78-0); (M+HCOO)-												20208									4577						
THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-07-1); (M-H)-			1161								1202							3300			2481						
N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6); (M+HCOO)-												3739									4581				1550		
RIBOSE 5-PHOSPHATE (CAS# 4300-28-1); (M-H)-																					1186	4126					
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)-		2094	1882								4330				1030			7967		8661	9416		2261				
2'-DEOXYINOSINE (CAS# 890-38-0); (M-H)-	2475	5810		1198								67208			2192					7851	13841		3961			5157	
GALACTARATE (CAS# 526-99-8); (M-H)-						1670																					
3,5-DIBROMO-4-HYDROXYBENZONITRILE (CAS# 1689-84-5); (M-H)-						3241																					
BENZALDEHYDE (CAS# 100-52-7); (M+HCOO)-						1500																					
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (2M-H)-					1981	1918	2594			1455														49502			
4-HYDROXYPHENYLACETATE (CAS# 156-38-7); (M-H)-						1500																					
2,5-DIOXOPIPERAZINE (CAS# 106-57-0); (M-H)-						12219																					
2-OXOADIPATE (CAS# 3184-35-8); (M-H)-										4862																	
SPHINGANINE (CAS# 764-22-7); (M+HCOO)-[-H2O]										1717																	
GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (M-H)-					1233		1372			1142	15440				16077												
2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-5); (M-H)-					6420					6385																	
3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CAS# 28822-73-3); (M-H)-[-H2O]					2884																					1051	
INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M-H)-			29509	6771	19129						53498	6062		5009	32898	4348						2787			1045		3449
5-HYDROXYINDOLEACETATE (CAS# 54-16-0); (M-H)-					19347																				2291		
PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M-H)-					1907																						
ARABITOL (CAS# 7643-75-6); (M+HCOO)-					3866		1459																				
MEVALONIC ACID (CAS# 674-26-0); (M-H)-					11429																						
PROTOPORPHYRIN (CAS# 553-12-8); (M-H)-							1448																				
THYMINE (CAS# 65-71-4); (M-H)-	7813		8570	6868							14953	81952		6438	5702	5360				1565					2510	2302	
L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (CAS#); (M-H)-			1776	2956							9525	2276	15331				1922			1900		6629		1158	71149		
RIBOFLAVIN (CAS# 83-88-5); (M+Cl)-																				1652							
BIOTIN (CAS# 58-85-5); (M-H)-	1025												4277				4746			2319			3520				
CAPRYLIC ACID (CAS# 124-07-2); (M-H)-																				1785							
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Cl)-[-H2O]																				3075							
LUMICHROME (CAS# 1086-80-2); (M-H)-																				1022							
CHOLINE PHOSPHATE (CAS# 107-73-3); (M+HCOO)-			5766	1504							17480	3032		9053		9816	1815					2231					
N-NITROSODIETHANOLAMINE (CAS# 1116-54-7); (M+Cl)-				3956																							
NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE (CAS# 22052-73-9); (M-H)-																		1707									
3-OXALOMALATE (CAS# 89304-26-7); (M-H)-[-H2O]																		2340									
METHYL VANILLATE (CAS# 3943-74-6); (M-H)-																		1250									
N-AMIDINO-L-ASPARTATE (CAS# 6133-30-8); (M+Cl)+[-H2O]																		10985									
GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M-H)-			4812											2543													
4-ACETAMIDOBUTANOATE (CAS# 3025-96-5); (M-H)-			6478																								
SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (M+HCOO)-			3858																								
S-CARBOXYMETHYL-L-CYSTEINE (CAS# 638-23-3); (M-H)-			2450																								
PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M-H)-																							13316	78702		129429	
PENTANOATE (CAS# 109-52-4); (M+HCOO)-																							2986				
1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 3436-44-0); (M+HCOO)-																							2529			2206	
5ALPHA-ANDROSTANE-3ALPHA,17BETA-DIOL (CAS# 1852-53-5); (M+Cl)-[-H2O]																							4512				4091
D-MANNOSAMINE (CAS# 14307-02-9); (M-H)-[-H2O]	7001										14649																
THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#); (M-H)-	455127											508785		542425		417029						533326			891806		575767
D-GALACTOSAMINE (CAS# 7535-00-4); (M-H)-[-H2O]	7001										14649																
N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M-H)-	7001										13505																
ADENOSINE 2',3'-CYCLIC MONOPHOSPHATE (CAS# 634-01-5); (M-H)-																								2534			
N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3); (M-H)-																								6349			
3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+Cl)-																										1845	
SULFADIMETHOXINE (CAS# 122-11-2); (M-H)-																										13856	
CYTIDINE (CAS# 65-46-3); (M+Cl)-													4836	10048		15398										34494	
LACTOSE (CAS# 63-42-3); (M-H)-													6522	9032			6054								11568		
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+HCOO)-															2121		1614										
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0); (M+Cl)-																	1848										
UDP-GALACTOSE (CAS# 2956-16-3); (M-H)-											12291	23729		17724	52043												
HOMOCYSTINE (CAS# 462-10-2); (M-H)-												7726															
MELIBIOSE (CAS# 585-99-9); (M+HCOO)-											3431	7760	10207	6248	10228										13195		6609
SUCROSE (CAS# 57-50-1); (M+HCOO)-											3431	7760	10207	6248	10228										13195		6609
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+HCOO)-												8208		2735	3011												
INDICAN (CAS# 487-60-5); (2M+Cl)-[-H2O]												1224															
BETA-MALTOSE (CAS# 69-79-4); (M+HCOO)-											3431	7760	10207	6248	10228										13195		6609
2',3'-CYCLIC CMP (CAS# 15718-51-1); (M-H)-											3890	6532	2722			6311						1299			1068		
MALTOSE (CAS# 69-79-4); (M+HCOO)-											3431	7760	10207	6248	10228										13195		6609
20:0 LYSO PC (CAS# 108341-80-6); (M+Cl)-												1201		1207	1301												
MALEAMATE (CAS# 557-24-4); (M-H)-												27011		2165	4254												
PALATINOSE (CAS# 343336-76-5); (M+HCOO)-											3431	7760	10207	6248	10228										13195		6609
DIHYDROXYMANDELIC ACID (CAS# 775-01-9); (M-H)-													3079	3477	2925												4020
XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8); (M-H)-											1456																
GLUCOSE (CAS# 50-99-7); (2M+HCOO)-[-H2O]											3431		10207		10228										13195		
UDP-GLUCOSE (CAS# 133-89-1); (M-H)-											11829			12326	19412												
PHENYLACETIC ACID (CAS# 103-82-2); (M+HCOO)-											2002				2651												
OXALOACETATE (CAS# 328-42-7); (M-H)-[-H2O]															6444												
4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-KRYNURENIC ACID (CAS# 492-27-3); (M-H)-															4326												
3-METHOXY-4-HYDROXYMANDELATE (CAS# 55-10-7); (M-H)-															3031												
DEHYDROASCORBATE (CAS# 490-83-5); (M+HCOO)-														10542	9162												
GULONO-1,4-LACTONE (CAS# 1128-23-0); (M-H)-															3321												
GLUCURONIC ACID (CAS# 6556-12-3); (M+Cl)-																						4302					
CREATINE (CAS# 57-00-1); (M-H)-													37345														
CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (M-H)-																									1380		
STACHYOSE (CAS# 54261-98-2); (M+HCOO)-																									2738		

Compound	Component 1 (37.24%)	Component 2 (13.61%)	Component 3 (10.51%)	Component 4 (5.96%)
C25 H21 P	2.9095829	-1.5176756	1.3550706	-0.4442433
C7 H2 Cl N O3	-0.92973745	1.9124476	-2.8615243	-1.0994081
C24 H32 P4	1.8123741	-1.301545	1.7106473	-0.26638404
C15 H16 N4 O S	4.0190306	-0.18727013	-0.4369481	0.92323244
C29 H56 N O6 P S2	3.0225453	1.2527548	1.4698542	0.17661786
C15 H24 N3 O6 P S	-0.92706263	1.2087747	-3.0098312	-0.86906993
C12 H12 N8 O4	1.8308519	-1.4556342	1.4812152	1.4511546
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5	1.0058311	-3.2212076	-2.4889061	-0.08095016
C20 H32 N4	3.7030432	-0.21990117	-0.115389	0.22820032
HIPPURATE (CAS# 495-69-2); (M-H)-	2.578053	0.043289166	1.1036228	-0.13798147
C37 H66 N5 P	-0.7772212	1.591213	-1.5529191	-1.6002204
C25 H41 Cl N8	-0.2905876	-2.259796	0.34260777	-2.188624
C7 H6 O3	3.4381456	0.9383171	-1.1108991	0.594332
C22 H44 N2 O5	0.75823164	-0.9092341	0.02325246	-0.0065415
MONO-METHYL GLUTARATE (CAS# 150	2.419259	-0.6695772	0.50572807	0.56806314
C22 H36 S4	1.5887928	-1.4847605	-0.0664134	0.6027702
C24 H34 N2 O10	0.4074364	-3.1477866	-2.720636	0.026651137
C14 H28 O2	4.0512524	0.015978936	-0.5914055	0.56994045
C4 H6 O5 P2 S	3.7918506	-0.76373667	-0.0462595	-0.23086733
C32 H47 N O5	0.505495	-0.18132524	0.98520195	0.24449769
C17 H22 N16 O2 P2	-1.5934886	-0.12986302	-1.3314605	-0.17578845
TRANS-ACONITATE (CAS# 4023-65-8); (	-0.063131884	-0.09000707	-0.3875204	-1.130566
C13 H16 N4 O5 S	0.5985997	-3.2118018	-2.5151443	0.2367287
C21 H33 N10 P S	0.99420124	0.14197636	-1.5845907	-0.19097537
C22 H4 N O P	1.9327415	-0.69347715	-1.6548119	-1.3113658
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5	1.0980802	-3.238939	-2.3603032	-0.12157878
C18 H34 O5	2.4311311	1.5727899	0.04336165	-0.7962984
C18 H34 O3	3.210258	-1.5054554	-0.7194229	0.1518901
C18 H34 O2	3.5058842	2.1514013	-0.8563204	0.26427227
C30 H54 N5 O2 P5	2.2103376	-0.7401854	1.2142252	-0.78029954
C14 H28 O3	3.9623713	-0.5031794	-0.1616907	0.9183198
C39 H63 N4 P S	3.390934	-0.8081601	-0.7840297	-1.4692159
C37 H64 O3 P6	0.3696073	-3.1070383	-2.7371757	0.083024085
C43 H58 S2	3.6217601	1.5336953	-0.2771824	-0.9206733
C25 H37 N10 O5 P5	3.4917686	2.1565747	-0.7667471	0.23969972
C21 H20 N6 O2	1.4133073	-0.25898582	-0.7947583	1.1698718
NONANOATE (CAS# 112-05-0); (M-H)-	3.713996	-0.057544164	-0.7762112	0.62189233
C13 H3 Cl O5	0.20193994	-1.0038491	2.1526237	-0.46273297
C42 H67 O4 P S	3.2982993	-0.96277326	0.3290416	-1.4289362
C25 H32 N8 O7 P4	-1.6345241	-0.8715806	0.41710296	0.079702854
C21 H33 N8 O P5	3.7924886	-0.59168315	-0.7624997	1.1111505
ARACHIDIC ACID (CAS# 506-30-9); (M-	2.7490644	1.8854482	-0.0165605	-0.15968323
ALPHA-LINOLENIC ACID (CAS# 463-40-1	3.120159	1.7699736	-0.8595416	0.32067752
C29 H27 N2 O P S2	0.61342186	-2.0879834	-0.0771603	0.74179035
C21 H38 O10 S	2.6914768	1.9531014	-1.2054634	-0.6889434
C7 H17 N6 P S	1.5546241	1.3233477	-0.1388995	-0.6787399
C7 H13 N2 O16 P3 S2	-3.3772151	0.87631255	-1.2457021	-0.6442168
C19 H25 N10 O4 P5	-0.39484164	-3.2131643	-2.5982902	-0.3138653
C17 H28 O3 S	-2.057154	-0.69228834	0.5626809	0.33478338
C26 H52 N3 O15 P	2.1156862	1.0811914	-0.9731474	0.796536
C30 H49 N5 P2 S3	3.8946476	0.73056227	0.70663166	-0.00138259
C36 H66 N2 O8	3.2141187	-0.61399955	-1.2351047	-1.2193938
C13 H19 N5 O4	1.6882055	-0.859952	0.6980978	-2.056979
C19 H14 N10 O2	0.79187906	-3.1751187	-2.612661	-0.29288295
C24 H43 N9 O S3	3.750796	0.24818338	0.8689045	-0.19763571
C12 H16 Cl N O S	2.1394832	-0.53550774	0.8762176	-0.63629097
C40 H81 N2 O8 P	3.3104303	-0.9665965	-0.2425537	-0.5668733
C31 H34 N2 O7 S	0.092250854	-3.060744	-2.827264	-0.03290175
C35 H65 O6 P S	1.4466879	0.84050643	-0.9304988	0.772924
C22 H36 O2	-1.6233733	-2.0178807	1.9754666	0.044044614
C28 H34 N2 O3 P2	3.8966913	1.3725114	-0.3925817	-0.22624546
C3 H10 N8	0.17422038	0.5921651	-0.8636341	-0.61715496
TYROSINE (CAS# 60-18-4); (M-H)-	3.3079436	1.4343963	-0.7583767	0.83857185
C36 H58 N6 O2	2.7616756	-0.6067186	0.37476555	-1.8793459
C14 H21 N O3	1.71317	-1.1780881	-2.090482	-0.45148867
C38 H74 O4 S	3.066508	-0.48545533	-1.3853773	-1.2420332
C24 H46 O2	0.7656844	-0.17989138	1.3737085	-1.9581671
C27 H56 N14 O2	2.538742	-0.5929662	-1.1779408	-2.1322691
C22 H41 N4 O4 P3 S	2.620018	2.0211077	-1.3243718	-0.51864505
C14 H16 N2 O4	2.8412714	-1.7695673	-0.5002058	0.9405061
C14 H16 N2 O5	3.5314975	-0.44335437	-0.6884661	1.538567
N-METHYL-D-ASPARTIC ACID (CAS# 638	1.0561614	2.7015269	-0.414319	0.6375896
C33 H54 N4 O2	2.3259845	0.58584416	-0.1141446	0.35693613
C34 H62 N6 O2	3.155409	-0.5506159	-1.2227318	-1.2268811
C39 H62 N2 O3 P2	3.619255	0.9640521	-0.255621	-0.5208039
C7 H19 N2 P S2	3.3880224	0.6985952	-0.4451168	1.1222725
ADIPIC ACID (CAS# 124-04-9); (M-H)-	2.4179063	-0.6713635	0.49865448	0.5665724
C35 H72 O4 S	3.5328774	0.68011194	-0.7610014	1.1180565
C22 H31 N7 O2 S	2.1081204	-0.011154316	-1.275929	-1.1619767
C27 H52 N O9 P	3.7665734	1.6309956	-0.1796895	0.22046983
C14 H24 N2 S4	1.0630442	-0.036345974	-1.5139408	-1.6104171
C39 H72 O3 S2	3.4520326	-1.467714	-1.1309358	0.8221662
C35 H40 N14	2.0524268	0.9100673	0.52853495	-0.30337912
C4 H9 N2 O4 P3 S2	-1.4655524	-1.5657094	0.34255823	-0.8032466
C8 H12 O18 P2 S3	-2.3828537	1.5507087	-2.366351	-1.4152783
C10 H11 N5	-1.160206	-2.7703087	-2.2253184	0.002753452
C18 H29 N18 O6 P5	-2.3603373	0.24317744	1.987346	-0.02282703
C15 H16 N10	1.7932631	-2.7870238	-1.3740647	-0.2904178
C9 H6 N2 O4	-0.40429837	-1.08007	-3.3660383	-0.960863
INOSINE (CAS# 58-63-9); (M-H)-	3.312049	1.5381843	-0.2848225	1.223047
RAFFINOSE (CAS# 512-69-6); (M+Cl)-	1.5410714	-1.5252476	-1.8942109	1.4105259
C4 H5 N2 P S2	-3.38803	-0.947048	-0.5761885	-1.5692719
TAURINE (CAS# 107-35-7); (M-H)-	-1.3256805	1.4057695	-2.1792696	-1.5083607
C12 H3 Cl N3 P	2.8617544	2.480801	-0.9136158	0.6776125
C16 H32 O3	2.341294	2.019011	-0.56868	-2.0704517
C16 H32 O2	3.4215047	1.2424207	-1.0639547	0.61866635
C32 H58 N8 O3 S2	2.5920272	0.61159617	0.5561951	0.44993293



C30 H62 N2 O S2	1.4841837	-1.0146921	0.94445795	-0.8610599
C40 H81 N O S2	2.3520603	-0.53475493	1.189105	-2.1844563
C9 H7 N O	2.6607933	-0.9859595	-1.1817598	1.2246265
C14 H30 N6 O	3.3765576	-1.2264273	0.10243321	0.56313
C21 H37 Cl N2 O S2	2.913383	1.9156418	-1.1560256	0.031858265
(S)-3-METHYL-2-OXOPENTANOATE (CA	0.8293569	-0.546312	-1.3466522	-0.08401507
C27 H44 O4	0.91097564	-0.34417686	-0.0244794	-0.13850754
C23 H30 N14 O5 P4	3.704626	0.5519471	0.34191686	-0.9549707
C16 H30 O2	3.719545	1.3309802	-0.7585695	-0.57175314
C16 H30 O3	3.8103757	-0.50589585	-0.4839931	0.8199588
C9 H20 N8 P2 S	3.1409533	1.8408121	-0.705718	-0.92130804
C25 H54 N O3 P	2.526528	-1.1226091	2.1982343	-0.34491444
C33 H66 Cl2 O P4	1.1489449	-3.127005	-2.446939	0.020296767
C26 H37 N15	0.8160888	-3.3446915	-2.1694095	0.36943743
2-HYDROXY-3-METHYLBUTYRIC ACID (	1.4282265	-0.64203316	1.3250433	0.13864112
C3 H4 O3	0.1579335	0.25180387	-0.7404964	-1.9176064
C28 H48 N6 O3	-0.09723484	0.40477496	-0.1437611	-0.8214557
CIS-7,10,13,16-DOCOSATETRAENOIC A	0.22896072	0.5437459	0.27558357	-1.5564929
CORTISONE (CAS# 53-06-5); (M+Cl)-	0.5878697	-0.53088266	0.82031393	0.031952314
HEXACOSANOIC ACID (CAS# 506-46-7);	2.3904262	-1.7741133	1.2861439	1.333958
C20 H35 N6 O2 P3	3.4919193	-1.0175602	-0.7636405	-0.9831668
C4 H11 O3 P	3.53538	-0.99550796	-0.1850097	0.9267955
C5 H9 N2 O8 P3	-1.501835	-0.59479266	1.1665821	1.8038409
C27 H55 N3 O3 S3	3.7549648	0.9672518	0.6376006	-0.39162666
DECANOATE (CAS# 334-48-5); (M-H)-	3.8263764	-2.31E-04	-0.5445048	0.89187866
C42 H73 N3 O6 S	1.5879736	-0.70844394	2.5888605	-0.21934797
C30 H25 N5	1.8005502	-0.60395646	0.12221614	1.2449884
C21 H28 N4 O S	0.93579507	2.9799573	-1.6843774	1.096765
C4 H6 N6 O3	1.7632349	-0.30076504	2.278101	-0.8077934
C25 H44 N6 O2 P6	-0.26472506	-2.9542158	-2.9324129	-0.06325959
C30 H24 N4 O4	1.655281	-1.3104218	0.07575839	1.6141992
STEARATE (CAS# 57-11-4); (M-H)-	2.851809	2.4501305	-1.2121315	-0.22614473
CIS-VACCENIC ACID (CAS# 506-17-2); (	3.4853206	2.1812465	-0.8498932	0.28669488
C22 H36 N12 O2 P6	-1.6753566	-0.06280492	-1.2112929	0.17672767
C27 H42 N4	1.3681483	-0.64953107	0.61222535	-0.44547015
C24 H36 N2 O3 S2	3.635725	1.072366	-0.6090415	-0.03460401
C20 H37 N6 O2 P3	3.6465127	1.9149685	-0.8286618	0.30867976
C29 H27 N19 O4	3.40783	1.129934	0.42969126	1.1193892
C20 H36 O2	2.9432857	-0.36004472	-1.1008431	-2.1649146
C13 H33 N4 O4 P	2.8650622	2.0726104	-1.0416964	-1.5095527
C38 H41 N10 P	1.1857443	-3.1511528	-2.3273733	0.06616692
C19 H38 O2	1.6506495	0.44070697	-1.1866575	0.789964
C21 H32 N6 O2	2.8791094	-0.593817	-0.5525306	-1.5725065
C21 H34 O P4	3.9794753	-0.94212157	-0.3210028	0.08534205
C18 H32 N4 O14	3.7076864	1.4110563	-1.0303473	0.40562642
C18 H14 N6	2.2030454	-1.2757623	1.2587644	-0.6158397
C32 H61 N4 O2 P S	3.7081006	1.4597007	-0.907773	0.5140908
C20 H31 N2 O5 P	3.8143816	1.4702915	-0.3543562	-0.21769905
C38 H67 Cl N2 O S2	3.2635012	1.2347413	-0.2668583	-0.4455006
OMEGA-HYDROXYDODECANOIC ACID (	3.031791	-1.151649	-0.3892591	1.5920932
C30 H50 N5 O5 P	1.2536291	-1.0415692	1.3123523	0.855168
C22 H40 N5 O3 P	0.042700984	0.7143715	1.8201442	-1.5588623
C23 H44 N6 O4 P4 S	2.5783143	2.2645752	-1.4773841	-0.3458627
C24 H17 N8 O2 P	2.039907	-2.7334943	-2.1402333	-0.27353048
CIS-ZEATIN (CAS# 1637-39-4); (M+Cl)-	0.20286918	-3.272086	-2.5154676	-0.01273819
THEOPHYLLINE (CAS# 58-55-9); (M-H)-	1.2723725	-0.3037756	1.1492589	-0.13530128
C17 H33 N4 O3 P	3.5093913	2.0566516	-0.6976173	0.011594176
C7 H18 N2 O15 P4 S4	-2.635144	1.3827685	-2.17821	-1.3971633
C37 H68 N2 O5 S2	1.2505623	-0.9210479	0.5385776	-0.08711729
C23 H30 N4 O2 S2	2.732984	-0.5738247	0.7517504	-2.0386026
C24 H28 N12 O12 S	-0.32957038	-2.9079053	-3.0004063	0.028137684
C28 H40 N5 O3 P	3.044262	-1.4670407	1.6044906	0.07432401
C9 H18 N P3	3.3545954	2.0054092	-0.5213807	0.75255704
6-CARBOXYHEXANOATE (CAS# 111-16-	2.3504992	-1.2541475	0.36524892	-1.1718516
C7 H8 N4 O2	1.2486684	-0.3242588	1.1490769	-0.09993561
C25 H53 N8 P	0.43068448	0.39248794	1.6177424	-0.65711164
THREONINE (CAS# 72-19-5); (M+HCO	1.5264148	1.8054847	-0.7776221	1.3122424
C15 H22 O2	0.6691487	-0.70459366	-1.3292574	1.259264
C46 H52 N8	1.9405904	0.11742642	0.778339	-0.20094761
C39 H65 N7 O2 S	3.077156	2.4254496	-1.1079211	0.38413584
C23 H42 S4	-2.5950065	-0.99561524	0.20681505	2.0943227
C15 H22 O6	2.2032728	-0.5125103	0.3895613	-0.40751135
C32 H60 O6	1.7759151	-1.0916803	1.86531	0.5544673
C21 H44 N4 O14 P4 S	2.256039	1.8305748	-0.6791603	1.1157196
C40 H73 N3 O6 S	3.312494	-1.2093858	0.7346033	-0.65418255
C19 H37 O2 P3	3.5478787	0.9689776	-0.2943882	-1.1358076
C24 H45 O18 P S3	2.1596408	1.980759	-0.8638068	-0.6741653
C25 H32 N6 O12 S	-0.150368	-2.889363	-3.0139308	-0.10045884
C30 H46 N4 O5	0.3558349	-3.4849102	-2.3305688	0.115295984
C30 H46 N4 O4	0.34837177	-3.5222702	-2.2497518	0.21642749
C20 H32 O2	3.4890327	2.081253	-0.605688	0.116841435
C20 H32 O3	3.814044	1.174183	-0.5146391	-0.23624462
C39 H60 N P3	1.8248299	0.730902	0.49468443	-0.01516896
C6 H13 Cl N6	2.9358647	-1.7324293	-0.1347199	0.47471267
C32 H56 N2 O P2	3.594326	0.12461074	-0.1236442	0.7747612
C20 H34 O3	1.5368146	-0.76111454	1.1044759	-1.4197406
C20 H18 N4 O2	1.036292	-3.2435136	-2.4627433	-0.13630243
C20 H34 O2	3.7401807	1.3774147	-0.8178405	0.036617577
C16 H28 O2	2.4300578	-1.6624938	1.3075216	0.5624993
CIS-ZEATIN (CAS# 1637-39-4); (M-H)-	-0.7070261	-3.1614103	-2.530493	0.071860254
C19 H38 S2	3.289783	2.0775814	-0.3438606	-0.16357619
C34 H48 Cl N2 O5 P3 S	0.97854424	-1.4013034	0.55938995	0.8034208
PALMITOLEIC ACID (CAS# 373-49-9); (	3.7165732	1.338217	-0.7494635	-0.5641878
C25 H55 N5 O7 S3	3.417593	-1.081649	0.10844592	-0.88933194
C28 H40 O13 S3	2.0204973	2.28743	-1.1201047	-0.3064189
C25 H52 N O2 P S3	2.6492991	-1.383302	1.634996	0.3250847
C25 H50 O2	2.6635263	-1.7358779	1.5930697	0.91085917
C13 H11 N2 O2 P	3.7152472	0.16562635	-0.7098758	0.92393595
C24 H48 N O2 P S2	3.5392334	1.0227516	-0.4780303	0.8797033
C24 H32 N2 O5	1.5444788	-1.3958981	-0.1380949	0.90266275
C28 H60 N O4 P S2	2.8824766	-1.2959429	0.97541475	-0.13035926
C18 H39 Cl N2 O S3	2.7941217	-1.319227	-0.7256676	0.11255978
C30 H25 N5 O	2.7626681	2.278918	-1.3362062	0.7023083
C27 H54 Cl2 O	3.3606534	1.1348214	-0.4089451	0.7870387
NORLEUCINE (CAS# 327-57-1); (M-H)-	3.1074562	1.6119579	-0.6049011	0.87738323

C12 H23 N O3	3.5464206	0.54255134	0.1253747	0.59816384
C30 H57 N O11 P2 S	3.4484432	-1.1384485	-0.1026353	-0.5895779
C23 H34 N6 O13 P2	3.2475667	1.9637334	-0.8489053	0.68239945
C14 H16 N12 O P4	3.6012006	0.33668166	-0.8562216	0.8193661
4-METHYL-2-OXOVALERIC ACID (CAS# 8	1.3701124	-1.3107976	0.15713114	0.53953314
C21 H32 N2 O8	3.6691787	1.8182548	-0.6108466	0.05077648
C12 H20 O3	1.4916493	-2.4258587	-0.7807425	-0.64380926
C27 H50 S2	0.027265161	2.1255634	-0.6142513	-0.93749404
JASMONIC ACID [ISTD] (CAS# 77026-92	1.0337055	-3.222711	-2.461313	0.0937442
C38 H63 Cl N2 O S2	3.1034627	-1.3606775	0.5047741	-0.9062777
C38 H60 N9 P	0.39621937	0.04728974	-2.0350564	-1.0493178
C21 H32 N6 O4 P6	-0.6297364	-3.0447516	-2.7447865	-0.34536582
C45 H49 N5	1.3359601	-0.43388432	0.55607474	-0.5231962
C41 H86 O2 P4	2.7064993	-1.0105758	1.5314084	-0.5215721
C5 H5 N5	-1.0442638	-2.809809	-2.2870767	-0.6799174
ISOCITRATE (CAS# 320-77-4); (M-H)-	0.38181812	0.085661255	0.85432106	-1.8851094
C24 H52 N O2 P S2	1.6815025	3.104583	0.3525998	-0.0846703
16:0 LYSO PC (CAS# 17364-16-8); (M+C	1.1754956	-0.82306236	0.8630892	-0.46198684
FRUCTOSE (CAS# 57-48-7); (M+HCOO)-	-1.7483454	-1.0286078	-0.3440309	-0.7825837
C36 H66 N2 O6 S	0.10926071	-0.6806238	-0.849384	-0.15460533
C24 H53 Cl N4 O3	2.6824045	0.4325876	-0.0322345	1.6997216
C27 H53 N2 P3	-0.7327864	-2.255781	0.10944522	-2.2851837
C16 H30 N6 O2	3.6921492	1.3269283	-1.0587572	0.18691593
C28 H52 N5 O5 P	2.2971916	-1.3192241	0.6378279	-0.35019493
C23 H37 O17 P	3.5363266	2.0656648	-0.9258818	0.34009314
C38 H35 N5 O4	0.03697662	-3.5582647	-1.8922555	-0.22232944
C30 H51 N O20	2.5930245	-1.1407356	2.048194	-0.22534454
18:0 LYSO-PE (CAS# 69747-55-3); (M-H	0.8764379	0.5830433	0.18042284	-1.4519467
C44 H89 N S2	1.4060892	0.5654392	-0.7395543	-2.4778023
C11 H18 N2 O S2	2.1064625	0.43953386	0.739927	2.3727612
C6 H10 N6 O4	0.8124427	-0.33666268	0.33971232	-0.7107551
C24 H42 N6 O3	2.5348175	-1.2040085	0.27257788	-0.4403572
C20 H31 N6 O17 P	0.24646062	0.65852267	1.2648745	-0.4488967
C17 H35 O2 P3	4.0586367	-0.22060023	-0.5009394	0.43281746
C22 H27 N2 O2 P	3.1837027	2.4289248	-0.8510786	0.4699991
C17 H30 N6 O3	3.4072723	-1.4276129	-0.8027192	0.05746436
C23 H47 Cl N3 O3 P	3.7155976	1.0140706	1.3468578	0.2709508
C37 H39 N10 P	1.457898	-0.97465587	1.687628	-0.20225939
PALMITATE (CAS# 57-10-3); (M-H)-	3.409565	1.3014966	-1.1170101	0.51619905
CITRATE (CAS# 77-92-9); (M-H)-	1.1009512	-0.38191587	1.2377483	-1.691081
C41 H49 N5	2.1034145	1.6016935	-0.6463052	0.73921776
C41 H85 N2 O P3 S	2.6680832	-0.75017893	1.5798554	-1.6485236
C25 H43 N13 P2	1.7726763	-0.48039612	0.40708098	-0.45338184
C18 H28 O3 P2	3.717762	1.6011992	-0.8306493	-0.19623369
C27 H24 N4 O2	3.2630646	-0.7414855	-0.6603554	-1.1576209
C33 H66 N2 O3 S2	3.6392257	1.4603213	-0.1906011	0.56961715
C24 H47 N5 O P4	3.3413284	0.15712036	0.61761326	1.3823197
C13 H23 N2 O P S	2.5604386	-1.1522459	0.87240404	1.8674617
C22 H28 O3 P2	1.7445078	-0.44810787	-0.4193063	-1.846092
C31 H37 N14 O P S	2.8306284	-1.2361215	1.3905399	-0.42352778
N-ACETYL-D-GLUCOSAMINE (CAS# 751	3.250693	-1.3343252	0.8074176	0.05715704
C43 H76 N O7 P	3.3466568	-1.0874403	0.57109815	-0.7447499
C40 H60 O12	3.685121	1.2169554	-1.1192889	0.48815787
C40 H53 N3 O P4	1.2988068	-3.1126997	-2.3418298	0.014060214
C16 H22 N6 O3	1.1987021	-2.708014	-2.700288	0.024933606
C19 H32 N2 O7 S	1.1526926	0.51996934	0.55316526	-1.6483523
C14 H18 O4	-1.0870042	-0.15485182	-1.0247387	0.53115124
C38 H75 N S2	2.246279	-1.2620568	2.4398842	-0.06092113
C14 H23 N6 O9 P3 S	-0.6788783	-2.5800512	-3.1268997	-0.14829071
C27 H50 O5	2.9781938	1.3970494	-1.2595171	0.6880472
C22 H24 N4 O4	-1.6620399	0.5955553	-0.729501	-0.68915766
C40 H46 O2	0.8296883	-0.99383605	-0.2034265	0.12929562
C17 H22 N12 O P4	3.8376005	0.018000469	-0.484156	0.9344889
C21 H30 N6 O2	2.2802463	-0.50860614	-0.2073181	-0.7710577
C19 H34 N2 O8	3.760679	1.5813833	-1.0473399	0.01907432
C25 H30 N O2 P5	2.4026186	-1.9759957	0.31054553	1.4184126
C41 H81 N3 O2 S3	3.2745163	-1.0822963	0.7653883	-0.9762685
C16 H23 N2 O11 P S	-0.7067021	-2.7605805	-2.937767	-0.40379953
LEUCINE (CAS# 328-39-2); (M-H)-	3.1066442	1.6126277	-0.6016468	0.87596345
C17 H32 N2 O8	3.7661042	1.4859433	-0.8822087	0.46029252
C20 H30 N6 O P4	3.7709832	-1.0209887	-0.4887231	0.52535343
C25 H55 N3 O3 S3	3.7494047	1.2618929	0.9016088	0.72121805
C15 H33 Cl N4 O2	2.831256	1.6335255	-0.9966699	0.66464746
C18 H17 N5 O4 P2	2.560046	-0.96252596	0.8673842	-0.7051033
C25 H44 N O7 P	3.790293	1.2990066	-0.4690138	0.7539482
C21 H18 N4 O	3.6172526	1.1293712	-1.1288052	0.37536603
C27 H48 N11 O5 P	1.6749709	-0.5411687	0.35890982	-1.0445685
C33 H37 N6 O2 P	-1.3845438	-2.9789665	-2.343764	0.2664119
C29 H50 N10	1.8131636	0.5283048	0.50647944	0.5481857
C25 H54 N O4 P S2	1.7807138	-0.06817525	0.60868824	-1.098634
C23 H36 O2 S2	2.580976	-1.0580634	0.80544907	-0.17015909
C18 H21 N2 O2 P	3.9793587	0.42163143	-0.7737009	0.6789172
C22 H26 N4 O22	3.853345	-0.5423416	-0.6746281	0.98620844
C36 H41 N7 O P4	2.7003832	-1.2161716	0.9079495	-0.5840627
C12 H27 N4 O P3 S	2.2884538	-0.2632875	-0.3127269	1.4756835
C36 H73 Cl P4	1.9356978	-1.1869895	0.9830562	0.31452078
GAMMA-BUTYROLACTONE (CAS# 96-4	1.0576098	-1.1977632	1.2588191	-0.36957172
C24 H40 N12 O2 P6	-0.27122924	-3.0132384	-2.8782809	0.015432298
C14 H23 O5 P S	2.034697	-0.73827505	0.1781825	-2.0357425
C21 H34 N2 O5 S2	3.1565375	-0.8185085	-1.1943027	-1.6301088
C42 H70 O3 S3	3.601084	1.3446983	-0.4273756	-0.22445488
C8 H15 N3 P2 S	1.3739945	1.1303586	0.49845022	0.25080794
C31 H46 N4 O	0.6655543	0.07088973	1.7127196	-0.07789502
C23 H9 Cl N6 O	2.5217447	-0.7834819	1.027835	-1.1228278
C23 H35 O17 P	3.1389656	1.3886577	-1.6017126	0.34155616
C28 H44 Cl N10 P S3	1.7314899	-0.97991836	0.7632207	-1.0449737
C9 H16 O3	3.5278902	0.11244121	-0.7953836	0.9232291
C9 H16 O4	3.3608813	0.3731517	0.1017355	-0.74763614
C15 H37 N4 O3 P	2.8319275	2.6959352	-1.0829933	-0.20899075
C18 H36 O4	4.046763	-0.2163691	-0.1908996	0.93795896
C9 H10 S	1.6791749	0.03262232	-1.5038557	-2.166298
L-HISTIDINE (CAS# 71-00-1); (M-H)-	2.0608287	0.17035915	-1.3531611	0.87586004
C28 H45 Cl N2	0.8072225	0.3335198	0.7051339	-1.0790335
C22 H44 O2	2.5572004	-1.3755487	1.034811	-0.07296276
C26 H32 O7 S2	3.6285183	1.3775616	-0.7630542	-1.0208445

C22 H37 O12 P S2	3.8448687	0.9523599	-0.5180157	-0.7546875
C38 H77 N S2	2.171835	-0.32506546	1.7388464	-2.3826504
C24 H38 N2 O17 P2	3.326412	-0.88837045	-1.2086582	-1.0067879
C25 H50 N2 S3	1.7473149	1.7303023	-0.7045281	-1.4761419
C18 H36 O3	3.4306836	-0.9643167	-0.8734599	0.7354002
C18 H36 O2	2.8333426	2.4644094	-1.2066383	-0.22815907
C32 H33 N6 O2 P S3	0.7976215	-0.73487884	-0.3589178	-0.4682654
SALICYLATE (CAS# 69-72-7); (M-H)-	3.4316702	0.9298079	-1.1106184	0.6082854
C42 H45 O P S	-1.0327206	-3.3679438	-1.738177	-0.35905668
C31 H58 N O6 P S2	2.8505194	1.5790272	-0.576264	-0.5145596
C7 H17 N2 O P S4	3.7971897	-0.84160835	-0.1318689	-0.19800079
C26 H54 N O4 P S2	2.6831238	2.4159212	-0.2572164	-1.2216475
C16 H18 N4 O4	2.1023233	-1.7773418	-0.0679664	0.8930594
C11 H19 N7 O	3.6423483	0.6030676	-0.2923747	0.3430724
C17 H33 N8 O P	1.7370024	-0.5924697	-0.6978442	0.2601606
C30 H55 N5 O3 P4	3.5908785	0.55290246	0.96210223	0.1947816
C27 H36 N2 O P2	2.1326747	1.1108801	0.3090402	1.2703936
LINOLEATE (CAS# 60-33-3); (M-H)-	3.6804283	1.7933507	-0.9496396	0.1570375
C25 H38 N6 O6 P2 S2	3.7146955	1.7717372	-0.6342154	0.16445631
C8 H8 O3	2.9069157	-0.06686228	1.5801721	1.5251259
C18 H30 O2	2.5465276	1.3231596	1.1229095	-0.04361486
SEBACIC ACID (CAS# 111-20-6); (M-H)-	3.533088	-0.08678086	0.7003573	-0.45462555
CORTISOL (CAS# 50-23-7); (M+Cl)-	0.10637342	-0.44776988	0.03187737	-0.2199469
C20 H24 N4 O4	3.2439263	-1.0052493	-0.9200591	-1.5898728
C28 H18 N9 O3 P	3.0697784	-1.2262706	-0.3899091	1.3591906
C40 H67 O4 P S	2.7267241	-0.89565015	-0.7374877	-0.29563522
C14 H26 O2	2.9657478	-1.8219793	0.4971508	-0.1449818
ERUCIC ACID (CAS# 112-86-7); (M-H)-	2.5498745	0.14765662	-1.2154626	-2.0839822
C40 H75 N3 O6 S	2.379355	-1.3324283	1.9671897	0.4744169
C24 H38 O13 P2	3.6954956	1.4192429	-0.9678755	0.2638595
C22 H27 N O2 P2	2.7407656	-0.8380943	0.1258824	-2.0632246
C17 H32 O2 S	0.8722237	-0.65351427	-0.4437047	-0.7914893
N-ACETYL-L-ALANINE (CAS# 97-69-8); (	2.621952	-0.47600827	-1.2251575	-0.9489778
C20 H25 N2 O2 P	2.035766	0.35674262	-0.6286541	2.3025818
C41 H79 N3 O2 S3	2.5788186	-1.0071554	0.4415384	0.028471291
C29 H45 Cl N4 O2	0.37140316	-3.5069811	-2.2382216	0.1265429
C20 H20 N4 O2	0.7309934	-3.2511082	-2.5673528	-0.14060245
C7 H8 N2 O17 P2	0.32907432	-1.3326886	2.1678746	2.104276
C17 H18 N4 O S	2.119394	-1.9407248	1.0042653	0.897944
C22 H34 O2	3.063731	-0.9382711	-0.8530227	-0.8314271
C30 H44 N4 O4	-0.10122151	-3.4934669	-1.9406707	-0.0265947
C19 H23 N8 O2 P5	-0.6327772	-2.952313	-2.7893555	-0.12693247
C13 H12 N10	2.5742514	-0.97395897	-1.1195018	1.1273559
C16 H34 O8 S	0.7718238	0.84690976	-0.2178336	1.0824146
C13 H22 O3	1.3009517	-0.5433161	1.1529453	-0.23456609
C24 H37 N2 O10 P S	3.359965	-0.87708175	-0.8725434	-1.13799
C21 H19 N18 O P	3.6263556	0.33459386	-0.9116963	-0.64007026
C22 H23 O3 P S2	2.495882	-1.0464488	0.7372278	-0.7334566
PHENYL ACETATE (CAS# 122-79-2); (M-	1.4072857	-0.79816365	2.0515046	-0.9709769
C24 H37 O4 P3	2.6772509	1.480058	0.28468704	-0.03234094
C19 H21 Cl N2 O10	0.32833755	-3.142314	-2.655311	-0.37701213
C29 H50 N11 O2 P5	1.930201	-1.2935929	1.9771192	0.37853146
3BETA-HYDROXYANDROST-5-EN-17-ON	2.4430382	-1.2967331	2.2109394	-0.25175512
C12 H24 O2	3.974087	-0.5019561	-0.3570074	0.80302536
C9 H13 O12 P3 S2	-3.175796	1.2543504	-1.6695951	-1.1052175
ZEATIN [ISTD] (CAS# 13114-27-7); (M+	0.20286918	-3.272086	-2.5154676	-0.01273819
PARAXANTHINE (CAS# 611-59-6); (M-H	1.2608191	-0.32040042	1.1835358	-0.10354349
C28 H58 N O4 P S2	3.4443297	2.2491355	-0.2692643	-0.29860216
C9 H9 N O3	2.4807858	0.01477871	1.2785048	-0.33109874
C8 H12 O3 S	1.052969	-0.7391399	1.0699708	-0.8408328
C33 H62 N4 O14	3.6413581	1.3935821	-1.0155566	0.6514591
C24 H49 Cl N8	0.21830565	0.042069085	0.5941077	0.21190247
C36 H75 N S2	0.9152937	-0.41524002	1.7895601	-1.3882234
TRIDECANOIC ACID (CAS# 638-53-9); (M	3.325826	-0.3396195	-0.9473757	1.7814878
C34 H55 N4 O4 P	2.6525445	-0.6638069	-0.2829176	-1.8939202
C22 H32 N2 O9 P2 S	3.8213835	-0.72762007	-0.8252152	0.8561713
C20 H34 N4 O14	3.9874988	0.55591154	-0.9863695	-0.36967182
C20 H32 N4 O14	3.4288023	1.634494	0.03366555	0.45358604
C12 H14 O4	1.7246138	-1.6128573	-1.320165	1.641927
C37 H42 N5 O2 P3 S	2.8022904	-1.2044611	1.3255963	-0.52453977
C37 H70 O S2	2.4943686	0.3777734	-0.5956213	0.057405174
C25 H43 N12 P	0.5869588	-3.0919428	-2.7194328	-0.29250363
MYRISTIC ACID (CAS# 544-63-8); (M-H)	4.061348	0.03934497	-0.5863788	0.52963066
C34 H47 N3 O10	3.934258	0.909782	-0.312752	-0.18639392
C22 H32 O2	3.035309	2.1832705	-0.0920031	0.1766147
C20 H36 N4 O14	2.4437811	2.0470617	-1.6057265	-0.37031895
C17 H18 N10 O	1.1589463	0.07030318	0.5199001	-0.31578863
C7 H8 O4 S	2.863937	-0.35518822	-0.0558741	0.88290095
C35 H69 O6 P S	3.397897	-1.5082041	-0.9714402	-0.5487814
C6 H10 N8 O4	1.8153322	0.16274229	-0.7493281	-2.6197386
C17 H25 Cl N10 O4 S	-2.7806265	-0.7523675	-2.1888452	-0.03606063
C26 H28 N4 O4	2.3552027	-1.9664563	-0.0328763	0.9012042
C36 H37 N O3	2.2204313	-1.6031469	1.6929158	0.43990788
C41 H54 O6 P2 S	0.19817725	-2.9855335	-2.863192	-0.00352703
C11 H20 Cl P3	3.6754901	1.531334	-0.4811886	0.5996988
C28 H55 N3 P2 S	0.8994508	-0.5450927	1.7920347	-0.30142087
C21 H44 O4 S	-1.4678596	1.730013	-0.398025	-1.0723673
C19 H36 O2	2.8013997	1.6014577	-1.1258061	-0.68121815
C18 H19 N14 O2 P5	-0.5171308	-3.0587204	-2.7254045	-0.14165516
C26 H38 O13 P2	3.467871	-1.0810957	-0.8644701	-0.83504784
CORTISONE (CAS# 53-06-5); (M+HCOO	3.3211572	-1.395321	0.9362683	-0.30172426
C12 H14 N8 O9	-0.51596963	-3.0664237	-2.7156696	-0.02670714
C21 H37 N25 P2	1.5473472	-0.50880307	-1.3102033	0.1471081
PALMITIC ACID-13,13,14,14,15,15,16,16	-2.1378474	1.2064911	-1.6726458	-1.3952223
C28 H46 N O2 P3	2.1123307	0.34656715	-1.0315899	-1.5515792
C18 H41 O P3	3.3035007	-1.5061731	-0.0550039	-0.02613968
C22 H52 N15 O4 P5	1.2192695	0.73862374	-1.0361838	0.3207518
C28 H26 N3 O2 P	-0.035326008	0.3660817	0.5803658	0.69487345
C37 H77 N3 O S	-1.8276712	0.087711826	-1.9940717	-0.8296207
C27 H54 N7 O2 P3 S	2.6525898	-1.1472086	1.9587625	0.43014994
C21 H26 N4 O3	1.3250692	2.971161	-1.9683952	1.3344126
C23 H37 O2 P3	0.23467083	-0.24746574	-1.9643289	1.0991945
C19 H18 N8 O12	-0.56511086	-3.1274323	-2.725172	-0.32100126
C15 H25 O4 P3	2.468978	-1.0042496	1.3834343	-1.6092732
CIS-7,10,13,16-DOCOSATETRAENOIC AC	2.889534	-0.31419215	-0.6770673	-2.0570302

C18 H30 Cl2 N4 O2	3.4756439	1.7754647	-0.1897736	0.47850108
C13 H31 N4 O3 P	3.667106	1.1255356	-0.7132405	-0.63466763
C33 H36 N20 O2	3.7372458	-0.2529986	-0.2093749	1.1506383
C26 H40 N5 O3 P	3.8021793	0.72663695	0.8746367	-0.09376144
C5 H9 N O4	0.99375045	2.8421013	-0.2125269	0.48180848
C46 H56 N4 O2	2.4011755	-0.27577722	-0.0289	-0.11332989
C31 H52 N8 O P2	3.750762	-0.26345047	-0.6762937	0.38439202
AZELAIC ACID (CAS# 123-99-9); (M-H)-	3.355292	0.3459315	0.09011759	-0.7245267
C13 H7 P S3	-1.3836331	-1.7335659	1.1733828	-1.1313701
C11 H17 O20 P3 S4	-2.095481	0.85033286	-1.5406748	-0.86989605
C15 H15 N7 O5	3.5025144	0.63702744	-1.073572	1.466088
C20 H42 O4 S	0.12150717	-0.5220503	-0.8895018	0.6785589
C30 H22 N2	0.614013	-0.4433789	0.56060046	-0.8656523
ISOLEUCINE (CAS# 73-32-5); (M-H)-	3.1071718	1.6138431	-0.6052561	0.8735872
C22 H40 N4 S	-0.64980495	1.013062	-0.5578651	-0.3966015
C9 H11 N O3	3.215127	1.3847541	-0.7273995	0.8029957
C30 H55 N3 O P2 S	1.3959979	2.3241475	-0.2044255	0.5237831
C35 H74 N2 O S2	2.5605974	1.62783	-0.3807263	1.3512824
XANTHINE (CAS# 69-89-6); (M-H)-	1.9014394	3.0741184	-0.6882891	-0.89192086
C21 H40 N6 O2 P6	3.110516	-0.2637014	-1.1113899	-0.94960713
C26 H55 N9 O P6	2.0074594	-0.48704553	0.93161136	-0.37967473
C22 H43 N3 O6 S	3.8643928	0.09919566	0.22983769	0.045584857
C36 H61 N O2 P6	3.1882734	-1.1411538	-0.4117286	-0.7233567
C39 H61 N7 O2 S	2.6770296	-0.8002422	-0.3344834	-1.2005894
C28 H33 N2 O9 P	-5.29E-04	-2.92461	-2.965708	-0.00770903
C37 H33 N S4	2.6781979	-1.5317264	0.67848843	-0.17561162
C4 H4 N3 P	-1.3445768	1.5203315	-2.4798577	-1.2372367
C17 H26 O3	0.08987504	-3.0676463	-2.5466535	0.5521173
C30 H56 S2	1.8445537	-1.5837026	1.6856265	1.5403639
C10 H12 N4 O5	3.4800189	1.0428815	-0.0963768	1.263454
2-METHYLGLUTARIC ACID (CAS# 18069	2.4212155	-0.67692065	0.5115098	0.5680899
C17 H24 N2 O6 P4	-0.53520435	-2.6456735	-3.0863352	0.16705349
3-METHYLADIPIC ACID (CAS# 3058-01-	2.3504992	-1.2541475	0.36524892	-1.1718516
C25 H48 O4	1.434623	-0.44242	-0.7908446	2.1047585
C17 H26 O4	2.4930146	-0.8900513	-1.486722	0.93652093
C17 H26 O5	-0.27160066	-0.19840439	-0.206765	2.3408132
C22 H38 O P2 S	3.6315572	1.8118348	-0.9973564	0.20497274
C26 H43 N O5	2.6748214	-1.8861696	1.0133362	0.7068163
C34 H65 O2 P3	3.286037	0.22739269	-0.3220813	-1.269714
C15 H24 N5 O3 P3	-2.9971611	0.004820951	-1.8370366	-1.2709895
C11 H14 O3	-1.6471661	0.76250225	-0.7105689	-0.16732228
C23 H39 O17 P	2.7684176	2.1083236	-1.4630138	-0.3469332
C13 H20 O4	2.8586535	-0.7912092	-1.1466027	1.2155452
HYODEOXYCHOLATE (CAS# 83-49-8); (	-1.5494032	1.2732561	-0.2161899	-0.2548074
C13 H20 O2	1.5344212	1.3787931	0.8080458	0.80507696
4-ACETAMINOPHEN SULFATE (CAS# 32	0.3415798	-0.4974979	0.25648344	0.42915717
C30 H48 N O2 P3	1.0902323	0.7681915	0.4522329	-1.9691664
C32 H45 N18 O P	1.3929846	-0.58448505	1.9793853	-0.8085704
C36 H25 N2 P S	2.8152518	-1.2642707	1.2941458	-0.48544568
C36 H67 N2 O P	4.0541997	0.60605097	-0.386574	0.16400504
C19 H23 N2 O2 P	3.8746204	0.7064514	-1.0880764	0.17000204
C32 H59 Cl N2 O	1.3136775	0.43004563	0.68084234	0.23311332
C19 H39 Cl S4	2.1308088	-1.579658	1.6131147	0.52305764
C18 H14 N10 O	0.9201748	-3.275366	-2.0141146	0.16272521
C5 H5 Cl N2 S	0.9018183	-1.5395628	2.014718	-0.48979065
C35 H67 Cl2 O3 P	-0.025669038	0.8381995	-0.4008457	-2.149218
URIDINE (CAS# 58-96-8); (M+HCOO)-	3.7365224	1.5239342	-0.6787088	0.8708929
TRICOSANOIC ACID (CAS# 2433-96-7);	2.6751635	-1.6714766	1.3362083	0.5478935
N-ACETYL-D-MANNOSAMINE (CAS# 36	3.248344	-1.3353956	0.8054964	0.052756608
C15 H31 N4 P S2	2.703464	-0.76666826	-1.175348	1.0019526
C22 H26 Cl N4 O5 P	1.400896	-1.4184406	1.4977654	1.2515374
C17 H34 O2	3.2050726	0.42082414	-0.0252709	0.5235112
C26 H28 N6 O P2	3.3374093	2.2165756	0.08636443	0.41230845
C5 H4 N4 O3	1.8022493	2.240119	1.174321	-0.41473886
C25 H52 O4 S	0.84011924	1.076574	-0.5008634	-0.6027467
C31 H27 N17	3.7243497	1.3488594	-0.6513942	0.67290235
C15 H31 N4 O3 P	-1.3450178	-1.5727322	1.1560141	0.41335273
C20 H38 O2	2.4422107	0.2025061	-1.3499655	-2.4753456
C24 H51 N3 O8 S	3.7236645	1.1756392	0.87818205	0.5805901
C44 H82 N O3 P S2	3.3214617	-1.080568	0.3804193	-1.1242318
C22 H44 O2 P6	3.2822382	-1.0892886	-0.767266	-1.5134413
C23 H48 N O9 P	2.8444555	-0.42970142	0.02630283	-2.367151
C23 H40 N6 O2 P6	1.3368186	2.510333	-0.3018737	-0.75886047
JASMONIC ACID [ISTD] (CAS# 77026-92	1.0535125	-3.2185483	-2.4510107	0.11477329
C29 H37 N7 S	1.0361419	-0.9153287	1.3888584	0.55390346
C36 H75 N9 O2 P2	1.5820595	-1.0796993	1.815834	0.1728567
C10 H16 N2 O4	3.3550673	-0.16818358	-0.7309856	1.5240726
HYPOXANTHINE (CAS# 68-94-0); (M-H)	3.1085396	1.9535642	-0.5037402	-0.01347944
3-METHYLGLUTARIC ACID (CAS# 626-51-	2.417884	-0.67130464	0.49806285	0.56681377
5-AMINOPENTANOATE (CAS# 660-88-8	1.7683823	-1.436594	-0.2235268	0.6110972
C17 H20 N10 O12 P4	-0.6105231	-2.7358682	-2.7556934	0.45351645
C30 H41 N7 O2 S	3.0005994	-1.1677026	1.4215126	-1.2378151
C38 H78 N2 P2 S3	3.162371	2.0797198	-1.3565016	-0.03612244
C26 H40 N6 O3	1.0050366	0.572415	1.0857587	-1.4555395
C6 H9 N3 O2	2.2751286	0.154394	-1.0992842	0.7279602
C16 H19 N P2	-1.8254024	-2.6274948	-2.4720228	0.21781468
C38 H76 O4 S	3.1579456	2.173863	-0.64701	1.0262468
C34 H60 N6 O2	2.9794354	0.7352077	-1.0902456	-0.1269998
C39 H33 N9	1.5936887	-0.5000314	1.0152425	-1.2169119
C15 H15 N9 O	1.4131433	-3.2525954	-2.0588763	0.32790542
C22 H17 N6 O5 P	0.74412596	-3.1848395	-2.6250257	0.19542971
C35 H37 N O	2.3782785	-1.7072434	2.0478902	0.3416993
PHYTANATE (CAS# 14721-66-5); (M-H)	1.9175606	0.987123	-1.0337534	0.73545384
C28 H38 N4	1.2737392	-0.94138974	1.0749813	-0.08416167
GLUTARATE (CAS# 110-94-1); (M-H)-	1.0576098	-1.1977632	1.2588191	-0.36957172
C10 H13 N5 O	-0.62487173	-3.1976185	-2.5543847	0.050267518
C9 H2 N2 O5 S	-3.1463764	1.0711012	-0.224963	0.36581355
EPIBRASSINOLIDE [ISTD] (CAS# 78821-	0.3484868	-3.5224726	-2.2494187	0.21597709
C18 H32 O2	3.6804137	1.7975616	-0.9469271	0.15657735
GIBBERELLIC ACID [ISTD] (CAS# 77-06-	1.0299956	-3.2389865	-2.4771023	-0.13392106
C18 H32 O3	3.889784	0.91339254	-0.1826482	-0.45794675
C29 H43 N3 O3 S2	3.5154467	1.4759895	-0.5002921	0.35096526
C11 H9 Cl N8 O	3.5505168	0.9670001	0.38696557	1.4080966
DOCOSAHEXAENOIC ACID (CAS# 6217-	2.5592313	-0.7462171	0.21388996	-1.6084168
C39 H62 N2 O5 S	3.5201828	1.4655677	-0.8895063	0.70564437

C14 H26 N6 O2	3.2132215	0.42719546	-1.0138229	0.10903782
C23 H36 O P4	3.2317898	-0.79571223	-0.8871923	-1.6970004
C36 H65 N5 O	2.2853365	-0.23617163	1.4623986	-2.4744368
C22 H33 N6 O17 P	3.0715067	2.3889	-1.0092317	0.42740887
C34 H25 N5 O3	1.1804094	-3.1331906	-2.4227202	0.003144741
C20 H26 N6 O4	-1.126969	1.5539242	-1.2674664	-0.17923225
HEPTADECANOATE (CAS# 506-12-7); (	3.2045765	0.28038457	-0.0376094	0.4441102
N-ACETYLGALACTOSAMINE (CAS# 1811	3.250162	-1.3362705	0.80851173	0.04778287
C24 H35 N6 O2 P3	3.0552852	-1.0306025	-0.7765322	-1.0195416
C40 H76 N2 O S3	-0.4125009	-0.16345838	-1.0207793	0.6064679
C8 H12 N2 O4	3.752519	-0.17580795	-0.4695178	1.2952743
C18 H26 N10 O2	-2.880111	-0.7002576	-0.2731314	-0.45314258
C16 H34 N14 O6 P6	3.7645063	-1.1653973	-0.7747716	0.5222439
C34 H66 N6 O2	2.703226	2.9047828	-0.9168848	0.06862825
N-ACETYL-DL-SERINE (CAS# 97-14-3); (	1.011768	2.3007717	-0.3506578	0.89052606
C19 H32 N3 O2 P	-2.7910597	0.8498511	-1.5079659	-1.2704952
C38 H67 Cl N2	1.4454114	0.028002558	1.1538473	-0.3537396
C24 H24 N4 O4	2.1449072	-2.5465183	0.04904719	1.4885755
ZEATIN [ISTD] (CAS# 13114-27-7); (M-	-0.7070261	-3.1614103	-2.530493	0.071860254
TRANS-VACCENIC ACID (CAS# 693-72-1	3.4857783	2.1807754	-0.8492428	0.28638774
NERVONIC ACID (CAS# 506-37-6); (M-	0.70920146	-0.12710509	1.3184097	-2.0516567
MALATE (CAS# 97-67-6); (M-H)-	-0.29305986	-0.004870629	-0.9242873	-1.951271
C15 H35 N4 O3 P	3.393397	2.2914374	-0.9240614	0.29374588
C15 H18 N6 P2	1.8733327	-2.8549154	-2.0115771	0.08436553
C31 H60 O S2	0.29793435	-0.28063297	-0.4346634	-0.24531247
C22 H25 N2 O2 P	2.019647	0.26564518	-0.1202649	-1.4368902
EPIBRASSINOLIDE [ISTD] (CAS# 78821-	0.35389483	-3.5076401	-2.241426	0.14225946
C39 H72 Cl O2 P S	3.1540177	1.9459867	-1.2136552	0.002885282
C31 H47 N O13 S2	3.053734	-1.2043117	1.6231987	-0.48404917
C30 H56 N O4 P S2	3.5633154	1.9014916	-0.0642582	0.3852101
CITRULLINE (CAS# 372-75-8); (M-H)-	1.0881143	0.24658853	-0.131769	1.7084477
BEHENIC ACID (CAS# 112-85-6); (M-H)-	2.5631032	-1.3781934	1.0419401	-0.08327133
C23 H33 N2 O7 P	3.810921	1.4464201	-1.0585669	-0.08204883
C10 H8 N3 O9 P	-0.7744913	-1.085178	0.23351867	-0.67195034
N-ACETYL-DL-METHIONINE (CAS# 1115	3.4923983	1.5784589	-0.5217328	-0.14252037
C10 H13 Cl N6 O	0.39319146	-3.3696554	-2.3921242	-0.2069311
C29 H29 P	1.1456442	1.924092	-1.0778965	0.1273764
C19 H32 N6 O2	2.5629773	-0.27124885	-1.5803107	-2.0137234
C25 H25 Cl N O P5	2.3732557	1.1433342	1.3456407	1.6078109
C22 H35 N6 O17 P	2.5044987	2.2469459	-1.6117353	-0.7429372
C27 H30 O12	3.4451106	-1.1697145	-0.6017244	-0.99784636
C24 H40 N2 O17 P2	-2.355788	1.1261809	-0.0084359	1.0366788
C38 H78 N3 O P5	-1.0278767	-0.100243986	-0.9794898	-0.60957026
GLUTAMATE (CAS# 56-86-0); (M-H)-	1.0558084	2.7206454	-0.3959324	0.63265795
C7 H13 N O3 S	3.4941027	1.579117	-0.5210577	-0.15553454
C43 H62 N2 O5 S	2.9537141	-0.9370103	0.21089043	-1.4074259
C20 H39 N19 P2	-0.05497095	0.7161654	-0.4526717	-2.1556659
C38 H64 O10 S	3.9873705	0.9067919	-0.7937706	-0.20358866
C27 H26 N4 O	-2.735599	1.675139	1.5944723	-0.72589177
C13 H33 N4 O3 P	3.142437	1.8219961	-0.8407832	0.3615836
C28 H23 N5	2.237652	2.8258471	-1.3372648	0.7939509
C26 H52 O2	2.4000704	-1.8028888	1.2936096	1.343435
C4 H6 O4	1.6957963	-0.6040092	1.9324672	-1.6415895
C25 H32 N8 O9 P2 S	2.9656048	1.9132712	-0.4682209	0.9602555
ARACHIDONATE (CAS# 506-32-1); (M-	3.5103452	2.037881	-0.6102682	0.08958703
C26 H50 N6 O2	3.5186558	-1.6777227	-0.6060703	0.15916407
C18 H24 N4 O12 P4	-0.43125963	-2.691231	-3.0718436	0.32682103
C26 H29 N6 O3 P	0.8775168	-3.079328	-2.571682	-0.02755521
C27 H39 N5 O	2.0261319	-0.8972181	0.75638115	-0.11342704
C8 H14 Cl N2 P	1.7744062	-1.459752	-0.2003274	-0.512368
C30 H50 N O2 P3	0.08015814	0.72961015	1.7207495	-1.4577396
GLUCARIC ACID (CAS# 87-73-0); (M-H)-	0.5200207	0.030879546	0.5508803	-2.021683
C23 H26 N10	0.7752032	-3.1690254	-2.6118872	-0.00434537
CIS-11-EICOSENOIC ACID (CAS# 5561-9	2.4729605	0.15148935	-1.3990386	-2.4050179
C36 H72 O4 S	1.969538	-1.4736108	0.61876166	-0.43955454
C38 H58 N6 O2	3.3574226	1.2838919	0.55080545	-0.9468158
C43 H65 N2 O2 P S2	3.5934584	1.0462064	0.2913816	-0.5444006
C30 H41 O5 P3 S2	3.2030036	2.3525605	0.07984042	0.38745546
C35 H45 Cl N2 O2 S3	1.7340314	-1.3130643	0.5353998	-0.13210577
C20 H41 N3 O P2	-1.7538737	1.490506	-1.444207	-1.4623573
C29 H37 N11	2.8564794	1.8313237	-0.580267	1.3490508
C18 H13 Cl N10	1.3562565	-3.1343513	-2.428168	-0.13162111
URATE (CAS# 69-93-2); (M-H)-	1.8570256	2.2458544	1.1841558	-0.36600047
C27 H22 N4 O3	3.1870337	1.5044097	-0.3725301	-0.6665264
C18 H23 N3 O9	3.1051803	-1.3670305	-0.7149172	0.23743388
C20 H20 N10 O2	1.3335199	-1.2403293	0.47261685	-0.1417707
C19 H33 N4 O3 P	2.9500613	0.99438375	0.02644087	0.8400047
C14 H33 N6 O9 P	3.776913	1.1894563	-1.0653207	0.28540593
C21 H35 O17 P	1.992326	1.8128818	-0.5514191	0.7566028
C39 H81 N2 O3 P S2	2.4272795	-1.9159529	1.212703	1.1038026
LYSINE (CAS# 56-87-1); (M-H)-	-0.44480175	0.21593088	-0.3377547	-1.2152808
C35 H70 N2 O P2	1.533247	-1.1805806	1.3841664	0.44328988
C9 H19 N4 O4 P	0.8240129	-3.0632627	-2.6610081	-0.01294329
C29 H45 N5 O5	1.3318028	-3.233487	-1.3218683	0.13161083
C16 H26 O2	-1.4170717	0.32425463	-2.418273	1.3424014
C34 H58 N6 O2	3.305373	-0.649624	-1.0563961	-1.481682
C39 H67 N2 O P5	3.230361	0.7406729	-0.3785961	-0.28250632
C38 H65 O2 P3	1.8072417	0.5564941	-1.1477629	0.58814913
C30 H58 N6 O2	3.4427066	1.3169945	-0.5819182	0.31751955
C26 H19 N5	-0.113506585	-0.45812297	1.6487311	0.6524896
4-HYDROXYBENZOATE (CAS# 99-96-7);	3.4332414	0.9294795	-1.107369	0.61429965
C38 H47 N O P2 S	1.5962943	-0.42124072	0.8753678	-1.2554002
C28 H19 N5	2.7393017	-0.5753044	0.9648831	-1.584558
C11 H22 N2 O3	1.5082772	-0.9480542	0.23053315	-1.3755987
C14 H20 O P2 S	0.92912066	-1.4675394	-3.453045	-0.57129645
C36 H67 Cl N2 O	1.3167703	0.058860853	-0.0248264	-0.16614264
C24 H42 N2 O17 P2	2.531666	2.0154157	-1.5275156	-0.4800313
C23 H39 N8 O7 P5 S	-2.1870391	-0.15534881	-0.6261076	1.0110152
C37 H66 Cl N11	2.960626	-1.662077	1.4801121	0.074086666
4-NITROPHENOL (CAS# 100-02-7); (M-	2.6863408	0.36834726	-0.8454549	-0.60157806
OLEIC ACID (CAS# 112-80-1); (M-H)-	3.4857783	2.1807754	-0.8492428	0.28638774
C24 H36 O10 P6	3.8053136	-0.2112391	-0.3327076	1.0917504
C19 H38 N2 O12 P2	3.665621	1.8631806	-0.8522182	0.31066382
C6 H10 O3	3.321935	-1.5232971	0.64488584	0.08708778
C30 H41 N2 O P5	2.934474	-0.6343128	-0.9621878	-1.1174991

C27 H56 N3 O10 P S2	3.744137	1.2006583	0.63613194	0.52533907
C23 H28 N12 O P4	-1.397875	0.06839957	-0.8237338	-0.82394934
C34 H29 Cl N6	0.24794503	-2.9800324	-2.8349285	-0.1726663
C32 H43 N O4	0.8265348	-0.31290063	1.6229365	0.024804726
C40 H69 Cl N2	2.949699	-0.9381982	0.14786811	-1.3960218
C30 H64 N10 S	1.8106192	0.58704513	1.0953165	0.38610685
C17 H44 Cl N9 O7 S	1.4248619	-0.6764475	1.7250029	-0.38339412
CORTISOL (CAS# 50-23-7); (M+HCOO)-	2.8083718	-1.3170288	0.82020277	0.37970603
METHYLMALONATE (CAS# 516-05-2); (	1.6924062	-0.6072041	1.9082522	-1.6490608
4-METHYL-2-OXOPENTANOATE (CAS#	2.2772317	-1.6686109	1.0048051	-0.01570413
16:0 LYSO PC (CAS# 17364-16-8); (M+	3.720935	1.2047147	0.8771271	0.5816772
C17 H36 N2 O12 P2	2.917808	0.53570163	-0.9113178	0.6920412
C33 H41 N11	1.4385625	-1.1882374	0.6305076	-0.56235605
C25 H36 N11 O3 P	3.8493085	0.8562822	-0.3828986	0.83237064
C11 H18 N2 O4	3.4882846	0.8322859	-0.8526957	0.8330169
C44 H69 N2 P S2	2.4518805	-0.56859756	0.12481329	-1.1370538
C20 H22 N2 O12	-0.2139411	-3.174626	-2.7636635	-0.27443376
C15 H30 O2	3.6268063	0.5964856	-1.2320408	-0.73504275
C21 H31 N2 O7 P	3.500039	1.2502675	-0.5202296	0.43726283
C29 H44 N4 O3	0.4356402	-3.540259	-2.215656	0.23365125
C36 H36 N8 O3	-0.67857456	-3.1934252	-1.787334	-0.4554711
C36 H62 N11 P	-0.15384121	1.712839	-1.8168457	-0.7207706
C22 H37 N2 O P5	3.662548	-0.41822425	-0.419759	1.2955526
C35 H62 N8 O8	3.8353417	1.421824	-0.9974214	-0.00610793
C34 H64 N2 O2 S4	2.2934604	0.9647889	1.4531277	0.4219486
C32 H67 O2 P S2	-0.16493669	-0.30219066	-0.6281762	2.3351893
C9 H8 O13 P2	-0.029210508	-1.0530652	2.1118038	2.16383
C28 H51 N3 O8 S	3.4143455	0.8087901	1.0885689	0.9708747
C27 H19 N9 O5	2.8389995	-1.2710112	1.3008685	-0.49604106
CYCLOHEPTANECARBOXYLIC ACID (CAS	3.354122	0.35396582	0.10241167	-0.7309668
C30 H50 O17	-1.3407484	1.5752438	0.66056895	-1.5715399
C11 H19 P3	3.8382132	1.1919614	-0.506254	0.77880716
C26 H40 O19 P2 S	2.150027	-0.42290136	-1.5657879	-1.0747461
C27 H31 N5 O2 P2	2.8533504	-1.4081017	1.3733647	-0.28976858
C25 H44 N11 O5 P	0.30601314	-0.44172177	0.9659904	1.6942871
C24 H48 N6 O3	2.2920825	-0.8049146	0.7563817	-1.385998
C24 H44 O2 P6	-0.25071096	0.346694	-0.9836464	0.12086585
3-(4-HYDROXYPHENYL)LACTATE (CAS#	1.4072857	-0.79816365	2.0515046	-0.9709769
C22 H38 S2	1.1929396	-0.9727392	0.7710807	0.83388615
C26 H34 N6 O P2	2.0062137	-2.9211564	-1.9814581	0.12504248
ELAIDIC ACID (CAS# 112-79-8); (M-H)-	3.4853075	2.181255	-0.8499124	0.28670573
URIDINE (CAS# 58-96-8); (M+Cl)-	3.3365297	-1.2050915	-0.4969089	-0.5648609
C20 H30 O2	3.4544437	0.3845294	0.00848264	-0.19559282
C13 H18 N2 O9	0.32317764	-3.163257	-2.6974545	0.17877713
C24 H38 O19 P2 S	3.2332616	-0.9788161	-0.973169	-1.4533067
C14 H13 N2 O2 P	3.744624	0.6926231	0.02213	1.0420913
MYRISTOLEIC ACID (CAS# 544-64-9); (	2.9965923	-1.777784	0.5724983	-0.25356317
C27 H52 N4 S2	0.5086032	0.19901958	0.36900613	-1.017306
L-[15N]ANTHRANILIC ACID [ISTD] (CAS	3.5304568	-1.0067921	-0.1618104	0.9468733
C17 H31 N4 O3 P	2.0119402	-0.85316396	-1.270138	0.98647875
C18 H37 N2 O14 P3 S	3.8129656	-0.6401682	-0.570877	0.9902754
C28 H52 O4	1.3273978	-0.38201213	0.593805	-0.54844797
C18 H21 N16 O4 P5	-0.15621938	-3.2616286	-2.5882378	-0.38424188
C38 H55 O P5 S	0.9436612	-3.203213	-2.5237868	-0.16146408
C22 H35 N5	2.5291207	0.9824897	0.30885834	-0.5003239
C18 H22 N4 O4	3.7382176	-0.8076307	-0.5619279	0.87970996
GAMMA-LINOLENIC ACID (CAS# 506-2	3.1202831	1.7694794	-0.8594717	0.3190968
C20 H40 N2 O3 S2	2.8458827	2.4974618	-1.195361	-0.31026053
LIGNOCERIC ACID (CAS# 557-59-5); (M	3.1281013	-1.2757708	-0.0665999	0.13826099
C30 H20 N2 O	2.9584286	0.9860613	-0.7342073	0.8934781
C17 H38 N2 P2 S	2.899837	-0.8065266	0.27713037	-1.7889326
C12 H18 O3	1.0346087	-3.2261984	-2.4574854	0.08868465
C9 H17 N O4	2.927373	-1.2620162	1.0732048	0.26108795
C9 H17 N O5	3.9029279	0.94147474	0.06163393	0.42519593
C29 H46 N10	2.1733077	-1.1282051	1.3478607	0.20982209
C42 H65 N2 P S2	2.7399175	-0.40222153	-1.4190392	-1.1493179
C32 H66 N6 O P2	2.3198924	-0.41410887	-1.7635367	-1.4665784
C40 H50 N3 O2 P3	1.2135991	-0.8463165	0.7042227	0.6730786
C36 H70 N2 O8	3.00138	2.6312919	-1.0077205	0.18556583
C26 H25 P	2.8469746	-0.6090919	-1.7110262	-1.7319939
VALINE (CAS# 72-18-4); (M-H)-	1.6221353	-1.5283015	-0.2344909	0.85426784
DIACETYL (CAS# 431-03-8); (M+HCOO)	1.0728003	-1.2081821	1.2886264	-0.34007064
C13 H24 N6 O2	4.014375	-0.47766626	-0.5121292	0.6974336
C13 H28 O6 S2	1.3170798	0.002667881	1.1050031	-0.86449045
C4 H8 O7	1.9709313	1.6455625	-0.0891783	-0.1575925
C13 H16 N2 O4	2.7217765	-0.9972651	0.22087735	-0.51077294
C43 H70 N2 O5 S	2.7645879	2.4489405	-1.3572623	-0.09880573
C19 H32 N2 O8	2.9540904	-1.0556761	0.2040229	-1.1712774
C24 H35 N10 O7 P5	3.7726464	0.26247692	-0.8729744	-0.78716904
C43 H67 O6 P S	3.008521	-1.0161638	0.52532816	-1.4904377
C23 H24 N4 O S	2.0461035	0.057120755	0.9389442	-2.189272
C13 H21 Cl3 N12 O S	0.9025714	-1.1060557	1.2884388	1.3043119
C13 H14 O P2	1.1964587	-0.28104585	0.4303298	-0.11502639
C26 H30 N4 O S	-2.5984142	-0.5882404	0.48689997	0.4880267
C20 H24 N18 O P4	3.6937926	0.6409011	-0.7320008	-0.30600297
C24 H48 O2	3.1284242	-1.2795203	-0.0732811	0.14154175
C28 H52 S2	1.6861176	-0.9837929	0.6728899	-0.04752296
C25 H49 N2 O2 P	0.75877124	0.7509977	0.48217773	-0.09038331
URIDINE (CAS# 58-96-8); (M-H)-	3.7043748	1.3734437	-0.5862576	0.822935
PANTOTHENATE (CAS# 79-83-4); (M-H	3.8960824	0.9699633	0.05286819	0.43844467
C17 H17 N2 O8 P	-0.15944561	-2.9657025	-2.9197302	0.004986145
C26 H40 O13 P2	4.020986	0.6446963	-0.4594034	-0.38639325
C18 H34 S4	3.1298132	-0.8252269	0.9610246	0.14007342
C17 H32 O2	3.1343703	-0.8820045	-1.1497349	-1.4487067
C13 H25 N O3	3.627405	0.59961694	-0.2681073	0.3719542
C9 H14 N2 O23 P4 S	-3.0500169	-0.11992133	0.05639967	0.54633915
C20 H29 N14 O P5	3.9326277	-0.52482986	-0.4441799	0.93881714
C16 H20 N4	-2.364387	0.34294152	-1.8549818	0.5541779
C30 H41 N O4	1.9122039	2.9271753	0.20592889	-0.5007815
C42 H67 N2 P S2	2.6550062	-0.29750416	-0.9622568	-1.2374735
C31 H45 N9 O10	3.2063735	-0.64329076	-0.4265223	-1.6482823
L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (	1.3477833	-1.9355996	-2.0690956	0.4900372
C15 H33 N4 O3 P	3.7262247	1.6347264	-0.9928753	0.002285123
C31 H27 P	1.3865799	-0.39967334	-1.3872584	0.85271627
SUCCINATE (CAS# 110-15-6); (M-H)-	1.6924062	-0.6072041	1.9082522	-1.6490608

C35 H57 N7 O2 S	2.166044	2.646319	-0.2334481	0.80750686
C33 H46 Cl N O4	1.3899344	-0.62234515	1.7227653	0.1162678
C26 H27 N8 O5 P5	-0.34898975	-3.2757163	-2.6090114	-0.09668136
C20 H36 N12 O2 P6	3.761347	1.2564223	-0.5755767	-0.7385696
C30 H54 O3 S2	0.40710163	-3.3111002	-2.510631	0.46154007
4-NITROBENZOIC ACID (CAS# 62-23-7);	-0.76112044	0.17569816	-1.2316654	-0.95360327
C17 H28 O5	2.6279619	-2.045515	-0.2603674	0.9324859
C29 H42 N4	1.6093806	-0.35962647	2.2388897	-0.68087804
RETINOATE (CAS# 302-79-4); (M-H)-	2.888102	0.05045106	-0.830991	0.87015
LAURIC ACID (CAS# 143-07-7); (M-H)-	4.0041285	-0.4135735	-0.3175506	0.7554733
C42 H85 N S2	2.849147	-1.3940029	1.8092462	-0.59553564
C26 H9 Cl N9 O2 P	2.009179	1.4892162	0.8614636	2.1123574
C8 H7 N O4 S	0.7506505	0.32850432	-1.539968	0.071068734
C19 H30 N6 O2	3.0201101	0.15272155	0.80108905	-0.7483052
C27 H26 N11 P5	2.8556392	-1.4279798	0.5798973	0.49137622
C36 H27 N2 O12 P S	-1.0102123	0.5776031	1.6937107	-1.270884
C42 H70 O3 P2 S	2.5218287	-0.9269197	-1.2483149	-1.6443739
ALLANTOIN (CAS# 97-59-6); (M-H)-	-1.3476741	-0.36552447	-0.578112	1.3827324
C7 H6 O2	3.303269	-0.7050364	-0.1017107	-0.04070443
C24 H33 N3 O2	2.880862	-0.24914032	1.6953205	1.5830572
D-GLUCOSE 6-PHOSPHATE (CAS# 56-73	-0.1324199	1.3934877	-0.3662897	-0.37509662
BENZOATE (CAS# 65-85-0); (M-H)-	3.302492	-0.70883787	-0.1030746	-0.02595019
C37 H80 N9 O P	2.645639	-1.0291162	1.0222558	-1.4989352
C11 H14 N6 O S3	2.9478216	1.3134844	-0.5206163	0.6729297
C40 H68 N3 O P S2	1.9900584	0.21843949	-1.232959	-2.1204875
C36 H72 Cl N3	2.8178043	-1.0515115	1.2828598	-1.613889
C32 H54 N8 P4	0.012874499	-3.083403	-2.1849136	0.14103758
C20 H35 N5 O7 P2 S	3.0933573	-1.4809391	-0.6054097	0.37707055
16:0-18:0 PC (CAS# 59403-51-9); (M+C	0.8793972	-0.8280072	0.7234053	0.47779778
5'-METHYLTHIOADENOSINE (CAS# 245	-0.072258145	0.2671495	1.1443529	-1.3572898
OXIDIZED GLUTATHIONE (CAS# 27025-	0.39319712	0.24654393	-0.0077107	-1.5858246
C26 H14 N2	2.5814347	-1.1794778	1.251524	-0.6280947
C13 H13 O28 P3 S	-2.1963925	-0.81147647	0.90342236	1.0730428
C10 H8 N2 O19 P2	0.6617268	-1.4390224	2.2333567	2.0926611
C26 H40 N6 O3 S2	1.5170524	-1.656635	0.403895	2.166733
PALATINOSE (CAS# 343336-76-5); (M+	1.2030311	0.20718269	-2.048124	-0.10045564
C8 H7 Cl2 N5 O4 P2	3.471129	0.9005426	-0.2412712	0.6006947
C7 H9 N4 O6 P3 S2	-3.0067687	1.3385302	-1.9556134	-1.3181726
MALEIC ACID (CAS# 110-16-7); (M-H)-	0.3193927	-0.974259	-1.289231	-0.15185562
C18 H33 Cl O16	1.531208	-1.492887	-1.921602	1.3827794
C3 H8 N O3 P	2.8894982	-0.10325524	1.5872092	1.496835
C23 H43 N O4 P2 S	2.0310097	-1.596253	0.5973399	2.2521033
C21 H36 S2	2.2983196	-0.41140392	0.26352853	-1.8698249
C31 H59 Cl2 N2 O3 P	2.212895	0.4223283	-0.4459548	-1.1103617
C26 H47 N O6 P2 S	1.9098806	-1.5596654	0.36985487	2.2901306
C17 H6 Cl N7 O4 S	1.4920162	0.92551064	1.1520876	1.7478521
C11 H14 O19 P4 S	-3.3285248	0.39501575	-0.5986405	-0.21569437
C42 H72 N3 P S2	1.3537985	0.33666623	1.1618519	-2.6257286
4-HYDROXYBENZALDEHYDE (CAS# 123-	3.302668	-0.711876	-0.1053905	-0.02186269
L-ARGININE (CAS# 74-79-3); (M-H)-	-1.0476792	-1.5281872	-1.6074399	0.39839482
C25 H27 Cl N4 O2	2.5549672	-1.8257923	-0.0206694	0.5181366
C27 H26 N4 O2	1.8298157	2.8684886	-0.6627441	-0.08964872
C38 H71 N O3 S3	0.6291885	0.8403217	0.13142386	-3.1101508
MANNOSE-6-PHOSPHATE (CAS# 3672-1	-0.132302	1.3934075	-0.3658104	-0.37663123
S-ADENOSYL-L-HOMOCYSTEINE (CAS#	1.5168115	-1.0442486	1.366917	-0.7650547
3-HYDROXYKYNURENINE (CAS# 2147-6	1.504455	-1.2740965	-0.3305674	1.0340102
C37 H61 N7 O2 S	2.7259858	2.4297383	-1.5015268	0.08444911
C39 H40 N9 O4 P	1.882082	-3.0170546	-1.9756639	0.30482343
C35 H71 N S2	1.3428503	0.20112535	-0.0094991	-2.623525
GLUCOSE (CAS# 50-99-7); (M+Cl)-	3.164924	-0.229921	0.03973783	1.4717561
GUANOSINE (CAS# 118-00-3); (M-H)-	3.5515058	0.34181023	-0.8906904	1.2708306
C5 H11 N O3 S2	0.28628758	-0.056874283	1.2334517	-0.62604266
D-PSICOSE (CAS# 551-68-8); (M+Cl)-	3.165604	-0.22995208	0.03993404	1.4706981
3-HYDROXYBENZALDEHYDE (CAS# 100-	3.3067212	-0.70639056	-0.0971908	-0.02760124
XANTHOSINE (CAS# 146-80-5); (M-H)-	0.17633402	0.7934376	-1.364512	-3.3020492
C19 H22 N14 O3 S2	3.1339622	-1.4756545	-0.1756385	0.41540086
C6 H13 Cl O6	3.1674469	-0.23469034	0.03703233	1.4648968
C17 H38 N6	2.5344112	0.8084494	-1.5082245	0.62095195
C44 H81 N S	2.900768	-1.612214	1.1365921	-0.07291102
C31 H67 N5 O5 P2	-0.2989675	1.8573904	0.39008418	-0.19688064
C14 H22 N2 O5 S	2.5804298	-0.5941384	1.7588553	1.084046
SUBERIC ACID (CAS# 505-48-6); (M-H)-	3.0261848	0.382388	-0.2635973	0.37378496
NAD (CAS# 53-84-9); (M-H)-	-0.39138484	0.96796125	-0.2503607	-2.8724346
C9 H14 N2 O5	1.7975085	-1.4426324	-0.1664234	-0.3590275
DEOXYCYTIDINE (CAS# 951-77-9); (M-	1.188916	-0.2939325	0.05442749	-1.0466777
C28 H28 N2 O15	2.9510157	-1.3986628	0.53137976	0.37940222
C25 H48 P2 S3	2.3247938	-1.4844211	0.602445	2.1534166
C13 H3 N2 O5 P	1.7319493	-0.72275627	0.33671528	-0.44587737
GUANINE (CAS# 73-40-5); (M-H)-	2.3928475	-0.27256173	-0.2649082	1.4601852
C42 H72 N3 O P S2	2.572225	-1.5213889	1.1190419	0.21384251
C14 H6 Cl2 N O5 P	0.5778755	0.19468552	-0.6995641	0.8455635
C47 H59 N5 O	2.5373995	2.6335516	-0.8986305	0.19965643
C32 H21 N7 O6 P2	3.037782	-0.002919292	1.4736471	1.5605966
16:0-18:0 PC (CAS# 59403-51-9); (M+H	1.5211176	-0.9738661	1.7337496	-0.7173408
STACHYOSE (CAS# 54261-98-2); (M+Cl)	0.46861705	-2.1324854	-2.1060805	1.2364223
C24 H19 N3 O9 P2	2.715528	0.09363114	1.5577846	1.64277
C18 H23 N9 O11 S	2.830196	0.60364234	-1.1480656	0.20669535
CMP (CAS# 63-37-6); (M-H)-	0.59097296	-0.6772405	-0.6042494	1.3785515
C25 H36 N5 O2 P	-1.0893487	0.8430797	-1.4204699	-1.0532203
C18 H27 N3 O2 P2	3.0227275	-1.3786632	-0.1309364	-0.45520276
RIBOFLAVIN (CAS# 83-88-5); (M+HCOC	1.2982999	-0.9421869	1.1718167	0.10554439
C42 H83 N O5	1.5980682	-0.25889128	1.1193529	-2.417091
C8 H15 N O4	2.9452791	-1.3597201	0.8117761	0.6485543
MELIBIOSE (CAS# 585-99-9); (M+Cl)-	1.1954015	0.26085708	-2.0602868	-0.11723737
GLUCOSE 1-PHOSPHATE (CAS# 59-56-3	-0.13232642	1.3934243	-0.3659104	-0.37631124
C42 H79 N5 O	2.4976099	-1.6195542	0.90244037	0.3017726
C29 H18 N8	1.245372	-1.7195059	-0.9097474	0.5692561
PROSTAGLANDIN E2 (CAS# 363-24-6);	2.5404725	-0.6450386	0.1662054	-1.6149349
UROCANATE (CAS# 104-98-3); (M-H)-	2.7544641	-0.45237306	0.43854782	1.7518545
C19 H16 N10 O8 S	0.1646223	-3.284565	-2.6098275	-0.16613382
INOSINE (CAS# 58-63-9); (M+Cl)-	3.7097096	0.7383733	0.37603298	1.0040616
THROMBOXANE B2 (CAS# 54397-85-2);	2.5671792	-0.6394979	0.09924638	-1.6046566
C8 H18 O20 P4 S	0.84274507	-1.4960891	2.2490056	2.0889945
C15 H28 N4 S2	2.2346869	-1.6737754	-0.0027631	2.246348
C35 H74 N9 O4 P	2.289106	-0.33638516	0.78692997	-2.152616

C23 H27 Cl O8 S	2.3408432	-1.4995764	1.1139308	0.67945987
MANDELIC ACID (CAS# 611-71-2); (M-H	2.9105973	-0.069534905	1.5828221	1.5212419
D-TAGATOSE (CAS# 87-81-0); (M+Cl)-	3.164924	-0.229921	0.03973783	1.4717561
C28 H14 N2	0.5287407	1.2791598	0.08091165	0.882109
BETA-MALTOSE (CAS# 69-79-4); (M+Cl	1.1996348	0.19164656	-2.067545	-0.11709042
5'-DEOXYADENOSINE (CAS# 4754-39-6)	0.043592542	0.6642311	-0.4401517	-1.1298872
CELLOBIOSE (CAS# 528-50-7); (M+Cl)-	1.2030311	0.20718269	-2.048124	-0.10045564
C23 H23 Cl N4 O2	2.4580078	-2.3932812	0.01387078	1.6539359
10-HYDROXYDECANOATE (CAS# 1679-5	2.33953	-0.5770947	-0.2286916	-1.24053
N-ACETYLNEURAMINATE (CAS# 131-48	-0.36916006	0.42500594	-1.7654452	-2.5398858
SERINE (CAS# 56-45-1); (M-H)-	0.8544042	-0.4610137	-1.6616898	1.626031
C35 H63 N5	1.0687101	0.5378887	0.42424816	-3.0369456
C11 H19 N3 O3	2.5711653	-1.5721489	0.48825422	1.3171647
C43 H85 N O6	2.1942928	-0.81812596	1.0643836	-1.827763
C8 H12 N2 O5	2.6879933	-0.89904153	0.07236133	2.2864676
C19 H39 Cl2 N4 O3 P3 S2	2.8606632	-1.2030072	-0.8649355	1.520688
C9 H10 O4	1.6239606	-1.0089104	1.4116502	-0.8537499
3'-CMP (CAS# 63-37-6); (M-H)-	0.8500412	-0.9637941	-0.5327459	1.340022
GUANOSINE (CAS# 118-00-3); (M+Cl)-	2.8354647	0.8930408	-0.5942115	1.6418308
C16 H18 N16	3.3883362	0.2865974	-0.8930495	-1.8338095
C22 H32 N4 O	2.6256702	-1.3578961	-0.4438723	0.9071621
C29 H26 N2 P4	1.3532835	-1.1990203	0.28751025	0.5106669
SUCROSE (CAS# 57-50-1); (M+Cl)-	1.1998528	0.1987197	-2.0682755	-0.12256241
C13 H19 N2 P S	1.9305794	-0.43810865	-0.4678042	2.5694778
C12 H15 N O4	2.1966808	-1.4304277	1.7627695	0.6568988
SN-GLYCERO-3-PHOSPHOCHOLINE (CAS	2.001791	1.6315641	0.2327474	0.40196958
ALPHA-D-GALACTOSE 1-PHOSPHATE (C	-0.13273567	1.3936917	-0.3675675	-0.37099844
BETA-MALTOSE (CAS# 69-79-4); (2M+C	0.4818462	-2.1471722	-2.106651	1.243191
C18 H34 N3 O P S4	-0.7401624	1.8098172	-3.0829031	-0.9695611
FUMARATE (CAS# 110-17-8); (M-H)-	0.1436427	-0.8701948	-0.2946073	-0.31395447
C16 H28 N13 O2 P5	2.5607047	-0.015508548	-1.3572712	-0.43193376
C35 H49 N7 O5 S2	0.5945167	-1.3447223	-0.0248941	1.9727967
C46 H93 N O S2	2.389697	-1.3534372	1.7168269	-0.5823402
C17 H33 N4 O4 P	2.86268	-1.2980514	0.7284461	-0.8122922
C14 H14 O22 P4	1.069714	-1.4875733	2.2361188	2.083927
MALTOSE (CAS# 69-79-4); (M+Cl)-	1.1869487	0.24326433	-2.0622153	-0.12503386
C40 H70 N3 O P S2	2.9275682	-1.352004	0.9491575	-0.6451574
C29 H22 N2	3.3962522	-0.29250142	0.13611491	-0.07803583
C6 H6 N2 O2	1.5188842	0.020996675	0.47710136	1.8665577
24:0 SM (D18:1/24:0) (CAS# 60037-60-	2.0056067	-1.3376863	2.2597537	0.34905684
C43 H89 N S2	2.4353676	-1.2204335	1.4122297	-0.8108321
C10 H13 N5 O5	3.5631018	0.5371945	-0.6889082	1.1167479
C24 H43 Cl O21	0.45318556	-2.123685	-2.1470625	1.2107718
C4 H7 N O4	0.18590316	1.2197578	-1.9076208	-0.20770893
ASPARTATE (CAS# 56-84-8); (M-H)-	-0.2757756	1.196712	-1.8715967	-0.46048537
URACIL (CAS# 66-22-8); (M-H)-	1.1179377	0.31749043	-0.8361426	-2.3412936
C37 H75 N S2	2.4013124	-0.32501885	1.3462524	-2.1880343
RIBOFLAVIN (CAS# 83-88-5); (M-H)-	0.87265414	-0.80076516	0.83259034	0.5761025
C24 H47 N7 O2 S2	1.4322913	-1.0825984	0.8249725	-0.07742421
PHENOL (CAS# 108-95-2); (M-H)-	1.1833808	-1.5971897	-0.0201962	1.2980952
METHIONINE (CAS# 63-68-3); (M-H)-	2.004013	1.0315694	-0.8616858	2.133198
GLUTATHIONE (CAS# 27025-41-8); (M-	0.39319712	0.24654393	-0.0077107	-1.5858246
C22 H19 P	0.88399863	-1.2542976	-0.2491695	1.5060735
C11 H13 N3 O5	1.3695567	-1.1761587	-0.7089964	-0.92652273
LEUKOTRIENE B4 (CAS# 71160-24-2); (	1.8554385	-0.47787592	0.09862879	-0.7279676
C42 H85 N O S2	2.311404	-0.52254504	0.8789779	-2.3284354
C17 H32 N6 O4 P2	1.5701796	-0.85554475	-0.6182217	0.35301435
C6 H13 N3 O3	1.1136719	0.27228984	-0.1385082	1.6951576
5-HYDROXYTRYPTOPHAN (CAS# 4350-0	1.9599204	-2.0229533	0.08430594	0.7055303
C21 H33 N3 O3	2.6619682	0.022825774	1.1057949	0.32489675
C35 H73 P S5	2.1952028	-0.36209193	-1.0854447	-1.1751089
GLUCOSE (CAS# 50-99-7); (2M+Cl)-[-H2	1.4529365	-0.20345105	-1.9507797	0.61174786
C34 H57 N4 O4 P	2.6048234	-1.9407119	0.08196321	0.4801459
C28 H25 N3 O P6	1.803575	1.297109	1.6474675	1.484905
C29 H31 N5 P4	2.6999016	-1.608936	0.41619807	0.25708044
FRUCTOSE (CAS# 57-48-7); (M+Cl)-	3.164924	-0.229921	0.03973783	1.4717561
ADENOSINE (CAS# 58-61-7); (M+HCOO	2.0881805	-0.027044212	0.92369044	-1.8591694
C5 H7 N O3	2.504966	0.25354385	-0.2413103	2.346775
C20 H15 O2 P	2.6953595	-1.3565253	-0.4843664	0.6729628
C33 H51 N O2 P2	3.9492872	0.25523645	-0.4409024	0.64041364
C25 H40 N2 O10 S4	-0.6501705	0.61235803	1.5055195	-1.3393428
C39 H84 N9 P	2.1813715	-0.17012165	-0.8543945	-1.1875701
C29 H48 N4 O3	2.0523252	1.4383874	-1.3655884	0.2440758
C33 H59 Cl N2 O6	3.3171768	1.5588627	-1.3228772	0.6696688
C31 H54 S2	2.7730815	-0.07837209	0.50573796	0.06476444
LACTOSE (CAS# 63-42-3); (M+Cl)-	1.1869487	0.24326433	-2.0622153	-0.12503386
C12 H23 Cl O11	1.0988057	0.34876624	-2.0584002	-0.2871719
C8 H3 N2 O9 P S	-2.7242367	1.4561313	-1.9825467	-1.6452816
5-OXOPROLINE (CAS# 4042-36-8); (M-H	3.0551467	0.058065873	-1.3118647	1.635052
PHENYLALANINE (CAS# 63-91-2); (M-H	3.4043505	1.4440855	-0.4579942	0.66773313
BETA-MALTOSE (CAS# 69-79-4); (2M-H	-0.5481323	-2.3340392	-2.3010015	0.39645433
ETHANOLAMINE PHOSPHATE (CAS# 10	-0.3426222	1.3910154	-2.1707752	-1.6757004
C4 H13 N2 O13 P3 S3	-2.2978845	1.3079827	-1.7711545	-1.7726468
C35 H65 Cl O7 S2	0.56788373	0.14125377	-1.2211764	-1.6469743
N-ACETYL-L-ASPARTIC ACID (CAS# 997-	1.8603165	1.4621199	-0.4907503	-0.7146819
RAFFINOSE (CAS# 512-69-6); (M+HCOO	-1.4003133	-0.73741144	-0.9883542	-0.6603539
C9 H11 N O2	3.4079812	1.4349029	-0.4555357	0.6675649
RIBOSE (CAS# 50-69-1); (M+Cl)-	1.3763602	-0.27266714	0.29828027	-0.44776523
D-LYXOSE (CAS# 1114-34-7); (M+Cl)-	1.3755687	-0.24668874	0.25733167	-0.44380304
STACHYOSE (CAS# 54261-98-2); (M-H)-	-0.75008786	-2.2134783	-2.3814507	0.57726896
C38 H66 O3 P2 S	-0.7809248	1.098153	-0.1230399	0.77490896
DEOXYCYTIDINE (CAS# 951-77-9); (M+H	0.37073976	0.59729105	-0.1075587	-0.5259298
C10 H11 N5 O4	2.1271493	2.2596009	-0.5616673	1.2449476
C27 H51 Cl N2 S	1.1768576	1.2875842	1.1015642	0.54164773
2-AMINOETHYL DIHYDROGEN PHOSPHA	-0.18139327	1.2145957	-2.1127045	-1.6194186
INOSINE 5'-PHOSPHATE (CAS# 131-99-	0.67928934	1.6374176	0.06710009	-1.126957
THYMINE (CAS# 65-71-4); (M-H)-	-0.054911718	1.1748505	-0.6560277	-0.96227163
MELIBIOSE (CAS# 585-99-9); (M+HCOO	-0.7172524	-1.317609	0.5270249	0.14474632
SUCROSE (CAS# 57-50-1); (M+HCOO)-	-0.7172524	-1.317609	0.5270249	0.14474632
BETA-MALTOSE (CAS# 69-79-4); (M+H	-0.7172524	-1.317609	0.5270249	0.14474632
MALTOSE (CAS# 69-79-4); (M+HCOO)-	-0.7172524	-1.317609	0.5270249	0.14474632
PALATINOSE (CAS# 343336-76-5); (M+H	-0.7172524	-1.317609	0.5270249	0.14474632
956.9781@0.67696446	3.3467562	-0.18338914	0.02788959	1.031241
196.8179@0.71062976	-1.0891166	1.1773318	-1.192393	1.4622684
840.3183@3.597034	2.1900585	-1.5868474	0.33971322	0.702875

869.2725@3.5984445	1.9544878	-1.0958017	1.0145665	-1.0524405
912.2129@8.460721	0.022381999	-3.1902177	-2.743192	-0.04886967
844.225@8.460042	0.33208287	-3.1830838	-2.722464	-0.11085244
850.2403@8.458829	0.20061556	-3.217857	-2.6983647	-0.18776464
782.2537@8.460257	0.314097	-3.226086	-2.6483195	-0.18052639
940.2718@13.098411	-0.13353845	-2.8784068	-2.9672585	-0.20689401
900.4308@13.097647	0.6348899	-3.050573	-2.7734802	-0.09913378
872.2861@13.0997305	-0.079549775	-2.8991194	-3.004357	0.029607423
968.4186@13.099865	0.31960583	-3.0629203	-2.806227	0.027376845
804.2994@13.099768	0.022713065	-2.968541	-2.9324558	-0.07955468
776.1531@13.099658	0.05594107	-2.9038486	-2.7717671	0.009364307
844.1401@13.100767	-0.30809265	-2.881521	-2.9917853	-0.13439679
810.3161@13.099784	0.12894487	-3.044302	-2.8756657	0.09234719
881.2764@22.30472	1.7081697	-0.9347537	2.3004541	0.47148448
813.2878@22.306946	2.6972022	-0.9471585	2.3230674	-0.5043928
880.3095@22.448568	3.8687725	-0.36277935	-0.6849484	1.1713091
766.091@22.448961	3.8992462	-0.45684874	-0.662634	0.93041027
772.1086@22.449924	3.5893073	-0.5329904	-0.8423203	1.1779503
970.0489@22.452425	2.788281	-1.0421122	-1.0268345	0.7888871
812.3241@22.450232	3.673087	-0.2554665	-0.2248895	1.7439437
834.0804@22.447712	3.6145983	-0.5587164	-0.5966486	1.0538888
932.3407@22.582136	1.2863579	-1.0250132	0.5506903	-0.9986744
796.3649@22.58109	1.5057782	-1.1349977	0.88562137	-0.7711449
798.126@22.58789	3.1536179	-0.7741111	-0.7365749	-1.9058796
792.1075@22.582975	3.6208978	1.7292345	-0.9194347	-0.06844485
928.0811@22.579584	3.6845818	1.5040575	-0.7843307	-0.37809312
860.0948@22.581999	2.998467	-0.89614546	-1.2915319	-1.377798
774.1318@22.694763	2.7791817	-0.39033678	-0.9668403	-1.2904632
834.4263@22.703411	2.2129683	-1.4327569	1.6031697	-0.18877488
766.4387@22.702051	2.1085281	-1.27312	1.5487878	-0.2719502
932.6817@22.702452	1.8781075	-1.0853288	1.4015499	-0.22835481
940.3804@22.708122	2.9425933	-0.98770463	0.78749645	-1.6023927
872.3943@22.709047	2.9914136	-1.0839386	0.7740195	-1.4130586
946.3981@22.709084	3.014352	-1.139599	0.8753128	-1.3340961
878.4136@22.711048	2.3731332	-1.6233315	1.2463243	0.23585723
810.4253@22.712088	2.3583963	-1.5615793	1.3353026	0.18744993
804.4079@22.715647	3.47349	-1.1182656	0.12986079	-1.3147328
970.6544@22.714334	1.4192928	-0.9786811	1.5233617	-0.07830606
976.6711@22.716951	1.8877501	-1.0955116	1.1994429	0.1466023
908.6825@22.715044	2.1714787	-1.373984	1.0885812	0.115117565
854.4134@22.721003	2.378795	-1.7391579	0.72379404	0.63581264
786.4252@22.721195	3.0263436	-1.174768	0.3177324	-1.064764
922.3991@22.722313	2.740062	-0.8007166	0.36412114	-1.315038
780.4092@22.723911	2.7675252	-0.7880381	0.46156397	-1.2943583
848.3947@22.723244	2.3841572	-1.7441365	0.72993016	0.5997146
952.6676@22.725416	1.5197451	-1.2996616	0.43120256	0.7814125
916.3827@22.726923	2.265891	-1.6317544	0.57241577	0.4518843
990.3873@22.72658	1.9642484	-1.6406319	0.19856367	0.801381
984.3693@22.730658	1.9239724	-1.3203887	0.6924207	0.6742404
756.1528@22.731094	3.4958928	2.0394945	-1.0395418	0.42045867
824.1386@22.73434	3.4757178	2.0092516	-1.1562123	0.30932385
818.1219@22.739376	3.3076274	2.150226	-1.13105	0.67949855
886.1106@22.738554	3.0947669	2.4195075	-1.1578096	0.64441526
265.2973@22.820448	-2.1175256	1.2330028	-1.7018793	-1.4064449
809.4521@22.830763	0.52147335	1.8111788	-1.772648	-0.85876703
815.4733@22.83448	1.1375315	1.7663093	-2.0445967	-0.57097083
948.6596@22.84815	3.6547804	1.1375948	-1.0913483	0.36286932
806.412@22.846617	3.6529832	1.4636828	-0.9718871	0.38369888
942.641@22.846617	3.719844	1.0477635	-1.0409267	0.3511852
880.6714@22.84751	3.6665378	0.94151825	-0.9165459	0.35590398
942.3879@22.852045	3.543615	1.7577759	-0.8230587	0.49845922
874.651@22.847902	3.6790617	0.975667	-0.8335142	0.47086823
874.4002@22.849009	3.7285056	1.4106778	-0.8937885	0.36929625
812.683@22.848618	3.2869377	0.74809736	-0.52048	0.35429478
800.3953@22.848757	3.7148638	1.4301634	-0.8510959	0.49299604
868.3824@22.852972	3.6835322	1.4895113	-0.7924866	0.54979837
936.3699@22.860899	3.4301267	1.7918681	-0.5368967	0.8319358
800.1383@22.869429	-1.8675253	0.7767363	0.67918056	0.1519914
868.1262@22.870573	-2.037264	0.961534	0.12069397	-0.74863803
794.1233@22.874426	-2.6270835	0.4559155	0.24194267	0.006973684
862.1093@22.87621	-2.906222	-0.09325349	0.48771444	0.27128127
958.7182@22.927029	2.346265	-1.7653129	0.7497993	0.88085884
790.4564@22.92349	2.8161306	-0.7741961	-0.007119	-1.6276565
858.4442@22.92771	2.3568869	-1.7769363	0.5866462	0.5681067
784.4399@22.926924	3.3720045	-0.8325129	-1.1000233	-1.297993
952.7013@22.91744	4.0362234	0.2811732	-0.6474679	-0.13952363
852.4268@22.929146	3.3540618	-0.8199158	-1.1355582	-1.2623713
926.4317@22.929146	2.9797387	-1.0635537	0.09087907	-1.2430836
890.7308@22.92085	3.2472174	-0.64715457	-1.0848534	-1.1878681
994.4194@22.931183	2.9222827	-1.1055231	-7.48E-04	-1.2351086
920.4147@22.931295	3.4001966	-0.87939256	-0.9799251	-1.368845
988.4018@22.932953	2.8316283	-0.86385137	-0.0699551	-1.5209711
914.4015@22.935183	2.806147	-0.87611556	-0.0946249	-1.3064084
752.1517@22.943537	3.3158817	2.3390594	-0.9962092	0.35687006
894.1401@22.941717	3.0521517	2.5288153	-1.1451137	0.39406285
820.1395@22.945572	3.133228	2.5264304	-1.0399643	0.3767922
888.126@22.948214	2.7707207	2.7009122	-1.1523957	0.5061153
956.1108@22.95032	2.507463	2.9857998	-1.1305554	0.38122195
888.5404@22.979513	2.1442363	-1.456884	0.98871297	0.642161
370.1825@23.004324	0.8889497	-0.8396027	-1.4341081	0.73373854
794.4872@23.182186	2.6916683	2.1960218	-1.4714828	-0.02116007
924.4461@23.183435	2.753267	1.9904519	-1.4154598	-0.32327133
896.1574@23.18372	2.521339	2.3438091	-1.5601429	-0.35591725
930.4617@23.18279	2.4141026	2.2238805	-1.5317132	-0.12363523
992.4333@23.181005	2.7695417	2.0932882	-1.3867326	-0.4573291
788.4697@23.181292	2.634633	1.9908841	-1.6579099	-0.24798226
856.4573@23.18165	2.6968894	1.9386331	-1.6383892	-0.6095155
828.1705@23.183365	2.5410814	2.3783977	-1.5018449	-0.06214237
986.4176@23.184006	2.725815	2.4707625	-1.4620991	-0.15454698
760.1843@23.183365	2.7957447	2.2440722	-1.4027956	-0.11089879
754.167@23.181934	2.4010344	2.4143205	-1.5805255	-0.2655195
816.1365@23.182901	2.7148695	1.1303781	-1.1802164	-0.3705625
822.1552@23.183685	2.5761778	2.5576544	-1.3562704	-0.26250637
958.1287@23.18668	2.3024962	3.0235636	-0.7195814	0.24119014
789.9837@23.188755	1.1122534	2.6309552	-1.9552343	0.29624668

890.14@23.186148	2.7902093	1.961146	-0.9879552	0.004472315
884.1239@23.18904	1.8954018	2.418368	-0.926226	0.23173788
856.5126@23.707132	1.1522595	-1.2308717	0.9794359	0.7981192
788.5303@23.708025	2.273074	-1.7603239	1.5700368	0.7273535
814.546@23.81533	2.3319256	-1.4484825	2.1200793	0.55625105
831.5205@23.83582	2.4581444	-0.485129	2.1485999	-1.6230053
789.9827@24.123894	0.59224045	-0.31622857	1.1041424	-0.22317958
878.5307@24.134247	3.0688303	-1.2804655	1.4014521	-0.70133036
946.519@24.131824	3.00773	-1.3156025	1.4789046	-0.4257806
816.5609@24.13103	3.31842	-0.9773444	-0.3639985	-0.5740688
884.5485@24.132364	3.020685	-1.3174521	1.3977534	-0.5004681
952.5352@24.13251	3.3024411	-0.9589317	-0.4089395	-0.5940883
827.5673@24.247963	1.4633931	-0.8905095	1.7966263	0.8118691
895.5529@24.245691	1.129825	-0.42322895	1.169376	-0.11396335
774.5898@24.286057	2.283948	-1.4918221	2.3875527	0.7227227
845.5383@24.346788	1.3007429	-0.5986912	2.203786	-0.450307
777.5507@24.352367	2.5754905	-0.6715234	1.6003275	-1.8282816
765.5312@24.455208	2.366247	-0.6917526	1.3104503	-1.5895951
963.5438@24.433931	1.1287508	-0.60734487	1.5491254	-0.16408297
895.5547@24.433441	2.8147807	-1.0511441	1.8690193	-1.2613987
827.5687@24.43402	2.7485108	-1.0169368	2.0862148	-1.184893
815.5134@24.467724	2.1343443	-1.5515238	2.024865	0.38546708
889.5122@24.501265	0.96451163	-0.7616128	1.7291541	0.18792276
803.5704@24.495302	2.9822412	-1.2911123	1.5108417	-0.7480018
871.5551@24.4953	2.9892774	-1.3073083	1.4853758	-0.7314601
939.5417@24.50164	3.0128822	-1.2553009	1.4635365	-0.7889416
791.5117@24.541157	2.8590689	-1.2390242	1.8660468	-0.8951534
853.5806@24.555206	2.2327566	-1.3413191	2.5504413	0.22812697
965.5593@24.655502	1.4629476	-1.1911925	0.7832421	0.44708803
897.5714@24.652512	2.2369125	-1.588531	1.6457112	0.63027537
829.5868@24.66468	3.0397377	-1.2764702	1.544624	-0.6273167
811.5692@24.689384	0.8874152	-0.41416025	1.9495542	-0.44064143
817.5255@24.673075	3.2547455	-0.9662762	-5.45E-04	-0.7027806
915.5349@24.771643	2.6612134	-0.9743976	1.5143874	-1.2232575
779.5681@24.801208	3.025343	-0.6865655	-0.592378	-0.9683904
847.5537@24.80091	2.7924054	-1.1469983	1.5103563	-1.2109281
785.5479@24.86617	2.7897086	-0.59834874	-0.3759948	-1.1161748
835.5342@24.885294	2.6807346	-1.1692837	1.9615984	-1.0846547
805.5843@24.927763	3.3049712	-0.9501905	0.0218201	-0.9368829
873.5701@24.92519	2.9465141	-1.1865512	1.6273345	-1.0261061
941.5576@24.924244	2.2106497	-1.5091246	2.215376	0.21200669
811.5413@24.925144	1.0552349	-0.45349148	2.1556537	-0.8859757
991.5681@25.086418	2.5463073	-0.7015948	1.8556511	-1.206982
923.5869@25.089668	2.0791216	-1.4091635	2.4003785	0.20149599
855.5999@25.083378	2.742302	-1.1491451	2.0436087	-0.94922197
775.5523@25.12754	1.8315461	-1.0710876	1.715649	0.16746658
831.5993@25.1719	3.3925152	-1.0381345	0.03732596	-0.5677923
899.5875@25.17249	2.9078712	-1.102896	1.2602537	-0.855505
967.5749@25.17143	2.2546525	-1.5001395	2.200879	0.7487425
751.5512@25.219986	3.2039015	-1.0463139	0.5723022	-0.8332868
819.5442@25.223696	2.8896432	-1.3104205	1.8415899	-1.0819948
769.5533@25.231102	1.99647	-0.23317826	1.0814133	-2.4579492
857.6148@25.444185	1.0486066	-0.9664071	1.4947871	1.1056921
833.6146@25.746096	2.951666	-1.312396	1.6736826	-0.4314981
856.6719@25.828072	2.7140572	-0.81502813	1.8851342	-1.040928
837.2864@22.020664	0.6112384	0.6882253	1.1403053	-0.7741501
769.3001@22.014704	1.2900038	-0.24762452	-0.4014926	-0.4489029
899.2533@22.1221	0.70946264	-0.102511145	1.9583097	-0.5241077
769.2982@22.117897	3.4128485	-0.9102787	-0.1315216	-1.2285619
837.2883@22.120522	2.7529144	-0.9484019	0.9565247	-1.1372707
905.2751@22.121227	3.1543503	-0.9690533	0.2693466	-1.0989394
831.2707@22.120157	1.7545592	-0.42821535	-0.3355152	-0.59087443
793.3004@22.121735	0.76537824	-0.50800335	1.2795419	-0.49828726
763.2823@22.120653	1.8361293	-0.97139454	1.8401845	0.27018422
973.2642@22.120821	1.6131082	-0.5320046	2.0977957	-0.4609074
943.2475@22.245485	0.35282353	-0.4827563	0.22053689	0.007083148
813.2876@22.269299	2.0319698	-0.6440108	1.5862168	-0.5603868
875.258@22.252308	1.133638	0.101075076	1.9292003	-1.0185883
949.2609@22.270824	1.436175	-0.97311115	2.3694448	0.1918931
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539.3414@22.447004	1.9972553	-0.9277863	-0.5110573	0.894877
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946.6513@22.727638	2.3519344	-1.6913424	0.7613589	0.52840537
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758.1685@22.93772	3.4966457	2.0736535	-1.0496345	0.2042259
826.1555@22.940037	3.3623307	2.2709084	-1.0165875	0.26617265
592.4751@23.119793	1.2074602	-0.56532675	1.6840664	-0.15116045
933.7588@23.180662	2.5003383	-0.034522276	-1.6032765	-1.7273438
862.4753@23.181692	2.5113587	1.8275985	-1.346022	-0.14990336
998.4517@23.18197	2.5667963	1.9118931	-1.7749996	-0.35046571
789.9832@23.233425	2.2080767	2.178063	-1.65644	0.83039665
882.5337@23.808203	1.2494435	-0.9015022	2.2247066	0.50256777
950.5183@23.81049	0.73598146	-0.55229694	1.4989758	0.33735016
775.5406@23.993422	1.8758539	-1.1054949	2.3442304	0.32806975
801.5529@24.113777	1.830056	-1.0489786	1.945245	0.6339266
851.5676@24.191595	1.635064	-0.7354381	1.8591878	0.23299515
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913.5176@24.37286	1.1508628	-0.7084743	1.8894682	-0.02618142
933.5284@24.497889	1.8423501	-1.1115621	1.9611728	0.7172562
773.5369@24.573845	2.073523	-1.340006	2.352433	-0.06312627
935.5416@24.914215	1.0285819	-0.4894974	1.3270802	-0.50698495

839.6043@24.974514	0.7283281	-0.30403247	1.3670301	-0.57806575
843.5413@25.124508	1.1668262	-1.199839	1.050261	0.9478682
961.5559@25.16651	0.68871784	-0.17217381	1.6120752	-0.00139126
881.6139@25.22479	0.38558304	-0.34101444	0.08507155	-0.50459707
793.4574@25.23036	2.8708746	-1.1845917	0.25916213	-0.6618521
969.5907@25.74866	2.2552888	-1.4497703	1.9329566	0.107786566
924.65@25.827486	0.5580062	0.028261334	1.4675771	-0.8748904
795.4708@25.864923	1.5155058	-1.0334272	2.2476504	0.71917695
954.0963@22.742481	2.9888196	2.350159	-1.5029973	0.41693407
862.3615@22.861217	2.7874026	1.3539507	0.15748116	0.6619983
930.3513@22.86497	2.1215355	1.2176869	-0.0152411	0.21421528
930.0965@22.88042	-3.228695	0.6066448	0.673212	-0.21245307
961.7809@0.58430463	-2.5256412	1.4464154	-1.2815484	-0.48902854
757.8295@0.5829288	-3.0090978	1.1990908	-1.6572148	-1.4544667
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785.5021@8.227946	2.81243	-0.5312158	-0.5013751	0.65942353
913.5596@8.419434	2.038636	-0.804615	-0.2539244	-0.92881036
896.534@10.775598	2.246083	-0.40485787	-0.0810043	0.85411334
663.4302@22.925947	2.6094558	-0.5772535	0.22271779	-1.6341788
847.5115@23.699986	1.9492834	-0.06460884	1.027059	-2.2534122
757.5168@24.177675	1.3515184	-0.071332924	0.84238005	-2.464288
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783.5687@25.759329	2.487403	-1.0151049	0.7648806	-0.99597365
827.5949@26.126913	1.8077592	-0.46339506	1.7770569	-1.0898242
801.58@26.247076	2.5116851	-1.5409918	0.97820956	0.4653167
797.5844@26.244934	3.0126388	2.2114964	-1.0417974	0.26254725
841.611@26.701244	2.7694674	2.2201946	-0.7987304	-0.15751523
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785.5833@26.954992	2.9385805	-1.621149	0.80106246	0.00804019
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841.7887@0.5935558	-1.3053546	1.5335566	-2.1048706	-1.1856056
745.5704@23.833296	1.4731804	-0.18391214	0.53492785	-1.4716289

Compound	p	p (Corr)	FC ([Healthy] vs [Lesional])	Log FC ([Healthy] vs [Lesional])	FC (abs) ([Healthy] vs [Lesional])	Regulation ([Healthy] vs [Lesional])	FC ([Healthy] vs [Nonlesional])	Log FC ([Healthy] vs [Nonlesional])	FC (abs) ([Healthy] vs [Nonlesional])	Regulation ([Healthy] vs [Nonlesional])	FC ([Lesional] vs [Nonlesional])	Log FC ([Lesional] vs [Nonlesional])	FC (abs) ([Lesional] vs [Nonlesional])	Regulation ([Lesional] vs [Nonlesional])
C32 H47 N O5	0	0	6.0151615	2.5886035	6.0151615	up	-101.709	-6.6683035	101.709	down	-611.79626	-9.256907	611.79626	down
TRANS-ACONITATE (CAS# 4023-65-8); (M-H)-	0	0	-40.634403	-5.34463	40.634403	down	-3731.4768	-11.865531	3731.4768	down	-91.83048	-6.520901	91.83048	down
C3 H10 N8	0	0	-607.7184	-9.247259	607.7184	down	-1.6517838	-0.7240249	1.6517838	down	367.91644	8.523234	367.91644	up
CORTISONE (CAS# 53-06-5); (M+Cl)-	0	0	16.09224	4.008293	16.09224	up	-22.195982	-4.4722266	22.195982	down	-357.18317	-8.48052	357.18317	down
C25 H53 N8 P	0	0	752.5651	9.555673	752.5651	up	2.5488894	1.3498688	2.5488894	up	-295.25217	-8.205804	295.25217	down
C6 H10 N6 O4	0	0	20.724504	4.3732657	20.724504	up	-86.65577	-6.437224	86.65577	down	-1795.898	-10.81049	1795.898	down
C40 H46 O2	0	0	24.019806	4.59E+00	24.019806	up	-16.039324	-4.0035415	16.039324	down	-385.26144	-8.589694	385.26144	down
C31 H46 N4 O	0	0	328.15628	8.358239	328.15628	up	2.0338306	1.0241995	2.0338306	up	-161.34888	-7.3340397	161.34888	down
C28 H44 Cl N10 P S3	0	0	169.85263	7.4081397	169.85263	up	-31.727089	-4.9876432	31.727089	down	-5388.9277	-12.395782	5388.9277	down
CORTISOL (CAS# 50-23-7); (M+Cl)-	0	0	15.776621	3.9797163	15.776621	up	-67.005646	-6.0662107	67.005646	down	-1057.1227	-10.045927	1057.1227	down
C24 H49 Cl N8	0	0	1361.6079	10.411096	1361.6079	up	15.147483	3.9210062	15.147483	up	-89.890045	-6.4900894	89.890045	down
C28 H55 N3 P2 S	0	0	271.41852	8.084375	271.41852	up	2.255019	1.1731396	2.255019	up	-120.36201	-6.9112363	120.36201	down
4-ACETAMINOPHEN SULFATE (CAS# 32113-41-0); (M-H)-	0	0	-98.3999	-6.620585	98.3999	down	46.430477	5.537	46.430477	up	4568.7544	12.157585	4568.7544	up
C32 H59 Cl N2 O	0	0	1199.326	10.228008	1199.326	up	8.959474	3.163414	8.959474	up	-133.86122	-7.0645943	133.86122	down
C39 H33 N9	0	0	63.909866	5.997967	63.909866	up	-74.969574	-6.2282333	74.969574	down	-4791.2954	-12.2262	4791.2954	down
C28 H38 N4	0	0	483.1842	8.9164295	483.1842	up	3.6845436	1.8814859	3.6845436	up	-131.13818	-7.034944	131.13818	down
CITRULLINE (CAS# 372-75-8); (M-H)-	0	0.00E+00	9.98E+03	13.285395	9983.947	up	67.19895	6.070367	67.19895	up	-148.57297	-7.215028	148.57297	down
C20 H20 N10 O2	0	0	1385.2249	10.4359045	1385.2249	up	1.0733435	0.10211182	1.0733435	up	-1290.57	-10.333793	1290.57	down
C38 H47 N O P2 S	0	0	65.65039	6.0367317	65.65039	up	-4.0038333	-2.0013819	4.0038333	down	-262.8532	-8.038114	262.8532	down
C30 H64 N10 S	0	0	1857.4663	10.85912	1857.4663	up	9.356867	3.2260256	9.356867	up	-198.51364	-7.6330943	198.51364	down
C28 H52 O4	0	0	410.80884	8.682323	410.80884	up	91.90448	6.5220633	91.90448	up	-4.4699545	-2.1602602	4.4699545	down
C40 H50 N3 O2 P3	0	0	-1237.6804	-10.273423	1237.6804	down	-724.7176	-9.501275	724.7176	down	1.7078108	0.77214813	1.7078108	up
C25 H49 N2 O2 P	0	0	1404.7128	10.456059	1404.7128	up	2.3544726	1.235404	2.3544726	up	-596.61456	-9.220655	596.61456	down
16:0-18:0 PC (CAS# 59403-51-9); (M+Cl)-	0	0	-697.8128	-9.446696	697.8128	down	1.0051904	0.0074687	1.0051904	up	701.43445	9.4541645	701.43445	up
L-ARGININE (CAS# 74-79-3); (M-H)-	0	0	4314.726	12.075053	4314.726	up	1.2211839	0.2882805	1.2211839	up	-3533.232	-11.786773	3533.232	down
C5 H11 N O3 S2	0	0	222.51262	7.7977433	222.51262	up	-102.17576	-6.674909	102.17576	down	-22735.395	-14.472652	22735.395	down
C9 H14 N2 O5	0	0	6044.9106	12.561505	6044.9106	up	-5.7155433	-2.5148907	5.7155433	down	-34549.95	-15.076396	34549.95	down
DEOXYCYTIDINE (CAS# 951-77-9); (M-H)-	0	0	4.9410067	2.304805	4.9410067	up	-524.29083	-9.034224	524.29083	down	-2590.5242	-11.339028	2590.5242	down
C13 H3 N2 O5 P	0	0	4.80E+01	5.585479	48.01718	up	-268.6656	-8.069668	268.6656	down	-12900.564	-13.655147	12900.564	down
C28 H14 N2	0	0	4030.9119	11.976891	4030.9119	up	26.264454	4.7150397	26.264454	up	-153.47404	-7.261851	153.47404	down
5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+HCOO)-	0	0	-1420.9368	-10.472627	1420.9368	down	2.2864847	1.1931312	2.2864847	up	3248.9507	11.665758	3248.9507	up
RIBOFLAVIN (CAS# 83-88-5); (M-H)-	0	0	70.943665	6.148602	70.943665	up	-5.2962356	-2.4049673	5.2962356	down	-375.7345	-8.55357	375.7345	down
C11 H13 N3 O5	0	0	2836.701	11.469998	2836.701	up	-2.4566298	-1.2966805	2.4566298	down	-6968.724	-12.766679	6968.724	down
C6 H13 N3 O3	0	0	10496.448	13.357614	10496.448	up	69.7124	6.1233435	69.7124	up	-150.56787	-7.23427	150.56787	down
RAFFINOSE (CAS# 512-69-6); (M+HCOO)-	0	0	196.22076	7.616334	196.22076	up	20.121296	4.3306513	20.121296	up	-9.751894	-3.2856824	9.751894	down
INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M-H)-	0.00E+00	0	-200.24379	-7.6456137	200.24379	down	3.3007457	1.722792	3.3007457	up	660.9537	9.368405	660.9537	up
THYMINE (CAS# 65-71-4); (M-H)-	0	0	-186.24103	-7.541027	186.24103	down	3.9313722	1.9750329	3.9313722	up	732.1827	9.51606	732.1827	up
MELIBIOSE (CAS# 585-99-9); (M+HCOO)-	0	0	-76.41781	-6.255837	76.41781	down	21.05834	4.39632	21.05834	up	1609.2322	10.652157	1609.2322	up
SUCROSE (CAS# 57-50-1); (M+HCOO)-	0	0	-76.41781	-6.255837	76.41781	down	21.05834	4.39632	21.05834	up	1609.2322	10.652157	1609.2322	up
BETA-MALTOSE (CAS# 69-79-4); (M+HCOO)-	0	0	-76.41781	-6.255837	76.41781	down	21.05834	4.39632	21.05834	up	1609.2322	10.652157	1609.2322	up
MALTOSE (CAS# 69-79-4); (M+HCOO)-	0	0	-76.41781	-6.255837	76.41781	down	21.05834	4.39632	21.05834	up	1609.2322	10.652157	1609.2322	up
PALATINOSE (CAS# 343336-76-5); (M+HCOO)-	0	0	-76.41781	-6.255837	76.41781	down	21.05834	4.39632	21.05834	up	1609.2322	10.652157	1609.2322	up
869.2725@3.5984445	0	0	1292.4371	10.335878	1292.4371	up	-7.8322153	-2.9694204	7.8322153	down	-10122.639	-13.305298	10122.639	down
789.9827@24.123894	0.00E+00	0	25.66566	4.6817675	25.66566	up	-27.966011	-4.8056026	27.966011	down	-717.76636	-9.4873705	717.76636	down
895.5529@24.245691	0	0	7.057112	2.819078	7.057112	up	-139.88445	-7.128092	139.88445	down	-987.1806	-9.94717	987.1806	down
811.5692@24.689384	0	0	111.66578	6.8030434	111.66578	up	-8.798099	-3.1371918	8.798099	down	-982.4466	-9.940235	982.4466	down
811.5413@24.925144	0	0	1461.788	10.513518	1461.788	up	-1.5356513	-0.6188507	1.5356513	down	-2244.7966	-11.132369	2244.7966	down
899.2533@22.1221	0	0	216.52953	7.75842	216.52953	up	2.8784258	1.52528	2.8784258	up	-75.22498	-6.23314	75.22498	down
907.2904@22.43314	0	0	-182.8187	-7.51427	182.8187	down	-14.052855	-3.8127913	14.052855	down	13.009363	3.7014785	13.009363	up
754.1354@22.516384	0	0	751.34534	9.553332	751.34534	up	2.9099622	1.5410004	2.9099622	up	-258.19763	-8.012332	258.19763	down
950.5183@23.81049	0	0	21.94982	4.456137	21.94982	up	-20.267328	-4.341084	20.267328	down	-444.8642	-8.797221	444.8642	down
910.5611@24.28466	0	0	189.93138	7.5693345	189.93138	up	-4.8240633	-2.270249	4.8240633	down	-916.241	-9.839583	916.241	down
935.5416@24.914215	0	0	4.970205	2.3133054	4.970205	up	-115.381714	-6.8502707	115.381714	down	-573.47076	-9.163576	573.47076	down
839.6043@24.974514	0	0	81.30709	6.3453093	81.30709	up	-7.881576	-2.9784842	7.881576	down	-640.828	-9.323793	640.828	down
961.5559@25.16651	0	0	87.6141	6.453091	87.6141	up	-6.804868	-2.7665672	6.804868	down	-596.2022	-9.219658	596.2022	down
881.6139@25.22479	0	0	4.3001857	2.10E+00	4.3001857	up	-162.23013	-7.341898	162.23013	down	-697.61957	-9.446297	697.61957	down
924.65@25.827486	0	0	704.42365	9.4602995	704.42365	up	-6.8642693	-2.7791061	6.8642693	down	-4835.3535	-12.239406	4835.3535	down
789.9816@24.124975	0.00E+00	0	4.4986563	2.1694942	4.4986563	up	-153.73245	-7.264278	153.73245	down	-691.5895	-9.433772	691.5895	down
830.6569@25.71992	0	0	148.28773	7.2122555	148.28773	up	-6.3605194	-2.6691446	6.3605194	down	-943.1871	-9.8814	943.1871	down
745.5704@23.833296	0	0	-684.1071	-9.418078	684.1071	down	-5.513754	-2.4630349	5.513754	down	124.07286	6.955044	124.07286	up
C8 H12 O18 P2 S3	1.31E-04	0.03453444	-1.892657	-0.920413	1.892657	down	1.4359629	0.52201843	1.4359629	up	2.7177851	1.4424314	2.7177851	up
HEXACOSANOIC ACID (CAS# 506-46-7); (M-H)-	2.33E-04	0.03453444	5.1831627	2.37E+00	5.1831627	up	-5.4293256	-2.440773	5.4293256	down	-28.141079	-4.8146057	28.141079	down
C7 H18 N2 O15 P4 S4	2.22E-04	0.03453444	-1.9629396	-0.9730158	1.9629396	down	1.4015306	0.48700333	1.4015306	up	2.75112	1.4600191	2.75112	up
C13 H23 N2 O P S	2.58E-04	0.03453444	432.60043	8.756891	432.60043	up	-1.2178127	-0.28429222	1.2178127	down	-526.8263	-9.041183	526.8263	down
C30 H56 S2	3.10E-04	0.03453444	14.539176	3.8618736	14.539176	up	-1.303434	-0.38231754	1.303434	down	-18.950857	-4.244191	18.950857	down
C26 H52 O2	2.05E-04	0.03453444	5.19E+00	2.3764553	5.1925936	up	-5.547017	-2.471712	5.547017	down	-28.803404	-4.8481674	28.803404	down
C39 H81 N2 O3 P S2	1.13E-04	0.03453444	-2.177453	-1.1226416	2.177453	down	-6.062491	-2.5999107	6.062491	down	-2.784212	-1.4772692	2.784212	down
C27 H26 N11 P5	2.91E-04	0.03453444	2.323109	1.2160568	2.323109	up	-88.26689	-6.4638004	88.26689	down	-205.0536	-7.6798573	205.0536	down
C8 H15 N O4	3.34E-04	0.03453444	-4.0555525	-2.0198984	4.0555525	down	-131.21115	-7.0357466	131.21115	down	-32.353462	-5.015848	32.353462	down
C8 H3 N2 O9 P S	1.81E-04	0.03453444	-1.9203776	-0.94139004	1.9203776	down	1.3247917	0.40576553	1.3247917	up	2.5441003	1.3471556	2.5441003	up
C4 H13 N2 O13 P3 S3	1.30E-04	0.03453444	-12.910292	-3.6904497	12.910292	down	-3.1517534	-1.6561546	3.1517534	down	4.0962253	2.034295	4.0962253	up
C12 H12 N8 O4	0.002211596	0.043720596	32.252823	5.01E+00	32.252823	up	3.9098015	1.9670954	3.9098015	up	-8.249223	-3.044258	8.249223	down
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M-H)-	0.001489234	0.043720596	2.1775393	1.1226988	2.1775393	up	1.89471	0.92197704	1.89471	up	-1.1492732	-0.20072174	1.1492732	down
C13 H16 N4 O5 S	0.002325022	0.043720596	1.2594186	0.33275795	1.2594186	up	1.2075518	0.2720852	1.2075518	up	-1.042952	-0.06067276	1.042952	down
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Cl)-	0.002494189	0.043720596	1.3893224	0.47438145	1.3893224	up	1.2868568	0.36385155	1.2868568	up	-1.0796247	-0.1105299	1.0796247	down
C37 H64 O3 P6	0.003736337	0.043720596	2.6913152	1.4283113	2.6913152	up	2.529874	1.3390656	2.529874	up	-1.0638139	-0.089245796	1.0638139	down
C19 H14 N10 O2	0.002487422	0.043720596	1.3614614	0.4451561	1.3614614	up	1.3133899	0.3932953	1.3133899	up	-1.0366011	-0.05186081	1.0366011	down
C14 H16 N2 O4	0.001778892	0.043720596	-1.0112401	-0.016125679	1.0112401	down	1.0271906	0.03870392	1.0271906	up	1.0387365	0.054829597	1.0387365	up
C33 H66 Cl2 O P4	0.003765043	0.043720596	2.445012	1.2898417	2.445012	up	1.9450631	0.95981693	1.9450631	up	-1.2570349	-0.33002472	1.2570349	down
C26 H37 N15	0.001888517	0.043720596	1.4148878	0.5006876	1.41E+00	up	1.2701478	0.34499645	1.2701478	up	-1.1139551	-0.15569115	1.1139551	down
C30 H24 N4 O4	0.003497948	0.043720596	1.5023949	5.87E-01	1.5023949	up	1.1806053	0.23952675	1.1806053	up	-1.2725632	-0.3477373	1.2725632	down
C38 H41 N10 P	0.003085356	0.043720596	2.4009354	1.2635965	2.4009354	up	1.8524098	0.88940334	1.8524098	up	-1.2961146	-0.3741932	1.2961146	down
C24 H17 N8 O2 P	0.002307482	0.043720596	1.417672	0.5035238	1.417672	up	1.299651	0.37812424	1.299651	up	-1.0908098	-0.12539959	1.0908098	down
C24 H28 N12 O12 S	0.003690786	0.043720596	1.5227438	6.07E-01	1.5227438	up	1.5885718	0.66773033	1.5885718	up	1.0432298	0.06105709	1.0432298	up
C30 H46 N4 O5	0.002259662	0.043720596	1.463516	0.5494385	1.463516	up	1.3559325	0.43928528	1.3559325	up	-1.0793428	-0.1101532	1.0793428	down
C30 H46 N4 O4	0.001792177	0.043720596	1.4216088	0.5075245	1.4216088	up	1.3151119	0.39518547	1.3151119	up	-1.0809793	-0.11233902	1.0809793	down
C20 H18 N4 O2	0.00198532	0.043720596	1.4333549	0.5193958	1.43E+00	up	1.3328449	0.41450882	1.3328449	up	-1.0754101	-0.10488701	1.0754101	down
C25 H50 O2	0.002216264	0.043720596	5.558032	2.474574	5.558032	up	-7.2537427	-2.8587255	7.2537427	down	-40.316532	-5.3332996	40.316532	down
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M-H)-	0.001969731	0.043720596	1.426072	0.5120468	1.426072	up	1.2988025	0.377182	1.2988025	up	-1.0979899	-0.1348648	1.0979899	down
N-ACETYL-D-GLUCOSAMINE (CAS# 7512-17-6); (M+Cl)-	0.003100195	0.043720596	-2.2717133	-1.1837807	2.2717133	down	-11.098347	-3.4722729	11.098347	down	-4.8854527	-2.2884922	4.8854527	down
C41 H79 N3 O2 S3	0.002683818	0.043720596	17.342964	4.1162786	17.342964	up	-2.0811357	-1.0573711	2.0811357	down	-36.093067	-5.17365	36.093067	down
C29 H45 Cl N4 O2	0.001511285	0.043720596	1.4887371	0.57408905	1.4887371	up	1.3707719	0.45498848	1.3707719	up	-1.0860575	-0.11910057	1.0860575	down
C20 H20 N4 O2	0.001913915	0.043720596	1.4289123	0.5149174	1.4289123	up	1.3682723	0.45235538	1.3682723	up	-1.0443187	-0.06256199	1.0443187	down
C30 H44 N4 O4	0.003675936	0.043720596	1.4300349	0.51605034	1.4300349	up	1.3245605	0.40551376	1.3245605	up	-1.0796297	-0.110536575	1.0796297	down
C19 H21 Cl N2 O10	0.003571315	0.043720596	1.3035012	0.38239193	1.3035012	up	1.2901906	0.36758423	1.2901906	up	-1.0103167	-0.014807701	1.0103167	down
C9 H13 O12 P3 S2	0.001871106	0.043720596	-1.5301936	-0.6137142	1.5301936	down	1.1637487	0.21877956	1.1637487	up	1.7807609	0.8324938	1.7807609	up
C12 H14 O4	0.003106083	0.043720596	3.1366472	1.6492233	3.1366472	up	2.0454743	1.0324354	2.0454743	up	-1.5334572	-0.6167879	1.5334572	down
N-ACETYL-D-MANNOSAMINE (CAS# 3615-17-6); (M+Cl)-	0.003169564	0.043720596	-2.2794013	-1.1886549	2.2794013	down	-11.110363	-3.473834	11.110363	down	-4.874246	-2.2851791	4.874246	down
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (2M-H)-	0.002934762	0.043720596	2.1935556	1.1332712	2.1935556	up	1.7802818	0.83210564	1.7802818	up	-1.2321395	-0.30116558	1.2321395	down

C17 H20 N10 O12 P4	0.003105738	0.043720596	1.1644766	0.21968174	1.1644766	up	1.179104	0.23769093	1.179104	up	1.0125612	0.018009186	1.0125612	up
C15 H15 N9 O	0.002140158	0.043720596	1.4677216	0.5535784	1.4677216	up	1.2524258	0.32472515	1.2524258	up	-1.171903	-0.22885323	1.171903	down
C22 H17 N6 O5 P	0.002475691	0.043720596	1.367915	0.45197868	1.367915	up	1.2658144	0.34006596	1.2658144	up	-1.08066	-0.11191273	1.08066	down
EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (M+HCOO)-	0.001793256	0.043720596	1.4215956	0.50751114	1.4215956	up	1.3150927	0.3951645	1.3150927	up	-1.0809851	-0.11234665	1.0809851	down
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M-H)-	0.00195093	0.043720596	1.4352207	0.52127266	1.4352207	up	1.3358985	0.41781044	1.3358985	up	-1.0743486	-0.10346222	1.0743486	down
N-ACETYLGALACTOSAMINE (CAS# 1811-31-0); (M+Cl)-	0.003196951	0.043720596	-2.2835908	-1.1913042	2.2835908	down	-11.127444	-3.4760504	11.127444	down	-4.8727837	-2.2847462	4.8727837	down
C24 H24 N4 O4	0.00271407	0.043720596	1.25E+00	0.32394028	1.2517446	up	1.0022553	0.003250122	1.0022553	up	-1.2489278	-0.32069016	1.2489278	down
C15 H18 N6 P2	2.40E-03	0.043720596	1.211943	0.27732182	1.211943	up	1.1319791	0.17884731	1.1319791	up	-1.0706408	-0.0984745	1.0706408	down
EPIBRASSINOLIDE [ISTD] (CAS# 78821-43-9); (M+Cl)-	0.001535118	0.043720596	1.4933105	0.5785141	1.4933105	up	1.3747592	0.45917892	1.3747592	up	-1.0862342	-0.119335175	1.0862342	down
C10 H13 Cl N6 O	0.00236889	0.043720596	1.3362465	0.4181862	1.3362465	up	1.2842038	0.36087418	1.2842038	up	-1.0405253	-0.05731201	1.0405253	down
C26 H50 N6 O2	0.003263773	0.043720596	1.042349	0.059838295	1.042349	up	-3.582591	-1.8410034	3.582591	down	-3.7343102	-1.9008417	3.7343102	down
C23 H26 N10	0.002923816	0.043720596	1.9552897	0.96738243	1.9552897	up	1.7499456	0.8073101	1.7499456	up	-1.1173432	-0.16007233	1.1173432	down
C18 H13 Cl N10	0.001458273	0.043720596	1.409781	0.495471	1.409781	up	1.286594	0.36355686	1.286594	up	-1.0957465	-0.13191414	1.0957465	down
C9 H19 N4 O4 P	3.49E-03	0.043720596	1.3068496	0.38609314	1.3068496	up	1.2524813	0.32478905	1.2524813	up	-1.0434085	-0.061304092	1.0434085	down
C6 H10 O3	0.002684098	0.043720596	1.0970178	0.13358688	1.0970178	up	-13.323462	-3.735897	13.323462	down	-14.616075	-3.869484	14.616075	down
C34 H29 Cl N6	0.003549906	0.043720596	1.537127	0.6202364	1.537127	up	1.5362941	0.6194544	1.5362941	up	-1.0005422	-7.82E-04	1.0005422	down
C29 H44 N4 O3	0.001303842	0.043720596	1.4619148	0.5478592	1.4619148	up	1.3426979	0.42513466	1.3426979	up	-1.0887891	-0.12272453	1.0887891	down
C30 H50 O17	0.003302497	4.37E-02	-5.220302	-2.3841333	5.220302	down	-2.3947885	-1.2598982	2.3947885	down	2.1798594	1.1242352	2.1798594	up
C26 H34 N6 O P2	0.003259051	0.043720596	1.7522734	0.80922794	1.7522734	up	1.3760393	0.4605217	1.3760393	up	-1.2734182	-0.34870625	1.2734182	down
C38 H55 O P5 S	0.002109765	0.043720596	2.2232127	1.1526461	2.2232127	up	1.982698	0.9874649	1.982698	up	-1.1213069	-0.16518116	1.1213069	down
LIGNOCERIC ACID (CAS# 557-59-5); (M-H)-	0.003620581	0.043720596	6.6391826	2.7310057	6.6391826	up	-8.241286	-3.0428696	8.241286	down	-54.71541	-5.773875	54.71541	down
C12 H18 O3	0.001945627	0.043720596	1.4243855	0.51033974	1.4243855	up	1.2972339	0.3754387	1.2972339	up	-1.0980175	-0.13490105	1.0980175	down
C9 H17 N O4	9.26E-04	0.043720596	-1.4631774	-0.5491047	1.4631774	down	-24.435804	-4.6109247	24.435804	down	-16.700508	-4.06182	16.700508	down
C24 H48 O2	0.003672949	0.043720596	6.60276	2.7230692	6.60276	up	-8.188266	-3.033558	8.188266	down	-54.06515	-5.756627	54.06515	down
C30 H54 O3 S2	6.63E-04	0.043720596	1.4735292	0.5592756	1.4735292	up	1.3519809	0.4350748	1.3519809	up	-1.0899038	-0.12420082	1.0899038	down
C7 H9 N4 O6 P3 S2	5.89E-04	0.043720596	-1.6916459	-0.7584276	1.6916459	down	1.252887	0.32525635	1.252887	up	2.1194413	1.083684	2.1194413	up
C23 H43 N O4 P2 S	0.003449571	0.043720596	2.783075	1.4766798	2.783075	up	-1.2603898	-0.33386993	1.2603898	down	-3.5077593	-1.8105497	3.5077593	down
C39 H40 N9 O4 P	0.002764458	0.043720596	2.4595757	1.2984095	2.4595757	up	1.5783547	0.6584215	1.5783547	up	-1.5583161	-0.63998795	1.5583161	down
GLUCOSE (CAS# 50-99-7); (M+Cl)-	0.003296553	0.043720596	3.2809014	1.7140923	3.2809014	up	-1.2900916	-0.3674736	1.2900916	down	-4.2326636	-2.0815659	4.2326636	down
D-PSICOSE (CAS# 551-68-8); (M+Cl)-	0.003301379	0.043720596	3.2809014	1.7140923	3.2809014	up	-1.2900507	-0.36742783	1.2900507	down	-4.232529	-2.08152	4.232529	down
C6 H13 Cl O6	0.003242508	0.043720596	3.2962577	1.720829	3.2962577	up	-1.29038	-0.36779594	1.29038	down	-4.2534246	-2.088625	4.2534246	down
C28 H28 N2 O15	6.44E-04	0.043720596	4.8455453	2.28E+00	4.8455453	up	-171.62021	-7.4230757	171.62021	down	-831.5935	-9.699735	831.5935	down
C25 H48 P2 S3	0.002629078	0.043720596	2.7910192	1.480792	2.7910192	up	-1.3938658	-0.47909164	1.3938658	down	-3.8903062	-1.9598837	3.8903062	down
C19 H16 N10 O8 S	0.003308749	0.043720596	1.2939247	0.3717537	1.2939247	up	1.2652665	0.3394413	1.2652665	up	-1.02265	-0.032312393	1.02265	down
C23 H27 Cl O8 S	0.00136037	0.043720596	8.15663	3.0279732	8.15663	up	-84.92112	-6.4080515	84.92112	down	-692.67017	-9.436025	692.67017	down
D-TAGATOSE (CAS# 87-81-0); (M+Cl)-	0.003296553	0.043720596	3.2809014	1.7140923	3.2809014	up	-1.2900916	-0.3674736	1.2900916	down	-4.2326636	-2.0815659	4.2326636	down
C23 H23 Cl N4 O2	4.68E-04	0.043720596	1.3906152	0.47572327	1.3906152	up	1.016041	0.022958755	1.016041	up	-1.3686604	-0.4527645	1.3686604	down
C11 H19 N3 O3	0.001523063	0.043720596	14.22387	3.8302422	14.22387	up	-1.0940399	-0.12966537	1.0940399	down	-15.561481	-3.9599075	15.561481	down
C22 H32 N4 O	0.002704005	0.043720596	-2.6089282	-1.3834572	2.6089282	down	-4.7787075	-2.2566204	4.7787075	down	-1.8316746	-0.8731632	1.8316746	down
C12 H15 N O4	0.002041055	0.043720596	11.526131	3.5268364	11.526131	up	-20.687637	-4.370697	20.687637	down	-238.44843	-7.8975334	238.44843	down
C14 H14 O22 P4	0.001952226	0.043720596	1.9399897	0.95604897	1.9399897	up	-1.2510067	-0.3230896	1.2510067	down	-2.4269402	-1.2791386	2.4269402	down
FRUCTOSE (CAS# 57-48-7); (M+Cl)-	0.003296553	0.043720596	3.2809014	1.7140923	3.2809014	up	-1.2900916	-0.3674736	1.2900916	down	-4.2326636	-2.0815659	4.2326636	down
912.2129@8.460721	0.003673614	0.043720596	1.8065094	0.8532047	1.8065094	up	1.830578	0.8722992	1.830578	up	1.0133233	0.019094467	1.0133233	up
844.225@8.460042	0.003069896	0.043720596	2.0805664	1.0569763	2.0805664	up	2.011349	1.0081635	2.011349	up	-1.0344135	-0.048812866	1.0344135	down
782.2537@8.460257	0.003626898	0.043720596	1.9310604	0.9493933	1.9310604	up	1.8985088	0.9248667	1.8985088	up	-1.0171459	-0.024526596	1.0171459	down
900.4308@13.097647	0.002770544	0.043720596	2.4495888	1.2925396	2.4495888	up	2.3109646	1.2084951	2.3109646	up	-1.0599854	-0.08404446	1.0599854	down
968.4186@13.099865	0.002947956	0.043720596	2.3739204	1.2472715	2.3739204	up	2.3094985	1.2075796	2.3094985	up	-1.0278943	-0.039691925	1.0278943	down
776.1531@13.099658	0.002939009	0.043720596	1.5744107	0.65481186	1.5744107	up	1.6236984	0.6992836	1.6236984	up	1.0313054	0.04447174	1.0313054	up
810.3161@13.099784	0.003070931	0.043720596	2.301461	1.2025499	2.301461	up	2.2729673	1.184577	2.2729673	up	-1.0125358	-0.017972946	1.0125358	down
827.5673@24.247963	0.002922999	0.043720596	185.63145	7.54E+00	185.63145	up	-2.109601	-1.0769701	2.109601	down	-391.6084	-8.613268	391.6084	down
774.5898@24.286057	0.002491812	0.043720596	2.1162844	1.0815334	2.1162844	up	-1.6167837	-0.6931267	1.6167837	down	-3.4215739	-1.7746601	3.4215739	down
967.5749@25.17143	0.001248663	0.043720596	2.1025271	1.0721245	2.1025271	up	-1.8875644	-0.91652584	1.8875644	down	-3.9686553	-1.9886503	3.9686553	down
857.6148@25.444185	9.73E-04	0.043720596	38.497406	5.2666893	38.497406	up	-7.5810394	-2.9223957	7.5810394	down	-291.85034	-8.189085	291.85034	down
807.2674@22.275352	6.68E-04	0.043720596	-1.9080013	-0.93206215	1.9080013	down	-1.2196592	-0.28647804	1.2196592	down	1.5643725	0.6455841	1.5643725	up
807.2695@22.306526	0.001455615	0.043720596	-1.8390754	-0.87898064	1.8390754	down	-4.783059	-2.2579336	4.783059	down	-2.6007955	-1.378953	2.6007955	down
757.8295@0.5829288	5.06E-04	0.043720596	-2.3773077	-1.25E+00	2.3773077	down	1.4154041	0.501214	1.4154041	up	3.364851	1.7505426	3.364851	up
893.8083@0.5906194	0.003689032	0.043720596	-8.798628	-3.1372786	8.798628	down	1.2665803	0.34093857	1.2665803	up	11.144169	3.4782171	11.144169	up
825.8165@0.5850002	0.001390864	0.043720596	-2.017585	-1.0126295	2.017585	down	1.507056	0.591733	1.507056	up	3.0406137	1.6043625	3.0406137	up
841.7887@0.5935558	0.002608982	0.043720596	-56.440163	-5.8186502	56.440163	down	1.4118886	0.4976263	1.4118886	up	79.687225	6.3162766	79.687225	up
C41 H54 O6 P2 S	0.003928671	0.044948332	2.0660033	1.0468426	2.0660033	up	2.099859	1.0702925	2.099859	up	1.0163871	0.023449898	1.0163871	up
C17 H24 N2 O6 P4	0.004013365	0.044948332	1.1624594	0.21718025	1.1624594	up	1.2042979	0.2681923	1.2042979	up	1.0359914	0.05101204	1.0359914	up
C29 H45 N5 O5	0.003976297	0.044948332	1.3081945	0.38757706	1.3081945	up	1.2032483	0.2669344	1.2032483	up	-1.0872191	-0.12064266	1.0872191	down
C19 H22 N14 O3 S2	0.004063975	0.044948332	-1.1563334	-0.20955753	1.1563334	down	-8.76318	-3.1314545	8.76318	down	-7.578419	-2.921897	7.578419	down
C19 H39 Cl2 N4 O3 P3 S2	0.004068259	0.044948332	19.420155	4.279483	19.420155	up	-1.0990545	-0.1362629	1.0990545	down	-21.34381	-4.4157457	21.34381	down
C24 H34 N2 O10	0.00429556	0.04543222	1.7448239	0.8030815	1.7448239	up	1.653981	0.7259426	1.653981	up	-1.0549239	-0.0771389	1.0549239	down
C36 H37 N O3	0.004400513	0.04543222	-2.3987365	-1.2622747	2.3987365	down	-8.364645	-3.0643044	8.364645	down	-3.4871044	-1.8020296	3.4871044	down
C13 H18 N2 O9	0.004402685	0.04543222	1.2471294	0.31861115	1.2471294	up	1.2058529	0.27005386	1.2058529	up	-1.0342301	-0.04855728	1.0342301	down
C20 H35 N5 O7 P2 S	0.004236332	0.04543222	1.1544646	0.20722389	1.1544646	up	-7.3793335	-2.8834906	7.3793335	down	-8.519179	-3.0907145	8.519179	down
C8 H18 O20 P4 S	0.004431438	0.04543222	1.782815	0.834157	1.782815	up	-1.229774	-0.29839325	1.229774	down	-2.1924596	-1.1325502	2.1924596	down
850.2403@8.458829	0.004230551	0.04543222	1.8420635	0.88132286	1.8420635	up	1.8004675	0.8483715	1.8004675	up	-1.023103	-0.032951355	1.023103	down
940.2718@13.098411	0.004337703	0.04543222	1.9690881	0.9775276	1.9690881	up	2.169297	1.1172276	2.169297	up	1.101676	0.13969994	1.101676	up
872.2861@13.0997305	0.004286767	0.04543222	2.0264778	1.0189743	2.03E+00	up	2.1122425	1.0787754	2.1122425	up	1.042322	0.0598011	1.042322	up
C25 H32 N6 O12 S	0.004559901	0.04633185	1.5097421	0.5943022	1.5097421	up	1.5952002	0.6737375	1.5952002	up	1.0566044	0.07943535	1.0566044	up

Sample ID	Name	GROUP	FILE
S00001201		POOLED PLASMA	Pos_Human Plasma Extraction_0
S00001201		POOLED PLASMA	Pos_Human Plasma Extraction_1
S00001201		POOLED PLASMA	Pos_Human Plasma Extraction_2
S00001201		POOLED PLASMA	Pos_Human Plasma Extraction_3
S00001201		POOLED PLASMA	Pos_Human Plasma Extraction_4
S00001201		POOLED PLASMA	Pos_Human Plasma Extraction_5
S00001201		POOLED PLASMA	Pos_Human Plasma Extraction_6
S00016763		POOLED	Pos_Pool QC 1
S00016763		POOLED	Pos_Pool QC 2
S00016763		POOLED	Pos_Pool QC 3
S00016763		POOLED	Pos_Pool QC 4
S00015447	5022PP	Lesional	Pos_S00015447_1
S00015448	5258PP	Lesional	Pos_S00015448_2
S00015449	5311PP	Lesional	Pos_S00015449_3
S00015450	5397PP	Lesional	Pos_S00015450_4
S00015451	TR PP	Lesional	Pos_S00015451_5
S00015452	KB PP	Lesional	Pos_S00015452_6
S00015453	5022PN	Nonlesional	Pos_S00015453_7
S00015454	5258PN	Nonlesional	Pos_S00015454_8
S00015455	5311PN	Nonlesional	Pos_S00015455_9
S00015456	5397PN	Nonlesional	Pos_S00015456_10
S00015457	TR PN	Nonlesional	Pos_S00015457_11
S00015458	KB PN	Nonlesional	Pos_S00015458_12
S00015459	6108 C	Healthy	Pos_S00015459_13
S00015460	5660 C	Healthy	Pos_S00015460_14
S00015461	4480 C	Healthy	Pos_S00015461_15
S00015462	6609 C	Healthy	Pos_S00015462_16
S00015463	6998 C	Healthy	Pos_S00015463_17
S00015464	DM NN	Healthy	Pos_S00015464_18

Compound	Alignment Value	Annotations	CAS Number	ChEBI ID	CompositeSpectrum	Compound Name	KEGG ID	CompoundAlgo	Frequency	Ionization mode	Mass	METLIN ID	PubChem ID	Retention Time
(-)-COTININE (CAS# 486-56-6); (M+H)+	(-)-COTININE (CAS# 486-56-6); (M+H)+	(-)-COTININE (CAS# 486-56-6); (M+H)+ [, tgt=80.41, overa	486-56-6		(177.10342, 9302.439)(178.10648, 1224.0325)(179.1041, 70.	(-)-COTININE (CAS# 486-56-6); (M+H)+		FindByFormula	4	+	176.0959			1.6822537
(-)-SALSOLINOL (CAS# 27740-96-1); (M+H)+	(-)-SALSOLINOL (CAS# 27740-96-1); (M+H)+	(-)-SALSOLINOL (CAS# 27740-96-1); (M+H)+ [, tgt=78.84, o	27740-96-1		(180.10257, 2244.7214)(181.09998, 240.59071)(182.10059, 4	(-)-SALSOLINOL (CAS# 27740-96-1); (M+H)+	C09642	FindByFormula	14	+	179.0951			1.2817202
(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-1	(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-1	(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-14-7); (M+H	2041-14-7		(126.03091, 9322.854)(127.03658, 241.1757)(128.0331, 1738	(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-14-7); (M+H)+	C03557	FindByFormula	7	+	125.023			0.79643
(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-1	(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-1	(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-14-7); (M+N	2041-14-7		(148.01378, 11158.859)(149.01619, 352.30997)(150.01944, 2	(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-14-7); (M+Na)+	C03557	FindByFormula	6	+	125.0248			0.6398333
(S)-2-AMINO-3-(3-HYDOXY-4-OXO-4H-PYRIDIN	(S)-2-AMINO-3-(3-HYDOXY-4-OXO-4H-PYRIDIN	(S)-2-AMINO-3-(3-HYDOXY-4-OXO-4H-PYRIDIN-1-YL)PROP	500-44-7		(221.0519, 818.43)(222.047, 55.53)	(S)-2-AMINO-3-(3-HYDOXY-4-OXO-4H-PYRIDIN-1-YL)PROPANOATI	C04771	FindByFormula	1	+	198.0622			0.73500246
(S)-DIHYDROOROTATE (CAS# 5988-19-2); (M+	(S)-DIHYDROOROTATE (CAS# 5988-19-2); (M+	(S)-DIHYDROOROTATE (CAS# 5988-19-2); (M+H)+ [, tgt=5	5988-19-2		(159.0392, 74892.72)(160.0421, 5204.82)	(S)-DIHYDROOROTATE (CAS# 5988-19-2); (M+H)+	C00337	FindByFormula	1	+	158.0319			1.0990059
1,2-DIPALMITOYL-SN-GLYCEROL (CAS# 30334-	1,2-DIPALMITOYL-SN-GLYCEROL (CAS# 30334-	1,2-DIPALMITOYL-SN-GLYCEROL (CAS# 30334-71-5); (M+N	30334-71-5		(591.4959, 15150.625)(592.499, 6019.6143)(593.5014, 1462.	1,2-DIPALMITOYL-SN-GLYCEROL (CAS# 30334-71-5); (M+Na)+		FindByFormula	7	+	568.5068			26.12479
1,3-DIAMINOPROPANE (CAS# 109-76-2); (M+	1,3-DIAMINOPROPANE (CAS# 109-76-2); (M+	1,3-DIAMINOPROPANE (CAS# 109-76-2); (M+H)+ [, tgt=84	109-76-2		(75.09192, 1171.334)(76.09416, 35.522)	1,3-DIAMINOPROPANE (CAS# 109-76-2); (M+H)+	C00986	FindByFormula	5	+	74.0848			0.53460157
1,3-DIELAIDIN (CAS# 98168-52-6); (M+Na)+	1,3-DIELAIDIN (CAS# 98168-52-6); (M+Na)+	1,3-DIELAIDIN (CAS# 98168-52-6); (M+Na)+ [, tgt=79.09, c	98168-52-6		(643.5289, 102873.17)(644.53174, 43497.97)(645.53534, 103	1,3-DIELAIDIN (CAS# 98168-52-6); (M+Na)+		FindByFormula	8	+	620.5392			26.76233
1,3-DIMETHYLURIC ACID (CAS# 944-73-0); (M	1,3-DIMETHYLURIC ACID (CAS# 944-73-0); (M	1,3-DIMETHYLURIC ACID (CAS# 944-73-0); (M+Na)+ [, tgt=	944-73-0		(219.0491, 3167.66)(220.0638, 327.05)	1,3-DIMETHYLURIC ACID (CAS# 944-73-0); (M+Na)+		FindByFormula	1	+	196.061			3.4470577
100.001@0.5352921					(101.00825, 14116.948)(102.008095, 2319.0413)(102.99985,	100.001@0.5352921		FindByFormula	24	+	100.001			0.5352921
1000.4479@18.6169					(501.23428, 2192.7717)(501.73337, 1050.7133)(502.2349, 33	1000.4479@18.6169		FindByFormula	6	+	1000.4479			18.6169
1005.4501@10.68129					(503.73355, 1151.4573)(504.23587, 744.1701)(504.7358, 291	1005.4501@10.68129		FindByFormula	19	+	1005.4501			10.68129
1006.652@22.587593					(504.3337, 1150.74)(504.8314, 741.1)(505.3263, 674.74)	1006.652@22.587593		FindByFormula	1	+	1006.652			22.587593
1006.6558@22.773655					(504.33047, 3067.8777)(504.82883, 1702.4606)(505.33456, 1	1006.6558@22.773655		FindByFormula	17	+	1006.6558			22.773655
1012.2439@16.705917					(507.1317, 1421.3766)(507.632, 655.03)	1012.2439@16.705917		FindByFormula	6	+	1012.2439			16.705917
1012.5953@22.298977					(507.3108, 43508.24)(507.805, 19835.748)(508.31665, 9395.	1012.5953@22.298977		FindByFormula	20	+	1012.5953			22.298977
1012.6042@22.069912					(507.3109, 2600.7324)(507.80695, 588.485)(508.31512, 744.	1012.6042@22.069912		FindByFormula	4	+	1012.6042			22.069912
1013.4035@16.89687					(507.71, 2094.7102)(508.213, 1146.495)(508.71155, 424.448	1013.4035@16.89687		FindByFormula	6	+	1013.4035			16.89687
1014.426@17.23685					(508.2237, 7295.779)(508.72144, 3614.6729)(509.21994, 165	1014.426@17.23685		FindByFormula	17	+	1014.426			17.23685
1016.3469@16.988739					(509.18124, 3240.567)(509.6809, 1584.2599)(510.18637, 644	1016.3469@16.988739		FindByFormula	7	+	1016.3469			16.988739
1018.4564@16.715847					(510.23578, 1625.7313)(510.7373, 741.2572)(511.23413, 462	1018.4564@16.715847		FindByFormula	7	+	1018.4564			16.715847
1018.4765@21.967066					(510.24832, 1433.383)(510.74658, 753.76605)	1018.4765@21.967066		FindByFormula	28	+	1018.4765			21.967066
1023.4739@24.431517					(512.7442, 1344.1454)(513.24786, 836.8173)	1023.4739@24.431517		FindByFormula	11	+	1023.4739			24.431517
1025.4164@20.84796					(513.71564, 1332.77)(514.21674, 869.25)(514.71936, 209.23	1025.4164@20.84796		FindByFormula	6	+	1025.4164			20.84796
1028.6036@22.069344					(515.31964, 618.8367)(515.8117, 102.456665)(516.3102, 421	1028.6036@22.069344		FindByFormula	3	+	1028.6036			22.069344
1028.6078@22.300411					(515.3113, 36240.188)(515.8107, 19995.305)(516.313, 8450.	1028.6078@22.300411		FindByFormula	11	+	1028.6078			22.300411
1028.608@22.469181					(515.3162, 5742.4707)(515.8099, 2356.5852)(516.30914, 123	1028.608@22.469181		FindByFormula	13	+	1028.608			22.469181
1028.6086@22.182531					(515.3131, 3786.3374)(515.8163, 2119.7925)(516.30945, 271	1028.6086@22.182531		FindByFormula	4	+	1028.6086			22.182531
1028.6116@22.4945					(515.31647, 2397.8901)(515.81586, 179.30666)(516.3123, 54	1028.6116@22.4945		FindByFormula	3	+	1028.6116			22.4945
1029.376@5.4622707					(515.7028, 227.29)(516.1978, 196.48)(526.6831, 182.07)(527.	1029.376@5.4622707		FindByFormula	1	+	1029.376			5.4622707
1029.3823@5.774042					(515.6991, 3926.6536)(516.20123, 1912.8634)(516.7022, 646	1029.3823@5.774042		FindByFormula	6	+	1029.3823			5.774042
1030.5504@14.407582					(516.2819, 1453.5466)(516.78674, 768.2212)(517.2751, 451.	1030.5504@14.407582		FindByFormula	27	+	1030.5504			14.407582
1034.6707@23.058197					(518.3438, 31007.36)(518.84393, 17539.94)(519.3481, 6704.	1034.6707@23.058197		FindByFormula	12	+	1034.6707			23.058197
1036.4094@20.84011					(519.2144, 2469.656)(519.7094, 1609.7839)(520.20935, 452.	1036.4094@20.84011		FindByFormula	5	+	1036.4094			20.84011
1036.6456@22.186314					(519.329, 5602.15)(519.8194, 324.23)(520.3402, 3132.7)	1036.6456@22.186314		FindByFormula	1	+	1036.6456			22.186314
1036.6469@22.822523					(519.3326, 3190.86)(519.8238, 228.13)	1036.6469@22.822523		FindByFormula	1	+	1036.6469			22.822523
1036.6488@22.501652					(519.33545, 4735.5146)(519.83374, 2138.795)(520.33606, 11	1036.6488@22.501652		FindByFormula	20	+	1036.6488			22.501652
1036.9066@20.835611					(519.46014, 1820.0083)(519.9577, 671.1017)	1036.9066@20.835611		FindByFormula	6	+	1036.9066			20.835611
1037.3947@10.2885					(519.70386, 7725.0063)(520.2054, 4353.2617)(520.7064, 149	1037.3947@10.2885		FindByFormula	6	+	1037.3947			10.2885
1039.5897@9.211685					(520.80255, 14969.488)(521.3033, 8893.641)(521.80414, 305	1039.5897@9.211685		FindByFormula	24	+	1039.5897			9.211685
1039.5977@8.992071					(542.7856, 163.7)(543.2983, 43.94)	1039.5977@8.992071		FindByFormula	1	+	1039.5977			8.992071
1044.4469@18.761848					(523.2378, 2682.85)(523.7368, 1390.49)(524.23413, 502.856	1044.4469@18.761848		FindByFormula	5	+	1044.4469			18.761848
1046.5753@21.991354					(524.2969, 249.25)(524.7941, 97.42)	1046.5753@21.991354		FindByFormula	1	+	1046.5753			21.991354
1046.5851@22.395437					(524.2959, 1594.9418)(524.79913, 707.93164)(525.2978, 133	1046.5851@22.395437		FindByFormula	6	+	1046.5851			22.395437
1051.5432@5.3152485					(526.7681, 122.46)(527.2704, 43.4)(537.7709, 154.46)(538.28	1051.5432@5.3152485		FindByFormula	1	+	1051.5432			5.3152485
1051.5522@4.9759607					(526.78345, 5678.013)(527.2844, 3210.7637)(527.7862, 1131	1051.5522@4.9759607		FindByFormula	6	+	1051.5522			4.9759607
1052.6097@22.204243					(527.3183, 1989.4355)(527.82214, 958.85144)(528.32043, 75	1052.6097@22.204243		FindByFormula	10	+	1052.6097			22.204243
1052.6198@22.489832					(527.3124, 911.13)(527.80725, 276.45502)(528.321, 846.97)(	1052.6198@22.489832		FindByFormula	2	+	1052.6198			22.489832
1053.3593@10.285832					(527.687, 1529.8501)(528.18964, 934.75336)	1053.3593@10.285832		FindByFormula	6	+	1053.3593			10.285832
1053.388@9.672932					(527.7013, 2339.0132)(528.20245, 1387.5518)	1053.388@9.672932		FindByFormula	6	+	1053.388			9.672932
1053.4802@7.6255107					(527.7481, 1136.6843)(528.24774, 692.6253)(528.7499, 278.	1053.4802@7.6255107		FindByFormula	21	+	1053.4802			7.6255107
1053.6014@10.078312					(527.8099, 2034.77)(528.3078, 1434.227)(528.81006, 459.58	1053.6014@10.078312		FindByFormula	18	+	1053.6014			10.078312
1053.6044@9.82568					(549.7888, 376.3)(550.2929, 230.23)(538.8051, 236.27)(539.2	1053.6044@9.82568		FindByFormula	1	+	1053.6044			9.82568
1054.419@18.06434					(528.2172, 6935.7)(528.71765, 3627.6104)(529.2272, 2082.6	1054.419@18.06434		FindByFormula	9	+	1054.419			18.06434
1054.5454@11.958135					(528.27954, 16226.8)(528.781, 9944.32)(529.2818, 3588.438	1054.5454@11.958135		FindByFormula	6	+	1054.5454			11.958135
1054.5469@12.156662					(539.2682, 202.01)(539.7729, 122.82)(540.2768, 159.2)	1054.5469@12.156662		FindByFormula	1	+	1054.5469			12.156662
1054.6086@22.301497					(529.31836, 21979.889)(529.81714, 12386.623)	1054.6086@22.301497		FindByFormula	28	+	1054.6086			22.301497
1055.5723@7.1004105					(528.7928, 1552.5616)(529.29346, 862.8367)	1055.5723@7.1004105		FindByFormula	6	+	1055.5723			7.1004105
1056.5461@22.146221					(529.2859, 200.27)(529.7693, 36.69)(530.2879, 89.95)	1056.5461@22.146221		FindByFormula	1	+	1056.5461			22.146221
1056.5503@21.995012					(529.7891, 113.04)(530.2869, 118.76)	1056.5503@21.995012		FindByFormula	1	+	1056.5503			21.995012
1056.6182@22.300308					(529.31824, 23229.92)(529.8175, 13130.1875)(530.32074, 61	1056.6182@22.300308		FindByFormula	27	+	1056.6182			22.300308
1056.6205@22.308039					(529.31726, 35172.504)(529.81805, 20054.953)(530.3212, 76	1056.6205@22.308039		FindByFormula	6	+	1056.6205			22.308039
1056.6208@22.051985					(529.3173, 1425.0647)(529.8185, 607.36926)(530.3213, 1193	1056.6208@22.051985		FindByFormula	15	+	1056.6208			22.051985
1057.4308@17.134548					(529.72394, 4908.4854)(530.22626, 2644.4382)(530.7276, 10	1057.4308@17.134548		FindByFormula	7	+	1057.4308			17.134548
1058.4427@17.132696					(530.2275, 327.85)(530.7363, 97.95)	1058.4427@17.132696		FindByFormula	1	+	1058.4427			17.132696
1058.4513@17.49708					(530.2343, 1996.5582)(530.7335, 975.6783)(531.24817, 804.	1058.4513@17.49708		FindByFormula	6	+	1058.4513			17.49708
1058.4529@17.437723					(530.23444, 2054.9717)(530.7364, 1105.3083)(531.2497, 674	1058.4529@17.437723		FindByFormula	6	+	1058.4529			17.437723
1059.5623@8.449423					(530.78723, 5129.6836)(531.2868, 3189.8884)(531.79034, 14	1059.5623@8.449423		FindByFormula	7	+	1059.5623			8.449423
1063.4921@12.495282					(532.75336, 1093.7484)(533.253, 794.7517)(554.7358, 3466.	1063.4921@12.495282		FindByFormula	6	+	1063.4921			12.495282
1066.6133@19.442995					(534.3173, 1079.6929)(534.82007, 596.93506)(535.31177, 35	1066.6133@19.442995		FindByFormula	14	+	1066.6133			19.442995
1066.6136@19.785637					(534.31757, 11006.907)(534.81964, 7178.7583)(535.3197, 30	1066.6136@19.785637		FindByFormula	26	+	1066.6136			19.785637
1066.617@19.785236					(534.318, 9340.542)(534.8202, 6096.215)(535.3197, 2596.34	1066.617@19.785236		FindByFormula	10	+	1066.617			19.785236
1066.6592@22.45198					(534.33954, 1950.8242)(534.84033, 992.33624)(535.34015, 1	1066.6592@22.45198		FindByFormula	19	+	1066.6592			22.45198
1074.5717@22.300463					(538.29425, 1451.1129)(538.795, 867.6262)(539.29584, 664.	1074.5717@22.300463		FindByFormula	21	+	1074.5717			22.300463
1076.614@22.132786					(539.31525, 9078.163)(539.81824, 5150.1396)(540.3091, 453	1076.614@22.132786		FindByFormula	10	+	1076.614			22.132786
1076.6147@22.279636					(539.31244, 652.42596)(539.81024, 102.138)(540.3062, 558.	1076.6147@22.279636		FindByFormula	7	+	1076.6147			22.279636
1078.6967@23.051666					(540.35626, 34142.14)(540.8571, 20153.85)(541.35925, 9052	1078.6967@23.051666		FindByFormula	18	+	1078.6967			23.051666
1080.5695@22.100702					(541.2937, 1661.0199)(541.7895, 631.90594)	1080.5695@22.100702		FindByFormula	5	+	1080.5695			22.100702
1080.592@22.3007					(541.3032, 1949.3984)(541.8018, 745.99054)(542.31836, 197	1080.592@22.3007		FindByFormula	21	+	1080.592			22.3007
1080.6711@22.493565					(541.3424, 3554.4175)(541.84393, 1957.2468)(542.3378, 143	1080.6711@22.493565		FindByFormula	20	+	1080.6711			22.493565
1084.3444@16.991095					(543.1766, 1830.5599)(543.67596, 941.8217)	1084.3444@16.991095		FindByFormula	6	+	1084.3444			16.991095
1088.493@18.905933					(545.26013, 1662.198)(545.76044, 826.0)(546.2618, 471.837	1088.493@18.905933		FindByFormula	5	+	1088.493			18.905933
1096.5903@22.225706					(549.30524, 2282.688)(549.8084, 1030.2781)	1096.5903@22.225706		FindByFormula	10	+	1096.5903			22.225706
1096.6002@22.0223					(549.30664, 1453.9268)(549.82086, 399.84)	1096.6002@22.0223		FindByFormula	3	+	1096.6002			22.0223
1097.5546@8.855887					(549.7857, 265.5)(550.2829, 158.155)(560.7742, 354.07)(561.	1097.5546@8.855887		FindByFormula	3	+	1097.5546			8.855887
1097.5607@8.660056					(549.78754, 16288.487)(550.28876, 9999.141)(550.7902, 364	1097.5607@8.660056		FindByFormula	7	+	1097.5607			8.660056
1098.4341@18.046814					(550.2266, 7672.07)(550.72864, 4209.3804)(551.2327, 1752.	1098.4341@18.046814		FindByFormula	6	+	1098.4341			18.046814
10-HYDROXYDECANOATE (CAS# 1679-53-4); (	10-HYDROXYDECANOATE (CAS# 1679-53-4); (	10-HYDROXYDECANOATE (CAS# 1679-53-4); (M+Na)+ [, t	1679-53-4		(211.13005, 3336.2131)(212.12622, 218.80334)(213.1185, 13	10-HYDROXYDECANOATE (CAS# 1679-53-4); (M+Na)+	C02774	FindByFormula	3	+	188.1401			13.504272
1100.4362@17.020802					(551.22943, 1525.198)(551.72986, 755.98)	1100.4362@17.020802		FindByFormula	5	+	1100.4362			17.020802
1102.6552@23.055687					(552.3394, 1716.1136)(552.8349, 916.59644)(553.3429, 572.	1102.6552@23.055687		FindByFormula	11	+	1102.6552			23.055687
1102.6676@22.750177					(552.3431, 672.56)(552.8405, 393.09335)	1102.6676@22.750177		FindByFormula	3	+	1102.6676			22.750177
1105.3809@10.285832					(553.6976, 3477.5117)(554.19934, 1994.2567)(554.699, 790.	1105.3809@10.285832		FindByFormula	6	+	1105.3809			10.285832
1110.4423@18.905958					(556.23206, 1852.1151)(556.7341, 1046.1901)(557.2355, 724	1110.4423@18.905958		FindByFormula	6	+	1110.4423			18.905958
1110.6819@22.456293					(556.3494, 1503.3403)(556.8515, 961.3148)(557.34894, 751.	1110.6819@22.456293		FindByFormula	23	+	1110.6819			22.456293
1110.685@22.736984					(556.3574, 1490.39)(556.8403, 743.38)	1110.685@22.736984		FindByFormula	1	+	1110.685			22.736984
1112.5656@22.133215					(557.29193, 795.4267)(557.77716, 232.89336)(558.2953, 524	1112.5656@22.133215		FindByFormula	3	+	1112.5656			22.133215
1112.5714@22.31866					(557.2905, 3785.4539)(557.7909, 2271.252)(558.2973, 1323.	1112.5714@22.31866		FindByFormula	5	+	1112.5714			22.31866
1117.4926@5.234659					(559.7573, 109.6575)(560.2559, 625.065)(560.7395, 47.29)(	1117.4926@5.234659		FindByFormula	4	+	1117.4926			5.234659
1117.4976@4.9856634					(559.7569, 9890.586)(560.25696, 5696.3633)(560.7584, 1942	1117.4976@4.9856634		FindByFormula	8	+	1117.4976			4.9856634
1118.5803@22.314342					(560.3, 2612.3489)(560.79816, 1022.59094)(561.2976, 725.4	1118.5803@22.314342		FindByFormula	9	+	1118.5803			22.314342
1119.4707@5.8832226					(560.7425, 1870.32)(561.2437, 1136.255)	1119.4707@5.8832226		FindByFormula	6	+	1119.4707			5.8832226
1120.4318@18.050985					(561.225, 3267.9065)(561.72534, 1800.6615)(562.2257, 776.	1120.4318@18.050985		FindByFormula	6	+	1120.4318			18.050985
1121.348@10.2873335					(561.6803, 1814.4584)(562.18243, 1096.4017)	1121.348@10.2873335		FindByFormula	6	+	1121.348			10.2873335
1122.7275@23.046068					(562.36914, 35688.523)(562.8697, 21873.828)(563.37213, 11	1122.7275@23.046068		FindByFormula	17	+	1122.7275			23.046068
1124.4612@19.968307					(563.23944, 33001.46)(563.74023, 17883.03)(564.24225, 713	1124.4612@19.968307		FindByFormula	7	+	1124.4612			19.968307
1124.6028@22.293247					(563.3204, 2176.9683)(563.8137, 1178.6995)(564.3214, 719.	1124.6028@22.293247		FindByFormula	18	+	1124.6028			22.293247
1124.6176@21.994186					(563.3209, 2030.095)(563.817, 185.95001)(564.3196, 957.54	1124.6176@21.994186		FindByFormula	2	+	1124.6176			21.994186
1124.6996@22.511711					(563.3624, 4244.2397)(563.8592, 2211.0366)(564.3614, 1201	1124.6996@22.511711		FindByFormula	26	+	1124.6996			22.511711
1125.5085@8.435857					(563.762, 9018.201)(564.2602, 5686.064)(564.7635, 2477.99	1125.5085@8.435857		FindByFormula	7	+	1125.5085			8.435857
1125.5096@8.545201					(563.7677, 138.09)(564.2591, 286.63)	1125.5096@8.545201		FindByFormula	1	+	1125.5096			8.545201
113.9797@0.5336199					(114.98739, 6525.4004)(115.98793, 1105.837)(116.9831, 317	113.9797@0.5336199		FindByFormula	21	+	113.9797			0.5336199
1133.4579@21.160587					(567.73834, 1725.48)(568.24097, 1453.0402)(568.74133, 434	1133.4579@21.160587		FindByFormula	6	+	1133.4579			21.160587
1133.9595@21.152266					(567.9879, 1736.1072)(568.4874, 665.26855)	1133.9595@21.152266		FindByFormula	7	+	1133.9595			21.152266
1134.606@19.783178					(568.3106, 5588.123)(568.8127, 2736.197)(569.3028, 3469.7	1134.606@19.783178		FindByFormula	27	+	1134.606			19.783178
1138.606@22.160442					(570.30963, 2402.3923)(570.8107, 1290.384)(571.3142, 1068	1138.606@22.160442		FindByFormula	20	+	1138.606			22.160442
1138.7039@23.056713					(570.3644, 865.16)(570.8544, 444.08)	1138.7039@23.056713		FindByFormula	1	+	1138.7039			23.056713
1138.7122@22.778687					(570.3656, 1562.1788)(570.86456, 844.19214)(571.36926, 68	1138.7122@22.778687		FindByFormula	9	+	1138.7122			22.778687
114.0774@0.6278321					(115.082924, 30235.541)(116.08633, 3558.6602)(137.06425,	114.0774@0.6278321		FindByFormula	6	+	114.0774			0.6278321
1142.4716@18.042645					(572.24493, 2641.04)(572.7474, 1489.4332)(573.25165, 609.	1142.4716@18.042645		FindByFormula	6	+	1142.4716			18.042645
1142.472@11.969642					(572.2437, 1853.515)(572.7454, 1142.9667)	1142.472@11.969642		FindByFormula	6	+	1142.472			11.969642
1142.4731@18.225863					(572.2444, 28324.11)(572.74585, 16009.193)(573.2489, 7192	1142.4731@18.225863		FindByFormula	8	+	1142.4731			18.225863
1142.483@18.21962					(572.2479, 854.025)(572.7483, 450.415)(573.257, 52.44)(583.	1142.483@18.21962		FindByFormula	2	+	1142.483			18.21962
1144.4542@21.159016					(573.23737, 2897.9075)(573.73267, 2209.9976)(574.2345, 99	1144.4542@21.159016		FindByFormula	4	+	1144.4542			21.159016
1144.6743@22.311687					(573.3431, 12156.923)(573.8433, 7544.207)(574.34485, 3070	1144.6743@22.311687		FindByFormula	23	+	1144.6743			22.311687
1144.9528@21.155699					(573.48254, 2103.01)(573.98236, 990.4301)(574.47815, 399.	1144.9528@21.155699		FindByFormula	7	+	1144.9528			21.155699
1146.5034@17.735426					(574.26166, 2462.6135)(574.7627, 1442.5668)(575.26154, 55	1146.5034@17.735426		FindByFormula	6	+	1146.5034			17.735426
1146.5802@22.40071					(574.30347, 813.73)(574.8017, 185.49666)(575.2917, 140.19)	1146.5802@22.40071		FindByFormula	3	+	1146.5802			22.40071
1146.5864@22.135443					(574.30475, 2007.7251)(574.80536, 1369.5449)(575.2992, 12	1146.5864@22.135443		FindByFormula	6	+	1146.5864			22.135443
1146.5872@21.792347					(574.3041, 524.35)(574.8037, 253.36)	1146.5872@21.792347		FindByFormula	1	+	1146.5872			21.792347
1153.4316@24.441654					(577.72015, 679.4686)(578.2223, 388.70712)	1153.4316@24.441654		FindByFormula	14	+	1153.4316			24.441654
1154.7118@22.453062					(578.36584, 1070.98)(578.85693, 688.94)(579.34845, 1529.4	1154.7118@22.453062		FindByFormula	3	+	1154.7118			22.453062
1156.4895@19.188068					(579.25555, 1977.8658)(579.7547, 1092.218)(580.2549, 631.	1156.4895@19.188068		FindByFormula	10	+	1156.4895			19.188068
1163.5018@8.604081					(582.755, 1003.85754)(583.2569, 627.5188)(604.7444, 687.3	1163.5018@8.604081		FindByFormula	9	+	1163.5018			8.604081
1164.4984@18.576044					(583.25665, 4458.91)(583.75745, 423.406)(584.25946, 1792.	1164.4984@18.576044		FindByFormula	5	+	1164.4984			18.576044
1164.5836@22.198692					(583.301, 2153.6548)(583.7979, 868.0826)	1164.5836@22.198692		FindByFormula	8	+	1164.5836			22.198692
1164.585@22.312641					(583.3006, 4717.2656)(583.801, 2470.1228)(584.2974, 2756.	1164.585@22.312641		FindByFormula	7	+	1164.585			22.312641
1166.3751@18.055323					(584.1958, 1599.3317)(584.6978, 874.74164)(585.2011, 349.	1166.3751@18.055323		FindByFormula	6	+	1166.3751			18.055323
1166.7499@23.045338					(584.3814, 42102.453)(584.8824, 26781.744)(585.3848, 1071	1166.7499@23.045338		FindByFormula	16	+	1166.7499			23.045338
1168.6298@22.010498					(585.3185, 893.88)(585.8376, 276.43)	1168.6298@22.010498		FindByFormula	1	+	1168.6298			22.010498
1168.6357@22.313885					(585.32764, 1872.9851)(585.82825, 914.32404)	1168.6357@22.313885		FindByFormula	20	+	1168.6357			22.313885
1168.7233@22.505514					(585.3699, 4431.131)(585.87177, 2520.8828)(586.3621, 1175	1168.7233@22.505514		FindByFormula	23	+	1168.7233			22.505514
117.0631@3.6138756					(118.07025, 17165.066)(119.066345, 3344.8318)	117.0631@3.6138756		FindByFormula	6	+	117.0631			3.6138756
1172.497@9.5336					(587.2529, 1588.1174)(587.7617, 134.3875)(588.2551, 556.2	1172.497@9.5336		FindByFormula	4	+	1172.497			9.5336
1172.5013@9.87934					(587.2569, 1942.8649)(587.7586, 1227.9066)(588.25854, 561	1172.5013@9.87934		FindByFormula	6	+	1172.5013			9.87934
1172.5085@10.09456					(587.2594, 687.18)(587.7567, 159.025)(588.2619, 338.65298)	1172.5085@10.09456		FindByFormula	10	+	1172.5085			10.09456
1172.5259@19.652117					(587.272, 2018.6473)(587.7704, 1087.4551)(588.2727, 562.0	1172.5259@19.652117		FindByFormula	4	+	1172.5259			19.652117
1175.449@12.495116					(588.73, 2009.5599)(589.2323, 1291.6517)(589.7287, 446.05)	1175.449@12.495116		FindByFormula	6	+	1175.449			12.495116
1177.9858@21.172935					(590.0007, 1436.475)(590.48724, 1260.4833)(590.9894, 760.	1177.9858@21.172935		FindByFormula	6	+	1177.9858			21.172935
1182.627@22.007689					(592.3262, 1397.45)(592.8186, 202.24)(593.3007, 44.32)	1182.627@22.007689		FindByFormula	1	+	1182.627			22.007689
1182.6368@22.152647					(592.331, 1981.6176)(592.82336, 864.038)(593.3345, 812.50	1182.6368@22.152647		FindByFormula	25	+	1182.6368			22.152647
1185.4738@5.250163					(593.7393, 72.26)(594.2485, 152.56)	1185.4738@5.250163		FindByFormula	1	+	1185.4738			5.250163
1185.4822@18.109724					(593.7468, 4567.946)(594.24945, 2823.062)(594.75385, 1250	1185.4822@18.109724		FindByFormula	5	+	1185.4822			18.109724
1185.4827@5.0349865					(593.7474, 636.9933)(594.2472, 428.7186)(604.7417, 393.26	1185.4827@5.0349865		FindByFormula	22	+	1185.4827			5.0349865
1186.4926@18.234165					(594.25653, 4113.241)(594.7591, 2447.3599)(595.26495, 130	1186.4926@18.234165		FindByFormula	7	+	1186.4926			18.234165
1186.498@18.216084					(594.25696, 5988.8726)(594.7602, 3588.5776)(595.2642, 211	1186.498@18.216084		FindByFormula	8	+	1186.498			18.216084
1186.5009@18.578032					(594.2563, 281.05334)(594.7586, 274.52667)(595.2633, 94.1	1186.5009@18.578032		FindByFormula	3	+	1186.5009			18.578032
1188.4261@18.052319					(595.22394, 1363.2434)(595.71967, 752.88165)(596.2268, 21	1188.4261@18.052319		FindByFormula	6	+	1188.4261			18.052319
1190.5253@17.855618					(596.2735, 1989.0157)(596.77594, 1096.9458)(597.28217, 61	1190.5253@17.855618		FindByFormula	7	+	1190.5253			17.855618
1190.7104@23.050585					(596.3623, 2666.108)(596.8605, 1706.8873)(597.3651, 952.7	1190.7104@23.050585		FindByFormula	15	+	1190.7104			23.050585
1192.4489@19.965733					(597.23566, 3729.6838)(597.7359, 2081.4998)(598.2437, 112	1192.4489@19.965733		FindByFormula	7	+	1192.4489			19.965733
1193.4915@8.418485					(597.7537, 1752.795)(598.2542, 1184.8683)(598.7546, 534.5	1193.4915@8.418485		FindByFormula	7	+	1193.4915			8.418485
1196.4637@16.426586					(599.2398, 4370.01)(599.74146, 3246.82)(600.2438, 1491.86	1196.4637@16.426586		FindByFormula	22	+	1196.4637			16.426586
1198.6483@22.548525					(600.3323, 2461.9624)(600.8296, 680.3388)(601.33563, 892.	1198.6483@22.548525		FindByFormula	17	+	1198.6483			22.548525
11BETA-HYDROXYANDROST-4-ENE-3,17-DION	11BETA-HYDROXYANDROST-4-ENE-3,17-DION	11BETA-HYDROXYANDROST-4-ENE-3,17-DIONE (CAS# 382	382-44-5		(325.1774, 1076.27)(326.17697, 167.85751)(327.17682, 432.	11BETA-HYDROXYANDROST-4-ENE-3,17-DIONE (CAS# 382-44-5); (M+Na)+		FindByFormula	4	+	302.187			14.564842
11-DEOXYCORTICOSTERONE (CAS# 64-85-7);	11-DEOXYCORTICOSTERONE (CAS# 64-85-7); (	11-DEOXYCORTICOSTERONE (CAS# 64-85-7); (M+Na)+ [, t	64-85-7		(353.2122, 2024.16)(354.2206, 455.46)(355.1965, 302.11)	11-DEOXYCORTICOSTERONE (CAS# 64-85-7); (M+Na)+		FindByFormula	1	+	330.2214			16.843922
11-DEOXYCORTISOL (CAS# 152-58-9); (M+H)+	11-DEOXYCORTISOL (CAS# 152-58-9); (M+H)+	11-DEOXYCORTISOL (CAS# 152-58-9); (M+H)+ [, tgt=73.36	152-58-9		(347.2204, 741.93)(348.2281, 217.81)	11-DEOXYCORTISOL (CAS# 152-58-9); (M+H)+		FindByFormula	1	+	346.2141			15.607649
11-DEOXYCORTISOL (CAS# 152-58-9); (M+Na)	11-DEOXYCORTISOL (CAS# 152-58-9); (M+Na)	11-DEOXYCORTISOL (CAS# 152-58-9); (M+Na)+ [, tgt=45.0	152-58-9		(369.20206, 1683.6183)(370.20264, 352.3567)(371.2064, 85.	11-DEOXYCORTISOL (CAS# 152-58-9); (M+Na)+		FindByFormula	6	+	346.213			15.367729
1210.4646@11.948796					(606.2392, 1390.4634)(606.7417, 834.47174)(617.231, 726.0	1210.4646@11.948796		FindByFormula	6	+	1210.4646			11.948796
1210.6334@10.541441					(628.3062, 320.79)(628.8079, 145.51)	1210.6334@10.541441		FindByFormula	1	+	1210.6334			10.541441
1210.6353@9.997115					(617.3337, 185.37)(617.8069, 295.52)(636.2962, 359.3)(636.7	1210.6353@9.997115		FindByFormula	1	+	1210.6353			9.997115
1210.6443@10.313508					(606.3293, 18019.514)(606.83044, 12566.843)(607.3317, 494	1210.6443@10.313508		FindByFormula	6	+	1210.6443			10.313508
1210.7787@23.040709					(606.3945, 32182.822)(606.89484, 21037.098)(607.3998, 887	1210.7787@23.040709		FindByFormula	19	+	1210.7787			23.040709
1211.5614@7.3494577					(606.78986, 1011.24133)(607.2889, 707.49286)(617.7817, 11	1211.5614@7.3494577		FindByFormula	7	+	1211.5614			7.3494577
1212.5859@22.133291					(607.3012, 2170.0398)(607.8017, 1064.4801)(608.29175, 201	1212.5859@22.133291		FindByFormula	7	+	1212.5859			22.133291
1212.753@22.50781					(607.3858, 4265.499)(607.8847, 2483.8281)(608.3865, 1333.	1212.753@22.50781		FindByFormula	21	+	1212.753			22.50781
1216.546@19.763077					(609.281, 1359.8627)(609.7779, 747.7888)(610.2844, 1120.1)	1216.546@19.763077		FindByFormula	8	+	1216.546			19.763077
1216.5483@19.507824					(609.281, 308.925)(609.77893, 83.97)(610.2761, 282.59)	1216.5483@19.507824		FindByFormula	2	+	1216.5483			19.507824
1220.4956@18.800629					(611.259, 1479.7902)(611.7601, 871.862)(612.2581, 512.116)	1220.4956@18.800629		FindByFormula	5	+	1220.4956			18.800629
1229.4987@18.098938					(615.7578, 2127.8257)(616.2581, 1363.9056)(616.75494, 63.	1229.4987@18.098938		FindByFormula	7	+	1229.4987			18.098938
1230.5209@18.384392					(616.2681, 9593.4795)(616.7773, 5622.312)(617.2734, 2654.	1230.5209@18.384392		FindByFormula	6	+	1230.5209			18.384392
1232.4283@18.235004					(617.21643, 6605.8604)(617.7304, 3163.5898)(618.22095, 18	1232.4283@18.235004		FindByFormula	4	+	1232.4283			18.235004

1232.7206@22.085045				(617.36566, 1314.3779)(617.86584, 940.746)(618.3637, 479.	1232.7206@22.085045		FindByFormula	5	+	1232.7206	22.085045
1232.7281@22.32031				(617.3695, 4247.3823)(617.86707, 2532.8572)(618.3665, 132	1232.7281@22.32031		FindByFormula	22	+	1232.7281	22.32031
1234.7437@23.039314				(618.3766, 3710.4304)(618.8742, 2517.6355)(619.3774, 1109	1234.7437@23.039314		FindByFormula	15	+	1234.7437	23.039314
1234.7458@22.752865				(618.3766, 1870.848)(618.8783, 767.12195)(619.3834, 80.39	1234.7458@22.752865		FindByFormula	5	+	1234.7458	22.752865
1242.0122@21.353111				(622.01215, 2301.0017)(622.50604, 1064.8649)(623.0118, 75	1242.0122@21.353111		FindByFormula	6	+	1242.0122	21.353111
1248.5905@10.296051				(625.3013, 1098.4257)(625.8028, 793.2115)(626.298, 376.27	1248.5905@10.296051		FindByFormula	7	+	1248.5905	10.296051
1252.4971@21.35066				(627.56, 2204.284)(628.0553, 1381.408)(628.5087, 600.1)(62	1252.4971@21.35066		FindByFormula	5	+	1252.4971	21.35066
1252.9946@21.345747				(627.5059, 1924.3641)(628.00397, 1100.4043)(628.499, 562.	1252.9946@21.345747		FindByFormula	7	+	1252.9946	21.345747
1254.8029@23.033033				(628.40643, 40907.98)(628.90674, 28866.967)(629.41, 11814	1254.8029@23.033033		FindByFormula	14	+	1254.8029	23.033033
1256.7773@22.507423				(629.39703, 3992.8467)(629.8954, 2448.5737)(630.3933, 150	1256.7773@22.507423		FindByFormula	22	+	1256.7773	22.507423
126.0297@1.4797589				(127.037704, 3013.0037)(149.01622, 302.82748)	126.0297@1.4797589		FindByFormula	8	+	126.0297	1.4797589
126.0305@1.7831684				(127.037415, 2957.2383)(149.01778, 629.6634)	126.0305@1.7831684		FindByFormula	6	+	126.0305	1.7831684
1269.5417@4.962292				(635.77765, 1602.335)(636.2784, 1058.5634)	1269.5417@4.962292		FindByFormula	6	+	1269.5417	4.962292
1270.505@18.84669				(647.252, 287.78)(647.7654, 49.02)(648.2598, 47.69)(648.741	1270.505@18.84669		FindByFormula	1	+	1270.505	18.84669
1270.5171@19.018045				(636.2673, 8996.859)(636.76935, 5806.3237)(637.27167, 266	1270.5171@19.018045		FindByFormula	6	+	1270.5171	19.018045
1273.5255@18.26263				(637.7729, 4475.12)(638.27246, 2989.0461)(638.77454, 1337	1273.5255@18.26263		FindByFormula	7	+	1273.5255	18.26263
1278.7646@23.037779				(640.3893, 4001.7305)(640.8868, 2785.0542)(641.3987, 1408	1278.7646@23.037779		FindByFormula	15	+	1278.7646	23.037779
1285.5272@21.354149				(643.7739, 1499.235)(644.26715, 1846.3275)(644.7711, 2232	1285.5272@21.354149		FindByFormula	4	+	1285.5272	21.354149
129.0578@3.6125422				(130.06506, 7570.9985)(131.06787, 1843.5768)	129.0578@3.6125422		FindByFormula	6	+	129.0578	3.6125422
1296.3391@18.052319				(649.17523, 1299.8483)(649.67694, 735.405)	1296.3391@18.052319		FindByFormula	6	+	1296.3391	18.052319
1298.8184@22.722378				(650.418, 656.44)(650.912, 224.45)	1298.8184@22.722378		FindByFormula	1	+	1298.8184	22.722378
1298.8292@23.027048				(650.4193, 27866.502)(650.9207, 19437.094)(651.4234, 9104	1298.8292@23.027048		FindByFormula	15	+	1298.8292	23.027048
1300.8066@22.50717				(651.4144, 3583.6162)(651.91174, 2170.9824)(652.4127, 125	1300.8066@22.50717		FindByFormula	23	+	1300.8066	22.50717
1304.5859@19.938639				(653.30536, 1373.9316)(653.8105, 911.9084)	1304.5859@19.938639		FindByFormula	6	+	1304.5859	19.938639
1306.6158@8.93452				(654.31525, 1157.6149)(654.81573, 865.73834)(655.31366, 4	1306.6158@8.93452		FindByFormula	6	+	1306.6158	8.93452
1314.5312@19.003178				(658.2744, 6135.718)(658.77893, 4202.064)(659.2807, 1954.	1314.5312@19.003178		FindByFormula	5	+	1314.5312	19.003178
1320.7703@22.341627				(661.3972, 1422.3145)(661.8941, 669.27997)(662.3944, 692.	1320.7703@22.341627		FindByFormula	18	+	1320.7703	22.341627
1320.7839@22.092813				(661.39453, 817.31995)(661.89655, 401.1914)(662.3903, 314	1320.7839@22.092813		FindByFormula	7	+	1320.7839	22.092813
1322.6031@18.199108				(662.3095, 1431.5)(662.81165, 1040.748)(663.31335, 478.5)	1322.6031@18.199108		FindByFormula	5	+	1322.6031	18.199108
1336.5323@19.000364				(669.2753, 2173.965)(669.7757, 1476.9966)(670.27386, 753.	1336.5323@19.000364		FindByFormula	6	+	1336.5323	19.000364
1340.5599@20.775043				(671.2881, 23283.527)(671.78906, 15764.542)(672.29065, 70	1340.5599@20.775043		FindByFormula	7	+	1340.5599	20.775043
1342.8453@23.021261				(672.43286, 20768.85)(672.93365, 15032.58)(673.4368, 7404	1342.8453@23.021261		FindByFormula	18	+	1342.8453	23.021261
1344.5762@20.427486				(673.3009, 1180.866)(673.8017, 689.502)(674.30023, 457.95	1344.5762@20.427486		FindByFormula	5	+	1344.5762	20.427486
1344.818@22.681278				(673.4201, 1263.73)(673.9207, 80.39)(674.4064, 398.49)	1344.818@22.681278		FindByFormula	1	+	1344.818	22.681278
1344.8298@22.509373				(673.4234, 2751.8872)(673.9245, 1568.7163)(674.41595, 153	1344.8298@22.509373		FindByFormula	27	+	1344.8298	22.509373
1350.0544@21.487574				(676.0379, 2738.43)(676.53613, 1461.1051)	1350.0544@21.487574		FindByFormula	6	+	1350.0544	21.487574
1358.568@18.97668				(680.2934, 1971.9183)(680.7969, 1612.1918)(681.297, 729.5	1358.568@18.97668		FindByFormula	6	+	1358.568	18.97668
1358.5696@19.134098				(680.2927, 16754.564)(680.7946, 11967.815)(681.29706, 521	1358.5696@19.134098		FindByFormula	8	+	1358.5696	19.134098
1358.5768@19.134363				(680.296, 905.68)(680.7979, 1007.87)(681.3003, 372.9)	1358.5768@19.134363		FindByFormula	1	+	1358.5768	19.134363
1360.539@21.790722				(681.2671, 459.86)(681.7832, 233.91)(682.2988, 197.29)	1360.539@21.790722		FindByFormula	1	+	1360.539	21.790722
1360.5453@21.476757				(681.3841, 1712.526)(681.8823, 1405.0579)(682.3848, 1120.	1360.5453@21.476757		FindByFormula	5	+	1360.5453	21.476757
1361.0408@21.484573				(681.5284, 2353.8499)(682.0297, 1554.6964)(682.5199, 876.	1361.0408@21.484573		FindByFormula	6	+	1361.0408	21.484573
1362.6011@18.73716				(682.309, 1881.3165)(682.80743, 1505.9233)(683.3098, 660.	1362.6011@18.73716		FindByFormula	6	+	1362.6011	18.73716
1366.7979@22.686644				(684.4123, 838.03)(684.8969, 119.06999)	1366.7979@22.686644		FindByFormula	2	+	1366.7979	22.686644
1366.8147@23.031672				(684.4155, 3070.01)(684.91095, 2268.733)(685.43024, 1968.	1366.8147@23.031672		FindByFormula	14	+	1366.8147	23.031672
1372.5957@19.969269				(687.30695, 888.66113)(687.8046, 717.3228)(688.30005, 417	1372.5957@19.969269		FindByFormula	18	+	1372.5957	19.969269
1382.4766@19.019548				(692.2473, 1417.3717)(692.7492, 907.87164)(693.2563, 528.	1382.4766@19.019548		FindByFormula	6	+	1382.4766	19.019548
1382.4806@19.1701				(692.2463, 373.06)(692.7572, 272.41)(693.2551, 111.96)	1382.4806@19.1701		FindByFormula	1	+	1382.4806	19.1701
1386.8802@23.00639				(694.44476, 12898.498)(694.9446, 9291.311)(695.4496, 5352	1386.8802@23.00639		FindByFormula	19	+	1386.8802	23.00639
1388.6174@20.494795				(695.3162, 1224.6615)(695.81445, 681.49506)(696.31464, 43	1388.6174@20.494795		FindByFormula	6	+	1388.6174	20.494795
1388.8488@22.735203				(695.4256, 1554.42)(695.9408, 223.5)(696.4201, 1005.41)	1388.8488@22.735203		FindByFormula	1	+	1388.8488	22.735203
1388.8547@22.314741				(695.4306, 2553.59)(695.9151, 284.72)(696.4255, 1618.68)	1388.8547@22.314741		FindByFormula	1	+	1388.8547	22.314741
1388.8752@22.508917				(695.4392, 2733.383)(695.9379, 1612.484)(696.42554, 1625.	1388.8752@22.508917		FindByFormula	22	+	1388.8752	22.508917
1394.0824@21.486767				(698.04877, 1119.936)(698.53577, 1067.8121)(699.044, 749.	1394.0824@21.486767		FindByFormula	5	+	1394.0824	21.486767
1401.5758@19.0491				(701.7953, 2500.492)(702.298, 1948.9978)(702.80273, 1050.	1401.5758@19.0491		FindByFormula	7	+	1401.5758	19.0491
1402.5927@19.115122				(702.3051, 4332.062)(702.80884, 3109.36)(703.30853, 1559.	1402.5927@19.115122		FindByFormula	6	+	1402.5927	19.115122
1404.5671@20.50224				(703.29156, 2630.0867)(703.79144, 1903.9432)(704.29047, 1	1404.5671@20.50224		FindByFormula	3	+	1404.5671	20.50224
1406.6229@18.831232				(704.32196, 1798.8434)(704.82056, 1364.3783)(705.32416, 7	1406.6229@18.831232		FindByFormula	6	+	1406.6229	18.831232
1408.5463@20.775045				(705.2828, 1903.1156)(705.7835, 1350.1686)(706.288, 1407.	1408.5463@20.775045		FindByFormula	7	+	1408.5463	20.775045
1410.8372@23.022943				(706.4295, 3287.0693)(706.9282, 2452.4265)(707.4438, 1647	1410.8372@23.022943		FindByFormula	11	+	1410.8372	23.022943
1430.9071@23.017159				(716.45795, 10501.235)(716.9589, 8106.398)(717.46014, 421	1430.9071@23.017159		FindByFormula	17	+	1430.9071	23.017159
1432.636@20.576471				(717.328, 1681.45)(717.82733, 1139.474)(718.3219, 639.787	1432.636@20.576471		FindByFormula	5	+	1432.636	20.576471
1432.8774@22.841396				(717.4449, 392.32)(717.9488, 177.59)	1432.8774@22.841396		FindByFormula	1	+	1432.8774	22.841396
1432.8842@22.508942				(717.4487, 1983.1917)(717.94934, 1104.9164)(718.4472, 107	1432.8842@22.508942		FindByFormula	19	+	1432.8842	22.508942
1435.7126@12.813649				(718.8647, 1258.8184)(719.36566, 1012.47833)(719.86694, 5	1435.7126@12.813649		FindByFormula	6	+	1435.7126	12.813649
1445.5927@19.002205				(723.7984, 1441.8151)(724.3083, 1054.0916)(724.80695, 809	1445.5927@19.002205		FindByFormula	6	+	1445.5927	19.002205
1446.6211@19.246643				(724.31885, 6314.7646)(724.8176, 4745.3604)(725.3254, 234	1446.6211@19.246643		FindByFormula	9	+	1446.6211	19.246643
1448.5474@19.139809				(725.2845, 1545.465)(725.7819, 1132.8016)(726.285, 739.90	1448.5474@19.139809		FindByFormula	6	+	1448.5474	19.139809
1450.6497@18.902102				(726.3325, 1846.9219)(726.83044, 1468.562)(727.3345, 828.	1450.6497@18.902102		FindByFormula	5	+	1450.6497	18.902102
1454.8629@22.74731				(728.4435, 1642.71)(728.9443, 1467.35)(729.4422, 931.22)(7	1454.8629@22.74731		FindByFormula	1	+	1454.8629	22.74731
1454.8632@23.030483				(728.44403, 2235.7295)(728.9401, 1653.6278)(729.4492, 121	1454.8632@23.030483		FindByFormula	14	+	1454.8632	23.030483
1474.927@23.01443				(738.4704, 10223.314)(738.97144, 8243.648)(739.4744, 4123	1474.927@23.01443		FindByFormula	19	+	1474.927	23.01443
1478.96@19.788363				(740.491, 1085.7458)(740.9952, 1017.99854)(741.48584, 602	1478.96@19.788363		FindByFormula	27	+	1478.96	19.788363
1484.9901@19.787737				(743.50256, 3721.9255)(744.0043, 3540.8215)(744.50476, 20	1484.9901@19.787737		FindByFormula	28	+	1484.9901	19.787737
1484.9976@19.447369				(743.5048, 1524.3987)(744.00696, 1448.6161)(744.508, 821.	1484.9976@19.447369		FindByFormula	28	+	1484.9976	19.447369
1486.6162@19.758654				(744.3127, 6485.7095)(744.81323, 5031.525)(745.3166, 2567	1486.6162@19.758654		FindByFormula	6	+	1486.6162	19.758654
1489.6285@19.128792				(745.8191, 2781.5117)(746.32275, 2100.9133)(746.81665, 13	1489.6285@19.128792		FindByFormula	6	+	1489.6285	19.128792
1494.6759@18.967403				(748.34607, 1588.765)(748.84314, 1239.28)(749.34326, 629.	1494.6759@18.967403		FindByFormula	4	+	1494.6759	18.967403
1501.6198@21.599972				(751.94037, 959.6975)(752.44385, 1290.735)	1501.6198@21.599972		FindByFormula	4	+	1501.6198	21.599972
1518.9471@23.276976				(760.4729, 173.44)(760.9838, 305.42)	1518.9471@23.276976		FindByFormula	1	+	1518.9471	23.276976
1518.9559@23.012383				(760.4847, 3895.421)(760.9841, 3128.3801)(761.4834, 2005.	1518.9559@23.012383		FindByFormula	12	+	1518.9559	23.012383
1518.9652@22.710419				(760.4869, 682.61)(760.9704, 108.3)(761.4957, 855.55)	1518.9652@22.710419		FindByFormula	1	+	1518.9652	22.710419
1523.924@22.07626				(762.9852, 125.99)(763.4568, 112.65)	1523.924@22.07626		FindByFormula	1	+	1523.924	22.07626
1523.9325@22.287415				(762.97504, 11545.587)(763.48004, 9628.307)(763.97797, 55	1523.9325@22.287415		FindByFormula	14	+	1523.9325	22.287415
1523.9374@22.582985				(762.9626, 107.6)(763.4806, 324.91)(763.9644, 209.57)(773.	1523.9374@22.582985		FindByFormula	2	+	1523.9374	22.582985
1529.95@22.317139				(765.98444, 20540.73)(766.48615, 17246.785)(766.9868, 848	1529.95@22.317139		FindByFormula	6	+	1529.95	22.317139
1530.6337@19.741968				(766.32275, 3350.2598)(766.8244, 2618.7717)(767.3257, 143	1530.6337@19.741968		FindByFormula	6	+	1530.6337	19.741968
1534.6768@19.455566				(768.3454, 1430.7916)(768.843, 1162.92)(769.343, 723.6401)	1534.6768@19.455566		FindByFormula	6	+	1534.6768	19.455566
1535.682@9.172261				(768.84863, 2862.8633)(769.34906, 2282.825)(769.8497, 109	1535.682@9.172261		FindByFormula	6	+	1535.682	9.172261
1546.945@19.785664				(774.4871, 5956.8306)(774.9888, 5782.981)(775.4897, 3301.	1546.945@19.785664		FindByFormula	28	+	1546.945	19.785664
1553.0778@24.505095				(777.54626, 11182.764)(778.0436, 10586.313)(778.5449, 691	1553.0778@24.505095		FindByFormula	10	+	1553.0778	24.505095
1555.9681@22.30349				(778.9931, 1118.4618)(779.4921, 1150.105)(779.9917, 646.1	1555.9681@22.30349		FindByFormula	6	+	1555.9681	22.30349
1556.659@21.285112				(779.3363, 15641.538)(779.8369, 11967.076)(780.3385, 6172	1556.659@21.285112		FindByFormula	7	+	1556.659	21.285112
1574.6628@19.832047				(788.34076, 13058.669)(788.8413, 10524.061)(789.34424, 53	1574.6628@19.832047		FindByFormula	6	+	1574.6628	19.832047
1577.0564@24.162605				(789.54156, 947.2867)(790.0449, 236.88167)(790.537, 1895.	1577.0564@24.162605		FindByFormula	6	+	1577.0564	24.162605
1577.0839@24.47486				(789.54645, 5344.3784)(790.04663, 3583.0369)(790.54987, 3	1577.0839@24.47486		FindByFormula	6	+	1577.0839	24.47486
1577.9546@22.163162				(789.98224, 2090.4817)(790.48486, 2247.6067)(790.9842, 10	1577.9546@22.163162		FindByFormula	6	+	1577.9546	22.163162
1578.6978@19.516186				(790.3583, 1433.3981)(790.8552, 1165.048)(791.35645, 619.	1578.6978@19.516186		FindByFormula	5	+	1578.6978	19.516186
1581.0741@24.434238				(792.5506, 8014.1484)(793.0518, 4124.7617)	1581.0741@24.434238		FindByFormula	10	+	1581.0741	24.434238
1583.0872@24.490883				(792.55096, 8283.944)(793.05176, 6189.4907)(793.55304, 85	1583.0872@24.490883		FindByFormula	11	+	1583.0872	24.490883
159.1285@0.87767106				(160.13902, 6697.3164)(161.14104, 919.57666)	159.1285@0.87767106		FindByFormula	3	+	159.1285	0.87767106
159.1288@0.7218033				(160.13806, 33902.22)(161.14073, 3209.974)	159.1288@0.7218033		FindByFormula	5	+	159.1288	0.7218033
1591.9208@22.310865				(796.96875, 12561.038)(797.4704, 10640.461)(797.9747, 532	1591.9208@22.310865		FindByFormula	7	+	1591.9208	22.310865
1591.9272@22.629114				(796.9715, 607.52997)(797.47015, 430.95334)(797.9591, 468	1591.9272@22.629114		FindByFormula	3	+	1591.9272	22.629114
1595.9323@22.416012				(810.4795, 318.56)(810.9647, 89.22)(811.4502, 171.98)	1595.9323@22.416012		FindByFormula	1	+	1595.9323	22.416012
1595.947@22.12218				(798.976, 1455.4398)(799.47906, 1353.8877)(799.98303, 154	1595.947@22.12218		FindByFormula	9	+	1595.947	22.12218
1597.939@22.312796				(799.97833, 11462.446)(800.4797, 9565.417)(800.98145, 464	1597.939@22.312796		FindByFormula	6	+	1597.939	22.312796
1597.951@22.57967				(799.96436, 204.275)(800.4817, 595.635)(800.9942, 180.01)(	1597.951@22.57967		FindByFormula	2	+	1597.951	22.57967
16:0 LYSO PC (CAS# 17364-16-8); (M+H)+	16:0 LYSO PC (CAS# 17364-16-8); (M+H)+	16:0 LYSO PC (CAS# 17364-16-8); (M+H)+ [, tgt=95.95, ove	17364-16-8	(496.3392, 156863.53)(497.3403, 42354.434)(498.33963, 793	16:0 LYSO PC (CAS# 17364-16-8); (M+H)+		FindByFormula	13	+	495.3292	22.295322
16:0 LYSO PC (CAS# 17364-16-8); (M+Na)+	16:0 LYSO PC (CAS# 17364-16-8); (M+Na)+	16:0 LYSO PC (CAS# 17364-16-8); (M+Na)+ [, tgt=94.05, o	17364-16-8	(518.3228, 237278.23)(519.32556, 65116.895)(520.3286, 123	16:0 LYSO PC (CAS# 17364-16-8); (M+Na)+		FindByFormula	28	+	495.3343	22.316336
16:0-18:0 PC (CAS# 59403-51-9); (M+H)+	16:0-18:0 PC (CAS# 59403-51-9); (M+H)+	16:0-18:0 PC (CAS# 59403-51-9); (M+H)+ [, tgt=52.78, ove	59403-51-9	(762.6017, 1797.76)(763.6141, 785.07)	16:0-18:0 PC (CAS# 59403-51-9); (M+H)+		FindByFormula	1	+	761.5971	25.594742
16:0-18:0 PC (CAS# 59403-51-9); (M+Na)+	16:0-18:0 PC (CAS# 59403-51-9); (M+Na)+	16:0-18:0 PC (CAS# 59403-51-9); (M+Na)+ [, tgt=44.28, ov	59403-51-9	(784.584, 12262.284)(785.59076, 5525.7397)(786.59595, 236	16:0-18:0 PC (CAS# 59403-51-9); (M+Na)+		FindByFormula	7	+	761.5943	25.60165
1601.0638@24.431795				(801.543, 2868.0068)(802.04266, 2825.9402)(802.54565, 457	1601.0638@24.431795		FindByFormula	6	+	1601.0638	24.431795
1601.9493@22.090096				(801.98413, 2418.1235)(802.4881, 2333.09)(802.9894, 1333.	1601.9493@22.090096		FindByFormula	9	+	1601.9493	22.090096
1603.0817@24.532478				(802.5493, 2705.87)(803.0477, 1603.14)	1603.0817@24.532478		FindByFormula	1	+	1603.0817	24.532478
1608.9333@19.784367				(805.4739, 3024.8616)(805.9738, 2827.8232)(806.475, 1876.	1608.9333@19.784367		FindByFormula	27	+	1608.9333	19.784367
1614.941@19.78335				(808.48016, 2376.0566)(808.98175, 2269.947)(809.48193, 13	1614.941@19.78335		FindByFormula	27	+	1614.941	19.78335
1618.6906@19.80102				(810.3538, 2123.8687)(810.85187, 1666.5)(811.35394, 889.8	1618.6906@19.80102		FindByFormula	7	+	1618.6906	19.80102
1621.0645@24.825544				(811.5452, 271.79)(812.0375, 375.94)(812.5365, 161.38)	1621.0645@24.825544		FindByFormula	1	+	1621.0645	24.825544
1621.0653@24.510847				(811.5334, 7288.695)(812.0369, 5804.266)(812.54846, 9854.	1621.0653@24.510847		FindByFormula	11	+	1621.0653	24.510847
1624.6503@21.286255				(813.333, 1511.0813)(813.8254, 1103.9828)(814.3295, 998.6	1624.6503@21.286255		FindByFormula	7	+	1624.6503	21.286255
1625.9518@22.15791				(814.2578, 3917.5413)(814.48706, 2577.6848)(814.9864, 120	1625.9518@22.15791		FindByFormula	13	+	1625.9518	22.15791
1631.0804@24.398626				(816.5519, 10995.355)(817.0537, 7863.3223)(817.55365, 725	1631.0804@24.398626		FindByFormula	8	+	1631.0804	24.398626
1635.1165@24.681023				(818.56464, 13901.415)(819.06464, 3763.2812)(819.5698, 73	1635.1165@24.681023		FindByFormula	11	+	1635.1165	24.681023
1635.1207@24.295227				(818.5668, 132.01)(819.0689, 63.6)	1635.1207@24.295227		FindByFormula	1	+	1635.1207	24.295227
1639.1426@25.157448				(820.58496, 10265.229)(821.0829, 9102.743)(821.58575, 592	1639.1426@25.157448		FindByFormula	5	+	1639.1426	25.157448
1645.0646@24.474503				(823.53534, 6233.687)(824.04004, 2602.98)(824.5406, 3472.	1645.0646@24.474503		FindByFormula	3	+	1645.0646	24.474503
1659.9058@22.308292				(830.964, 5009.6133)(831.46765, 4581.1143)(831.9649, 2315	1659.9058@22.308292		FindByFormula	7	+	1659.9058	22.308292
1662.72@19.908825				(832.3685, 4884.5063)(832.86365, 4321.6416)(833.37054, 23	1662.72@19.908825		FindByFormula	7	+	1662.72	19.908825
1665.9261@22.308792				(833.9715, 6624.4116)(834.47394, 5841.1016)(834.9755, 301	1665.9261@22.308792		FindByFormula	6	+	1665.9261	22.308792
1669.0471@24.240847				(835.5337, 7504.3403)(836.02124, 1219.405)(836.5335, 2564	1669.0471@24.240847		FindByFormula	2	+	1669.0471	24.240847
1669.0566@24.432535				(835.53644, 7215.3936)(836.0378, 7168.0444)(836.5394, 447	1669.0566@24.432535		FindByFormula	5	+	1669.0566	24.432535
1669.0571@24.6296				(835.5288, 135.93)(836.041, 295.56)	1669.0571@24.6296		FindByFormula	1	+	1669.0571	24.6296
1683.0399@24.510218				(842.52594, 10316.563)(843.02423, 1623.7942)(843.5296, 51	1683.0399@24.510218		FindByFormula	16	+	1683.0399	24.510218
1689.0492@24.522396				(845.5301, 6739.711)(846.0309, 6047.315)(846.53424, 6488.	1689.0492@24.522396		FindByFormula	10	+	1689.0492	24.522396
1689.0563@24.295227				(845.5343, 224.5)(846.043, 33.74)	1689.0563@24.295227		FindByFormula	1	+	1689.0563	24.295227
1702.7167@20.333158				(852.3643, 1770.6616)(852.8625, 1551.9517)(853.3669, 922.	1702.7167@20.333158		FindByFormula	6	+	1702.7167	20.333158
1705.7194@19.802855				(853.8686, 1279.9467)(854.36945, 1045.5566)(854.86707, 66	1705.7194@19.802855		FindByFormula	6	+	1705.7194	19.802855
1713.0625@24.46976				(857.53705, 2760.848)(858.02936, 2387.1533)(858.53735, 22	1713.0625@24.46976		FindByFormula	9	+	1713.0625	24.46976
1717.0374@24.148113				(859.5263, 1648.11)(860.0179, 459.88)(860.5382, 847.07)(86	1717.0374@24.148113		FindByFormula	1	+	1717.0374	24.148113
1717.0446@24.390936				(860.2017, 3013.3584)(860.7072, 644.4134)(861.206, 2210.0	1717.0446@24.390936		FindByFormula	6	+	1717.0446	24.390936
1727.8899@22.318472				(864.95685, 2886.0017)(865.45996, 2562.7766)(865.96063, 1	1727.8899@22.318472		FindByFormula	6	+	1727.8899	22.318472
1731.0343@24.437866				(866.52496, 6062.7896)(867.02124, 1035.4017)(867.5266, 21	1731.0343@24.437866		FindByFormula	6	+	1731.0343	24.437866
1733.9208@22.305954				(867.9658, 6028.85)(868.4676, 5356.487)(868.96783, 2806.2	1733.9208@22.305954		FindByFormula	6	+	1733.9208	22.305954
1737.0597@24.639109				(869.5414, 865.01)(870.0257, 242.0)(870.536, 861.12)(871.02	1737.0597@24.639109		FindByFormula	1	+	1737.0597	24.639109
1737.06@24.43337				(869.5292, 4503.6133)(870.03, 4123.3647)(870.5293, 3848.1	1737.06@24.43337		FindByFormula	9	+	1737.06	24.43337
1745.085@25.511362				(873.5495, 456.02)(874.0682, 139.47)	1745.085@25.511362		FindByFormula	1	+	1745.085	25.511362
1745.1005@25.172152				(873.55884, 7966.363)(874.05884, 6681.1177)	1745.1005@25.172152		FindByFormula	4	+	1745.1005	25.172152
1751.0331@24.530985				(876.6696, 3525.14)(877.1578, 2376.4116)(877.52325, 2005.	1751.0331@24.530985		FindByFormula	7	+	1751.0331	24.530985
1761.0497@24.610268				(881.5316, 730.285)(882.0392, 121.130005)	1761.0497@24.610268		FindByFormula	2	+	1761.0497	24.610268
1761.0632@24.385778				(881.5398, 2245.5366)(882.03253, 1411.4834)(882.5274, 137	1761.0632@24.385778		FindByFormula	3	+	1761.0632	24.385778
1785.0455@24.36731				(893.5305, 2280.3525)(894.02966, 2034.78)(894.5305, 1998.	1785.0455@24.36731		FindByFormula	4	+	1785.0455	24.36731
1785.0562@24.577515				(893.5378, 1863.04)(894.0217, 427.82)(894.5373, 1091.58)(	1785.0562@24.577515		FindByFormula	1	+	1785.0562	24.577515
1790.7694@20.384197				(896.3914, 3197.6218)(896.8901, 3007.8738)(897.39087, 163	1790.7694@20.384197		FindByFormula	6	+	1790.7694	20.384197
1799.0613@24.436441				(900.5356, 2303.23)(901.0161, 1312.44)(901.5227, 1102.25)(	1799.0613@24.436441		FindByFormula	1	+	1799.0613	24.436441
17ALPHA,20ALPHA-DIHYDROXYPREGN-4-EN-3	17ALPHA,20ALPHA-DIHYDROXYPREGN-4-EN-3	17ALPHA,20ALPHA-DIHYDROXYPREGN-4-EN-3-ONE (CAS#	652-69-7	(355.22308, 1181.24)(356.22803, 111.63)	17ALPHA,20ALPHA-DIHYDROXYPREGN-4-EN-3-ONE (CAS# 652-69-7); (M+Na)+		FindByFormula	2	+	332.2334	17.62857
17ALPHA-HYDROXYPROGESTERONE (CAS# 68-	17ALPHA-HYDROXYPROGESTERONE (CAS# 68-	17ALPHA-HYDROXYPROGESTERONE (CAS# 68-96-2); (M+N	68-96-2	(353.2168, 1156.1)(354.2167, 287.86)(355.2063, 559.41)	17ALPHA-HYDROXYPROGESTERONE (CAS# 68-96-2); (M+Na)+	C01176	FindByFormula	1	+	330.2224	17.727402
18:0 LYSO-PE (CAS# 69747-55-3); (2M+H)+	18:0 LYSO-PE (CAS# 69747-55-3); (2M+H)+	18:0 LYSO-PE (CAS# 69747-55-3); (2M+H)+ [, tgt=43.55, o	69747-55-3	(963.6501, 325.79)(964.6401, 148.29)(965.6481, 40.71)	18:0 LYSO-PE (CAS# 69747-55-3); (2M+H)+		FindByFormula	1	+	481.3215	22.949585
18:0 LYSO-PE (CAS# 69747-55-3); (2M+Na)+	18:0 LYSO-PE (CAS# 69747-55-3); (2M+Na)+	18:0 LYSO-PE (CAS# 69747-55-3); (2M+Na)+ [, tgt=59.31,	69747-55-3	(985.6322, 799.39)(986.6213, 329.02)(987.6015, 247.2)	18:0 LYSO-PE (CAS# 69747-55-3); (2M+Na)+		FindByFormula	1	+	481.3161	22.72806
18:0 LYSO-PE (CAS# 69747-55-3); (M+H)+	18:0 LYSO-PE (CAS# 69747-55-3); (M+H)+	18:0 LYSO-PE (CAS# 69747-55-3); (M+H)+ [, tgt=67.09, ov	69747-55-3	(482.32343, 2716.875)(483.32385, 1450.245)(484.325, 601.3	18:0 LYSO-PE (CAS# 69747-55-3); (M+H)+		FindByFormula	2	+	481.3124	22.74086
18:0 LYSO-PE (CAS# 69747-55-3); (M+Na)+	18:0 LYSO-PE (CAS# 69747-55-3); (M+Na)+	18:0 LYSO-PE (CAS# 69747-55-3); (M+Na)+ [, tgt=63.33, o	69747-55-3	(504.3071, 4591.98)(505.3205, 1661.89)(506.3255, 164.61)	18:0 LYSO-PE (CAS# 69747-55-3); (M+Na)+		FindByFormula	1	+	481.3208	22.691294
1805.02@24.618654				(903.5192, 145.35)(904.018, 188.45)	1805.02@24.618654		FindByFormula	1	+	1805.02	24.618654
1805.0333@24.410915				(903.5227, 2025.0913)(904.02386, 1959.4502)(904.52295, 16	1805.0333@24.410915		FindByFormula	8	+	1805.0333	24.410915
1819.008@24.514679				(910.512, 6923.7456)(911.0115, 1272.5687)(911.5142, 3660.	1819.008@24.514679		FindByFormula	15	+	1819.008	24.514679
1825.0208@24.524853				(913.5177, 1643.0145)(914.0172, 1159.9769)(914.51697, 896	1825.0208@24.524853		FindByFormula	13	+	1825.0208	24.524853
1834.7926@20.350834				(918.40173, 1469.468)(918.904, 1292.178)(919.4044, 883.49	1834.7926@20.350834		FindByFormula	5	+	1834.7926	20.350834
1849.0095@24.461954				(925.5189, 1048.217)(926.0146, 826.3343)(926.5088, 658.89	1849.0095@24.461954		FindByFormula	7	+	1849.0095	24.461954
1866.994@24.429123				(934.5035, 9094.385)(935.00946, 1416.4883)(935.5066, 5482	1866.994@24.429123		FindByFormula	6	+	1866.994	24.429123
1867.0255@24.184488				(934.5176, 1012.03503)(934.99536, 194.065)(935.51605, 609	1867.0255@24.184488		FindByFormula	2	+	1867.0255	24.184488
1873.0077@24.44233				(937.5149, 1900.8524)(938.0144, 1270.4974)(938.5129, 789.	1873.0077@24.44233		FindByFormula	8	+	1873.0077	24.44233
1873.0225@24.628525				(937.5176, 856.67505)(938.0113, 212.895)(938.51886, 534.1	1873.0225@24.628525		FindByFormula	2	+	1873.0225	24.628525
1875.0465@25.186728				(938.53845, 7161.3965)(939.0379, 1410.5775)(939.54285, 39	1875.0465@25.186728		FindByFormula	8	+	1875.0465	25.186728
1878.8181@20.440306				(940.41656, 2272.6128)(940.91754, 2170.0356)(941.4171, 13	1878.8181@20.440306		FindByFormula	7	+	1878.8181	20.440306
1910.9805@24.502874				(956.49976, 767.53375)(956.9988, 418.5791)(957.5021, 1242	1910.9805@24.502874		FindByFormula	11	+	1910.9805	24.502874
1935.0217@24.423288				(968.51746, 1506.9125)(968.9993, 936.01495)(969.4958, 509	1935.0217@24.423288		FindByFormula	4	+	1935.0217	24.423288
1959.3063@19.789024				(981.551, 3477.5654)(982.05414, 735.7256)(982.55396, 2622	1959.3063@19.789024		FindByFormula	9	+	1959.3063	19.789024
1988.8392@21.715416				(995.4325, 1703.6577)(995.9346, 1671.438)(996.4363, 1176.	1988.8392@21.715416		FindByFormula	9	+	1988.8392	21.715416
1-AMINOCYCLOPROPANE-1-CARBOXYLATE (C	1-AMINOCYCLOPROPANE-1-CARBOXYLATE (C	1-AMINOCYCLOPROPANE-1-CARBOXYLATE (CAS# 22059-2	22059-21-8	(102.05531, 1401.1544)(103.05335, 61.81572)	1-AMINOCYCLOPROPANE-1-CARBOXYLATE (CAS# 22059-21-8); (	C01234	FindByFormula	21	+	101.0475	1.0208106
1-METHYLADENOSINE (CAS# 15763-06-1); (M	1-METHYLADENOSINE (CAS# 15763-06-1); (M	1-METHYLADENOSINE (CAS# 15763-06-1); (M+H)+ [, tgt=	15763-06-1	(282.12097, 1361.6052)(283.11884, 342.675)(284.1146, 449.	1-METHYLADENOSINE (CAS# 15763-06-1); (M+H)+		FindByFormula	10	+	281.1118	3.0267305
1-METHYLADENOSINE (CAS# 15763-06-1); (M	1-METHYLADENOSINE (CAS# 15763-06-1); (M	1-METHYLADENOSINE (CAS# 15763-06-1); (M+Na)+ [, tgt	15763-06-1	(304.1024, 347.25)(305.098, 132.44)	1-METHYLADENOSINE (CAS# 15763-06-1); (M+Na)+		FindByFormula	1	+	281.1112	3.0130434
1-METHYLXANTHINE (CAS# 6136-37-4); (M+H	1-METHYLXANTHINE (CAS# 6136-37-4); (M+H	1-METHYLXANTHINE (CAS# 6136-37-4); (M+H)+ [, tgt=37.	6136-37-4	(167.0574, 5726.75)(168.06274, 1139.17)(169.0549, 104.64)	1-METHYLXANTHINE (CAS# 6136-37-4); (M+H)+		FindByFormula	2	+	166.0507	2.4305089
1-METHYLXANTHINE (CAS# 6136-37-4); (M+N	1-METHYLXANTHINE (CAS# 6136-37-4); (M+N	1-METHYLXANTHINE (CAS# 6136-37-4); (M+Na)+ [, tgt=7	6136-37-4	(189.03862, 1589.0625)(190.04218, 170.335)	1-METHYLXANTHINE (CAS# 6136-37-4); (M+Na)+		FindByFormula	4	+	166.0504	2.5780108
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+H)+ [, tgt=	111-03-5	(357.2983, 4404.5933)(358.29834, 1142.9166)(359.30798, 52	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+H)+		FindByFormula	3	+	356.2903	22.77241

1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+H)+[-H2O]	111-03-5	(339.28714, 10071.667)(340.28882, 2248.5935)(341.2917, 35	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+H)+[-H2O]		FindByFormula	3	+	356.2897	22.86943
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+Na)+ [, tgt	111-03-5	(379.2823, 47341.496)(380.28552, 10879.22)(381.2935, 5312	1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+Na)+		FindByFormula	26	+	356.294	22.700436
1-PHENYLETHANOL (CAS# 1445-91-6); (M+H)	1-PHENYLETHANOL (CAS# 1445-91-6); (M+H)+	1-PHENYLETHANOL (CAS# 1445-91-6); (M+H)+[-H2O] [, tg	1445-91-6	(105.0693, 655.21)(106.0738, 20.48)	1-PHENYLETHANOL (CAS# 1445-91-6); (M+H)+[-H2O]	C11348	FindByFormula	1	+	122.0726	2.8821123
2-(DIPHENYLMETHOXY)-N-METHYLETHYLAMI	2-(DIPHENYLMETHOXY)-N-METHYLETHYLAMI	2-(DIPHENYLMETHOXY)-N-METHYLETHYLAMINE (CAS# 17	17471-10-2	(242.15305, 396.49)(243.15495, 100.869995)	2-(DIPHENYLMETHOXY)-N-METHYLETHYLAMINE (CAS# 17471-10-2); (M+H)+		FindByFormula	2	+	241.1457	11.024316
2',3'-CYCLIC CMP (CAS# 0); (M+H)+	2',3'-CYCLIC CMP (CAS# 0); (M+H)+	2',3'-CYCLIC CMP (CAS# 0); (M+H)+ [, tgt=81.67, overall=81.67]		(306.0471, 445.98)(307.0486, 33.93)	2',3'-CYCLIC CMP (CAS# 0); (M+H)+		FindByFormula	1	+	305.0397	0.732002
2,4-DIHYDROXYPTERIDINE (CAS# 487-21-8); (M	2,4-DIHYDROXYPTERIDINE (CAS# 487-21-8); (M	2,4-DIHYDROXYPTERIDINE (CAS# 487-21-8); (M+Na)+ [, tg	487-21-8	(187.02252, 1270.6649)(188.02063, 65.183334)	2,4-DIHYDROXYPTERIDINE (CAS# 487-21-8); (M+Na)+	C03212	FindByFormula	6	+	164.0329	1.6853514
20:0 LYSO PC (CAS# 108341-80-6); (M+Na)+	20:0 LYSO PC (CAS# 108341-80-6); (M+Na)+	20:0 LYSO PC (CAS# 108341-80-6); (M+Na)+ [, tgt=15.20, c	108341-80-6	(574.3814, 2583.1965)(575.3921, 1556.41)(576.3822, 193.41)	20:0 LYSO PC (CAS# 108341-80-6); (M+Na)+		FindByFormula	6	+	551.4002	22.924753
226.0954@3.0594227				(227.10277, 1504.3165)(228.10336, 146.76477)(249.08623, 1	226.0954@3.0594227		FindByFormula	24	+	226.0954	3.0594227
24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M+	24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M+	24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M+Na)+ [, tgt=	60037-60-7	(837.68427, 56325.426)(838.68866, 29394.627)(839.69574, 9	24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M+Na)+		FindByFormula	3	+	814.6961	27.872147
25-HYDROXYCHOLESTEROL (CAS# 2140-46-7);	25-HYDROXYCHOLESTEROL (CAS# 2140-46-7);	25-HYDROXYCHOLESTEROL (CAS# 2140-46-7); (M+H)+[-H2	2140-46-7	(385.3475, 2053.92)(386.3475, 502.15)	25-HYDROXYCHOLESTEROL (CAS# 2140-46-7); (M+H)+[-H2O]	C15519	FindByFormula	1	+	402.3501	22.625874
25-HYDROXYCHOLESTEROL (CAS# 2140-46-7);	25-HYDROXYCHOLESTEROL (CAS# 2140-46-7);	25-HYDROXYCHOLESTEROL (CAS# 2140-46-7); (M+Na)+ [,	2140-46-7	(425.33786, 1104.7101)(426.3407, 382.9825)(427.3429, 1345	25-HYDROXYCHOLESTEROL (CAS# 2140-46-7); (M+Na)+	C15519	FindByFormula	4	+	402.348	22.973598
260.136@2.8055449				(261.14545, 375.91)(262.138, 112.85)(243.1365, 190.58)	260.136@2.8055449		FindByFormula	2	+	260.136	2.8055449
260.1374@3.1285338				(261.14447, 1836.6664)(262.1442, 334.84653)(243.1343, 142	260.1374@3.1285338		FindByFormula	23	+	260.1374	3.1285338
284.0765@2.291664				(285.08527, 1767.189)(286.08667, 261.81122)(307.06567, 18	284.0765@2.291664		FindByFormula	25	+	284.0765	2.291664
2-AMINOBUTANOATE (CAS# 2623-91-8); (M+	2-AMINOBUTANOATE (CAS# 2623-91-8); (M+	2-AMINOBUTANOATE (CAS# 2623-91-8); (M+H)+ [, tgt=4	2623-91-8	(104.07006, 733.8083)(105.07357, 41.148335)	2-AMINOBUTANOATE (CAS# 2623-91-8); (M+H)+	C02261	FindByFormula	6	+	103.0627	0.84966606
2-AMINOETHYL DIHYDROGEN PHOSPHATE (C	2-AMINOETHYL DIHYDROGEN PHOSPHATE (C	2-AMINOETHYL DIHYDROGEN PHOSPHATE (CAS# 1071-23	1071-23-4	(142.02654, 1908.6741)(143.02771, 54.988)(144.02275, 59.5	2-AMINOETHYL DIHYDROGEN PHOSPHATE (CAS# 1071-23-4); (M+H)+		FindByFormula	5	+	141.0195	0.8204009
2'-DEOXYCYTIDINE 5'-MONOPHOSPHATE (CAS	2'-DEOXYCYTIDINE 5'-MONOPHOSPHATE (CAS	2'-DEOXYCYTIDINE 5'-MONOPHOSPHATE (CAS# 1032-65-1	1032-65-1	(308.0631, 1230.27)(309.06958, 37.7)(310.07062, 37.4)	2'-DEOXYCYTIDINE 5'-MONOPHOSPHATE (CAS# 1032-65-1); (M+	C00239	FindByFormula	2	+	307.0571	1.0990279
2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Na	2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Na	2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Na)+ [, tgt=62.	154-17-6	(187.05919, 3442.3398)(188.0607, 290.09747)(189.0496, 497	2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Na)+	C00586	FindByFormula	4	+	164.0689	0.7237514
2'-DEOXYINOSINE (CAS# 890-38-0); (2M+Na)+	2'-DEOXYINOSINE (CAS# 890-38-0); (2M+Na)+	2'-DEOXYINOSINE (CAS# 890-38-0); (2M+Na)+ [, tgt=73.3	890-38-0	(527.16254, 687.02325)(528.16504, 175.19)(529.1679, 61.21)	2'-DEOXYINOSINE (CAS# 890-38-0); (2M+Na)+		FindByFormula	3	+	252.0862	2.0910187
2'-DEOXYINOSINE (CAS# 890-38-0); (M+Na)+	2'-DEOXYINOSINE (CAS# 890-38-0); (M+Na)+	2'-DEOXYINOSINE (CAS# 890-38-0); (M+Na)+ [, tgt=63.75,	890-38-0	(275.07706, 2848.0918)(276.0755, 418.57077)(277.07645, 10	2'-DEOXYINOSINE (CAS# 890-38-0); (M+Na)+		FindByFormula	14	+	252.0874	2.0788786
2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 40	2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 40	2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 4026-18-0); (M	4026-18-0	(141.0533, 6423.0195)(142.05457, 253.37334)(143.05597, 31	2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 4026-18-0); (M+Na)+		FindByFormula	3	+	118.064	3.5107143
2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (C	2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (C	2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-	583-91-5	(133.0316, 1188.38)(134.0287, 164.06)	2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-5); (M+H)+[-H2O]		FindByFormula	1	+	150.0342	3.0000594
2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (C	2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (C	2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-	583-91-5	(173.0237, 1053.9)(174.0294, 135.6)	2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-5); (M+Na)+		FindByFormula	1	+	150.0348	3.3930058
2-HYDROXYBUTYRATE (CAS#); (M+Na)+	2-HYDROXYBUTYRATE (CAS#); (M+Na)+	2-HYDROXYBUTYRATE (CAS#); (M+Na)+ [, tgt=85.02, overall=85.02]		(127.037254, 3337.6282)(128.03766, 157.058)(129.0437, 26.3	2-HYDROXYBUTYRATE (CAS#); (M+Na)+		FindByFormula	10	+	104.0478	1.6686058
2-METHYLGLUTARIC ACID (CAS# 18069-17-5);	2-METHYLGLUTARIC ACID (CAS# 18069-17-5);	2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M+H)+[-H2	18069-17-5	(129.05437, 560.3416)(130.05405, 63.535)	2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M+H)+[-H2O]		FindByFormula	6	+	146.0574	3.5264676
2-METHYLGLUTARIC ACID (CAS# 18069-17-5);	2-METHYLGLUTARIC ACID (CAS# 18069-17-5);	2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M+Na)+ [,	18069-17-5	(169.04782, 4079.1262)(170.04883, 118.23385)(171.0475, 44	2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M+Na)+		FindByFormula	13	+	146.0586	3.5313034
2-METHYLPROPANAL OXIME (CAS# 151-00-8);	2-METHYLPROPANAL OXIME (CAS# 151-00-8);	2-METHYLPROPANAL OXIME (CAS# 151-00-8); (M+H)+[-H	151-00-8	(70.0655, 17700.52)(71.06755, 889.1107)	2-METHYLPROPANAL OXIME (CAS# 151-00-8); (M+H)+[-H2O]	C03219	FindByFormula	14	+	87.0692	0.8236431
3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-9	3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-9	3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M+H)	6482-98-0	(183.06465, 1392.6278)(184.06938, 130.75357)(185.06744, 1	3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M+H)+	C03672	FindByFormula	14	+	182.0578	3.7124324
3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-9	3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-9	3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M+Na	6482-98-0	(205.04663, 2454.7344)(206.05011, 252.16556)(207.0416, 31	3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M+Na)+	C03672	FindByFormula	9	+	182.0576	3.7946167
3,3'-DITHIODIVALINE (PENICILLAMINE SS DIM	3,3'-DITHIODIVALINE (PENICILLAMINE SS DIM	3,3'-DITHIODIVALINE (PENICILLAMINE SS DIMER) (CAS# 2	20902-45-8	(297.091, 1356.32)(298.0938, 83.21)(299.1004, 45.7)	3,3'-DITHIODIVALINE (PENICILLAMINE SS DIMER) (CAS# 20902-45-8); (M+H)+		FindByFormula	1	+	296.0841	1.1320069
3,4-DICHLOROANILINE (CAS# 95-76-1); (M+H)	3,4-DICHLOROANILINE (CAS# 95-76-1); (M+H)	3,4-DICHLOROANILINE (CAS# 95-76-1); (M+H)+ [, tgt=43.8	95-76-1	(161.9858, 115.39)(162.9943, 36.4)	3,4-DICHLOROANILINE (CAS# 95-76-1); (M+H)+	C02791	FindByFormula	1	+	160.9799	11.68695
3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-9	3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-9	3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-92-7); (M+H)	59-92-7	(198.0755, 1711.77)(199.0874, 561.18)(200.0821, 239.93)	3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-92-7); (M+H)+		FindByFormula	1	+	197.0703	1.2760221
3,4-DIHYDROXYPHENYLACETATE (CAS# 102-3	3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32	3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+H)+	102-32-9	(169.04828, 4295.4443)(170.05219, 361.40887)	3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+H)+		FindByFormula	9	+	168.0406	3.5317616
3,4-DIHYDROXYPHENYLACETATE (CAS# 102-3	3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32	3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+Na	102-32-9	(191.03015, 603.08997)(192.03035, 62.73)	3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+Na)+		FindByFormula	2	+	168.0406	3.5320594
3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CA	3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CA	3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CAS# 28822-73	28822-73-3	(153.05513, 1076.14)(154.05717, 154.43333)	3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CAS# 28822-73-3); (M+H)+[-H2O]		FindByFormula	3	+	170.0585	1.0150005
3',5'-CYCLIC AMP (CAS# 60-92-4); (M+H)+	3',5'-CYCLIC AMP (CAS# 60-92-4); (M+H)+	3',5'-CYCLIC AMP (CAS# 60-92-4); (M+H)+ [, tgt=63.62, ov	60-92-4	(330.06073, 381.51202)(331.0705, 63.267998)	3',5'-CYCLIC AMP (CAS# 60-92-4); (M+H)+		FindByFormula	5	+	329.0552	1.9814253
359.3371@21.756748				(360.34683, 1200.2535)(361.34433, 440.21857)(382.32526, 2	359.3371@21.756748		FindByFormula	14	+	359.3371	21.756748
359.3533@21.494558				(360.36145, 4765.026)(361.36328, 1433.4275)(362.36142, 25	359.3533@21.494558		FindByFormula	27	+	359.3533	21.494558
367.417@22.331345				(368.42355, 2020.6481)(369.42407, 744.3164)(370.42282, 19	367.417@22.331345		FindByFormula	25	+	367.417	22.331345
3-AMINO-4-HYDROXYBENZOIC ACID (CAS# 15	3-AMINO-4-HYDROXYBENZOIC ACID (CAS# 15	3-AMINO-4-HYDROXYBENZOIC ACID (CAS# 1571-72-8); (M	1571-72-8	(154.049, 1742.73)(155.0441, 137.25)	3-AMINO-4-HYDROXYBENZOIC ACID (CAS# 1571-72-8); (M+H)+	C12115	FindByFormula	1	+	153.0411	1.2750062
3-AMINOISOBUTANOATE (CAS# 144-90-1); (M	3-AMINOISOBUTANOATE (CAS# 144-90-1); (M	3-AMINOISOBUTANOATE (CAS# 144-90-1); (M+H)+[-H2O]	144-90-1	(86.06009, 757.6337)(87.059, 39.2)	3-AMINOISOBUTANOATE (CAS# 144-90-1); (M+H)+[-H2O]	C05145	FindByFormula	8	+	103.0632	1.7318816
3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (	3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (	3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (CAS# 516-5	516-55-2	(341.2513, 726.16)(342.2408, 54.66)(343.2426, 328.28)	3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (CAS# 516-55-2); (M+Na)+		FindByFormula	1	+	318.2569	20.73819
3'-CMP (CAS# 63-37-6); (M+H)+	3'-CMP (CAS# 63-37-6); (M+H)+	3'-CMP (CAS# 63-37-6); (M+H)+ [, tgt=52.85, overall=52.8	63-37-6	(324.06058, 1337.6937)(325.0568, 132.88437)(326.05872, 10	3'-CMP (CAS# 63-37-6); (M+H)+	C00055	FindByFormula	16	+	323.0504	0.9640021
3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M	3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M+	3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M+H)+[-H2O] [	2922-42-1	(155.03433, 700.29504)(156.03287, 87.6725)	3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M+H)+[-H2O]	C02637	FindByFormula	4	+	172.0363	1.0877503
3-DEHYDROXYCARNITINE (CAS# 407-64-7); (M	3-DEHYDROXYCARNITINE (CAS# 407-64-7); (M	3-DEHYDROXYCARNITINE (CAS# 407-64-7); (M+H)+ [, tgt=	407-64-7	(146.11795, 21491.014)(147.11577, 2903.49)(148.11795, 300	3-DEHYDROXYCARNITINE (CAS# 407-64-7); (M+H)+	C05543	FindByFormula	7	+	145.11	0.7010001
3-HYDROXY-3-METHYLGLUTARATE (CAS# 503-	3-HYDROXY-3-METHYLGLUTARATE (CAS# 503-	3-HYDROXY-3-METHYLGLUTARATE (CAS# 503-49-1); (M+H	503-49-1	(163.06133, 1217.4233)(164.05856, 723.10333)	3-HYDROXY-3-METHYLGLUTARATE (CAS# 503-49-1); (M+H)+	C03761	FindByFormula	6	+	162.0516	1.9603457
3-HYDROXYANTHRANILATE (CAS# 548-93-6);	3-HYDROXYANTHRANILATE (CAS# 548-93-6); (	3-HYDROXYANTHRANILATE (CAS# 548-93-6); (M+H)+ [, tg	548-93-6	(154.0502, 840.39)(155.0575, 40.64)	3-HYDROXYANTHRANILATE (CAS# 548-93-6); (M+H)+		FindByFormula	1	+	153.0431	2.8092365
3-HYDROXYBENZALDEHYDE (CAS# 100-83-4);	3-HYDROXYBENZALDEHYDE (CAS# 100-83-4);	3-HYDROXYBENZALDEHYDE (CAS# 100-83-4); (M+H)+[-H2	100-83-4	(105.033516, 1658.6582)(106.03577, 103.10818)	3-HYDROXYBENZALDEHYDE (CAS# 100-83-4); (M+H)+[-H2O]	C03067	FindByFormula	11	+	122.037	4.797224
3-HYDROXYKYNURENINE (CAS# 2147-61-7); (M	3-HYDROXYKYNURENINE (CAS# 2147-61-7); (M	3-HYDROXYKYNURENINE (CAS# 2147-61-7); (M+H)+ [, tgt	2147-61-7	(225.0878, 748.18)(226.0922, 62.99)	3-HYDROXYKYNURENINE (CAS# 2147-61-7); (M+H)+		FindByFormula	1	+	224.0806	1.0740062
3-HYDROXYPHENYLACETATE (CAS# 621-37-4);	3-HYDROXYPHENYLACETATE (CAS# 621-37-4);	3-HYDROXYPHENYLACETATE (CAS# 621-37-4); (M+H)+ [, t	621-37-4	(153.0548, 441539.2)(154.05814, 37930.883)(155.06116, 470	3-HYDROXYPHENYLACETATE (CAS# 621-37-4); (M+H)+	C05593	FindByFormula	20	+	152.0474	8.665126
3-HYDROXYPROPANOATE (CAS# 503-66-2); (M	3-HYDROXYPROPANOATE (CAS# 503-66-2); (M	3-HYDROXYPROPANOATE (CAS# 503-66-2); (M+Na)+ [, tg	503-66-2	(113.02174, 1729.1)(114.01915, 28.35)	3-HYDROXYPROPANOATE (CAS# 503-66-2); (M+Na)+		FindByFormula	2	+	90.0324	0.9724995
3-METHOXY-4-HYDROXYMANDELATE (CAS# 5	3-METHOXY-4-HYDROXYMANDELATE (CAS# 5	3-METHOXY-4-HYDROXYMANDELATE (CAS# 55-10-7); (M	55-10-7	(221.0437, 884.38)(222.0457, 56.14)	3-METHOXY-4-HYDROXYMANDELATE (CAS# 55-10-7); (M+Na)+		FindByFormula	1	+	198.0544	1.6930073
3-METHOXYTYROSINE (CAS# 4214-13-5); (M+	3-METHOXYTYROSINE (CAS# 4214-13-5); (M+	3-METHOXYTYROSINE (CAS# 4214-13-5); (M+H)+ [, tgt=8	4214-13-5	(212.09253, 1929.4233)(213.09315, 343.31168)(214.09604, 1	3-METHOXYTYROSINE (CAS# 4214-13-5); (M+H)+		FindByFormula	6	+	211.0853	2.0146701
3-METHYGLUTARIC ACID (CAS# 626-51-7); (M	3-METHYGLUTARIC ACID (CAS# 626-51-7); (M	3-METHYGLUTARIC ACID (CAS# 626-51-7); (M+H)+[-H2O]	626-51-7	(129.05432, 534.02405)(130.05426, 65.028)	3-METHYGLUTARIC ACID (CAS# 626-51-7); (M+H)+[-H2O]		FindByFormula	5	+	146.0568	3.5389576
3-METHYGLUTARIC ACID (CAS# 626-51-7); (M	3-METHYGLUTARIC ACID (CAS# 626-51-7); (M	3-METHYGLUTARIC ACID (CAS# 626-51-7); (M+Na)+ [, tgt	626-51-7	(169.04782, 4079.1262)(170.04883, 118.23385)(171.0475, 44	3-METHYGLUTARIC ACID (CAS# 626-51-7); (M+Na)+		FindByFormula	13	+	146.0586	3.5313034
3-METHYL-2-BUTENAL (CAS# 107-86-8); (M+N	3-METHYL-2-BUTENAL (CAS# 107-86-8); (M+N	3-METHYL-2-BUTENAL (CAS# 107-86-8); (M+Na)+ [, tgt=6	107-86-8	(107.0466, 1489.16)(108.0517, 82.46)	3-METHYL-2-BUTENAL (CAS# 107-86-8); (M+Na)+		FindByFormula	2	+	84.0577	2.5299892
3-METHYLADENINE (CAS# 5142-23-4); (M+H)	3-METHYLADENINE (CAS# 5142-23-4); (M+H)	3-METHYLADENINE (CAS# 5142-23-4); (M+H)+ [, tgt=33.6	5142-23-4	(150.0758, 782.745)(151.08694, 160.065)	3-METHYLADENINE (CAS# 5142-23-4); (M+H)+	C00913	FindByFormula	2	+	149.0712	0.69900095
3-METHYLADIPIC ACID (CAS# 3058-01-3); (M+	3-METHYLADIPIC ACID (CAS# 3058-01-3); (M+	3-METHYLADIPIC ACID (CAS# 3058-01-3); (M+Na)+ [, tgt=	1/3/3058	(183.06271, 668.61005)(184.06505, 72.3)	3-METHYLADIPIC ACID (CAS# 3058-01-3); (M+Na)+		FindByFormula	7	+	160.0729	5.6614327
3-METHYLHISTAMINE (CAS# 644-42-8); (M+H	3-METHYLHISTAMINE (CAS# 644-42-8); (M+H)	3-METHYLHISTAMINE (CAS# 644-42-8); (M+H)+ [, tgt=80.	644-42-8	(126.10238, 4073.8848)(127.10382, 389.16885)(128.1032, 35	3-METHYLHISTAMINE (CAS# 644-42-8); (M+H)+	C15526	FindByFormula	17	+	125.0953	0.556531
3-METHYLXANTHINE (CAS# 1076-22-8); (M+H	3-METHYLXANTHINE (CAS# 1076-22-8); (M+H	3-METHYLXANTHINE (CAS# 1076-22-8); (M+H)+ [, tgt=45.	1076-22-8	(166.0482, 6719.0537)(167.05484, 426.58398)(168.051, 97.8)	3-METHYLXANTHINE (CAS# 1076-22-8); (M+H)+		FindByFormula	5	+	166.0484	2.4198217
3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (	3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (	3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (M+H)+ [, tgt	462-88-4	(133.06097, 2235.4866)(134.06636, 323.33667)	3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (M+H)+	C02642	FindByFormula	3	+	132.0538	0.798343
415.9055@18.622404				(416.91235, 6616.875)(417.91483, 797.3433)(418.9059, 1223	415.9055@18.622404		FindByFormula	6	+	415.9055	18.622404
445.2466@19.244831				(446.25385, 2683.5452)(447.2473, 1308.251)	445.2466@19.244831		FindByFormula	19	+	445.2466	19.244831
467.5116@19.133024				(468.51947, 7349.743)(469.52353, 871.4772)	467.5116@19.133024		FindByFormula	7	+	467.5116	19.133024
4-ACETAMIDOBUTANOATE (CAS# 3025-96-5);	4-ACETAMIDOBUTANOATE (CAS# 3025-96-5);	4-ACETAMIDOBUTANOATE (CAS# 3025-96-5); (M+Na)+ [,	3025-96-5	(168.064, 1677.3885)(169.06201, 280.39664)(170.0688, 24.2)	4-ACETAMIDOBUTANOATE (CAS# 3025-96-5); (M+Na)+	C02946	FindByFormula	21	+	145.0752	1.932588
4-ACETAMINOPHEN SULFATE (CAS# 32113-41	4-ACETAMINOPHEN SULFATE (CAS# 32113-41-	4-ACETAMINOPHEN SULFATE (CAS# 32113-41-0); (M+H)+	32113-41-0	(232.0271, 534.775)(233.03061, 81.277504)(234.0269, 44.67	4-ACETAMINOPHEN SULFATE (CAS# 32113-41-0); (M+H)+		FindByFormula	4	+	231.0213	2.3812733
4-AMINOBENZOATE (CAS# 150-13-0); (M+H)+	4-AMINOBENZOATE (CAS# 150-13-0); (M+H)+	4-AMINOBENZOATE (CAS# 150-13-0); (M+H)+ [, tgt=73.4	150-13-0	(138.05516, 1073.3717)(139.05057, 169.52834)	4-AMINOBENZOATE (CAS# 150-13-0); (M+H)+	C00568	FindByFormula	6	+	137.0468	2.753684
4-AMINOBUTANOATE (CAS# 56-12-2); (M+H)	4-AMINOBUTANOATE (CAS# 56-12-2); (M+H)+	4-AMINOBUTANOATE (CAS# 56-12-2); (M+H)+ [, tgt=49.5	56-12-2	(104.07004, 739.9783)(105.07355, 41.446667)	4-AMINOBUTANOATE (CAS# 56-12-2); (M+H)+		FindByFormula	6	+	103.0625	0.84966606
4-GUANIDINOBUTANOATE (CAS# 463-00-3); (	4-GUANIDINOBUTANOATE (CAS# 463-00-3); (	4-GUANIDINOBUTANOATE (CAS# 463-00-3); (M+H)+ [, tg	463-00-3	(146.0935, 2276.15)(147.098, 330.62)	4-GUANIDINOBUTANOATE (CAS# 463-00-3); (M+H)+		FindByFormula	1	+	145.0865	0.88899314
4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-K	4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-K	4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-KRYNURENIC	492-27-3	(190.05049, 620.79834)(191.05121, 66.92834)	4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-KRYNURENIC ACID (CAS# 492-27-		FindByFormula	6	+	189.0431	4.9724407
4-HYDROXY-3-METHOXY-BENZENEMETHANO	4-HYDROXY-3-METHOXY-BENZENEMETHANOL	4-HYDROXY-3-METHOXY-BENZENEMETHANOL (CAS# 498-	498-00-0	(137.06317, 2007.6234)(138.05629, 1032.0333)	4-HYDROXY-3-METHOXY-BENZENEMETHANOL (CAS# 498-00-0);	C06317	FindByFormula	3	+	154.0615	3.9003823
4-HYDROXYBENZALDEHYDE (CAS# 123-08-0);	4-HYDROXYBENZALDEHYDE (CAS# 123-08-0);	4-HYDROXYBENZALDEHYDE (CAS# 123-08-0); (M+H)+ [, tg	123-08-0	(123.04482, 2132.4678)(124.04451, 179.10799)(125.03695, 1	4-HYDROXYBENZALDEHYDE (CAS# 123-08-0); (M+H)+	C00633	FindByFormula	20	+	122.0374	4.932517
4-HYDROXY-L-PROLINE (CAS# 2584-71-6); (M+	4-HYDROXY-L-PROLINE (CAS# 2584-71-6); (M+	4-HYDROXY-L-PROLINE (CAS# 2584-71-6); (M+H)+ [, tgt=6	2584-71-6	(132.06696, 10858.069)(133.06458, 801.6425)(134.0635, 74.(	4-HYDROXY-L-PROLINE (CAS# 2584-71-6); (M+H)+	C03440	FindByFormula	4	+	131.0586	0.7009997
4-HYDROXYPHENYLACETATE (CAS# 156-38-7);	4-HYDROXYPHENYLACETATE (CAS# 156-38-7);	4-HYDROXYPHENYLACETATE (CAS# 156-38-7); (M+H)+ [, t	156-38-7	(153.05481, 889.93256)(154.05165, 97.02)	4-HYDROXYPHENYLACETATE (CAS# 156-38-7); (M+H)+		FindByFormula	4	+	152.047	4.5353403
4-METHYL-2-OXOVALERIC ACID (CAS# 816-66-	4-METHYL-2-OXOVALERIC ACID (CAS# 816-66-(	4-METHYL-2-OXOVALERIC ACID (CAS# 816-66-0); (M+Na)+	816-66-0	(153.0534, 931.51337)(154.0504, 92.57667)	4-METHYL-2-OXOVALERIC ACID (CAS# 816-66-0); (M+Na)+		FindByFormula	3	+	130.0636	4.5341105
4-PYRIDOXATE (CAS# 82-82-6); (M+H)+	4-PYRIDOXATE (CAS# 82-82-6); (M+H)+	4-PYRIDOXATE (CAS# 82-82-6); (M+H)+ [, tgt=77.45, overa	82-82-6	(184.06108, 4160.106)(185.06416, 327.45636)(186.06549, 27	4-PYRIDOXATE (CAS# 82-82-6); (M+H)+	C00847	FindByFormula	11	+	183.0529	1.9250102
4-PYRIDOXATE (CAS# 82-82-6); (M+H)+[-H2O]	4-PYRIDOXATE (CAS# 82-82-6); (M+H)+[-H2O]	4-PYRIDOXATE (CAS# 82-82-6); (M+H)+[-H2O] [, tgt=57.10	82-82-6	(166.0504, 981.165)(167.05975, 38.074997)	4-PYRIDOXATE (CAS# 82-82-6); (M+H)+[-H2O]	C00847	FindByFormula	2	+	183.0548	1.9705163
4-PYRIDOXATE (CAS# 82-82-6); (M+Na)+	4-PYRIDOXATE (CAS# 82-82-6); (M+Na)+	4-PYRIDOXATE (CAS# 82-82-6); (M+Na)+ [, tgt=63.43, ove	82-82-6	(206.0439, 1171.1517)(207.04268, 134.29333)(208.047, 32.5)	4-PYRIDOXATE (CAS# 82-82-6); (M+Na)+	C00847	FindByFormula	6	+	183.0548	1.8933382
504.0074@10.469363				(505.0144, 9811.302)(506.0175, 1784.1385)(507.0115, 15996	504.0074@10.469363		FindByFormula	7	+	504.0074	10.469363
511.8361@19.314745				(512.84344, 12964.861)(513.84735, 2112.4158)(514.8408, 25	511.8361@19.314745		FindByFormula	7	+	511.8361	19.314745
520.0013@9.197242				(521.3421, 457.77335)(522.3495, 110.31667)(523.00354, 88.8	520.0013@9.197242		FindByFormula	3	+	520.0013	9.197242
520.0016@9.493141				(521.0092, 15110.16)(522.01215, 2690.8284)(523.0065, 2501	520.0016@9.493141		FindByFormula	6	+	520.0016	9.493141
521.5911@22.722954				(522.5969, 8411.807)(523.59937, 3581.9016)(524.6037, 991.3	521.5911@22.722954		FindByFormula	22	+	521.5911	22.722954
532.5483@19.841719				(533.55786, 7742.6606)(534.5562, 747.44)	532.5483@19.841719		FindByFormula	6	+	532.5483	19.841719
539.5427@19.849634				(540.55133, 5948.1616)(541.5543, 1089.1742)	539.5427@19.849634		FindByFormula	7	+	539.5427	19.849634
541.8695@20.984104				(542.8758, 30872.455)(543.87915, 4304.196)(552.86017, 293	541.8695@20.984104		FindByFormula	7	+	541.8695	20.984104
561.568@19.914976				(562.57526, 5548.2515)(563.56793, 1314.5214)	561.568@19.914976		FindByFormula	7	+	561.568	19.914976
561.7977@22.134104				(562.8057, 4053.6982)(563.80835, 2015.0233)(564.793, 644.(	561.7977@22.134104		FindByFormula	6	+	561.7977	22.134104
580.276@19.786844				(581.85706, 1797.3947)(582.8607, 791.3661)(583.85443, 250	580.276@19.786844		FindByFormula	28	+	580.276	19.786844
586.7073@25.82004				(587.7132, 10765.253)(588.7159, 4467.364)(589.7161, 1232.4	586.7073@25.82004		FindByFormula	8	+	586.7073	25.82004
588.6146@25.369286				(589.6216, 19162.953)(590.62506, 7538.579)(591.6303, 1848	588.6146@25.369286		FindByFormula	21	+	588.6146	25.369286
589.5668@20.313803				(590.57404, 3259.9568)(591.57574, 771.1499)	589.5668@20.313803		FindByFormula	6	+	589.5668	20.313803
5ALPHA-CHOLEST-7-EN-3BETA-OL (CAS# 80-9	5ALPHA-CHOLEST-7-EN-3BETA-OL (CAS# 80-99	5ALPHA-CHOLEST-7-EN-3BETA-OL (CAS# 80-99-9); (M+H)+	80-99-9	(369.35153, 3760.924)(370.35507, 1177.4335)(371.3533, 251	5ALPHA-CHOLEST-7-EN-3BETA-OL (CAS# 80-99-9); (M+H)+[-H2O]	C01189	FindByFormula	17	+	386.3548	24.585417
5-AMINOLEVULINATE (CAS# 106-60-5); (M+H	5-AMINOLEVULINATE (CAS# 106-60-5); (M+H)	5-AMINOLEVULINATE (CAS# 106-60-5); (M+H)+ [, tgt=66.(	106-60-5	(132.06696, 10858.069)(133.06458, 801.6425)(134.0635, 74.(	5-AMINOLEVULINATE (CAS# 106-60-5); (M+H)+	C00430	FindByFormula	4	+	131.0586	0.7009997
5-AMINOPENTANOATE (CAS# 660-88-8); (M+	5-AMINOPENTANOATE (CAS# 660-88-8); (M+	5-AMINOPENTANOATE (CAS# 660-88-8); (M+H)+ [, tgt=9	660-88-8	(118.08656, 122273.29)(119.08843, 7520.3013)(120.08718, 6	5-AMINOPENTANOATE (CAS# 660-88-8); (M+H)+	C00431	FindByFormula	18	+	117.0786	0.6678897
5BETA-ANDROSTANE-3,17-DIONE (CAS# 1229	5BETA-ANDROSTANE-3,17-DIONE (CAS# 1229-	5BETA-ANDROSTANE-3,17-DIONE (CAS# 1229-12-5); (M+	1229-12-5	(311.1996, 1178.745)(312.20752, 157.045)	5BETA-ANDROSTANE-3,17-DIONE (CAS# 1229-12-5); (M+Na)+	C03772	FindByFormula	2	+	288.2107	18.691315
5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+	5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+H	5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+H)+ [, tgt=52.	4754-39-6	(252.1101, 648.74)(253.1053, 95.05)	5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+H)+	C05198	FindByFormula	1	+	251.1019	2.3861718
5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3);	5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3);	5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M+H)+ [, t	92340-57-3	(362.11728, 2068.365)(363.1162, 311.32834)(364.11862, 193	5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M+H)+		FindByFormula	6	+	361.1102	12.298663
5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3);	5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3);	5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M+Na)+ [,	92340-57-3	(384.09915, 2834.7317)(385.10327, 564.045)(386.10062, 250	5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M+Na)+		FindByFormula	6	+	361.1102	12.287659
5-HYDROXYINDOLEACETATE (CAS# 54-16-0); (	5-HYDROXYINDOLEACETATE (CAS# 54-16-0); (	5-HYDROXYINDOLEACETATE (CAS# 54-16-0); (M+Na)+ [, t	54-16-0	(214.0495, 742.34)(215.0473, 65.31)	5-HYDROXYINDOLEACETATE (CAS# 54-16-0); (M+Na)+		FindByFormula	1	+	191.0598	4.028034
5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (	5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (M	5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (M+H)+ [, tgt	9/8/4350	(221.0928, 3153.39)(222.0977, 555.8)(223.1, 406.7)	5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (M+H)+		FindByFormula	1	+	220.0859	1.8079946
5-METHYLCYTOSINE (CAS# 554-01-8); (2M+H)	5-METHYLCYTOSINE (CAS# 554-01-8); (2M+H)	5-METHYLCYTOSINE (CAS# 554-01-8); (2M+H)+ [, tgt=76.4	554-01-8	(251.1249, 1224.86)(252.1252, 106.24)	5-METHYLCYTOSINE (CAS# 554-01-8); (2M+H)+	C02376	FindByFormula	1	+	125.0585	0.667992
5-METHYLCYTOSINE (CAS# 554-01-8); (M+H)+	5-METHYLCYTOSINE (CAS# 554-01-8); (M+H)+	5-METHYLCYTOSINE (CAS# 554-01-8); (M+H)+ [, tgt=50.8	554-01-8	(126.066505, 1013.12195)(127.06694, 98.03999)	5-METHYLCYTOSINE (CAS# 554-01-8); (M+H)+	C02376	FindByFormula	5	+	125.0595	0.99920714
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9)	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9);	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+H)+ [,	2457-80-9	(298.09833, 949.2359)(299.09973, 163.08882)(300.0939, 81.1	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+H)+	C00170	FindByFormula	17	+	297.0914	4.4659886
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9)	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9);	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+Na)+ [	2457-80-9	(320.0803, 778.18884)(321.08218, 158.71834)(322.07944, 78	5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+Na)+	C00170	FindByFormula	18	+	297.0914	4.4622626
5-OXOPROLINE (CAS# 4042-36-8); (M+H)+	5-OXOPROLINE (CAS# 4042-36-8); (M+H)+	5-OXOPROLINE (CAS# 4042-36-8); (M+H)+ [, tgt=90.41, ov	4042-36-8	(130.0505, 267785.94)(131.05383, 15955.546)(132.06267, 22	5-OXOPROLINE (CAS# 4042-36-8); (M+H)+	C02237	FindByFormula	21	+	129.0437	1.190431
5-OXOPROLINE (CAS# 4042-36-8); (M+Na)+	5-OXOPROLINE (CAS# 4042-36-8); (M+Na)+	5-OXOPROLINE (CAS# 4042-36-8); (M+Na)+ [, tgt=62.37, c	4042-36-8	(152.0323, 75355.195)(153.03865, 8650.751)(154.04266, 113	5-OXOPROLINE (CAS# 4042-36-8); (M+Na)+	C02237	FindByFormula	4	+	129.0437	1.188245
5-VALEROLACTONE (CAS# 542-28-9); (M+H)+	5-VALEROLACTONE (CAS# 542-28-9); (M+H)+	5-VALEROLACTONE (CAS# 542-28-9); (M+H)+ [, tgt=75.48,	542-28-9	(101.05973, 6492.5234)(102.05793, 222.81)(103.06184, 53.3	5-VALEROLACTONE (CAS# 542-28-9); (M+H)+	C02240	FindByFormula	3	+	100.0522	2.0883348
602.6712@25.634558				(603.6699, 591.22)(604.6631, 76.58)	602.6712@25.634558		FindByFormula	1	+	602.6712	25.634558
602.6757@25.823212				(603.671, 4325.69)(604.676, 1842.7754)(605.6754, 638.76)	602.6757@25.823212		FindByFormula	9	+	602.6757	25.823212
604.5843@20.386108				(605.59076, 7776.933)(606.5892, 863.483)	604.5843@20.386108		FindByFormula	7	+	604.5843	20.386108
629.7354@26.437578				(630.7386, 1342.27)(631.73724, 673.05817)	629.7354@26.437578		FindByFormula	11	+	629.7354	26.437578
633.8659@21.435715				(638.8653, 78.07)(639.8515, 35.39)(640.8774, 59.12)(641.889	633.8659@21.435715		FindByFormula	1	+	633.8659	21.435715
633.8683@21.74444				(634.8771, 2618.5256)(635.8778, 549.55426)(636.8754, 5346	633.8683@21.74444		FindByFormula	7	+	633.8683	21.74444
644.697@27.795586				(645.7086, 10276.712)(646.71375, 4450.927)(647.72076, 174	644.697@27.795586		FindByFormula	18	+	644.697	27.795586
646.711@29.511913				(647.7226, 6887.62)(648.7256, 3125.84)(649.7179, 722.0)	646.711@29.511913		FindByFormula	1	+	646.711	29.511913
646.7123@29.322798				(647.72595, 26872.525)(648.7298, 11563.452)(649.73315, 28	646.7123@29.322798		FindByFormula	12	+	646.7123	29.322798
646.716@29.049877				(647.7242, 822.79504)(648.7276, 443.0)(649.73, 117.7)	646.716@29.049877		FindByFormula	2	+	646.716	29.049877
661.2191@21.898596				(662.51025, 6497.474)(663.51624, 2273.9385)(664.5072, 102	661.2191@21.898596		FindByFormula	7	+	661.2191	21.898596
676.6165@20.836817				(677.62354, 4966.4116)(678.6257, 751.6442)	676.6165@20.836817		FindByFormula	7	+	676.6165	20.836817
691.7938@26.276608				(692.7992, 2618.2498)(693.8004, 1311.6368)	691.7938@26.276608		FindByFormula	13	+	691.7938	26.276608
693.4089@22.273722				(695.4207, 2773.8867)(696.4143, 1693.2666)(696.92145, 218	693.4089@22.273722		FindByFormula	3	+	693.4089	22.273722
693.4115@22.520391				(695.21234, 1084.01)(696.22595, 917.6221)(696.75635, 230.1	693.4115@22.520391		FindByFormula	5	+	693.4115	22.520391
6-CARBOXYHEXANOATE (CAS# 111-16-0); (M+	6-CARBOXYHEXANOATE (CAS# 111-16-0); (M+	6-CARBOXYHEXANOATE (CAS# 111-16-0); (M+Na)+ [, tgt=	111-16-0	(183.06302, 710.6)(184.06535, 76.5475)	6-CARBOXYHEXANOATE (CAS# 111-16-0); (M+Na)+	C02656	FindByFormula	4	+	160.0729	5.6547337
719.4407@22.357714				(720.445, 1297.2273)(721.4492, 812.90564)(722.4397, 347.6	719.4407@22.357714		FindByFormula	14	+	719.4407	22.357714
731.7994@21.414972				(733.30756, 7649.3022)(734.3115, 1737.8351)(742.7967, 442	731.7994@21.414972		FindByFormula	8	+	731.7994	21.414972
748.44@22.25464				(375.22897, 18484.932)(375.72723, 7548.943)(376.22778, 24	748.44@22.25464		FindByFormula	28	+	748.44	22.25464
748.6456@21.157753				(749.65546, 4083.2615)(750.6552, 813.62994)(751.6571, 197	748.6456@21.157753		FindByFormula	6	+	748.6456	21.157753
749.3071@22.770224				(750.31647, 5077.13)(751.32434, 1484.304)(752.3178, 317.3	749.3071@22.770224		FindByFormula	5	+	749.3071	22.770224
749.3137@22.667034				(750.31775, 3116.0342)(751.3202, 1204.43)	749.3137@22.667034		FindByFormula	5	+	749.3137	22.667034
749.7589@25.361473				(750.76166, 8815.163)(751.7658, 4655.5356)(752.76794, 184	749.7589@25.361473		FindByFormula	18	+	749.7589	25.361473
750.4164@22.246555				(751.4252, 1679.9474)(752.42706, 855.0171)(753.4268, 516.(	750.4164@22.246555		FindByFormula	28	+	750.4164	22.246555
750.4748@22.106497				(751.48, 4534.6567)(752.48224, 2076.361)(753.47656, 919.5	750.4748@22.106497		FindByFormula	9	+	750.4748	22.106497
750.5098@22.407883				(751.5147, 2218.06)(752.51807, 954.26)(753.5055, 311.11)	750.5098@22.407883		FindByFormula	2	+	750.5098	22.407883
750.5114@22.61297				(751.5141, 3739.7698)(752.5084, 1744.0554)(753.5054, 621.9	750.5114@22.61297		FindByFormula	23	+	750.5114	22.61297
753.2803@15.102336				(377.64804, 2034.9349)(378.1521, 874.52826)(754.2951, 588	753.2803@15.102336		FindByFormula	6	+	753.2803	15.102336
754.3032@15.242076				(378.15854, 4824.616)(378.65952, 1818.1366)(379.165, 778.3	754.3032@15.242076		FindByFormula	6	+	754.3032	15.242076
755.6398@21.157751				(756.64966, 1638.625)(757.6457, 877.1184)	755.6398@21.157751		FindByFormula	6	+	755.6398	21.157751
756.3904@6.6820736				(379.20227, 8514.521)(379.70236, 3679.2427)(380.2025, 112	756.3904@6.6820736		FindByFormula	18	+	756.3904	6.6820736
756.3915@6.384316				(379.1969, 835.38)(379.7069, 139.82)(380.2044, 380.59)(390.	756.3915@6.384316		FindByFormula	1	+	756.3915	6.384316
756.3995@6.8234158				(379.2033, 332.68)(379.6926, 44.26)(380.2085, 179.45)(401.1	756.3995@6.8234158		FindByFormula	1	+	756.3995	6.8234158
756.4251@5.0011296				(379.22046, 6140.9233)(379.72208, 2476.5417)(380.21225, 9	756.4251@5.0011296		FindByFormula	6	+	756.4251	5.0011296
756.4574@21.98579				(757.46924, 11508.008)(758.47064, 4953.9385)(759.4706, 14	756.4574@21.98579		FindByFormula	27	+	756.4574	21.98579
757.5596@24.842958				(758.5585, 16906.81)(759.5608, 3088.95)(760.5651, 1181.9)(	757.5596@24.842958		FindByFormula	1	+	757.5596	24.842958
757.5616@24.534454				(758.5709, 36980.816)(759.57385, 17399.299)(760.57635, 49	757.5616@24.534454		FindByFormula	16	+	757.5616	24.534454
758.4818@22.426146				(380.24915, 6465.5938)(380.74802, 2649.6562)	758.4818@22.426146		FindByFormula	26	+	758.4818	22.426146
762.242@19.776638				(763.2496, 1982.2107)(764.2528, 815.1003)	762.242@19.776638		FindByFormula	27	+	762.242	19.776638
762.3666@16.903872				(763.3715, 3620.4531)(764.3742, 1519.0099)(765.3719, 611.2	762.3666@16.903872		FindByFormula	6	+	762.3666	16.903872
763.2595@22.065031				(764.2619, 1115.3556)(765.26373, 495.54608)	763.2595@22.065031		FindByFormula	23	+	763.2595	22.065031
763.4031@22.503992				(764.4111, 1622.9242)(765.41095, 729.5744)(766.4139, 417.(	763.4031@22.503992		FindByFormula	23	+	763.4031	22.503992
763.4113@22.724209				(764.4142, 1558.73)(765.4249, 424.94)	763.4113@22.724209		FindByFormula	1	+	763.4113	22.724209
764.3666@9.155757				(383.1915, 1936.445)(383.6934, 771.1784)	764.3666@9.155757		FindByFormula	6	+	764.3666	9.155757
764.412@22.092783				(765.4218, 1345.5092)(766.4196, 743.35205)(767.4198, 267.3	764.412@22.092783		FindByFormula	19	+	764.412	22.092783
764.5186@22.470398				(765.52844, 846.29)(766.5298, 432.04)(767.5227, 217.39)	764.5186@22.470398		FindByFormula	2	+	764.5186	22.470398
764.5205@22.788843				(765.53125, 8878.646)(766.5299, 4080.5366)(767.5262, 1420	764.5205@22.788843		FindByFormula	20	+	764.5205	22.788843
765.5647@24.971613				(766.56616, 4401.77)(767.5812, 2709.655)(768.5797, 1597.1	765.5647@24.971613		FindByFormula	2	+	765.5647	24.971613
765.5656@24.693314				(766.5687, 3940.9514)(767.569, 1746.628)(768.55505, 4389.5	765.5656@24.693314		FindByFormula	16	+	765.5656	24.693314
765.5674@25.264753				(766.57104, 7371.4966)(767.5769, 3642.4375)(768.5806, 323	765.5674@25.264753		FindByFormula	11	+	765.5674	25.264753
765.7701@25.607588				(766.7787, 896.22)(767.7721, 541.66)	765.7701@25.607588		FindByFormula	1	+	765.7701	25.607588
765.7811@25.317173				(766.7808, 4134.9478)(767.78845, 2137.986)(768.7882, 2239	765.7811@25.317173		FindByFormula	13	+	765.7811	25.317173
765.7823@24.985867				(766.7841, 20184.875)(767.7905, 9776.04)(768.7975, 5097.0	765.7823@24.985867		FindByFormula	2	+	765.7823	24.985867
766.3968@12.524396				(384.2051, 5259.481)(384.70682, 1941.0144)(385.20248, 102	766.3968@12.524396		FindByFormula	28	+	766.3968	12.524396
767.5366@24.270397				(768.5433, 1446.9)(769.549, 540.48)	767.5366@24.270397		FindByFormula	1	+	767.5366	24.270397
767.5439@24.62556				(768.55133, 13534.504)(769.5551, 6540.458)(770.55255, 233	767.5439@24.62556		FindByFormula	15	+	767.5439	24.62556
767.7954@25.46408				(768.7965, 7019.875)(769.8023, 3462.2449)(770.80066, 1321	767.7954@25.46408		FindByFormula	20	+	767.7954	25.46408
769.2738@22.124748				(770.2844, 1238.39)(771.28754, 528.5217)	769.2738@22.124748		FindByFormula	18	+	769.2738	22.124748
769.46@22.165522				(770.4664, 14108.393)(771.4742, 8582.899)(772.4784, 2977.9	769.46@22.165522		FindByFormula	20	+	769.46	22.165522
770.4795@22.26616				(771.4873, 76840.06)(772.49036, 32702.512)(773.4926, 9226	770.4795@22.26616		FindByFormula	28	+	770.4795	22.26616
772.3838@5.6205163				(409.1824, 156.37)(409.6812, 67.29)(398.1874, 236.75)(398.6	772.3838@5.6205163		FindByFormula	1	+	772.3838	5.6205163
772.3893@5.8998537				(387.20084, 3928.6743)(387.70285, 1737.7244)(388.20355, 5	772.3893@5.8998537		FindByFormula	8	+	772.3893	5.8998537
775.324@15.16887				(776.33154, 1650.5917)(777.3333, 748.7933)	775.324@15.16887		FindByFormula	6	+	775.324	15.16887
776.3455@15.591792				(777.35126, 7779.008)(778.3519, 3091.4614)(779.3526, 1101	776.3455@15.591792		FindByFormula	8	+	776.3455	15.591792
777.6613@21.185612				(778.67474, 2133.825)(779.666, 1433.4532)	777.6613@21.185612		FindByFormula	6	+	777.6613	21.185612
778.4451@21.968401				(390.23077, 8057.89)(390.7326, 3422.7295)(391.23187, 1224	778.4451@21.968401		FindByFormula	22	+	778.4451	21.968401
779.5456@24.53104				(780.5524, 533204.75)(781.55585, 251344.73)(782.55963, 75	779.5456@24.53104		FindByFormula	17	+	779.5456	24.53104
780.4258@4.246074				(391.21982, 2307.12)(391.7212, 986.86835)	780.4258@4.246074		FindByFormula	6	+	780.4258	4.246074
780.5207@22.436514				(781.52765, 6471.5576)(782.5287, 3025.703)(783.5165, 1466	780.5207@22.436514		FindByFormula	26	+	780.5207	22.436514
781.4594@22.326466				(782.47003, 1582.4325)(783.4692, 981.1995)(784.47577, 105	781.4594@22.326466		FindByFormula	20	+	781.4594	22.326466
783.2499@22.26301				(784.2569, 1629.0806)(785.25696, 643.7073)(786.25134, 438	783.2499@22.26301		FindByFormula	18	+	783.2499	22.26301
783.5801@24.648405				(784.58484, 20654.062)(785.5921, 9865.409)(786.59125, 310	783.5801@24.648405		FindByFormula	18	+	783.5801	24.648405
783.581@24.41983				(784.5801, 11339.63)(785.59, 3582.85)(786.5965, 721.84)(82	783.581@24.41983		FindByFormula	1	+	783.581	24.41983
783.7955@25.61029				(784.8074, 10324.577)(785.8126, 5040.4146)(786.8167, 1836	783.7955@25.61029		FindByFormula	13	+	783.7955	25.61029
784.3152@17.391024				(785.322, 1455.5265)(786.3238, 711.10175)	784.3152@17.391024		FindByFormula	6	+	784.3152	17.391024

784.4937@22.412384	(785.5006, 3401.2224)(786.5021, 1709.946)(787.4953, 643.6	784.4937@22.412384	FindByFormula	28 +	784.4937	22.412384
785.5006@8.232729	(393.7585, 5463.3647)(394.2588, 2543.9229)(394.76028, 675	785.5006@8.232729	FindByFormula	22 +	785.5006	8.232729
785.53@24.35946	(786.54156, 3232.5452)(787.5474, 1937.7084)(788.54474, 23	785.53@24.35946	FindByFormula	6 +	785.53	24.35946
785.5852@25.195345	(786.60065, 32949.438)(787.6046, 16397.129)(788.59894, 56	785.5852@25.195345	FindByFormula	15 +	785.5852	25.195345
785.5877@24.955555	(786.5924, 116.62)(787.553, 51.32)(824.5548, 192.37)(808.6	785.5877@24.955555	FindByFormula	1 +	785.5877	24.955555
786.5182@22.788322	(394.2638, 5242.5073)(394.76407, 2247.1687)(395.27478, 21	786.5182@22.788322	FindByFormula	16 +	786.5182	22.788322
786.5229@22.476688	(394.2681, 872.528)(394.7605, 247.43001)(395.2763, 1344.3	786.5229@22.476688	FindByFormula	5 +	786.5229	22.476688
787.5016@22.77321	(788.5157, 309.1)(789.5003, 292.92)(810.4937, 83.8)	787.5016@22.77321	FindByFormula	1 +	787.5016	22.77321
787.5026@22.468431	(788.5059, 1551.76)(789.5101, 1092.4568)(790.50446, 503.2	787.5026@22.468431	FindByFormula	11 +	787.5026	22.468431
788.5265@22.951626	(789.5304, 2576.4778)(790.5316, 1376.0228)(791.5298, 823.	788.5265@22.951626	FindByFormula	14 +	788.5265	22.951626
789.2611@22.251148	(790.2712, 1781.4532)(791.27374, 694.088)(792.2647, 209.6	789.2611@22.251148	FindByFormula	15 +	789.2611	22.251148
789.2642@22.332657	(790.27124, 2587.8555)(791.27545, 981.6931)(792.2751, 427	789.2642@22.332657	FindByFormula	16 +	789.2642	22.332657
790.996@21.349993	(792.0033, 1249.2)(793.01056, 782.19403)(794.01404, 438.4	790.996@21.349993	FindByFormula	5 +	790.996	21.349993
792.4642@22.26437	(397.2397, 34658.07)(397.7404, 15127.954)(398.244, 4595.2	792.4642@22.26437	FindByFormula	28 +	792.4642	22.26437
792.5548@22.774387	(793.5664, 2277.87)(794.5648, 984.51)(795.5425, 664.07)	792.5548@22.774387	FindByFormula	1 +	792.5548	22.774387
792.5564@23.077744	(793.56433, 7208.9053)(794.5667, 3402.4885)(795.5675, 132	792.5564@23.077744	FindByFormula	14 +	792.5564	23.077744
793.5193@22.47253	(794.5306, 6428.08)(795.5302, 4650.4316)(796.5303, 1607.6	793.5193@22.47253	FindByFormula	9 +	793.5193	22.47253
793.5283@22.272923	(794.52783, 279.3943)(795.5259, 215.46799)(796.527, 318.6	793.5283@22.272923	FindByFormula	7 +	793.5283	22.272923
794.2594@22.54076	(795.2646, 1742.3591)(796.2711, 780.85516)	794.2594@22.54076	FindByFormula	27 +	794.2594	22.54076
794.326@17.455503	(795.33545, 95137.68)(796.33856, 45573.34)(797.3407, 1310	794.326@17.455503	FindByFormula	28 +	794.326	17.455503
794.3295@16.810375	(795.33496, 34160.832)(796.3378, 16569.498)(797.34015, 49	794.3295@16.810375	FindByFormula	28 +	794.3295	16.810375
794.3422@6.6771693	(398.1769, 1366.5067)(398.6771, 634.7233)	794.3422@6.6771693	FindByFormula	6 +	794.3422	6.6771693
794.4457@22.256075	(795.45056, 1668.787)(796.4496, 828.3176)(797.444, 422.39	794.4457@22.256075	FindByFormula	25 +	794.4457	22.256075
795.5113@24.243965	(398.7615, 57.94)(399.2763, 45.93)(796.52686, 9927.225)(79	795.5113@24.243965	FindByFormula	2 +	795.5113	24.243965
795.5152@24.516008	(398.76248, 8418.239)(399.2623, 4077.2097)(399.76578, 120	795.5152@24.516008	FindByFormula	12 +	795.5152	24.516008
795.7901@25.479336	(796.7996, 4385.94)(797.8053, 2683.93)(798.8053, 1324.43)	795.7901@25.479336	FindByFormula	1 +	795.7901	25.479336
795.7949@25.335617	(796.80963, 6385.6465)(797.811, 3366.6934)(798.811, 1266.	795.7949@25.335617	FindByFormula	12 +	795.7949	25.335617
796.3903@21.512106	(797.3932, 1500.3534)(798.3943, 734.0576)(799.3939, 389.7	796.3903@21.512106	FindByFormula	26 +	796.3903	21.512106
796.4833@19.792416	(797.48816, 1115.8356)(798.491, 632.93304)(799.48413, 239	796.4833@19.792416	FindByFormula	27 +	796.4833	19.792416
798.3285@15.589261	(400.1719, 13145.6045)(400.6726, 5238.053)(401.1812, 2285	798.3285@15.589261	FindByFormula	6 +	798.3285	15.589261
800.2489@15.174374	(401.1326, 2864.485)(401.63217, 1053.8817)	800.2489@15.174374	FindByFormula	6 +	800.2489	15.174374
800.3571@6.6805854	(801.3602, 4562.161)(802.3642, 2063.056)(803.3694, 714.33	800.3571@6.6805854	FindByFormula	10 +	800.3571	6.6805854
800.4905@21.98228	(801.4961, 10543.395)(802.49774, 4744.088)(803.49457, 151	800.4905@21.98228	FindByFormula	15 +	800.4905	21.98228
801.6078@19.727795	(802.6141, 1375.0049)(803.6123, 851.07)	801.6078@19.727795	FindByFormula	6 +	801.6078	19.727795
802.5058@22.273735	(402.2656, 617.79)(402.7557, 81.83)(403.2589, 218.73)	802.5058@22.273735	FindByFormula	1 +	802.5058	22.273735
802.5088@22.430168	(402.26428, 9072.524)(402.76117, 2723.8286)(403.26736, 14	802.5088@22.430168	FindByFormula	21 +	802.5088	22.430168
803.4564@17.77778	(804.4643, 3635.8062)(805.4664, 1899.7551)(806.4677, 622.	803.4564@17.77778	FindByFormula	15 +	803.4564	17.77778
803.5417@24.245163	(804.5493, 21001.05)(805.5521, 10887.35)(806.5527, 3729.5	803.5417@24.245163	FindByFormula	1 +	803.5417	24.245163
803.5482@24.449387	(804.553, 310247.9)(805.5561, 154014.58)(806.56104, 51810	803.5482@24.449387	FindByFormula	17 +	803.5482	24.449387
805.0521@24.56559	(806.0569, 4980.847)(807.05884, 1341.7645)	805.0521@24.56559	FindByFormula	11 +	805.0521	24.56559
806.3896@17.155703	(807.3972, 2497.07)(808.39557, 1069.2284)(809.39667, 411.	806.3896@17.155703	FindByFormula	6 +	806.3896	17.155703
806.4853@22.410055	(404.24796, 2009.4862)(404.74692, 918.12854)	806.4853@22.410055	FindByFormula	28 +	806.4853	22.410055
807.2397@22.122429	(808.2526, 1242.1008)(809.2578, 593.38666)(810.2473, 338.	807.2397@22.122429	FindByFormula	13 +	807.2397	22.122429
807.2472@21.983837	(808.25726, 1259.96)(809.2516, 538.085)(810.2637, 222.885	807.2472@21.983837	FindByFormula	2 +	807.2472	21.983837
807.8033@25.364607	(808.80676, 136579.97)(809.81, 67569.38)(810.8097, 20351.	807.8033@25.364607	FindByFormula	2 +	807.8033	25.364607
807.8118@25.191593	(808.81323, 160849.84)(809.8172, 79347.9)(810.82, 23637.0	807.8118@25.191593	FindByFormula	19 +	807.8118	25.191593
808.4348@22.107382	(809.44586, 1283.9546)(810.4456, 710.21625)(811.4406, 366	808.4348@22.107382	FindByFormula	21 +	808.4348	22.107382
808.5483@22.446434	(809.557, 1116.85)(810.5491, 366.34)	808.5483@22.446434	FindByFormula	1 +	808.5483	22.446434
808.5553@22.77996	(809.5579, 4640.905)(810.5599, 2306.3674)(811.554, 951.94	808.5553@22.77996	FindByFormula	23 +	808.5553	22.77996
808.8757@26.516602	(809.8803, 16841.207)(810.88226, 9039.689)(811.8904, 3675	808.8757@26.516602	FindByFormula	15 +	808.8757	26.516602
809.2599@22.43519	(810.26733, 995.6367)(811.2715, 662.11835)(832.2549, 517.	809.2599@22.43519	FindByFormula	9 +	809.2599	22.43519
809.2637@22.120275	(810.26044, 189.87334)(811.2724, 80.875)(832.2507, 428.85	809.2637@22.120275	FindByFormula	3 +	809.2637	22.120275
810.295@16.42741	(406.15524, 17304.232)(406.6555, 8849.659)(407.15735, 323	810.295@16.42741	FindByFormula	26 +	810.295	16.42741
810.4211@12.899628	(406.21817, 4157.362)(406.71982, 1589.5492)(407.21683, 66	810.4211@12.899628	FindByFormula	28 +	810.4211	12.899628
811.5453@24.918062	(812.5515, 2007.98)(813.5631, 1264.59)	811.5453@24.918062	FindByFormula	1 +	811.5453	24.918062
811.5476@24.620996	(812.55707, 6670.9663)(813.56384, 3233.137)(814.57086, 42	811.5476@24.620996	FindByFormula	9 +	811.5476	24.620996
813.2642@22.13976	(814.2736, 720.70776)(815.2729, 337.10443)	813.2642@22.13976	FindByFormula	9 +	813.2642	22.13976
813.2651@22.035553	(814.2714, 1185.9546)(815.2775, 511.72638)	813.2651@22.035553	FindByFormula	11 +	813.2651	22.035553
813.488@22.168575	(814.4914, 6886.691)(815.49927, 4332.195)(816.50104, 1635	813.488@22.168575	FindByFormula	22 +	813.488	22.168575
814.5071@22.272953	(815.51355, 45199.688)(816.51666, 20511.66)(817.519, 6077	814.5071@22.272953	FindByFormula	28 +	814.5071	22.272953
815.2816@22.42304	(816.2865, 1455.4407)(817.29004, 665.5136)	815.2816@22.42304	FindByFormula	14 +	815.2816	22.42304
816.3386@16.701916	(817.34717, 3741.795)(818.3506, 1699.8485)(819.3498, 663.	816.3386@16.701916	FindByFormula	6 +	816.3386	16.701916
818.5481@24.287775	(819.5614, 12714.981)(820.5517, 8338.476)(821.54895, 3131	818.5481@24.287775	FindByFormula	8 +	818.5481	24.287775
819.3509@15.503695	(820.3569, 2671.2532)(821.3569, 1170.5886)(822.3587, 508.	819.3509@15.503695	FindByFormula	7 +	819.3509	15.503695
819.5066@24.406973	(410.76312, 6838.985)(411.26178, 3547.8015)(411.76547, 12	819.5066@24.406973	FindByFormula	15 +	819.5066	24.406973
819.5132@24.647125	(410.7637, 1051.8)(411.2616, 594.29)(411.7692, 630.69)(412	819.5132@24.647125	FindByFormula	1 +	819.5132	24.647125
820.6785@21.350441	(821.689, 2535.9385)(822.69073, 721.0267)	820.6785@21.350441	FindByFormula	6 +	820.6785	21.350441
822.3443@6.673502	(412.17804, 10017.323)(412.67767, 4465.3735)(413.17606, 1	822.3443@6.673502	FindByFormula	18 +	822.3443	6.673502
822.3579@17.51095	(823.36584, 2932.0254)(824.3693, 1602.7675)(825.37103, 61	822.3579@17.51095	FindByFormula	22 +	822.3579	17.51095
822.4739@21.999432	(412.24518, 7777.8145)(412.7449, 3447.5)(413.25546, 4571.	822.4739@21.999432	FindByFormula	26 +	822.4739	21.999432
823.5312@25.380026	(824.5422, 2607.65)(825.5548, 1504.11)(826.5547, 762.37)	823.5312@25.380026	FindByFormula	1 +	823.5312	25.380026
823.5383@25.18249	(412.77823, 8680.071)(413.27673, 5112.372)(413.7804, 1369	823.5383@25.18249	FindByFormula	11 +	823.5383	25.18249
824.5407@22.774292	(825.5465, 414.12)(826.5505, 617.29)	824.5407@22.774292	FindByFormula	1 +	824.5407	22.774292
824.546@22.43388	(825.5532, 4693.414)(826.55347, 2364.7083)(827.5431, 1003	824.546@22.43388	FindByFormula	21 +	824.546	22.43388
825.4823@22.123959	(826.4859, 837.89)(827.4947, 290.03)(828.486, 336.63)	825.4823@22.123959	FindByFormula	1 +	825.4823	22.123959
825.4897@22.337337	(826.49475, 1203.1309)(827.48645, 793.777)(828.4987, 847.	825.4897@22.337337	FindByFormula	20 +	825.4897	22.337337
827.4613@5.6203575	(414.73843, 2593.115)(415.23953, 1277.6583)	827.4613@5.6203575	FindByFormula	6 +	827.4613	5.6203575
827.4638@1.3281665	(414.73865, 2094.9915)(415.2389, 999.2316)(415.73837, 261	827.4638@1.3281665	FindByFormula	6 +	827.4638	1.3281665
827.5443@24.206425	(828.55347, 10677.324)(829.55774, 5813.015)(830.56116, 17	827.5443@24.206425	FindByFormula	2 +	827.5443	24.206425
827.5454@24.372906	(828.55286, 274820.8)(829.55676, 142283.02)(830.5608, 455	827.5454@24.372906	FindByFormula	13 +	827.5454	24.372906
828.3997@19.74982	(829.40906, 1637.2523)(830.4068, 912.1745)(831.40704, 452	828.3997@19.74982	FindByFormula	27 +	828.3997	19.74982
828.5102@22.623009	(829.5168, 589.87)(830.5112, 226.14)(831.5347, 303.29)	828.5102@22.623009	FindByFormula	1 +	828.5102	22.623009
828.5144@22.427803	(829.52563, 2287.3513)(830.52747, 1237.5259)(831.5221, 53	828.5144@22.427803	FindByFormula	27 +	828.5144	22.427803
829.5609@24.580767	(830.5682, 123214.2)(831.5714, 62735.85)(832.57306, 18716	829.5609@24.580767	FindByFormula	16 +	829.5609	24.580767
83.9528@0.5360841	(84.96017, 104432.71)(85.962, 2245.82)(106.94405, 1648.51	83.9528@0.5360841	FindByFormula	12 +	83.9528	0.5360841
83.9529@0.8059941	(84.9603, 1971.63)(106.9413, 67.61)	83.9529@0.8059941	FindByFormula	1 +	83.9529	0.8059941
830.5392@22.788803	(416.27634, 5145.3076)(416.7771, 2292.64)(417.2756, 1170.	830.5392@22.788803	FindByFormula	17 +	830.5392	22.788803
830.5403@22.445963	(416.2783, 991.6082)(416.7727, 349.86667)(417.2748, 374.4	830.5403@22.445963	FindByFormula	6 +	830.5403	22.445963
831.5684@24.859982	(832.5789, 10034.64)(833.586, 5149.6)(834.5849, 1957.02)(8	831.5684@24.859982	FindByFormula	1 +	831.5684	24.859982
831.5711@25.10127	(832.5834, 318533.1)(833.5867, 164783.31)(834.58905, 4905	831.5711@25.10127	FindByFormula	15 +	831.5711	25.10127
831.8173@25.115229	(832.82404, 95715.22)(833.8271, 49229.758)(834.8285, 1622	831.8173@25.115229	FindByFormula	21 +	831.8173	25.115229
832.9296@26.10271	(833.9213, 8386.97)(834.9255, 5262.46)(835.9268, 1494.71)	832.9296@26.10271	FindByFormula	1 +	832.9296	26.10271
832.9368@25.862532	(833.9258, 21924.773)(834.9277, 11567.679)(835.9304, 3740	832.9368@25.862532	FindByFormula	6 +	832.9368	25.862532
833.825@25.63534	(816.8048, 230.51)(817.7947, 117.0)(872.7903, 341.25)	833.825@25.63534	FindByFormula	1 +	833.825	25.63534
833.8331@25.473904	(834.8363, 45143.773)(835.84125, 22886.93)(836.8286, 1209	833.8331@25.473904	FindByFormula	17 +	833.8331	25.473904
836.4918@22.271847	(419.25302, 45635.73)(419.75327, 20262.682)(420.2581, 654	836.4918@22.271847	FindByFormula	28 +	836.4918	22.271847
838.3228@16.71113	(420.16928, 5148.767)(420.66943, 2037.68)(421.17545, 751.	838.3228@16.71113	FindByFormula	7 +	838.3228	16.71113
838.3332@5.899891	(420.17416, 6347.0815)(420.67587, 2734.3516)(421.177, 863	838.3332@5.899891	FindByFormula	6 +	838.3332	5.899891
838.4701@22.265482	(839.4773, 1418.1421)(840.4801, 799.4194)(841.48035, 450.	838.4701@22.265482	FindByFormula	27 +	838.4701	22.265482
840.3294@22.59082	(841.33954, 1281.4623)(842.34186, 639.25616)	840.3294@22.59082	FindByFormula	13 +	840.3294	22.59082
841.3327@15.513131	(421.67383, 4090.3384)(422.17743, 1752.6571)(422.67938, 5	841.3327@15.513131	FindByFormula	7 +	841.3327	15.513131
842.3543@15.861749	(422.1859, 1537.1099)(422.68555, 647.8466)	842.3543@15.861749	FindByFormula	6 +	842.3543	15.861749
842.3581@18.739824	(843.3649, 1792.2433)(844.366, 909.64496)	842.3581@18.739824	FindByFormula	6 +	842.3581	18.739824
843.5096@24.13249	(422.76233, 696.165)(423.2679, 415.41254)(423.75922, 235.	843.5096@24.13249	FindByFormula	7 +	843.5096	24.13249
843.5149@24.358906	(422.76312, 7146.245)(423.26447, 3871.6626)(423.76688, 14	843.5149@24.358906	FindByFormula	4 +	843.5149	24.358906
843.5152@24.449684	(422.7625, 9909.62)(423.2634, 5693.87)(423.7687, 1932.38)(	843.5152@24.449684	FindByFormula	2 +	843.5152	24.449684
843.5377@22.50305	(844.5406, 2022.0328)(845.5423, 1234.4701)(846.5488, 800.	843.5377@22.50305	FindByFormula	8 +	843.5377	22.50305
844.5074@22.009975	(845.5193, 4074.2244)(846.5241, 2010.0912)(847.52405, 694	844.5074@22.009975	FindByFormula	18 +	844.5074	22.009975
844.5132@22.242424	(845.5254, 275.18)(846.52, 232.5)	844.5132@22.242424	FindByFormula	1 +	844.5132	22.242424
845.5211@24.264343	(423.7716, 58.76)(424.2989, 70.71)(846.5272, 7516.13)(847.	845.5211@24.264343	FindByFormula	1 +	845.5211	24.264343
845.5264@24.562315	(423.76968, 1009.2729)(424.27124, 573.8529)(846.5358, 323	845.5264@24.562315	FindByFormula	7 +	845.5264	24.562315
846.3861@18.078674	(847.3935, 1315.2384)(848.394, 677.9816)	846.3861@18.078674	FindByFormula	6 +	846.3861	18.078674
846.533@22.45591	(424.27356, 5451.566)(424.77322, 2457.324)(425.27554, 575	846.533@22.45591	FindByFormula	24 +	846.533	22.45591
846.5334@22.230986	(424.27365, 912.22)(424.77646, 314.695)	846.5334@22.230986	FindByFormula	2 +	846.5334	22.230986
847.5322@24.538563	(848.54095, 239727.2)(849.5439, 115925.984)(850.5466, 321	847.5322@24.538563	FindByFormula	17 +	847.5322	24.538563
847.5361@24.92951	(424.77618, 1577.87)(425.27505, 960.308)(425.77466, 215.8	847.5361@24.92951	FindByFormula	8 +	847.5361	24.92951
847.5401@25.099321	(424.77878, 3220.096)(425.2777, 1960.6338)(425.78116, 629	847.5401@25.099321	FindByFormula	9 +	847.5401	25.099321
847.5656@23.07916	(848.5556, 148.53)(870.551, 513.44)	847.5656@23.07916	FindByFormula	1 +	847.5656	23.07916
847.5693@22.747322	(848.5723, 28996.346)(849.57245, 14388.121)(850.57056, 44	847.5693@22.747322	FindByFormula	9 +	847.5693	22.747322
849.6965@21.359217	(850.71, 1857.6934)(851.7034, 1351.6533)	849.6965@21.359217	FindByFormula	3 +	849.6965	21.359217
849.7948@25.00409	(850.8039, 129767.94)(851.8076, 62029.527)(852.8112, 1735	849.7948@25.00409	FindByFormula	19 +	849.7948	25.00409
850.4168@17.390692	(851.4231, 1385.3448)(852.41986, 675.5983)	850.4168@17.390692	FindByFormula	6 +	850.4168	17.390692
850.5027@22.625221	(426.2592, 423.57)(426.7498, 47.6)	850.5027@22.625221	FindByFormula	1 +	850.5027	22.625221
850.5065@22.444714	(426.2617, 2397.074)(426.76086, 1027.4224)(427.258, 2759.	850.5065@22.444714	FindByFormula	26 +	850.5065	22.444714
851.8118@25.594587	(852.81793, 12069.002)(853.8206, 5717.9404)(854.82336, 18	851.8118@25.594587	FindByFormula	19 +	851.8118	25.594587
851.8178@25.34311	(852.8266, 1009.76)(853.8443, 482.15)(854.8088, 363.27)	851.8178@25.34311	FindByFormula	1 +	851.8178	25.34311
852.5753@22.548275	(853.586, 1271.13)(854.5764, 976.93506)(855.5739, 557.71)	852.5753@22.548275	FindByFormula	2 +	852.5753	22.548275
852.5821@22.78476	(853.58575, 3653.547)(854.5838, 2064.4587)(855.5793, 768.	852.5821@22.78476	FindByFormula	14 +	852.5821	22.78476
853.5528@24.458563	(854.5634, 5241.3613)(855.56696, 2806.6204)(856.56055, 28	853.5528@24.458563	FindByFormula	12 +	853.5528	24.458563
854.4479@13.245994	(428.231, 3415.8792)(428.73297, 1410.0905)(429.22473, 721	854.4479@13.245994	FindByFormula	28 +	854.4479	13.245994
854.4511@22.263014	(428.23355, 2278.1858)(428.72595, 862.53687)	854.4511@22.263014	FindByFormula	26 +	854.4511	22.263014
856.2961@16.427088	(857.3055, 3859.8757)(858.30865, 2043.0132)(859.30994, 75	856.2961@16.427088	FindByFormula	22 +	856.2961	16.427088
857.2493@22.33704	(858.2549, 1455.0244)(859.25793, 602.4222)	857.2493@22.33704	FindByFormula	14 +	857.2493	22.33704
857.3804@13.576004	(858.38873, 1597.085)(859.38934, 1092.2301)	857.3804@13.576004	FindByFormula	6 +	857.3804	13.576004
857.7144@13.581676	(858.72363, 2377.1218)(859.7242, 566.01666)	857.7144@13.581676	FindByFormula	6 +	857.7144	13.581676
857.8393@25.265139	(858.8451, 12430.503)(859.8492, 6677.008)(860.84674, 3391	857.8393@25.265139	FindByFormula	14 +	857.8393	25.265139
857.8468@25.059256	(858.8514, 3295.23)(859.855, 1864.7)(860.8443, 1765.17)	857.8468@25.059256	FindByFormula	1 +	857.8468	25.059256
858.5306@22.280897	(859.5394, 24789.404)(860.54285, 11917.95)(861.5449, 3814	858.5306@22.280897	FindByFormula	28 +	858.5306	22.280897
860.3637@16.733767	(861.3716, 2757.9316)(862.3742, 1335.4099)(863.3755, 482.	860.3637@16.733767	FindByFormula	6 +	860.3637	16.733767
861.5069@22.45328	(862.5135, 3046.859)(863.5202, 1697.6558)(864.5299, 968.2	861.5069@22.45328	FindByFormula	9 +	861.5069	22.45328
861.5118@22.669655	(862.5224, 654.255)(863.50165, 311.53)(864.5109, 249.69)	861.5118@22.669655	FindByFormula	2 +	861.5118	22.669655
862.2494@22.540915	(863.2529, 1940.5226)(864.2589, 910.8612)(865.2613, 333.5	862.2494@22.540915	FindByFormula	26 +	862.2494	22.540915
863.5081@24.520555	(432.7557, 721.72)(433.25195, 357.76663)(864.5208, 2322.0	863.5081@24.520555	FindByFormula	12 +	863.5081	24.520555
866.3585@18.392859	(434.1873, 6604.929)(434.6875, 3870.19)(435.18964, 1797.6	866.3585@18.392859	FindByFormula	22 +	866.3585	18.392859
866.4949@22.026224	(434.25867, 7645.3936)(434.75882, 3418.0237)(435.2637, 16	866.4949@22.026224	FindByFormula	22 +	866.4949	22.026224
866.5028@21.646309	(434.2623, 613.35)(434.7577, 108.3)(435.2595, 86.38)	866.5028@21.646309	FindByFormula	1 +	866.5028	21.646309
868.2339@15.176519	(435.12515, 1847.0199)(435.62524, 708.20856)	868.2339@15.176519	FindByFormula	7 +	868.2339	15.176519
868.572@22.445438	(869.5792, 2752.1204)(870.57886, 1502.5358)(871.5715, 629	868.572@22.445438	FindByFormula	21 +	868.572	22.445438
871.5331@24.445992	(872.5408, 135821.39)(873.54376, 68753.55)(874.5472, 2016	871.5331@24.445992	FindByFormula	18 +	871.5331	24.445992
872.3645@17.680222	(873.3733, 1182.7567)(874.3737, 620.88007)	872.3645@17.680222	FindByFormula	6 +	872.3645	17.680222
872.544@22.427355	(873.5507, 1457.02)(874.5535, 879.7622)(875.54736, 417.05	872.544@22.427355	FindByFormula	24 +	872.544	22.427355
873.5456@24.969215	(874.5538, 8736.63)(875.5582, 4675.39)(876.5627, 4063.06)	873.5456@24.969215	FindByFormula	1 +	873.5456	24.969215
873.5459@24.643751	(874.5551, 171272.78)(875.56055, 85683.13)(876.56146, 278	873.5459@24.643751	FindByFormula	18 +	873.5459	24.643751
874.5523@22.484612	(438.29385, 1039.31)(438.78592, 242.49501)(439.29016, 542	874.5523@22.484612	FindByFormula	4 +	874.5523	22.484612
874.5603@22.785263	(438.28992, 3825.2998)(438.78912, 1718.1177)(439.29263, 9	874.5603@22.785263	FindByFormula	17 +	874.5603	22.785263
875.5576@25.349667	(876.5701, 36410.23)(877.5724, 18300.96)(878.574, 4878.05	875.5576@25.349667	FindByFormula	1 +	875.5576	25.349667
875.5589@25.197231	(876.57166, 274128.8)(877.5745, 139830.84)(878.57697, 397	875.5589@25.197231	FindByFormula	14 +	875.5589	25.197231
875.8166@25.536413	(876.824, 25622.26)(877.8274, 12777.44)(878.8302, 4333.39	875.8166@25.536413	FindByFormula	1 +	875.8166	25.536413
875.82@25.311146	(876.8243, 153989.78)(877.82837, 75583.85)(878.8307, 2133	875.82@25.311146	FindByFormula	2 +	875.82	25.311146
875.8232@25.200348	(876.82916, 116712.17)(877.8325, 58399.914)(878.83514, 16	875.8232@25.200348	FindByFormula	19 +	875.8232	25.200348
876.3051@19.871077	(877.3124, 1698.1827)(878.3203, 855.97705)(879.31165, 230	876.3051@19.871077	FindByFormula	7 +	876.3051	19.871077
879.7467@19.318176	(880.7538, 3134.0942)(881.757, 896.2757)(882.75226, 5596.	879.7467@19.318176	FindByFormula	7 +	879.7467	19.318176
880.5145@22.278997	(441.2651, 45437.82)(441.76645, 21443.926)(442.2685, 6978	880.5145@22.278997	FindByFormula	28 +	880.5145	22.278997
882.338@16.728094	(442.17844, 7324.285)(442.67868, 3080.4817)(443.19012, 16	882.338@16.728094	FindByFormula	6 +	882.338	16.728094
883.2687@22.436209	(884.2741, 1560.8851)(885.2757, 752.8384)	883.2687@22.436209	FindByFormula	6 +	883.2687	22.436209
885.5432@24.749071	(886.5498, 5472.4253)(887.5549, 3053.1008)(888.55255, 181	885.5432@24.749071	FindByFormula	11 +	885.5432	24.749071
886.3777@16.156132	(444.1968, 1530.1189)(444.69934, 590.44995)	886.3777@16.156132	FindByFormula	8 +	886.3777	16.156132
886.3806@16.197645	(444.1975, 1460.355)(444.69977, 553.6712)	886.3806@16.197645	FindByFormula	8 +	886.3806	16.197645
886.3831@18.827066	(887.38934, 66585.24)(888.3922, 29350.021)(889.3951, 9149	886.3831@18.827066	FindByFormula	7 +	886.3831	18.827066
887.515@24.447718	(888.5224, 1871.188)(889.01245, 710.2867)(889.52637, 1554	887.515@24.447718	FindByFormula	9 +	887.515	24.447718
888.5332@22.030827	(445.2747, 630.30115)(445.78278, 251.78777)(889.54553, 20	888.5332@22.030827	FindByFormula	20 +	888.5332	22.030827
888.5448@22.161186	(445.2768, 935.47)(445.7827, 308.98)(889.54126, 281.525)(8	888.5448@22.161186	FindByFormula	2 +	888.5448	22.161186
890.3263@6.6908507	(446.17102, 5571.6216)(446.6709, 2539.3867)(447.1707, 846	890.3263@6.6908507	FindByFormula	9 +	890.3263	6.6908507
890.4078@18.27498	(891.4182, 1852.1317)(892.4212, 964.24)	890.4078@18.27498	FindByFormula	6 +	890.4078	18.27498
890.5538@22.44111	(446.28458, 5786.736)(446.78726, 2796.4941)(447.28644, 17	890.5538@22.44111	FindByFormula	24 +	890.5538	22.44111
890.9112@27.177477	(891.92645, 5056.3403)(892.9321, 2755.4333)	890.9112@27.177477	FindByFormula	6 +	890.9112	27.177477
890.9204@27.34777	(891.9336, 8311.045)(892.9335, 4410.11)(893.92944, 1637.1	890.9204@27.34777	FindByFormula	2 +	890.9204	27.34777
894.3493@17.671717	(448.1836, 1635.5101)(448.68286, 740.4033)(449.18835, 292	894.3493@17.671717	FindByFormula	6 +	894.3493	17.671717
894.5349@22.419611	(448.27368, 2635.072)(448.7742, 1189.6517)(449.28027, 339	894.5349@22.419611	FindByFormula	17 +	894.5349	22.419611
895.4521@5.775376	(448.733, 11508.535)(449.23416, 5475.215)(449.7358, 1630.	895.4521@5.775376	FindByFormula	6 +	895.4521	5.775376
895.5347@24.199373	(896.54114, 10753.35)(897.54517, 6040.1953)(898.54456, 22	895.5347@24.199373	FindByFormula	2 +	895.5347	24.199373
895.5347@24.376024	(896.54034, 97880.61)(897.54364, 51729.438)(898.54816, 17	895.5347@24.376024	FindByFormula	15 +	895.5347	24.376024
897.5463@24.58501	(898.5553, 46699.97)(899.5588, 24472.648)(900.5612, 7832.	897.5463@24.58501	FindByFormula	16 +	897.5463	24.58501

898.4602@22.272749				(450.23972, 2269.4395)(450.74008, 1116.2069)(451.23746, 1	898.4602@22.272749		FindByFormula	26	+	898.4602	22.272749
898.4725@13.568503				(450.24368, 2737.8396)(450.74588, 1217.6472)(451.2417, 50	898.4725@13.568503		FindByFormula	28	+	898.4725	13.568503
899.5587@24.851969				(900.5716, 8647.79)(901.5766, 4587.22)(902.5718, 1666.22)	899.5587@24.851969		FindByFormula	1	+	899.5587	24.851969
899.5588@25.093525				(900.57074, 153688.6)(901.57367, 80495.21)(902.5763, 2398	899.5588@25.093525		FindByFormula	15	+	899.5588	25.093525
899.8235@25.351126				(900.8323, 25060.16)(901.8336, 13684.19)	899.8235@25.351126		FindByFormula	1	+	899.8235	25.351126
899.8317@25.102629				(900.8407, 69006.26)(901.8444, 36243.84)(902.84753, 11173	899.8317@25.102629		FindByFormula	18	+	899.8317	25.102629
902.5615@22.287943				(452.28445, 756.51086)(452.78268, 267.31082)(903.5654, 13	902.5615@22.287943		FindByFormula	28	+	902.5615	22.287943
902.5975@23.068104				(452.30408, 9989.753)(452.80423, 5037.613)(453.3162, 2592	902.5975@23.068104		FindByFormula	17	+	902.5975	23.068104
903.4606@10.295564				(452.73685, 5366.5933)(453.2384, 3055.186)(453.74097, 121	903.4606@10.295564		FindByFormula	8	+	903.4606	10.295564
904.3297@16.73777				(453.1757, 3425.577)(453.67484, 1426.3116)(454.17813, 511	904.3297@16.73777		FindByFormula	6	+	904.3297	16.73777
904.3867@16.983585				(905.3938, 562.72)(906.3992, 336.34)(907.4007, 190.48)	904.3867@16.983585		FindByFormula	1	+	904.3867	16.983585
904.3903@16.992311				(905.39795, 7816.4414)(906.40173, 3545.2415)(907.4034, 14	904.3903@16.992311		FindByFormula	7	+	904.3903	16.992311
904.3945@16.754278				(905.39886, 1384.5751)(906.3974, 654.50665)	904.3945@16.754278		FindByFormula	6	+	904.3945	16.754278
904.5756@22.50441				(453.29636, 2998.9392)(453.79434, 1081.4601)(454.2958, 74	904.5756@22.50441		FindByFormula	24	+	904.5756	22.50441
904.5778@22.660416				(453.29672, 2530.5735)(453.79892, 761.4734)(454.29916, 78	904.5778@22.660416		FindByFormula	3	+	904.5778	22.660416
906.2928@6.695007				(454.15283, 2161.9968)(454.65506, 1051.39)	906.2928@6.695007		FindByFormula	6	+	906.2928	6.695007
906.3227@5.9000583				(454.168, 2013.5018)(454.6694, 913.645)	906.3227@5.9000583		FindByFormula	6	+	906.3227	5.9000583
907.4604@24.366047				(908.47614, 2094.3909)(909.47925, 1366.7856)(910.48474, 8	907.4604@24.366047		FindByFormula	11	+	907.4604	24.366047
908.3653@18.828564				(455.19006, 29107.695)(455.69104, 13055.44)(456.19345, 43	908.3653@18.828564		FindByFormula	6	+	908.3653	18.828564
912.5968@22.448559				(913.6038, 1695.5007)(914.6061, 971.325)(915.5988, 385.02	912.5968@22.448559		FindByFormula	20	+	912.5968	22.448559
913.233@3.608588				(914.23926, 1107.4465)(915.2396, 798.42303)(916.2373, 100	913.233@3.608588		FindByFormula	20	+	913.233	3.608588
915.5211@24.535116				(916.52716, 11934.993)(917.5315, 6242.0254)(918.5354, 300	915.5211@24.535116		FindByFormula	12	+	915.5211	24.535116
918.4083@18.132708				(919.41437, 941.095)(920.41675, 498.59085)	918.4083@18.132708		FindByFormula	12	+	918.4083	18.132708
918.5902@22.784018				(460.3035, 4753.9497)(460.80237, 2443.7861)(461.30035, 13	918.5902@22.784018		FindByFormula	18	+	918.5902	22.784018
919.4562@9.677266				(460.73547, 1608.1382)(461.236, 961.1517)(482.71683, 2811	919.4562@9.677266		FindByFormula	6	+	919.4562	9.677266
923.4806@22.453142				(924.486, 1756.3267)(925.4917, 1277.5941)(926.4913, 588.2	923.4806@22.453142		FindByFormula	15	+	923.4806	22.453142
924.5438@22.285477				(463.2807, 42983.25)(463.77924, 20543.686)(464.28613, 748	924.5438@22.285477		FindByFormula	27	+	924.5438	22.285477
924.6388@22.730396				(925.6428, 1795.33)(926.6519, 781.48)	924.6388@22.730396		FindByFormula	1	+	924.6388	22.730396
924.6419@23.040983				(925.6491, 5782.7056)(926.6542, 3130.7446)(927.66174, 133	924.6419@23.040983		FindByFormula	15	+	924.6419	23.040983
925.4703@24.515404				(463.7422, 1208.8447)(464.24234, 660.6859)	925.4703@24.515404		FindByFormula	17	+	925.4703	24.515404
925.5725@25.451336				(926.5867, 22051.84)(927.5873, 13002.52)(928.5928, 5158.0	925.5725@25.451336		FindByFormula	1	+	925.5725	25.451336
925.573@25.266247				(926.5857, 7732.5986)(927.5886, 4320.9653)(928.5891, 2027	925.573@25.266247		FindByFormula	13	+	925.573	25.266247
925.8507@25.536413				(926.8481, 1807.43)(927.8577, 1055.97)(928.8708, 1478.32)	925.8507@25.536413		FindByFormula	1	+	925.8507	25.536413
925.8544@25.280811				(926.862, 6560.7183)(927.8644, 3706.9849)(928.8626, 1536.	925.8544@25.280811		FindByFormula	18	+	925.8544	25.280811
926.3723@16.754114				(464.1957, 2090.9417)(464.6958, 942.6718)(465.2002, 350.9	926.3723@16.754114		FindByFormula	6	+	926.3723	16.754114
926.3747@16.987732				(464.1947, 25419.428)(464.6963, 11482.429)(465.1982, 4470	926.3747@16.987732		FindByFormula	8	+	926.3747	16.987732
926.3777@16.978142				(464.19525, 1156.545)(464.69635, 527.71)(465.1944, 254.69)	926.3777@16.978142		FindByFormula	2	+	926.3777	16.978142
929.1763@0.6045015				(930.1887, 104.415)(931.1399, 176.16)(968.14996, 284.22)(	929.1763@0.6045015		FindByFormula	2	+	929.1763	0.6045015
929.1824@0.83849937				(930.1899, 19131.012)(931.19257, 7329.666)(932.1944, 2447	929.1824@0.83849937		FindByFormula	6	+	929.1824	0.83849937
929.4978@22.457798				(930.50287, 1890.4865)(931.5039, 1080.8182)(932.51074, 64	929.4978@22.457798		FindByFormula	11	+	929.4978	22.457798
930.2113@19.41068				(931.2194, 3592.0386)(932.2242, 1604.6584)(933.21716, 717	930.2113@19.41068		FindByFormula	7	+	930.2113	19.41068
934.4355@18.447943				(935.445, 1684.4868)(936.4467, 872.6416)	934.4355@18.447943		FindByFormula	6	+	934.4355	18.447943
934.5858@22.438871				(468.30167, 2203.9163)(468.79858, 980.90875)(469.3005, 12	934.5858@22.438871		FindByFormula	25	+	934.5858	22.438871
937.2088@19.411821				(938.2144, 1197.2487)(939.2103, 965.5142)	937.2088@19.411821		FindByFormula	7	+	937.2088	19.411821
938.564@22.436773				(470.2909, 2445.04)(470.7873, 872.1753)(471.2927, 1863.24	938.564@22.436773		FindByFormula	25	+	938.564	22.436773
939.5053@10.673127				(470.76157, 2542.0774)(471.2597, 1657.4637)(471.7576, 523	939.5053@10.673127		FindByFormula	19	+	939.5053	10.673127
939.5101@24.245163				(940.5189, 1827.71)(941.529, 962.92)(942.5172, 532.51)	939.5101@24.245163		FindByFormula	1	+	939.5101	24.245163
939.5172@24.440104				(940.5271, 8256.137)(941.5296, 4574.575)(942.53375, 1976.	939.5172@24.440104		FindByFormula	15	+	939.5172	24.440104
940.3933@18.134588				(471.20758, 2041.565)(471.70325, 897.3916)(472.20496, 484	940.3933@18.134588		FindByFormula	13	+	940.3933	18.134588
941.4594@10.395044				(471.73746, 8438.738)(472.23868, 4550.2803)(472.74142, 15	941.4594@10.395044		FindByFormula	6	+	941.4594	10.395044
941.5282@24.661093				(942.54, 11206.927)(943.5415, 6382.8823)(944.53827, 2721.	941.5282@24.661093		FindByFormula	12	+	941.5282	24.661093
942.2077@0.67785704				(943.2209, 1346.6067)(944.2171, 965.896)(981.17865, 1710.	942.2077@0.67785704		FindByFormula	7	+	942.2077	0.67785704
942.218@1.0000008				(943.2177, 347.35)(981.1988, 51.31)(982.2082, 22.06)	942.218@1.0000008		FindByFormula	1	+	942.218	1.0000008
942.4895@22.279886				(472.25198, 2055.1619)(472.75195, 1001.1525)(473.24118, 8	942.4895@22.279886		FindByFormula	24	+	942.4895	22.279886
942.4985@13.866499				(472.25623, 2287.242)(472.7602, 1083.2947)(473.2492, 614.	942.4985@13.866499		FindByFormula	27	+	942.4985	13.866499
943.5407@25.210548				(944.5576, 14942.606)(945.561, 8001.7095)(946.56274, 2770	943.5407@25.210548		FindByFormula	12	+	943.5407	25.210548
946.2066@18.899412				(947.2158, 1256.1628)(948.2183, 649.4872)(949.21027, 2236	946.2066@18.899412		FindByFormula	7	+	946.2066	18.899412
946.5839@22.293484				(947.5917, 8002.7837)(948.59454, 4355.015)(949.5922, 1644	946.5839@22.293484		FindByFormula	27	+	946.5839	22.293484
946.6215@23.066227				(474.3169, 19677.95)(474.8186, 10508.731)(475.32245, 3781	946.6215@23.066227		FindByFormula	14	+	946.6215	23.066227
948.4163@17.00477				(949.4238, 2626.84)(950.42725, 1345.6017)(951.4299, 555.0	948.4163@17.00477		FindByFormula	6	+	948.4163	17.00477
948.5966@22.215168				(475.305, 769.9)(475.8224, 146.96)	948.5966@22.215168		FindByFormula	1	+	948.5966	22.215168
948.6022@22.490602				(475.3102, 3323.5627)(475.80872, 1542.4784)(476.31073, 71	948.6022@22.490602		FindByFormula	24	+	948.6022	22.490602
949.4684@24.438002				(475.742, 1040.8651)(476.2436, 602.15717)	949.4684@24.438002		FindByFormula	14	+	949.4684	24.438002
950.3874@18.494951				(951.39594, 2147.9187)(952.4012, 1167.57)(953.4034, 472.0	950.3874@18.494951		FindByFormula	7	+	950.3874	18.494951
951.1641@0.78333265				(952.17065, 8015.0845)(953.1735, 3167.883)(954.1678, 1507	951.1641@0.78333265		FindByFormula	6	+	951.1641	0.78333265
951.1647@0.59233814				(952.1765, 227.87)(953.17145, 43.120003)(954.1859, 54.05)(	951.1647@0.59233814		FindByFormula	3	+	951.1647	0.59233814
953.4982@25.185356				(477.7582, 1720.7617)(478.25958, 1001.73004)	953.4982@25.185356		FindByFormula	11	+	953.4982	25.185356
954.5524@22.05358				(478.28867, 6653.0947)(478.7912, 2641.2998)(479.28818, 15	954.5524@22.05358		FindByFormula	15	+	954.5524	22.05358
956.4175@18.450941				(479.21982, 1797.6583)(479.7172, 784.79)	956.4175@18.450941		FindByFormula	6	+	956.4175	18.450941
958.3127@6.69148				(480.16342, 3890.9382)(480.66446, 1877.14)(481.16513, 662	958.3127@6.69148		FindByFormula	7	+	958.3127	6.69148
959.4948@24.635881				(960.5036, 5722.9966)(961.5066, 3619.0942)(962.5132, 1951	959.4948@24.635881		FindByFormula	18	+	959.4948	24.635881
961.3825@10.292669				(481.6968, 1337.6066)(482.19836, 782.35175)	961.3825@10.292669		FindByFormula	6	+	961.3825	10.292669
961.3955@5.7852254				(481.7067, 4723.815)(482.2063, 2280.82)(482.70865, 811.56	961.3955@5.7852254		FindByFormula	7	+	961.3955	5.7852254
961.5032@24.43698				(481.75833, 1274.1133)(482.26044, 789.66724)	961.5032@24.43698		FindByFormula	15	+	961.5032	24.43698
962.1421@0.81299925				(963.1512, 1785.6481)(964.15393, 1104.3201)(965.15515, 40	962.1421@0.81299925		FindByFormula	5	+	962.1421	0.81299925
962.1435@0.61450136				(963.1523, 441.13852)(964.147, 353.93597)(965.13513, 72.5	962.1435@0.61450136		FindByFormula	8	+	962.1435	0.61450136
962.6126@22.455866				(482.31216, 933.458)(482.8271, 415.494)(483.32022, 462.80	962.6126@22.455866		FindByFormula	5	+	962.6126	22.455866
962.62@22.774042				(482.31674, 3133.1365)(482.81882, 1465.4166)(483.32556, 1	962.62@22.774042		FindByFormula	15	+	962.62	22.774042
963.5163@24.194462				(964.5266, 3012.0752)(965.52094, 1883.1599)(966.5247, 128	963.5163@24.194462		FindByFormula	2	+	963.5163	24.194462
963.5231@24.37688				(964.528, 7203.79)(965.5285, 4198.1313)(966.5324, 1726.43	963.5231@24.37688		FindByFormula	10	+	963.5231	24.37688
965.9105@27.363674				(966.9309, 11322.48)(967.9337, 6939.43)(968.94, 2562.14)	965.9105@27.363674		FindByFormula	1	+	965.9105	27.363674
967.5352@24.838104				(968.5512, 4065.02)(969.55334, 2665.475)(970.5468, 1514.6	967.5352@24.838104		FindByFormula	2	+	967.5352	24.838104
967.546@25.10503				(968.5592, 9194.487)(969.5617, 5187.1904)(970.5601, 2101.	967.546@25.10503		FindByFormula	8	+	967.546	25.10503
968.5658@22.031195				(485.29242, 1415.8535)(485.79205, 519.49603)	968.5658@22.031195		FindByFormula	20	+	968.5658	22.031195
968.5665@22.293741				(485.29065, 52194.52)(485.79208, 27473.873)(486.29395, 76	968.5665@22.293741		FindByFormula	8	+	968.5665	22.293741
968.5668@22.29198				(485.2913, 34043.99)(485.792, 17911.98)(486.2951, 5909.23	968.5668@22.29198		FindByFormula	28	+	968.5668	22.29198
968.6634@23.068396				(969.67303, 4316.774)(970.6758, 2443.1401)(971.6836, 1015	968.6634@23.068396		FindByFormula	16	+	968.6634	23.068396
969.383@16.880194				(485.69687, 3955.3586)(486.20157, 2188.1467)(486.7015, 81	969.383@16.880194		FindByFormula	6	+	969.383	16.880194
969.4065@10.295565				(485.7104, 17180.607)(486.21198, 9494.433)(486.70953, 297	969.4065@10.295565		FindByFormula	8	+	969.4065	10.295565
970.3987@16.999172				(486.2081, 7747.624)(486.70822, 3777.1)(487.21472, 1834.5	970.3987@16.999172		FindByFormula	7	+	970.3987	16.999172
970.4013@17.192896				(486.20938, 1843.2164)(486.70947, 879.6833)	970.4013@17.192896		FindByFormula	6	+	970.4013	17.192896
970.4048@16.999598				(486.2115, 475.77)(486.7045, 115.14)	970.4048@16.999598		FindByFormula	1	+	970.4048	16.999598
972.3756@18.495142				(487.19662, 2183.125)(487.6954, 1054.6)(488.19168, 309.30	972.3756@18.495142		FindByFormula	6	+	972.3756	18.495142
976.3546@18.827229				(489.18787, 3407.8467)(489.68484, 1642.6766)(490.19156, 6	976.3546@18.827229		FindByFormula	6	+	976.3546	18.827229
980.6528@19.790384				(981.6629, 3384.4158)(982.667, 2170.7527)	980.6528@19.790384		FindByFormula	28	+	980.6528	19.790384
982.6736@19.445652				(983.68036, 27878.014)(984.6836, 17702.354)(985.6872, 638	982.6736@19.445652		FindByFormula	28	+	982.6736	19.445652
983.5043@24.547352				(984.5109, 4007.7444)(985.51355, 2298.8457)(986.5144, 128	983.5043@24.547352		FindByFormula	16	+	983.5043	24.547352
984.1201@0.9613991				(985.1292, 1180.43)(986.1331, 819.048)(987.1077, 29.12)	984.1201@0.9613991		FindByFormula	5	+	984.1201	0.9613991
984.1208@0.71400017				(985.1288, 1636.26)(986.1306, 1104.77)	984.1208@0.71400017		FindByFormula	1	+	984.1208	0.71400017
985.4018@9.678767				(493.7076, 5956.625)(494.20908, 3301.5215)(494.7113, 1086	985.4018@9.678767		FindByFormula	6	+	985.4018	9.678767
986.5193@22.290657				(494.27365, 1320.115)(494.77423, 757.66003)(495.276, 203.	986.5193@22.290657		FindByFormula	4	+	986.5193	22.290657
987.5345@7.6266623				(494.77448, 1467.4896)(495.2727, 847.9725)(495.77335, 303	987.5345@7.6266623		FindByFormula	20	+	987.5345	7.6266623
988.3911@21.79887				(989.4003, 1547.0177)(990.4025, 943.81)(991.4053, 491.305	988.3911@21.79887		FindByFormula	22	+	988.3911	21.79887
990.6147@22.29418				(991.61957, 4989.321)(992.6233, 2853.335)(993.6197, 1089.	990.6147@22.29418		FindByFormula	24	+	990.6147	22.29418
990.6445@23.054432				(496.33026, 20396.83)(496.8319, 10898.42)(497.3345, 4472.	990.6445@23.054432		FindByFormula	16	+	990.6445	23.054432
990.647@22.737679				(496.3389, 2720.17)(496.823, 210.83)(497.3386, 2083.51)(49	990.647@22.737679		FindByFormula	2	+	990.647	22.737679
992.4435@17.242594				(993.45044, 4094.1619)(994.45416, 2106.46)(995.45435, 844	992.4435@17.242594		FindByFormula	6	+	992.4435	17.242594
992.6181@22.166582				(497.32056, 1291.23)(497.819, 299.84)(498.32257, 385.7525)	992.6181@22.166582		FindByFormula	4	+	992.6181	22.166582
992.6256@22.509481				(497.32312, 3645.2234)(497.8202, 1539.8192)(498.32068, 82	992.6256@22.509481		FindByFormula	12	+	992.6256	22.509481
992.6305@22.746069				(497.32657, 1160.5233)(497.81348, 118.1)(498.31787, 417.1	992.6305@22.746069		FindByFormula	3	+	992.6305	22.746069
ABRINE (CAS# 526-31-8); (M+H)+	ABRINE (CAS# 526-31-8); (M+H)+	ABRINE (CAS# 526-31-8); (M+H)+ [, tgt=41.52, overall=41.	526-31-8	(219.1116, 1418.05)(220.1148, 313.2)	ABRINE (CAS# 526-31-8); (M+H)+	C02983	FindByFormula	2	+	218.1035	3.5466342
ACETAMINOPHEN (TN TYLENOL) (CAS# 103-9	ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90	ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M+H)	103-90-2	(152.07051, 17974.434)(153.07323, 1854.1443)(154.0711, 19	ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M+H)+	C06804	FindByFormula	14	+	151.0634	3.0716157
ACETAMINOPHEN (TN TYLENOL) (CAS# 103-9	ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90	ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M+Na	103-90-2	(174.05269, 31033.666)(175.05444, 3135.8452)(176.0591, 28	ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M+Na)+	C06804	FindByFormula	20	+	151.0635	3.0741389
ACETYLCHOLINE (CAS# 51-84-3); M+	ACETYLCHOLINE (CAS# 51-84-3); M+	ACETYLCHOLINE (CAS# 51-84-3); M+ [, tgt=62.10, overall=	51-84-3	(146.11722, 1218.7606)(147.11592, 141.64714)	ACETYLCHOLINE (CAS# 51-84-3); M+	C01996	FindByFormula	14	+	146.1172	3.9036748
ADENINE (CAS# 73-24-5); (M+H)+	ADENINE (CAS# 73-24-5); (M+H)+	ADENINE (CAS# 73-24-5); (M+H)+ [, tgt=72.33, overall=72	73-24-5	(136.06236, 1782.7538)(137.06117, 182.47272)	ADENINE (CAS# 73-24-5); (M+H)+		FindByFormula	11	+	135.0548	0.91836375
ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-	ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-7	ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-73-2); (M+H	1053-73-2	(428.03973, 1885.514)(429.04132, 465.148)(430.03613, 213.	ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-73-2); (M+H)+	C00054	FindByFormula	5	+	427.0323	1.1954027
ADENOSINE 5'-DIPHOSPHATE (CAS# 58-64-0);	ADENOSINE 5'-DIPHOSPHATE (CAS# 58-64-0);	ADENOSINE 5'-DIPHOSPHATE (CAS# 58-64-0); (M+H)+ [, t	58-64-0	(428.03973, 1885.514)(429.04132, 465.148)(430.03613, 213.	ADENOSINE 5'-DIPHOSPHATE (CAS# 58-64-0); (M+H)+		FindByFormula	5	+	427.0323	1.1954027
ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-1	ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-1	ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-19-8); (M+H)	61-19-8	(348.07062, 2162.8982)(349.06827, 317.1282)(350.06815, 15	ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-19-8); (M+H)+		FindByFormula	11	+	347.0604	1.232916
ADIPIC ACID (CAS# 124-04-9); (M+Na)+	ADIPIC ACID (CAS# 124-04-9); (M+Na)+	ADIPIC ACID (CAS# 124-04-9); (M+Na)+ [, tgt=71.53, over	124-04-9	(169.04782, 4079.1262)(170.04883, 118.23385)(171.0475, 44	ADIPIC ACID (CAS# 124-04-9); (M+Na)+	C06104	FindByFormula	13	+	146.0586	3.5313034
ADP-RIBOSE (CAS#); (M+H)+[-H2O]	ADP-RIBOSE (CAS#); (M+H)+[-H2O]	ADP-RIBOSE (CAS#); (M+H)+[-H2O] [, tgt=27.99, overall=27.99]		(542.068, 518.14)(543.0628, 129.08)(544.0491, 45.73)	ADP-RIBOSE (CAS#); (M+H)+[-H2O]		FindByFormula	1	+	559.0682	1.0160055
AHBA (CAS# 76045-71-1); (M+H)+	AHBA (CAS# 76045-71-1); (M+H)+	AHBA (CAS# 76045-71-1); (M+H)+ [, tgt=49.08, overall=49	76045-71-1	(154.04909, 6014.81)(155.05003, 320.26602)	AHBA (CAS# 76045-71-1); (M+H)+	C12107	FindByFormula	5	+	153.0413	1.4176052
ALANINE (CAS# 56-41-7); (M+H)+	ALANINE (CAS# 56-41-7); (M+H)+	ALANINE (CAS# 56-41-7); (M+H)+ [, tgt=31.44, overall=31.	56-41-7	(90.055336, 891.484)(91.05376, 133.894)	ALANINE (CAS# 56-41-7); (M+H)+		FindByFormula	5	+	89.0473	1.4403982
ALLANTOIN (CAS# 97-59-6); (M+H)+	ALLANTOIN (CAS# 97-59-6); (M+H)+	ALLANTOIN (CAS# 97-59-6); (M+H)+ [, tgt=45.92, overall=	97-59-6	(159.0502, 357.72)(160.0457, 24.13)	ALLANTOIN (CAS# 97-59-6); (M+H)+		FindByFormula	1	+	158.0425	0.38699895
ALLOSE (CAS# 2595-97-3); (M+H)+[-H2O]	ALLOSE (CAS# 2595-97-3); (M+H)+[-H2O]	ALLOSE (CAS# 2595-97-3); (M+H)+[-H2O] [, tgt=31.90, ove	2595-97-3	(163.06155, 1165.8672)(164.05824, 715.92145)	ALLOSE (CAS# 2595-97-3); (M+H)+[-H2O]	C01487	FindByFormula	7	+	180.0622	1.947869
ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 22	ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 22	ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 2255-14-3); (M	2255-14-3	(283.01758, 449.47498)(284.0216, 96.865)	ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 2255-14-3); (M+Na)+		FindByFormula	4	+	260.0273	0.89899933
ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+	ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+	ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+Na)+ [, tgt=	463-40-1	(301.2123, 17077.32)(302.21683, 3220.9236)(303.221, 1555.	ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+Na)+		FindByFormula	26	+	278.2223	22.704765
ALPHA-TOCOPHEROL (CAS# 59-02-9); (M+H)+	ALPHA-TOCOPHEROL (CAS# 59-02-9); (M+H)+	ALPHA-TOCOPHEROL (CAS# 59-02-9); (M+H)+ [, tgt=70.85	59-02-9	(431.38736, 583.62164)(432.39066, 219.03001)(433.3855, 80	ALPHA-TOCOPHEROL (CAS# 59-02-9); (M+H)+	C02477	FindByFormula	6	+	430.3778	24.490105
ANDROSTERONE (CAS# 53-41-8); (M+H)+[-H2	ANDROSTERONE (CAS# 53-41-8); (M+H)+[-H2	ANDROSTERONE (CAS# 53-41-8); (M+H)+[-H2O] [, tgt=68.	53-41-8	(273.2192, 849.45)(274.2218, 263.51)	ANDROSTERONE (CAS# 53-41-8); (M+H)+[-H2O]		FindByFormula	1	+	290.2223	19.64505
ANDROSTERONE (CAS# 53-41-8); (M+Na)+	ANDROSTERONE (CAS# 53-41-8); (M+Na)+	ANDROSTERONE (CAS# 53-41-8); (M+Na)+ [, tgt=37.44, o	53-41-8	(313.21268, 2024.4911)(314.21704, 473.66333)(315.2167, 32	ANDROSTERONE (CAS# 53-41-8); (M+Na)+		FindByFormula	12	+	290.2233	19.67865
ANTHRANILATE (CAS# 118-92-3); (M+H)+	ANTHRANILATE (CAS# 118-92-3); (M+H)+	ANTHRANILATE (CAS# 118-92-3); (M+H)+ [, tgt=65.75, ov	118-92-3	(138.055, 780.89)(139.0641, 126.53)	ANTHRANILATE (CAS# 118-92-3); (M+H)+		FindByFormula	1	+	137.0486	5.268
ARABINOSE (CAS# 147-81-9); (M+Na)+	ARABINOSE (CAS# 147-81-9); (M+Na)+	ARABINOSE (CAS# 147-81-9); (M+Na)+ [, tgt=63.88, overa	147-81-9	(173.04222, 14187.223)(174.04117, 1619.8125)(175.0391, 69	ARABINOSE (CAS# 147-81-9); (M+Na)+	C00259	FindByFormula	4	+	150.053	0.91000307
ARACHIDIC ACID (CAS# 506-30-9); (M+Na)+	ARACHIDIC ACID (CAS# 506-30-9); (M+Na)+	ARACHIDIC ACID (CAS# 506-30-9); (M+Na)+ [, tgt=33.08,	506-30-9	(335.29156, 1163.725)(336.29565, 132.3)	ARACHIDIC ACID (CAS# 506-30-9); (M+Na)+	C06425	FindByFormula	2	+	312.3012	23.25819
ASCORBATE (CAS# 50-81-7); (M+H)+[-H2O]	ASCORBATE (CAS# 50-81-7); (M+H)+[-H2O]	ASCORBATE (CAS# 50-81-7); (M+H)+[-H2O] [, tgt=96.70, o	50-81-7	(159.02876, 77616.54)(160.0313, 5346.4546)(161.03156, 256	ASCORBATE (CAS# 50-81-7); (M+H)+[-H2O]		FindByFormula	19	+	176.0323	1.1074787
ASPARAGINE (CAS# 70-47-3); (M+H)+	ASPARAGINE (CAS# 70-47-3); (M+H)+	ASPARAGINE (CAS# 70-47-3); (M+H)+ [, tgt=30.51, overall	70-47-3	(133.06113, 2080.2725)(134.06621, 273.19)	ASPARAGINE (CAS# 70-47-3); (M+H)+		FindByFormula	4	+	132.0538	0.7115079
ASPARAGINE (CAS# 70-47-3); (M+Na)+	ASPARAGINE (CAS# 70-47-3); (M+Na)+	ASPARAGINE (CAS# 70-47-3); (M+Na)+ [, tgt=89.85, overa	70-47-3	(155.0436, 1822.4)(156.03876, 125.630005)(157.0358, 51.52)	ASPARAGINE (CAS# 70-47-3); (M+Na)+		FindByFormula	2	+	132.0537	0.6315018
ASPARTATE (CAS# 56-84-8); (M+H)+	ASPARTATE (CAS# 56-84-8); (M+H)+	ASPARTATE (CAS# 56-84-8); (M+H)+ [, tgt=34.25, overall=	56-84-8	(134.04446, 2382.062)(135.04778, 272.514)(136.0495, 177.1)	ASPARTATE (CAS# 56-84-8); (M+H)+		FindByFormula	5	+	133.0363	0.7351997
ASPARTATE (CAS# 56-84-8); (M+Na)+	ASPARTATE (CAS# 56-84-8); (M+Na)+	ASPARTATE (CAS# 56-84-8); (M+Na)+ [, tgt=61.90, overall	56-84-8	(156.02782, 2609.1619)(157.0276, 164.982)(158.02374, 202.	ASPARTATE (CAS# 56-84-8); (M+Na)+		FindByFormula	5	+	133.0378	0.62699974
AZELAIC ACID (CAS# 123-99-9); (M+H)+[-H2O]	AZELAIC ACID (CAS# 123-99-9); (M+H)+[-H2O]	AZELAIC ACID (CAS# 123-99-9); (M+H)+[-H2O] [, tgt=82.2	123-99-9	(171.1003, 1830.96)(172.1022, 154.22)	AZELAIC ACID (CAS# 123-99-9); (M+H)+[-H2O]	C08261	FindByFormula	1	+	188.1034	10.691504
AZELAIC ACID (CAS# 123-99-9); (M+Na)+	AZELAIC ACID (CAS# 123-99-9); (M+Na)+	AZELAIC ACID (CAS# 123-99-9); (M+Na)+ [, tgt=68.24, ove	123-99-9	(211.09511, 12430.481)(212.09747, 1384.0619)(213.0952, 31	AZELAIC ACID (CAS# 123-99-9); (M+Na)+	C08261	FindByFormula	22	+	188.1055	10.6841955
BENZOATE (CAS# 65-85-0); (M+H)+	BENZOATE (CAS# 65-85-0); (M+H)+	BENZOATE (CAS# 65-85-0); (M+H)+ [, tgt=75.74, overall=7	65-85-0	(123.04482, 2126.4744)(124.04451, 178.40898)(125.03695, 1	BENZOATE (CAS# 65-85-0); (M+H)+	C00180	FindByFormula	20	+	122.0374	4.932517
BETA-ALANINE (CAS# 107-95-9); (M+H)+	BETA-ALANINE (CAS# 107-95-9); (M+H)+	BETA-ALANINE (CAS# 107-95-9); (M+H)+ [, tgt=78.33, ove	107-95-9	(90.05532, 2221.007)(91.05602, 66.617)	BETA-ALANINE (CAS# 107-95-9); (M+H)+		FindByFormula	10	+	89.048	0.67180026
BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (C	BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (C	BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (CAS# 584-85-	584-85-0	(241.1285, 478.35)(242.1297, 55.74)	BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (CAS# 584-85-0); (M+H)+		FindByFormula	1	+	240.1211	0.72700197
BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (C	BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (C	BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (CAS# 584-85-	584-85-0	(263.1119, 906.66)(264.1116, 254.52)	BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (CAS# 584-85-0); (M+Na)+		FindByFormula	1	+	240.122	0.73900026
BETAINE (CAS# 107-43-7); (M+H)+	BETAINE (CAS# 107-43-7); (M+H)+	BETAINE (CAS# 107-43-7); (M+H)+ [, tgt=98.04, overall=9	107-43-7	(118.08652, 105635.68)(119.08814, 6473.576)(120.08629, 54	BETAINE (CAS# 107-43-7); (M+H)+		FindByFormula	22	+	117.0786	0.6018646
BETAINE (CAS# 107-43-7); (M+Na)+	BETAINE (CAS# 107-43-7); (M+Na)+	BETAINE (CAS# 107-43-7); (M+Na)+ [, tgt=87.25, overall=	107-43-7	(140.06839, 3587.9434)(141.06947, 295.6158)(142.07195, 14	BETAINE (CAS# 107-43-7); (M+Na)+		FindByFormula	24	+	117.0789	0.59337544
BETA-MALTOSE (CAS# 69-79-4); (M+Na)+	BETA-MALTOSE (CAS# 69-79-4); (M+Na)+	BETA-MALTOSE (CAS# 69-79-4); (M+Na)+ [, tgt=81.32, ov	69-79-4	(365.1071, 1436.5284)(366.10913, 190.30142)(367.11215, 64	BETA-MALTOSE (CAS# 69-79-4); (M+Na)+	C00208	FindByFormula	14	+	342.1191	0.716929
BILIVERDIN (CAS# 114-25-0); (M+H)+	BILIVERDIN (CAS# 114-25-0); (M+H)+	BILIVERDIN (CAS# 114-25-0); (M+H)+ [, tgt=77.46, overall	114-25-0	(583.2564, 4673.0337)(584.25934, 1863.0548)(585.27167, 65	BILIVERDIN (CAS# 114-25-0); (M+H)+	C00500	FindByFormula	6	+	582.2508	18.577179
BILIVERDIN (CAS# 114-25-0); (M+Na)+	BILIVERDIN (CAS# 114-25-0); (M+Na)+	BILIVERDIN (CAS# 114-25-0); (M+Na)+ [, tgt=70.01, overal	114-25-0	(605.2403, 2573.125)(606.24347, 1057.3534)(607.24695, 185	BILIVERDIN (CAS# 114-25-0); (M+Na)+	C00500	FindByFormula	6	+	582.253	18.582687
BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-	BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7	BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7); (M+H)+ [	117-81-7	(391.28546, 7694.402)(392.2887, 1861.2874)(393.28787, 254	BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7); (M+H)+	C03690	FindByFormula	18	+	390.2792	23.170147
BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-	BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7	BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7); (M+Na)+	117-81-7	(413.2673, 406341.7)(414.2706, 107564.68)(415.27216, 1729	BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7); (M+Na)+	C03690	FindByFormula	19	+	390.2777	23.121073
BIURET (CAS# 108-19-0); (M+Na)+	BIURET (CAS# 108-19-0); (M+Na)+	BIURET (CAS# 108-19-0); (M+Na)+ [, tgt=71.20, overall=7	108-19-0	(126.02692, 5921.887)(127.02895, 247.98999)(128.0256, 275	BIURET (CAS# 108-19-0); (M+Na)+	C06555	FindByFormula	10	+	103.0373	0.6900028
C10 H10 N8	C10 H10 N8	[C10 H10 N8, tgt=78.95, overall=78.95]		(243.11118, 8308.9795)(244.10878, 1749.5184)(245.10555, 1	C10 H10 N8		FindByFormula	14	+	242.1033	11.618258
C10 H11 N3 O3 S	C10 H11 N3 O3 S	[C10 H11 N3 O3 S, tgt=99.31, overall=99.31]		(254.0598, 7493.85)(255.0648, 1101.955)(256.0585, 434.783	C10 H11 N3 O3 S		FindByFormula	6	+	253.0526	6.50981
C10 H11 N5	C10 H11 N5	[C10 H11 N5, tgt=90.79, overall=90.79]		(202.10893, 8439.675)(203.10966, 1015.1207)(204.11026, 12	C10 H11 N5		FindByFormula	28	+	201.1015	3.8876235
C10 H12 N2 O3	C10 H12 N2 O3	[C10 H12 N2 O3, tgt=95.95, overall=95.95]		(209.09244, 16531.42)(210.0958, 2172.1685)(211.08884, 116	C10 H12 N2 O3		FindByFormula	24	+	208.0851	2.2087314
C10 H12 N4 O5	C10 H12 N4 O5	[C10 H12 N4 O5, tgt=81.25, overall=81.25]		(269.09024, 50833.344)(270.0934, 6347.0093)(271.08853, 20	C10 H12 N4 O5		FindByFormula	27	+	268.0829	1.7902312
C10 H13 N	C10 H13 N	[C10 H13 N, tgt=99.51, overall=99.51]		(148.11186, 18553.652)(149.11423, 2160.1287)(150.11618, 1	C10 H13 N		FindByFormula	20	+	147.1047	10.88497
C10 H13 N P2 S2	C10 H13 N P2 S2	[C10 H13 N P2 S2, tgt=55.99, overall=55.99]		(274.0024, 2517.2573)(275.00272, 434.00388)(276.00266, 35	C10 H13 N P2 S2		FindByFormula	26	+	272.9959	1.0996577
C10 H13 N5	C10 H13 N5	[C10 H13 N5, tgt=96.58, overall=96.58]		(204.124, 46207.785)(205.12502, 5604.027)(206.12407, 730.	C10 H13 N5		FindByFormula	28	+	203.1163	2.2576559
C10 H13 N5 O	C10 H13 N5 O	[C10 H13 N5 O, tgt=99.18, overall=99.18]		(220.11983, 713129.6)(221.12254, 87747.234)(222.12509, 67	C10 H13 N5 O		FindByFormula	28	+	219.1124	3.888517
C10 H14 N2 O	C10 H14 N2 O	[C10 H14 N2 O, tgt=46.48, overall=46.48]		(179.11818, 33620.28)(180.11943, 4419.5073)(181.12067, 52	C10 H14 N2 O		FindByFormula	23	+	178.111	3.7206497
C10 H14 N2 O2	C10 H14 N2 O2	[C10 H14 N2 O2, tgt=98.72, overall=98.72]		(195.1131, 1498.3387)(196.11263, 113.726265)(197.10852, 1	C10 H14 N2 O2		FindByFormula	26	+	194.1056	4.161453
C10 H14 N6	C10 H14 N6	[C10 H14 N6, tgt=63.64, overall=63.64]		(219.13428, 4152.689)(220.13408, 602.3508)(221.138, 118.5	C10 H14 N6		FindByFormula	23	+	218.1267	2.690771
C10 H14 O	C10 H14 O	[C10 H14 O, tgt=78.89, overall=78.89]		(151.11137, 2795.0974)(152.11313, 323.23)(153.11546, 51.8	C10 H14 O		FindByFormula	28	+	150.1038	13.107524
C10 H15 N2 O P	C10 H15 N2 O P	[C10 H15 N2 O P, tgt=87.41, overall=87.41]		(211.10074, 4064.7344)(212.1001, 365.6664)(213.09996, 192	C10 H15 N2 O P		FindByFormula	28	+	210.0931	19.820889
C10 H15 N4 P	C10 H15 N4 P	[C10 H15 N4 P, tgt=83.52, overall=83.52]		(223.10913, 5906.5405)(224.1223, 3967.42)(225.113, 1280.8	C10 H15 N4 P		FindByFormula	17	+	222.1027	4.437573
C10 H16 Cl3 O10 P S4	C10 H16 Cl3 O10 P S4	[C10 H16 Cl3 O10 P S4, tgt=79.50, overall=79.50]		(560.8577, 4284.2896)(561.8527, 587.555)(562.84393, 3104.	C10 H16 Cl3 O10 P S4		FindByFormula	8	+	559.8416	21.046694
C10 H16 N2 O	C10 H16 N2 O	[C10 H16 N2 O, tgt=98.54, overall=98.54]		(181.1331, 9142.3955)(182.13605, 1096.3866)(183.13878, 26	C10 H16 N2 O		FindByFormula	6	+	180.1259	8.55958
C10 H16 N2 O2	C10 H16 N2 O2	[C10 H16 N2 O2, tgt=90.47, overall=90.47]		(197.12674, 2805.0547)(198.12653, 466.2617)(199.12328, 56	C10 H16 N2 O2		FindByFormula	12	+	196.1211	5.5833917
C10 H16 N6 O	C10 H16 N6 O	[C10 H16 N6 O, tgt=81.44, overall=81.44]		(237.1462, 4535.7153)(238.14818, 729.25757)(275.1099, 55.	C10 H16 N6 O		FindByFormula	8	+	236.14	18.722801
C10 H16 N6 O4	C10 H16 N6 O4	[C10 H16 N6 O4, tgt=93.32, overall=93.32]		(285.13174, 13838.784)(286.13486, 1994.8657)(287.1351, 48	C10 H16 N6 O4		FindByFormula	9	+	284.1241	18.135838
C10 H16 O5 P2	C10 H16 O5 P2	[C10 H16 O5 P2, tgt=95.64, overall=95.64]		(279.05548, 6015.7075)(280.05975, 744.53)(281.0582, 129.8	C10 H16 O5 P2		FindByFormula	8	+	278.0479	15.6367445
C10 H17 N2 O2 P	C10 H17 N2 O2 P	[C10 H17 N2 O2 P, tgt=66.60, overall=66.60]		(229.11137, 6645.5747)(230.11415, 852.6965)(231.11775, 12	C10 H17 N2 O2 P		FindByFormula	23	+	228.1042	18.3232
C10 H17 N7 O	C10 H17 N7 O	[C10 H17 N7 O, tgt=92.57, overall=92.57]		(252.15723, 8332.515)(253.15561, 1328.5874)(254.15762, 23	C10 H17 N7 O		FindByFormula	22	+	251.1492	8.9629965
C10 H18 N O6 P	C10 H18 N O6 P	[C10 H18 N O6 P, tgt=91.31, overall=91.31]		(280.09464, 13387.983)(281.09665, 1351.36)(282.09772, 341	C10 H18 N O6 P		FindByFormula	24	+	279.0885	0.6349594
C10 H18 N2 O	C10 H18 N2 O	[C10 H18 N2 O, tgt=99.48, overall=99.48]		(183.14886, 18461.02)(184.15175, 2309.1782)(185.15538, 23	C10 H18 N2 O		FindByFormula	13	+	182.1416	4.75942
C10 H18 N2 O5	C10 H18 N2 O5	[C10 H18 N2 O5, tgt=96.54, overall=96.54]		(247.1289, 7528.3413)(248.12737, 1076.65)(249.12439, 266.	C10 H18 N2 O5		FindByFormula	27	+	246.1213	2.438879
C10 H18 N6 O	C10 H18 N6 O	[C10 H18 N6 O, tgt=96.22, overall=96.22]		(239.162, 25409.676)(240.1653, 3520.4055)(241.16231, 535.	C10 H18 N6 O		FindByFormula	28	+	238.1548	17.960075
C10 H18 N6 O3	C10 H18 N6 O3	[C10 H18 N6 O3, tgt=97.96, overall=97.96]		(271.15158, 16702.736)(272.15384, 2385.814)(273.151, 431.	C10 H18 N6 O3		FindByFormula	15	+	270.1451	13.18361
C10 H18 O3 P2	C10 H18 O3 P2	[C10 H18 O3 P2, tgt=97.72, overall=97.72]		(249.08047, 38576.883)(250.08391, 5235.469)(251.08348, 61	C10 H18 O3 P2		FindByFormula	28	+	248.0731	13.103129
C10 H19 N O2	C10 H19 N O2	[C10 H19 N O2, tgt=96.30, overall=96.30]		(186.14845, 3758.8608)(187.15112, 728.0311)(188.14836, 85	C10 H19 N O2		FindByFormula	16	+	185.1415	1.9700129
C10 H19 N O3	C10 H19 N O3	[C10 H19 N O3, tgt=79.76, overall=79.76]		(202.14244, 1544.2156)(203.14293, 641.54333)(204.1425, 31	C10 H19 N O3		FindByFormula	23	+	201.1371	3.0003958
C10 H19 N4 O4 P	C10 H19 N4 O4 P	[C10 H19 N4 O4 P, tgt=97.22, overall=97.22]		(291.1212, 27106.67)(292.1248, 4262.8047)(293.13156, 1281	C10 H19 N4 O4 P		FindByFormula	6	+	290.1143	18.647776

C10 H19 N7 O	C10 H19 N7 O	[C10 H19 N7 O, tgt=78.59, overall=78.59]	(254.17265, 4944.878)(255.17014, 775.462)(256.17032, 85.1	C10 H19 N7 O	FindByFormula	25 +	253.1644	12.532163
C10 H20 N2 O3	C10 H20 N2 O3	[C10 H20 N2 O3, tgt=84.96, overall=84.96]	(217.1547, 5004.729)(218.1555, 665.5679)(219.15263, 107.0	C10 H20 N2 O3	FindByFormula	27 +	216.1466	2.3362834
C10 H20 N6 O	C10 H20 N6 O	[C10 H20 N6 O, tgt=94.92, overall=94.92]	(241.1768, 6764.8228)(242.18088, 983.1086)(243.1787, 124.	C10 H20 N6 O	FindByFormula	8 +	240.17	15.061917
C10 H21 N O2	C10 H21 N O2	[C10 H21 N O2, tgt=68.13, overall=68.13]	(188.1644, 9250.405)(189.16733, 1122.1439)(190.16707, 126	C10 H21 N O2	FindByFormula	6 +	187.1572	4.5474277
C10 H21 N4 O3 P	C10 H21 N4 O3 P	[C10 H21 N4 O3 P, tgt=86.19, overall=86.19]	(277.14154, 7379.288)(278.145, 1146.7596)(279.14594, 282.	C10 H21 N4 O3 P	FindByFormula	27 +	276.1345	14.845832
C10 H21 N6 P	C10 H21 N6 P	[C10 H21 N6 P, tgt=83.04, overall=83.04]	(257.16296, 336193.7)(258.16605, 52616.074)(259.1687, 450	C10 H21 N6 P	FindByFormula	18 +	256.1558	5.4793878
C10 H22 N2 O3	C10 H22 N2 O3	[C10 H22 N2 O3, tgt=88.42, overall=88.42]	(219.1704, 8061.5806)(220.17252, 1181.0192)(221.1718, 136	C10 H22 N2 O3	FindByFormula	15 +	218.162	0.7013341
C10 H22 O6	C10 H22 O6	[C10 H22 O6, tgt=99.16, overall=99.16]	(239.14803, 4431.4346)(240.15025, 558.8454)(241.1482, 149	C10 H22 O6	FindByFormula	28 +	238.1417	4.81987
C10 H24 N8 O3	C10 H24 N8 O3	[C10 H24 N8 O3, tgt=79.66, overall=79.66]	(305.20526, 2224.0146)(306.20425, 451.8813)(307.20132, 18	C10 H24 N8 O3	FindByFormula	10 +	304.1955	0.7742032
C10 H25 N3 O3 P2 S2	C10 H25 N3 O3 P2 S2	[C10 H25 N3 O3 P2 S2, tgt=90.94, overall=90.94]	(362.08862, 42977.215)(363.09268, 6418.405)(364.0889, 313	C10 H25 N3 O3 P2 S2	FindByFormula	14 +	361.0818	10.488086
C10 H26 N4	C10 H26 N4	[C10 H26 N4, tgt=38.67, overall=38.67]	(203.22305, 24387.25)(204.2253, 3236.9126)(205.229, 317.4	C10 H26 N4	FindByFormula	20 +	202.216	0.602752
C10 H28 N6 O S	C10 H28 N6 O S	[C10 H28 N6 O S, tgt=87.83, overall=87.83]	(281.21194, 3383.017)(282.2116, 539.19446)(283.20737, 200	C10 H28 N6 O S	FindByFormula	25 +	280.2048	21.63425
C10 H31 N12 O3 P3	C10 H31 N12 O3 P3	[C10 H31 N12 O3 P3, tgt=94.33, overall=94.33]	(461.19373, 5611.2627)(462.1961, 784.34863)(463.19955, 18	C10 H31 N12 O3 P3	FindByFormula	8 +	460.1854	19.16135
C10 H9 N	C10 H9 N	[C10 H9 N, tgt=72.69, overall=72.69]	(144.07999, 22222.297)(145.08092, 4181.9434)	C10 H9 N	FindByFormula	6 +	143.0723	3.6112087
C10 H9 N O2	C10 H9 N O2	[C10 H9 N O2, tgt=95.30, overall=95.30]	(176.06998, 2087.643)(177.07324, 329.76083)(178.07617, 12	C10 H9 N O2	FindByFormula	14 +	175.0641	8.35952
C10 H9 N O3	C10 H9 N O3	[C10 H9 N O3, tgt=98.30, overall=98.30]	(192.06595, 4668.9897)(193.06795, 690.8156)(194.06563, 70	C10 H9 N O3	FindByFormula	28 +	191.0585	2.2246635
C11 H10 N6 O2	C11 H10 N6 O2	[C11 H10 N6 O2, tgt=84.61, overall=84.61]	(259.0944, 15154.355)(260.0981, 2296.8584)(261.08734, 557	C11 H10 N6 O2	FindByFormula	6 +	258.0872	12.961578
C11 H10 N8 O3	C11 H10 N8 O3	[C11 H10 N8 O3, tgt=95.96, overall=95.96]	(303.09656, 4800.802)(304.09943, 792.395)(305.09955, 215.	C11 H10 N8 O3	FindByFormula	6 +	302.0887	9.321628
C11 H11 N O2	C11 H11 N O2	[C11 H11 N O2, tgt=63.26, overall=63.26]	(190.08643, 2997.3965)(191.09279, 505.78003)(192.09262, 1	C11 H11 N O2	FindByFormula	6 +	189.0793	10.35086
C11 H11 N O3	C11 H11 N O3	[C11 H11 N O3, tgt=83.33, overall=83.33]	(206.08202, 502.46793)(207.0807, 52.99)(244.03374, 140.29	C11 H11 N O3	FindByFormula	20 +	205.0758	7.385054
C11 H11 N6 P	C11 H11 N6 P	[C11 H11 N6 P, tgt=63.27, overall=63.27]	(259.0848, 8312.102)(260.08823, 1531.366)(261.08545, 593.	C11 H11 N6 P	FindByFormula	5 +	258.0776	13.30472
C11 H12 N10 O	C11 H12 N10 O	[C11 H12 N10 O, tgt=74.26, overall=74.26]	(301.12552, 3461.8489)(302.126, 504.73154)(303.12354, 367	C11 H12 N10 O	FindByFormula	20 +	300.1175	7.2863755
C11 H12 N5 O12 P3	C11 H12 N5 O12 P3	[C11 H12 N5 O12 P3, tgt=74.58, overall=74.58]	(499.97714, 7763.5146)(500.97662, 1225.9464)(501.98264, 6	C11 H12 N5 O12 P3	FindByFormula	16 +	498.9701	23.013447
C11 H12 N6	C11 H12 N6	[C11 H12 N6, tgt=96.73, overall=96.73]	(229.12071, 32014.76)(230.12299, 3832.5125)(231.12471, 73	C11 H12 N6	FindByFormula	26 +	228.1133	7.5549946
C11 H12 N6 O	C11 H12 N6 O	[C11 H12 N6 O, tgt=78.28, overall=78.28]	(245.11511, 17039.574)(246.11559, 4045.955)	C11 H12 N6 O	FindByFormula	28 +	244.1075	15.838597
C11 H12 N6 O2	C11 H12 N6 O2	[C11 H12 N6 O2, tgt=96.30, overall=96.30]	(261.11005, 26261.113)(262.11334, 3847.3562)(263.11792, 7	C11 H12 N6 O2	FindByFormula	28 +	260.1031	14.503946
C11 H13 N4 O2 P	C11 H13 N4 O2 P	[C11 H13 N4 O2 P, tgt=87.05, overall=87.05]	(265.08582, 4499.958)(266.08774, 746.6301)(303.0327, 79.7)	C11 H13 N4 O2 P	FindByFormula	13 +	264.078	15.805727
C11 H14 N2 O5	C11 H14 N2 O5	[C11 H14 N2 O5, tgt=97.38, overall=97.38]	(255.09764, 16704.787)(256.10104, 2327.2761)(257.09982, 2	C11 H14 N2 O5	FindByFormula	28 +	254.0902	13.103131
C11 H14 N6 O	C11 H14 N6 O	[C11 H14 N6 O, tgt=67.07, overall=67.07]	(247.13036, 7864.0156)(248.1318, 1167.0885)(249.13452, 23	C11 H14 N6 O	FindByFormula	27 +	246.123	15.771619
C11 H14 N6 O2	C11 H14 N6 O2	[C11 H14 N6 O2, tgt=84.71, overall=84.71]	(263.12607, 4428.175)(264.12808, 640.8926)(265.1291, 95.8	C11 H14 N6 O2	FindByFormula	23 +	262.1188	16.90376
C11 H15 N O3	C11 H15 N O3	[C11 H15 N O3, tgt=81.69, overall=81.69]	(210.11162, 2408.8384)(211.11205, 444.8364)(212.10556, 92	C11 H15 N O3	FindByFormula	28 +	209.1054	7.6829505
C11 H15 N5	C11 H15 N5	[C11 H15 N5, tgt=94.10, overall=94.10]	(218.13979, 17045.043)(219.1408, 2370.299)(220.13918, 361	C11 H15 N5	FindByFormula	28 +	217.132	1.6598674
C11 H16 N2 O	C11 H16 N2 O	[C11 H16 N2 O, tgt=63.77, overall=63.77]	(193.1325, 1514.73)(231.0879, 107.625)(215.11646, 1475.86)	C11 H16 N2 O	FindByFormula	3 +	192.1273	6.5062847
C11 H16 O4 P2	C11 H16 O4 P2	[C11 H16 O4 P2, tgt=91.66, overall=91.66]	(275.0601, 4292.543)(276.06424, 726.83496)(277.0619, 131.	C11 H16 O4 P2	FindByFormula	6 +	274.0528	12.9630785
C11 H17 N O2	C11 H17 N O2	[C11 H17 N O2, tgt=89.44, overall=89.44]	(196.13348, 6058.315)(197.1332, 998.2933)(198.1326, 59.76	C11 H17 N O2	FindByFormula	6 +	195.1255	4.6731033
C11 H18 N4 S	C11 H18 N4 S	[C11 H18 N4 S, tgt=95.57, overall=95.57]	(239.13287, 10377.684)(240.13577, 1481.2212)(241.13396, 3	C11 H18 N4 S	FindByFormula	28 +	238.1256	21.754715
C11 H19 N4 O4 P	C11 H19 N4 O4 P	[C11 H19 N4 O4 P, tgt=97.59, overall=97.59]	(303.12192, 4414.884)(304.12503, 775.8117)(305.1218, 119.	C11 H19 N4 O4 P	FindByFormula	6 +	302.1144	17.509623
C11 H19 N7 O	C11 H19 N7 O	[C11 H19 N7 O, tgt=76.32, overall=76.32]	(266.1729, 52686.85)(267.17538, 8244.713)(268.1789, 1164.	C11 H19 N7 O	FindByFormula	28 +	265.1656	15.769325
C11 H19 P3	C11 H19 P3	[C11 H19 P3, tgt=77.00, overall=77.00]	(245.07912, 7886.015)(246.08093, 937.06415)(247.08026, 21	C11 H19 P3	FindByFormula	27 +	244.0708	1.3617836
C11 H20 N2 O3	C11 H20 N2 O3	[C11 H20 N2 O3, tgt=81.78, overall=81.78]	(229.15472, 12270.338)(230.157, 1593.0227)(231.15385, 185	C11 H20 N2 O3	FindByFormula	22 +	228.1475	4.3258553
C11 H20 N4 O3	C11 H20 N4 O3	[C11 H20 N4 O3, tgt=84.72, overall=84.72]	(257.1618, 17923.191)(258.16434, 2935.6807)(259.15665, 66	C11 H20 N4 O3	FindByFormula	16 +	256.1547	8.657887
C11 H20 N6 O3	C11 H20 N6 O3	[C11 H20 N6 O3, tgt=97.17, overall=97.17]	(285.16623, 6082.7227)(286.16913, 963.275)(287.1661, 139.	C11 H20 N6 O3	FindByFormula	14 +	284.1598	15.257676
C11 H20 O3 P2 S	C11 H20 O3 P2 S	[C11 H20 O3 P2 S, tgt=92.01, overall=92.01]	(295.06796, 44520.88)(296.07053, 6281.727)(297.07098, 104	C11 H20 O3 P2 S	FindByFormula	22 +	294.0602	1.1050507
C11 H21 Cl N4 O3 S3	C11 H21 Cl N4 O3 S3	[C11 H21 Cl N4 O3 S3, tgt=81.86, overall=81.86]	(389.05487, 3821.4827)(390.05835, 820.77167)(391.05063, 1	C11 H21 Cl N4 O3 S3	FindByFormula	19 +	388.0466	8.663026
C11 H21 N O2	C11 H21 N O2	[C11 H21 N O2, tgt=89.91, overall=89.91]	(200.16457, 12046.648)(201.16563, 2051.0967)(202.16518, 1	C11 H21 N O2	FindByFormula	6 +	199.1568	2.0625043
C11 H21 N O4	C11 H21 N O4	[C11 H21 N O4, tgt=97.02, overall=97.02]	(232.15483, 24048.863)(233.15717, 4107.4233)(234.15738, 4	C11 H21 N O4	FindByFormula	26 +	231.1477	2.887653
C11 H21 N7	C11 H21 N7	[C11 H21 N7, tgt=82.27, overall=82.27]	(252.19328, 10075.863)(253.18965, 1981.7224)(254.1887, 21	C11 H21 N7	FindByFormula	18 +	251.186	16.24999
C11 H21 N7 O	C11 H21 N7 O	[C11 H21 N7 O, tgt=80.91, overall=80.91]	(268.1884, 25894.244)(269.1905, 4333.9067)(270.18893, 584	C11 H21 N7 O	FindByFormula	28 +	267.1813	14.445335
C11 H22 N2 O3	C11 H22 N2 O3	[C11 H22 N2 O3, tgt=99.27, overall=99.27]	(231.17004, 7941.824)(232.17162, 1092.1797)(233.16934, 28	C11 H22 N2 O3	FindByFormula	28 +	230.1627	4.090856
C11 H22 O4 P2	C11 H22 O4 P2	[C11 H22 O4 P2, tgt=88.23, overall=88.23]	(281.1072, 9419.623)(282.1107, 1440.3806)(283.1127, 161.3	C11 H22 O4 P2	FindByFormula	28 +	280.1001	13.10431
C11 H25 Cl N8 S	C11 H25 Cl N8 S	[C11 H25 Cl N8 S, tgt=85.07, overall=85.07]	(337.1675, 4644.5747)(338.16974, 1027.3129)(339.1646, 247	C11 H25 Cl N8 S	FindByFormula	14 +	336.1605	22.732662
C11 H25 N3 O2 P2	C11 H25 N3 O2 P2	[C11 H25 N3 O2 P2, tgt=96.20, overall=96.20]	(294.15094, 10711.595)(295.15387, 1530.0785)(296.15842, 1	C11 H25 N3 O2 P2	FindByFormula	7 +	293.143	1.9025759
C11 H28 N5 O3 P	C11 H28 N5 O3 P	[C11 H28 N5 O3 P, tgt=78.47, overall=78.47]	(310.2016, 1600.6001)(311.19827, 377.17468)(312.19995, 12	C11 H28 N5 O3 P	FindByFormula	17 +	309.193	11.4193
C11 H28 N8 O9	C11 H28 N8 O9	[C11 H28 N8 O9, tgt=89.79, overall=89.79]	(417.20605, 4706.4727)(418.2076, 557.3367)(419.20163, 184	C11 H28 N8 O9	FindByFormula	7 +	416.1977	10.304504
C11 H29 N4 P S2	C11 H29 N4 P S2	[C11 H29 N4 P S2, tgt=77.86, overall=77.86]	(313.16403, 3824.4414)(314.16617, 681.56757)(315.16138, 1	C11 H29 N4 P S2	FindByFormula	8 +	312.1564	19.935349
C11 H29 N6 P S2	C11 H29 N6 P S2	[C11 H29 N6 P S2, tgt=81.83, overall=81.83]	(341.1716, 4307.2783)(342.17496, 794.857)(343.16782, 458.	C11 H29 N6 P S2	FindByFormula	26 +	340.1646	22.470818
C11 H31 Cl N10	C11 H31 Cl N10	[C11 H31 Cl N10, tgt=40.56, overall=40.56]	(339.25082, 3799.6035)(340.25095, 750.92456)(341.2438, 66	C11 H31 Cl N10	FindByFormula	24 +	338.2433	22.422544
C11 H33 Cl N10 O	C11 H33 Cl N10 O	[C11 H33 Cl N10 O, tgt=29.86, overall=29.86]	(357.25964, 3564.7668)(358.26013, 642.7683)(359.25168, 10	C11 H33 Cl N10 O	FindByFormula	20 +	356.2494	21.551544
C11 H6	C11 H6	[C11 H6, tgt=86.88, overall=86.88]	(139.05406, 222137.53)(140.06053, 17048.484)(141.06789, 3	C11 H6	FindByFormula	9 +	138.0472	0.80944854
C11 H8 O S3	C11 H8 O S3	[C11 H8 O S3, tgt=81.48, overall=81.48]	(252.97984, 4579.7285)(253.98564, 735.35767)(254.98189, 3	C11 H8 O S3	FindByFormula	22 +	251.9735	8.656963
C11 H9 N O2	C11 H9 N O2	[C11 H9 N O2, tgt=88.09, overall=88.09]	(188.07126, 336034.56)(189.07129, 77184.75)(190.07353, 12	C11 H9 N O2	FindByFormula	17 +	187.0631	3.8534434
C11 H9 N9 O	C11 H9 N9 O	[C11 H9 N9 O, tgt=97.38, overall=97.38]	(284.10037, 72416.92)(285.10315, 9505.439)(286.10876, 144	C11 H9 N9 O	FindByFormula	22 +	283.0931	1.8241524
C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12	C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12	C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12:0) (CAS# 41 41613-14-3	(644.4983, 768.615)(645.5161, 994.6)(646.5202, 477.68)	C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12:0) (CAS# 41613-14-3); (M+H)+	FindByFormula	2 +	643.5007	23.053318
C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12	C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12	C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12:0) (CAS# 41 41613-14-3	(464.44724, 484.07248)(465.4488, 966.54504)(466.45285, 20	C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12:0) (CAS# 41613-14-3); M+[-C6H	FindByFormula	4 +	643.5075	23.080936
C12 H10 N6 O2	C12 H10 N6 O2	[C12 H10 N6 O2, tgt=71.41, overall=71.41]	(271.0937, 5008.63)(272.09802, 653.342)(273.09467, 219.37	C12 H10 N6 O2	FindByFormula	26 +	270.0867	2.1160967
C12 H11 N9 O	C12 H11 N9 O	[C12 H11 N9 O, tgt=32.13, overall=32.13]	(298.116, 2042.1552)(299.11755, 417.5391)(300.11597, 72.6	C12 H11 N9 O	FindByFormula	25 +	297.1086	2.5435116
C12 H12 N6 O2	C12 H12 N6 O2	[C12 H12 N6 O2, tgt=82.32, overall=82.32]	(273.11078, 2605.6902)(274.11142, 398.7735)(275.11115, 63	C12 H12 N6 O2	FindByFormula	20 +	272.1036	15.125981
C12 H12 N8	C12 H12 N8	[C12 H12 N8, tgt=97.53, overall=97.53]	(269.12643, 37593.676)(270.12906, 5957.4165)(271.1279, 72	C12 H12 N8	FindByFormula	28 +	268.1192	4.1318893
C12 H13 N2 P	C12 H13 N2 P	[C12 H13 N2 P, tgt=96.84, overall=96.84]	(217.09099, 1140.22)(218.08717, 109.62)(255.0415, 153.92)(	C12 H13 N2 P	FindByFormula	6 +	216.082	14.014497
C12 H14 N6 O	C12 H14 N6 O	[C12 H14 N6 O, tgt=96.16, overall=96.16]	(259.1309, 12279.858)(260.13428, 2010.418)(261.13376, 555	C12 H14 N6 O	FindByFormula	28 +	258.1237	17.52618
C12 H14 N8	C12 H14 N8	[C12 H14 N8, tgt=32.37, overall=32.37]	(271.142, 20664.703)(272.14465, 3582.3093)(273.1421, 495.	C12 H14 N8	FindByFormula	23 +	270.135	9.585915
C12 H14 N8 O	C12 H14 N8 O	[C12 H14 N8 O, tgt=86.27, overall=86.27]	(287.13605, 10596.6455)(288.13947, 1817.3141)(289.13705,	C12 H14 N8 O	FindByFormula	15 +	286.1287	1.4021434
C12 H14 O5	C12 H14 O5	[C12 H14 O5, tgt=94.19, overall=94.19]	(239.09047, 4812.2812)(240.09218, 502.77148)(241.09612, 1	C12 H14 O5	FindByFormula	13 +	238.0834	7.878431
C12 H15 N6 O3 P	C12 H15 N6 O3 P	[C12 H15 N6 O3 P, tgt=80.61, overall=80.61]	(323.10254, 4216.033)(324.1062, 599.88104)(325.10568, 176	C12 H15 N6 O3 P	FindByFormula	28 +	322.0953	4.8205132
C12 H16 O4	C12 H16 O4	[C12 H16 O4, tgt=97.72, overall=97.72]	(225.11234, 10681.318)(226.11407, 1106.0638)(227.11143, 1	C12 H16 O4	FindByFormula	14 +	224.1037	13.675164
C12 H17 N5	C12 H17 N5	[C12 H17 N5, tgt=96.49, overall=96.49]	(232.15477, 27687.549)(233.15907, 4755.91)(234.16017, 678	C12 H17 N5	FindByFormula	27 +	231.1477	2.9523768
C12 H18 N2 O	C12 H18 N2 O	[C12 H18 N2 O, tgt=99.42, overall=99.42]	(207.14948, 528864.56)(208.15254, 72507.47)(209.15454, 56	C12 H18 N2 O	FindByFormula	22 +	206.1422	4.692929
C12 H18 N2 S3	C12 H18 N2 S3	[C12 H18 N2 S3, tgt=90.62, overall=90.62]	(287.06985, 6455.7476)(288.07202, 956.16724)(289.06488, 1	C12 H18 N2 S3	FindByFormula	21 +	286.062	16.244211
C12 H18 N8	C12 H18 N8	[C12 H18 N8, tgt=81.95, overall=81.95]	(275.1721, 7409.7627)(276.17264, 1724.6866)(277.1742, 118	C12 H18 N8	FindByFormula	19 +	274.164	0.7584211
C12 H18 O3	C12 H18 O3	[C12 H18 O3, tgt=99.37, overall=99.37]	(211.13303, 39124.305)(212.1364, 5224.9346)(213.13477, 64	C12 H18 O3	FindByFormula	28 +	210.1261	13.107524
C12 H19 Cl3 O2 S3	C12 H19 Cl3 O2 S3	[C12 H19 Cl3 O2 S3, tgt=88.30, overall=88.30]	(396.9673, 8662.602)(397.9708, 1064.2114)(398.96426, 1114	C12 H19 Cl3 O2 S3	FindByFormula	7 +	395.9599	19.881657
C12 H19 N O2	C12 H19 N O2	[C12 H19 N O2, tgt=96.61, overall=96.61]	(210.1486, 6086.522)(211.14813, 851.5367)(212.14601, 94.0	C12 H19 N O2	FindByFormula	6 +	209.1409	9.544386
C12 H19 N O2 S2	C12 H19 N O2 S2	[C12 H19 N O2 S2, tgt=91.25, overall=91.25]	(274.09137, 14775.836)(275.10147, 2425.3003)(276.08963, 1	C12 H19 N O2 S2	FindByFormula	20 +	273.0845	17.629274
C12 H20 N6	C12 H20 N6	[C12 H20 N6, tgt=64.09, overall=64.09]	(249.18251, 12505.603)(250.18571, 2093.1145)(251.17647, 8	C12 H20 N6	FindByFormula	28 +	248.1748	19.033035
C12 H21 N O	C12 H21 N O	[C12 H21 N O, tgt=98.89, overall=98.89]	(196.16937, 13318.668)(197.17236, 1912.0801)(198.17113, 2	C12 H21 N O	FindByFormula	6 +	195.162	4.1820703
C12 H21 N3 O5	C12 H21 N3 O5	[C12 H21 N3 O5, tgt=63.14, overall=63.14]	(288.1546, 4312.929)(289.15512, 939.0301)(290.1511, 129.1	C12 H21 N3 O5	FindByFormula	25 +	287.1474	15.762071
C12 H21 N4 O3 P	C12 H21 N4 O3 P	[C12 H21 N4 O3 P, tgt=97.57, overall=97.57]	(301.14185, 314802.7)(302.14487, 53638.035)(303.14822, 74	C12 H21 N4 O3 P	FindByFormula	28 +	300.1346	20.777449
C12 H21 N4 O4 P	C12 H21 N4 O4 P	[C12 H21 N4 O4 P, tgt=95.97, overall=95.97]	(317.13907, 3839.8289)(318.1409, 697.19366)(319.1394, 122	C12 H21 N4 O4 P	FindByFormula	22 +	316.1319	17.051325
C12 H21 N7 O	C12 H21 N7 O	[C12 H21 N7 O, tgt=64.03, overall=64.03]	(280.1884, 2162.3545)(281.18884, 718.1146)(282.18704, 184	C12 H21 N7 O	FindByFormula	18 +	279.1803	17.897026
C12 H22 N2 S2	C12 H22 N2 S2	[C12 H22 N2 S2, tgt=85.20, overall=85.20]	(259.13037, 9892.831)(260.13156, 1610.9199)(261.1324, 307	C12 H22 N2 S2	FindByFormula	8 +	258.1237	15.258192
C12 H22 N4 P2	C12 H22 N4 P2	[C12 H22 N4 P2, tgt=97.07, overall=97.07]	(285.13776, 3446.272)(286.13962, 594.78143)(287.13354, 36	C12 H22 N4 P2	FindByFormula	28 +	284.1317	21.75672
C12 H22 N8	C12 H22 N8	[C12 H22 N8, tgt=68.26, overall=68.26]	(279.20377, 4434.582)(280.2041, 901.9474)(281.20663, 47.9	C12 H22 N8	FindByFormula	20 +	278.1967	15.06293
C12 H22 O2 S3	C12 H22 O2 S3	[C12 H22 O2 S3, tgt=80.91, overall=80.91]	(295.08646, 8235.826)(296.08456, 1976.8236)(297.0842, 101	C12 H22 O2 S3	FindByFormula	28 +	294.0783	13.106917
C12 H22 O3 P2	C12 H22 O3 P2	[C12 H22 O3 P2, tgt=89.41, overall=89.41]	(277.11295, 5810.3516)(278.116, 997.175)(279.1079, 215.21	C12 H22 O3 P2	FindByFormula	6 +	276.1053	18.855732
C12 H23 N O2	C12 H23 N O2	[C12 H23 N O2, tgt=68.21, overall=68.21]	(214.17941, 5929.1353)(215.18062, 892.9224)(216.17885, 12	C12 H23 N O2	FindByFormula	22 +	213.1721	11.3245
C12 H23 N O3	C12 H23 N O3	[C12 H23 N O3, tgt=70.12, overall=70.12]	(230.17467, 1009.279)(231.17639, 198.08958)(232.17609, 59	C12 H23 N O3	FindByFormula	27 +	229.1664	14.11986
C12 H23 N O4	C12 H23 N O4	[C12 H23 N O4, tgt=98.19, overall=98.19]	(246.17015, 46256.617)(247.17322, 6325.968)(248.17442, 83	C12 H23 N O4	FindByFormula	27 +	245.1628	4.591804
C12 H23 N7	C12 H23 N7	[C12 H23 N7, tgt=54.48, overall=54.48]	(266.20853, 17402.502)(267.206, 5047.0083)(268.20624, 614	C12 H23 N7	FindByFormula	15 +	265.2011	20.20861
C12 H23 N7 O	C12 H23 N7 O	[C12 H23 N7 O, tgt=92.02, overall=92.02]	(282.2044, 112109.61)(283.20663, 17327.234)(284.20776, 20	C12 H23 N7 O	FindByFormula	28 +	281.1974	16.102774
C12 H23 O2 P3	C12 H23 O2 P3	[C12 H23 O2 P3, tgt=94.56, overall=94.56]	(293.09854, 885238.7)(294.10168, 104620.28)(295.1033, 194	C12 H23 O2 P3	FindByFormula	6 +	292.0912	0.84699935
C12 H24 N2 O3	C12 H24 N2 O3	[C12 H24 N2 O3, tgt=97.77, overall=97.77]	(245.1853, 3426.0562)(246.18552, 538.9927)(247.18657, 111	C12 H24 N2 O3	FindByFormula	26 +	244.178	6.4525633
C12 H24 N6	C12 H24 N6	[C12 H24 N6, tgt=96.69, overall=96.69]	(253.21335, 4066.6914)(254.21545, 590.4911)(255.2161, 158	C12 H24 N6	FindByFormula	28 +	252.2048	22.21812
C12 H24 N6 O	C12 H24 N6 O	[C12 H24 N6 O, tgt=97.12, overall=97.12]	(269.2084, 4928.8545)(270.2106, 774.67633)(271.20895, 115	C12 H24 N6 O	FindByFormula	28 +	268.2011	20.824368
C12 H25 N O	C12 H25 N O	[C12 H25 N O, tgt=98.96, overall=98.96]	(200.20093, 4361.9917)(201.20378, 648.1293)(202.20374, 41	C12 H25 N O	FindByFormula	28 +	199.1934	18.666378
C12 H25 N O2	C12 H25 N O2	[C12 H25 N O2, tgt=58.46, overall=58.46]	(216.19545, 2687.6294)(217.19617, 444.73218)(218.19911, 7	C12 H25 N O2	FindByFormula	25 +	215.1884	14.633248
C12 H25 N3 O3	C12 H25 N3 O3	[C12 H25 N3 O3, tgt=91.53, overall=91.53]	(260.19638, 4178.847)(261.1951, 634.1805)(262.19806, 108.	C12 H25 N3 O3	FindByFormula	21 +	259.1884	1.3830087
C12 H25 N5 O3	C12 H25 N5 O3	[C12 H25 N5 O3, tgt=93.79, overall=93.79]	(288.2027, 2724.9868)(289.2057, 538.8933)(290.20294, 128.	C12 H25 N5 O3	FindByFormula	11 +	287.1957	5.311613
C12 H26 O7	C12 H26 O7	[C12 H26 O7, tgt=98.94, overall=98.94]	(283.1749, 4297.19)(284.1767, 610.2143)(285.17584, 152.06	C12 H26 O7	FindByFormula	28 +	282.1681	5.9879956
C12 H28 O2 S2	C12 H28 O2 S2	[C12 H28 O2 S2, tgt=75.60, overall=75.60]	(269.16132, 3313.3389)(270.15903, 551.9446)(271.15247, 34	C12 H28 O2 S2	FindByFormula	26 +	268.1528	1.3140444
C12 H29 N4 O3 P	C12 H29 N4 O3 P	[C12 H29 N4 O3 P, tgt=97.19, overall=97.19]	(309.20474, 96284.734)(310.2082, 16703.184)(311.2086, 520	C12 H29 N4 O3 P	FindByFormula	28 +	308.1975	21.728788
C12 H30 N2 O4 S2	C12 H30 N2 O4 S2	[C12 H30 N2 O4 S2, tgt=68.53, overall=68.53]	(331.1702, 3775.9963)(332.17285, 766.6481)(333.17596, 867	C12 H30 N2 O4 S2	FindByFormula	25 +	330.1627	21.536263
C12 H35 N14 O4 P3	C12 H35 N14 O4 P3	[C12 H35 N14 O4 P3, tgt=24.66, overall=24.66]	(533.2265, 7998.7314)(534.22473, 1212.54)(535.21924, 137.	C12 H35 N14 O4 P3	FindByFormula	7 +	532.2169	19.883741
C12 H5 Cl N6 O3 S	C12 H5 Cl N6 O3 S	[C12 H5 Cl N6 O3 S, tgt=96.54, overall=96.54]	(348.99042, 5605.19)(349.99265, 855.9359)(350.98935, 2072	C12 H5 Cl N6 O3 S	FindByFormula	22 +	347.9832	1.1886879
C12 H6 N4 O2 P2 S4	C12 H6 N4 O2 P2 S4	[C12 H6 N4 O2 P2 S4, tgt=63.51, overall=63.51]	(428.88867, 3873.3335)(429.8904, 868.59247)(430.88998, 26	C12 H6 N4 O2 P2 S4	FindByFormula	27 +	427.8854	19.32322
C12 H8 P2	C12 H8 P2	[C12 H8 P2, tgt=79.21, overall=79.21]	(215.01732, 5000.964)(216.01799, 361.5724)(217.01811, 216	C12 H8 P2	FindByFormula	13 +	214.0091	0.90669256
C13 H10	C13 H10	[C13 H10, tgt=88.90, overall=88.90]	(167.08592, 3417.4336)(168.08556, 342.55)(169.0823, 285.8	C13 H10	FindByFormula	13 +	166.0781	15.799264
C13 H10 N10	C13 H10 N10	[C13 H10 N10, tgt=73.99, overall=73.99]	(307.11578, 10757.417)(308.11948, 1789.9128)(309.12387, 4	C13 H10 N10	FindByFormula	28 +	306.1087	7.8878164
C13 H10 N2 O5	C13 H10 N2 O5	[C13 H10 N2 O5, tgt=97.61, overall=97.61]	(275.06702, 8381.066)(276.0706, 1388.2076)(277.0725, 126.	C13 H10 N2 O5	FindByFormula	8 +	274.0593	15.708372
C13 H10 N4 O	C13 H10 N4 O	[C13 H10 N4 O, tgt=94.42, overall=94.42]	(239.0926, 5866.905)(240.09618, 900.4749)(241.09605, 123.	C13 H10 N4 O	FindByFormula	6 +	238.0843	9.868003
C13 H11 O5 P	C13 H11 O5 P	[C13 H11 O5 P, tgt=91.22, overall=91.22]	(279.0411, 3158.6838)(280.04218, 342.49252)(281.0369, 108	C13 H11 O5 P	FindByFormula	12 +	278.0332	5.8844705
C13 H12 O	C13 H12 O	[C13 H12 O, tgt=93.95, overall=93.95]	(185.0969, 3460.186)(186.09839, 493.79623)(187.09904, 96.	C13 H12 O	FindByFormula	8 +	184.0898	15.708122
C13 H13 N9 O	C13 H13 N9 O	[C13 H13 N9 O, tgt=88.93, overall=88.93]	(312.13177, 1258.938)(313.1315, 301.27628)(314.12363, 132	C13 H13 N9 O	FindByFormula	26 +	311.1256	3.653269
C13 H14 N4 O P2	C13 H14 N4 O P2	[C13 H14 N4 O P2, tgt=61.61, overall=61.61]	(305.07123, 361.006)(306.06723, 44.674)	C13 H14 N4 O P2	FindByFormula	5 +	304.0623	16.429424
C13 H14 N4 O3 P2	C13 H14 N4 O3 P2	[C13 H14 N4 O3 P2, tgt=94.92, overall=94.92]	(337.0612, 15660.73)(338.06177, 3490.4182)(339.0623, 720.	C13 H14 N4 O3 P2	FindByFormula	10 +	336.055	0.8160001
C13 H14 O4 P2	C13 H14 O4 P2	[C13 H14 O4 P2, tgt=61.75, overall=61.75]	(297.0436, 5039.321)(298.0443, 586.29926)(299.0442, 149.1	C13 H14 O4 P2	FindByFormula	17 +	296.0363	1.1661247
C13 H15 N5 O2	C13 H15 N5 O2	[C13 H15 N5 O2, tgt=60.80, overall=60.80]	(274.12704, 2309.7249)(275.1333, 784.8)(276.1337, 180.8)(	C13 H15 N5 O2	FindByFormula	4 +	273.1202	1.048501
C13 H16 N4 O P2	C13 H16 N4 O P2	[C13 H16 N4 O P2, tgt=93.73, overall=93.73]	(307.0869, 4528.358)(308.09235, 615.9459)(309.09195, 31.6	C13 H16 N4 O P2	FindByFormula	6 +	306.08	18.654951
C13 H16 N4 P2	C13 H16 N4 P2	[C13 H16 N4 P2, tgt=98.21, overall=98.21]	(291.09238, 7703.9746)(292.09543, 1308.855)(293.09222, 39	C13 H16 N4 P2	FindByFormula	6 +	290.0856	18.859573
C13 H16 N6	C13 H16 N6	[C13 H16 N6, tgt=90.10, overall=90.10]	(257.15115, 19387.887)(258.1543, 3251.317)(259.14923, 745	C13 H16 N6	FindByFormula	26 +	256.1437	19.687395
C13 H16 N6 O3	C13 H16 N6 O3	[C13 H16 N6 O3, tgt=86.96, overall=86.96]	(305.13644, 12396.681)(306.13992, 2194.8816)(307.1557, 13	C13 H16 N6 O3	FindByFormula	6 +	304.1294	20.200287
C13 H16 N6 O4	C13 H16 N6 O4	[C13 H16 N6 O4, tgt=76.23, overall=76.23]	(321.13153, 14099.423)(322.13498, 2428.7534)(323.13522, 4	C13 H16 N6 O4	FindByFormula	28 +	320.1241	9.922751
C13 H17 P S	C13 H17 P S	[C13 H17 P S, tgt=71.36, overall=71.36]	(237.08784, 5871.9683)(238.09096, 893.74725)(239.08438, 1	C13 H17 P S	FindByFormula	22 +	236.0807	2.5448942
C13 H18 Cl N O2	C13 H18 Cl N O2	[C13 H18 Cl N O2, tgt=93.35, overall=93.35]	(256.1103, 8638.585)(257.1131, 1223.9412)(258.10785, 3044	C13 H18 Cl N O2	FindByFormula	9 +	255.103	7.967989
C13 H18 N2 O	C13 H18 N2 O	[C13 H18 N2 O, tgt=54.10, overall=54.10]	(219.14917, 61593.242)(220.15068, 9531.832)(221.1525, 964	C13 H18 N2 O	FindByFormula	26 +	218.1424	9.3564825
C13 H18 O2	C13 H18 O2	[C13 H18 O2, tgt=70.94, overall=70.94]	(207.1369, 1734.784)(208.13525, 50.751255)(209.13501, 63.	C13 H18 O2	FindByFormula	28 +	206.1302	17.768522
C13 H18 O3 S	C13 H18 O3 S	[C13 H18 O3 S, tgt=84.36, overall=84.36]	(255.10449, 5580.9614)(256.1077, 1012.32)(257.1066, 159.9	C13 H18 O3 S	FindByFormula	13 +	254.0954	0.7538487
C13 H19 N O	C13 H19 N O	[C13 H19 N O, tgt=94.60, overall=94.60]	(206.15462, 8132.759)(207.1566, 1718.1484)(208.15253, 325	C13 H19 N O	FindByFormula	9 +	205.1463	5.7772202
C13 H19 N3 O7 S	C13 H19 N3 O7 S	[C13 H19 N3 O7 S, tgt=91.17, overall=91.17]	(362.10135, 3681.7544)(363.1034, 636.22565)(364.09927, 18	C13 H19 N3 O7 S	FindByFormula	26 +	361.0942	1.3028138
C13 H20 Cl N O	C13 H20 Cl N O	[C13 H20 Cl N O, tgt=79.60, overall=79.60]	(242.13051, 6811.237)(243.13028, 1226.6318)(244.1248, 240	C13 H20 Cl N O	FindByFormula	12 +	241.1231	9.773616
C13 H20 N2	C13 H20 N2	[C13 H20 N2, tgt=99.08, overall=99.08]	(205.16962, 22109.912)(206.17262, 3445.322)(207.17253, 31	C13 H20 N2	FindByFormula	18 +	204.1623	6.663948
C13 H20 N2 O	C13 H20 N2 O	[C13 H20 N2 O, tgt=40.84, overall=40.84]	(221.1645, 11531.157)(222.16528, 1820.0032)(223.16533, 20	C13 H20 N2 O	FindByFormula	20 +	220.1576	4.9404793
C13 H20 O2	C13 H20 O2	[C13 H20 O2, tgt=87.60, overall=87.60]	(209.15225, 1435.8826)(210.1519, 166.175)(211.15259, 106.	C13 H20 O2	FindByFormula	28 +	208.1455	17.328909
C13 H20 O4	C13 H20 O4	[C13 H20 O4, tgt=78.44, overall=78.44]	(241.14316, 4729.5576)(242.14243, 532.2003)(243.1392, 143	C13 H20 O4	FindByFormula	28 +	240.1346	15.562848
C13 H21 N O2	C13 H21 N O2	[C13 H21 N O2, tgt=85.54, overall=85.54]	(224.16289, 10548.361)(225.16537, 1939.9059)(226.16402, 1	C13 H21 N O2	FindByFormula	16 +	223.1551	4.4997964
C13 H21 N4 O P3	C13 H21 N4 O P3	[C13 H21 N4 O P3, tgt=97.92, overall=97.92]	(343.10004, 7071.9795)(344.1015, 1111.792)(345.1014, 308.	C13 H21 N4 O P3	FindByFormula	10 +	342.0928	3.4985554
C13 H22 N4 S	C13 H22 N4 S	[C13 H22 N4 S, tgt=93.43, overall=93.43]	(267.16385, 14628.339)(268.16644, 2289.0715)(269.16098, 5	C13 H22 N4 S	FindByFormula	28 +	266.1563	22.459993
C13 H22 O3	C13 H22 O3	[C13 H22 O3, tgt=53.87, overall=53.87]	(227.1623, 1347.3302)(228.16487, 189.07747)(229.16592, 35	C13 H22 O3	FindByFormula	26 +	226.1555	14.583572
C13 H23 N4 O3 P	C13 H23 N4 O3 P	[C13 H23 N4 O3 P, tgt=94.59, overall=94.59]	(315.15717, 23794.168)(316.16058, 4569.2554)(317.16397, 5	C13 H23 N4 O3 P	FindByFormula	28 +	314.1501	18.91855
C13 H23 N4 P	C13 H23 N4 P	[C13 H23 N4 P, tgt=86.01, overall=86.01]	(267.17615, 3547.2488)(268.17563, 644.2972)(305.13284, 26	C13 H23 N4 P	FindByFormula	28 +	266.1652	20.705936
C13 H23 P S	C13 H23 P S	[C13 H23 P S, tgt=80.85, overall=80.85]	(243.13152, 3376.8186)(244.13136, 457.28958)(245.12704, 3	C13 H23 P S	FindByFormula	27 +	242.1259	6.479126
C13 H24 N2 O	C13 H24 N2 O	[C13 H24 N2 O, tgt=56.54, overall=56.54]	(225.19502, 1287.3712)(226.19458, 189.76874)(227.19466, 6	C13 H24 N2 O	FindByFormula	17 +	224.1877	16.377796
C13 H24 N2 O4	C13 H24 N2 O4	[C13 H24 N2 O4, tgt=97.55, overall=97.55]	(273.18036, 3911.8186)(274.1824, 638.77606)(275.1798, 170	C13 H24 N2 O4	FindByFormula	28 +	272.173	22.460562
C13 H24 N6 O2	C13 H24 N6 O2	[C13 H24 N6 O2, tgt=75.63, overall=75.63]	(297.2039, 3981.4592)(298.20587, 696.2435)(299.20197, 293	C13 H24 N6 O2	FindByFormula	28 +	296.1959	21.182726
C13 H24 N6 O3	C13 H24 N6 O3	[C13 H24 N6 O3, tgt=66.41, overall=66.41]	(313.19843, 3519.5498)(314.19974, 665.39844)(315.1969, 10	C13 H24 N6 O3	FindByFormula	13 +	312.1912	18.50734
C13 H25 N O2	C13 H25 N O2	[C13 H25 N O2, tgt=79.64, overall=79.64]	(228.19585, 8910.109)(229.19824, 1418.0677)(230.2002, 180	C13 H25 N O2	FindByFormula	24 +	227.1888	16.101969
C13 H25 N O3	C13 H25 N O3	[C13 H25 N O3, tgt=74.21, overall=74.21]	(244.19069, 7614.8164)(245.19067, 1237.3835)(246.19171, 2	C13 H25 N O3	FindByFormula	28 +	243.1834	15.769289
C13 H25 N O4	C13 H25 N O4	[C13 H25 N O4, tgt=96.47, overall=96.47]	(260.18585, 2887.2332)(261.18784, 513.6897)(262.18927, 94	C13 H25 N O4	FindByFormula	25 +	259.1782	7.065523
C13 H25 N7	C13 H25 N7	[C13 H25 N7, tgt=60.27, overall=60.27]	(280.22583, 33576.07)(281.22684, 6721.275)(282.22473, 895	C13 H25 N7	FindByFormula	20 +	279.2181	21.475279
C13 H25 N7 O	C13 H25 N7 O	[C13 H25 N7 O, tgt=55.51, overall=55.51]	(296.2197, 5724.692)(297.2188, 962.2032)(298.21674, 108.4	C13 H25 N7 O	FindByFormula	28 +	295.2121	18.637281
C13 H25 O P S	C13 H25 O P S	[C13 H25 O P S, tgt=96.31, overall=96.31]	(261.144, 8406.814)(262.14517, 1172.7897)(263.1444, 313.0	C13 H25 O P S	FindByFormula	26 +	260.137	4.57183
C13 H26 N6 O	C13 H26 N6 O	[C13 H26 N6 O, tgt=76.94, overall=76.94]	(283.22464, 9306.259)(284.2276, 1596.009)(285.22467, 337.	C13 H26 N6 O	FindByFormula	28 +	282.2173	21.919888
C13 H27 N S2	C13 H27 N S2	[C13 H27 N S2, tgt=76.90, overall=76.90]	(262.16464, 11961.858)(263.16586, 1789.818)(264.1595, 383	C13 H27 N S2	FindByFormula	26 +	261.1575	1.9766704
C13 H30 N2 O4 S	C13 H30 N2 O4 S	[C13 H30 N2 O4 S, tgt=83.92, overall=83.92]	(311.19977, 7432.897)(312.20163, 1529.7057)(313.19632, 30	C13 H30 N2 O4 S	FindByFormula	14 +	310.1928	20.323347
C13 H30 N8 O S2	C13 H30 N8 O S2	[C13 H30 N8 O S2, tgt=83.53, overall=83.53]	(379.2054, 5947.535)(380.20728, 1250.8434)(381.20374, 74.	C13 H30 N8 O S2	FindByFormula	12 +	378.1948	21.33153
C13 H31 N3 O3	C13 H31 N3 O3	[C13 H31 N3 O3, tgt=62.94, overall=62.94]	(278.24557, 10328.353)(279.24384, 2603.145)(280.24237, 37	C13 H31 N3 O3	FindByFormula	22 +	277.237	22.512506
C13 H31 N7	C13 H31 N7	[C13 H31 N7, tgt=60.38, overall=60.38]	(286.2735, 1108.4655)(287.27048, 316.72906)(288.27426, 10	C13 H31 N7	FindByFormula	22 +	285.2645	19.82374
C13 H32 N2 O P2 S	C13 H32 N2 O P2 S	[C13 H32 N2 O P2 S, tgt=86.19, overall=86.19]	(327.17828, 8432.587)(328.18033, 1529.06)(329.1738, 591.1	C13 H32 N2 O P2 S	FindByFormula	15 +	326.1711	16.213526
C13 H32 N6 P2	C13 H32 N6 P2	[C13 H32 N6 P2, tgt=81.94, overall=81.94]	(335.22458, 8331.685)(336.22824, 1693.3042)(373.17905, 38	C13 H32 N6 P2	FindByFormula	14 +	334.2162	21.551392
C13 H36 N8 O2	C13 H36 N8 O2	[C13 H36 N8 O2, tgt=93.81, overall=93.81]	(337.3038, 37043.03)(338.30704, 8050.507)(339.3055, 960.8	C13 H36 N8 O2	FindByFormula	9 +	336.2972	22.599716
C13 H8 N8	C13 H8 N8	[C13 H8 N8, tgt=96.47, overall=96.47]	(277.0954, 11021.012)(278.09906, 1947.3602)(279.10156, 20	C13 H8 N8	FindByFormula	6 +	276.0884	10.465574
C14 H10 N4 O3 S	C14 H10 N4 O3 S	[C14 H10 N4 O3 S, tgt=97.04, overall=97.04]	(315.05466, 8919.649)(316.05853, 1569.1483)(317.05814, 49	C14 H10 N4 O3 S	FindByFormula	11 +	314.0477	15.705484
C14 H12 N6	C14 H12 N6	[C14 H12 N6, tgt=97.36, overall=97.36]	(265.11847, 4394.4873)(266.12073, 817.4694)(267.12143, 46	C14 H12 N6	FindByFormula	21 +	264.1134	5.223565
C14 H12 O4	C14 H12 O4	[C14 H12 O4, tgt=32.05, overall=32.05]	(245.0826, 1241.04)(283.03632, 84.84875)(284.0285, 33.39)(	C14 H12 O4	FindByFormula	23 +	244.0733	14.452854
C14 H14 N4 P2	C14 H14 N4 P2	[C14 H14 N4 P2, tgt=97.48, overall=97.48]	(301.07632, 3941.4202)(302.08032, 733.97)(303.0795, 88.92	C14 H14 N4 P2	FindByFormula	8 +	300.0688	15.709249
C14 H14 O S	C14 H14 O S	[C14 H14 O S, tgt=89.50, overall=89.50]	(231.08435, 5192.7344)(232.08778, 528.86896)(233.08395, 2	C14 H14 O S	FindByFormula	28 +	230.0774	3.403134
C14 H14 O3	C14 H14 O3	[C14 H14 O3, tgt=97.93, overall=97.93]	(231.10216, 7289.1426)(232.10452, 1174.5801)(233.10233, 2	C14 H14 O3	FindByFormula	9 +	230.0947	15.707301
C14 H14 O6	C14 H14 O6	[C14 H14 O6, tgt=91.78, overall=91.78]	(279.08582, 6688.569)(280.09003, 1135.3075)(281.08844, 14	C14 H14 O6	FindByFormula	8 +	278.0779	9.865976
C14 H14 S	C14 H14 S	[C14 H14 S, tgt=65.92, overall=65.92]	(215.08914, 11952.6)(216.09554, 2157.6267)(217.09546, 554	C14 H14 S	FindByFormula	8 +	214.0825	3.863194
C14 H17 N O8	C14 H17 N O8	[C14 H17 N O8, tgt=96.89, overall=96.89]	(328.1037, 1132.2493)(329.10596, 302.5586)(330.10318, 104	C14 H17 N O8	FindByFormula	16 +	327.0957	2.2562647
C14 H18 N2 O2	C14 H18 N2 O2	[C14 H18 N2 O2, tgt=99.82, overall=99.82]	(247.14336, 24047.041)(248.1458, 3918.8423)(249.14755, 66	C14 H18 N2 O2	FindByFormula	28 +	246.1372	4.130389
C14 H18 N4 O3	C14 H18 N4 O3	[C14 H18 N4 O3, tgt=78.77, overall=78.77]	(291.14548, 3856.277)(292.15094, 858.8729)(293.1389, 187.	C14 H18 N4 O3	FindByFormula	7 +	290.1385	5.5520673
C14 H18 N6	C14 H18 N6	[C14 H18 N6, tgt=96.71, overall=96.71]	(271.16696, 9216.905)(272.1702, 1684.5642)(273.1698, 525.	C14 H18 N6	FindByFormula	28 +	270.16	20.056568
C14 H19 P S	C14 H19 P S	[C14 H19 P S, tgt=93.34, overall=93.34]	(251.10092, 24635.986)(252.10458, 3074.1719)(253.10606, 7	C14 H19 P S	FindByFormula	22 +	250.094	4.1621156

C14 H20 N2 O	C14 H20 N2 O	[C14 H20 N2 O, tgt=22.58, overall=22.58]	(233.16489, 49102.31)(234.16705, 7726.2017)(235.168, 243.	C14 H20 N2 O	FindByFormula	23 +	232.158	9.488219
C14 H20 N2 O2	C14 H20 N2 O2	[C14 H20 N2 O2, tgt=99.10, overall=99.10]	(249.16, 169020.14)(250.16295, 26016.545)(251.16368, 2984	C14 H20 N2 O2	FindByFormula	22 +	248.1531	4.3839498
C14 H21 N O4	C14 H21 N O4	[C14 H21 N O4, tgt=98.05, overall=98.05]	(268.15472, 4846.3853)(269.1533, 897.0323)(270.15863, 267	C14 H21 N O4	FindByFormula	13 +	267.1474	5.166599
C14 H22 N2 O	C14 H22 N2 O	[C14 H22 N2 O, tgt=66.61, overall=66.61]	(235.18047, 801762.5)(236.18274, 129891.78)(237.18686, 11	C14 H22 N2 O	FindByFormula	17 +	234.1732	5.685136
C14 H22 N2 O2	C14 H22 N2 O2	[C14 H22 N2 O2, tgt=99.06, overall=99.06]	(251.17593, 487039.62)(252.17894, 76939.48)(253.1809, 794	C14 H22 N2 O2	FindByFormula	22 +	250.1684	7.2353473
C14 H22 N2 O3	C14 H22 N2 O3	[C14 H22 N2 O3, tgt=95.24, overall=95.24]	(267.16946, 3572.7407)(268.17215, 430.83902)(269.17435, 9	C14 H22 N2 O3	FindByFormula	20 +	266.1617	3.487475
C14 H22 O3	C14 H22 O3	[C14 H22 O3, tgt=97.63, overall=97.63]	(239.16261, 1713.7533)(240.16228, 249.66333)(241.15395, 2	C14 H22 O3	FindByFormula	6 +	238.1555	20.92335
C14 H24 N3 O3 P	C14 H24 N3 O3 P	[C14 H24 N3 O3 P, tgt=69.41, overall=69.41]	(314.16473, 1471.6766)(315.16547, 122.47833)(316.1649, 65	C14 H24 N3 O3 P	FindByFormula	6 +	313.1574	4.2042384
C14 H24 N6	C14 H24 N6	[C14 H24 N6, tgt=87.78, overall=87.78]	(277.21375, 5013.626)(278.21976, 850.4239)(279.2162, 435.	C14 H24 N6	FindByFormula	28 +	276.2054	22.456211
C14 H24 N6 O	C14 H24 N6 O	[C14 H24 N6 O, tgt=79.68, overall=79.68]	(293.20883, 10223.399)(294.21216, 1982.948)(295.2106, 227	C14 H24 N6 O	FindByFormula	28 +	292.2036	20.822886
C14 H26 N4 P2	C14 H26 N4 P2	[C14 H26 N4 P2, tgt=87.23, overall=87.23]	(313.1723, 2848.8733)(314.17377, 575.37286)(315.18192, 27	C14 H26 N4 P2	FindByFormula	28 +	312.1643	22.462067
C14 H26 N6 O	C14 H26 N6 O	[C14 H26 N6 O, tgt=58.12, overall=58.12]	(295.22348, 5553.418)(296.2254, 1101.5187)(297.22174, 38.	C14 H26 N6 O	FindByFormula	23 +	294.2186	22.26261
C14 H27 N4 O2 P	C14 H27 N4 O2 P	[C14 H27 N4 O2 P, tgt=86.15, overall=86.15]	(315.19345, 66295.1)(316.19678, 13011.771)(317.20456, 447	C14 H27 N4 O2 P	FindByFormula	28 +	314.1866	21.533289
C14 H27 N4 O3 P	C14 H27 N4 O3 P	[C14 H27 N4 O3 P, tgt=80.38, overall=80.38]	(331.18845, 15973.297)(332.1923, 3237.387)(333.1951, 1953	C14 H27 N4 O3 P	FindByFormula	28 +	330.1818	19.57738
C14 H27 N4 P3	C14 H27 N4 P3	[C14 H27 N4 P3, tgt=84.81, overall=84.81]	(345.15323, 4760.7993)(346.15433, 788.6549)(347.1595, 974	C14 H27 N4 P3	FindByFormula	28 +	344.1452	8.477915
C14 H27 N7 O	C14 H27 N7 O	[C14 H27 N7 O, tgt=34.60, overall=34.60]	(310.23483, 5826.8955)(311.23184, 1267.2429)(312.23404, 2	C14 H27 N7 O	FindByFormula	23 +	309.2273	18.825037
C14 H28 N6 O	C14 H28 N6 O	[C14 H28 N6 O, tgt=93.25, overall=93.25]	(297.24017, 17899.121)(298.2437, 3245.8696)(299.2458, 605	C14 H28 N6 O	FindByFormula	26 +	296.2347	22.282335
C14 H28 N6 O2	C14 H28 N6 O2	[C14 H28 N6 O2, tgt=79.56, overall=79.56]	(313.2329, 6352.9844)(314.23465, 1187.827)(315.23764, 83.	C14 H28 N6 O2	FindByFormula	23 +	312.2253	21.481234
C14 H29 N O2	C14 H29 N O2	[C14 H29 N O2, tgt=98.74, overall=98.74]	(244.22705, 7274.871)(245.22867, 1649.7059)(246.23167, 31	C14 H29 N O2	FindByFormula	10 +	243.2199	14.8109
C14 H30 O2 P2	C14 H30 O2 P2	[C14 H30 O2 P2, tgt=87.00, overall=87.00]	(293.18005, 10206.198)(294.1832, 1852.4017)(295.18732, 16	C14 H30 O2 P2	FindByFormula	25 +	292.1727	22.603918
C14 H30 O8	C14 H30 O8	[C14 H30 O8, tgt=98.80, overall=98.80]	(327.20102, 4478.7036)(328.20508, 816.43427)(329.20078, 1	C14 H30 O8	FindByFormula	28 +	326.194	7.0196853
C14 H31 N O	C14 H31 N O	[C14 H31 N O, tgt=98.45, overall=98.45]	(230.2481, 71470.79)(231.25125, 10964.999)(232.25415, 101	C14 H31 N O	FindByFormula	28 +	229.2407	17.348188
C14 H31 N4 O2 P	C14 H31 N4 O2 P	[C14 H31 N4 O2 P, tgt=83.06, overall=83.06]	(319.22488, 24394.186)(320.23148, 3978.3977)(321.238, 879	C14 H31 N4 O2 P	FindByFormula	28 +	318.2185	21.69729
C14 H31 N6 O P S	C14 H31 N6 O P S	[C14 H31 N6 O P S, tgt=32.30, overall=32.30]	(363.20804, 38487.066)(364.21158, 9108.44)(365.2186, 4442	C14 H31 N6 O P S	FindByFormula	20 +	362.2008	22.396725
C14 H32 N2 S2	C14 H32 N2 S2	[C14 H32 N2 S2, tgt=91.71, overall=91.71]	(293.20923, 10188.087)(294.21265, 1997.443)(295.20404, 78	C14 H32 N2 S2	FindByFormula	27 +	292.2013	21.075058
C14 H33 N4 O2 P	C14 H33 N4 O2 P	[C14 H33 N4 O2 P, tgt=74.51, overall=74.51]	(321.24075, 21704.389)(322.24564, 4529.6787)(323.247, 536	C14 H33 N4 O2 P	FindByFormula	28 +	320.2344	21.880514
C14 H33 N4 P3	C14 H33 N4 P3	[C14 H33 N4 P3, tgt=78.96, overall=78.96]	(351.2001, 944.87396)(352.1987, 119.837204)(353.1928, 110	C14 H33 N4 P3	FindByFormula	25 +	350.1913	12.13333
C14 H33 N7	C14 H33 N7	[C14 H33 N7, tgt=67.90, overall=67.90]	(300.28967, 3912.0798)(301.2901, 437.7499)(302.29056, 303	C14 H33 N7	FindByFormula	26 +	299.2796	20.623753
C14 H34 N2 O6	C14 H34 N2 O6	[C14 H34 N2 O6, tgt=51.35, overall=51.35]	(327.24905, 9252.412)(328.25348, 1828.1093)(329.24677, 26	C14 H34 N2 O6	FindByFormula	24 +	326.244	21.95523
C14 H34 N2 S2	C14 H34 N2 S2	[C14 H34 N2 S2, tgt=76.11, overall=76.11]	(295.22256, 6493.0376)(296.22342, 1039.3623)(297.2183, 47	C14 H34 N2 S2	FindByFormula	27 +	294.2175	21.396212
C14 H35 N7	C14 H35 N7	[C14 H35 N7, tgt=88.59, overall=88.59]	(302.3035, 1499.3186)(303.30383, 351.4563)(304.3012, 127.	C14 H35 N7	FindByFormula	27 +	301.2971	20.990671
C14 H35 N7 O2	C14 H35 N7 O2	[C14 H35 N7 O2, tgt=88.67, overall=88.67]	(334.29373, 1449.0833)(335.29272, 350.77704)(336.29608, 6	C14 H35 N7 O2	FindByFormula	19 +	333.2859	19.021992
C14 H38 N4 O6 P2	C14 H38 N4 O6 P2	[C14 H38 N4 O6 P2, tgt=87.06, overall=87.06]	(421.23334, 176886.47)(422.2368, 35140.695)(423.2395, 618	C14 H38 N4 O6 P2	FindByFormula	28 +	420.2264	21.441587
C14 H39 Cl N10 O	C14 H39 Cl N10 O	[C14 H39 Cl N10 O, tgt=18.15, overall=18.15]	(399.30612, 16912.18)(400.3086, 4074.8672)(401.3037, 607.	C14 H39 Cl N10 O	FindByFormula	24 +	398.3004	22.53266
C14 H9 N4 O P S2	C14 H9 N4 O P S2	[C14 H9 N4 O P S2, tgt=81.23, overall=81.23]	(345.0029, 4500.5825)(346.00797, 1035.4768)(347.0044, 619	C14 H9 N4 O P S2	FindByFormula	22 +	343.9967	1.3651903
C14 H9 N6 O2 P	C14 H9 N6 O2 P	[C14 H9 N6 O2 P, tgt=96.73, overall=96.73]	(325.06113, 3738.2913)(326.06464, 660.1322)(327.0604, 332	C14 H9 N6 O2 P	FindByFormula	9 +	324.0544	15.642742
C15 H11 N9	C15 H11 N9	[C15 H11 N9, tgt=69.02, overall=69.02]	(318.1211, 3513.0854)(319.12125, 559.1481)(320.12292, 100	C15 H11 N9	FindByFormula	21 +	317.1141	1.2144347
C15 H13 N O2	C15 H13 N O2	[C15 H13 N O2, tgt=95.23, overall=95.23]	(240.10225, 4144.629)(241.10588, 913.97253)(242.10164, 14	C15 H13 N O2	FindByFormula	22 +	239.0954	2.6811726
C15 H14 N6	C15 H14 N6	[C15 H14 N6, tgt=93.20, overall=93.20]	(279.13452, 4395.7617)(280.13696, 781.94336)(281.1345, 17	C15 H14 N6	FindByFormula	21 +	278.1274	3.3665931
C15 H14 N6 O	C15 H14 N6 O	[C15 H14 N6 O, tgt=81.64, overall=81.64]	(295.12955, 3071.9226)(296.13202, 651.9537)(297.12796, 29	C15 H14 N6 O	FindByFormula	22 +	294.121	5.010121
C15 H14 P2	C15 H14 P2	[C15 H14 P2, tgt=92.98, overall=92.98]	(257.0643, 8033.184)(258.06833, 909.4991)(259.06955, 165.	C15 H14 P2	FindByFormula	22 +	256.0567	6.5851045
C15 H15 N3 O S	C15 H15 N3 O S	[C15 H15 N3 O S, tgt=27.31, overall=27.31]	(286.0993, 4487.3164)(287.1039, 644.13104)(288.1026, 506.	C15 H15 N3 O S	FindByFormula	22 +	285.0938	0.984003
C15 H16 N O3 P3	C15 H16 N O3 P3	[C15 H16 N O3 P3, tgt=79.40, overall=79.40]	(352.04288, 1743.8467)(353.05054, 290.66)(354.038, 170.57	C15 H16 N O3 P3	FindByFormula	6 +	351.0347	15.560501
C15 H16 N10 O3	C15 H16 N10 O3	[C15 H16 N10 O3, tgt=57.27, overall=57.27]	(385.1503, 3693.3362)(386.1507, 829.2614)(387.15027, 185.	C15 H16 N10 O3	FindByFormula	8 +	384.1418	11.1916685
C15 H18 N5 O2 P S3	C15 H18 N5 O2 P S3	[C15 H18 N5 O2 P S3, tgt=89.17, overall=89.17]	(428.0412, 3600.83)(429.044, 886.1834)(430.04254, 365.659	C15 H18 N5 O2 P S3	FindByFormula	21 +	427.0363	1.2062445
C15 H18 N6 O	C15 H18 N6 O	[C15 H18 N6 O, tgt=83.08, overall=83.08]	(299.16205, 4690.0977)(300.16495, 959.61505)(301.16147, 4	C15 H18 N6 O	FindByFormula	28 +	298.1542	19.550976
C15 H18 N6 O S	C15 H18 N6 O S	[C15 H18 N6 O S, tgt=95.93, overall=95.93]	(331.13263, 4587.3286)(332.13638, 906.5306)(333.13544, 43	C15 H18 N6 O S	FindByFormula	22 +	330.1258	4.550327
C15 H19 N4 O3 P	C15 H19 N4 O3 P	[C15 H19 N4 O3 P, tgt=96.49, overall=96.49]	(335.12616, 168424.2)(336.12933, 34937.45)(337.12967, 522	C15 H19 N4 O3 P	FindByFormula	28 +	334.1189	20.726429
C15 H19 N7 O2 S3	C15 H19 N7 O2 S3	[C15 H19 N7 O2 S3, tgt=73.73, overall=73.73]	(426.08273, 9233.079)(427.0842, 1885.7128)(428.0813, 130.	C15 H19 N7 O2 S3	FindByFormula	22 +	425.0754	1.1899602
C15 H20 N6 O	C15 H20 N6 O	[C15 H20 N6 O, tgt=93.46, overall=93.46]	(301.1774, 24461.55)(302.18082, 4687.4766)(303.18332, 112	C15 H20 N6 O	FindByFormula	28 +	300.1705	19.794386
C15 H20 N6 O2	C15 H20 N6 O2	[C15 H20 N6 O2, tgt=72.60, overall=72.60]	(317.17252, 5531.6455)(318.1755, 1104.8835)(319.17477, 59	C15 H20 N6 O2	FindByFormula	28 +	316.1661	17.42746
C15 H20 N6 O3	C15 H20 N6 O3	[C15 H20 N6 O3, tgt=86.08, overall=86.08]	(333.16812, 29721.479)(334.1718, 5706.872)(335.16803, 50.	C15 H20 N6 O3	FindByFormula	28 +	332.1613	17.268473
C15 H20 O3	C15 H20 O3	[C15 H20 O3, tgt=79.12, overall=79.12]	(249.14767, 5577.1284)(250.15176, 814.55316)(251.1477, 33	C15 H20 O3	FindByFormula	28 +	248.1404	17.400383
C15 H20 O4	C15 H20 O4	[C15 H20 O4, tgt=85.57, overall=85.57]	(265.14227, 4389.9272)(266.14468, 625.5264)(267.14163, 40	C15 H20 O4	FindByFormula	28 +	264.1344	14.923198
C15 H22 N2 O3	C15 H22 N2 O3	[C15 H22 N2 O3, tgt=95.70, overall=95.70]	(279.1695, 3533.7107)(280.16934, 649.74603)(281.17087, 12	C15 H22 N2 O3	FindByFormula	23 +	278.1621	7.866235
C15 H22 O2	C15 H22 O2	[C15 H22 O2, tgt=91.37, overall=91.37]	(235.1717, 6745.8037)(236.1768, 914.88824)(237.1677, 377.	C15 H22 O2	FindByFormula	28 +	234.1619	19.686005
C15 H22 S2	C15 H22 S2	[C15 H22 S2, tgt=64.23, overall=64.23]	(267.12476, 3843.4312)(268.127, 638.2296)(269.119, 327.20	C15 H22 S2	FindByFormula	28 +	266.1163	16.430653
C15 H23 N5 O3	C15 H23 N5 O3	[C15 H23 N5 O3, tgt=98.84, overall=98.84]	(322.1885, 3798.51)(323.18665, 804.18195)(324.18674, 147.	C15 H23 N5 O3	FindByFormula	25 +	321.1794	1.6108912
C15 H24 N2 O3	C15 H24 N2 O3	[C15 H24 N2 O3, tgt=77.21, overall=77.21]	(281.18503, 1606.5332)(282.18216, 383.95612)(283.18192, 7	C15 H24 N2 O3	FindByFormula	20 +	280.1778	4.373484
C15 H26 N2 O4	C15 H26 N2 O4	[C15 H26 N2 O4, tgt=96.04, overall=96.04]	(299.19604, 8729.965)(300.19772, 1506.6981)(301.1934, 388	C15 H26 N2 O4	FindByFormula	25 +	298.1888	22.582993
C15 H27 Cl O S	C15 H27 Cl O S	[C15 H27 Cl O S, tgt=90.83, overall=90.83]	(291.1574, 3868.2769)(292.16098, 681.4979)(293.146, 1147.	C15 H27 Cl O S	FindByFormula	28 +	290.1482	16.180622
C15 H27 Cl3 N2 O3 S3	C15 H27 Cl3 N2 O3 S3	[C15 H27 Cl3 N2 O3 S3, tgt=91.16, overall=91.16]	(485.0326, 4216.2534)(486.03516, 787.50494)(487.0298, 543	C15 H27 Cl3 N2 O3 S3	FindByFormula	6 +	484.0259	7.762642
C15 H27 N O4	C15 H27 N O4	[C15 H27 N O4, tgt=98.98, overall=98.98]	(286.20117, 6733.522)(287.20135, 1145.6136)(288.2005, 231	C15 H27 N O4	FindByFormula	25 +	285.1933	9.587813
C15 H28 N5 O P3	C15 H28 N5 O P3	[C15 H28 N5 O P3, tgt=98.00, overall=98.00]	(388.15845, 6766.844)(389.15985, 1431.3899)(390.16293, 39	C15 H28 N5 O P3	FindByFormula	7 +	387.1505	8.757385
C15 H28 N6 O	C15 H28 N6 O	[C15 H28 N6 O, tgt=72.71, overall=72.71]	(309.23834, 6313.7656)(310.2402, 1279.8207)(311.2344, 217	C15 H28 N6 O	FindByFormula	28 +	308.2325	22.239172
C15 H28 N6 O2	C15 H28 N6 O2	[C15 H28 N6 O2, tgt=54.15, overall=54.15]	(325.2353, 6101.631)(326.235, 1099.4933)(327.2299, 806.28	C15 H28 N6 O2	FindByFormula	27 +	324.2261	22.148258
C15 H29 N O4	C15 H29 N O4	[C15 H29 N O4, tgt=89.85, overall=89.85]	(288.2168, 2798.8396)(289.21844, 554.53)(290.22235, 150.1	C15 H29 N O4	FindByFormula	25 +	287.2102	11.739599
C15 H29 P S	C15 H29 P S	[C15 H29 P S, tgt=84.92, overall=84.92]	(273.18158, 3502.698)(274.1813, 518.1458)(275.17383, 443.	C15 H29 P S	FindByFormula	27 +	272.1729	19.15463
C15 H30 N14 O5 P2 S3	C15 H30 N14 O5 P2 S3	[C15 H30 N14 O5 P2 S3, tgt=83.26, overall=83.26]	(645.1247, 9491.868)(646.1269, 2484.0583)(647.1125, 3099.	C15 H30 N14 O5 P2 S3	FindByFormula	7 +	644.1123	0.6929998
C15 H30 N2 O	C15 H30 N2 O	[C15 H30 N2 O, tgt=85.69, overall=85.69]	(255.2424, 1011.1647)(256.24454, 204.6254)(257.24368, 77.	C15 H30 N2 O	FindByFormula	13 +	254.2351	20.729414
C15 H30 N6 O	C15 H30 N6 O	[C15 H30 N6 O, tgt=97.02, overall=97.02]	(311.25476, 9269.141)(312.25662, 1834.9419)(313.25854, 37	C15 H30 N6 O	FindByFormula	27 +	310.2486	22.429396
C15 H30 N6 O2	C15 H30 N6 O2	[C15 H30 N6 O2, tgt=72.85, overall=72.85]	(327.24878, 8999.751)(328.25504, 1835.819)(329.24963, 215	C15 H30 N6 O2	FindByFormula	27 +	326.2434	21.877695
C15 H31 N O2	C15 H31 N O2	[C15 H31 N O2, tgt=67.65, overall=67.65]	(258.24237, 1134.2343)(259.24286, 239.05301)(260.24573, 9	C15 H31 N O2	FindByFormula	22 +	257.2353	21.473295
C15 H31 N4 O2 P	C15 H31 N4 O2 P	[C15 H31 N4 O2 P, tgt=79.21, overall=79.21]	(331.22488, 14079.096)(332.22916, 3047.5325)(333.22888, 1	C15 H31 N4 O2 P	FindByFormula	28 +	330.2184	22.027658
C15 H33 Cl N4 O	C15 H33 Cl N4 O	[C15 H33 Cl N4 O, tgt=68.56, overall=68.56]	(321.24066, 23578.033)(322.2446, 5010.1226)(323.249, 9005	C15 H33 Cl N4 O	FindByFormula	27 +	320.2364	22.009363
C15 H34 N2 O5	C15 H34 N2 O5	[C15 H34 N2 O5, tgt=71.66, overall=71.66]	(323.25323, 10924.409)(324.25604, 2311.32)(325.26364, 229	C15 H34 N2 O5	FindByFormula	25 +	322.2467	22.100714
C15 H35 N2 O6 P S2	C15 H35 N2 O6 P S2	[C15 H35 N2 O6 P S2, tgt=58.56, overall=58.56]	(435.17426, 4347.898)(436.17715, 942.2018)(437.18793, 92.	C15 H35 N2 O6 P S2	FindByFormula	23 +	434.1662	22.595127
C15 H35 N4 O3 P	C15 H35 N4 O3 P	[C15 H35 N4 O3 P, tgt=86.00, overall=86.00]	(351.25174, 24074.26)(352.25528, 5302.423)(389.20337, 390	C15 H35 N4 O3 P	FindByFormula	28 +	350.2453	22.52334
C15 H35 N7	C15 H35 N7	[C15 H35 N7, tgt=74.06, overall=74.06]	(314.30392, 718.4785)(315.3013, 142.01857)(352.2553, 883.	C15 H35 N7	FindByFormula	7 +	313.2954	21.253128
C15 H35 N7 O	C15 H35 N7 O	[C15 H35 N7 O, tgt=75.19, overall=75.19]	(330.30008, 1296.6483)(331.3013, 368.0353)(332.30643, 95.	C15 H35 N7 O	FindByFormula	19 +	329.2898	19.864668
C15 H36 N2 O P2 S	C15 H36 N2 O P2 S	[C15 H36 N2 O P2 S, tgt=81.01, overall=81.01]	(355.2108, 7831.8657)(356.21295, 1404.3347)(357.20523, 80	C15 H36 N2 O P2 S	FindByFormula	19 +	354.2032	19.105982
C15 H36 N8 O7	C15 H36 N8 O7	[C15 H36 N8 O7, tgt=22.11, overall=22.11]	(441.27896, 10262.432)(442.2825, 1313.8314)(443.28104, 41	C15 H36 N8 O7	FindByFormula	14 +	440.2714	23.007828
C15 H40 N8 S2	C15 H40 N8 S2	[C15 H40 N8 S2, tgt=63.15, overall=63.15]	(397.2886, 18094.736)(398.29153, 4169.9624)(399.28967, 16	C15 H40 N8 S2	FindByFormula	10 +	396.2856	21.811718
C15 H5 Cl3 N2 O3 P2	C15 H5 Cl3 N2 O3 P2	[C15 H5 Cl3 N2 O3 P2, tgt=80.51, overall=80.51]	(428.89035, 1449.7684)(429.8909, 216.90714)(430.8968, 460	C15 H5 Cl3 N2 O3 P2	FindByFormula	7 +	427.884	18.931292
C16 H14 N2 O4 S2	C16 H14 N2 O4 S2	[C16 H14 N2 O4 S2, tgt=88.68, overall=88.68]	(363.0463, 5230.069)(364.04953, 1138.7854)(365.04916, 215	C16 H14 N2 O4 S2	FindByFormula	20 +	362.0389	16.325161
C16 H14 N2 P4	C16 H14 N2 P4	[C16 H14 N2 P4, tgt=20.58, overall=20.58]	(359.0171, 5469.305)(360.01837, 995.41644)(361.01932, 459	C16 H14 N2 P4	FindByFormula	26 +	358.0109	1.1405437
C16 H14 N8	C16 H14 N8	[C16 H14 N8, tgt=86.72, overall=86.72]	(319.1423, 2002.3174)(320.1449, 468.1389)(321.14026, 159.	C16 H14 N8	FindByFormula	12 +	318.1341	2.6614645
C16 H16 O3	C16 H16 O3	[C16 H16 O3, tgt=48.92, overall=48.92]	(257.11667, 2657.2434)(258.11493, 350.50717)(259.11285, 1	C16 H16 O3	FindByFormula	21 +	256.1087	16.732603
C16 H16 O4	C16 H16 O4	[C16 H16 O4, tgt=81.10, overall=81.10]	(273.11087, 3982.547)(274.11264, 576.3958)(275.1131, 182.	C16 H16 O4	FindByFormula	28 +	272.1032	17.15188
C16 H18 O2 P2	C16 H18 O2 P2	[C16 H18 O2 P2, tgt=88.79, overall=88.79]	(305.08685, 2900.02)(306.08853, 505.3329)(307.0843, 112.6	C16 H18 O2 P2	FindByFormula	27 +	304.0794	2.6622925
C16 H19 N O4	C16 H19 N O4	[C16 H19 N O4, tgt=91.19, overall=91.19]	(290.13937, 6061.048)(291.14026, 1123.7845)(292.14133, 23	C16 H19 N O4	FindByFormula	9 +	289.1318	6.8264465
C16 H19 N8 O3 P	C16 H19 N8 O3 P	[C16 H19 N8 O3 P, tgt=92.72, overall=92.72]	(403.13974, 2830.7546)(404.14313, 558.9704)(405.13974, 15	C16 H19 N8 O3 P	FindByFormula	28 +	402.1327	22.463861
C16 H20 N2 O3	C16 H20 N2 O3	[C16 H20 N2 O3, tgt=88.91, overall=88.91]	(289.15427, 26482.58)(290.1581, 3583.9656)(291.157, 517.0	C16 H20 N2 O3	FindByFormula	28 +	288.1472	20.706833
C16 H20 N4 O2 P2	C16 H20 N4 O2 P2	[C16 H20 N4 O2 P2, tgt=80.68, overall=80.68]	(363.11334, 3384.356)(364.11606, 672.7447)	C16 H20 N4 O2 P2	FindByFormula	28 +	362.1061	20.729465
C16 H20 O	C16 H20 O	[C16 H20 O, tgt=82.04, overall=82.04]	(229.15808, 1983.013)(230.15994, 321.09198)(231.15681, 78	C16 H20 O	FindByFormula	14 +	228.1513	0.7335745
C16 H20 P2	C16 H20 P2	[C16 H20 P2, tgt=88.43, overall=88.43]	(275.11063, 4462.879)(276.11343, 539.44446)(277.11334, 21	C16 H20 P2	FindByFormula	27 +	274.1044	4.692147
C16 H22 N2 P2 S	C16 H22 N2 P2 S	[C16 H22 N2 P2 S, tgt=80.69, overall=80.69]	(337.10516, 16737.432)(338.11057, 3303.3713)(339.11655, 4	C16 H22 N2 P2 S	FindByFormula	28 +	336.0982	18.143362
C16 H22 N6 O2	C16 H22 N6 O2	[C16 H22 N6 O2, tgt=79.68, overall=79.68]	(331.18832, 4245.0854)(332.19193, 892.5586)(333.19354, 16	C16 H22 N6 O2	FindByFormula	28 +	330.1815	19.358725
C16 H22 O4	C16 H22 O4	[C16 H22 O4, tgt=98.03, overall=98.03]	(279.16315, 6447.05)(280.16562, 1188.1561)(281.16882, 175	C16 H22 O4	FindByFormula	28 +	278.1526	20.777449
C16 H23 N5	C16 H23 N5	[C16 H23 N5, tgt=94.70, overall=94.70]	(286.2012, 2283.732)(287.20163, 423.52002)(288.2007, 102.	C16 H23 N5	FindByFormula	22 +	285.1936	9.736411
C16 H24 N6	C16 H24 N6	[C16 H24 N6, tgt=89.78, overall=89.78]	(301.2128, 16232.36)(302.219, 3239.3538)(303.2248, 2613.3	C16 H24 N6	FindByFormula	26 +	300.2077	22.539927
C16 H24 N6 O	C16 H24 N6 O	[C16 H24 N6 O, tgt=60.24, overall=60.24]	(317.20755, 14291.014)(318.2131, 2799.6853)(355.1682, 122	C16 H24 N6 O	FindByFormula	26 +	316.2016	21.480282
C16 H24 N8 O4	C16 H24 N8 O4	[C16 H24 N8 O4, tgt=98.54, overall=98.54]	(393.19965, 14936.764)(394.20395, 2864.1187)(395.209, 519	C16 H24 N8 O4	FindByFormula	20 +	392.1926	22.73602
C16 H24 O4 S	C16 H24 O4 S	[C16 H24 O4 S, tgt=85.23, overall=85.23]	(313.1478, 2772.106)(314.1472, 652.01)(315.15808, 1233.63	C16 H24 O4 S	FindByFormula	28 +	312.1373	20.725859
C16 H25 N O2	C16 H25 N O2	[C16 H25 N O2, tgt=89.95, overall=89.95]	(264.19528, 1513.2893)(265.19714, 411.1025)(266.19833, 78	C16 H25 N O2	FindByFormula	17 +	263.1885	6.804969
C16 H25 P3	C16 H25 P3	[C16 H25 P3, tgt=84.31, overall=84.31]	(311.12433, 3034.7153)(312.12595, 638.7964)(313.1228, 168	C16 H25 P3	FindByFormula	25 +	310.1185	2.794717
C16 H26 N2 S3	C16 H26 N2 S3	[C16 H26 N2 S3, tgt=94.09, overall=94.09]	(343.13385, 11872.004)(344.13605, 2271.5872)(345.13205, 2	C16 H26 N2 S3	FindByFormula	20 +	342.1261	21.410976
C16 H28 N P S	C16 H28 N P S	[C16 H28 N P S, tgt=59.60, overall=59.60]	(298.17776, 3124.7778)(299.17465, 934.6619)(300.17358, 35	C16 H28 N P S	FindByFormula	23 +	297.1698	16.102314
C16 H28 N4 P2	C16 H28 N4 P2	[C16 H28 N4 P2, tgt=92.89, overall=92.89]	(339.18436, 1522.0275)(340.18536, 339.1609)(341.17477, 10	C16 H28 N4 P2	FindByFormula	25 +	338.1788	22.613567
C16 H28 N6 O2	C16 H28 N6 O2	[C16 H28 N6 O2, tgt=82.06, overall=82.06]	(337.2352, 11698.822)(338.2436, 2508.7788)(339.2316, 947.	C16 H28 N6 O2	FindByFormula	28 +	336.228	19.7169
C16 H29 Cl N6 O4	C16 H29 Cl N6 O4	[C16 H29 Cl N6 O4, tgt=73.04, overall=73.04]	(405.2013, 1444.8966)(406.20316, 387.0117)(407.1991, 128.	C16 H29 Cl N6 O4	FindByFormula	7 +	404.1953	9.022879
C16 H29 N4 P3	C16 H29 N4 P3	[C16 H29 N4 P3, tgt=58.03, overall=58.03]	(371.16696, 1639.1765)(372.16757, 277.33075)(373.1686, 23	C16 H29 N4 P3	FindByFormula	27 +	370.1595	11.641187
C16 H30 N6 O S	C16 H30 N6 O S	[C16 H30 N6 O S, tgt=82.19, overall=82.19]	(355.22806, 3704.98)(356.23065, 983.7213)(357.22842, 580.	C16 H30 N6 O S	FindByFormula	15 +	354.2205	21.908052
C16 H30 N6 O2	C16 H30 N6 O2	[C16 H30 N6 O2, tgt=95.80, overall=95.80]	(339.24887, 5016.3213)(340.25623, 1166.0823)(341.25693, 1	C16 H30 N6 O2	FindByFormula	28 +	338.2428	21.164194
C16 H30 O2	C16 H30 O2	[C16 H30 O2, tgt=61.65, overall=61.65]	(255.2282, 119.13048)(256.23398, 24.656668)(293.18988, 28	C16 H30 O2	FindByFormula	28 +	254.2248	22.42848
C16 H30 O2 P2	C16 H30 O2 P2	[C16 H30 O2 P2, tgt=86.95, overall=86.95]	(317.1792, 7981.96)(318.1821, 2044.543)(319.176, 69.88)(33	C16 H30 O2 P2	FindByFormula	18 +	316.1725	22.628424
C16 H31 N O2 S	C16 H31 N O2 S	[C16 H31 N O2 S, tgt=81.96, overall=81.96]	(302.21454, 2303.215)(303.21292, 434.41876)(304.2111, 168	C16 H31 N O2 S	FindByFormula	8 +	301.2071	18.453106
C16 H31 N2 O4 P3	C16 H31 N2 O4 P3	[C16 H31 N2 O4 P3, tgt=80.32, overall=80.32]	(409.1578, 4396.28)(410.16287, 894.91437)(411.17102, 58.5	C16 H31 N2 O4 P3	FindByFormula	28 +	408.1511	22.459705
C16 H31 N7 O	C16 H31 N7 O	[C16 H31 N7 O, tgt=79.94, overall=79.94]	(338.26678, 29090.057)(339.26666, 6743.233)(340.26727, 11	C16 H31 N7 O	FindByFormula	21 +	337.2587	21.750107
C16 H31 O P3 S	C16 H31 O P3 S	[C16 H31 O P3 S, tgt=80.41, overall=80.41]	(365.13715, 18438.482)(366.14078, 4091.403)(367.14996, 74	C16 H31 O P3 S	FindByFormula	28 +	364.13	20.474852
C16 H31 P3	C16 H31 P3	[C16 H31 P3, tgt=84.05, overall=84.05]	(317.17007, 4172.4995)(318.17178, 764.56793)(355.1337, 51	C16 H31 P3	FindByFormula	28 +	316.163	19.756807
C16 H32 N6 O2	C16 H32 N6 O2	[C16 H32 N6 O2, tgt=47.37, overall=47.37]	(341.26544, 30538.057)(342.26883, 6162.351)(343.26547, 86	C16 H32 N6 O2	FindByFormula	28 +	340.2589	22.27565
C16 H32 N8 S5	C16 H32 N8 S5	[C16 H32 N8 S5, tgt=88.02, overall=88.02]	(497.14383, 1831.187)(498.14743, 465.19125)(499.13528, 11	C16 H32 N8 S5	FindByFormula	26 +	496.1336	22.598732
C16 H32 O2 P2	C16 H32 O2 P2	[C16 H32 O2 P2, tgt=90.03, overall=90.03]	(319.1956, 26175.08)(320.19907, 5154.3115)(357.15164, 751	C16 H32 O2 P2	FindByFormula	27 +	318.1873	22.681137
C16 H33 N O	C16 H33 N O	[C16 H33 N O, tgt=53.52, overall=53.52]	(256.2635, 3425.7456)(257.2639, 678.86774)(258.26608, 234	C16 H33 N O	FindByFormula	26 +	255.2562	17.093655
C16 H33 N O2	C16 H33 N O2	[C16 H33 N O2, tgt=70.32, overall=70.32]	(272.25836, 28098.914)(273.26028, 5188.217)(274.26178, 44	C16 H33 N O2	FindByFormula	24 +	271.2509	17.283117
C16 H33 N O3	C16 H33 N O3	[C16 H33 N O3, tgt=80.91, overall=80.91]	(288.25345, 1731.5947)(289.25208, 540.7538)(290.2557, 128	C16 H33 N O3	FindByFormula	27 +	287.2462	20.095352
C16 H33 N4 O2 P3	C16 H33 N4 O2 P3	[C16 H33 N4 O2 P3, tgt=79.67, overall=79.67]	(407.18948, 2841.3398)(408.19257, 587.9923)(409.18256, 60	C16 H33 N4 O2 P3	FindByFormula	26 +	406.1815	7.8027716
C16 H33 N4 O3 P	C16 H33 N4 O3 P	[C16 H33 N4 O3 P, tgt=41.94, overall=41.94]	(361.2362, 10268.667)(362.24075, 2440.456)(363.23917, 138	C16 H33 N4 O3 P	FindByFormula	25 +	360.2292	21.582708
C16 H34 O9	C16 H34 O9	[C16 H34 O9, tgt=99.33, overall=99.33]	(371.2274, 4190.6655)(372.22867, 859.3571)(373.2297, 194.	C16 H34 O9	FindByFormula	28 +	370.2202	7.9295387
C16 H35 N	C16 H35 N	[C16 H35 N, tgt=84.86, overall=84.86]	(242.28436, 1157.2562)(243.28432, 225.32098)(244.28627, 8	C16 H35 N	FindByFormula	21 +	241.277	19.471664
C16 H35 N O	C16 H35 N O	[C16 H35 N O, tgt=55.75, overall=55.75]	(258.27887, 5612.989)(259.2805, 1044.9392)(260.28278, 124	C16 H35 N O	FindByFormula	28 +	257.2711	19.72111
C16 H35 N O2	C16 H35 N O2	[C16 H35 N O2, tgt=99.71, overall=99.71]	(274.2747, 241492.47)(275.27765, 42645.19)(276.28033, 465	C16 H35 N O2	FindByFormula	28 +	273.2675	17.054022
C16 H35 N O3	C16 H35 N O3	[C16 H35 N O3, tgt=98.63, overall=98.63]	(290.26935, 53279.625)(291.2722, 9641.281)(292.2745, 1198	C16 H35 N O3	FindByFormula	28 +	289.262	17.471554
C16 H36 N2 O2 S2	C16 H36 N2 O2 S2	[C16 H36 N2 O2 S2, tgt=93.03, overall=93.03]	(353.22827, 3932.7217)(354.22977, 757.2601)(355.2273, 208	C16 H36 N2 O2 S2	FindByFormula	21 +	352.2231	16.915329
C16 H36 N2 O4 P2 S	C16 H36 N2 O4 P2 S	[C16 H36 N2 O4 P2 S, tgt=89.92, overall=89.92]	(415.19452, 3160.486)(416.19363, 621.7762)(417.20703, 688	C16 H36 N2 O4 P2 S	FindByFormula	13 +	414.1884	12.436209
C16 H36 N2 O5	C16 H36 N2 O5	[C16 H36 N2 O5, tgt=82.26, overall=82.26]	(337.27054, 9332.187)(338.27307, 2120.2249)(339.26486, 82	C16 H36 N2 O5	FindByFormula	28 +	336.2623	22.738707
C16 H36 N6 O2 S	C16 H36 N6 O2 S	[C16 H36 N6 O2 S, tgt=78.14, overall=78.14]	(377.26874, 19814.318)(378.27237, 4605.2627)(379.27386, 1	C16 H36 N6 O2 S	FindByFormula	28 +	376.2619	22.431772
C16 H37 N7	C16 H37 N7	[C16 H37 N7, tgt=59.96, overall=59.96]	(328.31967, 3302.397)(329.3217, 838.89136)(330.32297, 22	C16 H37 N7	FindByFormula	24 +	327.3128	21.70842
C16 H38 N2 O6	C16 H38 N2 O6	[C16 H38 N2 O6, tgt=74.86, overall=74.86]	(355.28036, 16426.576)(356.28394, 3456.04)(357.2805, 530.	C16 H38 N2 O6	FindByFormula	24 +	354.275	22.453653
C16 H38 N4 O4 S2	C16 H38 N4 O4 S2	[C16 H38 N4 O4 S2, tgt=72.34, overall=72.34]	(415.23975, 3778.5845)(416.24472, 1056.8693)(417.2408, 53	C16 H38 N4 O4 S2	FindByFormula	15 +	414.2308	22.563951
C16 H38 N6 O2 S	C16 H38 N6 O2 S	[C16 H38 N6 O2 S, tgt=81.50, overall=81.50]	(379.282, 45501.332)(380.28522, 10428.483)(381.2936, 5415	C16 H38 N6 O2 S	FindByFormula	27 +	378.2763	22.688883
C16 H39 N7	C16 H39 N7	[C16 H39 N7, tgt=41.17, overall=41.17]	(330.3355, 2595.3613)(331.33844, 697.52277)(332.33405, 14	C16 H39 N7	FindByFormula	22 +	329.3284	21.711294
C16 H42 N8 O S2	C16 H42 N8 O S2	[C16 H42 N8 O S2, tgt=28.53, overall=28.53]	(427.2994, 3143.8645)(428.30563, 1319.6616)(429.30103, 55	C16 H42 N8 O S2	FindByFormula	9 +	426.2896	22.58688
C16 H44 N14 O P4 S	C16 H44 N14 O P4 S	[C16 H44 N14 O P4 S, tgt=96.11, overall=96.11]	(605.2578, 9346.829)(606.2607, 2173.6848)(607.26917, 414.	C16 H44 N14 O P4 S	FindByFormula	6 +	604.2502	20.381363
C17 H10 N10 O3	C17 H10 N10 O3	[C17 H10 N10 O3, tgt=74.29, overall=74.29]	(403.09933, 1758.5181)(404.09842, 320.79)(405.09665, 107.	C17 H10 N10 O3	FindByFormula	16 +	402.0939	1.1930697
C17 H11 N7 O6 S	C17 H11 N7 O6 S	[C17 H11 N7 O6 S, tgt=95.72, overall=95.72]	(442.0559, 18423.936)(443.0583, 3830.1218)(444.0589, 1566	C17 H11 N7 O6 S	FindByFormula	19 +	441.0493	1.1935335
C17 H18 N10 O3	C17 H18 N10 O3	[C17 H18 N10 O3, tgt=88.78, overall=88.78]	(411.1639, 7468.81)(412.16806, 1629.9401)	C17 H18 N10 O3	FindByFormula	6 +	410.1564	13.777039
C17 H18 N12	C17 H18 N12	[C17 H18 N12, tgt=97.86, overall=97.86]	(391.1863, 3934.3594)(392.1887, 857.17505)(393.18668, 59.	C17 H18 N12	FindByFormula	12 +	390.1771	22.52833
C17 H18 N6 O3	C17 H18 N6 O3	[C17 H18 N6 O3, tgt=80.45, overall=80.45]	(355.15314, 3401.0767)(356.1551, 685.31726)(357.16156, 33	C17 H18 N6 O3	FindByFormula	28 +	354.1459	17.271973
C17 H19 N O3	C17 H19 N O3	[C17 H19 N O3, tgt=98.94, overall=98.94]	(286.14426, 5645.919)(287.1439, 2986.7185)(288.14102, 571	C17 H19 N O3	FindByFormula	22 +	285.137	17.815323
C17 H19 P S2	C17 H19 P S2	[C17 H19 P S2, tgt=66.47, overall=66.47]	(319.07254, 4296.3037)(320.07413, 964.71747)(321.07153, 4	C17 H19 P S2	FindByFormula	14 +	318.0649	1.1877195
C17 H20 N10 O4	C17 H20 N10 O4	[C17 H20 N10 O4, tgt=51.24, overall=51.24]	(429.17642, 5012.819)(430.1799, 1111.4244)(431.178, 408.0	C17 H20 N10 O4	FindByFormula	9 +	428.167	11.547521
C17 H21 N2 O P	C17 H21 N2 O P	[C17 H21 N2 O P, tgt=88.53, overall=88.53]	(301.14627, 10484.619)(302.1495, 1927.2883)(303.14703, 30	C17 H21 N2 O P	FindByFormula	7 +	300.139	20.045866
C17 H22 Cl N3 O3 P2 S2	C17 H22 Cl N3 O3 P2 S2	[C17 H22 Cl N3 O3 P2 S2, tgt=30.10, overall=30.10]	(478.0331, 1939.9639)(479.03702, 532.83624)(480.03116, 94	C17 H22 Cl N3 O3 P2 S2	FindByFormula	21 +	477.025	1.1870066
C17 H22 N10 P2	C17 H22 N10 P2	[C17 H22 N10 P2, tgt=86.99, overall=86.99]	(429.15903, 3217.6965)(430.1611, 709.63666)(431.16055, 13	C17 H22 N10 P2	FindByFormula	25 +	428.1508	22.599863
C17 H23 Cl O	C17 H23 Cl O	[C17 H23 Cl O, tgt=19.31, overall=19.31]	(279.15167, 3637.4175)(280.1542, 540.08264)(281.15262, 20	C17 H23 Cl O	FindByFormula	20 +	278.1439	17.344578
C17 H25 N12 P	C17 H25 N12 P	[C17 H25 N12 P, tgt=85.27, overall=85.27]	(429.2141, 3002.3179)(430.21487, 647.09467)(431.2137, 302	C17 H25 N12 P	FindByFormula	17 +	428.2094	23.036085
C17 H25 N8 P3 S2	C17 H25 N8 P3 S2	[C17 H25 N8 P3 S2, tgt=22.77, overall=22.77]	(499.08994, 309.9482)(500.08673, 99.142006)(501.079, 46.7	C17 H25 N8 P3 S2	FindByFormula	11 +	498.0808	8.468007
C17 H26 O4	C17 H26 O4	[C17 H26 O4, tgt=89.32, overall=89.32]	(295.18954, 1820.31)(296.19254, 278.15332)(297.1896, 145.	C17 H26 O4	FindByFormula	28 +	294.1837	17.63389
C17 H27 N O4	C17 H27 N O4	[C17 H27 N O4, tgt=71.79, overall=71.79]	(310.20135, 3200.2778)(311.19855, 682.44336)(312.2011, 25	C17 H27 N O4	FindByFormula	18 +	309.1928	11.636684
C17 H27 N5 O15 S	C17 H27 N5 O15 S	[C17 H27 N5 O15 S, tgt=92.90, overall=92.90]	(574.1292, 4062.9102)(575.13275, 996.8931)(576.13464, 272	C17 H27 N5 O15 S	FindByFormula	22 +	573.1229	3.002143
C17 H28 N2 O4	C17 H28 N2 O4	[C17 H28 N2 O4, tgt=90.06, overall=90.06]	(325.21225, 134864.2)(326.2153, 26262.285)(363.16928, 681	C17 H28 N2 O4	FindByFormula	25 +	324.2052	22.728767
C17 H29 N O S	C17 H29 N O S	[C17 H29 N O S, tgt=79.25, overall=79.25]	(296.2072, 2472.385)(297.20523, 1084.8833)(298.2004, 355.	C17 H29 N O S	FindByFormula	6 +	295.1955	21.502703
C17 H29 N O4	C17 H29 N O4	[C17 H29 N O4, tgt=91.69, overall=91.69]	(312.2164, 1747.99)(313.21762, 417.62125)(314.21854, 80.1	C17 H29 N O4	FindByFormula	9 +	311.2087	10.802419
C17 H30 N6 O5	C17 H30 N6 O5	[C17 H30 N6 O5, tgt=99.57, overall=99.57]	(399.23462, 3129.1672)(400.2365, 754.7922)(401.234, 274.2	C17 H30 N6 O5	FindByFormula	20 +	398.2279	3.979945
C17 H31 N O4	C17 H31 N O4	[C17 H31 N O4, tgt=99.09, overall=99.09]	(314.2322, 5915.9697)(315.23303, 1235.3036)(316.23322, 18	C17 H31 N O4	FindByFormula	11 +	313.2255	13.995471
C17 H31 N2 O3 P	C17 H31 N2 O3 P	[C17 H31 N2 O3 P, tgt=37.08, overall=37.08]	(343.21515, 4696.4507)(344.21918, 1029.0653)(345.2129, 38	C17 H31 N2 O3 P	FindByFormula	17 +	342.2064	22.212975
C17 H32 N6 O2	C17 H32 N6 O2	[C17 H32 N6 O2, tgt=97.04, overall=97.04]	(353.2668, 163748.22)(354.27005, 33944.688)(355.27408, 82	C17 H32 N6 O2	FindByFormula	27 +	352.2599	22.620455
C17 H32 N8 O	C17 H32 N8 O	[C17 H32 N8 O, tgt=96.69, overall=96.69]	(365.27728, 35732.574)(366.28012, 7621.1807)(367.2778, 14	C17 H32 N8 O	FindByFormula	28 +	364.2704	19.01262
C17 H33 N O4	C17 H33 N O4	[C17 H33 N O4, tgt=99.55, overall=99.55]	(316.24878, 6202.2383)(317.24945, 1307.4744)(318.25323, 4	C17 H33 N O4	FindByFormula	21 +	315.2411	15.357383
C17 H33 N2 O P S2	C17 H33 N2 O P S2	[C17 H33 N2 O P S2, tgt=72.15, overall=72.15]	(377.18527, 9085.927)(378.18918, 1987.3892)(379.18423, 37	C17 H33 N2 O P S2	FindByFormula	12 +	376.1792	21.531858
C17 H33 N7 O2	C17 H33 N7 O2	[C17 H33 N7 O2, tgt=88.57, overall=88.57]	(368.2778, 1651.085)(369.27435, 467.352)(370.2792, 166.04	C17 H33 N7 O2	FindByFormula	14 +	367.2704	17.904678
C17 H33 O2 P S2	C17 H33 O2 P S2	[C17 H33 O2 P S2, tgt=68.07, overall=68.07]	(365.1745, 3909.3086)(366.1747, 655.90576)(367.173, 190.8	C17 H33 O2 P S2	FindByFormula	20 +	364.1689	16.722118
C17 H34 N6 O S2	C17 H34 N6 O S2	[C17 H34 N6 O S2, tgt=88.47, overall=88.47]	(403.2302, 9131.489)(404.23172, 2049.0337)(405.22543, 491	C17 H34 N6 O S2	FindByFormula	22 +	402.2231	2.6234014
C17 H34 N6 O6 S2	C17 H34 N6 O6 S2	[C17 H34 N6 O6 S2, tgt=80.84, overall=80.84]	(483.2057, 6702.498)(484.2098, 1541.3383)(485.2162, 599.9	C17 H34 N6 O6 S2	FindByFormula	12 +	482.1977	21.444399
C17 H35 N O2	C17 H35 N O2	[C17 H35 N O2, tgt=33.60, overall=33.60]	(286.2738, 1299.0687)(287.2746, 365.1114)(288.2807, 89.44	C17 H35 N O2	FindByFormula	10 +	285.2665	22.199144
C17 H35 N O3	C17 H35 N O3	[C17 H35 N O3, tgt=91.41, overall=91.41]	(302.2696, 2881.0154)(303.26907, 670.3319)(304.2827, 130.	C17 H35 N O3	FindByFormula	21 +	301.2614	17.918627
C17 H35 N2 O P3 S	C17 H35 N2 O P3 S	[C17 H35 N2 O P3 S, tgt=92.03, overall=92.03]	(409.17276, 14585.199)(410.17618, 3240.8657)(411.18372, 1	C17 H35 N2 O P3 S	FindByFormula	22 +	408.165	18.969389
C17 H35 N4 O3 P	C17 H35 N4 O3 P	[C17 H35 N4 O3 P, tgt=92.73, overall=92.73]	(375.25107, 36316.082)(376.2548, 8463.784)(377.25745, 212	C17 H35 N4 O3 P	FindByFormula	28 +	374.2438	22.085455
C17 H35 N6 O P S2	C17 H35 N6 O P S2	[C17 H35 N6 O P S2, tgt=76.35, overall=76.35]	(435.213, 8665.498)(436.2165, 1796.138)(437.2037, 1893.46	C17 H35 N6 O P S2	FindByFormula	15 +	434.2035	20.46236
C17 H35 O3 P S2	C17 H35 O3 P S2	[C17 H35 O3 P S2, tgt=83.84, overall=83.84]	(383.18457, 3293.539)(384.18866, 835.9899)(385.1879, 606.	C17 H35 O3 P S2	FindByFormula	10 +	382.1778	13.384737
C17 H36 N4 O10 S	C17 H36 N4 O10 S	[C17 H36 N4 O10 S, tgt=83.86, overall=83.86]	(489.22275, 9411.598)(490.22485, 1954.4359)(491.2311, 812	C17 H36 N4 O10 S	FindByFormula	19 +	488.2139	21.43802

C17 H36 N6 O2 S	C17 H36 N6 O2 S	[C17 H36 N6 O2 S, tgt=81.72, overall=81.72]	(389.26715, 3430.6304)(390.27304, 1140.2307)(391.26852, 4	C17 H36 N6 O2 S	FindByFormula	19 +	388.2604	22.278864
C17 H37 N	C17 H37 N	[C17 H37 N, tgt=99.79, overall=99.79]	(256.30008, 14601.078)(257.30115, 2875.49)(258.3064, 683.4	C17 H37 N	FindByFormula	10 +	255.2928	21.164854
C17 H37 N O2	C17 H37 N O2	[C17 H37 N O2, tgt=87.29, overall=87.29]	(288.2899, 18246.025)(289.29248, 3757.2207)(290.29352, 46	C17 H37 N O2	FindByFormula	28 +	287.2825	16.768124
C17 H37 N O3	C17 H37 N O3	[C17 H37 N O3, tgt=87.81, overall=87.81]	(304.28534, 1797.0836)(305.28412, 205.37167)(306.2876, 62	C17 H37 N O3	FindByFormula	19 +	303.2765	19.57091
C17 H37 N4 O3 P	C17 H37 N4 O3 P	[C17 H37 N4 O3 P, tgt=97.07, overall=97.07]	(377.26724, 45984.492)(378.27182, 10283.982)(379.27744, 2	C17 H37 N4 O3 P	FindByFormula	28 +	376.2603	22.490538
C17 H38 N2 O2 S2	C17 H38 N2 O2 S2	[C17 H38 N2 O2 S2, tgt=38.58, overall=38.58]	(367.24478, 4137.187)(368.24606, 990.45703)(369.23697, 59	C17 H38 N2 O2 S2	FindByFormula	21 +	366.2382	18.823149
C17 H38 N2 S2	C17 H38 N2 S2	[C17 H38 N2 S2, tgt=55.60, overall=55.60]	(335.25592, 8519.094)(336.25873, 1944.3175)(337.25516, 42	C17 H38 N2 S2	FindByFormula	23 +	334.2499	22.516665
C17 H4 N4 O4	C17 H4 N4 O4	[C17 H4 N4 O4, tgt=49.60, overall=49.60]	(329.0307, 2824.5022)(330.028, 668.76605)(331.0259, 193.6	C17 H4 N4 O4	FindByFormula	26 +	328.0239	1.3601995
C17 H40 Cl2 N17 O P	C17 H40 Cl2 N17 O P	[C17 H40 Cl2 N17 O P, tgt=70.51, overall=70.51]	(600.2772, 1416.231)(601.283, 751.437)(602.2784, 2058.388)	C17 H40 Cl2 N17 O P	FindByFormula	12 +	599.2733	22.081186
C17 H40 N8 O8	C17 H40 N8 O8	[C17 H40 N8 O8, tgt=40.74, overall=40.74]	(485.30386, 13067.667)(486.31088, 1972.8567)(487.30234, 1	C17 H40 N8 O8	FindByFormula	18 +	484.297	22.955605
C17 H7 N6 O P	C17 H7 N6 O P	[C17 H7 N6 O P, tgt=94.61, overall=94.61]	(343.04938, 16761.572)(344.0527, 3084.603)(345.05603, 656	C17 H7 N6 O P	FindByFormula	19 +	342.0422	8.659447
C18 H12 N10	C18 H12 N10	[C18 H12 N10, tgt=95.08, overall=95.08]	(369.13156, 19005.24)(370.13574, 4216.2734)(371.1403, 765	C18 H12 N10	FindByFormula	28 +	368.1243	8.461625
C18 H15 N O3	C18 H15 N O3	[C18 H15 N O3, tgt=92.55, overall=92.55]	(294.11282, 16862.912)(295.11868, 3966.0735)(296.12204, 6	C18 H15 N O3	FindByFormula	6 +	293.106	17.988724
C18 H15 O P	C18 H15 O P	[C18 H15 O P, tgt=55.22, overall=55.22]	(279.0943, 48794.66)(280.0967, 9612.6045)(281.10263, 2103	C18 H15 O P	FindByFormula	25 +	278.0866	16.324305
C18 H18 O3	C18 H18 O3	[C18 H18 O3, tgt=77.70, overall=77.70]	(283.13422, 2235.8625)(284.1346, 459.5651)(285.13345, 488	C18 H18 O3	FindByFormula	27 +	282.1266	8.465743
C18 H20 N P	C18 H20 N P	[C18 H20 N P, tgt=64.11, overall=64.11]	(282.13992, 4596.6826)(283.14276, 1097.2931)(284.1382, 24	C18 H20 N P	FindByFormula	25 +	281.1326	15.768769
C18 H20 O3	C18 H20 O3	[C18 H20 O3, tgt=64.59, overall=64.59]	(285.14838, 1974.3174)(286.14755, 230.9825)(287.1413, 543	C18 H20 O3	FindByFormula	4 +	284.1385	8.462988
C18 H20 P2	C18 H20 P2	[C18 H20 P2, tgt=68.34, overall=68.34]	(299.11255, 4466.0913)(300.11557, 678.6188)(301.11264, 11	C18 H20 P2	FindByFormula	24 +	298.1041	12.651939
C18 H22 N4 O	C18 H22 N4 O	[C18 H22 N4 O, tgt=89.12, overall=89.12]	(311.1864, 3618.322)(312.18906, 754.58594)(313.1778, 774.	C18 H22 N4 O	FindByFormula	28 +	310.1783	17.265146
C18 H22 N6	C18 H22 N6	[C18 H22 N6, tgt=90.56, overall=90.56]	(323.1979, 17227.332)(324.2009, 3324.036)(361.15637, 129.	C18 H22 N6	FindByFormula	15 +	322.1906	22.526178
C18 H23 N15	C18 H23 N15	[C18 H23 N15, tgt=93.98, overall=93.98]	(450.23438, 2888.543)(451.23453, 1074.055)(452.233, 253.8	C18 H23 N15	FindByFormula	7 +	449.2266	14.116656
C18 H24 Cl N4 O4 P	C18 H24 Cl N4 O4 P	[C18 H24 Cl N4 O4 P, tgt=51.66, overall=51.66]	(427.1306, 6825.178)(428.13312, 1764.7612)(429.12845, 249	C18 H24 Cl N4 O4 P	FindByFormula	25 +	426.1228	19.014992
C18 H24 O8 P2	C18 H24 O8 P2	[C18 H24 O8 P2, tgt=96.27, overall=96.27]	(431.1018, 9136.597)(432.10538, 2161.771)(433.107, 512.06	C18 H24 O8 P2	FindByFormula	28 +	430.0945	8.464554
C18 H25 N4 O5 P	C18 H25 N4 O5 P	[C18 H25 N4 O5 P, tgt=88.51, overall=88.51]	(409.1634, 26686.256)(410.16656, 6524.3657)(411.1768, 201	C18 H25 N4 O5 P	FindByFormula	28 +	408.156	17.986454
C18 H26 N6	C18 H26 N6	[C18 H26 N6, tgt=95.96, overall=95.96]	(327.22937, 123210.414)(328.23297, 26509.73)(329.23868, 4	C18 H26 N6	FindByFormula	26 +	326.2237	22.723864
C18 H26 N6 O	C18 H26 N6 O	[C18 H26 N6 O, tgt=41.91, overall=41.91]	(343.2232, 18059.406)(344.2282, 4136.9775)(345.2261, 1357	C18 H26 N6 O	FindByFormula	23 +	342.2172	21.737436
C18 H28 N4 O10	C18 H28 N4 O10	[C18 H28 N4 O10, tgt=96.02, overall=96.02]	(461.1876, 8556.685)(462.19037, 2014.984)(463.19623, 342.	C18 H28 N4 O10	FindByFormula	20 +	460.1785	22.726627
C18 H28 O2	C18 H28 O2	[C18 H28 O2, tgt=79.25, overall=79.25]	(277.21393, 3730.1458)(278.22202, 743.538)(279.221, 844.7	C18 H28 O2	FindByFormula	27 +	276.2065	22.316008
C18 H28 O3	C18 H28 O3	[C18 H28 O3, tgt=68.16, overall=68.16]	(293.20972, 7431.2036)(294.21515, 1268.234)(295.2095, 117	C18 H28 O3	FindByFormula	26 +	292.2033	22.05788
C18 H30 O2	C18 H30 O2	[C18 H30 O2, tgt=91.52, overall=91.52]	(279.2303, 2310.8262)(280.2308, 561.1059)(281.23846, 597.	C18 H30 O2	FindByFormula	26 +	278.2234	22.564138
C18 H31 N7	C18 H31 N7	[C18 H31 N7, tgt=54.75, overall=54.75]	(346.27182, 32694.959)(347.2728, 8648.949)(348.28033, 303	C18 H31 N7	FindByFormula	19 +	345.2651	22.307264
C18 H32 N2 O S2	C18 H32 N2 O S2	[C18 H32 N2 O S2, tgt=94.12, overall=94.12]	(357.2013, 9264.855)(358.20312, 2106.1345)(359.19464, 779	C18 H32 N2 O S2	FindByFormula	11 +	356.1957	15.314035
C18 H32 N6 O3	C18 H32 N6 O3	[C18 H32 N6 O3, tgt=80.47, overall=80.47]	(381.25925, 4592.679)(382.26328, 1155.8282)(383.26706, 77	C18 H32 N6 O3	FindByFormula	23 +	380.2536	19.958311
C18 H32 O2	C18 H32 O2	[C18 H32 O2, tgt=49.99, overall=49.99]	(281.24307, 1230.5947)(282.2466, 256.85797)(283.2554, 239	C18 H32 O2	FindByFormula	17 +	280.2375	22.613745
C18 H33 N O4	C18 H33 N O4	[C18 H33 N O4, tgt=97.17, overall=97.17]	(328.2477, 2274.573)(329.2507, 537.07715)(330.25403, 96.2	C18 H33 N O4	FindByFormula	7 +	327.2404	15.35972
C18 H33 N3 O3	C18 H33 N3 O3	[C18 H33 N3 O3, tgt=74.90, overall=74.90]	(340.2617, 3536.483)(341.2609, 690.64325)(342.26105, 127.	C18 H33 N3 O3	FindByFormula	21 +	339.2538	20.707632
C18 H33 N6 O2 P5	C18 H33 N6 O2 P5	[C18 H33 N6 O2 P5, tgt=95.81, overall=95.81]	(521.14215, 1851.2642)(522.14514, 427.8366)(523.1416, 118	C18 H33 N6 O2 P5	FindByFormula	16 +	520.1354	22.514893
C18 H33 N7	C18 H33 N7	[C18 H33 N7, tgt=4.63, overall=4.63]	(348.28717, 22469.338)(349.2877, 7126.3145)(350.2835, 154	C18 H33 N7	FindByFormula	21 +	347.2797	22.614254
C18 H33 O P3	C18 H33 O P3	[C18 H33 O P3, tgt=92.55, overall=92.55]	(359.18112, 3548.135)(360.1868, 794.5129)(361.18616, 180.	C18 H33 O P3	FindByFormula	28 +	358.1734	3.889696
C18 H34 N6 O2	C18 H34 N6 O2	[C18 H34 N6 O2, tgt=62.72, overall=62.72]	(367.28156, 9113.3955)(368.28134, 2045.7107)(369.27698, 4	C18 H34 N6 O2	FindByFormula	15 +	366.2775	22.818756
C18 H34 N8 O2 P2	C18 H34 N8 O2 P2	[C18 H34 N8 O2 P2, tgt=73.81, overall=73.81]	(457.24008, 2065.0566)(458.24023, 486.17648)(459.2351, 73	C18 H34 N8 O2 P2	FindByFormula	17 +	456.2293	21.851349
C18 H34 N8 O4 S	C18 H34 N8 O4 S	[C18 H34 N8 O4 S, tgt=91.09, overall=91.09]	(459.24857, 3382.7048)(460.25595, 1226.695)(461.25378, 37	C18 H34 N8 O4 S	FindByFormula	19 +	458.2438	22.186195
C18 H36 N6 O9	C18 H36 N6 O9	[C18 H36 N6 O9, tgt=98.80, overall=98.80]	(481.26212, 50280.617)(482.26532, 11059.099)(483.26688, 2	C18 H36 N6 O9	FindByFormula	28 +	480.2545	9.44882
C18 H37 N O	C18 H37 N O	[C18 H37 N O, tgt=98.61, overall=98.61]	(284.295, 19211.723)(285.2954, 4018.5664)(286.3013, 636.4	C18 H37 N O	FindByFormula	5 +	283.2876	19.378275
C18 H37 N O2	C18 H37 N O2	[C18 H37 N O2, tgt=99.13, overall=99.13]	(300.28836, 26139.623)(301.292, 6753.2153)(302.29608, 111	C18 H37 N O2	FindByFormula	9 +	299.2816	19.656147
C18 H37 N O3	C18 H37 N O3	[C18 H37 N O3, tgt=33.32, overall=33.32]	(316.2855, 10786.851)(317.2881, 2440.4573)(318.2893, 367.	C18 H37 N O3	FindByFormula	22 +	315.2775	18.960228
C18 H37 N9 O S	C18 H37 N9 O S	[C18 H37 N9 O S, tgt=58.27, overall=58.27]	(428.2925, 5509.786)(429.2879, 1926.747)(430.28912, 430.8	C18 H37 N9 O S	FindByFormula	19 +	427.2862	21.802893
C18 H38 O10	C18 H38 O10	[C18 H38 O10, tgt=99.70, overall=99.70]	(415.25345, 3168.554)(416.2554, 722.0247)(417.25464, 188.	C18 H38 O10	FindByFormula	28 +	414.2464	8.73437
C18 H39 Cl N4 O3	C18 H39 Cl N4 O3	[C18 H39 Cl N4 O3, tgt=56.56, overall=56.56]	(395.27692, 16794.79)(396.27887, 3869.041)(397.27017, 710	C18 H39 Cl N4 O3	FindByFormula	21 +	394.268	21.724735
C18 H39 N	C18 H39 N	[C18 H39 N, tgt=99.32, overall=99.32]	(270.31512, 38489.562)(271.31738, 8344.665)(272.3231, 161	C18 H39 N	FindByFormula	11 +	269.307	21.115814
C18 H39 N O	C18 H39 N O	[C18 H39 N O, tgt=41.35, overall=41.35]	(286.31036, 6477.9)(287.3099, 1333.572)(288.31265, 453.69	C18 H39 N O	FindByFormula	25 +	285.3028	21.18289
C18 H39 N O3	C18 H39 N O3	[C18 H39 N O3, tgt=86.78, overall=86.78]	(318.3005, 22601.863)(319.3029, 4748.5625)(320.30377, 657	C18 H39 N O3	FindByFormula	28 +	317.2931	17.204626
C18 H39 N O4	C18 H39 N O4	[C18 H39 N O4, tgt=70.75, overall=70.75]	(334.29428, 3325.1516)(335.29544, 791.99585)(336.2963, 14	C18 H39 N O4	FindByFormula	12 +	333.2868	17.567514
C18 H39 N9 S	C18 H39 N9 S	[C18 H39 N9 S, tgt=17.28, overall=17.28]	(414.3138, 14570.0205)(415.30966, 4822.437)(416.30713, 95	C18 H39 N9 S	FindByFormula	22 +	413.3061	22.385607
C18 H39 O7 P	C18 H39 O7 P	[C18 H39 O7 P, tgt=78.29, overall=78.29]	(399.24985, 7254.3804)(400.2518, 1704.8815)(401.2443, 968	C18 H39 O7 P	FindByFormula	28 +	398.2437	21.4413
C18 H40 N2 O2 S2	C18 H40 N2 O2 S2	[C18 H40 N2 O2 S2, tgt=71.37, overall=71.37]	(381.25943, 4596.5024)(382.2628, 1105.0803)(383.26053, 53	C18 H40 N2 O2 S2	FindByFormula	24 +	380.2539	20.089962
C18 H40 N5 O2 P	C18 H40 N5 O2 P	[C18 H40 N5 O2 P, tgt=39.27, overall=39.27]	(390.29776, 4581.3945)(391.30026, 2221.4482)(392.3043, 70	C18 H40 N5 O2 P	FindByFormula	20 +	389.2937	22.20285
C18 H40 N5 P	C18 H40 N5 P	[C18 H40 N5 P, tgt=60.82, overall=60.82]	(358.30847, 18769.504)(359.30966, 6530.132)(360.31927, 24	C18 H40 N5 P	FindByFormula	22 +	357.3014	22.986853
C18 H41 Cl N6 O S	C18 H41 Cl N6 O S	[C18 H41 Cl N6 O S, tgt=55.93, overall=55.93]	(425.2839, 3472.4875)(426.2798, 1215.625)(427.2849, 2428.	C18 H41 Cl N6 O S	FindByFormula	16 +	424.2737	22.434223
C18 H41 N13 S	C18 H41 N13 S	[C18 H41 N13 S, tgt=58.53, overall=58.53]	(472.33945, 25873.213)(473.33972, 6553.0757)(474.34186, 1	C18 H41 N13 S	FindByFormula	27 +	471.3323	21.441084
C18 H41 N7	C18 H41 N7	[C18 H41 N7, tgt=77.56, overall=77.56]	(356.35114, 2955.5374)(357.3526, 920.43585)(358.35126, 21	C18 H41 N7	FindByFormula	15 +	355.3425	21.944525
C18 H42 N5 P	C18 H42 N5 P	[C18 H42 N5 P, tgt=96.67, overall=96.67]	(360.3244, 545996.0)(361.32785, 134809.64)(362.3311, 1720	C18 H42 N5 P	FindByFormula	17 +	359.3172	23.26016
C18 H43 Cl2 N13	C18 H43 Cl2 N13	[C18 H43 Cl2 N13, tgt=26.54, overall=26.54]	(512.3223, 1494.925)(513.326, 878.8907)(514.31506, 1388.7	C18 H43 Cl2 N13	FindByFormula	22 +	511.3134	22.348763
C18 H43 N7	C18 H43 N7	[C18 H43 N7, tgt=63.86, overall=63.86]	(358.36743, 3662.4207)(359.37082, 1022.79285)(360.36523,	C18 H43 N7	FindByFormula	21 +	357.3591	22.06254
C18 H43 N7 O	C18 H43 N7 O	[C18 H43 N7 O, tgt=63.32, overall=63.32]	(374.36145, 1792.0066)(375.36383, 578.35046)(376.36115, 1	C18 H43 N7 O	FindByFormula	22 +	373.3536	21.935926
C18 H46 N7 O2 P S2	C18 H46 N7 O2 P S2	[C18 H46 N7 O2 P S2, tgt=84.57, overall=84.57]	(488.29584, 5772.611)(489.29437, 1715.0874)(490.29517, 37	C18 H46 N7 O2 P S2	FindByFormula	18 +	487.2867	20.48997
C18 H48 N8 O2 S2	C18 H48 N8 O2 S2	[C18 H48 N8 O2 S2, tgt=68.12, overall=68.12]	(473.3431, 20941.342)(474.3443, 5928.3877)(475.3363, 1805	C18 H48 N8 O2 S2	FindByFormula	27 +	472.3385	22.303843
C19 H15 N2 O20 P3	C19 H15 N2 O20 P3	[C19 H15 N2 O20 P3, tgt=90.53, overall=90.53]	(684.9505, 3321.242)(685.941, 709.0916)(686.9422, 180.188	C19 H15 N2 O20 P3	FindByFormula	6 +	683.9422	20.832777
C19 H20 N10	C19 H20 N10	[C19 H20 N10, tgt=89.84, overall=89.84]	(389.1944, 12771.385)(390.19778, 2981.369)(391.20575, 448	C19 H20 N10	FindByFormula	28 +	388.1878	21.090849
C19 H21 N O3	C19 H21 N O3	[C19 H21 N O3, tgt=72.24, overall=72.24]	(312.1592, 806.99567)(313.15826, 355.5675)(314.15973, 107	C19 H21 N O3	FindByFormula	8 +	311.1528	19.52814
C19 H21 N9	C19 H21 N9	[C19 H21 N9, tgt=31.42, overall=31.42]	(376.2, 3734.621)(377.20316, 1350.9045)(378.20334, 243.14	C19 H21 N9	FindByFormula	18 +	375.1931	16.215292
C19 H22 Cl N5 O	C19 H22 Cl N5 O	[C19 H22 Cl N5 O, tgt=89.13, overall=89.13]	(372.15903, 3099.01)(373.16275, 861.36005)(374.15735, 112	C19 H22 Cl N5 O	FindByFormula	6 +	371.1523	9.545888
C19 H22 N10 P2	C19 H22 N10 P2	[C19 H22 N10 P2, tgt=94.19, overall=94.19]	(453.15704, 1406.9044)(454.15866, 385.18774)(455.15213, 3	C19 H22 N10 P2	FindByFormula	12 +	452.1526	22.539536
C19 H22 N6 O2	C19 H22 N6 O2	[C19 H22 N6 O2, tgt=82.48, overall=82.48]	(367.1886, 6495.5938)(368.1906, 1231.0538)(369.183, 166.8	C19 H22 N6 O2	FindByFormula	21 +	366.1818	22.596476
C19 H23 P	C19 H23 P	[C19 H23 P, tgt=52.99, overall=52.99]	(283.1639, 3667.1167)(284.15912, 1141.407)(285.15887, 130	C19 H23 P	FindByFormula	21 +	282.1551	18.645884
C19 H24 N10 O5	C19 H24 N10 O5	[C19 H24 N10 O5, tgt=81.64, overall=81.64]	(473.20065, 14000.151)(474.2051, 3130.109)(475.20718, 804	C19 H24 N10 O5	FindByFormula	28 +	472.1948	12.23018
C19 H24 N10 P2	C19 H24 N10 P2	[C19 H24 N10 P2, tgt=93.62, overall=93.62]	(455.17303, 2884.7551)(456.17603, 705.33954)(457.1784, 35	C19 H24 N10 P2	FindByFormula	22 +	454.165	22.740211
C19 H24 O4	C19 H24 O4	[C19 H24 O4, tgt=68.81, overall=68.81]	(317.17502, 3748.5251)(318.176, 655.0837)(319.16714, 40.9	C19 H24 O4	FindByFormula	28 +	316.1682	20.092325
C19 H25 N15	C19 H25 N15	[C19 H25 N15, tgt=68.22, overall=68.22]	(464.24844, 2104.302)(465.2456, 814.644)(466.24405, 304.3	C19 H25 N15	FindByFormula	5 +	463.2395	14.1
C19 H25 N5	C19 H25 N5	[C19 H25 N5, tgt=71.22, overall=71.22]	(324.21954, 4227.9165)(325.21875, 1303.6241)(326.21957, 1	C19 H25 N5	FindByFormula	27 +	323.212	20.715614
C19 H25 N6 P3	C19 H25 N6 P3	[C19 H25 N6 P3, tgt=91.50, overall=91.50]	(431.14163, 3551.4585)(432.14435, 707.40765)(433.14493, 1	C19 H25 N6 P3	FindByFormula	22 +	430.1342	2.0483391
C19 H27 N3 O P2	C19 H27 N3 O P2	[C19 H27 N3 O P2, tgt=95.57, overall=95.57]	(376.172, 1500.5437)(377.17273, 330.61737)(378.17245, 123	C19 H27 N3 O P2	FindByFormula	19 +	375.1638	9.585456
C19 H28 N6 O	C19 H28 N6 O	[C19 H28 N6 O, tgt=89.45, overall=89.45]	(357.2393, 5431.137)(358.23947, 1612.033)(359.23975, 540.	C19 H28 N6 O	FindByFormula	23 +	356.2292	20.789928
C19 H28 N6 O2	C19 H28 N6 O2	[C19 H28 N6 O2, tgt=76.50, overall=76.50]	(373.23447, 2420.8823)(374.23633, 674.645)(375.2311, 400.	C19 H28 N6 O2	FindByFormula	9 +	372.2254	21.205221
C19 H29 N3 O P2	C19 H29 N3 O P2	[C19 H29 N3 O P2, tgt=98.18, overall=98.18]	(378.18567, 1413.217)(379.18942, 574.2943)(380.18985, 116	C19 H29 N3 O P2	FindByFormula	10 +	377.1822	11.699418
C19 H29 O P3	C19 H29 O P3	[C19 H29 O P3, tgt=96.37, overall=96.37]	(367.15097, 4600.2114)(368.15427, 986.4055)(369.15524, 19	C19 H29 O P3	FindByFormula	11 +	366.1429	2.2888296
C19 H30 N6 O	C19 H30 N6 O	[C19 H30 N6 O, tgt=80.66, overall=80.66]	(359.25296, 2791.3225)(360.25543, 706.30005)(361.25644, 6	C19 H30 N6 O	FindByFormula	8 +	358.2499	22.426483
C19 H30 O4 P2	C19 H30 O4 P2	[C19 H30 O4 P2, tgt=97.17, overall=97.17]	(385.16974, 2935.0842)(386.16763, 712.4079)(387.1793, 196	C19 H30 O4 P2	FindByFormula	16 +	384.163	22.365778
C19 H34 N6 O2 S	C19 H34 N6 O2 S	[C19 H34 N6 O2 S, tgt=50.24, overall=50.24]	(411.25226, 10957.76)(412.2556, 3125.549)(413.26318, 2813	C19 H34 N6 O2 S	FindByFormula	11 +	410.2445	22.168913
C19 H35 N O4	C19 H35 N O4	[C19 H35 N O4, tgt=54.47, overall=54.47]	(342.2635, 1457.3462)(343.26288, 485.82568)(344.2649, 91.	C19 H35 N O4	FindByFormula	8 +	341.2542	16.856512
C19 H35 O P S	C19 H35 O P S	[C19 H35 O P S, tgt=89.74, overall=89.74]	(343.22235, 17178.05)(344.22702, 3930.557)(345.22253, 123	C19 H35 O P S	FindByFormula	26 +	342.2173	21.768127
C19 H36 N2 O S2	C19 H36 N2 O S2	[C19 H36 N2 O S2, tgt=90.03, overall=90.03]	(373.2323, 2537.1936)(374.23627, 720.93494)(375.22708, 26	C19 H36 N2 O S2	FindByFormula	11 +	372.2288	20.809021
C19 H36 S5	C19 H36 S5	[C19 H36 S5, tgt=89.41, overall=89.41]	(425.151, 1941.5881)(426.15314, 414.66238)(427.14575, 712	C19 H36 S5	FindByFormula	22 +	424.143	18.996483
C19 H37 N O4	C19 H37 N O4	[C19 H37 N O4, tgt=86.80, overall=86.80]	(344.27902, 2733.3293)(345.27966, 680.1025)(346.27933, 29	C19 H37 N O4	FindByFormula	16 +	343.2695	17.99751
C19 H37 O P S2	C19 H37 O P S2	[C19 H37 O P S2, tgt=54.43, overall=54.43]	(377.20908, 5607.8506)(378.21466, 1066.2948)(379.20972, 2	C19 H37 O P S2	FindByFormula	23 +	376.2	21.216402
C19 H37 P S	C19 H37 P S	[C19 H37 P S, tgt=30.65, overall=30.65]	(329.2435, 3109.0835)(330.24564, 699.926)(331.23834, 838.	C19 H37 P S	FindByFormula	23 +	328.2369	22.407274
C19 H38 N2 O3	C19 H38 N2 O3	[C19 H38 N2 O3, tgt=95.61, overall=95.61]	(343.29468, 3744.144)(344.2969, 854.35895)(345.2947, 216.	C19 H38 N2 O3	FindByFormula	28 +	342.288	19.011402
C19 H39 N4 O4 P	C19 H39 N4 O4 P	[C19 H39 N4 O4 P, tgt=89.95, overall=89.95]	(419.27664, 54076.055)(420.28088, 13371.493)(421.2877, 68	C19 H39 N4 O4 P	FindByFormula	28 +	418.2703	22.131775
C19 H39 N7 O2	C19 H39 N7 O2	[C19 H39 N7 O2, tgt=80.69, overall=80.69]	(398.32513, 5689.4106)(399.32388, 1647.7529)(400.3264, 33	C19 H39 N7 O2	FindByFormula	27 +	397.3181	20.526169
C19 H40 O2 S	C19 H40 O2 S	[C19 H40 O2 S, tgt=80.30, overall=80.30]	(333.27893, 3127.397)(334.28397, 853.9822)(371.23883, 762	C19 H40 O2 S	FindByFormula	18 +	332.2745	22.602531
C19 H41 N	C19 H41 N	[C19 H41 N, tgt=84.32, overall=84.32]	(284.33087, 1823.1581)(285.33292, 432.6289)(286.3315, 46.	C19 H41 N	FindByFormula	28 +	283.3232	20.961102
C19 H41 N3 O3	C19 H41 N3 O3	[C19 H41 N3 O3, tgt=68.20, overall=68.20]	(360.32147, 415448.72)(361.32312, 115986.336)(362.32816,	C19 H41 N3 O3	FindByFormula	18 +	359.3175	23.17075
C19 H41 N3 O5	C19 H41 N3 O5	[C19 H41 N3 O5, tgt=34.22, overall=34.22]	(392.3124, 3415.9011)(393.30704, 962.6387)(394.30252, 119	C19 H41 N3 O5	FindByFormula	24 +	391.3039	21.790808
C19 H43 N3 O5	C19 H43 N3 O5	[C19 H43 N3 O5, tgt=82.87, overall=82.87]	(394.3283, 6904.172)(395.32452, 1752.3372)(396.3282, 428.	C19 H43 N3 O5	FindByFormula	26 +	393.32	21.96204
C19 H44 N2 P2 S	C19 H44 N2 P2 S	[C19 H44 N2 P2 S, tgt=32.51, overall=32.51]	(395.27505, 8780.045)(396.27682, 2000.6487)(397.27267, 14	C19 H44 N2 P2 S	FindByFormula	23 +	394.2702	21.758654
C19 H44 N4 S2	C19 H44 N4 S2	[C19 H44 N4 S2, tgt=86.40, overall=86.40]	(393.30844, 19176.146)(394.31094, 4633.7026)(395.30615, 7	C19 H44 N4 S2	FindByFormula	28 +	392.3009	21.214914
C19 H45 N7	C19 H45 N7	[C19 H45 N7, tgt=81.84, overall=81.84]	(372.38126, 2034.2322)(373.38315, 667.94214)(374.37994, 1	C19 H45 N7	FindByFormula	18 +	371.375	22.18734
C19 H9 P	C19 H9 P	[C19 H9 P, tgt=94.48, overall=94.48]	(269.05063, 3198.1538)(270.05368, 570.6825)(271.05048, 36	C19 H9 P	FindByFormula	8 +	268.0434	15.715505
C20 H16 N4 O	C20 H16 N4 O	[C20 H16 N4 O, tgt=78.42, overall=78.42]	(329.14017, 1884.5494)(330.1425, 431.0864)(331.1404, 123.	C20 H16 N4 O	FindByFormula	28 +	328.1333	8.468162
C20 H19 N2 P	C20 H19 N2 P	[C20 H19 N2 P, tgt=84.22, overall=84.22]	(319.13556, 2879.6443)(320.14, 552.30084)(321.13086, 439.	C20 H19 N2 P	FindByFormula	24 +	318.1297	5.867054
C20 H23 N S	C20 H23 N S	[C20 H23 N S, tgt=76.02, overall=76.02]	(310.1633, 2680.805)(311.1553, 853.445)(312.15976, 78.02)(	C20 H23 N S	FindByFormula	6 +	309.1533	12.116223
C20 H23 O P	C20 H23 O P	[C20 H23 O P, tgt=52.02, overall=52.02]	(311.15536, 45215.145)(312.15637, 9682.121)(313.1587, 144	C20 H23 O P	FindByFormula	8 +	310.1483	11.081168
C20 H26 O3 P2	C20 H26 O3 P2	[C20 H26 O3 P2, tgt=94.18, overall=94.18]	(377.14383, 2229.6294)(378.14822, 412.10153)(379.13943, 9	C20 H26 O3 P2	FindByFormula	26 +	376.135	6.8039193
C20 H27 N4 P	C20 H27 N4 P	[C20 H27 N4 P, tgt=86.88, overall=86.88]	(355.2097, 7332.008)(356.2129, 1632.8707)(357.2021, 1271.	C20 H27 N4 P	FindByFormula	15 +	354.1985	21.790653
C20 H28 O2 P2	C20 H28 O2 P2	[C20 H28 O2 P2, tgt=83.28, overall=83.28]	(363.1631, 3653.9817)(364.16833, 701.56525)(365.15817, 29	C20 H28 O2 P2	FindByFormula	27 +	362.1555	6.90953
C20 H29 N4 O5 P	C20 H29 N4 O5 P	[C20 H29 N4 O5 P, tgt=86.95, overall=86.95]	(437.194, 31026.72)(438.19742, 8286.605)(439.2065, 2051.7	C20 H29 N4 O5 P	FindByFormula	26 +	436.1867	19.695414
C20 H30 N8 O P4	C20 H30 N8 O P4	[C20 H30 N8 O P4, tgt=95.27, overall=95.27]	(523.15765, 2987.769)(524.16144, 818.71954)(525.1614, 188	C20 H30 N8 O P4	FindByFormula	23 +	522.1512	22.700928
C20 H32 N12	C20 H32 N12	[C20 H32 N12, tgt=67.84, overall=67.84]	(441.2942, 2355.2021)(442.2937, 840.3144)(443.29715, 204.	C20 H32 N12	FindByFormula	20 +	440.2911	22.461704
C20 H32 O10	C20 H32 O10	[C20 H32 O10, tgt=57.44, overall=57.44]	(433.20786, 3569.0466)(434.20886, 828.5232)(435.20602, 32	C20 H32 O10	FindByFormula	16 +	432.2003	14.143953
C20 H32 O3	C20 H32 O3	[C20 H32 O3, tgt=62.46, overall=62.46]	(321.24094, 18655.756)(322.24603, 3973.4995)(323.24625, 4	C20 H32 O3	FindByFormula	28 +	320.2331	21.768877
C20 H33 N4 O2 P3	C20 H33 N4 O2 P3	[C20 H33 N4 O2 P3, tgt=98.12, overall=98.12]	(455.18924, 585138.2)(456.19272, 132724.19)(457.19577, 25	C20 H33 N4 O2 P3	FindByFormula	7 +	454.1824	14.09369
C20 H34 N2 S3	C20 H34 N2 S3	[C20 H34 N2 S3, tgt=82.34, overall=82.34]	(399.19644, 4418.383)(400.19775, 1019.63257)(401.1956, 77	C20 H34 N2 S3	FindByFormula	24 +	398.1883	22.651194
C20 H35 N4 O3 P3	C20 H35 N4 O3 P3	[C20 H35 N4 O3 P3, tgt=89.54, overall=89.54]	(473.19995, 4807.0767)(474.20508, 1170.6534)(475.2099, 40	C20 H35 N4 O3 P3	FindByFormula	6 +	472.1924	11.807282
C20 H35 N4 P3	C20 H35 N4 P3	[C20 H35 N4 P3, tgt=96.63, overall=96.63]	(425.21555, 17402.768)(426.2197, 4073.5547)(427.2211, 840	C20 H35 N4 P3	FindByFormula	28 +	424.2088	21.84982
C20 H35 N7	C20 H35 N7	[C20 H35 N7, tgt=78.57, overall=78.57]	(374.30328, 42844.055)(375.30518, 11381.093)(376.29718, 1	C20 H35 N7	FindByFormula	26 +	373.2962	22.388618
C20 H36 N2 S	C20 H36 N2 S	[C20 H36 N2 S, tgt=81.70, overall=81.70]	(337.26663, 9262.219)(338.26865, 2032.6442)(339.258, 1087	C20 H36 N2 S	FindByFormula	23 +	336.2597	22.58425
C20 H36 O4	C20 H36 O4	[C20 H36 O4, tgt=41.34, overall=41.34]	(341.26627, 36261.836)(342.26974, 7332.0186)(343.2653, 10	C20 H36 O4	FindByFormula	23 +	340.2589	22.322205
C20 H37 Cl N6 O3	C20 H37 Cl N6 O3	[C20 H37 Cl N6 O3, tgt=77.49, overall=77.49]	(445.26794, 1476.163)(446.27112, 469.6492)(447.26367, 975	C20 H37 Cl N6 O3	FindByFormula	13 +	444.2584	22.600882
C20 H37 N O4	C20 H37 N O4	[C20 H37 N O4, tgt=79.39, overall=79.39]	(356.2786, 1848.3143)(357.2784, 511.18857)(358.27805, 107	C20 H37 N O4	FindByFormula	8 +	355.2703	17.910961
C20 H37 N4 O2 P3	C20 H37 N4 O2 P3	[C20 H37 N4 O2 P3, tgt=38.37, overall=38.37]	(459.22006, 5843.0435)(460.22168, 1382.3276)(461.22824, 5	C20 H37 N4 O2 P3	FindByFormula	9 +	458.2133	13.036905
C20 H37 N4 O3 P	C20 H37 N4 O3 P	[C20 H37 N4 O3 P, tgt=98.32, overall=98.32]	(413.2672, 367649.25)(414.2706, 107564.68)(415.27216, 172	C20 H37 N4 O3 P	FindByFormula	21 +	412.2597	23.140995
C20 H37 N7	C20 H37 N7	[C20 H37 N7, tgt=34.59, overall=34.59]	(376.31818, 26687.91)(377.3198, 7778.895)(378.32187, 1065	C20 H37 N7	FindByFormula	26 +	375.311	22.370653
C20 H37 O P S	C20 H37 O P S	[C20 H37 O P S, tgt=79.31, overall=79.31]	(357.23813, 5159.954)(358.23752, 1390.681)(359.23947, 428	C20 H37 O P S	FindByFormula	21 +	356.2293	22.285252
C20 H38 N6 O5	C20 H38 N6 O5	[C20 H38 N6 O5, tgt=29.86, overall=29.86]	(443.29626, 7379.251)(444.2993, 2028.6836)(445.29837, 820	C20 H38 N6 O5	FindByFormula	19 +	442.2883	21.988895
C20 H39 Cl N10	C20 H39 Cl N10	[C20 H39 Cl N10, tgt=43.10, overall=43.10]	(455.31146, 4588.7075)(456.31226, 1379.3527)(457.3047, 15	C20 H39 Cl N10	FindByFormula	15 +	454.3012	22.52622
C20 H39 N O2 P2	C20 H39 N O2 P2	[C20 H39 N O2 P2, tgt=88.52, overall=88.52]	(388.25388, 2880.3022)(389.25494, 619.0731)(390.25275, 17	C20 H39 N O2 P2	FindByFormula	28 +	387.2456	7.9325404
C20 H39 N O4	C20 H39 N O4	[C20 H39 N O4, tgt=95.83, overall=95.83]	(358.29434, 1030.6061)(359.29352, 335.57846)(360.298, 74.	C20 H39 N O4	FindByFormula	15 +	357.2865	18.826668
C20 H40 N6 O10	C20 H40 N6 O10	[C20 H40 N6 O10, tgt=99.72, overall=99.72]	(525.2882, 31070.7)(526.2912, 7729.3687)(527.29236, 1778.	C20 H40 N6 O10	FindByFormula	28 +	524.281	10.091773
C20 H41 N O	C20 H41 N O	[C20 H41 N O, tgt=20.43, overall=20.43]	(312.32605, 5663.331)(313.3281, 1530.5813)(314.32977, 533	C20 H41 N O	FindByFormula	9 +	311.319	21.196806
C20 H41 N O2	C20 H41 N O2	[C20 H41 N O2, tgt=99.01, overall=99.01]	(328.3204, 7873.981)(329.32278, 1891.2837)(330.3224, 370.	C20 H41 N O2	FindByFormula	19 +	327.3118	21.50976
C20 H41 N O3	C20 H41 N O3	[C20 H41 N O3, tgt=86.26, overall=86.26]	(344.31738, 3984.5044)(345.31833, 1075.78)(346.31775, 237	C20 H41 N O3	FindByFormula	21 +	343.3085	20.667004
C20 H42 N8 O4 P4	C20 H42 N8 O4 P4	[C20 H42 N8 O4 P4, tgt=97.18, overall=97.18]	(583.23676, 3260.1084)(584.2371, 754.0267)(585.246, 180.6	C20 H42 N8 O4 P4	FindByFormula	6 +	582.2281	20.328815
C20 H42 O11	C20 H42 O11	[C20 H42 O11, tgt=99.47, overall=99.47]	(459.27737, 5486.0283)(460.27966, 1512.8914)(461.27908, 3	C20 H42 O11	FindByFormula	27 +	458.2727	9.448664
C20 H42 O7 P4	C20 H42 O7 P4	[C20 H42 O7 P4, tgt=95.52, overall=95.52]	(519.1959, 12323.753)(520.19977, 3315.6387)(521.2084, 778	C20 H42 O7 P4	FindByFormula	7 +	518.1886	13.706086
C20 H43 N O	C20 H43 N O	[C20 H43 N O, tgt=87.82, overall=87.82]	(314.34088, 2315.898)(315.3437, 799.58)(316.3449, 156.932	C20 H43 N O	FindByFormula	10 +	313.3334	21.768137
C20 H43 N O3	C20 H43 N O3	[C20 H43 N O3, tgt=67.60, overall=67.60]	(346.33057, 2206.2861)(347.33054, 762.07684)(348.3289, 12	C20 H43 N O3	FindByFormula	18 +	345.3232	21.512474
C20 H43 N O4	C20 H43 N O4	[C20 H43 N O4, tgt=62.71, overall=62.71]	(362.32626, 2800.8245)(363.32773, 714.55286)(364.32855, 1	C20 H43 N O4	FindByFormula	28 +	361.3185	17.336535
C20 H44 Cl N3	C20 H44 Cl N3	[C20 H44 Cl N3, tgt=65.18, overall=65.18]	(362.32425, 797.9167)(363.32745, 449.13998)(364.33197, 61	C20 H44 Cl N3	FindByFormula	3 +	361.319	20.735518
C20 H45 N3 O4 P2	C20 H45 N3 O4 P2	[C20 H45 N3 O4 P2, tgt=82.60, overall=82.60]	(454.2941, 1511.8962)(455.29477, 858.00494)(456.29666, 25	C20 H45 N3 O4 P2	FindByFormula	16 +	453.2861	22.266142
C20 H45 N3 S2	C20 H45 N3 S2	[C20 H45 N3 S2, tgt=19.18, overall=19.18]	(392.31216, 3174.0422)(393.31012, 1595.1809)(394.3104, 40	C20 H45 N3 S2	FindByFormula	19 +	391.3066	22.626785
C20 H46 N4 O P2	C20 H46 N4 O P2	[C20 H46 N4 O P2, tgt=50.85, overall=50.85]	(421.3208, 3160.3347)(422.3273, 886.78)(423.33487, 79.686)	C20 H46 N4 O P2	FindByFormula	15 +	420.3106	22.147524
C20 H47 N7 O2 S	C20 H47 N7 O2 S	[C20 H47 N7 O2 S, tgt=75.30, overall=75.30]	(450.35327, 840.8908)(451.35266, 297.46887)(452.35074, 10	C20 H47 N7 O2 S	FindByFormula	26 +	449.3493	21.44095
C20 H50 N22 P4	C20 H50 N22 P4	[C20 H50 N22 P4, tgt=77.89, overall=77.89]	(723.36316, 2823.467)(724.3587, 545.0817)(725.35986, 129.	C20 H50 N22 P4	FindByFormula	7 +	722.3518	13.006128
C20 H53 Cl N13 O2 P S2	C20 H53 Cl N13 O2 P S2	[C20 H53 Cl N13 O2 P S2, tgt=71.42, overall=71.42]	(638.3368, 5726.572)(639.33954, 2687.6797)(640.3231, 3117	C20 H53 Cl N13 O2 P S2	FindByFormula	9 +	637.3286	22.593637
C20 H8 S2	C20 H8 S2	[C20 H8 S2, tgt=66.83, overall=66.83]	(313.01352, 14759.246)(314.01715, 3189.987)(315.0163, 276	C20 H8 S2	FindByFormula	24 +	312.0074	1.1926306
C20 H9 N O2	C20 H9 N O2	[C20 H9 N O2, tgt=88.17, overall=88.17]	(296.0722, 5446.1616)(297.07706, 1070.3182)(298.0748, 361	C20 H9 N O2	FindByFormula	6 +	295.0653	12.026507
C21 H16 N10	C21 H16 N10	[C21 H16 N10, tgt=66.29, overall=66.29]	(409.16293, 358702.9)(410.16602, 86324.08)(411.16916, 146	C21 H16 N10	FindByFormula	28 +	408.1557	16.701239
C21 H17 N	C21 H17 N	[C21 H17 N, tgt=80.43, overall=80.43]	(284.14294, 2851.98)(285.1453, 705.2463)(286.145, 136.451	C21 H17 N	FindByFormula	8 +	283.1338	20.262638
C21 H18 O5	C21 H18 O5	[C21 H18 O5, tgt=85.74, overall=85.74]	(351.12137, 2423.8318)(352.126, 527.7183)(353.13043, 62.9	C21 H18 O5	FindByFormula	6 +	350.1143	16.971045
C21 H19 N O3	C21 H19 N O3	[C21 H19 N O3, tgt=64.52, overall=64.52]	(334.14447, 1948.3601)(335.1428, 521.75)(336.1392, 129.09	C21 H19 N O3	FindByFormula	8 +	333.1344	19.845999
C21 H20 N8 P4	C21 H20 N8 P4	[C21 H20 N8 P4, tgt=51.24, overall=51.24]	(509.08478, 350.92572)(510.0842, 126.109276)(547.04407, 8	C21 H20 N8 P4	FindByFormula	14 +	508.0768	16.434662
C21 H21 N5	C21 H21 N5	[C21 H21 N5, tgt=73.27, overall=73.27]	(344.1863, 2808.5764)(345.1892, 828.07104)(346.18484, 167	C21 H21 N5	FindByFormula	21 +	343.18	20.727072
C21 H23 N O2	C21 H23 N O2	[C21 H23 N O2, tgt=82.35, overall=82.35]	(322.18063, 3942.0886)(323.17938, 1174.6416)(324.18015, 1	C21 H23 N O2	FindByFormula	12 +	321.1725	12.087467
C21 H23 N2 O9 P S2	C21 H23 N2 O9 P S2	[C21 H23 N2 O9 P S2, tgt=66.65, overall=66.65]	(543.06635, 2297.6167)(544.06866, 617.7495)(545.0682, 361	C21 H23 N2 O9 P S2	FindByFormula	22 +	542.0586	1.3691897
C21 H24 N4 O4	C21 H24 N4 O4	[C21 H24 N4 O4, tgt=78.73, overall=78.73]	(397.189, 3327.2964)(398.19336, 266.4382)(435.14752, 60.2	C21 H24 N4 O4	FindByFormula	27 +	396.1814	17.201393
C21 H25 N11	C21 H25 N11	[C21 H25 N11, tgt=55.79, overall=55.79]	(432.23746, 5047.9077)(433.23883, 1778.9874)(434.24014, 4	C21 H25 N11	FindByFormula	28 +	431.2305	17.24263
C21 H25 O P	C21 H25 O P	[C21 H25 O P, tgt=75.73, overall=75.73]	(325.17078, 58831.625)(326.17273, 13217.306)(327.1703, 19	C21 H25 O P	FindByFormula	11 +	324.1643	11.009614
C21 H26 S2	C21 H26 S2	[C21 H26 S2, tgt=79.74, overall=79.74]	(343.15576, 3991.0198)(344.159, 914.0204)(345.15704, 627.	C21 H26 S2	FindByFormula	28 +	342.1477	12.559182
C21 H27 N O4	C21 H27 N O4	[C21 H27 N O4, tgt=59.52, overall=59.52]	(358.20166, 4080.0366)(359.2032, 1406.7794)(360.2043, 267	C21 H27 N O4	FindByFormula	16 +	357.1942	20.727041
C21 H28 N10 P6	C21 H28 N10 P6	[C21 H28 N10 P6, tgt=69.46, overall=69.46]	(607.1011, 1787.5199)(608.1001, 583.52167)(609.1028, 190.	C21 H28 N10 P6	FindByFormula	23 +	606.096	22.463522
C21 H28 N11 P	C21 H28 N11 P	[C21 H28 N11 P, tgt=40.41, overall=40.41]	(466.23154, 909.0543)(467.23453, 274.98856)(468.2277, 66.	C21 H28 N11 P	FindByFormula	7 +	465.2221	2.6523168
C21 H29 O4 P	C21 H29 O4 P	[C21 H29 O4 P, tgt=96.75, overall=96.75]	(377.18768, 24099.271)(378.19122, 5058.001)(379.19113, 77	C21 H29 O4 P	FindByFormula	16 +	376.18	21.792387
C21 H30 N2 O3	C21 H30 N2 O3	[C21 H30 N2 O3, tgt=61.89, overall=61.89]	(359.23102, 2806.2898)(360.23422, 760.00555)(361.23294, 1	C21 H30 N2 O3	FindByFormula	11 +	358.2243	17.789465
C21 H30 O3	C21 H30 O3	[C21 H30 O3, tgt=46.79, overall=46.79]	(331.22592, 11482.873)(332.2297, 2455.2847)(333.22913, 12	C21 H30 O3	FindByFormula	28 +	330.2184	22.154955
C21 H30 O5	C21 H30 O5	[C21 H30 O5, tgt=95.65, overall=95.65]	(363.21542, 945.86005)(364.21536, 310.94455)(365.21265, 2	C21 H30 O5	FindByFormula	19 +	362.2096	13.769689
C21 H30 S2	C21 H30 S2	[C21 H30 S2, tgt=70.01, overall=70.01]	(347.1844, 3211.4963)(348.18774, 675.9614)(349.18936, 69.	C21 H30 S2	FindByFormula	27 +	346.1772	18.998055
C21 H31 N3 O P2	C21 H31 N3 O P2	[C21 H31 N3 O P2, tgt=98.51, overall=98.51]	(404.20255, 1952.3551)(405.20398, 530.22205)(406.20898, 1	C21 H31 N3 O P2	FindByFormula	10 +	403.195	13.951529
C21 H32 Cl N2 O P	C21 H32 Cl N2 O P	[C21 H32 Cl N2 O P, tgt=62.27, overall=62.27]	(395.2005, 4476.3223)(396.20166, 989.5556)(397.19492, 50.	C21 H32 Cl N2 O P	FindByFormula	16 +	394.1901	21.219172
C21 H32 N6 O2	C21 H32 N6 O2	[C21 H32 N6 O2, tgt=74.66, overall=74.66]	(401.26767, 12803.1)(402.2686, 4951.517)(403.27518, 1502.	C21 H32 N6 O2	FindByFormula	23 +	400.2606	22.486109
C21 H32 O3	C21 H32 O3	[C21 H32 O3, tgt=86.45, overall=86.45]	(333.2413, 4242.0503)(334.24408, 890.94214)(335.25256, 55	C21 H32 O3	FindByFormula	15 +	332.2353	22.17484
C21 H33 N2 P3	C21 H33 N2 P3	[C21 H33 N2 P3, tgt=92.91, overall=92.91]	(407.1926, 2637.7166)(408.1948, 680.425)(409.18967, 181.6	C21 H33 N2 P3	FindByFormula	7 +	406.1842	6.155378
C21 H33 N3 O P2	C21 H33 N3 O P2	[C21 H33 N3 O P2, tgt=93.76, overall=93.76]	(406.2162, 2284.4822)(407.21744, 1106.3777)(408.21982, 29	C21 H33 N3 O P2	FindByFormula	21 +	405.2103	15.433974
C21 H33 N3 O3	C21 H33 N3 O3	[C21 H33 N3 O3, tgt=75.39, overall=75.39]	(376.25995, 3578.8306)(377.25903, 999.2129)(378.25656, 23	C21 H33 N3 O3	FindByFormula	24 +	375.2524	17.273245

C21 H34 O6	C21 H34 O6	[C21 H34 O6, tgt=30.57, overall=30.57]	(383.24237, 6730.373)(384.2477, 1610.1139)(385.2429, 1546	C21 H34 O6	FindByFormula	16	+	382.2335	21.130386
C21 H34 S5	C21 H34 S5	[C21 H34 S5, tgt=90.88, overall=90.88]	(447.13522, 1288.5396)(448.13885, 365.15308)(449.13116, 6	C21 H34 S5	FindByFormula	23	+	446.127	3.6152515
C21 H36 O9 P2 S	C21 H36 O9 P2 S	[C21 H36 O9 P2 S, tgt=49.33, overall=49.33]	(527.16156, 4287.808)(528.1667, 1011.1862)(529.1657, 314.	C21 H36 O9 P2 S	FindByFormula	22	+	526.157	0.7275024
C21 H37 N	C21 H37 N	[C21 H37 N, tgt=68.59, overall=68.59]	(304.29977, 38810.754)(305.3011, 9131.721)(306.30338, 107	C21 H37 N	FindByFormula	28	+	303.2919	18.71229
C21 H37 N4 O3 P3	C21 H37 N4 O3 P3	[C21 H37 N4 O3 P3, tgt=72.03, overall=72.03]	(487.21765, 4342.8213)(488.21835, 1092.9863)(489.22626, 6	C21 H37 N4 O3 P3	FindByFormula	17	+	486.2113	14.094331
C21 H37 N8 P3	C21 H37 N8 P3	[C21 H37 N8 P3, tgt=82.10, overall=82.10]	(495.24124, 1685.8868)(496.2436, 489.44965)(497.2369, 370	C21 H37 N8 P3	FindByFormula	27	+	494.234	9.356114
C21 H38 N2 O S3	C21 H38 N2 O S3	[C21 H38 N2 O S3, tgt=89.46, overall=89.46]	(431.2236, 3336.9412)(432.2265, 854.0672)(433.22513, 670.	C21 H38 N2 O S3	FindByFormula	7	+	430.218	21.53188
C21 H38 N6 O4 S2	C21 H38 N6 O4 S2	[C21 H38 N6 O4 S2, tgt=43.13, overall=43.13]	(503.2455, 4769.105)(504.24698, 1415.361)(505.25278, 669.	C21 H38 N6 O4 S2	FindByFormula	11	+	502.2404	13.615742
C21 H39 N O4	C21 H39 N O4	[C21 H39 N O4, tgt=90.31, overall=90.31]	(370.29547, 3032.4268)(371.29492, 1001.3286)(372.29825, 2	C21 H39 N O4	FindByFormula	9	+	369.2867	18.965944
C21 H39 N3 O3 S2	C21 H39 N3 O3 S2	[C21 H39 N3 O3 S2, tgt=61.13, overall=61.13]	(446.25113, 5224.9395)(447.25186, 1724.5392)(448.24332, 7	C21 H39 N3 O3 S2	FindByFormula	24	+	445.2429	16.433338
C21 H39 N3 S	C21 H39 N3 S	[C21 H39 N3 S, tgt=81.21, overall=81.21]	(366.29608, 5980.855)(367.29037, 1933.6001)(368.29605, 36	C21 H39 N3 S	FindByFormula	18	+	365.285	22.386663
C21 H40 N17 P	C21 H40 N17 P	[C21 H40 N17 P, tgt=89.69, overall=89.69]	(562.34656, 2528.2444)(563.3459, 1121.1166)(564.34045, 28	C21 H40 N17 P	FindByFormula	8	+	561.3348	21.196547
C21 H40 N2 O S	C21 H40 N2 O S	[C21 H40 N2 O S, tgt=44.22, overall=44.22]	(369.2941, 16263.687)(370.29648, 3902.1873)(371.2899, 488	C21 H40 N2 O S	FindByFormula	16	+	368.2887	22.796227
C21 H40 N2 O2 S	C21 H40 N2 O2 S	[C21 H40 N2 O2 S, tgt=38.41, overall=38.41]	(385.2883, 8804.9)(386.29025, 2193.3906)(387.2885, 549.33	C21 H40 N2 O2 S	FindByFormula	26	+	384.2841	22.272686
C21 H40 N2 O3 S	C21 H40 N2 O3 S	[C21 H40 N2 O3 S, tgt=65.04, overall=65.04]	(401.28354, 4983.7207)(402.2859, 1277.5664)(403.27692, 34	C21 H40 N2 O3 S	FindByFormula	24	+	400.2772	21.63189
C21 H41 N O4	C21 H41 N O4	[C21 H41 N O4, tgt=92.74, overall=92.74]	(372.31036, 2803.5566)(373.31183, 790.868)(374.31525, 264	C21 H41 N O4	FindByFormula	25	+	371.3019	19.977531
C21 H41 N2 O3 P S	C21 H41 N2 O3 P S	[C21 H41 N2 O3 P S, tgt=66.57, overall=66.57]	(433.2637, 8702.857)(434.2668, 2136.1113)(435.2657, 508.8	C21 H41 N2 O3 P S	FindByFormula	27	+	432.2579	19.014357
C21 H41 P S	C21 H41 P S	[C21 H41 P S, tgt=86.30, overall=86.30]	(357.27213, 2273.3071)(358.27585, 519.32855)(359.26044, 1	C21 H41 P S	FindByFormula	11	+	356.2665	21.58559
C21 H42 Cl N	C21 H42 Cl N	[C21 H42 Cl N, tgt=31.69, overall=31.69]	(344.31006, 4487.727)(345.3113, 1369.4811)(346.30264, 236	C21 H42 Cl N	FindByFormula	12	+	343.3035	21.37147
C21 H42 N5 O3 P3	C21 H42 N5 O3 P3	[C21 H42 N5 O3 P3, tgt=42.88, overall=42.88]	(506.2529, 176.99)(544.2133, 348.97)(545.2241, 1371.65)(52	C21 H42 N5 O3 P3	FindByFormula	1	+	505.2547	21.471
C21 H42 N5 P3	C21 H42 N5 P3	[C21 H42 N5 P3, tgt=97.99, overall=97.99]	(458.27222, 5600.759)(459.2753, 1417.293)(460.2742, 268.1	C21 H42 N5 P3	FindByFormula	7	+	457.265	2.1585774
C21 H43 N O	C21 H43 N O	[C21 H43 N O, tgt=89.68, overall=89.68]	(326.34198, 24249.84)(327.34406, 5853.688)(328.3336, 929.	C21 H43 N O	FindByFormula	5	+	325.3341	21.194342
C21 H43 N O3	C21 H43 N O3	[C21 H43 N O3, tgt=70.30, overall=70.30]	(358.33215, 629.2818)(359.33228, 268.17902)(360.33063, 47	C21 H43 N O3	FindByFormula	11	+	357.3229	21.27722
C21 H43 N4 O5 P	C21 H43 N4 O5 P	[C21 H43 N4 O5 P, tgt=97.61, overall=97.61]	(463.303, 80458.75)(464.30667, 21615.309)(465.31052, 4465	C21 H43 N4 O5 P	FindByFormula	28	+	462.2961	22.163181
C21 H43 N4 P S	C21 H43 N4 P S	[C21 H43 N4 P S, tgt=44.79, overall=44.79]	(415.30197, 6862.648)(416.30383, 1859.0565)(417.29742, 27	C21 H43 N4 P S	FindByFormula	24	+	414.2966	22.03438
C21 H43 N5 O10 S	C21 H43 N5 O10 S	[C21 H43 N5 O10 S, tgt=91.35, overall=91.35]	(558.27936, 27810.098)(559.284, 7718.005)(560.2857, 1737.	C21 H43 N5 O10 S	FindByFormula	27	+	557.2727	21.588364
C21 H44 N6 S2	C21 H44 N6 S2	[C21 H44 N6 S2, tgt=57.59, overall=57.59]	(445.31195, 3256.507)(446.31412, 1309.866)(447.3121, 335.	C21 H44 N6 S2	FindByFormula	25	+	444.3073	21.63131
C21 H46 N O P S	C21 H46 N O P S	[C21 H46 N O P S, tgt=34.04, overall=34.04]	(392.31314, 4457.1523)(393.30676, 1550.2174)(394.30225, 1	C21 H46 N O P S	FindByFormula	23	+	391.3054	21.883797
C21 H49 N2 P5	C21 H49 N2 P5	[C21 H49 N2 P5, tgt=97.37, overall=97.37]	(485.26654, 10334.685)(486.2736, 3104.443)(487.26245, 85.	C21 H49 N2 P5	FindByFormula	9	+	484.2588	22.413736
C21 H5 O8 P5 S4	C21 H5 O8 P5 S4	[C21 H5 O8 P5 S4, tgt=59.52, overall=59.52]	(668.7636, 6004.895)(669.7685, 2904.0625)(670.774, 843.17	C21 H5 O8 P5 S4	FindByFormula	14	+	667.7596	26.306545
C22 H12 N2 O3	C22 H12 N2 O3	[C22 H12 N2 O3, tgt=94.50, overall=94.50]	(353.09274, 2962.5332)(354.0945, 641.7367)(355.08835, 132	C22 H12 N2 O3	FindByFormula	6	+	352.0834	18.654951
C22 H17 N17 O	C22 H17 N17 O	[C22 H17 N17 O, tgt=95.53, overall=95.53]	(536.18866, 2079.302)(537.19, 613.73627)(538.1938, 243.68	C22 H17 N17 O	FindByFormula	9	+	535.181	2.3220208
C22 H2 O S5	C22 H2 O S5	[C22 H2 O S5, tgt=85.73, overall=85.73]	(442.8727, 1657.6201)(443.87402, 410.596)(444.868, 697.38	C22 H2 O S5	FindByFormula	22	+	441.8701	0.5798186
C22 H20 O5	C22 H20 O5	[C22 H20 O5, tgt=66.11, overall=66.11]	(365.13947, 3377.872)(366.14285, 818.84875)(367.14972, 57	C22 H20 O5	FindByFormula	26	+	364.1315	20.063076
C22 H22 N12 O4	C22 H22 N12 O4	[C22 H22 N12 O4, tgt=94.19, overall=94.19]	(519.1967, 4777.7095)(520.2018, 1380.4833)(521.20795, 354	C22 H22 N12 O4	FindByFormula	6	+	518.1888	12.667587
C22 H22 N6 O2 P4	C22 H22 N6 O2 P4	[C22 H22 N6 O2 P4, tgt=95.93, overall=95.93]	(527.08386, 3717.1638)(528.085, 1197.0157)(529.0864, 378.	C22 H22 N6 O2 P4	FindByFormula	8	+	526.0755	1.3352544
C22 H23 N3	C22 H23 N3	[C22 H23 N3, tgt=91.80, overall=91.80]	(330.19653, 10643.831)(331.19547, 2756.004)(332.19495, 37	C22 H23 N3	FindByFormula	16	+	329.1882	14.94095
C22 H24 N6 O4	C22 H24 N6 O4	[C22 H24 N6 O4, tgt=90.23, overall=90.23]	(437.19415, 134456.4)(438.19733, 34961.97)(439.20233, 652	C22 H24 N6 O4	FindByFormula	28	+	436.187	18.718328
C22 H24 N8 O P4	C22 H24 N8 O P4	[C22 H24 N8 O P4, tgt=82.19, overall=82.19]	(541.1101, 2235.069)(542.1061, 625.9347)(543.1093, 38.783	C22 H24 N8 O P4	FindByFormula	18	+	540.1005	1.2016743
C22 H25 N4 O2 P3	C22 H25 N4 O2 P3	[C22 H25 N4 O2 P3, tgt=94.18, overall=94.18]	(471.12677, 2865.7112)(472.12997, 687.6068)(473.12805, 12	C22 H25 N4 O2 P3	FindByFormula	22	+	470.1202	22.465849
C22 H26 N O P	C22 H26 N O P	[C22 H26 N O P, tgt=97.00, overall=97.00]	(352.18338, 22742.68)(353.18497, 5825.1846)(354.1867, 825	C22 H26 N O P	FindByFormula	18	+	351.1755	16.324806
C22 H26 O6	C22 H26 O6	[C22 H26 O6, tgt=97.83, overall=97.83]	(387.18063, 23936.05)(388.18402, 5900.788)(389.18793, 127	C22 H26 O6	FindByFormula	28	+	386.1734	16.430906
C22 H27 N11	C22 H27 N11	[C22 H27 N11, tgt=62.04, overall=62.04]	(446.25366, 4644.805)(447.25156, 1519.7717)(448.25287, 40	C22 H27 N11	FindByFormula	28	+	445.2467	18.224787
C22 H27 N2 O3 P	C22 H27 N2 O3 P	[C22 H27 N2 O3 P, tgt=72.07, overall=72.07]	(399.18472, 3522.4727)(400.18768, 860.7225)(401.1812, 70.	C22 H27 N2 O3 P	FindByFormula	9	+	398.1744	14.440693
C22 H27 N3 S	C22 H27 N3 S	[C22 H27 N3 S, tgt=63.58, overall=63.58]	(366.19977, 2016.6918)(367.20416, 1177.45)(368.19998, 288	C22 H27 N3 S	FindByFormula	28	+	365.1948	16.425505
C22 H27 N4 O9 P S	C22 H27 N4 O9 P S	[C22 H27 N4 O9 P S, tgt=33.20, overall=33.20]	(555.1389, 89.32)(577.1132, 79.53)	C22 H27 N4 O9 P S	FindByFormula	1	+	554.128	1.3970242
C22 H28 O2	C22 H28 O2	[C22 H28 O2, tgt=91.02, overall=91.02]	(325.2174, 12319.719)(326.2198, 2676.9863)(327.22006, 148	C22 H28 O2	FindByFormula	24	+	324.2073	22.534262
C22 H29 N3 O2	C22 H29 N3 O2	[C22 H29 N3 O2, tgt=91.29, overall=91.29]	(368.23242, 3251.8262)(369.22818, 1075.633)(370.2279, 188	C22 H29 N3 O2	FindByFormula	17	+	367.2249	15.124695
C22 H32 N9 P3	C22 H32 N9 P3	[C22 H32 N9 P3, tgt=55.75, overall=55.75]	(516.20544, 3815.5552)(517.2129, 1154.7957)(518.21155, 33	C22 H32 N9 P3	FindByFormula	8	+	515.1992	12.263922
C22 H34 N2 O P2 S	C22 H34 N2 O P2 S	[C22 H34 N2 O P2 S, tgt=80.57, overall=80.57]	(437.1939, 46683.574)(438.19748, 12395.651)(439.20233, 31	C22 H34 N2 O P2 S	FindByFormula	28	+	436.1871	17.532684
C22 H34 N2 O15 P2	C22 H34 N2 O15 P2	[C22 H34 N2 O15 P2, tgt=97.81, overall=97.81]	(629.1519, 25630.107)(630.15485, 6203.313)(631.15436, 174	C22 H34 N2 O15 P2	FindByFormula	6	+	628.1435	0.71266603
C22 H34 N4	C22 H34 N4	[C22 H34 N4, tgt=88.60, overall=88.60]	(355.28058, 12326.17)(356.28427, 2700.2449)(357.28125, 30	C22 H34 N4	FindByFormula	28	+	354.2773	22.486643
C22 H34 N6 O2	C22 H34 N6 O2	[C22 H34 N6 O2, tgt=91.27, overall=91.27]	(415.2802, 5455.746)(416.2859, 1798.9032)(417.27838, 425.	C22 H34 N6 O2	FindByFormula	10	+	414.2729	21.615824
C22 H36 N P	C22 H36 N P	[C22 H36 N P, tgt=82.68, overall=82.68]	(346.26874, 4144.4023)(347.26224, 1448.8756)(348.26422, 1	C22 H36 N P	FindByFormula	12	+	345.2596	21.91334
C22 H36 N6 O11	C22 H36 N6 O11	[C22 H36 N6 O11, tgt=73.36, overall=73.36]	(561.25415, 5233.051)(562.25433, 1505.681)(563.25824, 532	C22 H36 N6 O11	FindByFormula	27	+	560.2449	13.035853
C22 H37 N7 O2	C22 H37 N7 O2	[C22 H37 N7 O2, tgt=88.42, overall=88.42]	(432.30716, 2024.4591)(433.3087, 657.897)(434.3086, 152.3	C22 H37 N7 O2	FindByFormula	11	+	431.3003	20.257433
C22 H38 N10 O2	C22 H38 N10 O2	[C22 H38 N10 O2, tgt=67.79, overall=67.79]	(475.32452, 1806.982)(476.32587, 536.2707)(477.3239, 134.	C22 H38 N10 O2	FindByFormula	28	+	474.3174	10.700096
C22 H38 N8 O	C22 H38 N8 O	[C22 H38 N8 O, tgt=64.84, overall=64.84]	(431.3221, 2590.9841)(432.32434, 905.1778)(433.32086, 207	C22 H38 N8 O	FindByFormula	21	+	430.3149	20.664064
C22 H39 N4 O4 P3	C22 H39 N4 O4 P3	[C22 H39 N4 O4 P3, tgt=63.25, overall=63.25]	(517.22784, 4752.464)(518.22876, 1243.0468)(519.23334, 71	C22 H39 N4 O4 P3	FindByFormula	19	+	516.219	12.456337
C22 H41 N3 O6	C22 H41 N3 O6	[C22 H41 N3 O6, tgt=7.69, overall=7.69]	(444.30914, 6164.187)(445.30573, 1863.2043)(446.3068, 951	C22 H41 N3 O6	FindByFormula	18	+	443.3002	21.469604
C22 H42 N2 O3 S	C22 H42 N2 O3 S	[C22 H42 N2 O3 S, tgt=33.54, overall=33.54]	(415.30136, 6798.326)(416.3044, 1791.9531)(417.29788, 319	C22 H42 N2 O3 S	FindByFormula	24	+	414.2939	21.957481
C22 H43 N7 O4 S2	C22 H43 N7 O4 S2	[C22 H43 N7 O4 S2, tgt=63.00, overall=63.00]	(534.28973, 4245.1353)(535.29553, 1862.7826)(536.29047, 7	C22 H43 N7 O4 S2	FindByFormula	15	+	533.2869	22.09289
C22 H44 N2 P2	C22 H44 N2 P2	[C22 H44 N2 P2, tgt=38.28, overall=38.28]	(399.30557, 11536.482)(400.30737, 2892.1868)(401.30734, 7	C22 H44 N2 P2	FindByFormula	28	+	398.2998	22.430899
C22 H44 N4 S2	C22 H44 N4 S2	[C22 H44 N4 S2, tgt=48.51, overall=48.51]	(429.3094, 4243.116)(430.30737, 1214.7385)(431.3123, 195.	C22 H44 N4 S2	FindByFormula	21	+	428.301	22.25785
C22 H44 N6 O11	C22 H44 N6 O11	[C22 H44 N6 O11, tgt=99.57, overall=99.57]	(569.31415, 16738.793)(570.317, 4637.508)(571.317, 1160.3	C22 H44 N6 O11	FindByFormula	28	+	568.3069	10.671227
C22 H44 O6 P6 S	C22 H44 O6 P6 S	[C22 H44 O6 P6 S, tgt=80.51, overall=80.51]	(623.1376, 3345.9033)(624.13794, 1037.9579)(625.1357, 356	C22 H44 O6 P6 S	FindByFormula	6	+	622.1285	0.70016646
C22 H45 N O	C22 H45 N O	[C22 H45 N O, tgt=89.08, overall=89.08]	(340.35687, 4850.2383)(341.36023, 1681.37)(342.34753, 366	C22 H45 N O	FindByFormula	8	+	339.3491	21.918463
C22 H45 N3 O3 S2	C22 H45 N3 O3 S2	[C22 H45 N3 O3 S2, tgt=42.88, overall=42.88]	(464.2955, 16541.607)(465.30844, 5221.973)(466.29984, 134	C22 H45 N3 O3 S2	FindByFormula	6	+	463.2867	22.511736
C22 H45 N4 P S	C22 H45 N4 P S	[C22 H45 N4 P S, tgt=25.65, overall=25.65]	(429.31754, 47351.59)(430.31995, 11891.804)(431.3156, 219	C22 H45 N4 P S	FindByFormula	26	+	428.3114	22.325062
C22 H46 N O7 P	C22 H46 N O7 P	[C22 H46 N O7 P, tgt=99.46, overall=99.46]	(468.30438, 2503.723)(469.30167, 1720.502)(470.3054, 466.	C22 H46 N O7 P	FindByFormula	28	+	467.3013	21.593801
C22 H46 N2 O P2 S	C22 H46 N2 O P2 S	[C22 H46 N2 O P2 S, tgt=51.27, overall=51.27]	(449.28802, 18839.88)(450.291, 5012.8867)(451.28513, 1320	C22 H46 N2 O P2 S	FindByFormula	28	+	448.2804	21.737194
C22 H46 N6 S2	C22 H46 N6 S2	[C22 H46 N6 S2, tgt=30.74, overall=30.74]	(459.32886, 5774.381)(460.32993, 1638.549)(461.32367, 653	C22 H46 N6 S2	FindByFormula	26	+	458.3218	22.058817
C22 H46 N8 O S3	C22 H46 N8 O S3	[C22 H46 N8 O S3, tgt=85.23, overall=85.23]	(535.30255, 2361.5198)(536.30554, 864.0047)(537.29755, 46	C22 H46 N8 O S3	FindByFormula	28	+	534.2957	18.26301
C22 H46 O12	C22 H46 O12	[C22 H46 O12, tgt=99.43, overall=99.43]	(503.30502, 1852.8009)(504.30588, 536.42395)(505.30423, 1	C22 H46 O12	FindByFormula	28	+	502.2986	10.091773
C22 H47 N	C22 H47 N	[C22 H47 N, tgt=98.75, overall=98.75]	(326.37778, 4352.318)(327.38016, 1160.3451)(328.37875, 20	C22 H47 N	FindByFormula	28	+	325.37	21.430243
C22 H48 N2 O S3	C22 H48 N2 O S3	[C22 H48 N2 O S3, tgt=76.02, overall=76.02]	(453.29678, 2650.1968)(454.29666, 926.45166)(455.30444, 1	C22 H48 N2 O S3	FindByFormula	21	+	452.292	21.93805
C22 H48 N2 O7 P2 S	C22 H48 N2 O7 P2 S	[C22 H48 N2 O7 P2 S, tgt=32.08, overall=32.08]	(547.2714, 3446.6135)(548.2713, 1101.0187)(549.27264, 497	C22 H48 N2 O7 P2 S	FindByFormula	14	+	546.2656	13.03385
C22 H49 N5 O3 P2 S2	C22 H49 N5 O3 P2 S2	[C22 H49 N5 O3 P2 S2, tgt=74.63, overall=74.63]	(558.2821, 8560.333)(559.2851, 2642.261)(560.2877, 811.56	C22 H49 N5 O3 P2 S2	FindByFormula	28	+	557.2733	21.390654
C22 H49 N7	C22 H49 N7	[C22 H49 N7, tgt=61.72, overall=61.72]	(412.413, 1064.2058)(413.41296, 472.59595)(414.41006, 161	C22 H49 N7	FindByFormula	20	+	411.4032	22.37505
C22 H50 Cl2 N8 O	C22 H50 Cl2 N8 O	[C22 H50 Cl2 N8 O, tgt=50.55, overall=50.55]	(513.3544, 2670.7778)(514.35345, 1152.919)(515.3627, 3207	C22 H50 Cl2 N8 O	FindByFormula	17	+	512.3519	22.709736
C22 H50 N7 P S3	C22 H50 N7 P S3	[C22 H50 N7 P S3, tgt=87.95, overall=87.95]	(540.3075, 12575.563)(541.3064, 4152.022)(542.3129, 2427.	C22 H50 N7 P S3	FindByFormula	20	+	539.3014	21.797802
C22 H8 N2 O3	C22 H8 N2 O3	[C22 H8 N2 O3, tgt=85.35, overall=85.35]	(349.06036, 13630.279)(350.06412, 2696.0845)(351.06503, 4	C22 H8 N2 O3	FindByFormula	28	+	348.0528	19.703207
C23 H10 O2	C23 H10 O2	[C23 H10 O2, tgt=70.24, overall=70.24]	(319.07565, 1545.6084)(320.07803, 299.215)(321.07443, 493	C23 H10 O2	FindByFormula	7	+	318.0657	18.462927
C23 H20 N10	C23 H20 N10	[C23 H20 N10, tgt=95.99, overall=95.99]	(437.19412, 310302.84)(438.19724, 82659.55)(439.2009, 146	C23 H20 N10	FindByFormula	28	+	436.187	19.253677
C23 H20 N4 O	C23 H20 N4 O	[C23 H20 N4 O, tgt=68.44, overall=68.44]	(369.17145, 2924.789)(370.17365, 675.08044)(371.17245, 25	C23 H20 N4 O	FindByFormula	23	+	368.1638	16.431044
C23 H24 N8 P4	C23 H24 N8 P4	[C23 H24 N8 P4, tgt=70.50, overall=70.50]	(537.1131, 347.13995)(538.1117, 120.29701)(575.0714, 71.2	C23 H24 N8 P4	FindByFormula	10	+	536.1107	18.405094
C23 H25 N3	C23 H25 N3	[C23 H25 N3, tgt=98.91, overall=98.91]	(344.21204, 33913.094)(345.21286, 9416.791)(346.2147, 125	C23 H25 N3	FindByFormula	19	+	343.2052	15.897032
C23 H25 N5 O2	C23 H25 N5 O2	[C23 H25 N5 O2, tgt=83.76, overall=83.76]	(404.20703, 9822.307)(405.2112, 2882.4263)(406.2097, 155.	C23 H25 N5 O2	FindByFormula	28	+	403.1997	16.431513
C23 H26 N3 P	C23 H26 N3 P	[C23 H26 N3 P, tgt=88.59, overall=88.59]	(376.19516, 2139.2527)(377.1937, 628.29877)(378.19443, 15	C23 H26 N3 P	FindByFormula	24	+	375.1874	3.8888738
C23 H28 N2 O3 S	C23 H28 N2 O3 S	[C23 H28 N2 O3 S, tgt=78.59, overall=78.59]	(413.19006, 18382.264)(414.19177, 5287.7783)(415.19577, 1	C23 H28 N2 O3 S	FindByFormula	22	+	412.1848	22.586988
C23 H28 O3	C23 H28 O3	[C23 H28 O3, tgt=84.10, overall=84.10]	(353.2113, 16574.266)(354.21396, 3796.8704)(355.21524, 25	C23 H28 O3	FindByFormula	15	+	352.203	21.528545
C23 H29 N11	C23 H29 N11	[C23 H29 N11, tgt=57.63, overall=57.63]	(460.26865, 2610.7476)(461.27026, 943.7611)(462.26913, 21	C23 H29 N11	FindByFormula	24	+	459.2614	17.547285
C23 H30 N10 P6	C23 H30 N10 P6	[C23 H30 N10 P6, tgt=82.15, overall=82.15]	(633.11755, 1692.7042)(634.12054, 524.53906)(635.12256, 3	C23 H30 N10 P6	FindByFormula	23	+	632.1097	22.586956
C23 H30 O3	C23 H30 O3	[C23 H30 O3, tgt=88.06, overall=88.06]	(355.22635, 5181.805)(356.23105, 1231.4368)(357.23236, 76	C23 H30 O3	FindByFormula	28	+	354.2194	20.56461
C23 H31 N O6	C23 H31 N O6	[C23 H31 N O6, tgt=97.92, overall=97.92]	(418.22272, 63548.406)(419.22586, 16603.803)(420.22903, 2	C23 H31 N O6	FindByFormula	28	+	417.2155	16.430655
C23 H32 O4	C23 H32 O4	[C23 H32 O4, tgt=64.39, overall=64.39]	(373.23813, 3831.9724)(374.23395, 416.68268)(375.2341, 94	C23 H32 O4	FindByFormula	26	+	372.2319	22.525383
C23 H34 O2 P2	C23 H34 O2 P2	[C23 H34 O2 P2, tgt=80.41, overall=80.41]	(405.21207, 2442.7927)(406.21014, 596.5061)(407.20715, 11	C23 H34 O2 P2	FindByFormula	21	+	404.2024	0.7662409
C23 H36 N17 O P	C23 H36 N17 O P	[C23 H36 N17 O P, tgt=85.79, overall=85.79]	(598.3106, 4007.7651)(599.3118, 1381.5793)(600.3089, 423.	C23 H36 N17 O P	FindByFormula	18	+	597.3012	22.187508
C23 H37 N3 O P2	C23 H37 N3 O P2	[C23 H37 N3 O P2, tgt=84.48, overall=84.48]	(434.24823, 1324.4862)(435.24823, 463.70197)(436.24557, 1	C23 H37 N3 O P2	FindByFormula	18	+	433.2418	18.036144
C23 H39 N4 O4 P	C23 H39 N4 O4 P	[C23 H39 N4 O4 P, tgt=78.12, overall=78.12]	(467.2805, 1381.7146)(468.2809, 483.88113)(469.2795, 524.	C23 H39 N4 O4 P	FindByFormula	11	+	466.2687	22.148945
C23 H39 N4 P3	C23 H39 N4 P3	[C23 H39 N4 P3, tgt=98.59, overall=98.59]	(465.24597, 9041.077)(466.24878, 2378.4834)(467.2512, 485	C23 H39 N4 P3	FindByFormula	6	+	464.2383	2.1038382
C23 H39 O7 P	C23 H39 O7 P	[C23 H39 O7 P, tgt=89.30, overall=89.30]	(459.25034, 10169.96)(460.25992, 2638.7458)(461.25677, 75	C23 H39 O7 P	FindByFormula	22	+	458.2419	22.291925
C23 H40 N4 O3	C23 H40 N4 O3	[C23 H40 N4 O3, tgt=44.49, overall=44.49]	(421.31677, 3095.8562)(422.31784, 908.5822)(423.31467, 23	C23 H40 N4 O3	FindByFormula	23	+	420.3086	17.283815
C23 H40 N8 O9	C23 H40 N8 O9	[C23 H40 N8 O9, tgt=98.06, overall=98.06]	(573.29626, 1659.2589)(574.3017, 918.25507)(575.3018, 265	C23 H40 N8 O9	FindByFormula	16	+	572.2908	3.6589952
C23 H40 O P2 S2	C23 H40 O P2 S2	[C23 H40 O P2 S2, tgt=85.17, overall=85.17]	(459.20633, 7178.454)(460.20996, 2005.217)(461.2171, 630.	C23 H40 O P2 S2	FindByFormula	28	+	458.1997	13.106881
C23 H41 N	C23 H41 N	[C23 H41 N, tgt=91.67, overall=91.67]	(332.33096, 17799.928)(333.33316, 4646.528)(334.33353, 60	C23 H41 N	FindByFormula	28	+	331.3236	20.426218
C23 H41 N7 O2	C23 H41 N7 O2	[C23 H41 N7 O2, tgt=88.23, overall=88.23]	(448.3382, 2229.753)(449.3376, 651.2061)(450.34186, 211.2	C23 H41 N7 O2	FindByFormula	25	+	447.3306	21.129475
C23 H43 N O2	C23 H43 N O2	[C23 H43 N O2, tgt=92.81, overall=92.81]	(366.33426, 3017.2776)(367.33435, 947.1284)(368.33286, 16	C23 H43 N O2	FindByFormula	13	+	365.3261	22.062456
C23 H43 N3 O3 S2	C23 H43 N3 O3 S2	[C23 H43 N3 O3 S2, tgt=78.58, overall=78.58]	(474.28198, 6630.068)(475.28333, 2223.1118)(476.2789, 800	C23 H43 N3 O3 S2	FindByFormula	24	+	473.2745	18.393456
C23 H43 N8 O P	C23 H43 N8 O P	[C23 H43 N8 O P, tgt=85.41, overall=85.41]	(479.33493, 1044.1183)(480.33514, 434.75604)(481.33694, 1	C23 H43 N8 O P	FindByFormula	28	+	478.3294	19.575678
C23 H43 O2 P S	C23 H43 O2 P S	[C23 H43 O2 P S, tgt=82.21, overall=82.21]	(415.2811, 7275.172)(416.2817, 2343.5942)(417.28043, 498.	C23 H43 O2 P S	FindByFormula	16	+	414.2743	21.734884
C23 H44 N2 O2 S	C23 H44 N2 O2 S	[C23 H44 N2 O2 S, tgt=39.84, overall=39.84]	(413.32166, 18157.287)(414.32343, 4662.92)(415.3176, 985.	C23 H44 N2 O2 S	FindByFormula	21	+	412.3153	22.763992
C23 H45 Cl N4 O3	C23 H45 Cl N4 O3	[C23 H45 Cl N4 O3, tgt=29.34, overall=29.34]	(461.3249, 1277.5663)(462.32672, 402.25925)(463.32193, 10	C23 H45 Cl N4 O3	FindByFormula	20	+	460.3157	22.559372
C23 H45 N O4	C23 H45 N O4	[C23 H45 N O4, tgt=92.24, overall=92.24]	(400.34146, 6609.599)(401.3415, 1812.7852)(402.34747, 110	C23 H45 N O4	FindByFormula	26	+	399.3351	21.363081
C23 H45 N2 O3 P S	C23 H45 N2 O3 P S	[C23 H45 N2 O3 P S, tgt=66.80, overall=66.80]	(461.29587, 6055.677)(462.29813, 1653.7145)(463.2921, 461	C23 H45 N2 O3 P S	FindByFormula	25	+	460.2883	21.212801
C23 H46 N O2 P3	C23 H46 N O2 P3	[C23 H46 N O2 P3, tgt=57.36, overall=57.36]	(462.28156, 2070.6934)(463.28085, 519.3656)(464.28384, 19	C23 H46 N O2 P3	FindByFormula	23	+	461.2744	19.977787
C23 H46 N5 O3 P3	C23 H46 N5 O3 P3	[C23 H46 N5 O3 P3, tgt=48.79, overall=48.79]	(534.2901, 2719.4275)(535.295, 1218.1769)(536.28925, 457.	C23 H46 N5 O3 P3	FindByFormula	19	+	533.2843	22.032547
C23 H47 N O4	C23 H47 N O4	[C23 H47 N O4, tgt=56.79, overall=56.79]	(402.3553, 1494.132)(403.35776, 545.9874)(404.35782, 121.	C23 H47 N O4	FindByFormula	28	+	401.3532	21.200068
C23 H47 N4 O P S	C23 H47 N4 O P S	[C23 H47 N4 O P S, tgt=38.42, overall=38.42]	(459.32907, 5949.0293)(460.3302, 1686.9243)(461.32404, 70	C23 H47 N4 O P S	FindByFormula	24	+	458.3192	22.001955
C23 H47 N5 S3	C23 H47 N5 S3	[C23 H47 N5 S3, tgt=34.09, overall=34.09]	(490.30746, 4474.5117)(491.31094, 1406.4954)(492.30865, 6	C23 H47 N5 S3	FindByFormula	23	+	489.3009	21.379593
C23 H47 O P S2	C23 H47 O P S2	[C23 H47 O P S2, tgt=28.98, overall=28.98]	(435.28876, 1458.4706)(436.28665, 594.87537)(437.28796, 1	C23 H47 O P S2	FindByFormula	22	+	434.2809	22.533506
C23 H48 N O7 P	C23 H48 N O7 P	[C23 H48 N O7 P, tgt=97.54, overall=97.54]	(482.32083, 1985.2869)(483.31686, 761.3507)(484.31662, 26	C23 H48 N O7 P	FindByFormula	20	+	481.3171	21.969944
C23 H49 N5 O9 S	C23 H49 N5 O9 S	[C23 H49 N5 O9 S, tgt=89.06, overall=89.06]	(572.3323, 20433.277)(573.3327, 7942.223)(574.33575, 1972	C23 H49 N5 O9 S	FindByFormula	12	+	571.325	22.520761
C23 H53 N5 O P2 S2	C23 H53 N5 O P2 S2	[C23 H53 N5 O P2 S2, tgt=89.46, overall=89.46]	(542.3221, 88442.04)(543.32526, 25904.11)(544.3314, 7557.	C23 H53 N5 O P2 S2	FindByFormula	28	+	541.3163	21.98287
C23 H55 N10 O7 P S2	C23 H55 N10 O7 P S2	[C23 H55 N10 O7 P S2, tgt=49.45, overall=49.45]	(679.36224, 109.884995)(717.3178, 283.21335)(718.31036, 1	C23 H55 N10 O7 P S2	FindByFormula	3	+	678.3497	11.785446
C23 H8 N2 O5 P6 S3	C23 H8 N2 O5 P6 S3	[C23 H8 N2 O5 P6 S3, tgt=72.80, overall=72.80]	(674.8051, 3062.1516)(675.8077, 1486.5785)(676.8112, 463.	C23 H8 N2 O5 P6 S3	FindByFormula	9	+	673.8013	25.828064
C24 H10 N2 O4	C24 H10 N2 O4	[C24 H10 N2 O4, tgt=83.50, overall=83.50]	(391.07257, 2067.152)(392.0752, 432.84213)(393.07285, 79.	C24 H10 N2 O4	FindByFormula	28	+	390.0654	13.105702
C24 H19 N12 O4 P	C24 H19 N12 O4 P	[C24 H19 N12 O4 P, tgt=80.89, overall=80.89]	(571.14923, 1718.4792)(572.1524, 468.9448)(573.15, 358.48	C24 H19 N12 O4 P	FindByFormula	23	+	570.1396	22.597445
C24 H19 N6 O3 P	C24 H19 N6 O3 P	[C24 H19 N6 O3 P, tgt=80.61, overall=80.61]	(471.13412, 3506.5825)(472.13614, 1013.71497)(473.13654,	C24 H19 N6 O3 P	FindByFormula	28	+	470.1261	17.456757
C24 H20 N8 O5 P4	C24 H20 N8 O5 P4	[C24 H20 N8 O5 P4, tgt=32.69, overall=32.69]	(625.0593, 86.69)(626.0383, 25.27)(663.033, 95.83)(664.024	C24 H20 N8 O5 P4	FindByFormula	2	+	624.0539	8.45948
C24 H27 N3	C24 H27 N3	[C24 H27 N3, tgt=99.05, overall=99.05]	(358.22787, 40295.61)(359.2289, 10994.263)(360.22797, 157	C24 H27 N3	FindByFormula	21	+	357.2202	16.71751
C24 H27 N5 O2	C24 H27 N5 O2	[C24 H27 N5 O2, tgt=44.38, overall=44.38]	(418.2227, 4144.1816)(419.2246, 1343.0354)(420.2246, 254.	C24 H27 N5 O2	FindByFormula	23	+	417.2144	17.368351
C24 H28 O2	C24 H28 O2	[C24 H28 O2, tgt=86.15, overall=86.15]	(349.21402, 62985.668)(350.21802, 13770.299)(387.1794, 53	C24 H28 O2	FindByFormula	21	+	348.2076	22.628002
C24 H28 O3	C24 H28 O3	[C24 H28 O3, tgt=46.72, overall=46.72]	(365.21155, 5165.481)(366.21457, 1251.84)(403.17105, 488.	C24 H28 O3	FindByFormula	21	+	364.203	21.726414
C24 H29 N2 P3 S	C24 H29 N2 P3 S	[C24 H29 N2 P3 S, tgt=85.69, overall=85.69]	(471.13358, 25535.324)(472.13596, 7120.543)(473.13614, 17	C24 H29 N2 P3 S	FindByFormula	28	+	470.1255	16.429333
C24 H29 O6 P S	C24 H29 O6 P S	[C24 H29 O6 P S, tgt=85.21, overall=85.21]	(477.14996, 6825.348)(478.1538, 1878.7487)(479.1536, 487.	C24 H29 O6 P S	FindByFormula	28	+	476.1429	16.428724
C24 H30 O6	C24 H30 O6	[C24 H30 O6, tgt=98.69, overall=98.69]	(415.21198, 20235.277)(416.21555, 5493.6284)(417.21744, 1	C24 H30 O6	FindByFormula	28	+	414.2049	18.39348
C24 H31 O4 P3	C24 H31 O4 P3	[C24 H31 O4 P3, tgt=88.76, overall=88.76]	(477.15054, 4031.3777)(478.15414, 1103.0803)(479.15546, 2	C24 H31 O4 P3	FindByFormula	28	+	476.143	16.811878
C24 H32 N11 O P	C24 H32 N11 O P	[C24 H32 N11 O P, tgt=71.69, overall=71.69]	(522.2598, 3880.841)(523.2644, 1199.4868)(524.2584, 85.39)	C24 H32 N11 O P	FindByFormula	14	+	521.2553	22.047415
C24 H32 O3 P6	C24 H32 O3 P6	[C24 H32 O3 P6, tgt=69.13, overall=69.13]	(555.08453, 2119.2336)(556.08777, 656.9715)(557.08704, 28	C24 H32 O3 P6	FindByFormula	27	+	554.0776	16.432497
C24 H33 N O6	C24 H33 N O6	[C24 H33 N O6, tgt=98.54, overall=98.54]	(432.23837, 47084.926)(433.24142, 12783.531)(434.24414, 2	C24 H33 N O6	FindByFormula	28	+	431.231	16.436518
C24 H33 N3 O2	C24 H33 N3 O2	[C24 H33 N3 O2, tgt=99.03, overall=99.03]	(396.26474, 37750.176)(397.26648, 10522.774)(398.26797, 1	C24 H33 N3 O2	FindByFormula	22	+	395.2575	13.137409
C24 H33 N4 P	C24 H33 N4 P	[C24 H33 N4 P, tgt=90.64, overall=90.64]	(409.25098, 3826.9333)(410.2568, 1104.2264)(411.25458, 23	C24 H33 N4 P	FindByFormula	26	+	408.2439	17.777147
C24 H35 N O S2	C24 H35 N O S2	[C24 H35 N O S2, tgt=58.81, overall=58.81]	(418.22263, 3428.4268)(419.22397, 1132.5526)(420.2247, 27	C24 H35 N O S2	FindByFormula	24	+	417.216	16.81257
C24 H35 N11 O5	C24 H35 N11 O5	[C24 H35 N11 O5, tgt=38.77, overall=38.77]	(558.29224, 2079.9365)(559.29016, 875.28906)(560.29315, 7	C24 H35 N11 O5	FindByFormula	12	+	557.2877	22.20092
C24 H35 N9 O P2	C24 H35 N9 O P2	[C24 H35 N9 O P2, tgt=63.37, overall=63.37]	(528.2479, 299.42715)(529.246, 144.40001)(530.2415, 59.08	C24 H35 N9 O P2	FindByFormula	7	+	527.2394	3.733916
C24 H36 N6 O4 P6	C24 H36 N6 O4 P6	[C24 H36 N6 O4 P6, tgt=86.54, overall=86.54]	(659.13104, 1480.2087)(660.13257, 549.7044)(661.13086, 27	C24 H36 N6 O4 P6	FindByFormula	20	+	658.1221	22.704548
C24 H36 N6 S2	C24 H36 N6 S2	[C24 H36 N6 S2, tgt=76.95, overall=76.95]	(473.24893, 1651.63)(474.25336, 640.1229)(475.25064, 266.	C24 H36 N6 S2	FindByFormula	14	+	472.246	21.87506
C24 H36 N9 O P3	C24 H36 N9 O P3	[C24 H36 N9 O P3, tgt=91.19, overall=91.19]	(560.2326, 3579.7852)(561.2404, 1130.0101)(562.2409, 359.	C24 H36 N9 O P3	FindByFormula	6	+	559.2254	12.478017
C24 H36 O5	C24 H36 O5	[C24 H36 O5, tgt=55.18, overall=55.18]	(405.26187, 14156.975)(406.26862, 3630.3857)(407.26614, 1	C24 H36 O5	FindByFormula	26	+	404.2562	21.670973
C24 H37 N11 O5	C24 H37 N11 O5	[C24 H37 N11 O5, tgt=35.44, overall=35.44]	(560.30383, 2281.7192)(561.3004, 628.7805)(562.30383, 413	C24 H37 N11 O5	FindByFormula	21	+	559.2979	22.30058
C24 H37 N7 O3	C24 H37 N7 O3	[C24 H37 N7 O3, tgt=98.74, overall=98.74]	(472.3019, 5899.842)(473.3083, 1899.045)(474.3002, 488.1)(	C24 H37 N7 O3	FindByFormula	19	+	471.2945	20.323118
C24 H38 N2 O6 S	C24 H38 N2 O6 S	[C24 H38 N2 O6 S, tgt=86.37, overall=86.37]	(483.25223, 6212.0854)(484.25656, 1733.014)(485.2512, 297	C24 H38 N2 O6 S	FindByFormula	15	+	482.2464	22.109795
C24 H4 N O11 P3	C24 H4 N O11 P3	[C24 H4 N O11 P3, tgt=94.61, overall=94.61]	(575.90607, 2174.6465)(576.909, 500.15503)(577.90894, 76.	C24 H4 N O11 P3	FindByFormula	8	+	574.8984	20.331482
C24 H40 N5 O3 P	C24 H40 N5 O3 P	[C24 H40 N5 O3 P, tgt=93.43, overall=93.43]	(478.29196, 3710.6091)(479.2938, 1289.3958)(480.29163, 33	C24 H40 N5 O3 P	FindByFormula	26	+	477.2873	22.051981
C24 H42 N2 O3 P4	C24 H42 N2 O3 P4	[C24 H42 N2 O3 P4, tgt=84.95, overall=84.95]	(531.22235, 4814.59)(532.2265, 1471.585)(533.2356, 361.78	C24 H42 N2 O3 P4	FindByFormula	6	+	530.2144	20.124163
C24 H45 P	C24 H45 P	[C24 H45 P, tgt=43.85, overall=43.85]	(365.33255, 18684.15)(366.33646, 4659.0)(367.33374, 2162.	C24 H45 P	FindByFormula	22	+	364.3227	22.81859
C24 H46 N2 O3 S	C24 H46 N2 O3 S	[C24 H46 N2 O3 S, tgt=61.28, overall=61.28]	(443.33258, 8367.243)(444.3356, 2301.6755)(445.32858, 700	C24 H46 N2 O3 S	FindByFormula	26	+	442.3257	22.541536
C24 H46 N3 O11 P	C24 H46 N3 O11 P	[C24 H46 N3 O11 P, tgt=98.50, overall=98.50]	(584.29376, 30566.5)(585.2985, 9179.749)(586.30554, 2748.	C24 H46 N3 O11 P	FindByFormula	28	+	583.2889	21.884008
C24 H47 N4 O2 P S	C24 H47 N4 O2 P S	[C24 H47 N4 O2 P S, tgt=43.30, overall=43.30]	(487.32242, 7033.732)(488.32477, 2132.4722)(489.3226, 738	C24 H47 N4 O2 P S	FindByFormula	24	+	486.3175	22.015398
C24 H47 N4 O6 P	C24 H47 N4 O6 P	[C24 H47 N4 O6 P, tgt=96.99, overall=96.99]	(519.3298, 141699.23)(520.3328, 43006.145)(521.3351, 8695	C24 H47 N4 O6 P	FindByFormula	28	+	518.3225	18.842287
C24 H48 N O7 P	C24 H48 N O7 P	[C24 H48 N O7 P, tgt=96.01, overall=96.01]	(494.32108, 3183.081)(495.31577, 1230.6819)(496.32034, 41	C24 H48 N O7 P	FindByFormula	27	+	493.3163	21.865917
C24 H48 N3 O11 P	C24 H48 N3 O11 P	[C24 H48 N3 O11 P, tgt=99.70, overall=99.70]	(586.30994, 101556.51)(587.3135, 28643.846)(588.31744, 60	C24 H48 N3 O11 P	FindByFormula	28	+	585.3025	22.312761
C24 H48 N3 O12 P	C24 H48 N3 O12 P	[C24 H48 N3 O12 P, tgt=98.31, overall=98.31]	(602.30475, 5853.4766)(603.3062, 2593.3616)(604.3076, 746	C24 H48 N3 O12 P	FindByFormula	16	+	601.2987	19.41835
C24 H49 N2 O P S	C24 H49 N2 O P S	[C24 H49 N2 O P S, tgt=86.09, overall=86.09]	(445.3376, 10204.609)(446.33908, 3186.214)(447.33496, 651	C24 H49 N2 O P S	FindByFormula	17	+	444.3278	21.32454
C24 H49 N4 O P S	C24 H49 N4 O P S	[C24 H49 N4 O P S, tgt=72.23, overall=72.23]	(473.3443, 35075.035)(474.3473, 9822.804)(475.34003, 2487	C24 H49 N4 O P S	FindByFormula	28	+	472.3383	22.368017
C24 H49 N5 O5 S3	C24 H49 N5 O5 S3	[C24 H49 N5 O5 S3, tgt=84.54, overall=84.54]	(584.2945, 9558.926)(585.29956, 3103.9504)(586.30365, 132	C24 H49 N5 O5 S3	FindByFormula	27	+	583.2878	21.697273
C24 H49 N5 O6 P2	C24 H49 N5 O6 P2	[C24 H49 N5 O6 P2, tgt=93.78, overall=93.78]	(566.32275, 71438.14)(567.3263, 23118.312)(568.33075, 676	C24 H49 N5 O6 P2	FindByFormula	28	+	565.3177	22.125158
C24 H5 O11 P5 S2	C24 H5 O11 P5 S2	[C24 H5 O11 P5 S2, tgt=69.87, overall=69.87]	(688.8033, 10929.211)(689.8067, 5592.931)(690.8095, 1496.	C24 H5 O11 P5 S2	FindByFormula	17	+	687.8027	26.270306
C24 H50 N O6 P	C24 H50 N O6 P	[C24 H50 N O6 P, tgt=54.49, overall=54.49]	(480.3429, 2152.524)(481.3456, 1612.9185)(482.35095, 1320	C24 H50 N O6 P	FindByFormula	15	+	479.3378	22.491398
C24 H50 N O7 P	C24 H50 N O7 P	[C24 H50 N O7 P, tgt=99.28, overall=99.28]	(496.33798, 17664.525)(497.3332, 5614.1655)(498.3337, 132	C24 H50 N O7 P	FindByFormula	28	+	495.3319	22.316944
C24 H50 N O8 P	C24 H50 N O8 P	[C24 H50 N O8 P, tgt=98.89, overall=98.89]	(512.33356, 850.6579)(513.332, 493.05167)(514.33136, 150.	C24 H50 N O8 P	FindByFormula	25	+	511.3247	19.425518
C24 H50 N2 O2 P2 S	C24 H50 N2 O2 P2 S	[C24 H50 N2 O2 P2 S, tgt=35.01, overall=35.01]	(493.3143, 32710.746)(494.31784, 9848.501)(495.31372, 219	C24 H50 N2 O2 P2 S	FindByFormula	24	+	492.3061	21.822737
C24 H50 N6 S2	C24 H50 N6 S2	[C24 H50 N6 S2, tgt=45.21, overall=45.21]	(487.36, 15098.728)(488.36258, 4425.1113)(489.35922, 1238	C24 H50 N6 S2	FindByFormula	24	+	486.3538	22.585878
C24 H50 O13	C24 H50 O13	[C24 H50 O13, tgt=98.87, overall=98.87]	(547.3301, 1176.8392)(548.32996, 362.8986)(549.3307, 134.	C24 H50 O13	FindByFormula	28	+	546.3239	10.671549
C24 H51 N O2	C24 H51 N O2	[C24 H51 N O2, tgt=96.63, overall=96.63]	(386.39886, 16382.95)(387.40186, 4473.3164)(388.4037, 769	C24 H51 N O2	FindByFormula	20	+	385.3924	22.285465
C24 H52 N O6 P	C24 H52 N O6 P	[C24 H52 N O6 P, tgt=98.42, overall=98.42]	(482.3578, 2534.0386)(483.3544, 1291.0475)(484.34933, 415	C24 H52 N O6 P	FindByFormula	16	+	481.354	22.538605
C24 H52 N2 O8 P2 S	C24 H52 N2 O8 P2 S	[C24 H52 N2 O8 P2 S, tgt=16.56, overall=16.56]	(591.2945, 462.16113)(592.29376, 200.48001)(593.2945, 130	C24 H52 N2 O8 P2 S	FindByFormula	9	+	590.287	10.816693
C24 H52 N2 P2 S	C24 H52 N2 P2 S	[C24 H52 N2 P2 S, tgt=95.87, overall=95.87]	(463.34064, 7413.968)(464.34406, 2424.3784)(465.34372, 62	C24 H52 N2 P2 S	FindByFormula	28	+	462.3333	19.787811
C24 H53 N3 O P2 S3	C24 H53 N3 O P2 S3	[C24 H53 N3 O P2 S3, tgt=23.12, overall=23.12]	(558.291, 925.7564)(559.29034, 529.44714)(560.28796, 331.	C24 H53 N3 O P2 S3	FindByFormula	11	+	557.2865	22.181053
C24 H54 N12 S2	C24 H54 N12 S2	[C24 H54 N12 S2, tgt=35.80, overall=35.80]	(575.4123, 11071.135)(576.4137, 3769.453)(577.4057, 1198.	C24 H54 N12 S2	FindByFormula	23	+	574.4037	22.61057
C25 H14 N2 O3	C25 H14 N2 O3	[C25 H14 N2 O3, tgt=97.86, overall=97.86]	(391.10782, 9602.539)(392.11148, 2336.9292)(393.1142, 392	C25 H14 N2 O3	FindByFormula	28	+	390.1009	21.68426
C25 H15 N O2	C25 H15 N O2	[C25 H15 N O2, tgt=78.69, overall=78.69]	(362.11728, 2140.8816)(363.11624, 318.86502)(364.11844, 2	C25 H15 N O2	FindByFormula	6	+	361.1097	12.286324

C25 H18 O2	C25 H18 O2	[C25 H18 O2, tgt=91.68, overall=91.68]	(351.13834, 2782.8916)(352.1418, 786.635)(353.14328, 126.	C25 H18 O2	FindByFormula	6	+	350.1311	19.878769
C25 H20 O	C25 H20 O	[C25 H20 O, tgt=98.28, overall=98.28]	(337.15796, 29038.354)(338.16052, 7503.703)(339.16733, 14	C25 H20 O	FindByFormula	7	+	336.1509	21.907867
C25 H24 N8 P2	C25 H24 N8 P2	[C25 H24 N8 P2, tgt=61.83, overall=61.83]	(499.16635, 2240.2866)(500.16827, 733.73615)(501.16757, 1	C25 H24 N8 P2	FindByFormula	23	+	498.1596	19.252739
C25 H26 N12	C25 H26 N12	[C25 H26 N12, tgt=79.70, overall=79.70]	(495.24847, 2051.503)(496.2513, 769.0404)(497.24802, 384.	C25 H26 N12	FindByFormula	28	+	494.2409	16.442123
C25 H26 N4 O2	C25 H26 N4 O2	[C25 H26 N4 O2, tgt=91.73, overall=91.73]	(415.2132, 3476.4766)(416.21588, 957.9715)(417.21515, 868	C25 H26 N4 O2	FindByFormula	28	+	414.2051	18.717722
C25 H28 N6 O	C25 H28 N6 O	[C25 H28 N6 O, tgt=51.99, overall=51.99]	(429.23627, 868.7015)(430.24112, 871.3725)(431.2243, 790.	C25 H28 N6 O	FindByFormula	14	+	428.2291	16.427258
C25 H29 N3	C25 H29 N3	[C25 H29 N3, tgt=42.75, overall=42.75]	(372.2434, 16182.577)(373.24225, 4659.038)(374.2443, 878.	C25 H29 N3	FindByFormula	22	+	371.2337	17.436047
C25 H29 N5 O2	C25 H29 N5 O2	[C25 H29 N5 O2, tgt=83.59, overall=83.59]	(432.23846, 5184.434)(433.24103, 1959.6527)(434.23987, 13	C25 H29 N5 O2	FindByFormula	22	+	431.2312	18.397682
C25 H30 N10	C25 H30 N10	[C25 H30 N10, tgt=73.97, overall=73.97]	(471.27197, 1666.1139)(472.27643, 628.614)(473.2688, 264.	C25 H30 N10	FindByFormula	5	+	470.2631	21.500217
C25 H32 O3	C25 H32 O3	[C25 H32 O3, tgt=60.52, overall=60.52]	(381.243, 7508.3833)(382.2465, 2072.5918)(383.25552, 1836	C25 H32 O3	FindByFormula	7	+	380.2366	22.26147
C25 H33 N11	C25 H33 N11	[C25 H33 N11, tgt=64.59, overall=64.59]	(488.2988, 2237.0386)(489.29498, 825.76996)(490.29355, 21	C25 H33 N11	FindByFormula	16	+	487.2893	18.333035
C25 H33 N25 O	C25 H33 N25 O	[C25 H33 N25 O, tgt=96.68, overall=96.68]	(700.3385, 2911.2527)(701.34064, 1042.5886)(702.34247, 35	C25 H33 N25 O	FindByFormula	7	+	699.3303	2.5423071
C25 H34 N19 P3	C25 H34 N19 P3	[C25 H34 N19 P3, tgt=79.32, overall=79.32]	(694.2545, 2046.8937)(695.2593, 870.41003)(696.26666, 389	C25 H34 N19 P3	FindByFormula	8	+	693.25	21.593277
C25 H34 N4	C25 H34 N4	[C25 H34 N4, tgt=97.06, overall=97.06]	(391.28745, 4612.9785)(392.29236, 1311.4452)(393.2899, 21	C25 H34 N4	FindByFormula	23	+	390.2794	23.135899
C25 H34 O3 P2	C25 H34 O3 P2	[C25 H34 O3 P2, tgt=86.85, overall=86.85]	(445.2066, 3682.3784)(446.20535, 752.35876)(447.21582, 11	C25 H34 O3 P2	FindByFormula	28	+	444.1964	22.412455
C25 H35 N O6	C25 H35 N O6	[C25 H35 N O6, tgt=97.72, overall=97.72]	(446.25412, 65635.2)(447.257, 18698.486)(448.25977, 3336.	C25 H35 N O6	FindByFormula	28	+	445.2467	18.397379
C25 H37 N16 O2 P3	C25 H37 N16 O2 P3	[C25 H37 N16 O2 P3, tgt=42.47, overall=42.47]	(687.2648, 1009.93)(688.2565, 96.72)(689.2769, 146.79)(725.	C25 H37 N16 O2 P3	FindByFormula	1	+	686.2553	17.097448
C25 H38 S	C25 H38 S	[C25 H38 S, tgt=37.58, overall=37.58]	(371.27524, 9599.475)(372.28012, 2380.7144)(373.27335, 26	C25 H38 S	FindByFormula	26	+	370.269	21.974281
C25 H39 N O6 S2	C25 H39 N O6 S2	[C25 H39 N O6 S2, tgt=29.00, overall=29.00]	(514.2279, 3473.4785)(515.2322, 1198.4904)(516.2349, 300.	C25 H39 N O6 S2	FindByFormula	24	+	513.2208	7.766027
C25 H39 O7 P	C25 H39 O7 P	[C25 H39 O7 P, tgt=86.77, overall=86.77]	(483.25208, 3637.611)(484.25467, 973.44086)(485.25787, 16	C25 H39 O7 P	FindByFormula	12	+	482.2434	22.059784
C25 H40 N10	C25 H40 N10	[C25 H40 N10, tgt=96.73, overall=96.73]	(481.352, 56073.438)(482.35516, 17220.504)(483.3567, 3478	C25 H40 N10	FindByFormula	28	+	480.3449	19.786806
C25 H41 N7 O2 S	C25 H41 N7 O2 S	[C25 H41 N7 O2 S, tgt=76.78, overall=76.78]	(504.31186, 19523.553)(505.3141, 5801.045)(506.31302, 135	C25 H41 N7 O2 S	FindByFormula	25	+	503.3059	22.021889
C25 H41 N9 O4 S	C25 H41 N9 O4 S	[C25 H41 N9 O4 S, tgt=96.03, overall=96.03]	(564.30505, 17992.814)(565.3089, 5878.132)(566.3043, 1908	C25 H41 N9 O4 S	FindByFormula	10	+	563.2998	21.778545
C25 H42 N6 O5	C25 H42 N6 O5	[C25 H42 N6 O5, tgt=98.18, overall=98.18]	(507.3289, 109296.1)(508.33234, 31409.65)(509.33456, 6547	C25 H42 N6 O5	FindByFormula	28	+	506.3211	22.186571
C25 H44 N4 O3	C25 H44 N4 O3	[C25 H44 N4 O3, tgt=31.31, overall=31.31]	(449.34842, 5004.39)(450.3512, 1548.15)(451.3502, 337.542	C25 H44 N4 O3	FindByFormula	23	+	448.3407	17.285015
C25 H45 N O4	C25 H45 N O4	[C25 H45 N O4, tgt=98.98, overall=98.98]	(424.342, 17825.191)(425.34412, 5130.193)(426.34634, 940.	C25 H45 N O4	FindByFormula	28	+	423.335	21.08845
C25 H45 N O8	C25 H45 N O8	[C25 H45 N O8, tgt=82.04, overall=82.04]	(488.3197, 1036.3833)(489.32098, 742.95135)(490.31894, 12	C25 H45 N O8	FindByFormula	20	+	487.3098	5.327489
C25 H45 N14 P3	C25 H45 N14 P3	[C25 H45 N14 P3, tgt=89.41, overall=89.41]	(635.32056, 2017.5798)(636.3257, 1030.1917)(637.3229, 501	C25 H45 N14 P3	FindByFormula	9	+	634.313	14.880903
C25 H46 N7 O2 P S2	C25 H46 N7 O2 P S2	[C25 H46 N7 O2 P S2, tgt=82.20, overall=82.20]	(572.296, 13280.448)(573.30457, 4290.0435)(574.30414, 111	C25 H46 N7 O2 P S2	FindByFormula	21	+	571.2885	21.969872
C25 H47 N O4	C25 H47 N O4	[C25 H47 N O4, tgt=97.75, overall=97.75]	(426.3578, 12169.553)(427.359, 3696.0928)(428.3644, 1362.	C25 H47 N O4	FindByFormula	27	+	425.3499	21.559666
C25 H47 N3 O S3	C25 H47 N3 O S3	[C25 H47 N3 O S3, tgt=64.64, overall=64.64]	(502.29303, 1711.8961)(503.29904, 86.9125)(540.2469, 1597	C25 H47 N3 O S3	FindByFormula	27	+	501.2899	22.004158
C25 H47 N3 O5 S	C25 H47 N3 O5 S	[C25 H47 N3 O5 S, tgt=65.59, overall=65.59]	(502.329, 20521.48)(503.33157, 6785.014)(504.34012, 20868	C25 H47 N3 O5 S	FindByFormula	17	+	501.327	22.494976
C25 H48 N2 O3 S	C25 H48 N2 O3 S	[C25 H48 N2 O3 S, tgt=51.83, overall=51.83]	(457.34604, 25331.607)(458.3492, 7250.972)(459.34558, 248	C25 H48 N2 O3 S	FindByFormula	22	+	456.3404	22.75945
C25 H49 N O4	C25 H49 N O4	[C25 H49 N O4, tgt=84.96, overall=84.96]	(428.37195, 1702.7853)(429.37344, 665.62695)(430.38144, 8	C25 H49 N O4	FindByFormula	23	+	427.3633	21.881723
C25 H51 N O4	C25 H51 N O4	[C25 H51 N O4, tgt=89.88, overall=89.88]	(430.3885, 4073.2844)(431.38998, 1337.4008)(432.38797, 30	C25 H51 N O4	FindByFormula	27	+	429.381	21.826797
C25 H51 N2 O P S	C25 H51 N2 O P S	[C25 H51 N2 O P S, tgt=72.69, overall=72.69]	(459.35443, 22832.83)(460.35745, 6700.9727)(461.35394, 12	C25 H51 N2 O P S	FindByFormula	28	+	458.3483	21.708578
C25 H51 N5 O10 S	C25 H51 N5 O10 S	[C25 H51 N5 O10 S, tgt=87.87, overall=87.87]	(614.3422, 32051.613)(615.34503, 9975.589)(616.3477, 2599	C25 H51 N5 O10 S	FindByFormula	26	+	613.3389	22.64319
C25 H51 O2 P3	C25 H51 O2 P3	[C25 H51 O2 P3, tgt=1.84, overall=1.84]	(477.31552, 816.6625)(478.31665, 337.666)(479.31796, 394.	C25 H51 O2 P3	FindByFormula	14	+	476.313	21.872295
C25 H52 N6 O7 S2	C25 H52 N6 O7 S2	[C25 H52 N6 O7 S2, tgt=92.15, overall=92.15]	(613.33997, 8245.895)(614.34283, 2535.0396)(615.34094, 71	C25 H52 N6 O7 S2	FindByFormula	28	+	612.3333	11.198398
C25 H52 O3 P2	C25 H52 O3 P2	[C25 H52 O3 P2, tgt=92.38, overall=92.38]	(463.3437, 2351.142)(464.34317, 935.5086)(465.33963, 933.	C25 H52 O3 P2	FindByFormula	11	+	462.3346	22.779625
C25 H53 N O2	C25 H53 N O2	[C25 H53 N O2, tgt=95.21, overall=95.21]	(400.41312, 7808.608)(401.41556, 2429.0288)(402.41812, 57	C25 H53 N O2	FindByFormula	20	+	399.4067	22.383675
C25 H54 N4 O2 S2	C25 H54 N4 O2 S2	[C25 H54 N4 O2 S2, tgt=12.07, overall=12.07]	(507.37564, 3019.7498)(508.3784, 1013.4087)(509.3742, 261	C25 H54 N4 O2 S2	FindByFormula	24	+	506.3681	21.028948
C25 H55 N5 O3 P2 S2	C25 H55 N5 O3 P2 S2	[C25 H55 N5 O3 P2 S2, tgt=81.42, overall=81.42]	(600.32935, 9816.214)(601.3335, 3090.7092)(602.3306, 1598	C25 H55 N5 O3 P2 S2	FindByFormula	23	+	599.326	22.550123
C25 H56 N12 P2 S	C25 H56 N12 P2 S	[C25 H56 N12 P2 S, tgt=44.07, overall=44.07]	(619.4029, 10644.549)(620.4041, 4376.837)(621.39813, 1467	C25 H56 N12 P2 S	FindByFormula	22	+	618.3911	22.09414
C26 H20 N2 O4	C26 H20 N2 O4	[C26 H20 N2 O4, tgt=65.01, overall=65.01]	(425.14667, 2893.3298)(426.14532, 606.812)(427.1621, 53.5	C26 H20 N2 O4	FindByFormula	5	+	424.1384	17.99406
C26 H23 N6 O3 P	C26 H23 N6 O3 P	[C26 H23 N6 O3 P, tgt=90.09, overall=90.09]	(499.16473, 14611.394)(500.16733, 4405.0107)(501.17044, 1	C26 H23 N6 O3 P	FindByFormula	28	+	498.1568	18.394302
C26 H24 O2	C26 H24 O2	[C26 H24 O2, tgt=84.62, overall=84.62]	(369.18457, 3820.854)(370.18793, 962.93427)(371.1904, 177	C26 H24 O2	FindByFormula	8	+	368.1774	21.019737
C26 H26 N10 S	C26 H26 N10 S	[C26 H26 N10 S, tgt=61.14, overall=61.14]	(511.2138, 8028.909)(512.2159, 2741.4075)(513.2259, 647.8	C26 H26 N10 S	FindByFormula	27	+	510.205	21.990845
C26 H26 N2 O3 P2	C26 H26 N2 O3 P2	[C26 H26 N2 O3 P2, tgt=86.82, overall=86.82]	(477.14996, 3548.2698)(478.15387, 988.2878)(479.1539, 243	C26 H26 N2 O3 P2	FindByFormula	28	+	476.1426	17.457865
C26 H27 Cl O5	C26 H27 Cl O5	[C26 H27 Cl O5, tgt=53.71, overall=53.71]	(455.16226, 3984.2031)(456.16605, 1103.8689)(457.1616, 14	C26 H27 Cl O5	FindByFormula	26	+	454.1554	20.600939
C26 H28 N6 O S2	C26 H28 N6 O S2	[C26 H28 N6 O S2, tgt=65.03, overall=65.03]	(505.1829, 4137.5283)(506.18747, 1256.924)(507.1892, 193.	C26 H28 N6 O S2	FindByFormula	28	+	504.1755	18.720728
C26 H30 N14 O P2	C26 H30 N14 O P2	[C26 H30 N14 O P2, tgt=99.39, overall=99.39]	(617.22833, 2030.565)(618.22845, 772.86285)(619.2311, 210	C26 H30 N14 O P2	FindByFormula	8	+	616.2196	4.250602
C26 H31 N2 O3 P	C26 H31 N2 O3 P	[C26 H31 N2 O3 P, tgt=76.81, overall=76.81]	(451.21625, 1911.0643)(452.2205, 483.19565)(453.21155, 35	C26 H31 N2 O3 P	FindByFormula	28	+	450.206	8.634918
C26 H33 O6 P S	C26 H33 O6 P S	[C26 H33 O6 P S, tgt=66.88, overall=66.88]	(505.182, 8140.5425)(506.1851, 2397.9155)(507.18588, 714.	C26 H33 O6 P S	FindByFormula	27	+	504.174	18.405497
C26 H35 N11	C26 H35 N11	[C26 H35 N11, tgt=62.91, overall=62.91]	(502.3153, 12677.458)(503.31766, 4445.737)(504.31714, 112	C26 H35 N11	FindByFormula	27	+	501.3072	18.39347
C26 H35 N19 O	C26 H35 N19 O	[C26 H35 N19 O, tgt=76.70, overall=76.70]	(630.3325, 2080.3772)(631.3337, 950.0429)(632.32996, 325.	C26 H35 N19 O	FindByFormula	9	+	629.3257	21.225883
C26 H35 O4 P3	C26 H35 O4 P3	[C26 H35 O4 P3, tgt=72.67, overall=72.67]	(505.18295, 4800.9756)(506.18637, 1445.1868)(507.19247, 2	C26 H35 O4 P3	FindByFormula	28	+	504.1756	19.248352
C26 H36 O5	C26 H36 O5	[C26 H36 O5, tgt=77.36, overall=77.36]	(429.26416, 4177.6733)(430.26868, 1359.2064)(431.26828, 2	C26 H36 O5	FindByFormula	12	+	428.2566	22.335665
C26 H37 N O6	C26 H37 N O6	[C26 H37 N O6, tgt=99.17, overall=99.17]	(460.2697, 57484.758)(461.27274, 16609.879)(462.27554, 31	C26 H37 N O6	FindByFormula	28	+	459.2623	18.391119
C26 H37 N12 O P	C26 H37 N12 O P	[C26 H37 N12 O P, tgt=92.34, overall=92.34]	(565.30383, 96106.766)(566.3068, 30639.576)(567.3084, 730	C26 H37 N12 O P	FindByFormula	28	+	564.2975	19.783804
C26 H38 N10	C26 H38 N10	[C26 H38 N10, tgt=84.41, overall=84.41]	(491.33612, 665276.0)(492.3395, 217331.89)(493.34186, 365	C26 H38 N10	FindByFormula	17	+	490.329	5.498165
C26 H39 N3 O6	C26 H39 N3 O6	[C26 H39 N3 O6, tgt=96.60, overall=96.60]	(490.29117, 36682.98)(491.29468, 9365.21)(492.2977, 1856.	C26 H39 N3 O6	FindByFormula	28	+	489.2836	21.593554
C26 H40 S	C26 H40 S	[C26 H40 S, tgt=47.53, overall=47.53]	(385.29187, 43118.81)(386.2938, 10974.433)(387.28635, 278	C26 H40 S	FindByFormula	25	+	384.2854	22.35329
C26 H42 N6 O4	C26 H42 N6 O4	[C26 H42 N6 O4, tgt=98.06, overall=98.06]	(503.33414, 14103.052)(504.33734, 4550.0347)(505.3364, 10	C26 H42 N6 O4	FindByFormula	28	+	502.3261	17.901081
C26 H42 N6 O5	C26 H42 N6 O5	[C26 H42 N6 O5, tgt=99.59, overall=99.59]	(519.3295, 112282.33)(520.3326, 33958.586)(521.3348, 6963	C26 H42 N6 O5	FindByFormula	28	+	518.3217	17.782179
C26 H44 N14 P4	C26 H44 N14 P4	[C26 H44 N14 P4, tgt=91.21, overall=91.21]	(677.29095, 5252.632)(678.2911, 1813.0034)(679.2901, 568.	C26 H44 N14 P4	FindByFormula	6	+	676.2832	20.835445
C26 H44 N23 P	C26 H44 N23 P	[C26 H44 N23 P, tgt=45.83, overall=45.83]	(710.389, 123.972)(711.3939, 79.994)(748.35846, 89.326)(74	C26 H44 N23 P	FindByFormula	6	+	709.3865	3.6179829
C26 H44 N7 O5 P	C26 H44 N7 O5 P	[C26 H44 N7 O5 P, tgt=96.85, overall=96.85]	(566.3223, 40746.05)(567.3258, 12975.851)(568.3287, 3086.	C26 H44 N7 O5 P	FindByFormula	28	+	565.3155	22.004192
C26 H44 O4	C26 H44 O4	[C26 H44 O4, tgt=25.46, overall=25.46]	(421.32935, 5506.914)(422.33572, 1660.911)(423.337, 137.4	C26 H44 O4	FindByFormula	11	+	420.3241	22.17224
C26 H47 N4 O14 P	C26 H47 N4 O14 P	[C26 H47 N4 O14 P, tgt=96.15, overall=96.15]	(671.29095, 175628.48)(672.2937, 58555.617)(673.29407, 16	C26 H47 N4 O14 P	FindByFormula	9	+	670.2811	17.09928
C26 H47 N6 O4 P S	C26 H47 N6 O4 P S	[C26 H47 N6 O4 P S, tgt=92.69, overall=92.69]	(571.3204, 24209.006)(572.32367, 8014.1562)(573.32245, 21	C26 H47 N6 O4 P S	FindByFormula	28	+	570.313	19.78502
C26 H48 N O7 P	C26 H48 N O7 P	[C26 H48 N O7 P, tgt=76.28, overall=76.28]	(518.32294, 234098.9)(519.32574, 64265.57)(520.329, 12238	C26 H48 N O7 P	FindByFormula	28	+	517.3151	22.311293
C26 H48 N10 S3	C26 H48 N10 S3	[C26 H48 N10 S3, tgt=71.23, overall=71.23]	(597.33, 2741.7434)(598.3326, 1057.0549)(599.32275, 564.7	C26 H48 N10 S3	FindByFormula	28	+	596.3233	19.442717
C26 H48 N2 O2 S3	C26 H48 N2 O2 S3	[C26 H48 N2 O2 S3, tgt=64.93, overall=64.93]	(517.29254, 2904.1775)(518.2967, 1034.0997)(555.2606, 203	C26 H48 N2 O2 S3	FindByFormula	28	+	516.2854	19.587566
C26 H48 N3 O11 P	C26 H48 N3 O11 P	[C26 H48 N3 O11 P, tgt=99.24, overall=99.24]	(610.3097, 68304.28)(611.314, 20564.514)(612.3172, 4712.2	C26 H48 N3 O11 P	FindByFormula	28	+	609.3028	22.117825
C26 H50 N O2 P S2	C26 H50 N O2 P S2	[C26 H50 N O2 P S2, tgt=79.09, overall=79.09]	(504.31113, 4416.9277)(505.31378, 1850.3217)(506.3145, 58	C26 H50 N O2 P S2	FindByFormula	25	+	503.3031	21.893631
C26 H50 N O7 P	C26 H50 N O7 P	[C26 H50 N O7 P, tgt=95.39, overall=95.39]	(520.3373, 26170.385)(521.3318, 7390.89)(522.3358, 1661.6	C26 H50 N O7 P	FindByFormula	28	+	519.3333	22.129704
C26 H50 N3 O11 P	C26 H50 N3 O11 P	[C26 H50 N3 O11 P, tgt=99.26, overall=99.26]	(612.3253, 73599.3)(613.33, 22842.906)(614.3366, 5123.162	C26 H50 N3 O11 P	FindByFormula	28	+	611.3179	22.444288
C26 H50 P6	C26 H50 P6	[C26 H50 P6, tgt=96.25, overall=96.25]	(549.2403, 4337.1753)(550.2432, 1307.805)(551.24286, 296.	C26 H50 P6	FindByFormula	6	+	548.2331	4.28041
C26 H51 N3 O S2	C26 H51 N3 O S2	[C26 H51 N3 O S2, tgt=22.88, overall=22.88]	(486.35425, 5994.217)(487.35422, 1810.2073)(488.35092, 44	C26 H51 N3 O S2	FindByFormula	21	+	485.3467	21.442598
C26 H51 N4 O2 P S	C26 H51 N4 O2 P S	[C26 H51 N4 O2 P S, tgt=52.60, overall=52.60]	(515.3507, 7015.813)(516.35736, 2313.5952)(517.3615, 2130	C26 H51 N4 O2 P S	FindByFormula	19	+	514.3488	22.540384
C26 H51 N4 O3 P S	C26 H51 N4 O3 P S	[C26 H51 N4 O3 P S, tgt=60.89, overall=60.89]	(531.3495, 12771.375)(532.3512, 4095.139)(533.347, 1265.6	C26 H51 N4 O3 P S	FindByFormula	21	+	530.341	22.025705
C26 H51 N7 O4	C26 H51 N7 O4	[C26 H51 N7 O4, tgt=81.76, overall=81.76]	(526.40875, 2988.6719)(527.4112, 1169.3086)(528.4115, 302	C26 H51 N7 O4	FindByFormula	28	+	525.4007	19.786808
C26 H52 N O7 P	C26 H52 N O7 P	[C26 H52 N O7 P, tgt=99.84, overall=99.84]	(522.3534, 11682.776)(523.35345, 4237.892)(524.35394, 102	C26 H52 N O7 P	FindByFormula	28	+	521.3485	22.44872
C26 H52 N2 O2 P2 S	C26 H52 N2 O2 P2 S	[C26 H52 N2 O2 P2 S, tgt=96.21, overall=96.21]	(519.32886, 7913.934)(520.3321, 2595.6365)(521.32874, 632	C26 H52 N2 O2 P2 S	FindByFormula	28	+	518.321	17.410748
C26 H52 N2 O2 S2	C26 H52 N2 O2 S2	[C26 H52 N2 O2 S2, tgt=77.84, overall=77.84]	(489.3554, 3202.3367)(490.3546, 1198.0643)(491.35144, 177	C26 H52 N2 O2 S2	FindByFormula	21	+	488.3457	22.736023
C26 H52 N2 S3	C26 H52 N2 S3	[C26 H52 N2 S3, tgt=49.82, overall=49.82]	(489.3375, 2872.375)(490.3364, 989.5863)(491.3307, 518.17	C26 H52 N2 S3	FindByFormula	23	+	488.3304	21.735903
C26 H52 N3 O11 P	C26 H52 N3 O11 P	[C26 H52 N3 O11 P, tgt=96.54, overall=96.54]	(614.3421, 51933.23)(615.3458, 15854.354)(616.3496, 4063.	C26 H52 N3 O11 P	FindByFormula	25	+	613.3341	22.700445
C26 H53 N4 O P S	C26 H53 N4 O P S	[C26 H53 N4 O P S, tgt=49.91, overall=49.91]	(501.37582, 23502.1)(502.3789, 7024.1885)(503.37567, 2244	C26 H53 N4 O P S	FindByFormula	24	+	500.3675	22.7097
C26 H54 N O7 P	C26 H54 N O7 P	[C26 H54 N O7 P, tgt=96.58, overall=96.58]	(524.36804, 6531.595)(525.365, 2813.731)(526.3605, 1536.6	C26 H54 N O7 P	FindByFormula	25	+	523.3639	22.696367
C26 H54 N6 O S2	C26 H54 N6 O S2	[C26 H54 N6 O S2, tgt=41.68, overall=41.68]	(531.38605, 14600.092)(532.3859, 4702.071)(533.37915, 149	C26 H54 N6 O S2	FindByFormula	20	+	530.3765	22.559984
C26 H55 N O2	C26 H55 N O2	[C26 H55 N O2, tgt=55.24, overall=55.24]	(414.43054, 18545.764)(415.43243, 5933.0474)(416.4329, 10	C26 H55 N O2	FindByFormula	24	+	413.4234	22.465693
C26 H55 N12 O2 P	C26 H55 N12 O2 P	[C26 H55 N12 O2 P, tgt=99.42, overall=99.42]	(599.4357, 43918.785)(600.4379, 21203.762)(601.4427, 6270	C26 H55 N12 O2 P	FindByFormula	20	+	598.4307	22.427238
C26 H55 N5 S5	C26 H55 N5 S5	[C26 H55 N5 S5, tgt=55.46, overall=55.46]	(598.3112, 1609.7476)(599.31555, 822.2988)(600.3089, 439.	C26 H55 N5 S5	FindByFormula	20	+	597.3027	22.09432
C26 H56 N2 O9 P2 S	C26 H56 N2 O9 P2 S	[C26 H56 N2 O9 P2 S, tgt=24.99, overall=24.99]	(635.3306, 62.93)(673.28314, 268.7575)(674.28845, 357.949	C26 H56 N2 O9 P2 S	FindByFormula	4	+	634.3183	11.45142
C26 H58 N P3 S	C26 H58 N P3 S	[C26 H58 N P3 S, tgt=89.97, overall=89.97]	(510.34973, 306.21667)(548.3183, 963.07996)(549.3213, 198	C26 H58 N P3 S	FindByFormula	10	+	509.3503	22.520315
C26 H58 N4 O2 S2	C26 H58 N4 O2 S2	[C26 H58 N4 O2 S2, tgt=47.46, overall=47.46]	(523.4056, 1856.1204)(524.409, 698.1734)(525.40375, 202.6	C26 H58 N4 O2 S2	FindByFormula	23	+	522.3986	21.242743
C27 H18 N4 O S3	C27 H18 N4 O S3	[C27 H18 N4 O S3, tgt=37.96, overall=37.96]	(511.0682, 227.59001)(512.06964, 93.57666)(513.06824, 55.	C27 H18 N4 O S3	FindByFormula	7	+	510.0601	8.641913
C27 H25 N6 O4 P	C27 H25 N6 O4 P	[C27 H25 N6 O4 P, tgt=19.47, overall=19.47]	(529.17474, 2292.5308)(530.1778, 644.3974)(531.1736, 90.8	C27 H25 N6 O4 P	FindByFormula	19	+	528.1678	22.744892
C27 H30 N6 O2 P4	C27 H30 N6 O2 P4	[C27 H30 N6 O2 P4, tgt=28.59, overall=28.59]	(595.14746, 195.75713)(596.1457, 99.23334)(633.10614, 236	C27 H30 N6 O2 P4	FindByFormula	9	+	594.1411	22.390451
C27 H32 N6 O2 P4	C27 H32 N6 O2 P4	[C27 H32 N6 O2 P4, tgt=91.86, overall=91.86]	(597.1599, 1974.7943)(598.16394, 624.83405)(599.1639, 183	C27 H32 N6 O2 P4	FindByFormula	21	+	596.1526	22.75801
C27 H33 N5 O2	C27 H33 N5 O2	[C27 H33 N5 O2, tgt=64.12, overall=64.12]	(460.26944, 7794.5547)(461.27286, 2406.6914)(462.27228, 5	C27 H33 N5 O2	FindByFormula	28	+	459.2624	18.659868
C27 H34 N2 O P2	C27 H34 N2 O P2	[C27 H34 N2 O P2, tgt=66.00, overall=66.00]	(465.22162, 3069.9526)(466.22433, 886.35956)(467.22208, 3	C27 H34 N2 O P2	FindByFormula	28	+	464.2157	13.103666
C27 H34 N7 P	C27 H34 N7 P	[C27 H34 N7 P, tgt=96.07, overall=96.07]	(488.2684, 4943.7524)(489.26996, 2040.3727)(490.26904, 52	C27 H34 N7 P	FindByFormula	10	+	487.2603	20.282703
C27 H35 N23 P2	C27 H35 N23 P2	[C27 H35 N23 P2, tgt=73.86, overall=73.86]	(744.29724, 1423.0342)(745.3033, 716.54)(746.29553, 491.6	C27 H35 N23 P2	FindByFormula	8	+	743.2919	22.642082
C27 H36 N10	C27 H36 N10	[C27 H36 N10, tgt=85.11, overall=85.11]	(501.3188, 30391.303)(502.32175, 9834.539)(503.3339, 3959	C27 H36 N10	FindByFormula	28	+	500.3119	19.571444
C27 H37 N11 P2	C27 H37 N11 P2	[C27 H37 N11 P2, tgt=76.08, overall=76.08]	(578.27936, 1795.7542)(579.28564, 1133.8667)(580.28326, 6	C27 H37 N11 P2	FindByFormula	6	+	577.2765	21.843561
C27 H38 N10	C27 H38 N10	[C27 H38 N10, tgt=99.13, overall=99.13]	(503.3353, 311269.66)(504.33832, 96929.49)(505.3406, 1804	C27 H38 N10	FindByFormula	28	+	502.3281	19.443829
C27 H39 N5 O12	C27 H39 N5 O12	[C27 H39 N5 O12, tgt=95.87, overall=95.87]	(626.2617, 6165.689)(627.2705, 2026.3248)(628.2655, 1151.	C27 H39 N5 O12	FindByFormula	14	+	625.2552	21.744442
C27 H40 N12 O4	C27 H40 N12 O4	[C27 H40 N12 O4, tgt=79.46, overall=79.46]	(597.3352, 490.1162)(598.3368, 234.77002)(599.33844, 55.1	C27 H40 N12 O4	FindByFormula	11	+	596.3255	6.4351063
C27 H41 N5	C27 H41 N5	[C27 H41 N5, tgt=91.09, overall=91.09]	(436.34424, 10906.289)(437.34476, 4237.307)(438.34305, 85	C27 H41 N5	FindByFormula	18	+	435.3343	23.086964
C27 H41 N8 O P3	C27 H41 N8 O P3	[C27 H41 N8 O P3, tgt=81.05, overall=81.05]	(587.26953, 2286.7642)(588.27386, 846.22003)(589.27655, 3	C27 H41 N8 O P3	FindByFormula	5	+	586.2628	15.602768
C27 H41 N9 O12 S	C27 H41 N9 O12 S	[C27 H41 N9 O12 S, tgt=94.99, overall=94.99]	(716.26874, 2626.9531)(717.27094, 946.0175)(718.2698, 469	C27 H41 N9 O12 S	FindByFormula	25	+	715.2594	22.277546
C27 H43 N3 P2	C27 H43 N3 P2	[C27 H43 N3 P2, tgt=87.42, overall=87.42]	(472.3011, 1477.328)(473.2996, 553.41895)(474.29947, 92.9	C27 H43 N3 P2	FindByFormula	10	+	471.293	17.686605
C27 H43 N7 O16	C27 H43 N7 O16	[C27 H43 N7 O16, tgt=91.65, overall=91.65]	(722.2849, 2925.153)(723.28955, 1060.714)(724.2866, 314.7	C27 H43 N7 O16	FindByFormula	23	+	721.276	22.236998
C27 H44	C27 H44	[C27 H44, tgt=97.49, overall=97.49]	(369.35184, 3650.7256)(370.3554, 1144.643)(371.3544, 240.	C27 H44	FindByFormula	17	+	368.3442	24.587894
C27 H46 N6 O6	C27 H46 N6 O6	[C27 H46 N6 O6, tgt=95.56, overall=95.56]	(551.3551, 128912.06)(552.35846, 40279.9)(553.361, 8479.5	C27 H46 N6 O6	FindByFormula	28	+	550.3498	22.205137
C27 H47 N4 O P3 S2	C27 H47 N4 O P3 S2	[C27 H47 N4 O P3 S2, tgt=32.30, overall=32.30]	(601.24866, 6376.999)(602.2524, 1951.8828)(603.2576, 1150	C27 H47 N4 O P3 S2	FindByFormula	7	+	600.2409	14.664668
C27 H48 N3 O13 P	C27 H48 N3 O13 P	[C27 H48 N3 O13 P, tgt=85.76, overall=85.76]	(654.29926, 9243.919)(655.3072, 3003.9487)(656.3095, 805.	C27 H48 N3 O13 P	FindByFormula	26	+	653.2899	22.31194
C27 H48 N6 O S2	C27 H48 N6 O S2	[C27 H48 N6 O S2, tgt=47.08, overall=47.08]	(537.3396, 37530.41)(538.3426, 11795.687)(539.33966, 2712	C27 H48 N6 O S2	FindByFormula	25	+	536.3341	21.829859
C27 H49 N4 O2 P5	C27 H49 N4 O2 P5	[C27 H49 N4 O2 P5, tgt=91.97, overall=91.97]	(617.2643, 1357.5277)(618.26794, 594.9036)(619.2657, 330.	C27 H49 N4 O2 P5	FindByFormula	22	+	616.2541	3.5981607
C27 H50 N O2 P S2	C27 H50 N O2 P S2	[C27 H50 N O2 P S2, tgt=85.44, overall=85.44]	(516.30634, 41607.324)(517.3106, 11552.201)(518.3143, 435	C27 H50 N O2 P S2	FindByFormula	27	+	515.2986	21.871777
C27 H50 N O4 P S	C27 H50 N O4 P S	[C27 H50 N O4 P S, tgt=76.10, overall=76.10]	(516.32526, 9507.402)(517.3261, 3038.8625)(518.326, 1269.	C27 H50 N O4 P S	FindByFormula	25	+	515.3191	21.562124
C27 H50 N7 P S2	C27 H50 N7 P S2	[C27 H50 N7 P S2, tgt=90.60, overall=90.60]	(568.3374, 14943.574)(569.338, 5109.027)(570.3401, 1922.8	C27 H50 N7 P S2	FindByFormula	27	+	567.3332	22.359367
C27 H51 N3 O6 S	C27 H51 N3 O6 S	[C27 H51 N3 O6 S, tgt=79.69, overall=79.69]	(546.3554, 84456.88)(547.3582, 24961.055)(548.35974, 5749	C27 H51 N3 O6 S	FindByFormula	27	+	545.3473	22.6788
C27 H51 N5 O3 S3	C27 H51 N5 O3 S3	[C27 H51 N5 O3 S3, tgt=63.27, overall=63.27]	(590.3212, 14635.371)(591.3242, 4977.263)(592.32764, 2814	C27 H51 N5 O3 S3	FindByFormula	12	+	589.3173	22.076927
C27 H51 O2 P3	C27 H51 O2 P3	[C27 H51 O2 P3, tgt=81.82, overall=81.82]	(501.31778, 9307.244)(502.3209, 3228.343)(539.2747, 278.8	C27 H51 O2 P3	FindByFormula	28	+	500.3096	19.77492
C27 H51 O3 P S2	C27 H51 O3 P S2	[C27 H51 O3 P S2, tgt=98.74, overall=98.74]	(519.3083, 19537.691)(520.3114, 6334.999)(521.3092, 2799.	C27 H51 O3 P S2	FindByFormula	28	+	518.3008	19.44808
C27 H51 O4 P S2	C27 H51 O4 P S2	[C27 H51 O4 P S2, tgt=93.51, overall=93.51]	(535.30316, 7282.214)(536.3062, 2409.6833)(537.3023, 1264	C27 H51 O4 P S2	FindByFormula	28	+	534.295	18.692492
C27 H52 S2	C27 H52 S2	[C27 H52 S2, tgt=39.56, overall=39.56]	(441.359, 8171.5024)(442.36362, 1200.7275)(443.356, 945.3	C27 H52 S2	FindByFormula	10	+	440.3506	22.941399
C27 H54 N2 O2 P4 S2	C27 H54 N2 O2 P4 S2	[C27 H54 N2 O2 P4 S2, tgt=91.53, overall=91.53]	(627.2651, 3335.0073)(628.2668, 1190.7285)(629.26886, 380	C27 H54 N2 O2 P4 S2	FindByFormula	7	+	626.2576	16.910398
C27 H54 N2 S3	C27 H54 N2 S3	[C27 H54 N2 S3, tgt=17.22, overall=17.22]	(503.35193, 5873.354)(504.35, 1767.2905)(505.35446, 398.6	C27 H54 N2 S3	FindByFormula	22	+	502.3445	22.033274
C27 H54 N5 P S	C27 H54 N5 P S	[C27 H54 N5 P S, tgt=84.16, overall=84.16]	(512.39325, 3780.2947)(513.3947, 1478.6075)(514.3929, 398	C27 H54 N5 P S	FindByFormula	28	+	511.3856	19.785803
C27 H56 Cl3 N P2 S2	C27 H56 Cl3 N P2 S2	[C27 H56 Cl3 N P2 S2, tgt=81.08, overall=81.08]	(626.2472, 10420.782)(627.2531, 3752.405)(628.2445, 13711	C27 H56 Cl3 N P2 S2	FindByFormula	6	+	625.2413	21.86531
C27 H57 N O2	C27 H57 N O2	[C27 H57 N O2, tgt=82.09, overall=82.09]	(428.44473, 1298.3275)(429.4476, 588.2592)(430.44727, 141	C27 H57 N O2	FindByFormula	17	+	427.4383	22.517113
C28 H19 N8 P3	C28 H19 N8 P3	[C28 H19 N8 P3, tgt=65.58, overall=65.58]	(561.1011, 1970.4479)(562.1047, 614.9434)(563.1018, 218.4	C28 H19 N8 P3	FindByFormula	24	+	560.0932	16.432028
C28 H24 N9 O P	C28 H24 N9 O P	[C28 H24 N9 O P, tgt=94.30, overall=94.30]	(534.1924, 1797.8295)(535.1951, 629.20776)(536.1917, 174.	C28 H24 N9 O P	FindByFormula	26	+	533.1824	2.5186064
C28 H34 O S	C28 H34 O S	[C28 H34 O S, tgt=79.67, overall=79.67]	(419.24002, 3960.6897)(420.24484, 1057.6595)(421.23975, 3	C28 H34 O S	FindByFormula	28	+	418.2325	18.594587
C28 H36 O4 P2	C28 H36 O4 P2	[C28 H36 O4 P2, tgt=89.21, overall=89.21]	(499.21695, 2681.05)(500.22, 785.44336)(501.21893, 280.45	C28 H36 O4 P2	FindByFormula	6	+	498.2089	14.735652
C28 H37 N15 O	C28 H37 N15 O	[C28 H37 N15 O, tgt=77.66, overall=77.66]	(600.3341, 374.742)(601.3384, 142.86398)(602.3399, 40.976	C28 H37 N15 O	FindByFormula	6	+	599.3287	2.963043
C28 H37 N4 O P S2	C28 H37 N4 O P S2	[C28 H37 N4 O P S2, tgt=66.36, overall=66.36]	(541.22125, 5474.025)(542.225, 1987.6185)(543.2337, 504.4	C28 H37 N4 O P S2	FindByFormula	23	+	540.2152	21.637371
C28 H38 O6 P6	C28 H38 O6 P6	[C28 H38 O6 P6, tgt=77.65, overall=77.65]	(657.1143, 716.41174)(658.11237, 299.24252)(659.11224, 15	C28 H38 O6 P6	FindByFormula	21	+	656.1129	22.496696
C28 H40 O8	C28 H40 O8	[C28 H40 O8, tgt=86.98, overall=86.98]	(505.27698, 2067.5383)(506.27795, 688.89667)(507.2786, 16	C28 H40 O8	FindByFormula	7	+	504.2689	4.2823663
C28 H41 N O6	C28 H41 N O6	[C28 H41 N O6, tgt=92.91, overall=92.91]	(488.3011, 83888.625)(489.3038, 26245.494)(490.30524, 547	C28 H41 N O6	FindByFormula	28	+	487.2935	18.393124
C28 H41 N5 S	C28 H41 N5 S	[C28 H41 N5 S, tgt=65.77, overall=65.77]	(480.31293, 1710.5302)(481.31824, 1000.31274)(482.31302,	C28 H41 N5 S	FindByFormula	22	+	479.3113	22.326628
C28 H41 N8 O2 P3	C28 H41 N8 O2 P3	[C28 H41 N8 O2 P3, tgt=32.78, overall=32.78]	(615.26514, 1479.7699)(616.2729, 605.74854)(617.2689, 229	C28 H41 N8 O2 P3	FindByFormula	7	+	614.2591	16.206585
C28 H43 N O8 S2	C28 H43 N O8 S2	[C28 H43 N O8 S2, tgt=47.77, overall=47.77]	(586.24994, 4379.2715)(587.25323, 1541.6932)(588.2541, 55	C28 H43 N O8 S2	FindByFormula	24	+	585.2416	9.536348
C28 H44 N4 O7 S	C28 H44 N4 O7 S	[C28 H44 N4 O7 S, tgt=73.92, overall=73.92]	(581.29913, 5689.261)(582.3024, 1969.8894)(583.3011, 758.	C28 H44 N4 O7 S	FindByFormula	28	+	580.2919	18.841715
C28 H44 N6 O14	C28 H44 N6 O14	[C28 H44 N6 O14, tgt=99.43, overall=99.43]	(689.3, 21264.816)(690.30255, 7251.252)(691.306, 2307.966	C28 H44 N6 O14	FindByFormula	9	+	688.2932	15.171871
C28 H44 O4	C28 H44 O4	[C28 H44 O4, tgt=96.58, overall=96.58]	(445.33124, 9038.958)(446.3344, 2988.0437)(447.33292, 682	C28 H44 O4	FindByFormula	28	+	444.3236	19.445618
C28 H45 N7 O4 P2	C28 H45 N7 O4 P2	[C28 H45 N7 O4 P2, tgt=91.91, overall=91.91]	(606.30804, 5809.9873)(607.3108, 2952.5422)(608.31256, 13	C28 H45 N7 O4 P2	FindByFormula	15	+	605.3024	22.287672
C28 H46 N3 O11 P	C28 H46 N3 O11 P	[C28 H46 N3 O11 P, tgt=98.95, overall=98.95]	(632.2974, 11117.661)(633.2999, 4510.7563)(634.3018, 1548	C28 H46 N3 O11 P	FindByFormula	21	+	631.2893	21.773819
C28 H47 N4 O15 P	C28 H47 N4 O15 P	[C28 H47 N4 O15 P, tgt=84.17, overall=84.17]	(711.28217, 3799.0513)(712.2861, 1459.5642)(713.2893, 457	C28 H47 N4 O15 P	FindByFormula	7	+	710.2745	15.175375
C28 H47 N4 O7 P3	C28 H47 N4 O7 P3	[C28 H47 N4 O7 P3, tgt=94.57, overall=94.57]	(645.27325, 5291.7676)(646.2769, 1852.7389)(647.28485, 79	C28 H47 N4 O7 P3	FindByFormula	9	+	644.2681	14.742915
C28 H47 N4 P S	C28 H47 N4 P S	[C28 H47 N4 P S, tgt=95.85, overall=95.85]	(503.33398, 8781.877)(504.33682, 2898.0854)(505.33237, 68	C28 H47 N4 P S	FindByFormula	28	+	502.3262	18.984655
C28 H48 N3 O11 P	C28 H48 N3 O11 P	[C28 H48 N3 O11 P, tgt=99.37, overall=99.37]	(634.31, 23469.44)(635.3139, 7952.95)(636.318, 2014.5096)(	C28 H48 N3 O11 P	FindByFormula	28	+	633.3033	22.00562
C28 H48 N6 O S	C28 H48 N6 O S	[C28 H48 N6 O S, tgt=37.45, overall=37.45]	(517.37085, 49316.43)(518.3636, 16598.18)(519.356, 6058.8	C28 H48 N6 O S	FindByFormula	20	+	516.3611	22.371302
C28 H49 N4 P3	C28 H49 N4 P3	[C28 H49 N4 P3, tgt=77.69, overall=77.69]	(535.32336, 4217.958)(536.3263, 1412.067)(537.3212, 346.0	C28 H49 N4 P3	FindByFormula	28	+	534.316	16.26977
C28 H49 N5 O2 S3	C28 H49 N5 O2 S3	[C28 H49 N5 O2 S3, tgt=68.92, overall=68.92]	(584.31024, 1776.5189)(585.3151, 1045.6215)(586.3138, 807	C28 H49 N5 O2 S3	FindByFormula	10	+	583.3074	21.528076
C28 H50 N O7 P	C28 H50 N O7 P	[C28 H50 N O7 P, tgt=93.37, overall=93.37]	(544.3376, 193433.9)(545.34393, 57504.23)(546.3481, 11498	C28 H50 N O7 P	FindByFormula	28	+	543.3304	22.449045
C28 H52 N O2 P S2	C28 H52 N O2 P S2	[C28 H52 N O2 P S2, tgt=84.93, overall=84.93]	(530.3229, 5173.884)(531.3299, 1692.2062)(532.3252, 714.0	C28 H52 N O2 P S2	FindByFormula	18	+	529.3172	22.193663
C28 H52 N3 P S3	C28 H52 N3 P S3	[C28 H52 N3 P S3, tgt=81.17, overall=81.17]	(558.3117, 1751.4376)(559.3109, 881.3167)(560.3132, 438.2	C28 H52 N3 P S3	FindByFormula	22	+	557.3063	19.87142
C28 H53 Cl O P2	C28 H53 Cl O P2	[C28 H53 Cl O P2, tgt=74.80, overall=74.80]	(503.33267, 2922.7173)(504.33548, 984.5893)(505.3291, 691	C28 H53 Cl O P2	FindByFormula	28	+	502.3256	18.745874
C28 H53 N5 O5 S3	C28 H53 N5 O5 S3	[C28 H53 N5 O5 S3, tgt=71.51, overall=71.51]	(636.3265, 4733.983)(637.3344, 1795.0128)(638.3343, 1083.	C28 H53 N5 O5 S3	FindByFormula	25	+	635.3155	22.309586
C28 H54 N2 O	C28 H54 N2 O	[C28 H54 N2 O, tgt=41.28, overall=41.28]	(435.43225, 8109.4272)(436.43448, 2632.3271)(437.44293, 2	C28 H54 N2 O	FindByFormula	12	+	434.4247	23.58483
C28 H55 N4 O4 P S	C28 H55 N4 O4 P S	[C28 H55 N4 O4 P S, tgt=38.19, overall=38.19]	(575.3752, 11382.867)(576.3764, 3957.8486)(577.3728, 1270	C28 H55 N4 O4 P S	FindByFormula	23	+	574.3696	22.048056
C28 H56 N2 O6 S2	C28 H56 N2 O6 S2	[C28 H56 N2 O6 S2, tgt=60.40, overall=60.40]	(581.3648, 35234.277)(582.3659, 11815.715)(583.36456, 272	C28 H56 N2 O6 S2	FindByFormula	27	+	580.3596	21.860317
C28 H57 Cl O P2	C28 H57 Cl O P2	[C28 H57 Cl O P2, tgt=68.30, overall=68.30]	(507.3619, 4753.9)(508.36465, 1669.9618)(509.3664, 1928.4	C28 H57 Cl O P2	FindByFormula	6	+	506.3545	22.542145
C28 H57 N O5 P4	C28 H57 N O5 P4	[C28 H57 N O5 P4, tgt=76.27, overall=76.27]	(612.32574, 60166.31)(613.3305, 18739.48)(614.3343, 4362.	C28 H57 N O5 P4	FindByFormula	28	+	611.3196	22.363247
C28 H57 N3 P4 S4	C28 H57 N3 P4 S4	[C28 H57 N3 P4 S4, tgt=50.15, overall=50.15]	(688.2462, 920.83203)(689.24554, 389.82333)(690.2411, 382	C28 H57 N3 P4 S4	FindByFormula	16	+	687.2451	22.133482
C28 H57 N4 O3 P S	C28 H57 N4 O3 P S	[C28 H57 N4 O3 P S, tgt=65.99, overall=65.99]	(561.3976, 34694.406)(562.3983, 11375.93)(563.392, 3881.9	C28 H57 N4 O3 P S	FindByFormula	27	+	560.3894	22.400608
C28 H57 N4 O9 P S	C28 H57 N4 O9 P S	[C28 H57 N4 O9 P S, tgt=97.71, overall=97.71]	(657.36566, 3750.4304)(658.3674, 1279.2307)(659.3636, 394	C28 H57 N4 O9 P S	FindByFormula	28	+	656.3576	11.6789255
C28 H59 N P2 S3	C28 H59 N P2 S3	[C28 H59 N P2 S3, tgt=87.45, overall=87.45]	(568.3362, 8289.192)(569.33453, 3027.3672)(570.3348, 1298	C28 H59 N P2 S3	FindByFormula	26	+	567.3301	22.273794
C29 H15 N8 O2 P	C29 H15 N8 O2 P	[C29 H15 N8 O2 P, tgt=72.59, overall=72.59]	(539.1136, 1429.2316)(540.1152, 398.88037)(541.1119, 106.	C29 H15 N8 O2 P	FindByFormula	26	+	538.1047	22.464914
C29 H30	C29 H30	[C29 H30, tgt=70.34, overall=70.34]	(379.24274, 1377.0852)(380.24542, 430.08337)(381.23746, 5	C29 H30	FindByFormula	21	+	378.2384	19.761353
C29 H32 N18 P2	C29 H32 N18 P2	[C29 H32 N18 P2, tgt=90.29, overall=90.29]	(695.2621, 3649.7163)(696.2661, 1443.166)(697.2694, 538.5	C29 H32 N18 P2	FindByFormula	28	+	694.255	19.784197
C29 H42 N18	C29 H42 N18	[C29 H42 N18, tgt=39.48, overall=39.48]	(643.39154, 792.30133)(644.3936, 652.8884)(645.3823, 323.	C29 H42 N18	FindByFormula	15	+	642.3828	22.560907
C29 H42 N8 S2	C29 H42 N8 S2	[C29 H42 N8 S2, tgt=93.89, overall=93.89]	(567.30505, 1713.0553)(568.30554, 633.3352)(569.3003, 449	C29 H42 N8 S2	FindByFormula	19	+	566.2954	20.688675
C29 H43 O P	C29 H43 O P	[C29 H43 O P, tgt=60.58, overall=60.58]	(439.31207, 1940.9408)(440.31488, 702.088)(441.32184, 318	C29 H43 O P	FindByFormula	12	+	438.3044	21.89984
C29 H45 N3 O P2	C29 H45 N3 O P2	[C29 H45 N3 O P2, tgt=96.57, overall=96.57]	(514.3108, 13483.456)(515.3136, 4377.1685)(516.3141, 1003	C29 H45 N3 O P2	FindByFormula	26	+	513.3033	21.079475
C29 H45 N4 O P5	C29 H45 N4 O P5	[C29 H45 N4 O P5, tgt=93.90, overall=93.90]	(621.2347, 1632.2725)(622.24255, 617.88104)(623.2402, 131	C29 H45 N4 O P5	FindByFormula	12	+	620.2298	21.590067
C29 H46 N2 O2 S2	C29 H46 N2 O2 S2	[C29 H46 N2 O2 S2, tgt=93.15, overall=93.15]	(519.3078, 20962.396)(520.31116, 6831.3564)(521.3086, 304	C29 H46 N2 O2 S2	FindByFormula	28	+	518.3006	19.837225
C29 H46 N6 O14	C29 H46 N6 O14	[C29 H46 N6 O14, tgt=58.85, overall=58.85]	(703.317, 1919.0674)(704.3166, 760.2634)(705.3209, 348.09	C29 H46 N6 O14	FindByFormula	20	+	702.3075	16.59345

C29 H46 N7 O P3	C29 H46 N7 O P3	[C29 H46 N7 O P3, tgt=93.20, overall=93.20]	(602.3043, 1811.0023)(603.30646, 824.80145)(604.30334, 31	C29 H46 N7 O P3	FindByFormula	8 +	601.2963	18.945698
C29 H46 O4	C29 H46 O4	[C29 H46 O4, tgt=87.82, overall=87.82]	(459.34604, 2092.8608)(460.34702, 750.98035)(461.34476, 1	C29 H46 O4	FindByFormula	28 +	458.3378	19.447906
C29 H47 N5 O3 P2 S	C29 H47 N5 O3 P2 S	[C29 H47 N5 O3 P2 S, tgt=77.73, overall=77.73]	(608.295, 8022.244)(609.2961, 2802.8435)(610.3056, 1790.0	C29 H47 N5 O3 P2 S	FindByFormula	19 +	607.2872	21.76849
C29 H47 O3 P S3	C29 H47 O3 P S3	[C29 H47 O3 P S3, tgt=25.38, overall=25.38]	(571.2488, 4395.209)(572.2535, 1478.9712)(573.25494, 461.	C29 H47 O3 P S3	FindByFormula	24 +	570.2419	7.7273707
C29 H48 N O8 P	C29 H48 N O8 P	[C29 H48 N O8 P, tgt=85.75, overall=85.75]	(570.3189, 13343.787)(571.32324, 4346.2324)(572.3297, 226	C29 H48 N O8 P	FindByFormula	15 +	569.3109	22.466986
C29 H49 N3 P2 S	C29 H49 N3 P2 S	[C29 H49 N3 P2 S, tgt=59.44, overall=59.44]	(534.31995, 3557.5574)(535.3228, 1375.92)(536.3176, 377.3	C29 H49 N3 P2 S	FindByFormula	24 +	533.3128	21.824152
C29 H49 N4 O P S3	C29 H49 N4 O P S3	[C29 H49 N4 O P S3, tgt=66.78, overall=66.78]	(597.2899, 2812.4185)(598.2901, 932.72925)(599.29114, 529	C29 H49 N4 O P S3	FindByFormula	26 +	596.2821	20.11911
C29 H50 N5 O2 P S3	C29 H50 N5 O2 P S3	[C29 H50 N5 O2 P S3, tgt=81.99, overall=81.99]	(628.2942, 2506.2427)(629.2975, 1092.6958)(630.2959, 608.	C29 H50 N5 O2 P S3	FindByFormula	19 +	627.2884	22.108198
C29 H50 N6 O7	C29 H50 N6 O7	[C29 H50 N6 O7, tgt=99.12, overall=99.12]	(595.382, 147048.36)(596.38513, 49834.73)(597.38715, 1107	C29 H50 N6 O7	FindByFormula	28 +	594.3754	22.220516
C29 H50 N7 P S2	C29 H50 N7 P S2	[C29 H50 N7 P S2, tgt=88.31, overall=88.31]	(592.33466, 4999.924)(593.33795, 1908.0178)(594.33527, 77	C29 H50 N7 P S2	FindByFormula	20 +	591.3342	22.219652
C29 H55 N3 O3 S3	C29 H55 N3 O3 S3	[C29 H55 N3 O3 S3, tgt=58.06, overall=58.06]	(590.3473, 2597.9207)(591.35016, 1411.2784)(592.342, 1233	C29 H55 N3 O3 S3	FindByFormula	28 +	589.3361	22.40359
C29 H56 S4	C29 H56 S4	[C29 H56 S4, tgt=40.50, overall=40.50]	(533.3319, 50.59)(571.2873, 177.51)(555.3072, 116.01)	C29 H56 S4	FindByFormula	1 +	532.3222	3.6031847
C29 H58 N2 O S3	C29 H58 N2 O S3	[C29 H58 N2 O S3, tgt=66.72, overall=66.72]	(547.3785, 4486.8755)(548.37805, 1612.5128)(549.37695, 23	C29 H58 N2 O S3	FindByFormula	22 +	546.3694	22.071815
C29 H60 N11 O2 P3	C29 H60 N11 O2 P3	[C29 H60 N11 O2 P3, tgt=40.05, overall=40.05]	(688.4158, 2087.109)(689.42017, 1031.5049)(690.4306, 2141	C29 H60 N11 O2 P3	FindByFormula	21 +	687.4086	22.564327
C29 H61 N O P2 S3	C29 H61 N O P2 S3	[C29 H61 N O P2 S3, tgt=87.76, overall=87.76]	(598.3476, 11672.598)(599.35034, 4297.727)(600.34674, 164	C29 H61 N O P2 S3	FindByFormula	22 +	597.3411	22.661362
C29 H61 N23	C29 H61 N23	[C29 H61 N23, tgt=94.22, overall=94.22]	(732.5552, 3024.6013)(733.5588, 1546.6887)(734.5597, 524.	C29 H61 N23	FindByFormula	17 +	731.5488	24.352007
C29 H62 N8 O S3	C29 H62 N8 O S3	[C29 H62 N8 O S3, tgt=24.42, overall=24.42]	(635.4296, 2938.9675)(636.429, 1172.7855)(637.4308, 128.6	C29 H62 N8 O S3	FindByFormula	25 +	634.4218	22.138348
C29 H64 N12 O3 S2	C29 H64 N12 O3 S2	[C29 H64 N12 O3 S2, tgt=28.05, overall=28.05]	(693.4741, 14900.701)(694.47656, 5999.735)(695.4655, 2844	C29 H64 N12 O3 S2	FindByFormula	27 +	692.4675	22.438261
C3 H10 N3 O2 P	C3 H10 N3 O2 P	[C3 H10 N3 O2 P, tgt=92.75, overall=92.75]	(152.05824, 19421.959)(153.06065, 1622.8419)(154.05824, 4	C3 H10 N3 O2 P	FindByFormula	16 +	151.0511	0.9337519
C3 H12 N4 O4	C3 H12 N4 O4	[C3 H12 N4 O4, tgt=86.29, overall=86.29]	(169.0942, 3267.5977)(170.09372, 711.6741)(171.09508, 118	C3 H12 N4 O4	FindByFormula	25 +	168.0868	0.57720083
C3 H13 N7 O S	C3 H13 N7 O S	[C3 H13 N7 O S, tgt=17.32, overall=17.32]	(196.09709, 3011.4944)(197.0935, 492.82)(198.08911, 449.5	C3 H13 N7 O S	FindByFormula	20 +	195.0893	3.0510094
C3 H7 N	C3 H7 N	[C3 H7 N, tgt=33.68, overall=33.68]	(58.065517, 11715.69)(59.06838, 407.24936)(60.0685, 34.05)	C3 H7 N	FindByFormula	16 +	57.0583	4.187526
C3 H9 N2 O2 P	C3 H9 N2 O2 P	[C3 H9 N2 O2 P, tgt=74.04, overall=74.04]	(137.04677, 471498.28)(138.0499, 31616.63)(139.05063, 519	C3 H9 N2 O2 P	FindByFormula	28 +	136.0398	1.2527206
C3 H9 N2 O4 P	C3 H9 N2 O4 P	[C3 H9 N2 O4 P, tgt=92.98, overall=92.98]	(169.0369, 51599.06)(170.04153, 4617.5986)(171.03905, 537	C3 H9 N2 O4 P	FindByFormula	23 +	168.0288	1.0356109
C3 H9 N3 O2	C3 H9 N3 O2	[C3 H9 N3 O2, tgt=55.66, overall=55.66]	(120.07666, 12472.331)(121.080414, 891.69)(122.08048, 193	C3 H9 N3 O2	FindByFormula	15 +	119.0696	0.6619355
C3 H9 N5 O	C3 H9 N5 O	[C3 H9 N5 O, tgt=82.26, overall=82.26]	(132.08757, 170225.88)(133.09033, 9722.79)(134.08876, 136	C3 H9 N5 O	FindByFormula	11 +	131.0813	0.6856373
C30 H10 N3 O5 P5	C30 H10 N3 O5 P5	[C30 H10 N3 O5 P5, tgt=88.98, overall=88.98]	(647.93866, 2449.02)(648.93994, 807.678)(649.94446, 147.8	C30 H10 N3 O5 P5	FindByFormula	5 +	646.933	20.786028
C30 H28 P2	C30 H28 P2	[C30 H28 P2, tgt=70.42, overall=70.42]	(451.1751, 3132.39)(452.17874, 917.15546)(453.18185, 399.	C30 H28 P2	FindByFormula	22 +	450.1686	17.910492
C30 H33 N7 O2	C30 H33 N7 O2	[C30 H33 N7 O2, tgt=71.02, overall=71.02]	(524.27655, 3163.4736)(525.283, 1235.982)(526.2841, 1790.	C30 H33 N7 O2	FindByFormula	26 +	523.2698	22.26755
C30 H36 O6 S	C30 H36 O6 S	[C30 H36 O6 S, tgt=48.88, overall=48.88]	(525.23016, 6499.4937)(526.2346, 1909.1539)(527.246, 298.	C30 H36 O6 S	FindByFormula	18 +	524.2222	22.217936
C30 H37 N13 O8 S	C30 H37 N13 O8 S	[C30 H37 N13 O8 S, tgt=96.65, overall=96.65]	(740.26935, 1845.665)(741.2723, 761.2829)(742.26965, 299.	C30 H37 N13 O8 S	FindByFormula	24 +	739.2638	22.040712
C30 H38 N6 O6	C30 H38 N6 O6	[C30 H38 N6 O6, tgt=91.64, overall=91.64]	(579.2929, 10864.861)(580.2961, 4032.2383)(581.2982, 1226	C30 H38 N6 O6	FindByFormula	28 +	578.2855	20.754572
C30 H39 N5 P2	C30 H39 N5 P2	[C30 H39 N5 P2, tgt=38.45, overall=38.45]	(532.2778, 329.567)(533.27576, 237.99284)(534.2856, 151.3	C30 H39 N5 P2	FindByFormula	10 +	531.2718	21.675259
C30 H40 N13 P3	C30 H40 N13 P3	[C30 H40 N13 P3, tgt=83.03, overall=83.03]	(676.28345, 1317.246)(677.2877, 708.2051)(678.283, 636.81)	C30 H40 N13 P3	FindByFormula	16 +	675.2775	21.798235
C30 H40 S	C30 H40 S	[C30 H40 S, tgt=31.08, overall=31.08]	(433.29282, 3030.6765)(434.2904, 1065.995)(435.29242, 692	C30 H40 S	FindByFormula	21 +	432.2855	22.286541
C30 H41 N14 O3 P3	C30 H41 N14 O3 P3	[C30 H41 N14 O3 P3, tgt=86.84, overall=86.84]	(739.2769, 1843.1266)(740.2811, 907.954)(741.28564, 396.7	C30 H41 N14 O3 P3	FindByFormula	6 +	738.2684	17.094496
C30 H41 N6 O3 P	C30 H41 N6 O3 P	[C30 H41 N6 O3 P, tgt=94.65, overall=94.65]	(565.3048, 17942.209)(566.30804, 6028.6133)(567.30896, 16	C30 H41 N6 O3 P	FindByFormula	28 +	564.2977	19.4424
C30 H43 N18 P3	C30 H43 N18 P3	[C30 H43 N18 P3, tgt=75.72, overall=75.72]	(749.3211, 3341.6748)(750.3213, 1549.7667)(751.3227, 564.	C30 H43 N18 P3	FindByFormula	6 +	748.3147	21.15525
C30 H44 N O2 P S2	C30 H44 N O2 P S2	[C30 H44 N O2 P S2, tgt=47.45, overall=47.45]	(546.25977, 3490.3848)(547.2657, 1128.0116)(548.27386, 21	C30 H44 N O2 P S2	FindByFormula	25 +	545.2544	22.022856
C30 H44 N4 O11	C30 H44 N4 O11	[C30 H44 N4 O11, tgt=97.10, overall=97.10]	(637.31024, 4264.832)(638.31964, 2032.2281)(639.3199, 542	C30 H44 N4 O11	FindByFormula	28 +	636.2994	22.538685
C30 H45 N5 O7 S2	C30 H45 N5 O7 S2	[C30 H45 N5 O7 S2, tgt=90.94, overall=90.94]	(652.28326, 3330.9614)(653.29047, 1119.926)(654.2936, 574	C30 H45 N5 O7 S2	FindByFormula	26 +	651.2753	21.892303
C30 H48 N6 O15	C30 H48 N6 O15	[C30 H48 N6 O15, tgt=97.17, overall=97.17]	(733.3261, 4611.3833)(734.32916, 2196.7197)(735.3318, 776	C30 H48 N6 O15	FindByFormula	11 +	732.3181	15.33319
C30 H48 N7 P S	C30 H48 N7 P S	[C30 H48 N7 P S, tgt=78.94, overall=78.94]	(570.3512, 13239.536)(571.3548, 4955.2705)(572.34863, 542	C30 H48 N7 P S	FindByFormula	14 +	569.3454	22.469193
C30 H50 N2 P2	C30 H50 N2 P2	[C30 H50 N2 P2, tgt=56.03, overall=56.03]	(501.3514, 898.8767)(502.35077, 319.62997)(539.30756, 529	C30 H50 N2 P2	FindByFormula	9 +	500.3418	21.91917
C30 H50 N7 O2 P S2	C30 H50 N7 O2 P S2	[C30 H50 N7 O2 P S2, tgt=84.56, overall=84.56]	(636.3264, 5661.85)(637.3329, 1984.5176)(638.3336, 714.96	C30 H50 N7 O2 P S2	FindByFormula	26 +	635.3224	22.23822
C30 H51 N O16	C30 H51 N O16	[C30 H51 N O16, tgt=86.53, overall=86.53]	(682.3251, 6702.9355)(683.32587, 3124.4077)(684.3351, 877	C30 H51 N O16	FindByFormula	17 +	681.3206	22.69649
C30 H51 O6 P S	C30 H51 O6 P S	[C30 H51 O6 P S, tgt=85.42, overall=85.42]	(571.32117, 5861.9775)(572.3241, 2044.3154)(573.3171, 725	C30 H51 O6 P S	FindByFormula	28 +	570.3144	19.447369
C30 H53 N4 O P5	C30 H53 N4 O P5	[C30 H53 N4 O P5, tgt=98.37, overall=98.37]	(641.2964, 6478.0786)(642.30023, 2191.8801)(643.30426, 56	C30 H53 N4 O P5	FindByFormula	8 +	640.291	6.487411
C30 H53 N4 O2 P S	C30 H53 N4 O2 P S	[C30 H53 N4 O2 P S, tgt=67.09, overall=67.09]	(565.3707, 6707.558)(566.3689, 2540.9473)(567.36115, 1002	C30 H53 N4 O2 P S	FindByFormula	22 +	564.3601	22.374556
C30 H55 N O5 P4	C30 H55 N O5 P4	[C30 H55 N O5 P4, tgt=77.79, overall=77.79]	(634.3099, 19596.418)(635.31396, 6807.202)(636.3235, 2932	C30 H55 N O5 P4	FindByFormula	28 +	633.3019	22.102978
C30 H56 N2 P6	C30 H56 N2 P6	[C30 H56 N2 P6, tgt=89.41, overall=89.41]	(631.2951, 2703.8699)(632.2987, 960.5571)(633.30066, 532.	C30 H56 N2 P6	FindByFormula	7 +	630.2862	15.934827
C30 H57 N O2 S4	C30 H57 N O2 S4	[C30 H57 N O2 S4, tgt=61.80, overall=61.80]	(592.3328, 4076.604)(593.33795, 1634.3705)(594.3327, 623.	C30 H57 N O2 S4	FindByFormula	22 +	591.3251	22.205902
C30 H57 N O4 P2 S3	C30 H57 N O4 P2 S3	[C30 H57 N O4 P2 S3, tgt=79.61, overall=79.61]	(654.29944, 7003.0454)(655.3078, 2161.5889)(656.3083, 700	C30 H57 N O4 P2 S3	FindByFormula	25 +	653.2916	22.203882
C30 H58 Cl N O P4	C30 H58 Cl N O P4	[C30 H58 Cl N O P4, tgt=63.14, overall=63.14]	(608.32416, 2361.1936)(609.32935, 877.2337)(610.314, 2252	C30 H58 Cl N O P4	FindByFormula	9 +	607.3172	22.7373
C30 H58 Cl N2 O3 P	C30 H58 Cl N2 O3 P	[C30 H58 Cl N2 O3 P, tgt=27.42, overall=27.42]	(561.3961, 13665.849)(562.39435, 4668.7476)(563.3973, 144	C30 H58 Cl N2 O3 P	FindByFormula	26 +	560.3894	22.303495
C30 H59 N O4 S5	C30 H59 N O4 S5	[C30 H59 N O4 S5, tgt=73.47, overall=73.47]	(658.3139, 2386.3743)(659.31445, 1186.0939)(660.3147, 776	C30 H59 N O4 S5	FindByFormula	27 +	657.3012	22.130384
C30 H61 N4 O3 P S	C30 H61 N4 O3 P S	[C30 H61 N4 O3 P S, tgt=74.78, overall=74.78]	(589.42755, 19544.965)(590.4306, 6659.3804)(591.42847, 20	C30 H61 N4 O3 P S	FindByFormula	23 +	588.42	22.772724
C30 H61 N4 O4 P S	C30 H61 N4 O4 P S	[C30 H61 N4 O4 P S, tgt=77.67, overall=77.67]	(605.42316, 28548.803)(606.42444, 9620.787)(607.41565, 31	C30 H61 N4 O4 P S	FindByFormula	28 +	604.4153	22.41099
C30 H62 N2 O5 P2 S	C30 H62 N2 O5 P2 S	[C30 H62 N2 O5 P2 S, tgt=46.22, overall=46.22]	(625.39075, 43715.105)(626.3934, 15667.526)(627.3917, 373	C30 H62 N2 O5 P2 S	FindByFormula	20 +	624.3829	21.88175
C30 H62 N6 O3 S2	C30 H62 N6 O3 S2	[C30 H62 N6 O3 S2, tgt=32.17, overall=32.17]	(619.4386, 8526.325)(620.44116, 3159.892)(621.4312, 1131.	C30 H62 N6 O3 S2	FindByFormula	23 +	618.4308	22.63486
C30 H63 N8 O P S2	C30 H63 N8 O P S2	[C30 H63 N8 O P S2, tgt=43.74, overall=43.74]	(647.43915, 5660.9175)(648.4391, 2253.1677)(649.4351, 133	C30 H63 N8 O P S2	FindByFormula	23 +	646.4322	22.606495
C30 H64 N O2 P5 S3	C30 H64 N O2 P5 S3	[C30 H64 N O2 P5 S3, tgt=79.55, overall=79.55]	(722.2857, 4872.0)(723.29193, 1695.9708)(724.29236, 457.7	C30 H64 N O2 P5 S3	FindByFormula	24 +	721.2796	22.324274
C31 H27 N4 O P S3	C31 H27 N4 O P S3	[C31 H27 N4 O P S3, tgt=71.20, overall=71.20]	(599.1162, 4781.878)(600.1189, 1667.1173)(601.11896, 526.	C31 H27 N4 O P S3	FindByFormula	22 +	598.1104	21.43821
C31 H30 N2	C31 H30 N2	[C31 H30 N2, tgt=71.72, overall=71.72]	(431.24557, 2072.04)(432.24875, 557.8755)(433.24918, 605.	C31 H30 N2	FindByFormula	9 +	430.2405	21.735
C31 H32 N O P	C31 H32 N O P	[C31 H32 N O P, tgt=82.75, overall=82.75]	(466.2301, 1750.1504)(467.2323, 672.2391)(468.2317, 183.3	C31 H32 N O P	FindByFormula	22 +	465.222	17.273285
C31 H35 N5	C31 H35 N5	[C31 H35 N5, tgt=84.19, overall=84.19]	(478.29196, 3037.2456)(479.29364, 1017.6416)(480.2927, 26	C31 H35 N5	FindByFormula	26 +	477.2898	22.025257
C31 H37 N9 O2 P2	C31 H37 N9 O2 P2	[C31 H37 N9 O2 P2, tgt=82.16, overall=82.16]	(630.2637, 1468.4357)(631.2685, 663.0967)(632.27325, 132.	C31 H37 N9 O2 P2	FindByFormula	7 +	629.2584	20.274014
C31 H37 N9 O6	C31 H37 N9 O6	[C31 H37 N9 O6, tgt=91.13, overall=91.13]	(632.29584, 3936.5645)(633.30145, 1665.5989)(634.30194, 6	C31 H37 N9 O6	FindByFormula	20 +	631.286	21.689053
C31 H38 N7 O P3	C31 H38 N7 O P3	[C31 H38 N7 O P3, tgt=42.00, overall=42.00]	(618.24963, 943.42505)(619.24976, 351.8675)(620.2486, 204	C31 H38 N7 O P3	FindByFormula	4 +	617.2393	22.322273
C31 H38 O6 S	C31 H38 O6 S	[C31 H38 O6 S, tgt=64.77, overall=64.77]	(539.2446, 5404.3325)(540.25006, 1749.634)(541.2533, 257.	C31 H38 O6 S	FindByFormula	22 +	538.2354	22.382992
C31 H39 N O S	C31 H39 N O S	[C31 H39 N O S, tgt=58.92, overall=58.92]	(474.28366, 6792.85)(475.2847, 2260.1523)(476.28247, 680.	C31 H39 N O S	FindByFormula	24 +	473.274	16.43164
C31 H39 O2 P5 S	C31 H39 O2 P5 S	[C31 H39 O2 P5 S, tgt=32.63, overall=32.63]	(631.1419, 5692.424)(632.1462, 2014.4252)(633.14575, 562.	C31 H39 O2 P5 S	FindByFormula	27 +	630.1351	20.245632
C31 H41 N8 P	C31 H41 N8 P	[C31 H41 N8 P, tgt=64.31, overall=64.31]	(557.3273, 2689.1575)(558.3266, 870.37915)(559.3189, 374.	C31 H41 N8 P	FindByFormula	16 +	556.3197	21.44721
C31 H43 Cl2 N	C31 H43 Cl2 N	[C31 H43 Cl2 N, tgt=29.48, overall=29.48]	(500.28088, 3015.5447)(501.289, 1241.4686)(502.29453, 288	C31 H43 Cl2 N	FindByFormula	21 +	499.2772	22.078817
C31 H43 N O7 P2	C31 H43 N O7 P2	[C31 H43 N O7 P2, tgt=96.33, overall=96.33]	(604.25867, 6028.6436)(605.2627, 1958.8945)(606.2661, 624	C31 H43 N O7 P2	FindByFormula	7 +	603.2509	13.031228
C31 H43 N3 O3 S	C31 H43 N3 O3 S	[C31 H43 N3 O3 S, tgt=68.98, overall=68.98]	(538.31177, 1913.1324)(539.3094, 907.46783)(540.3089, 299	C31 H43 N3 O3 S	FindByFormula	24 +	537.3029	21.16156
C31 H43 N5 O12	C31 H43 N5 O12	[C31 H43 N5 O12, tgt=96.86, overall=96.86]	(678.29755, 7938.044)(679.30426, 2839.9158)(680.30597, 71	C31 H43 N5 O12	FindByFormula	28 +	677.2916	22.131382
C31 H44 N9 O4 P3	C31 H44 N9 O4 P3	[C31 H44 N9 O4 P3, tgt=84.49, overall=84.49]	(700.2804, 1521.2528)(701.2854, 764.25226)(702.28613, 848	C31 H44 N9 O4 P3	FindByFormula	10 +	699.2739	21.799786
C31 H47 N4 O P5	C31 H47 N4 O P5	[C31 H47 N4 O P5, tgt=73.62, overall=73.62]	(647.25323, 841.85895)(648.25726, 455.60266)(649.2569, 18	C31 H47 N4 O P5	FindByFormula	18 +	646.2473	21.873596
C31 H47 N8 O5 P S	C31 H47 N8 O5 P S	[C31 H47 N8 O5 P S, tgt=94.74, overall=94.74]	(675.3206, 3223.4834)(676.3253, 1202.6968)(677.3215, 535.	C31 H47 N8 O5 P S	FindByFormula	9 +	674.3134	16.271744
C31 H52 O2 P4	C31 H52 O2 P4	[C31 H52 O2 P4, tgt=69.71, overall=69.71]	(581.2986, 2214.7534)(582.3001, 857.56744)(583.2985, 409.	C31 H52 O2 P4	FindByFormula	28 +	580.2889	17.792894
C31 H53 N O9 P2 S	C31 H53 N O9 P2 S	[C31 H53 N O9 P2 S, tgt=96.39, overall=96.39]	(678.2977, 5581.9224)(679.305, 2025.6373)(680.30145, 582.	C31 H53 N O9 P2 S	FindByFormula	28 +	677.294	21.995356
C31 H53 N P6	C31 H53 N P6	[C31 H53 N P6, tgt=95.41, overall=95.41]	(626.26996, 3100.8904)(627.2751, 1325.8817)(628.2804, 454	C31 H53 N P6	FindByFormula	8 +	625.2618	21.358389
C31 H54 N2 O P6	C31 H54 N2 O P6	[C31 H54 N2 O P6, tgt=92.98, overall=92.98]	(657.27356, 1967.1201)(658.2739, 645.024)(659.27814, 232.	C31 H54 N2 O P6	FindByFormula	5 +	656.2709	15.815107
C31 H55 N5 S4	C31 H55 N5 S4	[C31 H55 N5 S4, tgt=65.80, overall=65.80]	(626.3443, 1252.5525)(627.3395, 1174.1775)(628.33875, 619	C31 H55 N5 S4	FindByFormula	11 +	625.334	22.54058
C31 H56 N2 O P6	C31 H56 N2 O P6	[C31 H56 N2 O P6, tgt=98.37, overall=98.37]	(659.2887, 278963.28)(660.29205, 100861.984)(661.2957, 21	C31 H56 N2 O P6	FindByFormula	28 +	658.2828	22.5384
C31 H58 N2 P2 S2	C31 H58 N2 P2 S2	[C31 H58 N2 P2 S2, tgt=30.48, overall=30.48]	(585.36163, 2423.57)(586.3603, 1142.1637)(587.35944, 256.	C31 H58 N2 P2 S2	FindByFormula	18 +	584.355	22.048117
C31 H60 N O7 P5 S	C31 H60 N O7 P5 S	[C31 H60 N O7 P5 S, tgt=98.01, overall=98.01]	(746.2861, 2136.2644)(747.2888, 840.4758)(748.2889, 361.9	C31 H60 N O7 P5 S	FindByFormula	26 +	745.2767	22.040709
C31 H60 N8 O5 S2	C31 H60 N8 O5 S2	[C31 H60 N8 O5 S2, tgt=64.65, overall=64.65]	(689.4156, 304.17908)(690.4158, 127.3491)(691.41864, 47.0	C31 H60 N8 O5 S2	FindByFormula	11 +	688.4067	4.1129637
C31 H62 Cl2 N2 O2 P2	C31 H62 Cl2 N2 O2 P2	[C31 H62 Cl2 N2 O2 P2, tgt=50.58, overall=50.58]	(627.3671, 2025.7849)(628.366, 760.72815)(629.3791, 1484.	C31 H62 Cl2 N2 O2 P2	FindByFormula	17 +	626.3686	20.229921
C31 H62 N O7 P5 S	C31 H62 N O7 P5 S	[C31 H62 N O7 P5 S, tgt=94.67, overall=94.67]	(748.3019, 3033.7837)(749.3039, 1112.3774)(750.3072, 466.	C31 H62 N O7 P5 S	FindByFormula	25 +	747.294	22.41502
C31 H63 N4 O10 P	C31 H63 N4 O10 P	[C31 H63 N4 O10 P, tgt=98.29, overall=98.29]	(683.43506, 142106.05)(684.4383, 54149.543)(685.4405, 135	C31 H63 N4 O10 P	FindByFormula	28 +	682.4274	22.244768
C31 H64 N2 O2 P2 S	C31 H64 N2 O2 P2 S	[C31 H64 N2 O2 P2 S, tgt=93.57, overall=93.57]	(591.4212, 11817.166)(592.4244, 3971.382)(593.4259, 919.7	C31 H64 N2 O2 P2 S	FindByFormula	10 +	590.4141	6.2476234
C31 H64 N2 O3 S4	C31 H64 N2 O3 S4	[C31 H64 N2 O3 S4, tgt=72.41, overall=72.41]	(641.38434, 1999.9225)(642.3875, 826.9474)(643.38257, 414	C31 H64 N2 O3 S4	FindByFormula	20 +	640.3749	20.830484
C31 H64 N6 O2	C31 H64 N6 O2	[C31 H64 N6 O2, tgt=85.94, overall=85.94]	(553.5168, 8599.976)(554.5189, 3086.4958)(555.51605, 1337	C31 H64 N6 O2	FindByFormula	12 +	552.5075	23.881002
C31 H64 N6 O4 S2	C31 H64 N6 O4 S2	[C31 H64 N6 O4 S2, tgt=84.15, overall=84.15]	(649.4489, 22488.611)(650.4523, 8241.46)(651.44165, 3148.	C31 H64 N6 O4 S2	FindByFormula	28 +	648.4407	22.410479
C31 H66 N8 O S3	C31 H66 N8 O S3	[C31 H66 N8 O S3, tgt=42.52, overall=42.52]	(663.4617, 5031.736)(664.4642, 2144.4434)(665.4524, 921.3	C31 H66 N8 O S3	FindByFormula	28 +	662.4541	22.460886
C31 H66 N8 O2 S3	C31 H66 N8 O2 S3	[C31 H66 N8 O2 S3, tgt=56.13, overall=56.13]	(679.4551, 1673.2062)(680.45447, 671.9078)(681.45734, 180	C31 H66 N8 O2 S3	FindByFormula	23 +	678.4491	22.15724
C31 H68 N12 O4 S2	C31 H68 N12 O4 S2	[C31 H68 N12 O4 S2, tgt=50.74, overall=50.74]	(737.50073, 10675.699)(738.5008, 4553.859)(739.4925, 2105	C31 H68 N12 O4 S2	FindByFormula	25 +	736.4941	22.429445
C32 H2 O5 P2 S5	C32 H2 O5 P2 S5	[C32 H2 O5 P2 S5, tgt=65.14, overall=65.14]	(688.80225, 6077.8823)(689.8048, 3050.7976)(690.81635, 29	C32 H2 O5 P2 S5	FindByFormula	8 +	687.8016	27.687904
C32 H30 O7	C32 H30 O7	[C32 H30 O7, tgt=56.85, overall=56.85]	(527.2063, 6897.2275)(528.20935, 2365.9053)(529.21765, 39	C32 H30 O7	FindByFormula	26 +	526.1972	21.233053
C32 H33 N5 O4	C32 H33 N5 O4	[C32 H33 N5 O4, tgt=95.03, overall=95.03]	(552.2611, 2163.7844)(553.2642, 869.81995)(554.2673, 332.	C32 H33 N5 O4	FindByFormula	7 +	551.2535	21.544504
C32 H36 N8 O3	C32 H36 N8 O3	[C32 H36 N8 O3, tgt=75.51, overall=75.51]	(581.2983, 1398.7626)(582.29974, 566.2743)(583.2942, 310.	C32 H36 N8 O3	FindByFormula	28 +	580.2907	18.10958
C32 H37 N20 P	C32 H37 N20 P	[C32 H37 N20 P, tgt=72.21, overall=72.21]	(733.3315, 1146.0045)(734.33344, 555.49274)(735.3315, 260	C32 H37 N20 P	FindByFormula	11 +	732.326	15.495528
C32 H38 N10 O3 S2	C32 H38 N10 O3 S2	[C32 H38 N10 O3 S2, tgt=77.18, overall=77.18]	(675.2637, 16125.874)(676.2675, 6078.196)(677.26685, 3076	C32 H38 N10 O3 S2	FindByFormula	27 +	674.2577	22.539019
C32 H40 Cl N3	C32 H40 Cl N3	[C32 H40 Cl N3, tgt=56.50, overall=56.50]	(502.29575, 1646.8129)(503.30298, 117.64571)(504.29184, 1	C32 H40 Cl N3	FindByFormula	27 +	501.2898	22.117546
C32 H40 O6 S	C32 H40 O6 S	[C32 H40 O6 S, tgt=63.95, overall=63.95]	(553.2616, 5535.8975)(554.2638, 2208.2832)(555.2673, 714.	C32 H40 O6 S	FindByFormula	28 +	552.2549	22.569843
C32 H44 N13 P3	C32 H44 N13 P3	[C32 H44 N13 P3, tgt=53.81, overall=53.81]	(704.31036, 757.4093)(705.3098, 299.94455)(706.3031, 186.	C32 H44 N13 P3	FindByFormula	18 +	703.3013	22.330965
C32 H44 O S	C32 H44 O S	[C32 H44 O S, tgt=9.21, overall=9.21]	(477.3202, 4040.2998)(478.3223, 1416.2454)(479.31885, 701	C32 H44 O S	FindByFormula	23 +	476.3145	22.331541
C32 H45 N O8 S	C32 H45 N O8 S	[C32 H45 N O8 S, tgt=95.92, overall=95.92]	(604.2934, 2926.7036)(605.2999, 1095.6525)(606.2924, 578.	C32 H45 N O8 S	FindByFormula	17 +	603.2913	22.021204
C32 H45 P3	C32 H45 P3	[C32 H45 P3, tgt=42.09, overall=42.09]	(523.2799, 2165.7788)(524.2829, 861.36743)(525.27783, 416	C32 H45 P3	FindByFormula	23 +	522.2714	18.405018
C32 H46 O8 S	C32 H46 O8 S	[C32 H46 O8 S, tgt=89.68, overall=89.68]	(591.2975, 3075.206)(592.3026, 1490.597)(593.30115, 588.5	C32 H46 O8 S	FindByFormula	10 +	590.2924	14.5371475
C32 H48 N2 O4 P2	C32 H48 N2 O4 P2	[C32 H48 N2 O4 P2, tgt=51.79, overall=51.79]	(587.3151, 2135.9143)(588.3171, 814.2528)(589.311, 404.83	C32 H48 N2 O4 P2	FindByFormula	27 +	586.3047	18.843035
C32 H50 N O P S	C32 H50 N O P S	[C32 H50 N O P S, tgt=71.67, overall=71.67]	(528.34076, 1781.1273)(529.3432, 1797.5785)(530.3342, 712	C32 H50 N O P S	FindByFormula	16 +	527.3368	22.557005
C32 H50 N10 O4	C32 H50 N10 O4	[C32 H50 N10 O4, tgt=98.83, overall=98.83]	(639.40875, 154077.77)(640.41174, 55712.285)(641.41425, 1	C32 H50 N10 O4	FindByFormula	28 +	638.4003	22.23418
C32 H51 N O4 P2 S2	C32 H51 N O4 P2 S2	[C32 H51 N O4 P2 S2, tgt=61.49, overall=61.49]	(640.2847, 1489.1805)(641.2857, 555.12195)(642.2887, 215.	C32 H51 N O4 P2 S2	FindByFormula	15 +	639.2784	22.01043
C32 H52 O6 S2	C32 H52 O6 S2	[C32 H52 O6 S2, tgt=86.23, overall=86.23]	(597.3306, 13735.548)(598.3334, 5149.817)(599.31866, 2347	C32 H52 O6 S2	FindByFormula	28 +	596.3221	19.785913
C32 H54 N2 O3 P2 S	C32 H54 N2 O3 P2 S	[C32 H54 N2 O3 P2 S, tgt=43.19, overall=43.19]	(609.34094, 18174.074)(610.33923, 8072.427)(611.33655, 27	C32 H54 N2 O3 P2 S	FindByFormula	16 +	608.3297	21.93081
C32 H55 N3 O S3	C32 H55 N3 O S3	[C32 H55 N3 O S3, tgt=67.32, overall=67.32]	(594.35425, 8504.35)(595.3598, 4887.998)(596.3521, 2079.9	C32 H55 N3 O S3	FindByFormula	13 +	593.3462	22.386536
C32 H55 N5 O6 P2	C32 H55 N5 O6 P2	[C32 H55 N5 O6 P2, tgt=87.78, overall=87.78]	(668.3712, 857.50494)(669.373, 349.31168)(670.37256, 106.	C32 H55 N5 O6 P2	FindByFormula	6 +	667.3624	6.6383305
C32 H58 N2 O2 P6	C32 H58 N2 O2 P6	[C32 H58 N2 O2 P6, tgt=91.04, overall=91.04]	(689.3001, 2528.3022)(690.30347, 1013.1744)(691.306, 390.	C32 H58 N2 O2 P6	FindByFormula	9 +	688.2939	14.9447365
C32 H59 N O4 P2 S3	C32 H59 N O4 P2 S3	[C32 H59 N O4 P2 S3, tgt=73.96, overall=73.96]	(680.31525, 7904.3467)(681.31903, 2528.7185)(682.3164, 89	C32 H59 N O4 P2 S3	FindByFormula	27 +	679.3063	22.441454
C32 H61 N O4 P6 S	C32 H61 N O4 P6 S	[C32 H61 N O4 P6 S, tgt=98.39, overall=98.39]	(742.2803, 1906.7095)(743.2836, 1056.4329)(744.28546, 680	C32 H61 N O4 P6 S	FindByFormula	23 +	741.2737	22.29331
C32 H63 N4 O6 P S	C32 H63 N4 O6 P S	[C32 H63 N4 O6 P S, tgt=13.00, overall=13.00]	(663.42834, 6693.6104)(664.4298, 2664.123)(665.4231, 998.	C32 H63 N4 O6 P S	FindByFormula	20 +	662.4226	22.112461
C32 H63 O3 P S2	C32 H63 O3 P S2	[C32 H63 O3 P S2, tgt=24.91, overall=24.91]	(591.4029, 4071.4307)(592.4028, 1395.314)(593.4083, 331.1	C32 H63 O3 P S2	FindByFormula	23 +	590.3935	22.119892
C32 H64 N O2 P5 S3	C32 H64 N O2 P5 S3	[C32 H64 N O2 P5 S3, tgt=90.70, overall=90.70]	(746.2856, 3402.503)(747.2895, 1299.4546)(748.2905, 479.0	C32 H64 N O2 P5 S3	FindByFormula	26 +	745.2813	22.131134
C32 H65 N4 O4 P S	C32 H65 N4 O4 P S	[C32 H65 N4 O4 P S, tgt=66.17, overall=66.17]	(633.4543, 15698.874)(634.4556, 5669.8765)(635.45435, 191	C32 H65 N4 O4 P S	FindByFormula	24 +	632.4486	22.74067
C32 H66 N8 S4	C32 H66 N8 S4	[C32 H66 N8 S4, tgt=61.02, overall=61.02]	(691.44165, 1946.2682)(692.44415, 928.89966)(693.44165, 2	C32 H66 N8 S4	FindByFormula	27 +	690.4348	19.804712
C32 H67 O5 P S3	C32 H67 O5 P S3	[C32 H67 O5 P S3, tgt=17.41, overall=17.41]	(659.3953, 2068.5583)(660.39636, 828.4077)(661.3901, 250.	C32 H67 O5 P S3	FindByFormula	17 +	658.3858	20.258732
C32 H69 N4 P S4	C32 H69 N4 P S4	[C32 H69 N4 P S4, tgt=63.82, overall=63.82]	(669.42285, 2072.0376)(670.42163, 1242.1907)(671.42334, 8	C32 H69 N4 P S4	FindByFormula	21 +	668.4102	22.711
C32 H69 O7 P3 S2	C32 H69 O7 P3 S2	[C32 H69 O7 P3 S2, tgt=23.93, overall=23.93]	(723.37665, 187.72002)(724.3723, 70.745)(761.318, 236.805)	C32 H69 O7 P3 S2	FindByFormula	4 +	722.3699	11.820706
C32 H70 N2 O10 S2	C32 H70 N2 O10 S2	[C32 H70 N2 O10 S2, tgt=29.91, overall=29.91]	(707.45337, 3650.7612)(708.45593, 1664.5175)(709.4542, 68	C32 H70 N2 O10 S2	FindByFormula	24 +	706.4487	22.18483
C32 H8 N2 O P6 S3	C32 H8 N2 O P6 S3	[C32 H8 N2 O P6 S3, tgt=73.63, overall=73.63]	(718.82886, 3418.6768)(719.82965, 1743.7999)(720.83246, 5	C32 H8 N2 O P6 S3	FindByFormula	13 +	717.8187	26.120016
C33 H27 N7 O2 P2	C33 H27 N7 O2 P2	[C33 H27 N7 O2 P2, tgt=79.23, overall=79.23]	(616.1768, 13704.134)(617.1793, 5262.641)(618.1817, 1308.	C33 H27 N7 O2 P2	FindByFormula	22 +	615.1703	18.267918
C33 H30	C33 H30	[C33 H30, tgt=68.33, overall=68.33]	(427.24677, 5606.674)(428.23953, 2440.1787)(429.2566, 618	C33 H30	FindByFormula	9 +	426.2342	22.278574
C33 H33 N3 O2	C33 H33 N3 O2	[C33 H33 N3 O2, tgt=80.09, overall=80.09]	(504.26196, 1024.574)(505.26486, 738.0843)(506.2614, 220.	C33 H33 N3 O2	FindByFormula	13 +	503.2564	18.90729
C33 H36 N4 O6	C33 H36 N4 O6	[C33 H36 N4 O6, tgt=95.09, overall=95.09]	(585.27075, 4942.312)(586.27423, 1971.4166)(587.28, 622.9	C33 H36 N4 O6	FindByFormula	6 +	584.265	15.308764
C33 H38 N7 O P3	C33 H38 N7 O P3	[C33 H38 N7 O P3, tgt=19.79, overall=19.79]	(642.2441, 197.924)(643.24084, 101.817505)(644.2505, 281.	C33 H38 N7 O P3	FindByFormula	9 +	641.2293	21.953138
C33 H39 N3	C33 H39 N3	[C33 H39 N3, tgt=98.82, overall=98.82]	(478.32196, 33781.87)(479.32498, 12378.318)(480.32684, 23	C33 H39 N3	FindByFormula	22 +	477.3142	20.442385
C33 H44 N O6 P	C33 H44 N O6 P	[C33 H44 N O6 P, tgt=9.55, overall=9.55]	(582.29767, 1998.5902)(583.2988, 883.9631)(584.3045, 489.	C33 H44 N O6 P	FindByFormula	21 +	581.2901	21.09341
C33 H44 O12	C33 H44 O12	[C33 H44 O12, tgt=90.85, overall=90.85]	(633.29095, 9702.399)(634.2945, 3429.827)(635.29816, 1132	C33 H44 O12	FindByFormula	28 +	632.2831	19.786879
C33 H44 O2 S3	C33 H44 O2 S3	[C33 H44 O2 S3, tgt=35.96, overall=35.96]	(569.257, 3994.3806)(570.2618, 1843.7003)(571.26666, 325.	C33 H44 O2 S3	FindByFormula	22 +	568.2509	22.098299
C33 H45 N O4 P2	C33 H45 N O4 P2	[C33 H45 N O4 P2, tgt=31.27, overall=31.27]	(582.29364, 1319.8408)(583.2957, 502.12915)(584.28955, 13	C33 H45 N O4 P2	FindByFormula	12 +	581.2791	22.093637
C33 H46 N10 P2	C33 H46 N10 P2	[C33 H46 N10 P2, tgt=77.06, overall=77.06]	(645.3449, 1618.606)(646.3486, 757.0546)(647.3451, 239.76	C33 H46 N10 P2	FindByFormula	15 +	644.3379	5.3624783
C33 H46 N11 O P3	C33 H46 N11 O P3	[C33 H46 N11 O P3, tgt=65.73, overall=65.73]	(706.3196, 143.72833)(707.3259, 62.205)(744.2738, 62.1550	C33 H46 N11 O P3	FindByFormula	6 +	705.3125	6.639883
C33 H47 N5 O5 S2	C33 H47 N5 O5 S2	[C33 H47 N5 O5 S2, tgt=91.22, overall=91.22]	(658.30865, 2738.8367)(659.3119, 1189.6421)(660.30566, 32	C33 H47 N5 O5 S2	FindByFormula	25 +	657.3001	22.043146
C33 H47 N7 S2	C33 H47 N7 S2	[C33 H47 N7 S2, tgt=4.74, overall=4.74]	(606.34204, 1284.9467)(607.3442, 843.0512)(608.3468, 187.	C33 H47 N7 S2	FindByFormula	19 +	605.3303	21.86837
C33 H49 N O3 S3	C33 H49 N O3 S3	[C33 H49 N O3 S3, tgt=82.89, overall=82.89]	(604.2928, 8018.7656)(605.2985, 2959.661)(606.2921, 1143.	C33 H49 N O3 S3	FindByFormula	19 +	603.2897	22.102634
C33 H5 O9 P5 S	C33 H5 O9 P5 S	[C33 H5 O9 P5 S, tgt=73.17, overall=73.17]	(732.8444, 5876.087)(733.8463, 2957.1392)(734.85065, 1042	C33 H5 O9 P5 S	FindByFormula	14 +	731.8396	26.737598
C33 H50 Cl N O6	C33 H50 Cl N O6	[C33 H50 Cl N O6, tgt=44.04, overall=44.04]	(592.33386, 4383.859)(593.336, 1644.3575)(594.332, 641.53	C33 H50 Cl N O6	FindByFormula	25 +	591.3305	22.203537
C33 H50 N O10 P S2	C33 H50 N O10 P S2	[C33 H50 N O10 P S2, tgt=83.42, overall=83.42]	(716.2693, 5187.7144)(717.27216, 1705.0714)(718.27203, 60	C33 H50 N O10 P S2	FindByFormula	26 +	715.2636	22.311838
C33 H50 N5 O3 P5	C33 H50 N5 O3 P5	[C33 H50 N5 O3 P5, tgt=65.35, overall=65.35]	(720.2644, 1750.1405)(721.26886, 607.22375)(722.27045, 26	C33 H50 N5 O3 P5	FindByFormula	16 +	719.2603	21.938229
C33 H54 N2 P2	C33 H54 N2 P2	[C33 H54 N2 P2, tgt=53.73, overall=53.73]	(541.38116, 3656.4163)(542.3788, 1274.3601)(543.3819, 209	C33 H54 N2 P2	FindByFormula	24 +	540.3732	22.525946
C33 H55 N P6	C33 H55 N P6	[C33 H55 N P6, tgt=75.99, overall=75.99]	(652.28345, 1855.4768)(653.291, 626.4763)(654.2953, 422.3	C33 H55 N P6	FindByFormula	27 +	651.278	21.805958
C33 H57 N O P6	C33 H57 N O P6	[C33 H57 N O P6, tgt=91.04, overall=91.04]	(670.2931, 2368.8628)(671.2995, 925.6357)(672.3007, 324.4	C33 H57 N O P6	FindByFormula	7 +	669.2866	19.37801
C33 H57 N O4 S4	C33 H57 N O4 S4	[C33 H57 N O4 S4, tgt=50.02, overall=50.02]	(660.32477, 1697.7582)(661.328, 842.70996)(662.33276, 317	C33 H57 N O4 S4	FindByFormula	22 +	659.311	22.385254
C33 H58 N5 O2 P5	C33 H58 N5 O2 P5	[C33 H58 N5 O2 P5, tgt=95.86, overall=95.86]	(712.33575, 2076.3442)(713.33325, 879.885)(714.33813, 295	C33 H58 N5 O2 P5	FindByFormula	9 +	711.3283	6.6554203
C33 H59 N3 O3 P6	C33 H59 N3 O3 P6	[C33 H59 N3 O3 P6, tgt=50.97, overall=50.97]	(732.30554, 2362.3374)(733.3108, 1170.265)(734.30664, 427	C33 H59 N3 O3 P6	FindByFormula	7 +	731.2983	15.085779
C33 H64 N12 O3 S2	C33 H64 N12 O3 S2	[C33 H64 N12 O3 S2, tgt=75.22, overall=75.22]	(741.47406, 4599.302)(742.47314, 2166.5881)(743.4715, 723	C33 H64 N12 O3 S2	FindByFormula	26 +	740.4662	22.416412
C33 H67 N4 O11 P	C33 H67 N4 O11 P	[C33 H67 N4 O11 P, tgt=98.19, overall=98.19]	(727.4613, 111780.44)(728.46436, 45323.668)(729.4665, 118	C33 H67 N4 O11 P	FindByFormula	28 +	726.4539	22.255535
C33 H67 N4 O5 P S	C33 H67 N4 O5 P S	[C33 H67 N4 O5 P S, tgt=56.10, overall=56.10]	(663.4635, 6764.585)(664.4646, 2726.6438)(665.4564, 1005.	C33 H67 N4 O5 P S	FindByFormula	23 +	662.4555	22.610485
C33 H73 Cl N4 O3 P2 S2	C33 H73 Cl N4 O3 P2 S2	[C33 H73 Cl N4 O3 P2 S2, tgt=35.15, overall=35.15]	(735.43805, 138.39168)(736.4442, 73.455)(737.43, 401.12)(	C33 H73 Cl N4 O3 P2 S2	FindByFormula	8 +	734.4233	21.938173
C34 H19 Cl O	C34 H19 Cl O	[C34 H19 Cl O, tgt=23.09, overall=23.09]	(517.07, 172.39667)(518.0764, 36.14)(501.1033, 83.776665)(	C34 H19 Cl O	FindByFormula	3 +	478.1083	8.890849
C34 H33 N17 O4	C34 H33 N17 O4	[C34 H33 N17 O4, tgt=87.28, overall=87.28]	(744.2988, 1101.5957)(745.3091, 719.028)(746.29535, 196.5	C34 H33 N17 O4	FindByFormula	10 +	743.2864	22.783909
C34 H34 O7	C34 H34 O7	[C34 H34 O7, tgt=44.07, overall=44.07]	(555.2382, 5441.14)(556.2416, 2061.4285)(557.2477, 477.92)	C34 H34 O7	FindByFormula	23 +	554.2298	21.864191
C34 H40 N6 O S2	C34 H40 N6 O S2	[C34 H40 N6 O S2, tgt=50.19, overall=50.19]	(613.27997, 2501.4175)(614.2823, 1120.5176)(615.2856, 540	C34 H40 N6 O S2	FindByFormula	16 +	612.2718	20.713306
C34 H43 N3 O6	C34 H43 N3 O6	[C34 H43 N3 O6, tgt=98.75, overall=98.75]	(590.3217, 10919.204)(591.32404, 3645.8347)(592.3272, 209	C34 H43 N3 O6	FindByFormula	13 +	589.3164	22.07023
C34 H43 N4 O3 P	C34 H43 N4 O3 P	[C34 H43 N4 O3 P, tgt=51.47, overall=51.47]	(587.31415, 1576.4862)(588.31586, 626.8111)(589.3083, 438	C34 H43 N4 O3 P	FindByFormula	28 +	586.3053	17.796982
C34 H44 O S	C34 H44 O S	[C34 H44 O S, tgt=77.51, overall=77.51]	(501.31793, 6647.383)(502.3208, 2267.9148)(503.32675, 198	C34 H44 O S	FindByFormula	28 +	500.3113	19.317814
C34 H45 N O3 S2	C34 H45 N O3 S2	[C34 H45 N O3 S2, tgt=87.76, overall=87.76]	(580.2917, 7491.895)(581.2945, 3255.344)(582.2944, 2562.5	C34 H45 N O3 S2	FindByFormula	9 +	579.2868	22.196402
C34 H45 N4 O8 P S	C34 H45 N4 O8 P S	[C34 H45 N4 O8 P S, tgt=73.32, overall=73.32]	(701.2792, 4157.447)(702.28253, 1620.7617)(703.2868, 567.	C34 H45 N4 O8 P S	FindByFormula	28 +	700.2712	19.786772
C34 H45 N9 O S3	C34 H45 N9 O S3	[C34 H45 N9 O S3, tgt=84.45, overall=84.45]	(692.2971, 1654.1367)(693.3042, 936.98)(694.3046, 395.16)(	C34 H45 N9 O S3	FindByFormula	3 +	691.2908	20.803833
C34 H46 N12	C34 H46 N12	[C34 H46 N12, tgt=51.32, overall=51.32]	(623.40607, 1546.8665)(624.4088, 640.31006)(625.40314, 62	C34 H46 N12	FindByFormula	17 +	622.3937	22.570017
C34 H46 N3 O3 P	C34 H46 N3 O3 P	[C34 H46 N3 O3 P, tgt=59.26, overall=59.26]	(576.3326, 2222.3586)(577.33606, 1312.6517)(578.3341, 563	C34 H46 N3 O3 P	FindByFormula	24 +	575.3259	22.23343
C34 H48 O2 S	C34 H48 O2 S	[C34 H48 O2 S, tgt=51.20, overall=51.20]	(521.344, 14435.264)(522.34595, 3946.8105)(523.34106, 916	C34 H48 O2 S	FindByFormula	28 +	520.3362	22.288136
C34 H49 Cl P2 S3	C34 H49 Cl P2 S3	[C34 H49 Cl P2 S3, tgt=83.07, overall=83.07]	(651.22546, 1290.4178)(652.226, 662.13446)(653.21985, 911	C34 H49 Cl P2 S3	FindByFormula	23 +	650.2153	3.609651
C34 H52 N3 O6 P S	C34 H52 N3 O6 P S	[C34 H52 N3 O6 P S, tgt=91.69, overall=91.69]	(662.3388, 3290.7456)(663.3376, 1320.8271)(664.3399, 502.	C34 H52 N3 O6 P S	FindByFormula	10 +	661.3269	22.560833
C34 H52 N6 O2 S	C34 H52 N6 O2 S	[C34 H52 N6 O2 S, tgt=75.97, overall=75.97]	(609.396, 6138.388)(610.394, 2474.5278)(611.3902, 771.884	C34 H52 N6 O2 S	FindByFormula	26 +	608.3875	22.385002
C34 H52 O3 P4	C34 H52 O3 P4	[C34 H52 O3 P4, tgt=82.68, overall=82.68]	(633.2935, 2459.9941)(634.2968, 970.289)(635.30237, 434.4	C34 H52 O3 P4	FindByFormula	28 +	632.2872	19.445295
C34 H55 N5 O11	C34 H55 N5 O11	[C34 H55 N5 O11, tgt=94.55, overall=94.55]	(710.396, 30270.418)(711.4015, 12771.234)(712.40424, 3693	C34 H55 N5 O11	FindByFormula	28 +	709.3888	22.54051
C34 H56 O2 P2	C34 H56 O2 P2	[C34 H56 O2 P2, tgt=30.55, overall=30.55]	(559.3813, 9201.108)(560.3856, 3060.5356)(561.3892, 2071.	C34 H56 O2 P2	FindByFormula	16 +	558.3745	22.54949
C34 H59 N4 P5	C34 H59 N4 P5	[C34 H59 N4 P5, tgt=25.90, overall=25.90]	(679.3494, 1471.8473)(680.3488, 697.61163)(681.34125, 332	C34 H59 N4 P5	FindByFormula	7 +	678.3416	15.347618
C34 H61 N4 O5 P S	C34 H61 N4 O5 P S	[C34 H61 N4 O5 P S, tgt=68.05, overall=68.05]	(669.4165, 26185.64)(670.4183, 10182.68)(671.41516, 2690.	C34 H61 N4 O5 P S	FindByFormula	28 +	668.4097	21.920824

C34 H62 N10 O S2	C34 H62 N10 O S2	[C34 H62 N10 O S2, tgt=40.77, overall=40.77]	(691.46484, 5402.4175)(692.46564, 2366.9758)(693.4624, 14	C34 H62 N10 O S2	FindByFormula	15 +	690.4555	22.59458
C34 H64 N4 P2 S	C34 H64 N4 P2 S	[C34 H64 N4 P2 S, tgt=96.69, overall=96.69]	(623.43854, 3874.6714)(624.4379, 2370.094)(625.4424, 1172	C34 H64 N4 P2 S	FindByFormula	22 +	622.4317	22.202614
C34 H65 N4 O P S3	C34 H65 N4 O P S3	[C34 H65 N4 O P S3, tgt=60.80, overall=60.80]	(673.41077, 1963.9186)(674.411, 792.923)(675.4086, 264.09	C34 H65 N4 O P S3	FindByFormula	20 +	672.4042	20.838493
C34 H68 N2 O9 S2	C34 H68 N2 O9 S2	[C34 H68 N2 O9 S2, tgt=57.94, overall=57.94]	(713.4425, 19198.203)(714.4437, 7878.6655)(715.4423, 2313	C34 H68 N2 O9 S2	FindByFormula	27 +	712.4334	21.960007
C34 H68 N2 S	C34 H68 N2 S	[C34 H68 N2 S, tgt=59.20, overall=59.20]	(537.517, 11834.537)(538.51996, 4068.5007)(539.5186, 1749	C34 H68 N2 S	FindByFormula	22 +	536.5105	25.34427
C34 H69 N4 O5 P S	C34 H69 N4 O5 P S	[C34 H69 N4 O5 P S, tgt=66.90, overall=66.90]	(677.47925, 15894.215)(678.48236, 6442.351)(679.47986, 23	C34 H69 N4 O5 P S	FindByFormula	22 +	676.4716	22.774195
C34 H70 N2 O9 S2	C34 H70 N2 O9 S2	[C34 H70 N2 O9 S2, tgt=70.34, overall=70.34]	(715.4558, 322.5389)(716.44666, 503.5175)(717.4557, 225.0	C34 H70 N2 O9 S2	FindByFormula	12 +	714.4513	22.581968
C34 H73 N2 O2 P5 S	C34 H73 N2 O2 P5 S	[C34 H73 N2 O2 P5 S, tgt=66.08, overall=66.08]	(729.4132, 900.42)(730.4124, 351.25467)(731.41583, 107.38	C34 H73 N2 O2 P5 S	FindByFormula	15 +	728.404	4.3133225
C34 H74 N7 P	C34 H74 N7 P	[C34 H74 N7 P, tgt=79.75, overall=79.75]	(612.584, 6296.197)(613.5798, 1708.9485)(614.58154, 173.8	C34 H74 N7 P	FindByFormula	7 +	611.5753	20.388397
C34 H9 N5 O5 P4	C34 H9 N5 O5 P4	[C34 H9 N5 O5 P4, tgt=77.53, overall=77.53]	(691.96295, 1680.3685)(692.9581, 718.55)(693.96515, 411.4	C34 H9 N5 O5 P4	FindByFormula	7 +	690.9554	20.803358
C35 H35 N5	C35 H35 N5	[C35 H35 N5, tgt=35.01, overall=35.01]	(526.2897, 1682.6371)(527.29114, 738.487)(528.29395, 256.	C35 H35 N5	FindByFormula	14 +	525.2899	22.06322
C35 H37 N8 P3	C35 H37 N8 P3	[C35 H37 N8 P3, tgt=90.55, overall=90.55]	(663.24384, 845.4825)(664.2471, 449.61432)(665.2472, 168.	C35 H37 N8 P3	FindByFormula	8 +	662.2378	21.87172
C35 H40 N2 O4	C35 H40 N2 O4	[C35 H40 N2 O4, tgt=91.30, overall=91.30]	(553.30597, 8269.608)(554.3088, 2913.21)(555.3088, 791.44	C35 H40 N2 O4	FindByFormula	17 +	552.2986	5.4224534
C35 H40 N5 O4 P3	C35 H40 N5 O4 P3	[C35 H40 N5 O4 P3, tgt=82.00, overall=82.00]	(688.23816, 1106.259)(689.2454, 615.39996)(690.2467, 247.	C35 H40 N5 O4 P3	FindByFormula	10 +	687.23	21.566454
C35 H45 N3 O2 P2	C35 H45 N3 O2 P2	[C35 H45 N3 O2 P2, tgt=52.34, overall=52.34]	(602.3051, 3064.8647)(603.30994, 1256.8679)(604.3055, 432	C35 H45 N3 O2 P2	FindByFormula	20 +	601.297	21.811262
C35 H49 N17	C35 H49 N17	[C35 H49 N17, tgt=87.46, overall=87.46]	(708.44214, 1574.0367)(709.44354, 776.1534)(710.4424, 252	C35 H49 N17	FindByFormula	6 +	707.4343	17.541792
C35 H50 N O10 P S2	C35 H50 N O10 P S2	[C35 H50 N O10 P S2, tgt=87.80, overall=87.80]	(740.2685, 3094.846)(741.2711, 1193.5535)(742.27045, 427.	C35 H50 N O10 P S2	FindByFormula	25 +	739.2656	22.129185
C35 H52 N O P3	C35 H52 N O P3	[C35 H52 N O P3, tgt=62.49, overall=62.49]	(596.3354, 2248.7773)(597.33417, 1111.5276)(598.34216, 10	C35 H52 N O P3	FindByFormula	10 +	595.3315	22.698963
C35 H60 S3	C35 H60 S3	[C35 H60 S3, tgt=82.83, overall=82.83]	(577.3916, 2777.2605)(578.39233, 1038.56)(579.3909, 267.5	C35 H60 S3	FindByFormula	20 +	576.38	21.81161
C35 H62 N7 O4 P S2	C35 H62 N7 O4 P S2	[C35 H62 N7 O4 P S2, tgt=76.36, overall=76.36]	(740.4101, 7358.6523)(741.4149, 3239.4478)(742.418, 1439.	C35 H62 N7 O4 P S2	FindByFormula	21 +	739.4033	22.66002
C35 H64 N6 S3	C35 H64 N6 S3	[C35 H64 N6 S3, tgt=47.01, overall=47.01]	(665.4422, 1499.9268)(666.4413, 692.60895)(667.4351, 292.	C35 H64 N6 S3	FindByFormula	20 +	664.4331	21.840641
C35 H70 O2 P4	C35 H70 O2 P4	[C35 H70 O2 P4, tgt=84.88, overall=84.88]	(647.4355, 1188.3943)(648.44086, 640.77374)(649.43713, 46	C35 H70 O2 P4	FindByFormula	23 +	646.4271	21.990572
C36 H38 N2 O4	C36 H38 N2 O4	[C36 H38 N2 O4, tgt=45.91, overall=45.91]	(563.2898, 1429.4753)(564.2918, 492.80252)(565.29755, 133	C36 H38 N2 O4	FindByFormula	28 +	562.2828	19.610945
C36 H41 N3 O S	C36 H41 N3 O S	[C36 H41 N3 O S, tgt=84.21, overall=84.21]	(564.3039, 6180.4595)(565.3073, 2237.326)(566.30884, 723.	C36 H41 N3 O S	FindByFormula	21 +	563.3013	21.675138
C36 H43 N2 P	C36 H43 N2 P	[C36 H43 N2 P, tgt=1.83, overall=1.83]	(535.32306, 1723.3307)(536.3243, 647.6984)(537.32104, 160	C36 H43 N2 P	FindByFormula	26 +	534.3152	16.909172
C36 H47 N3 O5 S3	C36 H47 N3 O5 S3	[C36 H47 N3 O5 S3, tgt=66.04, overall=66.04]	(698.27167, 2359.2097)(699.2756, 1137.1311)(700.2738, 596	C36 H47 N3 O5 S3	FindByFormula	25 +	697.2688	22.377487
C36 H52 N3 O3 P S3	C36 H52 N3 O3 P S3	[C36 H52 N3 O3 P S3, tgt=58.73, overall=58.73]	(702.29767, 2697.0579)(703.30316, 1140.57)(704.29803, 463	C36 H52 N3 O3 P S3	FindByFormula	22 +	701.2954	22.052397
C36 H54 N5 O4 P	C36 H54 N5 O4 P	[C36 H54 N5 O4 P, tgt=44.56, overall=44.56]	(652.40265, 338.79)(653.3912, 846.94)(654.3794, 365.85)(69	C36 H54 N5 O4 P	FindByFormula	12 +	651.3941	22.315908
C36 H54 N7 O4 P3	C36 H54 N7 O4 P3	[C36 H54 N7 O4 P3, tgt=59.94, overall=59.94]	(742.34766, 344.57874)(743.345, 194.82875)(744.3491, 50.3	C36 H54 N7 O4 P3	FindByFormula	8 +	741.3416	6.631085
C36 H56 N6 O3 S	C36 H56 N6 O3 S	[C36 H56 N6 O3 S, tgt=83.30, overall=83.30]	(653.4216, 5674.822)(654.421, 2383.3225)(655.4179, 778.49	C36 H56 N6 O3 S	FindByFormula	28 +	652.4147	22.41174
C36 H64 S2	C36 H64 S2	[C36 H64 S2, tgt=79.62, overall=79.62]	(561.44934, 8021.74)(562.4562, 2467.0938)(563.46136, 693.	C36 H64 S2	FindByFormula	16 +	560.443	24.627373
C36 H66 N O P	C36 H66 N O P	[C36 H66 N O P, tgt=33.27, overall=33.27]	(560.4976, 2411.616)(561.49524, 1065.1914)(562.5027, 452.	C36 H66 N O P	FindByFormula	25 +	559.4897	22.695585
C36 H66 N6 O4 P2	C36 H66 N6 O4 P2	[C36 H66 N6 O4 P2, tgt=35.82, overall=35.82]	(709.46814, 1265.239)(710.4684, 579.9269)(711.4702, 221.9	C36 H66 N6 O4 P2	FindByFormula	18 +	708.4571	21.936747
C36 H69 N2 O3 P S3	C36 H69 N2 O3 P S3	[C36 H69 N2 O3 P S3, tgt=65.32, overall=65.32]	(705.42737, 781.3554)(706.431, 528.5262)(707.4279, 199.87	C36 H69 N2 O3 P S3	FindByFormula	19 +	704.4277	22.299662
C36 H71 O P S4	C36 H71 O P S4	[C36 H71 O P S4, tgt=39.35, overall=39.35]	(679.4212, 2642.8716)(680.4179, 1361.391)(681.41864, 1206	C36 H71 O P S4	FindByFormula	22 +	678.4153	22.50999
C36 H74 N4	C36 H74 N4	[C36 H74 N4, tgt=73.72, overall=73.72]	(563.5975, 2092.8225)(564.60095, 805.1331)(565.5999, 265.	C36 H74 N4	FindByFormula	16 +	562.5889	25.149458
C36 H78 N9 O P	C36 H78 N9 O P	[C36 H78 N9 O P, tgt=89.03, overall=89.03]	(684.6177, 3104.5935)(685.61346, 1339.1167)(686.6147, 287	C36 H78 N9 O P	FindByFormula	6 +	683.6062	20.832613
C37 H33 N10 P	C37 H33 N10 P	[C37 H33 N10 P, tgt=74.90, overall=74.90]	(649.27026, 1449.1642)(650.2742, 605.6652)(651.27106, 157	C37 H33 N10 P	FindByFormula	26 +	648.2642	22.302975
C37 H34 N O P	C37 H34 N O P	[C37 H34 N O P, tgt=54.02, overall=54.02]	(540.2463, 2045.8761)(541.2501, 686.94165)(578.1988, 104.	C37 H34 N O P	FindByFormula	18 +	539.2395	22.023575
C37 H36 N5 P3	C37 H36 N5 P3	[C37 H36 N5 P3, tgt=71.62, overall=71.62]	(644.22833, 1881.5754)(645.2319, 801.5918)(646.2357, 170.	C37 H36 N5 P3	FindByFormula	11 +	643.22	21.590168
C37 H39 N2 P3	C37 H39 N2 P3	[C37 H39 N2 P3, tgt=85.54, overall=85.54]	(605.2412, 2081.1228)(606.2417, 862.09143)(607.2513, 203.	C37 H39 N2 P3	FindByFormula	7 +	604.2337	18.578955
C37 H39 N5 O P2	C37 H39 N5 O P2	[C37 H39 N5 O P2, tgt=57.82, overall=57.82]	(632.26855, 851.16)(633.2694, 355.34668)(670.2282, 615.14	C37 H39 N5 O P2	FindByFormula	3 +	631.2583	21.86347
C37 H45 O3 P S	C37 H45 O3 P S	[C37 H45 O3 P S, tgt=69.75, overall=69.75]	(601.2923, 2204.8596)(602.2925, 899.1162)(603.2945, 515.4	C37 H45 O3 P S	FindByFormula	16 +	600.2812	20.718426
C37 H47 N2 O P5	C37 H47 N2 O P5	[C37 H47 N2 O P5, tgt=75.70, overall=75.70]	(713.2304, 77.5)(714.223, 28.16)	C37 H47 N2 O P5	FindByFormula	1 +	690.2383	16.411476
C37 H47 N5 S	C37 H47 N5 S	[C37 H47 N5 S, tgt=25.79, overall=25.79]	(594.3595, 3800.6392)(595.3679, 2971.7227)(596.3603, 819.	C37 H47 N5 S	FindByFormula	19 +	593.3576	22.095547
C37 H49 N O8 S	C37 H49 N O8 S	[C37 H49 N O8 S, tgt=84.10, overall=84.10]	(668.3256, 1567.4042)(669.32837, 855.73)(670.32605, 629.8	C37 H49 N O8 S	FindByFormula	10 +	667.323	22.484985
C37 H51 O11 P S	C37 H51 O11 P S	[C37 H51 O11 P S, tgt=94.22, overall=94.22]	(735.2956, 6842.885)(736.29926, 2724.7)(737.3023, 891.113	C37 H51 O11 P S	FindByFormula	7 +	734.2885	16.754726
C37 H51 O3 P S2	C37 H51 O3 P S2	[C37 H51 O3 P S2, tgt=91.33, overall=91.33]	(639.3099, 2697.08)(640.3124, 1051.4028)(641.30865, 505.3	C37 H51 O3 P S2	FindByFormula	28 +	638.3034	19.785593
C37 H52 S3	C37 H52 S3	[C37 H52 S3, tgt=35.34, overall=35.34]	(593.33093, 1402.2585)(594.33057, 566.6205)(595.3263, 308	C37 H52 S3	FindByFormula	21 +	592.3223	20.574137
C37 H56 N2 O2 P4	C37 H56 N2 O2 P4	[C37 H56 N2 O2 P4, tgt=46.54, overall=46.54]	(685.3384, 1699.9702)(686.3384, 808.03766)(687.3456, 405.	C37 H56 N2 O2 P4	FindByFormula	28 +	684.3261	22.05907
C37 H69 N8 O P S	C37 H69 N8 O P S	[C37 H69 N8 O P S, tgt=63.72, overall=63.72]	(705.5116, 3986.2444)(706.51294, 1790.5076)(707.50287, 87	C37 H69 N8 O P S	FindByFormula	17 +	704.5027	23.084253
C37 H74 N4 O4 S3	C37 H74 N4 O4 S3	[C37 H74 N4 O4 S3, tgt=40.95, overall=40.95]	(735.49615, 3267.1746)(736.49475, 1512.0039)(737.48535, 1	C37 H74 N4 O4 S3	FindByFormula	22 +	734.4912	22.61624
C37 H77 N2 O P5	C37 H77 N2 O P5	[C37 H77 N2 O P5, tgt=72.90, overall=72.90]	(721.4792, 1717.544)(722.4891, 923.742)(723.4831, 34.36)(7	C37 H77 N2 O P5	FindByFormula	6 +	720.4721	24.53446
C37 H77 N4 O P S3	C37 H77 N4 O P S3	[C37 H77 N4 O P S3, tgt=67.60, overall=67.60]	(721.50555, 12771.756)(722.50635, 5619.4326)(723.50134, 1	C37 H77 N4 O P S3	FindByFormula	22 +	720.5011	22.772738
C37 H77 N9 O2 P2	C37 H77 N9 O2 P2	[C37 H77 N9 O2 P2, tgt=33.59, overall=33.59]	(742.56354, 993.63)(743.5757, 598.14)(744.5637, 594.56)(78	C37 H77 N9 O2 P2	FindByFormula	5 +	741.5682	24.903864
C37 H80 N4 O2	C37 H80 N4 O2	[C37 H80 N4 O2, tgt=98.61, overall=98.61]	(613.6325, 6079.2246)(614.6379, 2490.0671)(615.6423, 796.	C37 H80 N4 O2	FindByFormula	19 +	612.6261	25.04851
C38 H23 N17	C38 H23 N17	[C38 H23 N17, tgt=75.50, overall=75.50]	(718.23883, 930.62286)(719.244, 507.98288)(756.1937, 97.6	C38 H23 N17	FindByFormula	7 +	717.2328	21.820951
C38 H27 N15	C38 H27 N15	[C38 H27 N15, tgt=49.25, overall=49.25]	(694.2617, 408.655)(695.26666, 94.4425)(732.2182, 329.243	C38 H27 N15	FindByFormula	6 +	693.2574	22.048185
C38 H35 N6 O5 P	C38 H35 N6 O5 P	[C38 H35 N6 O5 P, tgt=99.58, overall=99.58]	(687.24866, 47725.875)(688.2522, 21061.482)(689.25555, 53	C38 H35 N6 O5 P	FindByFormula	22 +	686.2421	16.375317
C38 H43 N O S	C38 H43 N O S	[C38 H43 N O S, tgt=60.24, overall=60.24]	(562.3187, 2570.3296)(563.321, 1608.6346)(564.3134, 906.4	C38 H43 N O S	FindByFormula	28 +	561.3046	21.892351
C38 H45 N P2	C38 H45 N P2	[C38 H45 N P2, tgt=56.04, overall=56.04]	(578.3113, 1545.3912)(579.31244, 925.5433)(580.30896, 314	C38 H45 N P2	FindByFormula	16 +	577.3016	21.237465
C38 H46 N2 O6 P2 S	C38 H46 N2 O6 P2 S	[C38 H46 N2 O6 P2 S, tgt=19.45, overall=19.45]	(721.2619, 4009.8489)(722.2665, 1800.9606)(723.26984, 562	C38 H46 N2 O6 P2 S	FindByFormula	26 +	720.2535	22.53896
C38 H46 O12 S	C38 H46 O12 S	[C38 H46 O12 S, tgt=84.51, overall=84.51]	(727.2769, 9610.635)(728.28033, 3761.1018)(729.2848, 1013	C38 H46 O12 S	FindByFormula	28 +	726.271	22.53747
C38 H47 N2 O8 P	C38 H47 N2 O8 P	[C38 H47 N2 O8 P, tgt=93.95, overall=93.95]	(691.31415, 7096.657)(692.3162, 2766.3777)(693.32355, 162	C38 H47 N2 O8 P	FindByFormula	19 +	690.3071	22.570475
C38 H49 N5 P2 S2	C38 H49 N5 P2 S2	[C38 H49 N5 P2 S2, tgt=89.00, overall=89.00]	(702.2977, 2842.1228)(703.30225, 1202.7876)(704.29834, 50	C38 H49 N5 P2 S2	FindByFormula	23 +	701.2951	22.031898
C38 H54 N O P S	C38 H54 N O P S	[C38 H54 N O P S, tgt=22.01, overall=22.01]	(604.36755, 3034.3762)(605.374, 2047.2263)(606.3753, 1017	C38 H54 N O P S	FindByFormula	15 +	603.37	22.608318
C38 H54 O11 S	C38 H54 O11 S	[C38 H54 O11 S, tgt=97.23, overall=97.23]	(719.3433, 3317.5886)(720.3428, 1327.4976)(721.34607, 558	C38 H54 O11 S	FindByFormula	8 +	718.3388	16.586794
C38 H57 N O3 P2	C38 H57 N O3 P2	[C38 H57 N O3 P2, tgt=32.73, overall=32.73]	(638.3885, 17495.982)(639.3946, 9645.319)(640.3981, 2788.	C38 H57 N O3 P2	FindByFormula	21 +	637.3808	22.115591
C38 H58 N5 O2 P S	C38 H58 N5 O2 P S	[C38 H58 N5 O2 P S, tgt=96.74, overall=96.74]	(680.4106, 3832.7114)(681.4139, 1699.4672)(682.4126, 617.	C38 H58 N5 O2 P S	FindByFormula	7 +	679.4049	17.523386
C38 H60 N6 O4 S	C38 H60 N6 O4 S	[C38 H60 N6 O4 S, tgt=74.16, overall=74.16]	(697.44855, 4807.789)(698.44666, 2172.1292)(699.443, 819.	C38 H60 N6 O4 S	FindByFormula	28 +	696.4386	22.412247
C38 H62 O S2	C38 H62 O S2	[C38 H62 O S2, tgt=88.28, overall=88.28]	(599.4299, 4200.3486)(600.4329, 2001.4363)(601.4288, 1078	C38 H62 O S2	FindByFormula	23 +	598.4269	22.750732
C38 H65 O9 P S	C38 H65 O9 P S	[C38 H65 O9 P S, tgt=59.41, overall=59.41]	(729.4132, 937.2958)(730.414, 370.45428)(731.4163, 113.40	C38 H65 O9 P S	FindByFormula	14 +	728.4058	4.309766
C38 H66 N2 O2 S4	C38 H66 N2 O2 S4	[C38 H66 N2 O2 S4, tgt=31.45, overall=31.45]	(711.4072, 1403.1361)(712.4127, 976.47577)(713.405, 546.3	C38 H66 N2 O2 S4	FindByFormula	21 +	710.4052	21.829311
C38 H75 N7 O2	C38 H75 N7 O2	[C38 H75 N7 O2, tgt=81.43, overall=81.43]	(662.6076, 2243.2234)(663.60675, 737.2067)(664.6085, 146.	C38 H75 N7 O2	FindByFormula	6 +	661.6001	20.796747
C38 H82 N6 P2	C38 H82 N6 P2	[C38 H82 N6 P2, tgt=82.07, overall=82.07]	(685.6148, 84776.42)(686.6184, 38846.46)(687.6223, 9505.4	C38 H82 N6 P2	FindByFormula	21 +	684.609	25.369633
C38 H84 N7 O4 P	C38 H84 N7 O4 P	[C38 H84 N7 O4 P, tgt=84.77, overall=84.77]	(734.63995, 1297.7686)(735.63916, 530.95)(736.637, 217.56	C38 H84 N7 O4 P	FindByFormula	7 +	733.631	21.14526
C39 H30 N6	C39 H30 N6	[C39 H30 N6, tgt=86.51, overall=86.51]	(583.26373, 2214.8271)(584.2633, 886.2828)(585.2736, 252.	C39 H30 N6	FindByFormula	7 +	582.257	21.172495
C39 H31 N9	C39 H31 N9	[C39 H31 N9, tgt=65.83, overall=65.83]	(626.2779, 3994.4858)(627.2873, 1586.5759)(628.2899, 2228	C39 H31 N9	FindByFormula	14 +	625.275	21.98866
C39 H35 N9	C39 H35 N9	[C39 H35 N9, tgt=67.48, overall=67.48]	(630.3079, 1839.6031)(631.31366, 802.63995)(632.3043, 424	C39 H35 N9	FindByFormula	7 +	629.301	22.40607
C39 H36 N5 O2 P S	C39 H36 N5 O2 P S	[C39 H36 N5 O2 P S, tgt=55.85, overall=55.85]	(670.242, 1375.8451)(671.2459, 531.5617)(672.24255, 211.5	C39 H36 N5 O2 P S	FindByFormula	12 +	669.237	21.878372
C39 H37 N3 O2	C39 H37 N3 O2	[C39 H37 N3 O2, tgt=74.66, overall=74.66]	(580.293, 19904.938)(581.3015, 6741.5435)(582.3016, 2326.	C39 H37 N3 O2	FindByFormula	14 +	579.2855	22.292969
C39 H38 N11 O P	C39 H38 N11 O P	[C39 H38 N11 O P, tgt=31.56, overall=31.56]	(746.2578, 111.89)(730.30316, 174.14)	C39 H38 N11 O P	FindByFormula	2 +	707.3061	22.850624
C39 H44	C39 H44	[C39 H44, tgt=63.57, overall=63.57]	(513.3482, 1586.1213)(514.35315, 760.35834)(515.3617, 133	C39 H44	FindByFormula	11 +	512.342	22.369844
C39 H47 N P2	C39 H47 N P2	[C39 H47 N P2, tgt=38.77, overall=38.77]	(592.32605, 1287.6151)(593.3279, 656.2253)(594.32587, 310	C39 H47 N P2	FindByFormula	15 +	591.3198	21.650618
C39 H48 O2 P4	C39 H48 O2 P4	[C39 H48 O2 P4, tgt=81.01, overall=81.01]	(673.26746, 1712.2283)(674.26984, 787.58185)(675.276, 233	C39 H48 O2 P4	FindByFormula	27 +	672.2619	22.120438
C39 H62 N O4 P S	C39 H62 N O4 P S	[C39 H62 N O4 P S, tgt=88.71, overall=88.71]	(672.42163, 7624.0054)(673.4257, 3608.6748)(674.4268, 139	C39 H62 N O4 P S	FindByFormula	15 +	671.4152	22.654451
C39 H73 O P S3	C39 H73 O P S3	[C39 H73 O P S3, tgt=73.50, overall=73.50]	(685.46014, 274.6082)(686.4675, 120.98)(687.4541, 42.7979	C39 H73 O P S3	FindByFormula	11 +	684.4529	7.610805
C39 H77 N2 O P5	C39 H77 N2 O P5	[C39 H77 N2 O P5, tgt=55.77, overall=55.77]	(745.4808, 1818.1167)(746.4909, 1133.92)(747.4966, 431.80	C39 H77 N2 O P5	FindByFormula	4 +	744.4688	24.423143
C39 H79 O P S4	C39 H79 O P S4	[C39 H79 O P S4, tgt=17.32, overall=17.32]	(723.48157, 1333.504)(724.4837, 658.7989)(725.4852, 245.0	C39 H79 O P S4	FindByFormula	19 +	722.469	22.19733
C39 H83 N4 O P	C39 H83 N4 O P	[C39 H83 N4 O P, tgt=75.78, overall=75.78]	(655.63776, 1843.104)(656.6409, 800.5978)(657.6417, 520.0	C39 H83 N4 O P	FindByFormula	20 +	654.6322	25.311987
C39 H83 N9 O	C39 H83 N9 O	[C39 H83 N9 O, tgt=67.79, overall=67.79]	(694.68024, 1820.3644)(695.683, 962.5207)(696.67975, 275.	C39 H83 N9 O	FindByFormula	14 +	693.674	25.352184
C4 H11 N	C4 H11 N	[C4 H11 N, tgt=90.42, overall=90.42]	(74.09686, 15256.905)(75.09977, 718.9899)(76.1001, 22.23)(	C4 H11 N	FindByFormula	27 +	73.0895	16.430122
C4 H11 N3 O	C4 H11 N3 O	[C4 H11 N3 O, tgt=94.78, overall=94.78]	(118.09709, 122313.914)(119.10011, 7446.6943)(120.10649,	C4 H11 N3 O	FindByFormula	14 +	117.0896	0.6835022
C4 H11 O2 P	C4 H11 O2 P	[C4 H11 O2 P, tgt=46.45, overall=46.45]	(123.05631, 115552.25)(124.0597, 8913.112)(125.05983, 472	C4 H11 O2 P	FindByFormula	20 +	122.0488	1.124254
C4 H11 O3 P	C4 H11 O3 P	[C4 H11 O3 P, tgt=90.09, overall=90.09]	(139.05188, 190305.3)(140.0584, 15563.805)(141.06018, 231	C4 H11 O3 P	FindByFormula	25 +	138.0451	1.9087833
C4 H13 N2 O3 P S	C4 H13 N2 O3 P S	[C4 H13 N2 O3 P S, tgt=80.13, overall=80.13]	(201.04507, 11028.432)(202.04982, 1210.0157)(203.04442, 1	C4 H13 N2 O3 P S	FindByFormula	7 +	200.0387	3.7184944
C4 H13 N3	C4 H13 N3	[C4 H13 N3, tgt=98.60, overall=98.60]	(104.11794, 27784.674)(105.1211, 1677.2755)(106.11832, 76	C4 H13 N3	FindByFormula	11 +	103.111	0.6441832
C4 H13 N3 S2	C4 H13 N3 S2	[C4 H13 N3 S2, tgt=65.01, overall=65.01]	(168.06386, 1886.3649)(169.06024, 383.3725)(170.06404, 33	C4 H13 N3 S2	FindByFormula	16 +	167.0552	1.932457
C4 H14 N2 P2 S	C4 H14 N2 P2 S	[C4 H14 N2 P2 S, tgt=84.57, overall=84.57]	(185.04262, 19425.36)(186.04716, 1457.5703)(187.04974, 26	C4 H14 N2 P2 S	FindByFormula	28 +	184.0357	3.1729808
C4 H4 N2 O2	C4 H4 N2 O2	[C4 H4 N2 O2, tgt=91.91, overall=91.91]	(113.035, 22644.416)(114.03977, 1015.0747)(115.03939, 492	C4 H4 N2 O2	FindByFormula	17 +	112.0281	1.3682989
C4 H4 N4 O3 S	C4 H4 N4 O3 S	[C4 H4 N4 O3 S, tgt=95.71, overall=95.71]	(189.00792, 3475.5247)(190.00635, 252.29297)(191.0044, 79	C4 H4 N4 O3 S	FindByFormula	27 +	188	1.7671235
C4 H5 N O	C4 H5 N O	[C4 H5 N O, tgt=86.01, overall=86.01]	(84.04495, 7019.67)(85.04334, 279.05917)(86.05203, 40.313	C4 H5 N O	FindByFormula	12 +	83.0376	1.1404165
C4 H6 N6	C4 H6 N6	[C4 H6 N6, tgt=83.80, overall=83.80]	(139.0728, 88098.23)(140.07272, 17640.928)(141.06987, 710	C4 H6 N6	FindByFormula	8 +	138.0656	3.7829337
C4 H7 N	C4 H7 N	[C4 H7 N, tgt=91.51, overall=91.51]	(70.06534, 13968.5625)(71.067055, 745.5468)(92.0458, 133.	C4 H7 N	FindByFormula	14 +	69.0579	0.6452145
C4 H7 N3 O	C4 H7 N3 O	[C4 H7 N3 O, tgt=76.97, overall=76.97]	(114.066246, 6190.9917)(115.06705, 3220.865)(152.0238, 15	C4 H7 N3 O	FindByFormula	6 +	113.0598	0.7291682
C4 H7 N3 O2	C4 H7 N3 O2	[C4 H7 N3 O2, tgt=88.10, overall=88.10]	(130.06064, 14252.267)(131.06302, 870.1908)(132.07565, 37	C4 H7 N3 O2	FindByFormula	13 +	129.0536	0.64100206
C4 H8 N6 O	C4 H8 N6 O	[C4 H8 N6 O, tgt=84.12, overall=84.12]	(157.08371, 39080.72)(158.087, 2792.3772)(159.08464, 541.	C4 H8 N6 O	FindByFormula	28 +	156.0767	3.8138702
C4 H8 N6 O2	C4 H8 N6 O2	[C4 H8 N6 O2, tgt=93.77, overall=93.77]	(173.07858, 30818.654)(174.08049, 2381.6323)(175.07986, 3	C4 H8 N6 O2	FindByFormula	27 +	172.0715	2.2496517
C4 H9 N	C4 H9 N	[C4 H9 N, tgt=78.21, overall=78.21]	(72.08118, 58783.375)(73.0833, 2834.08)(74.08656, 108.334	C4 H9 N	FindByFormula	12 +	71.0741	0.7453347
C4 H9 N O3 S	C4 H9 N O3 S	[C4 H9 N O3 S, tgt=80.09, overall=80.09]	(152.03789, 2646.9119)(153.04402, 74.020004)(154.04008, 6	C4 H9 N O3 S	FindByFormula	6 +	151.0305	5.2168164
C4 H9 N S	C4 H9 N S	[C4 H9 N S, tgt=96.47, overall=96.47]	(104.053764, 11483.065)(105.05398, 846.11993)(106.049385	C4 H9 N S	FindByFormula	18 +	103.0466	0.98655725
C4 H9 N3 O2	C4 H9 N3 O2	[C4 H9 N3 O2, tgt=76.27, overall=76.27]	(132.07686, 49716.734)(133.0789, 4260.64)(134.07916, 670.	C4 H9 N3 O2	FindByFormula	16 +	131.07	0.7131891
C4 H9 O2 P	C4 H9 O2 P	[C4 H9 O2 P, tgt=88.70, overall=88.70]	(121.04103, 63433.438)(122.04504, 4763.7607)(123.04715, 1	C4 H9 O2 P	FindByFormula	20 +	120.0332	1.0639545
C40 H38 N5 P3	C40 H38 N5 P3	[C40 H38 N5 P3, tgt=57.46, overall=57.46]	(682.2386, 1577.1012)(683.2461, 578.6776)(684.24347, 353.	C40 H38 N5 P3	FindByFormula	18 +	681.2286	22.034716
C40 H41 N7 O S2	C40 H41 N7 O S2	[C40 H41 N7 O S2, tgt=64.38, overall=64.38]	(700.287, 2276.3015)(701.2912, 1050.6533)(702.28955, 588.	C40 H41 N7 O S2	FindByFormula	24 +	699.2821	22.641504
C40 H51 N3 O4 S3	C40 H51 N3 O4 S3	[C40 H51 N3 O4 S3, tgt=34.40, overall=34.40]	(734.3116, 1604.607)(735.3129, 776.6996)(736.3153, 331.39	C40 H51 N3 O4 S3	FindByFormula	23 +	733.3052	9.306369
C40 H53 N O2 P4	C40 H53 N O2 P4	[C40 H53 N O2 P4, tgt=72.17, overall=72.17]	(704.3105, 780.7151)(705.3093, 343.28305)(706.3064, 189.9	C40 H53 N O2 P4	FindByFormula	19 +	703.3	22.240902
C40 H59 Cl N5 O3 P	C40 H59 Cl N5 O3 P	[C40 H59 Cl N5 O3 P, tgt=76.93, overall=76.93]	(724.41046, 4087.7869)(725.4207, 2232.2222)(726.40454, 25	C40 H59 Cl N5 O3 P	FindByFormula	24 +	723.3987	22.526573
C40 H61 N O4 P2	C40 H61 N O4 P2	[C40 H61 N O4 P2, tgt=52.11, overall=52.11]	(682.41327, 21956.002)(683.42096, 11971.072)(684.42456, 3	C40 H61 N O4 P2	FindByFormula	20 +	681.4073	22.138145
C40 H76 O12	C40 H76 O12	[C40 H76 O12, tgt=56.68, overall=56.68]	(749.539, 5513.3633)(750.54474, 2671.3882)(751.54126, 112	C40 H76 O12	FindByFormula	17 +	748.5319	23.06269
C40 H86 N2 O4	C40 H86 N2 O4	[C40 H86 N2 O4, tgt=83.56, overall=83.56]	(659.6678, 4023.3606)(660.67145, 1819.8362)(661.67285, 83	C40 H86 N2 O4	FindByFormula	21 +	658.6625	26.767502
C41 H45 N3 O3 S	C41 H45 N3 O3 S	[C41 H45 N3 O3 S, tgt=86.03, overall=86.03]	(660.32605, 2104.2349)(661.3312, 781.1925)(662.3304, 382.	C41 H45 N3 O3 S	FindByFormula	21 +	659.316	22.288052
C41 H45 N7 S	C41 H45 N7 S	[C41 H45 N7 S, tgt=67.85, overall=67.85]	(668.3519, 3697.2104)(669.35443, 1796.4885)(670.35944, 71	C41 H45 N7 S	FindByFormula	22 +	667.3447	22.540356
C41 H50 N4 O S2	C41 H50 N4 O S2	[C41 H50 N4 O S2, tgt=24.95, overall=24.95]	(679.3501, 2091.8284)(680.347, 1203.4075)(681.34607, 398.	C41 H50 N4 O S2	FindByFormula	20 +	678.3415	22.251549
C41 H51 N3 O4 S	C41 H51 N3 O4 S	[C41 H51 N3 O4 S, tgt=73.06, overall=73.06]	(682.3653, 7828.289)(683.3713, 3557.1343)(684.3766, 1204.	C41 H51 N3 O4 S	FindByFormula	20 +	681.3599	22.536898
C41 H53 N2 P S2	C41 H53 N2 P S2	[C41 H53 N2 P S2, tgt=25.14, overall=25.14]	(669.3449, 2740.588)(670.34894, 1419.1215)(671.3524, 673.	C41 H53 N2 P S2	FindByFormula	22 +	668.3374	22.371529
C41 H62 N5 O P S	C41 H62 N5 O P S	[C41 H62 N5 O P S, tgt=63.19, overall=63.19]	(704.44775, 4258.803)(705.4525, 1908.3639)(706.4532, 833.	C41 H62 N5 O P S	FindByFormula	26 +	703.4455	22.619617
C41 H66 N6 S2	C41 H66 N6 S2	[C41 H66 N6 S2, tgt=44.97, overall=44.97]	(707.4892, 4757.9663)(708.48785, 2163.2515)(709.47943, 88	C41 H66 N6 S2	FindByFormula	21 +	706.4792	22.611
C41 H69 Cl N O4 P S	C41 H69 Cl N O4 P S	[C41 H69 Cl N O4 P S, tgt=29.10, overall=29.10]	(738.44415, 1583.3019)(739.4413, 1124.3926)(740.4487, 124	C41 H69 Cl N O4 P S	FindByFormula	22 +	737.4342	22.32538
C41 H80 N O P	C41 H80 N O P	[C41 H80 N O P, tgt=73.39, overall=73.39]	(634.6078, 4283.8345)(635.59906, 1800.6172)(636.60223, 12	C41 H80 N O P	FindByFormula	7 +	633.5965	20.441591
C41 H82 O	C41 H82 O	[C41 H82 O, tgt=94.19, overall=94.19]	(591.64136, 9034.043)(592.64526, 3553.4993)(593.6472, 902	C41 H82 O	FindByFormula	18 +	590.632	26.125309
C41 H85 N2 P S2	C41 H85 N2 P S2	[C41 H85 N2 P S2, tgt=63.35, overall=63.35]	(701.5975, 3595.157)(702.60187, 1757.5645)(703.59717, 838	C41 H85 N2 P S2	FindByFormula	21 +	700.5911	25.359436
C41 H88 N6	C41 H88 N6	[C41 H88 N6, tgt=67.46, overall=67.46]	(665.7105, 10252.145)(666.7155, 5355.1704)(667.7233, 1798	C41 H88 N6	FindByFormula	11 +	664.713	25.791222
C42 H19 N2 O P5	C42 H19 N2 O P5	[C42 H19 N2 O P5, tgt=83.84, overall=83.84]	(723.02466, 1942.7451)(724.02496, 957.8971)(725.02765, 10	C42 H19 N2 O P5	FindByFormula	8 +	722.0182	13.028126
C42 H38 N3 O2 P	C42 H38 N3 O2 P	[C42 H38 N3 O2 P, tgt=66.42, overall=66.42]	(648.2807, 1733.5066)(649.27515, 1321.2662)(650.27576, 24	C42 H38 N3 O2 P	FindByFormula	17 +	647.2661	22.188076
C42 H41 N O3 S2	C42 H41 N O3 S2	[C42 H41 N O3 S2, tgt=75.58, overall=75.58]	(672.25964, 2399.1096)(673.2624, 1174.7753)(674.268, 455.	C42 H41 N O3 S2	FindByFormula	28 +	671.2524	22.3118
C42 H44 N O4 P3	C42 H44 N O4 P3	[C42 H44 N O4 P3, tgt=20.92, overall=20.92]	(720.25385, 1107.9153)(721.25885, 519.1869)(722.2599, 192	C42 H44 N O4 P3	FindByFormula	25 +	719.2476	22.081514
C42 H51 N7 O S	C42 H51 N7 O S	[C42 H51 N7 O S, tgt=45.67, overall=45.67]	(702.3859, 222.98332)(703.3975, 106.09332)(704.4037, 32.9	C42 H51 N7 O S	FindByFormula	3 +	701.3828	6.40544
C42 H65 N O5 P2	C42 H65 N O5 P2	[C42 H65 N O5 P2, tgt=31.55, overall=31.55]	(726.4394, 16598.764)(727.44727, 10479.07)(728.451, 3303.	C42 H65 N O5 P2	FindByFormula	25 +	725.4348	22.124836
C42 H86 N2	C42 H86 N2	[C42 H86 N2, tgt=65.63, overall=65.63]	(619.6837, 10467.347)(620.6876, 4340.8066)(621.691, 1131.	C42 H86 N2	FindByFormula	13 +	618.6755	27.454855
C42 H87 O P	C42 H87 O P	[C42 H87 O P, tgt=70.65, overall=70.65]	(639.65686, 27235.412)(640.66064, 11816.94)(641.66504, 30	C42 H87 O P	FindByFormula	23 +	638.6521	25.315159
C43 H82 O	C43 H82 O	[C43 H82 O, tgt=73.49, overall=73.49]	(615.64734, 88449.32)(616.6505, 35703.684)(617.6545, 8137	C43 H82 O	FindByFormula	16 +	614.6425	25.62627
C43 H83 P	C43 H83 P	[C43 H83 P, tgt=68.30, overall=68.30]	(631.6302, 5799.135)(632.634, 2477.7705)(633.6353, 1158.1	C43 H83 P	FindByFormula	20 +	630.6225	25.66457
C43 H84 N2	C43 H84 N2	[C43 H84 N2, tgt=74.17, overall=74.17]	(629.6697, 4955.9233)(630.6746, 2176.9934)(631.678, 654.8	C43 H84 N2	FindByFormula	15 +	628.6617	26.152166
C43 H84 O	C43 H84 O	[C43 H84 O, tgt=85.44, overall=85.44]	(617.66205, 118784.336)(618.6658, 48169.35)(619.66943, 10	C43 H84 O	FindByFormula	13 +	616.6556	26.373833
C43 H85 P	C43 H85 P	[C43 H85 P, tgt=79.84, overall=79.84]	(633.6459, 4933.418)(634.64954, 2101.658)(635.64996, 959.	C43 H85 P	FindByFormula	22 +	632.6337	26.363934
C43 H90 N5 P	C43 H90 N5 P	[C43 H90 N5 P, tgt=91.78, overall=91.78]	(708.70044, 4091.022)(709.7044, 2118.5825)(710.7071, 665.	C43 H90 N5 P	FindByFormula	19 +	707.6955	25.360773
C43 H91 N2 P	C43 H91 N2 P	[C43 H91 N2 P, tgt=30.67, overall=30.67]	(667.6998, 27768.973)(668.7045, 12716.639)(669.70685, 365	C43 H91 N2 P	FindByFormula	22 +	666.6937	26.660067
C44 H41 N O3 S2	C44 H41 N O3 S2	[C44 H41 N O3 S2, tgt=95.29, overall=95.29]	(696.2599, 2176.4675)(697.26605, 1246.9724)(698.2662, 556	C44 H41 N O3 S2	FindByFormula	27 +	695.2532	22.029663
C44 H58 O P2 S	C44 H58 O P2 S	[C44 H58 O P2 S, tgt=49.19, overall=49.19]	(697.37573, 2187.6587)(698.3791, 1261.0787)(699.3813, 425	C44 H58 O P2 S	FindByFormula	13 +	696.3691	22.669436
C44 H86 N2	C44 H86 N2	[C44 H86 N2, tgt=77.84, overall=77.84]	(643.68854, 62186.598)(644.6918, 26112.342)(645.6961, 637	C44 H86 N2	FindByFormula	24 +	642.6833	26.741798
C44 H86 O3	C44 H86 O3	[C44 H86 O3, tgt=63.13, overall=63.13]	(663.6629, 2909.8735)(664.6679, 1388.1222)(665.67413, 891	C44 H86 O3	FindByFormula	16 +	662.6585	25.398943
C45 H15 N3 P2	C45 H15 N3 P2	[C45 H15 N3 P2, tgt=85.77, overall=85.77]	(660.0811, 4916.84)(661.0891, 2277.1433)(662.089, 697.396	C45 H15 N3 P2	FindByFormula	7 +	659.076	0.8081425
C45 H61 N O3 S2	C45 H61 N O3 S2	[C45 H61 N O3 S2, tgt=64.35, overall=64.35]	(728.41876, 1660.4727)(729.4233, 887.7267)(730.4165, 492.	C45 H61 N O3 S2	FindByFormula	20 +	727.4165	22.546223
C46 H78 N O2 P S	C46 H78 N O2 P S	[C46 H78 N O2 P S, tgt=70.70, overall=70.70]	(740.5569, 5883.2603)(741.56036, 2796.1677)(742.55817, 14	C46 H78 N O2 P S	FindByFormula	12 +	739.5502	25.125711
C46 H88	C46 H88	[C46 H88, tgt=56.92, overall=56.92]	(641.6948, 55477.082)(642.699, 23275.98)(643.7031, 5725.1	C46 H88	FindByFormula	12 +	640.6847	25.904549
C47 H34 N3 P	C47 H34 N3 P	[C47 H34 N3 P, tgt=66.38, overall=66.38]	(672.2579, 2746.996)(673.2616, 1456.6272)(674.2677, 599.8	C47 H34 N3 P	FindByFormula	25 +	671.2524	22.285461
C47 H37 N O3 S	C47 H37 N O3 S	[C47 H37 N O3 S, tgt=97.50, overall=97.50]	(696.2576, 2346.778)(697.2631, 1449.366)(698.2634, 526.55	C47 H37 N O3 S	FindByFormula	25 +	695.2506	22.112951
C47 H66 S	C47 H66 S	[C47 H66 S, tgt=76.47, overall=76.47]	(663.4949, 3259.5654)(664.4987, 1468.4901)(665.5049, 582.	C47 H66 S	FindByFormula	16 +	662.485	25.253006
C48 H102 P2	C48 H102 P2	[C48 H102 P2, tgt=22.41, overall=22.41]	(741.75104, 11559.908)(742.75385, 5175.9575)(743.7562, 19	C48 H102 P2	FindByFormula	16 +	740.7456	23.937004
C48 H59 N3 S2	C48 H59 N3 S2	[C48 H59 N3 S2, tgt=75.54, overall=75.54]	(742.4212, 1041.7787)(743.4227, 1246.21)(744.42017, 509.1	C48 H59 N3 S2	FindByFormula	27 +	741.4164	22.549889
C48 H86 N2	C48 H86 N2	[C48 H86 N2, tgt=69.49, overall=69.49]	(691.6864, 2523.1406)(692.6888, 1102.3262)(693.68506, 876	C48 H86 N2	FindByFormula	17 +	690.6771	22.90598
C49 H101 N	C49 H101 N	[C49 H101 N, tgt=81.33, overall=81.33]	(704.804, 14696.709)(705.80676, 7126.2466)(706.81006, 196	C49 H101 N	FindByFormula	15 +	703.7977	25.593035
C49 H71 N O4	C49 H71 N O4	[C49 H71 N O4, tgt=71.69, overall=71.69]	(738.54224, 2306.8374)(739.554, 1509.2213)(740.55286, 121	C49 H71 N O4	FindByFormula	9 +	737.5402	24.59163
C5 H10 N2 O S	C5 H10 N2 O S	[C5 H10 N2 O S, tgt=92.75, overall=92.75]	(147.05855, 5672.204)(148.06177, 516.44403)(149.06224, 16	C5 H10 N2 O S	FindByFormula	20 +	146.0512	3.6085312
C5 H10 N4 O2	C5 H10 N4 O2	[C5 H10 N4 O2, tgt=47.08, overall=47.08]	(159.08699, 21478.168)(160.09181, 1716.3478)(161.09358, 2	C5 H10 N4 O2	FindByFormula	15 +	158.0804	0.680535
C5 H10 N6 O	C5 H10 N6 O	[C5 H10 N6 O, tgt=78.08, overall=78.08]	(171.09741, 4432.0464)(172.09648, 277.8275)(173.10086, 45	C5 H10 N6 O	FindByFormula	25 +	170.0906	6.37367
C5 H10 P2	C5 H10 P2	[C5 H10 P2, tgt=78.88, overall=78.88]	(133.03316, 47909.9)(134.0387, 3431.0623)(135.03214, 2962	C5 H10 P2	FindByFormula	25 +	132.0251	0.9991629
C5 H11 Cl O2	C5 H11 Cl O2	[C5 H11 Cl O2, tgt=75.44, overall=75.44]	(177.00873, 133.155)(178.0159, 23.755001)(161.03105, 166.	C5 H11 Cl O2	FindByFormula	4 +	138.0436	4.8256674
C5 H11 N	C5 H11 N	[C5 H11 N, tgt=79.17, overall=79.17]	(86.09703, 255227.31)(87.1, 14437.43)(88.102905, 440.8946	C5 H11 N	FindByFormula	18 +	85.0898	1.6014527
C5 H11 N O2	C5 H11 N O2	[C5 H11 N O2, tgt=97.84, overall=97.84]	(118.08652, 155747.36)(119.08866, 9695.345)(120.08741, 94	C5 H11 N O2	FindByFormula	18 +	117.0794	0.8428344
C5 H11 N O2 S	C5 H11 N O2 S	[C5 H11 N O2 S, tgt=98.52, overall=98.52]	(150.05911, 145442.95)(151.06116, 10414.496)(152.05533, 1	C5 H11 N O2 S	FindByFormula	18 +	149.0522	1.0135013
C5 H11 N P2	C5 H11 N P2	[C5 H11 N P2, tgt=77.13, overall=77.13]	(148.04514, 24459.45)(149.0443, 1816.7571)(186.0022, 84.2	C5 H11 N P2	FindByFormula	7 +	147.0381	1.0367149
C5 H12 N3 O P	C5 H12 N3 O P	[C5 H12 N3 O P, tgt=98.94, overall=98.94]	(162.07881, 11732.515)(163.07967, 785.3561)(164.07924, 17	C5 H12 N3 O P	FindByFormula	10 +	161.0708	0.853706
C5 H12 O6 P2	C5 H12 O6 P2	[C5 H12 O6 P2, tgt=89.43, overall=89.43]	(231.01805, 5181.9336)(232.02022, 435.78665)(233.01671, 2	C5 H12 O6 P2	FindByFormula	6 +	230.0105	2.0775044
C5 H13 N O	C5 H13 N O	[C5 H13 N O, tgt=99.79, overall=99.79]	(104.10701, 9178.789)(105.11033, 1157.7864)(106.11029, 85	C5 H13 N O	FindByFormula	23 +	103.0995	22.226835
C5 H13 N4 O5 P	C5 H13 N4 O5 P	[C5 H13 N4 O5 P, tgt=79.14, overall=79.14]	(241.0703, 25338.828)(242.0718, 3086.4148)(243.06381, 777	C5 H13 N4 O5 P	FindByFormula	14 +	240.0619	8.240111
C5 H15 N4 O3 P	C5 H15 N4 O3 P	[C5 H15 N4 O3 P, tgt=82.46, overall=82.46]	(211.09534, 7962.188)(212.09572, 762.90265)(213.10002, 26	C5 H15 N4 O3 P	FindByFormula	28 +	210.0888	10.668622
C5 H4 N4 O2	C5 H4 N4 O2	[C5 H4 N4 O2, tgt=71.44, overall=71.44]	(153.04054, 29687.217)(154.04404, 2499.652)(155.04056, 26	C5 H4 N4 O2	FindByFormula	25 +	152.0332	1.2740453
C5 H4 O4 P2	C5 H4 O4 P2	[C5 H4 O4 P2, tgt=83.50, overall=83.50]	(190.96516, 11891.592)(191.96617, 917.3341)(192.96829, 11	C5 H4 O4 P2	FindByFormula	17 +	189.9574	1.068063
C5 H5 N5	C5 H5 N5	[C5 H5 N5, tgt=95.44, overall=95.44]	(136.06192, 55128.996)(137.06427, 4210.2915)(138.0598, 66	C5 H5 N5	FindByFormula	28 +	135.0546	3.8887308
C5 H5 N5 O	C5 H5 N5 O	[C5 H5 N5 O, tgt=73.85, overall=73.85]	(152.05727, 34365.63)(153.05984, 4749.8833)(154.05815, 70	C5 H5 N5 O	FindByFormula	14 +	151.05	1.7709391
C5 H6 O3 P2	C5 H6 O3 P2	[C5 H6 O3 P2, tgt=72.43, overall=72.43]	(176.98682, 7986.1963)(177.99033, 1129.2922)(178.9881, 90	C5 H6 O3 P2	FindByFormula	13 +	175.9793	0.9698492

C5 H7 N O3	C5 H7 N O3	[C5 H7 N O3, tgt=91.00, overall=91.00]		(130.05046, 257425.7)(131.0538, 15341.034)(132.06252, 247	C5 H7 N O3		FindByFormula	20	+	129.0433	1.1893021
C5 H9 N O2	C5 H9 N O2	[C5 H9 N O2, tgt=90.46, overall=90.46]		(116.07065, 81583.266)(117.0718, 5213.206)(118.0771, 29.8	C5 H9 N O2		FindByFormula	21	+	115.0636	0.63614416
C5 H9 N3	C5 H9 N3	[C5 H9 N3, tgt=31.25, overall=31.25]		(112.087006, 35692.633)(113.0898, 4602.913)(114.08943, 15	C5 H9 N3		FindByFormula	23	+	111.0798	0.5667404
C50 H93 N3	C50 H93 N3	[C50 H93 N3, tgt=73.18, overall=73.18]		(736.7431, 40120.75)(737.7468, 20551.217)(738.7499, 5749.	C50 H93 N3		FindByFormula	20	+	735.7375	25.353846
C54 H54 O2	C54 H54 O2	[C54 H54 O2, tgt=34.71, overall=34.71]		(735.42114, 2577.6567)(736.42456, 1506.6334)(737.4276, 92	C54 H54 O2		FindByFormula	18	+	734.418	22.744984
C6 H10 N6 O	C6 H10 N6 O	[C6 H10 N6 O, tgt=86.22, overall=86.22]		(183.09871, 2386.7368)(184.0961, 222.55214)(185.09396, 53	C6 H10 N6 O		FindByFormula	28	+	182.0912	4.775186
C6 H10 O4	C6 H10 O4	[C6 H10 O4, tgt=98.83, overall=98.83]		(147.06555, 1991.7778)(148.06511, 104.55428)(149.06209, 2	C6 H10 O4		FindByFormula	16	+	146.0583	2.083396
C6 H11 N O	C6 H11 N O	[C6 H11 N O, tgt=95.01, overall=95.01]		(114.09137, 53106.758)(115.09388, 4297.3765)(116.0932, 25	C6 H11 N O		FindByFormula	28	+	113.0842	4.487415
C6 H11 N O2 S	C6 H11 N O2 S	[C6 H11 N O2 S, tgt=97.49, overall=97.49]		(162.0595, 5170.5913)(163.05779, 397.29736)(164.05391, 32	C6 H11 N O2 S		FindByFormula	16	+	161.0521	1.9606452
C6 H12 N4 O4	C6 H12 N4 O4	[C6 H12 N4 O4, tgt=62.23, overall=62.23]		(205.09087, 2671.7336)(206.08994, 201.46696)(207.09735, 7	C6 H12 N4 O4		FindByFormula	23	+	204.0847	7.933327
C6 H12 N6	C6 H12 N6	[C6 H12 N6, tgt=89.68, overall=89.68]		(169.1191, 5658.017)(170.12021, 456.94504)(171.1217, 53.8	C6 H12 N6		FindByFormula	24	+	168.1126	8.039098
C6 H12 N6 O	C6 H12 N6 O	[C6 H12 N6 O, tgt=97.15, overall=97.15]		(185.11485, 39278.402)(186.11806, 3590.627)(187.11668, 35	C6 H12 N6 O		FindByFormula	28	+	184.1078	10.045829
C6 H12 N6 O3	C6 H12 N6 O3	[C6 H12 N6 O3, tgt=95.18, overall=95.18]		(217.10501, 49453.426)(218.1084, 4619.847)(219.10791, 800	C6 H12 N6 O3		FindByFormula	28	+	216.098	3.548355
C6 H13 Cl N6	C6 H13 Cl N6	[C6 H13 Cl N6, tgt=75.06, overall=75.06]		(205.09769, 442335.0)(206.10004, 58660.777)(207.09248, 13	C6 H13 Cl N6		FindByFormula	27	+	204.0902	3.610258
C6 H13 N O	C6 H13 N O	[C6 H13 N O, tgt=91.54, overall=91.54]		(116.107086, 84411.73)(117.11026, 6366.4883)(154.06235, 5	C6 H13 N O		FindByFormula	9	+	115.0997	0.9952239
C6 H13 N O2	C6 H13 N O2	[C6 H13 N O2, tgt=95.67, overall=95.67]		(132.10233, 660114.06)(133.10524, 47666.457)(134.10574, 4	C6 H13 N O2		FindByFormula	28	+	131.095	1.6275455
C6 H14 N5 O P S	C6 H14 N5 O P S	[C6 H14 N5 O P S, tgt=91.45, overall=91.45]		(236.072, 15255.868)(237.07758, 1810.1981)(238.0712, 960.	C6 H14 N5 O P S		FindByFormula	27	+	235.0652	13.485321
C6 H14 O3	C6 H14 O3	[C6 H14 O3, tgt=89.03, overall=89.03]		(135.10065, 1017.71405)(136.10379, 65.409546)(173.05826,	C6 H14 O3		FindByFormula	25	+	134.0943	4.349765
C6 H14 O4	C6 H14 O4	[C6 H14 O4, tgt=92.07, overall=92.07]		(151.09521, 1927.4374)(152.09706, 160.27333)(153.09552, 4	C6 H14 O4		FindByFormula	28	+	150.089	2.2495933
C6 H15 N3 O	C6 H15 N3 O	[C6 H15 N3 O, tgt=60.40, overall=60.40]		(184.08527, 1616.6068)(185.0782, 204.72)(186.0863, 419.33)	C6 H15 N3 O		FindByFormula	3	+	145.1202	0.64600646
C6 H15 N3 O2	C6 H15 N3 O2	[C6 H15 N3 O2, tgt=95.10, overall=95.10]		(162.1234, 90191.82)(163.12642, 7324.6753)(164.12996, 120	C6 H15 N3 O2		FindByFormula	15	+	161.1169	0.661202
C6 H4 O	C6 H4 O	[C6 H4 O, tgt=87.75, overall=87.75]		(93.033646, 8628.143)(94.039375, 1008.67267)(95.041855, 5	C6 H4 O		FindByFormula	19	+	92.0267	8.663448
C6 H4 O6 S	C6 H4 O6 S	[C6 H4 O6 S, tgt=89.19, overall=89.19]		(204.98094, 1905.4059)(205.98038, 273.61655)(206.97812, 2	C6 H4 O6 S		FindByFormula	25	+	203.973	1.7537737
C6 H6 N4 O2	C6 H6 N4 O2	[C6 H6 N4 O2, tgt=76.82, overall=76.82]		(167.05675, 5183.846)(168.05453, 497.13715)(169.0495, 701	C6 H6 N4 O2		FindByFormula	8	+	166.049	2.1888824
C6 H6 O5	C6 H6 O5	[C6 H6 O5, tgt=98.33, overall=98.33]		(159.0288, 74227.25)(160.03131, 5118.746)(161.03137, 2419	C6 H6 O5		FindByFormula	19	+	158.0217	1.1088475
C6 H8 O3	C6 H8 O3	[C6 H8 O3, tgt=83.80, overall=83.80]		(129.05501, 2165.7615)(130.05269, 415.5928)(131.0545, 57.	C6 H8 O3		FindByFormula	7	+	128.0473	2.0527208
C6 H8 O3 P2	C6 H8 O3 P2	[C6 H8 O3 P2, tgt=97.34, overall=97.34]		(191.00168, 15219.508)(192.00441, 1401.7445)(193.00189, 2	C6 H8 O3 P2		FindByFormula	20	+	189.9944	8.662489
C6 H9 N O4	C6 H9 N O4	[C6 H9 N O4, tgt=76.81, overall=76.81]		(160.06015, 107715.266)(161.06342, 8813.637)(162.06541, 1	C6 H9 N O4		FindByFormula	7	+	159.0535	0.88642865
C6 H9 N O4 S	C6 H9 N O4 S	[C6 H9 N O4 S, tgt=98.10, overall=98.10]		(192.03255, 6372.6885)(193.03365, 1095.4581)(194.03265, 7	C6 H9 N O4 S		FindByFormula	21	+	191.0257	0.90109724
C7 H10 N5 O2 P	C7 H10 N5 O2 P	[C7 H10 N5 O2 P, tgt=90.78, overall=90.78]		(228.06377, 19807.555)(229.06787, 2816.8835)(230.07137, 3	C7 H10 N5 O2 P		FindByFormula	8	+	227.0568	4.953084
C7 H10 N6 O	C7 H10 N6 O	[C7 H10 N6 O, tgt=73.76, overall=73.76]		(195.0999, 22353.738)(196.10144, 2310.1401)(197.09497, 53	C7 H10 N6 O		FindByFormula	23	+	194.0925	11.904942
C7 H10 N6 O2	C7 H10 N6 O2	[C7 H10 N6 O2, tgt=89.41, overall=89.41]		(211.09343, 19114.664)(212.09529, 2039.12)(213.10153, 889	C7 H10 N6 O2		FindByFormula	8	+	210.0873	8.573759
C7 H10 O2 S3	C7 H10 O2 S3	[C7 H10 O2 S3, tgt=75.05, overall=75.05]		(222.99182, 4297.511)(223.9875, 693.693)(224.98515, 1070.	C7 H10 O2 S3		FindByFormula	20	+	221.983	4.067561
C7 H12 N2 O2 S	C7 H12 N2 O2 S	[C7 H12 N2 O2 S, tgt=92.74, overall=92.74]		(189.06923, 127311.61)(190.07219, 14658.383)(191.07474, 1	C7 H12 N2 O2 S		FindByFormula	20	+	188.0627	3.6117263
C7 H12 N6 O	C7 H12 N6 O	[C7 H12 N6 O, tgt=98.88, overall=98.88]		(197.11446, 27087.848)(198.11734, 2843.3416)(199.11436, 3	C7 H12 N6 O		FindByFormula	7	+	196.1073	6.65654
C7 H12 O4 P2	C7 H12 O4 P2	[C7 H12 O4 P2, tgt=97.27, overall=97.27]		(223.02835, 22090.031)(224.03143, 2386.728)(225.0312, 478	C7 H12 O4 P2		FindByFormula	21	+	222.0209	8.6664505
C7 H13 N O2	C7 H13 N O2	[C7 H13 N O2, tgt=90.86, overall=90.86]		(144.10217, 127609.664)(145.10376, 11801.664)(146.10349,	C7 H13 N O2		FindByFormula	18	+	143.096	0.78905606
C7 H13 N7	C7 H13 N7	[C7 H13 N7, tgt=90.10, overall=90.10]		(196.12996, 4002.9673)(197.1283, 1011.7933)(198.12646, 89	C7 H13 N7		FindByFormula	20	+	195.1225	8.1156
C7 H14 N2 O	C7 H14 N2 O	[C7 H14 N2 O, tgt=97.42, overall=97.42]		(143.11743, 4199.447)(144.11845, 541.3306)(145.1194, 87.8	C7 H14 N2 O		FindByFormula	28	+	142.1098	3.2588062
C7 H14 N6 O2	C7 H14 N6 O2	[C7 H14 N6 O2, tgt=82.03, overall=82.03]		(215.12532, 3856.0337)(216.12146, 319.517)(217.12367, 61.	C7 H14 N6 O2		FindByFormula	27	+	214.1182	7.2612743
C7 H14 P2	C7 H14 P2	[C7 H14 P2, tgt=82.25, overall=82.25]		(161.06528, 2134.9565)(162.06523, 78.770004)(199.02448, 7	C7 H14 P2		FindByFormula	26	+	160.0581	5.990581
C7 H15 N O2	C7 H15 N O2	[C7 H15 N O2, tgt=22.67, overall=22.67]		(146.11725, 5002.692)(147.11342, 1884.5234)(148.1256, 365	C7 H15 N O2		FindByFormula	12	+	145.1091	0.7967517
C7 H15 N O3	C7 H15 N O3	[C7 H15 N O3, tgt=97.03, overall=97.03]		(162.11269, 59214.324)(163.11456, 4583.0645)(164.11546, 5	C7 H15 N O3		FindByFormula	24	+	161.1052	0.6997514
C7 H16 N8 O S	C7 H16 N8 O S	[C7 H16 N8 O S, tgt=79.63, overall=79.63]		(261.12357, 9289.571)(262.1265, 1697.9567)(263.11557, 139	C7 H16 N8 O S		FindByFormula	6	+	260.1162	5.22365
C7 H17 N5 S	C7 H17 N5 S	[C7 H17 N5 S, tgt=95.29, overall=95.29]		(204.12773, 210826.55)(205.13033, 22098.557)(206.13203, 2	C7 H17 N5 S		FindByFormula	13	+	203.1212	0.7530034
C7 H18 Cl N5 O	C7 H18 Cl N5 O	[C7 H18 Cl N5 O, tgt=69.89, overall=69.89]		(224.12865, 3604.6223)(225.12892, 527.7308)(226.12244, 26	C7 H18 Cl N5 O		FindByFormula	24	+	223.1215	0.9957517
C7 H18 O2 P2	C7 H18 O2 P2	[C7 H18 O2 P2, tgt=80.34, overall=80.34]		(197.08513, 12717.712)(198.08809, 1395.2916)(199.0862, 35	C7 H18 O2 P2		FindByFormula	28	+	196.0777	18.32577
C7 H19 N3	C7 H19 N3	[C7 H19 N3, tgt=94.97, overall=94.97]		(146.1651, 56402.586)(147.16617, 5530.445)(148.16664, 241	C7 H19 N3		FindByFormula	22	+	145.1577	0.5299556
C7 H20 N5 O2 P	C7 H20 N5 O2 P	[C7 H20 N5 O2 P, tgt=60.96, overall=60.96]		(238.14156, 5178.6655)(239.14238, 1028.1906)(240.14365, 1	C7 H20 N5 O2 P		FindByFormula	22	+	237.1342	12.217126
C7 H21 N3 O3 P2	C7 H21 N3 O3 P2	[C7 H21 N3 O3 P2, tgt=93.91, overall=93.91]		(258.11334, 15733.461)(259.11685, 1578.6357)(260.11697, 3	C7 H21 N3 O3 P2		FindByFormula	16	+	257.104	0.64868903
C7 H3 N O6 S	C7 H3 N O6 S	[C7 H3 N O6 S, tgt=95.61, overall=95.61]		(229.97594, 16800.072)(230.97923, 1748.4807)(231.97795, 1	C7 H3 N O6 S		FindByFormula	21	+	228.9688	1.2030535
C7 H3 P S3	C7 H3 P S3	[C7 H3 P S3, tgt=69.10, overall=69.10]		(214.9176, 74369.39)(215.9177, 2950.65)(216.92154, 1804.2	C7 H3 P S3		FindByFormula	2	+	213.9114	0.54300094
C7 H4 O2	C7 H4 O2	[C7 H4 O2, tgt=99.05, overall=99.05]		(121.02867, 99834.07)(122.032455, 7383.5015)(123.034645,	C7 H4 O2		FindByFormula	20	+	120.0214	8.662018
C7 H6 O2	C7 H6 O2	[C7 H6 O2, tgt=99.10, overall=99.10]		(123.04468, 22285.73)(124.04799, 1936.9875)(125.046265, 1	C7 H6 O2		FindByFormula	10	+	122.0372	1.2647005
C7 H6 O4	C7 H6 O4	[C7 H6 O4, tgt=83.84, overall=83.84]		(155.0327, 6104.115)(156.04083, 920.01105)(157.0321, 190.	C7 H6 O4		FindByFormula	10	+	154.0254	2.9770322
C7 H7 N O	C7 H7 N O	[C7 H7 N O, tgt=32.77, overall=32.77]		(122.0595, 500.92)(144.0393, 206.41)	C7 H7 N O		FindByFormula	1	+	121.0516	2.4820294
C7 H8 N2 O2	C7 H8 N2 O2	[C7 H8 N2 O2, tgt=89.77, overall=89.77]		(153.06549, 34035.05)(154.0654, 2229.4224)(155.06648, 508	C7 H8 N2 O2		FindByFormula	8	+	152.0579	1.859384
C7 H8 N4 O2	C7 H8 N4 O2	[C7 H8 N4 O2, tgt=98.85, overall=98.85]		(181.07285, 34666.434)(182.076, 3883.964)(183.08177, 411.	C7 H8 N4 O2		FindByFormula	25	+	180.0659	4.1075425
C7 H8 O	C7 H8 O	[C7 H8 O, tgt=72.02, overall=72.02]		(109.06486, 5467.136)(110.06793, 440.6142)(111.07314, 44.	C7 H8 O		FindByFormula	21	+	108.0576	8.66063
C7 H8 O2	C7 H8 O2	[C7 H8 O2, tgt=34.66, overall=34.66]		(125.060425, 609.575)(126.060455, 96.065)	C7 H8 O2		FindByFormula	4	+	124.0534	2.1430173
C7 H9 Cl N2 O3	C7 H9 Cl N2 O3	[C7 H9 Cl N2 O3, tgt=73.53, overall=73.53]		(205.03555, 3374.6414)(206.03638, 347.612)(207.0331, 861.	C7 H9 Cl N2 O3		FindByFormula	7	+	204.029	1.0412881
C7 H9 N O	C7 H9 N O	[C7 H9 N O, tgt=63.82, overall=63.82]		(124.07571, 3722.2734)(125.07317, 936.6567)(146.05847, 14	C7 H9 N O		FindByFormula	3	+	123.0675	1.7106673
C7 H9 N O3 P2	C7 H9 N O3 P2	[C7 H9 N O3 P2, tgt=97.51, overall=97.51]		(218.01305, 3461.7202)(219.01787, 424.15646)(220.01588, 1	C7 H9 N O3 P2		FindByFormula	15	+	217.0065	4.8053684
C8 H10 N4 O2	C8 H10 N4 O2	[C8 H10 N4 O2, tgt=98.83, overall=98.83]		(195.08832, 49364.164)(196.09038, 5056.4688)(197.0873, 99	C8 H10 N4 O2		FindByFormula	23	+	194.0807	5.883894
C8 H10 N8 O6	C8 H10 N8 O6	[C8 H10 N8 O6, tgt=96.15, overall=96.15]		(315.08047, 415305.97)(316.08334, 48487.676)(317.08328, 9	C8 H10 N8 O6		FindByFormula	7	+	314.0738	0.80599964
C8 H10 O6	C8 H10 O6	[C8 H10 O6, tgt=93.74, overall=93.74]		(203.05428, 36624.61)(204.05798, 2633.096)(205.06139, 671	C8 H10 O6		FindByFormula	25	+	202.0465	0.63852096
C8 H11 N	C8 H11 N	[C8 H11 N, tgt=49.65, overall=49.65]		(122.09654, 12318.351)(123.09829, 1275.7567)(124.10015, 5	C8 H11 N		FindByFormula	13	+	121.0891	3.7069361
C8 H11 N O	C8 H11 N O	[C8 H11 N O, tgt=97.75, overall=97.75]		(138.09135, 28342.55)(139.0943, 2766.4739)(140.10257, 684	C8 H11 N O		FindByFormula	5	+	137.0842	2.6776164
C8 H12 N6 O	C8 H12 N6 O	[C8 H12 N6 O, tgt=91.64, overall=91.64]		(209.11417, 5438.955)(210.11526, 595.79425)(211.11246, 35	C8 H12 N6 O		FindByFormula	17	+	208.1067	12.033246
C8 H12 N6 O4	C8 H12 N6 O4	[C8 H12 N6 O4, tgt=75.35, overall=75.35]		(257.10025, 6252.543)(258.10098, 805.0024)(259.1045, 411.	C8 H12 N6 O4		FindByFormula	16	+	256.0928	6.470496
C8 H12 O S3	C8 H12 O S3	[C8 H12 O S3, tgt=43.99, overall=43.99]		(221.01251, 5962.8623)(222.01309, 686.7735)(223.01106, 84	C8 H12 O S3		FindByFormula	21	+	220.006	1.0015279
C8 H12 P2 S2	C8 H12 P2 S2	[C8 H12 P2 S2, tgt=56.53, overall=56.53]		(234.9922, 8378.252)(235.99449, 1033.4937)(236.98924, 169	C8 H12 P2 S2		FindByFormula	26	+	233.985	1.0300035
C8 H14 N2 O3	C8 H14 N2 O3	[C8 H14 N2 O3, tgt=44.03, overall=44.03]		(187.1082, 3835.142)(188.1069, 475.61505)(189.10909, 33.6	C8 H14 N2 O3		FindByFormula	21	+	186.1012	1.041528
C8 H14 N6 O	C8 H14 N6 O	[C8 H14 N6 O, tgt=95.84, overall=95.84]		(211.12982, 5414.6294)(212.13124, 659.7836)(213.13338, 23	C8 H14 N6 O		FindByFormula	22	+	210.1233	7.7368336
C8 H14 N6 O2	C8 H14 N6 O2	[C8 H14 N6 O2, tgt=84.00, overall=84.00]		(227.12526, 6625.389)(228.12816, 508.54965)(229.12842, 24	C8 H14 N6 O2		FindByFormula	28	+	226.119	11.035869
C8 H14 N6 O3	C8 H14 N6 O3	[C8 H14 N6 O3, tgt=93.76, overall=93.76]		(243.12018, 12676.469)(244.12096, 1730.2886)(245.1208, 32	C8 H14 N6 O3		FindByFormula	18	+	242.1131	7.719796
C8 H15 N O	C8 H15 N O	[C8 H15 N O, tgt=71.22, overall=71.22]		(142.12238, 42727.71)(143.12543, 4779.62)(180.07985, 381.	C8 H15 N O		FindByFormula	8	+	141.1156	0.9863749
C8 H15 N O2	C8 H15 N O2	[C8 H15 N O2, tgt=74.19, overall=74.19]		(158.11664, 2435.3284)(159.11574, 439.9173)(196.07518, 15	C8 H15 N O2		FindByFormula	17	+	157.1098	1.0140007
C8 H15 N O4	C8 H15 N O4	[C8 H15 N O4, tgt=87.98, overall=87.98]		(190.1071, 1258.1107)(191.10768, 131.60786)(192.1088, 37.	C8 H15 N O4		FindByFormula	15	+	189.1005	5.775409
C8 H15 N4 O4 P	C8 H15 N4 O4 P	[C8 H15 N4 O4 P, tgt=95.52, overall=95.52]		(263.09103, 19590.383)(264.09268, 2642.467)(265.09216, 84	C8 H15 N4 O4 P		FindByFormula	15	+	262.0825	15.638879
C8 H16 N2 O2	C8 H16 N2 O2	[C8 H16 N2 O2, tgt=90.73, overall=90.73]		(173.12817, 8569.583)(174.13542, 1026.9979)(175.13857, 73	C8 H16 N2 O2		FindByFormula	7	+	172.1219	4.1530714
C8 H16 N2 O3	C8 H16 N2 O3	[C8 H16 N2 O3, tgt=77.25, overall=77.25]		(189.12334, 9305.387)(190.12585, 897.97174)(191.12373, 13	C8 H16 N2 O3		FindByFormula	27	+	188.1161	2.4838424
C8 H16 N2 O3 S	C8 H16 N2 O3 S	[C8 H16 N2 O3 S, tgt=72.59, overall=72.59]		(221.0949, 9375.416)(222.10649, 2958.9167)(223.09596, 107	C8 H16 N2 O3 S		FindByFormula	11	+	220.0899	1.3844609
C8 H16 N6 O	C8 H16 N6 O	[C8 H16 N6 O, tgt=98.12, overall=98.12]		(213.1463, 28800.74)(214.14804, 3383.3547)(215.1459, 412.	C8 H16 N6 O		FindByFormula	28	+	212.1392	14.635643
C8 H16 N6 O2	C8 H16 N6 O2	[C8 H16 N6 O2, tgt=97.50, overall=97.50]		(229.14082, 7982.6655)(230.14275, 916.0782)(231.14189, 13	C8 H16 N6 O2		FindByFormula	28	+	228.1337	10.307273
C8 H16 N6 O4	C8 H16 N6 O4	[C8 H16 N6 O4, tgt=97.13, overall=97.13]		(261.13113, 52463.555)(262.1348, 6025.652)(263.13568, 105	C8 H16 N6 O4		FindByFormula	28	+	260.124	4.8199058
C8 H16 N7 O P	C8 H16 N7 O P	[C8 H16 N7 O P, tgt=90.67, overall=90.67]		(258.1218, 17348.826)(259.12436, 1722.3741)(260.12335, 40	C8 H16 N7 O P		FindByFormula	14	+	257.1135	0.6515022
C8 H17 N O2	C8 H17 N O2	[C8 H17 N O2, tgt=84.58, overall=84.58]		(160.13367, 15077.506)(161.133, 1474.9904)(162.1375, 45.9	C8 H17 N O2		FindByFormula	26	+	159.1258	1.8328228
C8 H17 O2 P	C8 H17 O2 P	[C8 H17 O2 P, tgt=94.83, overall=94.83]		(177.10529, 8161.446)(178.10814, 1047.4833)(179.10815, 14	C8 H17 O2 P		FindByFormula	13	+	176.0971	1.6620852
C8 H19 N	C8 H19 N	[C8 H19 N, tgt=77.27, overall=77.27]		(130.15886, 15402.956)(131.16116, 1411.4738)(132.16183, 1	C8 H19 N		FindByFormula	28	+	129.1516	4.856587
C8 H20 N8 O2	C8 H20 N8 O2	[C8 H20 N8 O2, tgt=87.08, overall=87.08]		(261.17755, 5546.018)(262.18085, 1170.7025)(263.17776, 33	C8 H20 N8 O2		FindByFormula	15	+	260.1727	0.7411998
C8 H21 N3 O4	C8 H21 N3 O4	[C8 H21 N3 O4, tgt=90.81, overall=90.81]		(224.15935, 4057.9443)(225.15828, 749.51666)(226.15799, 1	C8 H21 N3 O4		FindByFormula	14	+	223.152	5.622151
C8 H4 N4 O3 S	C8 H4 N4 O3 S	[C8 H4 N4 O3 S, tgt=92.78, overall=92.78]		(237.0075, 44016.65)(238.01024, 4800.031)(239.00706, 1689	C8 H4 N4 O3 S		FindByFormula	22	+	236.0003	8.686199
C8 H6	C8 H6	[C8 H6, tgt=99.12, overall=99.12]		(103.054375, 8901.285)(104.05753, 764.91254)(105.06015, 4	C8 H6		FindByFormula	24	+	102.0471	2.519654
C8 H8 O	C8 H8 O	[C8 H8 O, tgt=72.15, overall=72.15]		(121.0646, 5340.8047)(122.0594, 1020.89496)(123.05465, 68	C8 H8 O		FindByFormula	2	+	120.0567	16.438858
C8 H8 O3	C8 H8 O3	[C8 H8 O3, tgt=99.54, overall=99.54]		(153.0548, 440830.7)(154.05815, 37882.094)(155.061, 4651.	C8 H8 O3		FindByFormula	22	+	152.0474	8.662739
C8 H9 N	C8 H9 N	[C8 H9 N, tgt=99.81, overall=99.81]		(120.080986, 469869.5)(121.08395, 42535.777)(122.08625, 1	C8 H9 N		FindByFormula	28	+	119.0735	2.5183504
C8 H9 N O	C8 H9 N O	[C8 H9 N O, tgt=94.89, overall=94.89]		(136.07593, 74457.18)(137.07457, 6279.079)(138.07649, 232	C8 H9 N O		FindByFormula	26	+	135.0682	1.3566598
C8 H9 N O2	C8 H9 N O2	[C8 H9 N O2, tgt=96.77, overall=96.77]		(152.07013, 14088.186)(153.07204, 1644.1587)(154.07115, 1	C8 H9 N O2		FindByFormula	22	+	151.0633	3.074215
C9 H10	C9 H10	[C9 H10, tgt=78.10, overall=78.10]		(119.08534, 6089.145)(120.088356, 693.54663)(121.08926, 4	C9 H10		FindByFormula	25	+	118.0781	18.39419
C9 H11 N	C9 H11 N	[C9 H11 N, tgt=97.38, overall=97.38]		(134.09618, 9618.921)(135.0963, 1006.1101)(136.09991, 62.	C9 H11 N		FindByFormula	19	+	133.089	9.359957
C9 H11 N O2	C9 H11 N O2	[C9 H11 N O2, tgt=99.93, overall=99.93]		(166.08656, 722440.5)(167.08974, 73962.17)(168.09183, 677	C9 H11 N O2		FindByFormula	28	+	165.0792	2.5183146
C9 H11 N O3	C9 H11 N O3	[C9 H11 N O3, tgt=98.92, overall=98.92]		(182.08191, 409196.72)(183.08492, 41508.75)(184.08371, 55	C9 H11 N O3		FindByFormula	28	+	181.0746	1.3917221
C9 H12 N6 P2	C9 H12 N6 P2	[C9 H12 N6 P2, tgt=94.95, overall=94.95]		(267.06674, 6660.1577)(268.0706, 898.579)(269.06403, 37.5	C9 H12 N6 P2		FindByFormula	20	+	266.0596	4.163518
C9 H13 N O	C9 H13 N O	[C9 H13 N O, tgt=99.57, overall=99.57]		(152.10664, 18436.791)(153.1097, 2258.1584)(154.11078, 13	C9 H13 N O		FindByFormula	7	+	151.0998	3.9044774
C9 H13 N8 O2 P3	C9 H13 N8 O2 P3	[C9 H13 N8 O2 P3, tgt=94.33, overall=94.33]		(359.04373, 4448.26)(360.0473, 700.60803)(361.05078, 152.	C9 H13 N8 O2 P3		FindByFormula	7	+	358.0351	0.712286
C9 H14 N2 O3	C9 H14 N2 O3	[C9 H14 N2 O3, tgt=68.56, overall=68.56]		(199.10632, 1527.4)(200.10388, 200.91669)(221.09076, 1641	C9 H14 N2 O3		FindByFormula	6	+	198.1003	2.8603506
C9 H14 N4 O2 S	C9 H14 N4 O2 S	[C9 H14 N4 O2 S, tgt=56.54, overall=56.54]		(243.09149, 7045.713)(244.09258, 1326.4706)(245.08981, 79	C9 H14 N4 O2 S		FindByFormula	24	+	242.0837	18.321093
C9 H15 Cl	C9 H15 Cl	[C9 H15 Cl, tgt=48.80, overall=48.80]		(159.08995, 281.975)(181.07475, 2550.9417)(182.07831, 419	C9 H15 Cl		FindByFormula	6	+	158.0848	3.4867527
C9 H15 N O2	C9 H15 N O2	[C9 H15 N O2, tgt=85.24, overall=85.24]		(170.11711, 6348.588)(171.11565, 633.2167)(172.11621, 66.	C9 H15 N O2		FindByFormula	6	+	169.1089	5.418836
C9 H15 N O3	C9 H15 N O3	[C9 H15 N O3, tgt=86.37, overall=86.37]		(186.11264, 4861.14)(187.11163, 701.3416)(188.10876, 189.	C9 H15 N O3		FindByFormula	9	+	185.1051	0.91733426
C9 H15 O P S	C9 H15 O P S	[C9 H15 O P S, tgt=81.80, overall=81.80]		(203.0643, 30145.05)(204.06876, 2012.9637)(205.0737, 514.	C9 H15 O P S		FindByFormula	14	+	202.0578	0.64664584
C9 H16 N2 O2	C9 H16 N2 O2	[C9 H16 N2 O2, tgt=99.27, overall=99.27]		(185.12755, 3327.8374)(186.12708, 386.60742)(187.13158, 9	C9 H16 N2 O2		FindByFormula	19	+	184.1215	3.9195247
C9 H16 N6 O2	C9 H16 N6 O2	[C9 H16 N6 O2, tgt=88.92, overall=88.92]		(241.14153, 3267.2014)(242.14265, 406.79715)(243.14174, 1	C9 H16 N6 O2		FindByFormula	28	+	240.1339	14.124199
C9 H17 N O	C9 H17 N O	[C9 H17 N O, tgt=94.72, overall=94.72]		(156.13863, 308686.47)(157.14159, 31119.303)(158.14357, 2	C9 H17 N O		FindByFormula	7	+	155.1313	1.5350012
C9 H17 N O2	C9 H17 N O2	[C9 H17 N O2, tgt=92.99, overall=92.99]		(172.13315, 9372.548)(173.13472, 1257.12)(174.13205, 27.5	C9 H17 N O2		FindByFormula	20	+	171.1273	4.092002
C9 H17 N O4	C9 H17 N O4	[C9 H17 N O4, tgt=76.56, overall=76.56]		(204.12383, 115812.95)(205.12473, 14810.478)(206.12465, 1	C9 H17 N O4		FindByFormula	18	+	203.1161	0.82044435
C9 H17 N2 O3 P	C9 H17 N2 O3 P	[C9 H17 N2 O3 P, tgt=84.74, overall=84.74]		(233.10532, 31080.8)(234.10811, 5046.1416)(235.09735, 149	C9 H17 N2 O3 P		FindByFormula	22	+	232.0973	11.046119
C9 H17 N6 O P	C9 H17 N6 O P	[C9 H17 N6 O P, tgt=95.81, overall=95.81]		(257.12747, 46603.465)(258.1303, 6860.179)(259.13498, 914	C9 H17 N6 O P		FindByFormula	21	+	256.12	8.859121
C9 H18 N2 O3	C9 H18 N2 O3	[C9 H18 N2 O3, tgt=38.44, overall=38.44]		(203.13875, 4574.6978)(204.13681, 626.12256)(205.13335, 1	C9 H18 N2 O3		FindByFormula	21	+	202.1312	2.9428082
C9 H19 Cl2 N5 O2 S	C9 H19 Cl2 N5 O2 S	[C9 H19 Cl2 N5 O2 S, tgt=72.18, overall=72.18]		(332.07162, 650.54144)(333.07135, 161.88713)(334.061, 70.	C9 H19 Cl2 N5 O2 S		FindByFormula	7	+	331.0647	13.118105
C9 H19 N O	C9 H19 N O	[C9 H19 N O, tgt=98.01, overall=98.01]		(158.15382, 4081.743)(159.1555, 447.31253)(160.15892, 31.	C9 H19 N O		FindByFormula	28	+	157.1466	15.252436
C9 H19 N O2	C9 H19 N O2	[C9 H19 N O2, tgt=89.01, overall=89.01]		(174.14915, 8627.353)(175.1494, 1275.4233)(212.10448, 377	C9 H19 N O2		FindByFormula	12	+	173.1414	1.4732562
C9 H19 N2 O3 P	C9 H19 N2 O3 P	[C9 H19 N2 O3 P, tgt=32.28, overall=32.28]		(235.12015, 70040.73)(236.12253, 9731.301)(237.1232, 1266	C9 H19 N2 O3 P		FindByFormula	21	+	234.1128	1.383151
C9 H19 N4 O2 P	C9 H19 N4 O2 P	[C9 H19 N4 O2 P, tgt=74.40, overall=74.40]		(247.13138, 5259.3228)(248.13536, 867.2675)(249.13304, 16	C9 H19 N4 O2 P		FindByFormula	14	+	246.1239	4.0840163
C9 H20 N8 O2 S	C9 H20 N8 O2 S	[C9 H20 N8 O2 S, tgt=91.29, overall=91.29]		(305.14984, 17519.816)(306.1543, 2482.2024)(307.1517, 829	C9 H20 N8 O2 S		FindByFormula	4	+	304.1429	17.153719
C9 H23 Cl N8 O	C9 H23 Cl N8 O	[C9 H23 Cl N8 O, tgt=31.34, overall=31.34]		(295.1753, 594.338)(296.1722, 508.04)(297.1805, 244.73)(31	C9 H23 Cl N8 O		FindByFormula	6	+	294.166	20.7698
C9 H23 N5 O P2 S	C9 H23 N5 O P2 S	[C9 H23 N5 O P2 S, tgt=30.48, overall=30.48]		(312.1171, 2876.5388)(313.1153, 889.60803)(314.10513, 577	C9 H23 N5 O P2 S		FindByFormula	7	+	311.1098	8.6359625
C9 H24 N4 O2	C9 H24 N4 O2	[C9 H24 N4 O2, tgt=67.57, overall=67.57]		(221.19687, 35101.215)(222.19968, 4190.1104)(223.19994, 5	C9 H24 N4 O2		FindByFormula	15	+	220.1889	0.6770691
C9 H24 N6 O2 S	C9 H24 N6 O2 S	[C9 H24 N6 O2 S, tgt=92.95, overall=92.95]		(281.17484, 7833.344)(282.17798, 1265.1343)(283.1737, 394	C9 H24 N6 O2 S		FindByFormula	27	+	280.1687	20.001839
C9 H29 N6 O2 P3	C9 H29 N6 O2 P3	[C9 H29 N6 O2 P3, tgt=73.51, overall=73.51]		(347.167, 657.2918)(348.1652, 191.72626)(385.11795, 67.75	C9 H29 N6 O2 P3		FindByFormula	14	+	346.1581	13.902952
C9 H5 N O4	C9 H5 N O4	[C9 H5 N O4, tgt=75.86, overall=75.86]		(192.0296, 6330.973)(193.03017, 635.25006)(194.03291, 107	C9 H5 N O4		FindByFormula	23	+	191.0202	0.62060976
C9 H5 N5	C9 H5 N5	[C9 H5 N5, tgt=85.31, overall=85.31]		(184.06097, 3787.13)(185.06502, 335.28464)(186.06499, 284	C9 H5 N5		FindByFormula	13	+	183.0548	1.9320872
C9 H6 O2	C9 H6 O2	[C9 H6 O2, tgt=90.73, overall=90.73]		(147.04497, 8407.445)(148.05092, 995.01886)(149.04865, 12	C9 H6 O2		FindByFormula	10	+	146.0379	1.334798
C9 H7 Cl2 N5	C9 H7 Cl2 N5	[C9 H7 Cl2 N5, tgt=96.36, overall=96.36]		(256.01566, 27099.203)(257.0181, 3231.9675)(258.0128, 176	C9 H7 Cl2 N5		FindByFormula	12	+	255.0083	7.173172
C9 H7 N O	C9 H7 N O	[C9 H7 N O, tgt=84.80, overall=84.80]		(146.06076, 11854.916)(147.05858, 2737.3438)(148.06071, 4	C9 H7 N O		FindByFormula	26	+	145.0529	6.3968344
C9 H8 N5 O11 P3	C9 H8 N5 O11 P3	[C9 H8 N5 O11 P3, tgt=63.70, overall=63.70]		(455.95193, 9357.753)(456.95535, 1214.3029)(457.9567, 69.	C9 H8 N5 O11 P3		FindByFormula	19	+	454.9447	23.02384
C9 H8 N6 O2	C9 H8 N6 O2	[C9 H8 N6 O2, tgt=67.80, overall=67.80]		(233.07852, 8681.903)(234.08167, 1240.6248)(235.08722, 97	C9 H8 N6 O2		FindByFormula	28	+	232.0717	10.606597
C9 H8 O2	C9 H8 O2	[C9 H8 O2, tgt=98.22, overall=98.22]		(149.05997, 13737.687)(150.06271, 1511.6344)(151.0622, 49	C9 H8 O2		FindByFormula	27	+	148.0525	2.5196218
C9 H8 O3	C9 H8 O3	[C9 H8 O3, tgt=94.73, overall=94.73]		(165.05508, 93495.21)(166.05959, 9588.25)(167.06276, 1079	C9 H8 O3		FindByFormula	22	+	164.0479	1.3336402
C9 H9 N	C9 H9 N	[C9 H9 N, tgt=84.67, overall=84.67]		(132.08104, 11718.505)(133.08043, 1728.509)(134.08061, 24	C9 H9 N		FindByFormula	10	+	131.0732	3.6369357
C9 H9 N O3	C9 H9 N O3	[C9 H9 N O3, tgt=96.71, overall=96.71]		(180.06703, 5185.688)(181.07445, 1339.2826)(182.0718, 159	C9 H9 N O3		FindByFormula	17	+	179.0594	4.793853
CAFFEINE (CAS# 58-08-2); (M+H)+	CAFFEINE (CAS# 58-08-2); (M+H)+	CAFFEINE (CAS# 58-08-2); (M+H)+ [, tgt=94.79, overall=9	58-08-2	(195.08838, 48278.957)(196.09006, 4949.3145)(197.0882, 10	CAFFEINE (CAS# 58-08-2); (M+H)+	C07481	FindByFormula	23	+	194.0807	5.885069
CAFFEINE (CAS# 58-08-2); (M+Na)+	CAFFEINE (CAS# 58-08-2); (M+Na)+	CAFFEINE (CAS# 58-08-2); (M+Na)+ [, tgt=96.01, overall=	58-08-2	(217.0705, 13399.348)(218.07164, 1455.9714)(219.06557, 53	CAFFEINE (CAS# 58-08-2); (M+Na)+	C07481	FindByFormula	22	+	194.0807	5.890636
CALCIDIOL (CAS# 19356-17-3); (M+H)+	CALCIDIOL (CAS# 19356-17-3); (M+H)+	CALCIDIOL (CAS# 19356-17-3); (M+H)+ [, tgt=41.63, overa	19356-17-3	(401.34247, 1196.8619)(402.34415, 238.526)(403.33792, 117	CALCIDIOL (CAS# 19356-17-3); (M+H)+	C01561	FindByFormula	5	+	400.3336	22.822208
CALCIDIOL (CAS# 19356-17-3); (M+Na)+	CALCIDIOL (CAS# 19356-17-3); (M+Na)+	CALCIDIOL (CAS# 19356-17-3); (M+Na)+ [, tgt=61.42, over	19356-17-3	(423.32297, 1297.1683)(424.3247, 404.5883)(425.3227, 42.4	CALCIDIOL (CAS# 19356-17-3); (M+Na)+	C01561	FindByFormula	6	+	400.3314	22.61956
CARNOSINE (CAS# 305-84-0); (M+H)+	CARNOSINE (CAS# 305-84-0); (M+H)+	CARNOSINE (CAS# 305-84-0); (M+H)+ [, tgt=72.18, overall	305-84-0	(227.1163, 411.99)(228.117, 63.37)	CARNOSINE (CAS# 305-84-0); (M+H)+		FindByFormula	1	+	226.1088	0.6270017
CELLOBIOSE (CAS# 528-50-7); (M+Na)+	CELLOBIOSE (CAS# 528-50-7); (M+Na)+	CELLOBIOSE (CAS# 528-50-7); (M+Na)+ [, tgt=81.72, overa	528-50-7	(365.1071, 1436.5284)(366.10913, 190.30142)(367.11215, 64	CELLOBIOSE (CAS# 528-50-7); (M+Na)+	C06422	FindByFormula	14	+	342.1189	0.716929
CHOLATE (CAS# 81-25-4); (M+Na)+	CHOLATE (CAS# 81-25-4); (M+Na)+	CHOLATE (CAS# 81-25-4); (M+Na)+ [, tgt=71.50, overall=7	81-25-4	(431.27496, 3725.032)(432.28094, 319.072)(433.27548, 167.	CHOLATE (CAS# 81-25-4); (M+Na)+		FindByFormula	5	+	408.2854	20.312107
CHOLESTEROL (CAS# 57-88-5); (M+H)+[-H2O]	CHOLESTEROL (CAS# 57-88-5); (M+H)+[-H2O]	CHOLESTEROL (CAS# 57-88-5); (M+H)+[-H2O] [, tgt=96.21	57-88-5	(369.35168, 3844.5173)(370.35522, 1212.5852)(371.35364, 2	CHOLESTEROL (CAS# 57-88-5); (M+H)+[-H2O]	C00187	FindByFormula	17	+	386.3548	24.587894
CHOLESTEROL HYDROGEN SULFATE (CAS# 12	CHOLESTEROL HYDROGEN SULFATE (CAS# 125	CHOLESTEROL HYDROGEN SULFATE (CAS# 1256-86-6); M	1256-86-6	(369.3464, 457.29)(370.3563, 191.29)	CHOLESTEROL HYDROGEN SULFATE (CAS# 1256-86-6); M+[-HSO	C18043	FindByFormula	1	+	466.3084	23.771051
CHOLINE (CAS# 62-49-7); M+	CHOLINE (CAS# 62-49-7); M+	CHOLINE (CAS# 62-49-7); M+ [, tgt=90.61, overall=90.61]	62-49-7	(104.1072, 31938.941)(105.11066, 1865.5302)(106.10985, 20	CHOLINE (CAS# 62-49-7); M+	C00114	FindByFormula	18	+	104.1075	0.64489
CHOLINE PHOSPHATE (CAS# 107-73-3); (M+H	CHOLINE PHOSPHATE (CAS# 107-73-3); (M+H)	CHOLINE PHOSPHATE (CAS# 107-73-3); (M+H)+ [, tgt=58.	107-73-3	(184.07422, 2294.0698)(185.07437, 121.997505)(186.07484,	CHOLINE PHOSPHATE (CAS# 107-73-3); (M+H)+	C00588	FindByFormula	16	+	183.0673	0.7759377
CHOLINE PHOSPHATE (CAS# 107-73-3); (M+N	CHOLINE PHOSPHATE (CAS# 107-73-3); (M+N	CHOLINE PHOSPHATE (CAS# 107-73-3); (M+Na)+ [, tgt=64	107-73-3	(206.05696, 1273.25)(207.05142, 327.42804)(208.0475, 232.	CHOLINE PHOSPHATE (CAS# 107-73-3); (M+Na)+	C00588	FindByFormula	5	+	183.0655	0.7606009
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CA	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CA	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-5	28874-58-0	(355.25952, 5945.7593)(356.26465, 1554.7407)(357.2626, 57	CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0); (M+Na)+		FindByFormula	16	+	332.2703	23.061665
CIS-VACCENIC ACID (CAS# 506-17-2); (M+H)+	CIS-VACCENIC ACID (CAS# 506-17-2); (M+H)+	CIS-VACCENIC ACID (CAS# 506-17-2); (M+H)+ [, tgt=93.35	506-17-2	(283.2624, 2493.1482)(284.26862, 454.0408)(285.26895, 84.	CIS-VACCENIC ACID (CAS# 506-17-2); (M+H)+		FindByFormula	12	+	282.256	22.937103
CIS-ZEATIN (CAS# 1637-39-4); (M+H)+	CIS-ZEATIN (CAS# 1637-39-4); (M+H)+	CIS-ZEATIN (CAS# 1637-39-4); (M+H)+ [, tgt=83.36, overal	1637-39-4	(220.1198, 741028.6)(221.12254, 91246.125)(222.1251, 7037	CIS-ZEATIN (CAS# 1637-39-4); (M+H)+	C00371	FindByFormula	28	+	219.1125	3.888838
CITRAMALATE (CAS# 2306-22-1); (2M+Na)+	CITRAMALATE (CAS# 2306-22-1); (2M+Na)+	CITRAMALATE (CAS# 2306-22-1); (2M+Na)+ [, tgt=33.50,	2306-22-1	(319.0654, 555.1)(320.0595, 198.67)	CITRAMALATE (CAS# 2306-22-1); (2M+Na)+	C00815	FindByFormula	1	+	148.0365	1.1570071
CITRAMALATE (CAS# 2306-22-1); (M+Na)+	CITRAMALATE (CAS# 2306-22-1); (M+Na)+	CITRAMALATE (CAS# 2306-22-1); (M+Na)+ [, tgt=83.01, o	2306-22-1	(171.02673, 919.485)(172.02414, 49.165)	CITRAMALATE (CAS# 2306-22-1); (M+Na)+	C00815	FindByFormula	4	+	148.0367	1.3977485
CITRATE (CAS# 77-92-9); (M+H)+[-H2O]	CITRATE (CAS# 77-92-9); (M+H)+[-H2O]	CITRATE (CAS# 77-92-9); (M+H)+[-H2O] [, tgt=47.78, over	77-92-9	(175.02254, 1549.8033)(176.02776, 146.69333)(177.0285, 16	CITRATE (CAS# 77-92-9); (M+H)+[-H2O]		FindByFormula	3	+	192.0251	1.0810028
CITRATE (CAS# 77-92-9); (M+Na)+	CITRATE (CAS# 77-92-9); (M+Na)+	CITRATE (CAS# 77-92-9); (M+Na)+ [, tgt=88.16, overall=8	77-92-9	(215.01689, 4903.98)(216.01945, 343.08252)(217.01881, 181	CITRATE (CAS# 77-92-9); (M+Na)+		FindByFormula	12	+	192.0274	0.9046669
CITRULLINE (CAS# 372-75-8); (M+Na)+	CITRULLINE (CAS# 372-75-8); (M+Na)+	CITRULLINE (CAS# 372-75-8); (M+Na)+ [, tgt=81.44, overa	372-75-8	(198.08638, 1642.4049)(199.08385, 153.55)	CITRULLINE (CAS# 372-75-8); (M+Na)+		FindByFormula	6	+	175.0969	0.66449946
CMP (CAS# 63-37-6); (M+H)+	CMP (CAS# 63-37-6); (M+H)+	CMP (CAS# 63-37-6); (M+H)+ [, tgt=37.31, overall=37.31]	63-37-6	(324.06058, 1190.6901)(325.05835, 116.66249)(326.06357, 1	CMP (CAS# 63-37-6); (M+H)+	C00055	FindByFormula	16	+	323.0547	0.917877
CORTICOSTERONE (CAS# 50-22-6); (M+Na)+	CORTICOSTERONE (CAS# 50-22-6); (M+Na)+	CORTICOSTERONE (CAS# 50-22-6); (M+Na)+ [, tgt=75.44,	50-22-6	(369.2029, 1623.1416)(370.20517, 376.12833)(371.20816, 95	CORTICOSTERONE (CAS# 50-22-6); (M+Na)+		FindByFormula	6	+	346.2117	15.33152
CORTISOL (CAS# 50-23-7); (M+H)+	CORTISOL (CAS# 50-23-7); (M+H)+	CORTISOL (CAS# 50-23-7); (M+H)+ [, tgt=55.83, overall=5	50-23-7	(363.2153, 2052.3)(364.2164, 465.10168)(365.21216, 234.53	CORTISOL (CAS# 50-23-7); (M+H)+	C00735	FindByFormula	6	+	362.2063	13.771148
CORTISOL (CAS# 50-23-7); (M+Na)+	CORTISOL (CAS# 50-23-7); (M+Na)+	CORTISOL (CAS# 50-23-7); (M+Na)+ [, tgt=95.55, overall=	50-23-7	(385.19778, 16665.139)(386.2007, 3905.826)(387.203, 1282.	CORTISOL (CAS# 50-23-7); (M+Na)+	C00735	FindByFormula	17	+	362.2099	13.766018
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)+ [, tgt=41.	50-03-3	(405.23093, 855.23145)(406.23148, 225.87715)(407.22592, 2	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)+	C02821	FindByFormula	7	+	404.2231	15.962064
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)+[-H2O] [, t	50-03-3	(387.21954, 821.20496)(388.21515, 280.88)(389.21265, 146.	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)+[-H2O]	C02821	FindByFormula	2	+	404.2219	15.690936
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+N	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+N	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+Na)+ [, tgt=41	50-03-3	(427.2101, 750.8233)(428.20956, 210.99)(429.2098, 450.395)	CORTISOL 21-ACETATE (CAS# 50-03-3); (M+Na)+	C02821	FindByFormula	6	+	404.2177	15.681273
CORTISONE (CAS# 53-06-5); (M+H)+	CORTISONE (CAS# 53-06-5); (M+H)+	CORTISONE (CAS# 53-06-5); (M+H)+ [, tgt=63.85, overall=	53-06-5	(361.19995, 646.99493)(362.20303, 168.12834)(363.20248, 1	CORTISONE (CAS# 53-06-5); (M+H)+	C00762	FindByFormula	6	+	360.1907	13.360181
CORTISONE (CAS# 53-06-5); (M+Na)+	CORTISONE (CAS# 53-06-5); (M+Na)+	CORTISONE (CAS# 53-06-5); (M+Na)+ [, tgt=83.43, overall	53-06-5	(383.18533, 3164.3728)(384.1885, 791.2609)(385.18784, 621	CORTISONE (CAS# 53-06-5); (M+Na)+	C00762	FindByFormula	12	+	360.1949	13.344338
CREATINE (CAS# 57-00-1); (M+H)+	CREATINE (CAS# 57-00-1); (M+H)+	CREATINE (CAS# 57-00-1); (M+H)+ [, tgt=90.39, overall=9	57-00-1	(132.07666, 80073.445)(133.07889, 4827.94)(134.07918, 755	CREATINE (CAS# 57-00-1); (M+H)+		FindByFormula	8	+	131.0702	0.69724965
CREATININE (CAS# 60-27-5); (M+H)+	CREATININE (CAS# 60-27-5); (M+H)+	CREATININE (CAS# 60-27-5); (M+H)+ [, tgt=57.12, overall=	60-27-5	(114.0668, 22513.01)(115.0705, 6135.85)	CREATININE (CAS# 60-27-5); (M+H)+		FindByFormula	1	+	113.0599	0.6810001
CREATININE (CAS# 60-27-5); (M+Na)+	CREATININE (CAS# 60-27-5); (M+Na)+	CREATININE (CAS# 60-27-5); (M+Na)+ [, tgt=78.54, overal	60-27-5	(136.04831, 3483.825)(137.05371, 61.85)	CREATININE (CAS# 60-27-5); (M+Na)+		FindByFormula	2	+	113.059	0.6914995
CREATININE-(GUANIDINO-13C) [ISTD] (CAS#);	CREATININE-(GUANIDINO-13C) [ISTD] (CAS#);	CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (2M+H)+ [, tgt=75.40, overall=75.40]		(229.1326, 589.94)(230.1356, 51.44)	CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (2M+H)+		FindByFormula	1	+	114.0632	0.7010001
CREATININE-(GUANIDINO-13C) [ISTD] (CAS#);	CREATININE-(GUANIDINO-13C) [ISTD] (CAS#);	CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (2M+Na)+ [, tgt=49.18, overall=49.18		(251.1152, 483.38)(252.1093, 171.62)	CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (2M+Na)+		FindByFormula	1	+	114.0617	0.71400017
CYSTATHIONINE (CAS# 56-88-2); (M+H)+[-H2	CYSTATHIONINE (CAS# 56-88-2); (M+H)+[-H2	CYSTATHIONINE (CAS# 56-88-2); (M+H)+[-H2O] [, tgt=68.	56-88-2	(205.06482, 1876.4032)(206.06285, 179.415)(207.0537, 48.9	CYSTATHIONINE (CAS# 56-88-2); (M+H)+[-H2O]		FindByFormula	6	+	222.0678	0.66149944
CYSTINE (CAS# 56-89-3); (M+Na)+	CYSTINE (CAS# 56-89-3); (M+Na)+	CYSTINE (CAS# 56-89-3); (M+Na)+ [, tgt=59.78, overall=5	56-89-3	(263.0125, 969.56433)(264.01215, 120.31715)(265.01297, 22	CYSTINE (CAS# 56-89-3); (M+Na)+		FindByFormula	7	+	240.022	0.6762858
CYTIDINE (CAS# 65-46-3); (M+H)+	CYTIDINE (CAS# 65-46-3); (M+H)+	CYTIDINE (CAS# 65-46-3); (M+H)+ [, tgt=64.07, overall=64	65-46-3	(244.09473, 1354.7267)(245.09187, 429.30002)(246.0825, 41	CYTIDINE (CAS# 65-46-3); (M+H)+		FindByFormula	3	+	243.0866	0.8289997
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-7	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-7	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+H)	987-78-0	(489.1151, 652.01996)(490.11737, 140.475)(491.11725, 46.5	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+H)+	C00307	FindByFormula	4	+	488.1089	0.7020007
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-7	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-7	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+N	987-78-0	(511.0978, 481.79663)(512.0925, 74.333336)(513.0932, 189.	CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+Na)+	C00307	FindByFormula	3	+	488.1107	0.5583351
CYTOSINE (CAS# 71-30-7); (M+H)+	CYTOSINE (CAS# 71-30-7); (M+H)+	CYTOSINE (CAS# 71-30-7); (M+H)+ [, tgt=47.38, overall=4	71-30-7	(112.050705, 1193.6328)(113.0558, 57.31286)	CYTOSINE (CAS# 71-30-7); (M+H)+		FindByFormula	7	+	111.0443	0.79657173
CYTOSINE (CAS# 71-30-7); (M+Na)+	CYTOSINE (CAS# 71-30-7); (M+Na)+	CYTOSINE (CAS# 71-30-7); (M+Na)+ [, tgt=63.93, overall=	71-30-7	(134.03212, 4160.484)(135.03809, 347.875)	CYTOSINE (CAS# 71-30-7); (M+Na)+		FindByFormula	8	+	111.0428	0.705127

D-(-)-ARABINOSE (CAS# 10323-20-3); (M+Na)	D-(-)-ARABINOSE (CAS# 10323-20-3); (M+Na)+	D-(-)-ARABINOSE (CAS# 10323-20-3); (M+Na)+ [, tgt=71.2	10323-20-3	(173.04222, 14187.223)(174.04117, 1619.8125)(175.0391, 69	D-(-)-ARABINOSE (CAS# 10323-20-3); (M+Na)+		FindByFormula	4	+	150.0531	0.91000307
DEBRISOQUIN (CAS# 581-88-4); (M+H)+	DEBRISOQUIN (CAS# 581-88-4); (M+H)+	DEBRISOQUIN (CAS# 581-88-4); (M+H)+ [, tgt=66.88, over	581-88-4	(176.1182, 16063.765)(177.12074, 2064.0566)(178.11942, 20	DEBRISOQUIN (CAS# 581-88-4); (M+H)+		FindByFormula	21	+	175.1109	5.154356
DECANOATE (CAS# 334-48-5); (2M+Na)+	DECANOATE (CAS# 334-48-5); (2M+Na)+	DECANOATE (CAS# 334-48-5); (2M+Na)+ [, tgt=64.22, ove	334-48-5	(367.28293, 20502.516)(368.2857, 4521.676)(369.28525, 884	DECANOATE (CAS# 334-48-5); (2M+Na)+	C01571	FindByFormula	5	+	172.1476	22.855198
DEHYDROASCORBATE (CAS# 490-83-5); (M+H	DEHYDROASCORBATE (CAS# 490-83-5); (M+H)	DEHYDROASCORBATE (CAS# 490-83-5); (M+H)+[-H2O] [, t	490-83-5	(157.0142, 1474.0533)(158.01259, 61.066666)	DEHYDROASCORBATE (CAS# 490-83-5); (M+H)+[-H2O]		FindByFormula	3	+	174.0174	0.7326668
DEOXYADENOSINE (CAS# 16373-93-6); (M+H)	DEOXYADENOSINE (CAS# 16373-93-6); (M+H)	DEOXYADENOSINE (CAS# 16373-93-6); (M+H)+ [, tgt=39.5	16373-93-6	(252.1089, 524.38)(253.1145, 166.34)	DEOXYADENOSINE (CAS# 16373-93-6); (M+H)+		FindByFormula	1	+	251.1024	1.7239971
DEOXYCHOLIC ACID (CAS# 83-44-3); (2M+Na)	DEOXYCHOLIC ACID (CAS# 83-44-3); (2M+Na)	DEOXYCHOLIC ACID (CAS# 83-44-3); (2M+Na)+ [, tgt=30.2	83-44-3	(807.57336, 407.735)(808.5808, 648.465)(809.5831, 403.0)	DEOXYCHOLIC ACID (CAS# 83-44-3); (2M+Na)+	C04483	FindByFormula	2	+	392.2959	21.791275
DEOXYCHOLIC ACID (CAS# 83-44-3); (M+H)+	DEOXYCHOLIC ACID (CAS# 83-44-3); (M+H)+	DEOXYCHOLIC ACID (CAS# 83-44-3); (M+H)+ [, tgt=25.74,	83-44-3	(393.30237, 2401.32)(394.29654, 321.66666)	DEOXYCHOLIC ACID (CAS# 83-44-3); (M+H)+	C04483	FindByFormula	3	+	392.2962	21.840897
DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Na)+	DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Na)+	DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Na)+ [, tgt=95.67	83-44-3	(415.2816, 10732.028)(416.28467, 2998.3145)(417.2819, 447	DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Na)+	C04483	FindByFormula	9	+	392.2916	21.728048
DEOXYCORTICOSTERONE ACETATE (CAS# 56-	DEOXYCORTICOSTERONE ACETATE (CAS# 56-4	DEOXYCORTICOSTERONE ACETATE (CAS# 56-47-3); (M+N	56-47-3	(395.21942, 2038.3336)(396.22296, 587.35095)(397.2212, 13	DEOXYCORTICOSTERONE ACETATE (CAS# 56-47-3); (M+Na)+	C14554	FindByFormula	11	+	372.229	18.913774
DEOXYCYTIDINE (CAS# 951-77-9); (2M+H)+	DEOXYCYTIDINE (CAS# 951-77-9); (2M+H)+	DEOXYCYTIDINE (CAS# 951-77-9); (2M+H)+ [, tgt=86.00, o	951-77-9	(455.1881, 388.7)(456.1893, 78.36)	DEOXYCYTIDINE (CAS# 951-77-9); (2M+H)+		FindByFormula	1	+	227.0899	0.94900566
DEOXYCYTIDINE (CAS# 951-77-9); (M+H)+	DEOXYCYTIDINE (CAS# 951-77-9); (M+H)+	DEOXYCYTIDINE (CAS# 951-77-9); (M+H)+ [, tgt=28.25, ov	951-77-9	(228.1017, 757.4)(229.0948, 177.62)	DEOXYCYTIDINE (CAS# 951-77-9); (M+H)+		FindByFormula	1	+	227.0926	1.2310096
DEOXYURIDINE (CAS# 951-78-0); (M+Na)+	DEOXYURIDINE (CAS# 951-78-0); (M+Na)+	DEOXYURIDINE (CAS# 951-78-0); (M+Na)+ [, tgt=64.02, o	951-78-0	(251.06517, 1057.9325)(252.06718, 61.5475)(253.0706, 34.2	DEOXYURIDINE (CAS# 951-78-0); (M+Na)+		FindByFormula	4	+	228.0769	1.6922476
DESMOSTEROL (CAS# 313-04-2); (M+H)+[-H2	DESMOSTEROL (CAS# 313-04-2); (M+H)+[-H2	DESMOSTEROL (CAS# 313-04-2); (M+H)+[-H2O] [, tgt=57.	313-04-2	(367.3335, 542.23596)(368.33945, 163.044)(369.3406, 131.6	DESMOSTEROL (CAS# 313-04-2); (M+H)+[-H2O]	C01802	FindByFormula	5	+	384.3366	24.278065
DETHIOBIOTIN (CAS# 533-48-2); (M+H)+[-H2	DETHIOBIOTIN (CAS# 533-48-2); (M+H)+[-H2O	DETHIOBIOTIN (CAS# 533-48-2); (M+H)+[-H2O] [, tgt=51.5	533-48-2	(197.12863, 1731.1827)(198.12796, 145.75285)	DETHIOBIOTIN (CAS# 533-48-2); (M+H)+[-H2O]	C01909	FindByFormula	7	+	214.1305	8.026037
DETHIOBIOTIN (CAS# 533-48-2); (M+Na)+	DETHIOBIOTIN (CAS# 533-48-2); (M+Na)+	DETHIOBIOTIN (CAS# 533-48-2); (M+Na)+ [, tgt=42.02, ov	533-48-2	(237.1199, 639.475)(238.11835, 89.5)	DETHIOBIOTIN (CAS# 533-48-2); (M+Na)+	C01909	FindByFormula	2	+	214.1299	8.456674
DEXTROMETHORPHAN (CAS# 125-69-9); (M+	DEXTROMETHORPHAN (CAS# 125-69-9); (M+	DEXTROMETHORPHAN (CAS# 125-69-9); (M+H)+ [, tgt=54	125-69-9	(272.20062, 1290.3099)(273.2026, 290.01715)(274.20355, 76	DEXTROMETHORPHAN (CAS# 125-69-9); (M+H)+	C08028	FindByFormula	7	+	271.1932	11.140906
D-GALACTOSAMINE (CAS# 7535-00-4); (M+H)	D-GALACTOSAMINE (CAS# 7535-00-4); (M+H)	D-GALACTOSAMINE (CAS# 7535-00-4); (M+H)+[-H2O] [, t	7535-00-4	(162.0765, 11212.352)(163.07689, 611.11676)(164.07655, 15	D-GALACTOSAMINE (CAS# 7535-00-4); (M+H)+[-H2O]	C02262	FindByFormula	9	+	179.0794	0.7990006
D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (M	D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (M	D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (M+Na)+ [, tgt	56-73-5	(283.01758, 449.47498)(284.0216, 96.865)	D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (M+Na)+	C00092	FindByFormula	4	+	260.0274	0.89899933
DGMP (CAS# 902-04-5); (M+H)+	DGMP (CAS# 902-04-5); (M+H)+	DGMP (CAS# 902-04-5); (M+H)+ [, tgt=43.77, overall=43.7	902-04-5	(348.07043, 1840.3301)(349.07074, 183.03998)(350.06665, 1	DGMP (CAS# 902-04-5); (M+H)+		FindByFormula	9	+	347.0637	1.2783384
DIETHANOLAMINE (CAS# 111-42-2); (M+Na)+	DIETHANOLAMINE (CAS# 111-42-2); (M+Na)+	DIETHANOLAMINE (CAS# 111-42-2); (M+Na)+ [, tgt=51.3	111-42-2	(128.0693, 774.57)(129.0624, 45.33)	DIETHANOLAMINE (CAS# 111-42-2); (M+Na)+	C06772	FindByFormula	1	+	105.0796	0.9079873
DIETHYLSTILBESTROL (CAS# 56-53-1); (M+Na)	DIETHYLSTILBESTROL (CAS# 56-53-1); (M+Na)	DIETHYLSTILBESTROL (CAS# 56-53-1); (M+Na)+ [, tgt=24.8	56-53-1	(291.1334, 2473.0)(292.127, 460.29)(293.1436, 749.15)	DIETHYLSTILBESTROL (CAS# 56-53-1); (M+Na)+		FindByFormula	1	+	268.1437	18.638031
DIHYDRO-4,4-DIMETHYL-2,3-FURANDIONE (C	DIHYDRO-4,4-DIMETHYL-2,3-FURANDIONE (C	DIHYDRO-4,4-DIMETHYL-2,3-FURANDIONE (CAS# 13031-0	13031-04-4	(151.03712, 6240.3867)(152.04063, 215.24333)(153.0507, 11	DIHYDRO-4,4-DIMETHYL-2,3-FURANDIONE (CAS# 13031-04-4); (	C01125	FindByFormula	3	+	128.048	3.3850257
DIPHENHYDRAMINE (CAS# 147-24-0); (M+H)+	DIPHENHYDRAMINE (CAS# 147-24-0); (M+H)+	DIPHENHYDRAMINE (CAS# 147-24-0); (M+H)+ [, tgt=37.8	147-24-0	(256.169, 1446.845)(257.16602, 300.95248)(258.16058, 94.0	DIPHENHYDRAMINE (CAS# 147-24-0); (M+H)+	C07784	FindByFormula	8	+	255.161	11.046461
DI-TERT-BUTYL DICARBONATE (CAS# 24424-9	DI-TERT-BUTYL DICARBONATE (CAS# 24424-9	DI-TERT-BUTYL DICARBONATE (CAS# 24424-99-5); (M+Na	24424-99-5	(241.10475, 2638.07)(242.10681, 845.615)	DI-TERT-BUTYL DICARBONATE (CAS# 24424-99-5); (M+Na)+		FindByFormula	2	+	218.1162	5.63809
D-LYXOSE (CAS# 1114-34-7); (M+Na)+	D-LYXOSE (CAS# 1114-34-7); (M+Na)+	D-LYXOSE (CAS# 1114-34-7); (M+Na)+ [, tgt=35.37, overal	1114-34-7	(173.0426, 7193.75)(174.0406, 1444.72)	D-LYXOSE (CAS# 1114-34-7); (M+Na)+	C00476	FindByFormula	1	+	150.0525	0.966005
D-MANNOSAMINE (CAS# 14307-02-9); (M+H)	D-MANNOSAMINE (CAS# 14307-02-9); (M+H)	D-MANNOSAMINE (CAS# 14307-02-9); (M+H)+[-H2O] [, t	14307-02-9	(162.0765, 11212.352)(163.07689, 611.11676)(164.07655, 15	D-MANNOSAMINE (CAS# 14307-02-9); (M+H)+[-H2O]	C03570	FindByFormula	9	+	179.0794	0.7990006
D-ORNITHINE (CAS# 348-66-3); (M+H)+	D-ORNITHINE (CAS# 348-66-3); (M+H)+	D-ORNITHINE (CAS# 348-66-3); (M+H)+ [, tgt=70.20, over	348-66-3	(133.09676, 3906.4395)(134.0965, 287.4969)(135.09633, 147	D-ORNITHINE (CAS# 348-66-3); (M+H)+	C00515	FindByFormula	16	+	132.0894	0.5542505
D-ORNITHINE (CAS# 348-66-3); (M+H)+[-H2O]	D-ORNITHINE (CAS# 348-66-3); (M+H)+[-H2O]	D-ORNITHINE (CAS# 348-66-3); (M+H)+[-H2O] [, tgt=80.4	348-66-3	(115.08565, 1039.765)(116.0972, 35.355)	D-ORNITHINE (CAS# 348-66-3); (M+H)+[-H2O]	C00515	FindByFormula	2	+	132.0893	0.5560005
D-PSICOSE (CAS# 551-68-8); (2M+Na)+[-H2O]	D-PSICOSE (CAS# 551-68-8); (2M+Na)+[-H2O]	D-PSICOSE (CAS# 551-68-8); (2M+Na)+[-H2O] [, tgt=69.49	551-68-8	(365.10623, 1344.1718)(366.10654, 139.50499)(367.11322, 8	D-PSICOSE (CAS# 551-68-8); (2M+Na)+[-H2O]	C06468	FindByFormula	6	+	180.0644	0.7264996
DUMP (CAS# 964-26-1); (M+H)+	DUMP (CAS# 964-26-1); (M+H)+	DUMP (CAS# 964-26-1); (M+H)+ [, tgt=70.27, overall=70.2	964-26-1	(309.05118, 1430.2506)(310.0511, 261.54465)(311.0446, 314	DUMP (CAS# 964-26-1); (M+H)+	C00365	FindByFormula	15	+	308.044	1.0257353
DUMP (CAS# 964-26-1); (M+K)+	DUMP (CAS# 964-26-1); (M+K)+	DUMP (CAS# 964-26-1); (M+K)+ [, tgt=42.23, overall=42.2	964-26-1	(347.0049, 706.2673)(348.00998, 80.62091)(348.9997, 86.31	DUMP (CAS# 964-26-1); (M+K)+	C00365	FindByFormula	11	+	308.0416	1.2170027
DUMP (CAS# 964-26-1); (M+Na)+	DUMP (CAS# 964-26-1); (M+Na)+	DUMP (CAS# 964-26-1); (M+Na)+ [, tgt=43.01, overall=43.	964-26-1	(331.0299, 328.26)(332.0389, 61.55)	DUMP (CAS# 964-26-1); (M+Na)+	C00365	FindByFormula	1	+	308.0417	1.2250075
EDTA (CAS# 60-00-4); (M+H)+	EDTA (CAS# 60-00-4); (M+H)+	EDTA (CAS# 60-00-4); (M+H)+ [, tgt=69.26, overall=69.26	60-00-4	(293.09848, 895221.7)(294.10165, 105809.43)(295.10327, 19	EDTA (CAS# 60-00-4); (M+H)+	C00284	FindByFormula	6	+	292.0912	0.8693326
EDTA (CAS# 60-00-4); (M+Na)+	EDTA (CAS# 60-00-4); (M+Na)+	EDTA (CAS# 60-00-4); (M+Na)+ [, tgt=84.80, overall=84.8	60-00-4	(315.08057, 154445.75)(316.08353, 17875.182)(317.0801, 42	EDTA (CAS# 60-00-4); (M+Na)+	C00284	FindByFormula	6	+	292.0912	1.1939995
ELAIDIC ACID (CAS# 112-79-8); (M+H)+	ELAIDIC ACID (CAS# 112-79-8); (M+H)+	ELAIDIC ACID (CAS# 112-79-8); (M+H)+ [, tgt=88.59, overa	112-79-8	(283.2624, 2493.1482)(284.26862, 454.0408)(285.26895, 84.	ELAIDIC ACID (CAS# 112-79-8); (M+H)+		FindByFormula	12	+	282.256	22.937103
ELAIDIC ACID (CAS# 112-79-8); (M+Na)+	ELAIDIC ACID (CAS# 112-79-8); (M+Na)+	ELAIDIC ACID (CAS# 112-79-8); (M+Na)+ [, tgt=48.18, ove	112-79-8	(305.245, 6830.2793)(306.2526, 1349.4669)(307.25006, 2165	ELAIDIC ACID (CAS# 112-79-8); (M+Na)+		FindByFormula	19	+	282.2561	22.849539
EPIANDROSTERONE (CAS# 481-29-8); (M+H)+	EPIANDROSTERONE (CAS# 481-29-8); (M+H)+[	EPIANDROSTERONE (CAS# 481-29-8); (M+H)+[-H2O] [, tgt	481-29-8	(273.22278, 388.075)(274.21674, 63.12)	EPIANDROSTERONE (CAS# 481-29-8); (M+H)+[-H2O]		FindByFormula	2	+	290.224	18.47712
EPINEPHRINE (CAS# 51-43-4); (M+H)+	EPINEPHRINE (CAS# 51-43-4); (M+H)+	EPINEPHRINE (CAS# 51-43-4); (M+H)+ [, tgt=68.28, overal	51-43-4	(184.09625, 1943.9226)(185.09613, 143.38)(186.0927, 111.1	EPINEPHRINE (CAS# 51-43-4); (M+H)+		FindByFormula	4	+	183.0878	0.652251
EPINEPHRINE (CAS# 51-43-4); (M+H)+[-H2O]	EPINEPHRINE (CAS# 51-43-4); (M+H)+[-H2O]	EPINEPHRINE (CAS# 51-43-4); (M+H)+[-H2O] [, tgt=65.34,	51-43-4	(166.08595, 1618.393)(167.08585, 246.38354)(168.0909, 41.8	EPINEPHRINE (CAS# 51-43-4); (M+H)+[-H2O]		FindByFormula	14	+	183.0888	0.84257185
ERYTHRITOL (CAS# 149-32-6); (M+Na)+	ERYTHRITOL (CAS# 149-32-6); (M+Na)+	ERYTHRITOL (CAS# 149-32-6); (M+Na)+ [, tgt=49.22, over	149-32-6	(145.04796, 2209.2358)(146.04517, 293.91714)	ERYTHRITOL (CAS# 149-32-6); (M+Na)+	C00503	FindByFormula	7	+	122.0568	0.93371594
ESTRONE (CAS# 53-16-7); (M+H)+	ESTRONE (CAS# 53-16-7); (M+H)+	ESTRONE (CAS# 53-16-7); (M+H)+ [, tgt=77.27, overall=77	53-16-7	(271.16855, 902.495)(272.1681, 124.759995)	ESTRONE (CAS# 53-16-7); (M+H)+		FindByFormula	2	+	270.1613	16.320076
ETHANOLAMINE PHOSPHATE (CAS# 1071-23-	ETHANOLAMINE PHOSPHATE (CAS# 1071-23-4	ETHANOLAMINE PHOSPHATE (CAS# 1071-23-4); (M+H)+ [	1071-23-4	(142.02638, 1884.6466)(143.02867, 104.54)(144.02275, 59.5	ETHANOLAMINE PHOSPHATE (CAS# 1071-23-4); (M+H)+		FindByFormula	6	+	141.0195	0.87416524
ETHYLMALONIC ACID (CAS# 601-75-2); (M+N	ETHYLMALONIC ACID (CAS# 601-75-2); (M+N	ETHYLMALONIC ACID (CAS# 601-75-2); (M+Na)+ [, tgt=52	601-75-2	(155.03206, 13064.695)(156.03938, 1262.0829)(157.03122, 3	ETHYLMALONIC ACID (CAS# 601-75-2); (M+Na)+		FindByFormula	14	+	132.0428	2.9776378
FERULATE (CAS# 1135-24-6); (M+H)+	FERULATE (CAS# 1135-24-6); (M+H)+	FERULATE (CAS# 1135-24-6); (M+H)+ [, tgt=70.72, overall	1135-24-6	(195.06606, 2243.442)(196.06711, 174.72406)(197.06232, 13	FERULATE (CAS# 1135-24-6); (M+H)+	C01494	FindByFormula	27	+	194.0594	8.323253
FERULATE (CAS# 1135-24-6); (M+Na)+	FERULATE (CAS# 1135-24-6); (M+Na)+	FERULATE (CAS# 1135-24-6); (M+Na)+ [, tgt=67.93, overal	1135-24-6	(217.04565, 744.21)(218.05405, 41.805)	FERULATE (CAS# 1135-24-6); (M+Na)+	C01494	FindByFormula	2	+	194.0564	8.118361
FRUCTOSE (CAS# 57-48-7); (M+Na)+	FRUCTOSE (CAS# 57-48-7); (M+Na)+	FRUCTOSE (CAS# 57-48-7); (M+Na)+ [, tgt=61.79, overall=	57-48-7	(203.05351, 35500.13)(204.0574, 2545.1973)(205.06061, 668	FRUCTOSE (CAS# 57-48-7); (M+Na)+	C00095	FindByFormula	23	+	180.0647	0.64047945
GALACTITOL OR DULCITOL (CAS# 608-66-2); (	GALACTITOL OR DULCITOL (CAS# 608-66-2); (	GALACTITOL OR DULCITOL (CAS# 608-66-2); (M+Na)+ [, t	608-66-2	(205.07092, 1554.0834)(206.06844, 505.3033)	GALACTITOL OR DULCITOL (CAS# 608-66-2); (M+Na)+		FindByFormula	3	+	182.08	0.6489997
GALACTURONIC ACID (CAS# 91510-62-2); (M+	GALACTURONIC ACID (CAS# 91510-62-2); (M+	GALACTURONIC ACID (CAS# 91510-62-2); (M+Na)+[-H2O]	91510-62-2	(199.02197, 831.39996)(200.02147, 69.675)	GALACTURONIC ACID (CAS# 91510-62-2); (M+Na)+[-H2O]		FindByFormula	6	+	194.0436	0.8303327
GAMMA-BUTYROLACTONE (CAS# 96-48-0); (	GAMMA-BUTYROLACTONE (CAS# 96-48-0); (	GAMMA-BUTYROLACTONE (CAS# 96-48-0); (M+H)+ [, tgt	96-48-0	(87.0441, 461.49)(88.04, 55.81)	GAMMA-BUTYROLACTONE (CAS# 96-48-0); (M+H)+		FindByFormula	1	+	86.036	2.0640104
GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-	GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-	GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M+H	686-58-8	(251.06854, 651.025)(252.07375, 86.235)(253.0709, 35.8)	GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M+H)+	C03320	FindByFormula	2	+	250.0611	0.9499971
GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-	GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-	GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M+H	686-58-8	(233.0611, 344.76)(234.0655, 25.75)	GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M+H)+[-H2	C03320	FindByFormula	1	+	250.0645	0.82300264
GAMMA-LINOLENIC ACID (CAS# 506-26-3); (	GAMMA-LINOLENIC ACID (CAS# 506-26-3); (	GAMMA-LINOLENIC ACID (CAS# 506-26-3); (M+Na)+ [, tg	506-26-3	(301.2123, 17077.32)(302.21683, 3220.9236)(303.221, 1555.	GAMMA-LINOLENIC ACID (CAS# 506-26-3); (M+Na)+		FindByFormula	26	+	278.2223	22.704765
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M+Na)+ [, tgt=	77-06-5	(715.2718, 331.51334)(716.2774, 242.96999)(717.26984, 146	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M+Na)+	C01699	FindByFormula	3	+	346.1391	8.456676
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Na)+ [, tgt=	77-06-5	(369.13135, 19506.691)(370.13577, 4324.6875)(371.1403, 77	GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Na)+	C01699	FindByFormula	26	+	346.1422	8.462518
GLUCOSE (CAS# 50-99-7); (2M+Na)+	GLUCOSE (CAS# 50-99-7); (2M+Na)+	GLUCOSE (CAS# 50-99-7); (2M+Na)+ [, tgt=66.65, overall=	50-99-7	(383.11676, 818.00574)(384.1154, 138.89143)(385.11884, 64	GLUCOSE (CAS# 50-99-7); (2M+Na)+		FindByFormula	7	+	180.0632	0.6495711
GLUCOSE (CAS# 50-99-7); (2M+Na)+[-H2O]	GLUCOSE (CAS# 50-99-7); (2M+Na)+[-H2O]	GLUCOSE (CAS# 50-99-7); (2M+Na)+[-H2O] [, tgt=73.14, o	50-99-7	(365.10663, 1126.3812)(366.10504, 124.50749)(367.10974, 5	GLUCOSE (CAS# 50-99-7); (2M+Na)+[-H2O]		FindByFormula	8	+	180.0651	0.71824974
GLUCOSE (CAS# 50-99-7); (M+Na)+	GLUCOSE (CAS# 50-99-7); (M+Na)+	GLUCOSE (CAS# 50-99-7); (M+Na)+ [, tgt=77.43, overall=7	50-99-7	(203.05354, 32703.375)(204.05702, 2343.2085)(205.06071, 6	GLUCOSE (CAS# 50-99-7); (M+Na)+		FindByFormula	23	+	180.0651	0.6556099
GLUTAMATE (CAS# 56-86-0); (M+H)+	GLUTAMATE (CAS# 56-86-0); (M+H)+	GLUTAMATE (CAS# 56-86-0); (M+H)+ [, tgt=64.90, overall	56-86-0	(148.0613, 11122.051)(149.06343, 731.95337)(150.06015, 18	GLUTAMATE (CAS# 56-86-0); (M+H)+		FindByFormula	12	+	147.0522	0.78558725
GLUTAMATE (CAS# 56-86-0); (M+H)+[-H2O]	GLUTAMATE (CAS# 56-86-0); (M+H)+[-H2O]	GLUTAMATE (CAS# 56-86-0); (M+H)+[-H2O] [, tgt=84.19,	56-86-0	(130.05014, 17605.625)(131.05174, 1047.9553)(132.06358, 6	GLUTAMATE (CAS# 56-86-0); (M+H)+[-H2O]		FindByFormula	13	+	147.0532	0.6529233
GLUTAMINE (CAS# 56-85-9); (M+Na)+	GLUTAMINE (CAS# 56-85-9); (M+Na)+	GLUTAMINE (CAS# 56-85-9); (M+Na)+ [, tgt=79.92, overal	56-85-9	(169.0588, 20549.1)(170.0541, 3001.54)(171.0485, 189.45)	GLUTAMINE (CAS# 56-85-9); (M+Na)+		FindByFormula	1	+	146.0686	0.6280017
GLUTARATE (CAS# 110-94-1); (M+Na)+	GLUTARATE (CAS# 110-94-1); (M+Na)+	GLUTARATE (CAS# 110-94-1); (M+Na)+ [, tgt=75.01, overa	110-94-1	(155.0321, 2749.95)(156.0312, 347.94)	GLUTARATE (CAS# 110-94-1); (M+Na)+	C00489	FindByFormula	1	+	132.0424	2.0440307
GLUTATHIONE (CAS# 27025-41-8); (M+H)+	GLUTATHIONE (CAS# 27025-41-8); (M+H)+	GLUTATHIONE (CAS# 27025-41-8); (M+H)+ [, tgt=65.36, o	27025-41-8	(613.1585, 499.3256)(614.1579, 158.82689)(615.15405, 88.8	GLUTATHIONE (CAS# 27025-41-8); (M+H)+	C00127	FindByFormula	16	+	612.1512	1.3712608
GLUTATHIONE (CAS# 27025-41-8); (M+H2)+2	GLUTATHIONE (CAS# 27025-41-8); (M+H2)+2	GLUTATHIONE (CAS# 27025-41-8); (M+H2)+2 [, tgt=76.76	27025-41-8	(307.0852, 1925.8469)(307.58527, 507.82874)(308.08514, 28	GLUTATHIONE (CAS# 27025-41-8); (M+H2)+2	C00127	FindByFormula	16	+	612.1569	1.3847575
GLYCERALDEHYDE (CAS# 367-47-5); (2M+H)+[	GLYCERALDEHYDE (CAS# 367-47-5); (2M+H)+[	GLYCERALDEHYDE (CAS# 367-47-5); (2M+H)+[-H2O] [, tgt	367-47-5	(163.06145, 1486.95)(164.0581, 716.95996)	GLYCERALDEHYDE (CAS# 367-47-5); (2M+H)+[-H2O]	C02154	FindByFormula	2	+	90.031	1.9555033
GLYCINE (CAS# 56-40-6); (M+H)+	GLYCINE (CAS# 56-40-6); (M+H)+	GLYCINE (CAS# 56-40-6); (M+H)+ [, tgt=88.15, overall=88.	56-40-6	(76.0386, 1560.17)(77.0403, 36.63)	GLYCINE (CAS# 56-40-6); (M+H)+		FindByFormula	1	+	75.0313	0.62600183
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-	GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9	GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+H)+ [	640-79-9	(450.32007, 845.6766)(451.31625, 303.13998)(452.31583, 60	GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+H)+	C05462	FindByFormula	3	+	449.311	20.61986
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-	GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9	GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+H)+[-	640-79-9	(432.30954, 2287.7751)(433.31033, 749.81665)(434.30972, 1	GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+H)+[-H2O]	C05462	FindByFormula	6	+	449.3105	20.497957
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-	GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9	GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+Na)+	640-79-9	(472.30237, 6476.9883)(473.30743, 2074.7637)(474.30176, 5	GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+Na)+	C05462	FindByFormula	17	+	449.3134	20.291916
GLYCOCHOLATE (CAS# 475-31-0); (M+H)+	GLYCOCHOLATE (CAS# 475-31-0); (M+H)+	GLYCOCHOLATE (CAS# 475-31-0); (M+H)+ [, tgt=55.37, ov	475-31-0	(466.3168, 398.195)(467.31348, 120.06999)(468.30273, 54.4	GLYCOCHOLATE (CAS# 475-31-0); (M+H)+	C01921	FindByFormula	2	+	465.3065	18.868454
GLYCOCHOLATE (CAS# 475-31-0); (M+H)+[-H2	GLYCOCHOLATE (CAS# 475-31-0); (M+H)+[-H2	GLYCOCHOLATE (CAS# 475-31-0); (M+H)+[-H2O] [, tgt=34	475-31-0	(448.3022, 752.17)(449.301, 192.17)(450.3155, 79.3)	GLYCOCHOLATE (CAS# 475-31-0); (M+H)+[-H2O]	C01921	FindByFormula	1	+	465.3052	18.64078
GLYCOCHOLATE (CAS# 475-31-0); (M+Na)+	GLYCOCHOLATE (CAS# 475-31-0); (M+Na)+	GLYCOCHOLATE (CAS# 475-31-0); (M+Na)+ [, tgt=78.74, o	475-31-0	(488.29868, 3032.1157)(489.29453, 1128.1221)(490.29428, 2	GLYCOCHOLATE (CAS# 475-31-0); (M+Na)+	C01921	FindByFormula	10	+	465.3073	18.794794
GLYCOLITHOCHOLATE (CAS# 474-74-8); (M+	GLYCOLITHOCHOLATE (CAS# 474-74-8); (M+	GLYCOLITHOCHOLATE (CAS# 474-74-8); (M+Na)+ [, tgt=7	474-74-8	(456.30856, 697.02997)(457.31183, 356.9025)(458.3098, 102	GLYCOLITHOCHOLATE (CAS# 474-74-8); (M+Na)+	C15557	FindByFormula	4	+	433.3234	21.601706
GUAIFENESIN (CAS# 93-14-1); (M+Na)+	GUAIFENESIN (CAS# 93-14-1); (M+Na)+	GUAIFENESIN (CAS# 93-14-1); (M+Na)+ [, tgt=67.80, over	93-14-1	(221.07901, 3379.2598)(222.08585, 58.519997)(223.0891, 20	GUAIFENESIN (CAS# 93-14-1); (M+Na)+	C07033	FindByFormula	2	+	198.0904	7.704035
GUANIDINOACETATE (CAS# 352-97-6); (M+H)	GUANIDINOACETATE (CAS# 352-97-6); (M+H)	GUANIDINOACETATE (CAS# 352-97-6); (M+H)+ [, tgt=88.5	352-97-6	(118.0614, 1197.72)(119.0605, 59.2)	GUANIDINOACETATE (CAS# 352-97-6); (M+H)+		FindByFormula	1	+	117.054	0.6340019
GUANINE (CAS# 73-40-5); (2M+H)+	GUANINE (CAS# 73-40-5); (2M+H)+	GUANINE (CAS# 73-40-5); (2M+H)+ [, tgt=77.10, overall=	73-40-5	(303.1068, 661.46497)(304.09833, 149.06)	GUANINE (CAS# 73-40-5); (2M+H)+		FindByFormula	2	+	151.0484	0.9349989
GUANINE (CAS# 73-40-5); (2M+Na)+	GUANINE (CAS# 73-40-5); (2M+Na)+	GUANINE (CAS# 73-40-5); (2M+Na)+ [, tgt=35.71, overall=	73-40-5	(325.09076, 12688.305)(326.09058, 1871.225)(327.08588, 64	GUANINE (CAS# 73-40-5); (2M+Na)+		FindByFormula	8	+	151.0504	0.768503
GUANINE (CAS# 73-40-5); (M+H)+	GUANINE (CAS# 73-40-5); (M+H)+	GUANINE (CAS# 73-40-5); (M+H)+ [, tgt=77.60, overall=77	73-40-5	(152.05756, 14087.1045)(153.05943, 1155.5966)(154.05661,	GUANINE (CAS# 73-40-5); (M+H)+		FindByFormula	9	+	151.0506	0.9263345
GUANINE (CAS# 73-40-5); (M+Na)+	GUANINE (CAS# 73-40-5); (M+Na)+	GUANINE (CAS# 73-40-5); (M+Na)+ [, tgt=76.59, overall=	73-40-5	(174.0399, 5704.7837)(175.04207, 400.6467)(176.0412, 251.	GUANINE (CAS# 73-40-5); (M+Na)+		FindByFormula	3	+	151.0506	0.90433186
GUANOSINE (CAS# 118-00-3); (M+H)+	GUANOSINE (CAS# 118-00-3); (M+H)+	GUANOSINE (CAS# 118-00-3); (M+H)+ [, tgt=90.27, overal	118-00-3	(284.10037, 69147.71)(285.10312, 9088.608)(286.10825, 141	GUANOSINE (CAS# 118-00-3); (M+H)+	C00387	FindByFormula	22	+	283.0931	1.8177426
GUANOSINE (CAS# 118-00-3); (M+Na)+	GUANOSINE (CAS# 118-00-3); (M+Na)+	GUANOSINE (CAS# 118-00-3); (M+Na)+ [, tgt=75.54, over	118-00-3	(306.082, 5068.195)(307.08167, 67.11)(308.07837, 81.635)	GUANOSINE (CAS# 118-00-3); (M+Na)+	C00387	FindByFormula	2	+	283.0929	1.7360139
GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (	GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (	GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (M+H)+ [, tgt	85-32-5	(364.06476, 686.33746)(365.0657, 94.05125)(366.057, 44.33)	GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (M+H)+		FindByFormula	8	+	363.0578	1.0029992
GULONO-1,4-LACTONE (CAS# 1128-23-0); (M	GULONO-1,4-LACTONE (CAS# 1128-23-0); (M+	GULONO-1,4-LACTONE (CAS# 1128-23-0); (M+H)+[-H2O] [	1128-23-0	(161.0428, 2629.64)(162.041, 109.15)(163.0495, 88.18)	GULONO-1,4-LACTONE (CAS# 1128-23-0); (M+H)+[-H2O]	C05410	FindByFormula	1	+	178.046	0.7250004
HIPPURATE (CAS# 495-69-2); (M+H)+	HIPPURATE (CAS# 495-69-2); (M+H)+	HIPPURATE (CAS# 495-69-2); (M+H)+ [, tgt=70.22, overall	495-69-2	(180.0668, 3707.59)(181.0664, 39.41)(182.0649, 68.72)	HIPPURATE (CAS# 495-69-2); (M+H)+	C01586	FindByFormula	1	+	179.0594	4.8271275
HIPPURATE (CAS# 495-69-2); (M+Na)+	HIPPURATE (CAS# 495-69-2); (M+Na)+	HIPPURATE (CAS# 495-69-2); (M+Na)+ [, tgt=93.56, overal	495-69-2	(202.04802, 16679.127)(203.05127, 2199.7036)(204.05313, 3	HIPPURATE (CAS# 495-69-2); (M+Na)+	C01586	FindByFormula	14	+	179.0587	4.7967744
HISTAMINE (CAS# 51-45-6); (M+H)+	HISTAMINE (CAS# 51-45-6); (M+H)+	HISTAMINE (CAS# 51-45-6); (M+H)+ [, tgt=91.07, overall=	51-45-6	(112.08702, 36509.594)(113.0898, 4710.6133)(114.090256, 1	HISTAMINE (CAS# 51-45-6); (M+H)+		FindByFormula	21	+	111.0798	0.5419061
HISTAMINE (CAS# 51-45-6); (M+Na)+	HISTAMINE (CAS# 51-45-6); (M+Na)+	HISTAMINE (CAS# 51-45-6); (M+Na)+ [, tgt=49.00, overall	51-45-6	(134.0691, 5853.5244)(135.06778, 579.93787)(136.0681, 66.	HISTAMINE (CAS# 51-45-6); (M+Na)+		FindByFormula	19	+	111.0796	0.57463324
HOMOCYSTINE (CAS# 462-10-2); (M+Na)+	HOMOCYSTINE (CAS# 462-10-2); (M+Na)+	HOMOCYSTINE (CAS# 462-10-2); (M+Na)+ [, tgt=38.20, o	462-10-2	(291.0415, 595.41)(292.0479, 253.0)(293.041, 65.77)	HOMOCYSTINE (CAS# 462-10-2); (M+Na)+	C01817	FindByFormula	1	+	268.0536	0.5629992
HOMOGENTISATE (CAS# 451-13-8); (M+H)+	HOMOGENTISATE (CAS# 451-13-8); (M+H)+	HOMOGENTISATE (CAS# 451-13-8); (M+H)+ [, tgt=60.90,	451-13-8	(169.04968, 1071.172)(170.04654, 80.564)	HOMOGENTISATE (CAS# 451-13-8); (M+H)+		FindByFormula	5	+	168.0412	2.0342329
HOMOSERINE (CAS# 672-15-1); (M+H)+	HOMOSERINE (CAS# 672-15-1); (M+H)+	HOMOSERINE (CAS# 672-15-1); (M+H)+ [, tgt=80.47, over	672-15-1	(120.06592, 5246.264)(121.06698, 243.81334)(122.06771, 17	HOMOSERINE (CAS# 672-15-1); (M+H)+	C00263	FindByFormula	9	+	119.0582	0.66333336
HOMOSERINE (CAS# 672-15-1); (M+Na)+	HOMOSERINE (CAS# 672-15-1); (M+Na)+	HOMOSERINE (CAS# 672-15-1); (M+Na)+ [, tgt=70.58, ov	672-15-1	(142.04807, 2092.151)(143.04944, 108.97099)(144.04669, 98	HOMOSERINE (CAS# 672-15-1); (M+Na)+	C00263	FindByFormula	10	+	119.0591	0.63840073
HOMOVANILLATE (CAS# 306-08-1); (M+H)+	HOMOVANILLATE (CAS# 306-08-1); (M+H)+	HOMOVANILLATE (CAS# 306-08-1); (M+H)+ [, tgt=65.23,	306-08-1	(183.0657, 708.71)(184.0641, 88.22)	HOMOVANILLATE (CAS# 306-08-1); (M+H)+		FindByFormula	1	+	182.0579	5.6473885
HYPOXANTHINE (CAS# 68-94-0); (M+H)+	HYPOXANTHINE (CAS# 68-94-0); (M+H)+	HYPOXANTHINE (CAS# 68-94-0); (M+H)+ [, tgt=95.92, ove	68-94-0	(137.04639, 410091.94)(138.04936, 27629.63)(139.04955, 30	HYPOXANTHINE (CAS# 68-94-0); (M+H)+		FindByFormula	21	+	136.0393	1.0941917
HYPOXANTHINE (CAS# 68-94-0); (M+Na)+	HYPOXANTHINE (CAS# 68-94-0); (M+Na)+	HYPOXANTHINE (CAS# 68-94-0); (M+Na)+ [, tgt=93.31, ov	68-94-0	(159.0284, 68187.21)(160.03085, 4693.1514)(161.03093, 223	HYPOXANTHINE (CAS# 68-94-0); (M+Na)+		FindByFormula	13	+	136.0398	1.1079254
IBUPROFEN (CAS# 15687-27-1); (M+Na)+	IBUPROFEN (CAS# 15687-27-1); (M+Na)+	IBUPROFEN (CAS# 15687-27-1); (M+Na)+ [, tgt=98.99, ov	15687-27-1	(229.11986, 22164.191)(230.12215, 3289.889)(231.12927, 84	IBUPROFEN (CAS# 15687-27-1); (M+Na)+	C01588	FindByFormula	8	+	206.131	18.860949
IBUPROFEN CARBOXYLIC ACID (CAS# 15935-5	IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54	IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M+H)+	15935-54-3	(219.10162, 2135.2383)(220.09874, 258.0717)(221.09906, 75	IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M+H)+[-H2O]		FindByFormula	6	+	236.1046	12.958744
IBUPROFEN CARBOXYLIC ACID (CAS# 15935-5	IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54	IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M+Na	15935-54-3	(259.09433, 13705.41)(260.0981, 2080.9817)(261.0871, 448.	IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M+Na)+		FindByFormula	6	+	236.1047	12.961578
IMIDAZOLE-4-ACETATE (CAS# 645-65-8); (M+	IMIDAZOLE-4-ACETATE (CAS# 645-65-8); (M+	IMIDAZOLE-4-ACETATE (CAS# 645-65-8); (M+H)+ [, tgt=84	645-65-8	(127.0503, 1801.915)(128.05345, 59.29)	IMIDAZOLE-4-ACETATE (CAS# 645-65-8); (M+H)+	C02835	FindByFormula	2	+	126.0437	0.670001
INDOLE (CAS# 120-72-9); (2M+Na)+	INDOLE (CAS# 120-72-9); (2M+Na)+	INDOLE (CAS# 120-72-9); (2M+Na)+ [, tgt=55.04, overall=	120-72-9	(257.1037, 1043.58)(258.1077, 200.39)	INDOLE (CAS# 120-72-9); (2M+Na)+	C00463	FindByFormula	1	+	117.0568	6.485379
INDOLE-3-ACETATE (CAS# 87-51-4); (M+H)+	INDOLE-3-ACETATE (CAS# 87-51-4); (M+H)+	INDOLE-3-ACETATE (CAS# 87-51-4); (M+H)+ [, tgt=94.57,	87-51-4	(176.07094, 3715.5374)(177.07538, 473.21875)(178.07361, 1	INDOLE-3-ACETATE (CAS# 87-51-4); (M+H)+	C00954	FindByFormula	8	+	175.0637	8.350184
INDOLE-3-ACETATE (CAS# 87-51-4); (M+Na)+	INDOLE-3-ACETATE (CAS# 87-51-4); (M+Na)+	INDOLE-3-ACETATE (CAS# 87-51-4); (M+Na)+ [, tgt=80.88	87-51-4	(198.05376, 8769.405)(199.05789, 1066.4172)(200.06076, 10	INDOLE-3-ACETATE (CAS# 87-51-4); (M+Na)+	C00954	FindByFormula	7	+	175.0645	8.352206
INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M	INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M	INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M+Na)+ [, tgt=	392-12-1	(226.0492, 813.425)(227.04144, 96.25)	INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M+Na)+	C00331	FindByFormula	2	+	203.0588	10.501239
INOSINE (CAS# 58-63-9); (M+H)+	INOSINE (CAS# 58-63-9); (M+H)+	INOSINE (CAS# 58-63-9); (M+H)+ [, tgt=73.45, overall=73.	58-63-9	(269.09003, 66785.19)(270.0928, 8271.822)(271.08893, 2155	INOSINE (CAS# 58-63-9); (M+H)+		FindByFormula	23	+	268.0823	1.8162243
INOSINE (CAS# 58-63-9); (M+Na)+	INOSINE (CAS# 58-63-9); (M+Na)+	INOSINE (CAS# 58-63-9); (M+Na)+ [, tgt=81.25, overall=81	58-63-9	(291.07132, 31615.336)(292.0739, 4069.6125)(293.07693, 94	INOSINE (CAS# 58-63-9); (M+Na)+		FindByFormula	27	+	268.0817	1.7643087
INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+	INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+	INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+H)+ [, tgt=7	131-99-7	(349.05457, 2406.0933)(350.05203, 382.1244)(351.05792, 71	INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+H)+		FindByFormula	9	+	348.0457	0.9932216
INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+	INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+	INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+Na)+ [, tgt=	131-99-7	(371.0334, 753.06)(372.0445, 126.18)	INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+Na)+		FindByFormula	1	+	348.0454	0.98300076
ISOLEUCINE (CAS# 73-32-5); (M+H)+	ISOLEUCINE (CAS# 73-32-5); (M+H)+	ISOLEUCINE (CAS# 73-32-5); (M+H)+ [, tgt=76.97, overall=	73-32-5	(132.10233, 630677.1)(133.10526, 45568.41)(134.10574, 404	ISOLEUCINE (CAS# 73-32-5); (M+H)+		FindByFormula	28	+	131.095	1.610081
ISOLEUCINE (CAS# 73-32-5); (M+Na)+	ISOLEUCINE (CAS# 73-32-5); (M+Na)+	ISOLEUCINE (CAS# 73-32-5); (M+Na)+ [, tgt=64.18, overall	73-32-5	(154.08403, 15611.794)(155.08476, 1282.0553)(156.07822, 6	ISOLEUCINE (CAS# 73-32-5); (M+Na)+		FindByFormula	24	+	131.0943	1.600718
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+H)+ [, tgt=	77026-92-7	(211.13298, 34690.61)(212.1363, 4593.674)(213.13509, 574.	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+H)+		FindByFormula	27	+	210.1256	13.105898
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+Na)+ [, tgt	77026-92-7	(233.11534, 148948.28)(234.11845, 19191.844)(235.11874, 2	JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+Na)+		FindByFormula	28	+	210.126	13.105774
KYNURENINE (CAS# 343-65-7); (M+H)+	KYNURENINE (CAS# 343-65-7); (M+H)+	KYNURENINE (CAS# 343-65-7); (M+H)+ [, tgt=91.30, overa	343-65-7	(209.09242, 15655.315)(210.09517, 2028.1714)(211.08897, 1	KYNURENINE (CAS# 343-65-7); (M+H)+	C00328	FindByFormula	24	+	208.0851	2.2084394
KYNURENINE (CAS# 343-65-7); (M+Na)+	KYNURENINE (CAS# 343-65-7); (M+Na)+	KYNURENINE (CAS# 343-65-7); (M+Na)+ [, tgt=68.97, ove	343-65-7	(231.07367, 1299.5665)(232.0705, 43.963333)	KYNURENINE (CAS# 343-65-7); (M+Na)+	C00328	FindByFormula	3	+	208.0847	2.2080047
L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M+	L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M+	L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M+H)+ [, tgt=69.47, overall=69.47]		(139.05203, 74045.58)(140.06215, 10171.96)(141.06148, 902	L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M+H)+		FindByFormula	4	+	138.046	5.307653
L-2,3-DIAMINOPROPANOATE (CAS# 4033-39-	L-2,3-DIAMINOPROPANOATE (CAS# 4033-39-0	L-2,3-DIAMINOPROPANOATE (CAS# 4033-39-0); (M+Na)+	4033-39-0	(127.0479, 1751.2051)(128.0457, 86.69)	L-2,3-DIAMINOPROPANOATE (CAS# 4033-39-0); (M+Na)+	C03401	FindByFormula	2	+	104.0593	0.64999926
LACTOSE (CAS# 63-42-3); (M+K)+	LACTOSE (CAS# 63-42-3); (M+K)+	LACTOSE (CAS# 63-42-3); (M+K)+ [, tgt=56.32, overall=56.	63-42-3	(381.08188, 487.59497)(382.0812, 82.5575)(383.07376, 66.0	LACTOSE (CAS# 63-42-3); (M+K)+		FindByFormula	4	+	342.1186	0.734
LACTOSE (CAS# 63-42-3); (M+Na)+	LACTOSE (CAS# 63-42-3); (M+Na)+	LACTOSE (CAS# 63-42-3); (M+Na)+ [, tgt=68.10, overall=6	63-42-3	(365.1071, 1439.8563)(366.10944, 194.09572)(367.11264, 72	LACTOSE (CAS# 63-42-3); (M+Na)+		FindByFormula	14	+	342.1191	0.716929
L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)	L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)	L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)+ [, tgt=81.0	28954-12-3	(120.06592, 5246.264)(121.06698, 243.81334)(122.06771, 17	L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)+	C05519	FindByFormula	9	+	119.0582	0.66333336
L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)	L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)	L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)+[-H2O] [, t	28954-12-3	(102.05574, 1586.134)(103.05416, 146.24002)	L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)+[-H2O]	C05519	FindByFormula	5	+	119.0581	0.745999
LANOSTEROL (CAS# 79-63-0); (M+Na)+	LANOSTEROL (CAS# 79-63-0); (M+Na)+	LANOSTEROL (CAS# 79-63-0); (M+Na)+ [, tgt=28.72, over	79-63-0	(449.3806, 667.37)(450.3801, 350.55)(451.3698, 45.68)	LANOSTEROL (CAS# 79-63-0); (M+Na)+		FindByFormula	1	+	426.3893	23.324097
LANTHIONINE (CAS# 3183-08-2); (M+H)+	LANTHIONINE (CAS# 3183-08-2); (M+H)+	LANTHIONINE (CAS# 3183-08-2); (M+H)+ [, tgt=43.96, ove	8/2/3183	(209.05771, 667.86)(210.0665, 135.24)	LANTHIONINE (CAS# 3183-08-2); (M+H)+		FindByFormula	2	+	208.0509	0.83150053
L-ARGININE (CAS# 74-79-3); (M+H)+	L-ARGININE (CAS# 74-79-3); (M+H)+	L-ARGININE (CAS# 74-79-3); (M+H)+ [, tgt=68.27, overall=	74-79-3	(175.1193, 12965.135)(176.11581, 3718.3)	L-ARGININE (CAS# 74-79-3); (M+H)+	C02385	FindByFormula	2	+	174.1111	0.63550186
L-ARGININE (CAS# 74-79-3); (M+Na)+	L-ARGININE (CAS# 74-79-3); (M+Na)+	L-ARGININE (CAS# 74-79-3); (M+Na)+ [, tgt=78.93, overall	74-79-3	(197.10138, 2246.4856)(198.10583, 208.74937)(199.0954, 11	L-ARGININE (CAS# 74-79-3); (M+Na)+	C02385	FindByFormula	16	+	174.1128	0.61793894
L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (	L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (	L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (CAS#); (M+H)+ [, tgt=72.33, overall=7		(177.11392, 12225.956)(178.11264, 1049.9241)(179.11711, 8	L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (CAS#); (M+H)+		FindByFormula	15	+	176.1065	0.6254007
LAUROYLCARNITINE (CAS# 25518-54-1); (M+H	LAUROYLCARNITINE (CAS# 25518-54-1); (M+H	LAUROYLCARNITINE (CAS# 25518-54-1); (M+H)+ [, tgt=55	25518-54-1	(344.27863, 1819.5453)(345.28036, 459.15475)(346.27887, 4	LAUROYLCARNITINE (CAS# 25518-54-1); (M+H)+		FindByFormula	25	+	343.2708	17.970499
LAUROYLCARNITINE (CAS# 25518-54-1); (M+N	LAUROYLCARNITINE (CAS# 25518-54-1); (M+N	LAUROYLCARNITINE (CAS# 25518-54-1); (M+Na)+ [, tgt=4	25518-54-1	(366.26077, 2817.0713)(367.2597, 690.3689)(368.259, 105.1	LAUROYLCARNITINE (CAS# 25518-54-1); (M+Na)+		FindByFormula	9	+	343.2699	17.999672
L-CARNITINE (CAS# 541-15-1); (M+H)+	L-CARNITINE (CAS# 541-15-1); (M+H)+	L-CARNITINE (CAS# 541-15-1); (M+H)+ [, tgt=95.86, overa	541-15-1	(162.11282, 61621.594)(163.11497, 4786.0107)(164.11543, 5	L-CARNITINE (CAS# 541-15-1); (M+H)+		FindByFormula	21	+	161.1052	0.6938584
LEUCINE (CAS# 328-39-2); (M+H)+	LEUCINE (CAS# 328-39-2); (M+H)+	LEUCINE (CAS# 328-39-2); (M+H)+ [, tgt=98.05, overall=9	328-39-2	(132.10233, 654500.56)(133.10522, 47270.957)(134.10573, 4	LEUCINE (CAS# 328-39-2); (M+H)+	C16439	FindByFormula	28	+	131.095	1.631117
LEUCINE (CAS# 328-39-2); (M+Na)+	LEUCINE (CAS# 328-39-2); (M+Na)+	LEUCINE (CAS# 328-39-2); (M+Na)+ [, tgt=85.26, overall=	328-39-2	(154.08415, 16926.865)(155.08528, 1515.7133)(156.07893, 5	LEUCINE (CAS# 328-39-2); (M+Na)+	C16439	FindByFormula	24	+	131.0943	1.6180102
LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+	LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+	LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+ [, tgt=47.31	71160-24-2	(337.23615, 4381.663)(338.23907, 1233.9595)(339.23987, 18	LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+		FindByFormula	17	+	336.23	20.648716
LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+[	LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+[	LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+[-H2O] [, tgt	71160-24-2	(319.2248, 4098.937)(320.23047, 928.1043)	LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+[-H2O]		FindByFormula	7	+	336.2285	20.678883
LEUKOTRIENE B4 (CAS# 71160-24-2); (M+Na)	LEUKOTRIENE B4 (CAS# 71160-24-2); (M+Na)+	LEUKOTRIENE B4 (CAS# 71160-24-2); (M+Na)+ [, tgt=40.9	71160-24-2	(359.21664, 2687.135)(360.22336, 607.0125)(361.21585, 336	LEUKOTRIENE B4 (CAS# 71160-24-2); (M+Na)+		FindByFormula	4	+	336.2277	20.838001
L-HISTIDINE (CAS# 71-00-1); (M+H)+	L-HISTIDINE (CAS# 71-00-1); (M+H)+	L-HISTIDINE (CAS# 71-00-1); (M+H)+ [, tgt=79.83, overall=	71-00-1	(156.07631, 7290.6826)(157.07904, 567.90643)(158.08417, 8	L-HISTIDINE (CAS# 71-00-1); (M+H)+		FindByFormula	25	+	155.0695	0.6389614
L-HISTIDINE (CAS# 71-00-1); (M+Na)+	L-HISTIDINE (CAS# 71-00-1); (M+Na)+	L-HISTIDINE (CAS# 71-00-1); (M+Na)+ [, tgt=85.52, overall	71-00-1	(178.05876, 3374.7686)(179.06071, 91.92477)(180.06589, 57	L-HISTIDINE (CAS# 71-00-1); (M+Na)+		FindByFormula	21	+	155.0698	0.62352556
LITHOCHOLIC ACID (CAS# 434-13-9); (M+Na)+	LITHOCHOLIC ACID (CAS# 434-13-9); (M+Na)+	LITHOCHOLIC ACID (CAS# 434-13-9); (M+Na)+ [, tgt=66.1	434-13-9	(399.2889, 3074.14)(400.29327, 919.9)	LITHOCHOLIC ACID (CAS# 434-13-9); (M+Na)+		FindByFormula	4	+	376.3011	22.325008
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-9	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-9	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+H)	583-93-7	(191.10234, 1032.6733)(192.11006, 58.459995)	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+H)+	C00666	FindByFormula	3	+	190.0946	0.72233194
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-9	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-9	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+H)	583-93-7	(173.09265, 4443.2026)(174.0903, 706.1568)	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+H)+[-H2O	C00666	FindByFormula	19	+	190.0939	0.7825282
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-9	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-9	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+N	583-93-7	(213.08426, 940.19)(214.0887, 300.34)	LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+Na)+	C00666	FindByFormula	2	+	190.0943	0.90651613
L-METHIONINE SULFOXIMINE (CAS# 15985-39	L-METHIONINE SULFOXIMINE (CAS# 15985-39	L-METHIONINE SULFOXIMINE (CAS# 15985-39-4); (M+H)+	15985-39-4	(181.0645, 501.02)(182.0676, 148.56)	L-METHIONINE SULFOXIMINE (CAS# 15985-39-4); (M+H)+	C03510	FindByFormula	1	+	180.0574	0.89302784
LOPERAMIDE (CAS# 34552-83-5); (M+H)+	LOPERAMIDE (CAS# 34552-83-5); (M+H)+	LOPERAMIDE (CAS# 34552-83-5); (M+H)+ [, tgt=42.04, ov	34552-83-5	(477.23022, 806.4466)(478.225, 154.78667)(479.23618, 472.	LOPERAMIDE (CAS# 34552-83-5); (M+H)+	C07873	FindByFormula	3	+	476.2242	15.36012
L-ORNITHINE (CAS# 70-26-8); (M+H)+	L-ORNITHINE (CAS# 70-26-8); (M+H)+	L-ORNITHINE (CAS# 70-26-8); (M+H)+ [, tgt=69.21, overall=	70-26-8	(133.09677, 3878.3362)(134.09644, 288.0675)(135.09644, 15	L-ORNITHINE (CAS# 70-26-8); (M+H)+	C00077	FindByFormula	16	+	132.0894	0.5542505
L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M+H)+	L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M+H)+	L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M+H)+ [, tgt=89.40, overall=89.40]		(207.09232, 133307.73)(208.09547, 16272.8125)(209.09663,	L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M+H)+		FindByFormula	28	+	206.0846	3.6105363
LUMICHROME (CAS# 1086-80-2); (M+Na)+	LUMICHROME (CAS# 1086-80-2); (M+Na)+	LUMICHROME (CAS# 1086-80-2); (M+Na)+ [, tgt=73.51, o	1086-80-2	(265.0703, 711.705)(266.0697, 109.645004)	LUMICHROME (CAS# 1086-80-2); (M+Na)+	C01727	FindByFormula	2	+	242.0826	10.883367
LYSINE (CAS# 56-87-1); (M+H)+	LYSINE (CAS# 56-87-1); (M+H)+	LYSINE (CAS# 56-87-1); (M+H)+ [, tgt=94.07, overall=94.0	56-87-1	(147.11269, 30503.936)(148.11514, 2434.2979)(149.11671, 2	LYSINE (CAS# 56-87-1); (M+H)+	C00047	FindByFormula	25	+	146.1055	0.553601
LYSINE (CAS# 56-87-1); (M+Na)+	LYSINE (CAS# 56-87-1); (M+Na)+	LYSINE (CAS# 56-87-1); (M+Na)+ [, tgt=63.45, overall=63.	56-87-1	(169.09433, 3217.5002)(170.09421, 572.67053)(171.0956, 11	LYSINE (CAS# 56-87-1); (M+Na)+	C00047	FindByFormula	20	+	146.1049	0.5685009
MALATE (CAS# 636-61-3); (M+Na)+	MALATE (CAS# 636-61-3); (M+Na)+	MALATE (CAS# 636-61-3); (M+Na)+ [, tgt=81.07, overall=	636-61-3	(157.0102, 676.87)(158.0123, 25.65)	MALATE (CAS# 636-61-3); (M+Na)+	C00497	FindByFormula	1	+	134.0209	0.7619988
MALEAMATE (CAS# 557-24-4); (M+H)+	MALEAMATE (CAS# 557-24-4); (M+H)+	MALEAMATE (CAS# 557-24-4); (M+H)+ [, tgt=51.52, overa	557-24-4	(116.0343, 1497.4567)(117.03433, 108.11001)	MALEAMATE (CAS# 557-24-4); (M+H)+	C01596	FindByFormula	3	+	115.0263	0.63133335
MALTOSE (CAS# 69-79-4); (M+Na)+	MALTOSE (CAS# 69-79-4); (M+Na)+	MALTOSE (CAS# 69-79-4); (M+Na)+ [, tgt=75.32, overall=	69-79-4	(365.1071, 1436.5284)(366.10913, 190.30142)(367.11215, 64	MALTOSE (CAS# 69-79-4); (M+Na)+	C00208	FindByFormula	14	+	342.1189	0.716929
MANDELIC ACID (CAS# 611-71-2); (M+Na)+	MANDELIC ACID (CAS# 611-71-2); (M+Na)+	MANDELIC ACID (CAS# 611-71-2); (M+Na)+ [, tgt=40.21,	611-71-2	(175.03531, 601.775)(176.0404, 77.705)	MANDELIC ACID (CAS# 611-71-2); (M+Na)+	C01983	FindByFormula	2	+	152.0464	5.2228355
MANNITOL (CAS# 69-65-8); (M+Na)+	MANNITOL (CAS# 69-65-8); (M+Na)+	MANNITOL (CAS# 69-65-8); (M+Na)+ [, tgt=60.18, overall	69-65-8	(205.07074, 1350.5825)(206.06747, 444.7125)	MANNITOL (CAS# 69-65-8); (M+Na)+	C00392	FindByFormula	4	+	182.0807	0.6497503
MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (	MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (	MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (M+Na)+ [, t	3672-15-9	(283.01758, 449.47498)(284.0216, 96.865)	MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (M+Na)+	C00275	FindByFormula	4	+	260.0274	0.89899933
MELANIN (CAS# 8049-97-6); (M+H)+	MELANIN (CAS# 8049-97-6); (M+H)+	MELANIN (CAS# 8049-97-6); (M+H)+ [, tgt=35.84, overall=	8049-97-6	(319.0731, 5002.691)(320.07166, 1168.3236)(321.07068, 483	MELANIN (CAS# 8049-97-6); (M+H)+		FindByFormula	11	+	318.0635	1.1909124
MELATONIN (CAS# 73-31-4); (M+Na)+	MELATONIN (CAS# 73-31-4); (M+Na)+	MELATONIN (CAS# 73-31-4); (M+Na)+ [, tgt=46.58, overa	73-31-4	(255.114, 1011.4)(256.1075, 163.0)	MELATONIN (CAS# 73-31-4); (M+Na)+		FindByFormula	1	+	232.1234	8.982716
MELIBIOSE (CAS# 585-99-9); (M+K)+	MELIBIOSE (CAS# 585-99-9); (M+K)+	MELIBIOSE (CAS# 585-99-9); (M+K)+ [, tgt=68.35, overal	585-99-9	(381.08188, 487.59497)(382.0812, 82.5575)(383.07376, 66.0	MELIBIOSE (CAS# 585-99-9); (M+K)+	C05402	FindByFormula	4	+	342.1186	0.734
MELIBIOSE (CAS# 585-99-9); (M+Na)+	MELIBIOSE (CAS# 585-99-9); (M+Na)+	MELIBIOSE (CAS# 585-99-9); (M+Na)+ [, tgt=74.11, overal	585-99-9	(365.10718, 1451.3671)(366.10904, 190.23071)(367.11322, 6	MELIBIOSE (CAS# 585-99-9); (M+Na)+	C05402	FindByFormula	14	+	342.1188	0.716929
MENAQUINONE (CAS# 11032-49-8); (M+Na)+	MENAQUINONE (CAS# 11032-49-8); (M+Na)+	MENAQUINONE (CAS# 11032-49-8); (M+Na)+ [, tgt=35.0	11032-49-8	(467.2958, 321.25)(468.2922, 175.21)	MENAQUINONE (CAS# 11032-49-8); (M+Na)+		FindByFormula	1	+	444.3041	24.397156
METHIONINE (CAS# 63-68-3); (M+H)+	METHIONINE (CAS# 63-68-3); (M+H)+	METHIONINE (CAS# 63-68-3); (M+H)+ [, tgt=97.16, overal	63-68-3	(150.05914, 150361.78)(151.0612, 10764.675)(152.05545, 12	METHIONINE (CAS# 63-68-3); (M+H)+		FindByFormula	19	+	149.0522	1.0133696
METHYL BETA-D-GALACTOSIDE (CAS# 1824-9	METHYL BETA-D-GALACTOSIDE (CAS# 1824-94	METHYL BETA-D-GALACTOSIDE (CAS# 1824-94-8); (M+Na)	1824-94-8	(217.0688, 529.5)(218.067, 103.62)	METHYL BETA-D-GALACTOSIDE (CAS# 1824-94-8); (M+Na)+	C03619	FindByFormula	1	+	194.0787	0.8309938
METHYL INDOLE-3-ACETATE (CAS# 1912-33-0)	METHYL INDOLE-3-ACETATE (CAS# 1912-33-0)	METHYL INDOLE-3-ACETATE (CAS# 1912-33-0); (M+H)+ [,	1912-33-0	(190.08815, 445.575)(191.08511, 69.975)	METHYL INDOLE-3-ACETATE (CAS# 1912-33-0); (M+H)+		FindByFormula	1	+	189.0799	11.634063
METHYL INDOLE-3-ACETATE (CAS# 1912-33-0)	METHYL INDOLE-3-ACETATE (CAS# 1912-33-0)	METHYL INDOLE-3-ACETATE (CAS# 1912-33-0); (M+Na)+ [	1912-33-0	(212.06982, 2176.5215)(213.06909, 277.24374)(214.0689, 57	METHYL INDOLE-3-ACETATE (CAS# 1912-33-0); (M+Na)+		FindByFormula	16	+	189.0804	11.618435
METHYL JASMONATE (CAS# 1211-29-6); (M+	METHYL JASMONATE (CAS# 1211-29-6); (M+	METHYL JASMONATE (CAS# 1211-29-6); (M+Na)+ [, tgt=6	1211-29-6	(247.13036, 6622.0874)(248.13115, 998.83746)(249.13274, 9	METHYL JASMONATE (CAS# 1211-29-6); (M+Na)+	C11512	FindByFormula	27	+	224.1409	15.845716
METHYLGUANIDINE (CAS# 471-29-4); (M+H)+	METHYLGUANIDINE (CAS# 471-29-4); (M+H)+	METHYLGUANIDINE (CAS# 471-29-4); (M+H)+ [, tgt=90.8	471-29-4	(74.0711, 3595.8723)(75.072914, 116.950005)	METHYLGUANIDINE (CAS# 471-29-4); (M+H)+	C02294	FindByFormula	8	+	73.0635	0.6495038
METHYLMALONATE (CAS# 516-05-2); (M+Na)	METHYLMALONATE (CAS# 516-05-2); (M+Na)	METHYLMALONATE (CAS# 516-05-2); (M+Na)+ [, tgt=58.0	516-05-2	(141.01651, 2344.546)(142.01819, 197.64226)(143.01418, 70	METHYLMALONATE (CAS# 516-05-2); (M+Na)+	C02170	FindByFormula	18	+	118.027	1.5120099
MEVALONIC ACID (CAS# 674-26-0); (M+Na)+	MEVALONIC ACID (CAS# 674-26-0); (M+Na)+	MEVALONIC ACID (CAS# 674-26-0); (M+Na)+ [, tgt=59.03,	674-26-0	(171.0635, 2643.62)(172.0681, 205.8)(173.0658, 146.26)	MEVALONIC ACID (CAS# 674-26-0); (M+Na)+		FindByFormula	1	+	148.0742	1.8620198
MONO-METHYL GLUTARATE (CAS# 1501-27-5	MONO-METHYL GLUTARATE (CAS# 1501-27-5)	MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M+H)+[-	1501-27-5	(129.05432, 534.02405)(130.05426, 65.028)	MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M+H)+[-H2O]		FindByFormula	5	+	146.0568	3.5389576
MONO-METHYL GLUTARATE (CAS# 1501-27-5	MONO-METHYL GLUTARATE (CAS# 1501-27-5)	MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M+Na)+	1501-27-5	(169.04782, 4079.1262)(170.04883, 118.23385)(171.0475, 44	MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M+Na)+		FindByFormula	13	+	146.0586	3.5313034
MYO-INOSITOL (CAS# 87-89-8); (M+Na)+	MYO-INOSITOL (CAS# 87-89-8); (M+Na)+	MYO-INOSITOL (CAS# 87-89-8); (M+Na)+ [, tgt=77.24, ov	87-89-8	(203.05351, 35500.13)(204.0574, 2545.1973)(205.06061, 668	MYO-INOSITOL (CAS# 87-89-8); (M+Na)+	C00137	FindByFormula	23	+	180.0647	0.64047945
N(PAI)-METHYL-L-HISTIDINE (CAS# 332-80-9);	N(PAI)-METHYL-L-HISTIDINE (CAS# 332-80-9);	N(PAI)-METHYL-L-HISTIDINE (CAS# 332-80-9); (M+H)+ [, t	332-80-9	(170.09242, 1414.7751)(171.09271, 159.61667)	N(PAI)-METHYL-L-HISTIDINE (CAS# 332-80-9); (M+H)+	C01152	FindByFormula	15	+	169.0847	0.60233474
N,N-DIMETHYLGLYCINE (CAS# 1118-68-9); (M	N,N-DIMETHYLGLYCINE (CAS# 1118-68-9); (M	N,N-DIMETHYLGLYCINE (CAS# 1118-68-9); (M+H)+ [, tgt=	1118-68-9	(104.07006, 733.8083)(105.07357, 41.148335)	N,N-DIMETHYLGLYCINE (CAS# 1118-68-9); (M+H)+	C01026	FindByFormula	6	+	103.0627	0.84966606
N1-ACETYLSPERMINE (CAS# 77928-70-2); (M	N1-ACETYLSPERMINE (CAS# 77928-70-2); (M	N1-ACETYLSPERMINE (CAS# 77928-70-2); (M+H)+ [, tgt=6	77928-70-2	(245.23335, 487.7782)(246.23105, 105.62092)	N1-ACETYLSPERMINE (CAS# 77928-70-2); (M+H)+		FindByFormula	11	+	244.2242	0.57681996
N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+	N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+H	N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+H)+ [, tgt=78.62, overall=78.62]		(189.15924, 2156.421)(190.16156, 207.8378)(191.15656, 147	N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+H)+		FindByFormula	9	+	188.1511	0.6302232
N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+	N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+N	N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+Na)+ [, tgt=74.21, overall=74.21]		(211.14171, 846.16144)(212.14143, 120.618576)	N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+Na)+		FindByFormula	7	+	188.1516	0.6231427
N-ACETYL-DL-GLUTAMIC ACID (CAS# 5817-08-	N-ACETYL-DL-GLUTAMIC ACID (CAS# 5817-08-	N-ACETYL-DL-GLUTAMIC ACID (CAS# 5817-08-3); (M+H)+[	8/3/5817	(172.06181, 564.56665)(173.06242, 111.37667)	N-ACETYL-DL-GLUTAMIC ACID (CAS# 5817-08-3); (M+H)+[-H2O]		FindByFormula	3	+	189.064	1.5810083
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5);	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5);	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+H)+ [, t	1115-47-5	(192.06892, 1444.5222)(193.07072, 172.6561)(194.06618, 74	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+H)+		FindByFormula	18	+	191.0616	4.068232
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5);	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5);	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+H)+[-H	1115-47-5	(174.05722, 848.66003)(175.0644, 101.83401)(176.0664, 90.	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+H)+[-H2O]		FindByFormula	5	+	191.063	4.0662637
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5);	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5);	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+Na)+ [,	1115-47-5	(214.05185, 4273.2183)(215.05252, 289.73773)(216.04803, 1	N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+Na)+		FindByFormula	26	+	191.0621	4.065639
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+ [, tgt=53.99	97-14-3	(148.0614, 11167.735)(149.06352, 728.1709)(150.06015, 18	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+		FindByFormula	12	+	147.0522	0.8160041
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+[	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+[-H2O] [, tgt	97-14-3	(130.05022, 116268.59)(131.05156, 6934.001)(132.0632, 234	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+[-H2O]		FindByFormula	21	+	147.0534	0.85533506
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+Na)+	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+Na)+	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+Na)+ [, tgt=55.1	97-14-3	(170.04291, 2373.0874)(171.03983, 124.833336)(172.04182,	N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+Na)+		FindByFormula	15	+	147.0526	0.8395346
N-ACETYLGLYCINE (CAS# 543-24-8); (M+Na)+	N-ACETYLGLYCINE (CAS# 543-24-8); (M+Na)+	N-ACETYLGLYCINE (CAS# 543-24-8); (M+Na)+ [, tgt=57.7	543-24-8	(140.0324, 2267.4)(141.0345, 67.71)	N-ACETYLGLYCINE (CAS# 543-24-8); (M+Na)+		FindByFormula	1	+	117.0431	1.1700028
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+ [, tgt=54.5	97-69-8	(132.06552, 6663.742)(133.06488, 187.42)	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+		FindByFormula	5	+	131.0583	1.1950121
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+[	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+[-H2O] [, tgt	97-69-8	(114.0546, 667.46)(115.0517, 74.84)	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+[-H2O]		FindByFormula	1	+	131.0573	1.7230163
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+Na)+	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+Na)	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+Na)+ [, tgt=79.2	97-69-8	(154.0483, 4595.9097)(155.04878, 225.6952)(156.04295, 168	N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+Na)+		FindByFormula	23	+	131.0588	1.4541374
N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M+N	N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M+N	N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M+Na)+ [, tgt=6	1188-21-2	(196.09644, 1144.7899)(197.09315, 197.67)(198.0885, 164.9	N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M+Na)+		FindByFormula	6	+	173.1063	7.3519807
N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-	N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-3	N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-3); (M+Na)+	2018-61-3	(230.07922, 545.26666)(231.07683, 133.42499)	N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-3); (M+Na)+	C03519	FindByFormula	6	+	207.0876	7.65419

N-ACETYLNEURAMINATE (CAS# 131-48-6); (M	N-ACETYLNEURAMINATE (CAS# 131-48-6); (M	N-ACETYLNEURAMINATE (CAS# 131-48-6); (M+H)+ [, tgt=	131-48-6	(310.1162, 487.515)(311.1139, 126.195)	N-ACETYLNEURAMINATE (CAS# 131-48-6); (M+H)+		FindByFormula	2	+	309.108	0.7430016
N-ACETYLNEURAMINATE (CAS# 131-48-6); (M	N-ACETYLNEURAMINATE (CAS# 131-48-6); (M	N-ACETYLNEURAMINATE (CAS# 131-48-6); (M+Na)+ [, tgt	131-48-6	(332.0944, 407.86)(333.0869, 66.21)	N-ACETYLNEURAMINATE (CAS# 131-48-6); (M+Na)+		FindByFormula	1	+	309.1037	0.8280009
N-ACETYLSEROTONIN (CAS# 1210-83-9); (M+	N-ACETYLSEROTONIN (CAS# 1210-83-9); (M+	N-ACETYLSEROTONIN (CAS# 1210-83-9); (M+Na)+ [, tgt=2	1210-83-9	(241.0964, 3204.53)(242.0877, 799.85)(243.0905, 687.41)	N-ACETYLSEROTONIN (CAS# 1210-83-9); (M+Na)+		FindByFormula	1	+	218.1035	5.0831614
NAD (CAS# 53-84-9); (M+2H)+2	NAD (CAS# 53-84-9); (M+2H)+2	NAD (CAS# 53-84-9); (M+2H)+2 [, tgt=73.58, overall=73.5	53-84-9	(332.56387, 591.6889)(333.06165, 247.03554)(333.5628, 58.	NAD (CAS# 53-84-9); (M+2H)+2		FindByFormula	9	+	663.1116	1.0223353
NAD (CAS# 53-84-9); (M+H)+	NAD (CAS# 53-84-9); (M+H)+	NAD (CAS# 53-84-9); (M+H)+ [, tgt=44.80, overall=44.80]	53-84-9	(664.1166, 789.783)(665.1177, 231.66153)(666.11597, 84.42	NAD (CAS# 53-84-9); (M+H)+		FindByFormula	20	+	663.1092	1.0091053
N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3);	N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3); (	N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3); (M+H)+ [, tg	1946-82-3	(189.12415, 3128.3289)(190.12012, 508.2525)(191.12419, 10	N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3); (M+H)+		FindByFormula	16	+	188.1179	1.0030053
NAPROXEN (CAS# 22204-53-1); (M+H)+	NAPROXEN (CAS# 22204-53-1); (M+H)+	NAPROXEN (CAS# 22204-53-1); (M+H)+ [, tgt=95.92, overa	22204-53-1	(231.1018, 7073.015)(232.10509, 1172.7644)(233.10387, 279	NAPROXEN (CAS# 22204-53-1); (M+H)+	C01517	FindByFormula	9	+	230.0946	15.708742
NAPROXEN (CAS# 22204-53-1); (M+Na)+	NAPROXEN (CAS# 22204-53-1); (M+Na)+	NAPROXEN (CAS# 22204-53-1); (M+Na)+ [, tgt=96.85, ove	22204-53-1	(253.08426, 52551.598)(254.08765, 8181.41)(255.09555, 889	NAPROXEN (CAS# 22204-53-1); (M+Na)+	C01517	FindByFormula	8	+	230.0951	15.709124
N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8); (	N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8); (	N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8); (M+Na)+ [, t	75251-80-8	(302.1217, 325.37)(303.1148, 140.22)	N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8); (M+Na)+		FindByFormula	1	+	279.1294	4.724168
N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8);	N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8);	N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8); (M+H)+ [, t	766-93-8	(128.10698, 370.94833)(129.10487, 38.706665)	N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8); (M+H)+	C11519	FindByFormula	6	+	127.0996	7.898964
N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8);	N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8);	N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8); (M+Na)+ [,	766-93-8	(150.08899, 999.8806)(151.08684, 117.21178)	N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8); (M+Na)+	C11519	FindByFormula	17	+	127.0995	7.902938
N-ETHYLMALEIMIDE (CAS# 128-53-0); (M+H)+	N-ETHYLMALEIMIDE (CAS# 128-53-0); (M+H)+	N-ETHYLMALEIMIDE (CAS# 128-53-0); (M+H)+ [, tgt=79.2	128-53-0	(126.05514, 807.00665)(127.05737, 75.200005)	N-ETHYLMALEIMIDE (CAS# 128-53-0); (M+H)+	C02441	FindByFormula	6	+	125.0473	3.390033
NICOTINAMIDE (CAS# 98-92-0); (M+H)+	NICOTINAMIDE (CAS# 98-92-0); (M+H)+	NICOTINAMIDE (CAS# 98-92-0); (M+H)+ [, tgt=92.87, over	98-92-0	(123.05541, 78915.67)(124.05817, 5756.9976)(125.05769, 26	NICOTINAMIDE (CAS# 98-92-0); (M+H)+	C00153	FindByFormula	24	+	122.0482	1.131627
NICOTINAMIDE HYPOXANTHINE DINUCLEOTI	NICOTINAMIDE HYPOXANTHINE DINUCLEOTID	NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE (CAS# 22	22052-73-9	(665.0905, 337.07)(666.1102, 91.24)(667.105, 809.63)	NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE (CAS# 22052-73-9); (M+H)+		FindByFormula	1	+	664.0907	0.95900065
NICOTINAMIDE MONONUCLEOTIDE (CAS# 10	NICOTINAMIDE MONONUCLEOTIDE (CAS# 10	NICOTINAMIDE MONONUCLEOTIDE (CAS# 1094-61-7); (M	1094-61-7	(335.0659, 908.0475)(336.0651, 190.2175)(337.06876, 63.3)	NICOTINAMIDE MONONUCLEOTIDE (CAS# 1094-61-7); (M+H)+		FindByFormula	4	+	334.0579	0.8014968
NICOTINAMIDE MONONUCLEOTIDE (CAS# 10	NICOTINAMIDE MONONUCLEOTIDE (CAS# 10	NICOTINAMIDE MONONUCLEOTIDE (CAS# 1094-61-7); (M	1094-61-7	(357.0514, 590.61)(358.043, 298.52)	NICOTINAMIDE MONONUCLEOTIDE (CAS# 1094-61-7); (M+Na)+		FindByFormula	1	+	334.0584	0.6030015
NICOTINATE (CAS# 59-67-6); (M+H)+	NICOTINATE (CAS# 59-67-6); (M+H)+	NICOTINATE (CAS# 59-67-6); (M+H)+ [, tgt=76.72, overall	59-67-6	(124.03957, 2279.905)(125.039375, 264.8125)	NICOTINATE (CAS# 59-67-6); (M+H)+	C00253	FindByFormula	4	+	123.0331	1.0527518
NICOTINE (CAS# 54-11-5); (M+H)+	NICOTINE (CAS# 54-11-5); (M+H)+	NICOTINE (CAS# 54-11-5); (M+H)+ [, tgt=81.92, overall=8	54-11-5	(163.12279, 2105.44)(164.12143, 256.16177)(165.1184, 24.8	NICOTINE (CAS# 54-11-5); (M+H)+	C00745	FindByFormula	11	+	162.1149	1.2853671
N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5	N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5	N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M+H)+ [,	6384-92-5	(148.0613, 11122.051)(149.06343, 731.95337)(150.06015, 18	N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M+H)+	C12269	FindByFormula	12	+	147.0522	0.78558725
N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5	N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5	N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M+Na)+	6384-92-5	(170.04308, 2200.9568)(171.04173, 107.38307)(172.04308, 2	N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M+Na)+	C12269	FindByFormula	13	+	147.0526	0.77307737
N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (	N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (	N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M+H)+[-H2	6753-62-4	(144.06575, 1075.3885)(145.06628, 177.32288)	N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M+H)+[-H2O]	C01046	FindByFormula	14	+	161.069	2.01774
N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (	N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (	N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M+Na)+ [, t	6753-62-4	(184.05815, 1605.785)(185.06241, 231.0)	N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M+Na)+	C01046	FindByFormula	2	+	161.07	2.0030105
N-METHYLNICOTINATE (CAS# 535-83-1); (M+	N-METHYLNICOTINATE (CAS# 535-83-1); (M+	N-METHYLNICOTINATE (CAS# 535-83-1); (M+H)+ [, tgt=8	535-83-1	(138.05412, 11865.578)(139.05656, 1066.295)	N-METHYLNICOTINATE (CAS# 535-83-1); (M+H)+	C01004	FindByFormula	6	+	137.0467	0.7003328
N-OLEOYLGLYCINE (CAS# 2601-90-3); (M+Na)	N-OLEOYLGLYCINE (CAS# 2601-90-3); (M+Na)	N-OLEOYLGLYCINE (CAS# 2601-90-3); (M+Na)+ [, tgt=49.2	2601-90-3	(362.2706, 638.295)(363.266, 370.555)(364.2537, 75.72)	N-OLEOYLGLYCINE (CAS# 2601-90-3); (M+Na)+		FindByFormula	2	+	339.2755	22.577133
NORADRENALINE (CAS# 51-41-2); (M+H)+[-H	NORADRENALINE (CAS# 51-41-2); (M+H)+[-H2	NORADRENALINE (CAS# 51-41-2); (M+H)+[-H2O] [, tgt=72	51-41-2	(152.06985, 10423.97)(153.0728, 982.53503)(154.07251, 189	NORADRENALINE (CAS# 51-41-2); (M+H)+[-H2O]		FindByFormula	2	+	169.0725	0.76399994
NORLEUCINE (CAS# 327-57-1); (M+H)+	NORLEUCINE (CAS# 327-57-1); (M+H)+	NORLEUCINE (CAS# 327-57-1); (M+H)+ [, tgt=91.74, overa	327-57-1	(132.10228, 594771.8)(133.10513, 42909.02)(134.10536, 392	NORLEUCINE (CAS# 327-57-1); (M+H)+	C01933	FindByFormula	28	+	131.0949	1.6551889
NORMETANEPHRINE (CAS# 0); (M+H)+	NORMETANEPHRINE (CAS# 0); (M+H)+	NORMETANEPHRINE (CAS# 0); (M+H)+ [, tgt=51.19, overall=51.19]		(184.0967, 1128.38)(185.1072, 93.44)	NORMETANEPHRINE (CAS# 0); (M+H)+		FindByFormula	1	+	183.09	2.9570556
NORMETANEPHRINE (CAS# 0); (M+H)+[-H2O]	NORMETANEPHRINE (CAS# 0); (M+H)+[-H2O]	NORMETANEPHRINE (CAS# 0); (M+H)+[-H2O] [, tgt=82.57, overall=82.57]		(166.08656, 721051.06)(167.08974, 73820.266)(168.09183, 6	NORMETANEPHRINE (CAS# 0); (M+H)+[-H2O]		FindByFormula	28	+	183.0898	2.5183146
NORVALINE (CAS# 6600-40-4); (M+H)+	NORVALINE (CAS# 6600-40-4); (M+H)+	NORVALINE (CAS# 6600-40-4); (M+H)+ [, tgt=99.58, overa	6600-40-4	(118.086586, 175130.17)(119.08914, 10872.538)(120.08798,	NORVALINE (CAS# 6600-40-4); (M+H)+	C01826	FindByFormula	13	+	117.079	0.90300053
NORVALINE (CAS# 6600-40-4); M+[-CO2H]	NORVALINE (CAS# 6600-40-4); M+[-CO2H]	NORVALINE (CAS# 6600-40-4); M+[-CO2H] [, tgt=88.32, o	6600-40-4	(72.081474, 90479.65)(73.08459, 4404.11)(74.08853, 137.11)	NORVALINE (CAS# 6600-40-4); M+[-CO2H]	C01826	FindByFormula	12	+	117.0799	0.8904166
O-ACETYLCARNITINE (CAS# 461-77-8); (M+H)	O-ACETYLCARNITINE (CAS# 461-77-8); (M+H)+	O-ACETYLCARNITINE (CAS# 461-77-8); (M+H)+ [, tgt=92.3	461-77-8	(204.124, 64539.812)(205.12514, 7637.2524)(206.1238, 883.	O-ACETYLCARNITINE (CAS# 461-77-8); (M+H)+	C02571	FindByFormula	18	+	203.1161	0.9375556
OCTACOSANOIC ACID (CAS# 506-48-9); (M+H	OCTACOSANOIC ACID (CAS# 506-48-9); (M+H)	OCTACOSANOIC ACID (CAS# 506-48-9); (M+H)+ [, tgt=84.	506-48-9	(425.43393, 2543.9583)(426.43817, 762.82996)(427.43594, 1	OCTACOSANOIC ACID (CAS# 506-48-9); (M+H)+		FindByFormula	5	+	424.4273	23.519966
OLEAMIDE (CAS# 301-02-0); (M+H)+	OLEAMIDE (CAS# 301-02-0); (M+H)+	OLEAMIDE (CAS# 301-02-0); (M+H)+ [, tgt=47.15, overall=	301-02-0	(282.27795, 1251.0973)(283.27856, 260.4891)(284.28302, 74	OLEAMIDE (CAS# 301-02-0); (M+H)+		FindByFormula	11	+	281.2702	22.637827
OLEAMIDE (CAS# 301-02-0); (M+Na)+	OLEAMIDE (CAS# 301-02-0); (M+Na)+	OLEAMIDE (CAS# 301-02-0); (M+Na)+ [, tgt=54.55, overal	301-02-0	(304.26163, 64676.207)(305.25754, 19568.594)(306.25803, 3	OLEAMIDE (CAS# 301-02-0); (M+Na)+		FindByFormula	4	+	281.2716	22.62983
OLEIC ACID (CAS# 112-80-1); (M+H)+	OLEIC ACID (CAS# 112-80-1); (M+H)+	OLEIC ACID (CAS# 112-80-1); (M+H)+ [, tgt=74.71, overall	112-80-1	(283.26138, 719.1563)(284.26373, 138.93124)	OLEIC ACID (CAS# 112-80-1); (M+H)+		FindByFormula	8	+	282.2556	22.557022
OLEIC ACID (CAS# 112-80-1); (M+Na)+	OLEIC ACID (CAS# 112-80-1); (M+Na)+	OLEIC ACID (CAS# 112-80-1); (M+Na)+ [, tgt=69.34, overal	112-80-1	(305.24548, 20373.324)(306.24908, 4145.9536)(307.25317, 5	OLEIC ACID (CAS# 112-80-1); (M+Na)+		FindByFormula	27	+	282.2563	22.510567
OMEGA-HYDROXYDODECANOIC ACID (CAS# 5	OMEGA-HYDROXYDODECANOIC ACID (CAS# 5	OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M	505-95-3	(199.1688, 390.05)(200.1621, 53.32)	OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M+H)+[-H2O]		FindByFormula	1	+	216.1709	17.000687
OMEGA-HYDROXYDODECANOIC ACID (CAS# 5	OMEGA-HYDROXYDODECANOIC ACID (CAS# 5	OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M	505-95-3	(239.16045, 3223.4531)(240.16266, 486.26334)(241.1706, 35	OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M+Na)+		FindByFormula	3	+	216.1713	16.980742
OMEPRAZOLE (CAS# 73590-58-6); (M+H)+	OMEPRAZOLE (CAS# 73590-58-6); (M+H)+	OMEPRAZOLE (CAS# 73590-58-6); (M+H)+ [, tgt=77.51, ov	73590-58-6	(346.12335, 699.1279)(347.12506, 125.254005)(348.11325, 7	OMEPRAZOLE (CAS# 73590-58-6); (M+H)+	C07324	FindByFormula	5	+	345.1144	11.1288395
OMEPRAZOLE SULFONE (CAS# 88546-55-8); (M	OMEPRAZOLE SULFONE (CAS# 88546-55-8); (M	OMEPRAZOLE SULFONE (CAS# 88546-55-8); (M+H)+ [, tgt	88546-55-8	(362.11728, 2131.4133)(363.11642, 329.07834)(364.11856, 2	OMEPRAZOLE SULFONE (CAS# 88546-55-8); (M+H)+		FindByFormula	6	+	361.1102	12.298663
O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (2	O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (2	O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (2M+H)+ [, tg	17885-08-4	(371.02716, 855.83575)(372.0223, 177.30286)(373.0249, 127	O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (2M+H)+		FindByFormula	7	+	185.0091	0.8814282
O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (M	O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (M	O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (M+Na)+ [, tg	17885-08-4	(207.99864, 994.4133)(209.00233, 259.97336)(209.9994, 175	O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (M+Na)+		FindByFormula	3	+	185.0072	0.8833387
O-PHOSPHOSERINE (CAS# 407-41-0); (M+Na)+	O-PHOSPHOSERINE (CAS# 407-41-0); (M+Na)+	O-PHOSPHOSERINE (CAS# 407-41-0); (M+Na)+ [, tgt=61.3	407-41-0	(207.99796, 1193.0)(209.0045, 126.47)(209.9994, 175.62)	O-PHOSPHOSERINE (CAS# 407-41-0); (M+Na)+		FindByFormula	2	+	185.0072	0.7510048
OPHTHALMIC ACID (CAS# 495-27-2); (M+H)+	OPHTHALMIC ACID (CAS# 495-27-2); (M+H)+	OPHTHALMIC ACID (CAS# 495-27-2); (M+H)+ [, tgt=34.33,	495-27-2	(290.13605, 1338.3821)(291.13525, 309.23746)(292.1283, 14	OPHTHALMIC ACID (CAS# 495-27-2); (M+H)+		FindByFormula	20	+	289.1264	1.1964055
O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5	O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5	O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5); (M+H)+ [,	1492-23-5	(220.08089, 6124.689)(221.08144, 705.05005)(222.08359, 67	O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5); (M+H)+	C01118	FindByFormula	6	+	219.0737	0.740338
OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (	OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (	OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M+2H)+2 [,	27025-41-8	(307.0852, 1925.8469)(307.58527, 507.82874)(308.08514, 28	OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M+2H)+2	C00127	FindByFormula	16	+	612.1569	1.3847575
OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (	OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (	OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M+H)+ [, tg	27025-41-8	(613.1585, 499.3256)(614.1579, 158.82689)(615.15405, 88.8	OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M+H)+	C00127	FindByFormula	16	+	612.1512	1.3712608
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 1205	120595-80-4	(655.1973, 1383.05)(656.2006, 479.29)(657.2072, 164.48)	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (2M+H)+		FindByFormula	1	+	327.0949	2.2550676
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 1205	120595-80-4	(328.10498, 1719.7999)(329.10513, 365.79364)(330.10068, 9	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (M+H)+		FindByFormula	11	+	327.0967	2.257109
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 1205	120595-80-4	(350.08514, 6617.425)(351.09073, 1146.0812)(352.09036, 24	P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (M+Na)+		FindByFormula	16	+	327.096	2.2572649
PALATINOSE (CAS# 343336-76-5); (M+Na)+	PALATINOSE (CAS# 343336-76-5); (M+Na)+	PALATINOSE (CAS# 343336-76-5); (M+Na)+ [, tgt=81.10, o	343336-76-5	(365.1071, 1436.5284)(366.10913, 190.30142)(367.11215, 64	PALATINOSE (CAS# 343336-76-5); (M+Na)+		FindByFormula	14	+	342.1191	0.716929
PALMITOYLCARNITINE (CAS# 2364-67-2); (M+	PALMITOYLCARNITINE (CAS# 2364-67-2); (M+	PALMITOYLCARNITINE (CAS# 2364-67-2); (M+H)+ [, tgt=6	2364-67-2	(400.3415, 6855.297)(401.34146, 1867.814)(402.3475, 1020.	PALMITOYLCARNITINE (CAS# 2364-67-2); (M+H)+	C02990	FindByFormula	26	+	399.335	21.36389
PALMITOYLCARNITINE (CAS# 2364-67-2); (M+	PALMITOYLCARNITINE (CAS# 2364-67-2); (M+	PALMITOYLCARNITINE (CAS# 2364-67-2); (M+Na)+ [, tgt=	2364-67-2	(422.32297, 5548.687)(423.3243, 1593.5911)(424.32635, 528	PALMITOYLCARNITINE (CAS# 2364-67-2); (M+Na)+	C02990	FindByFormula	25	+	399.3346	21.359108
PANTOTHENATE (CAS# 79-83-4); (M+H)+	PANTOTHENATE (CAS# 79-83-4); (M+H)+	PANTOTHENATE (CAS# 79-83-4); (M+H)+ [, tgt=71.03, ove	79-83-4	(220.1186, 5143.5156)(221.11902, 665.43555)(222.11464, 96	PANTOTHENATE (CAS# 79-83-4); (M+H)+	C02349	FindByFormula	20	+	219.1106	3.2639565
PANTOTHENATE (CAS# 79-83-4); (M+Na)+	PANTOTHENATE (CAS# 79-83-4); (M+Na)+	PANTOTHENATE (CAS# 79-83-4); (M+Na)+ [, tgt=87.89, o	79-83-4	(242.10051, 5123.531)(243.10226, 605.4684)(244.09662, 417	PANTOTHENATE (CAS# 79-83-4); (M+Na)+	C02349	FindByFormula	25	+	219.1116	3.2632458
PARAXANTHINE (CAS# 611-59-6); (M+H)+	PARAXANTHINE (CAS# 611-59-6); (M+H)+	PARAXANTHINE (CAS# 611-59-6); (M+H)+ [, tgt=82.39, ov	611-59-6	(181.07289, 16202.633)(182.07668, 2006.3063)(183.08765, 1	PARAXANTHINE (CAS# 611-59-6); (M+H)+	C13747	FindByFormula	19	+	180.066	4.2879405
PARAXANTHINE (CAS# 611-59-6); (M+Na)+	PARAXANTHINE (CAS# 611-59-6); (M+Na)+	PARAXANTHINE (CAS# 611-59-6); (M+Na)+ [, tgt=89.17, o	611-59-6	(203.05453, 5345.0435)(204.05827, 638.5138)(205.06213, 57	PARAXANTHINE (CAS# 611-59-6); (M+Na)+	C13747	FindByFormula	18	+	180.0658	4.420745
PHENYL ACETATE (CAS# 122-79-2); (M+H)+	PHENYL ACETATE (CAS# 122-79-2); (M+H)+	PHENYL ACETATE (CAS# 122-79-2); (M+H)+ [, tgt=39.47, o	122-79-2	(137.0633, 2419.76)(138.0568, 1112.515)	PHENYL ACETATE (CAS# 122-79-2); (M+H)+	C00548	FindByFormula	2	+	136.0531	3.9150338
PHENYLACETIC ACID (CAS# 103-82-2); (M+H)+	PHENYLACETIC ACID (CAS# 103-82-2); (M+H)+	PHENYLACETIC ACID (CAS# 103-82-2); (M+H)+ [, tgt=64.8	103-82-2	(137.0633, 2419.76)(138.0568, 1112.515)	PHENYLACETIC ACID (CAS# 103-82-2); (M+H)+	C07086	FindByFormula	2	+	136.0531	3.9150338
PHENYLALANINE (CAS# 63-91-2); (M+H)+	PHENYLALANINE (CAS# 63-91-2); (M+H)+	PHENYLALANINE (CAS# 63-91-2); (M+H)+ [, tgt=94.40, ov	63-91-2	(166.08656, 721051.06)(167.08974, 73820.266)(168.09183, 6	PHENYLALANINE (CAS# 63-91-2); (M+H)+	C00079	FindByFormula	28	+	165.0792	2.5183146
PHENYLALANINE (CAS# 63-91-2); (M+Na)+	PHENYLALANINE (CAS# 63-91-2); (M+Na)+	PHENYLALANINE (CAS# 63-91-2); (M+Na)+ [, tgt=94.48, o	63-91-2	(188.06851, 32711.28)(189.07152, 3625.2378)(190.07394, 26	PHENYLALANINE (CAS# 63-91-2); (M+Na)+	C00079	FindByFormula	28	+	165.0793	2.519279
PHENYLEPHRINE (CAS# 59-42-7); (M+H)+	PHENYLEPHRINE (CAS# 59-42-7); (M+H)+	PHENYLEPHRINE (CAS# 59-42-7); (M+H)+ [, tgt=46.87, ov	59-42-7	(168.10255, 1268.21)(169.10126, 111.505005)(170.1103, 20.	PHENYLEPHRINE (CAS# 59-42-7); (M+H)+	C07441	FindByFormula	4	+	167.0954	1.0457554
PHTHALATE (CAS# 88-99-3); (M+Na)+	PHTHALATE (CAS# 88-99-3); (M+Na)+	PHTHALATE (CAS# 88-99-3); (M+Na)+ [, tgt=67.62, overall	88-99-3	(189.01689, 1007.68994)(190.01497, 49.806667)	PHTHALATE (CAS# 88-99-3); (M+Na)+	C01606	FindByFormula	3	+	166.0282	4.846525
PICOLINIC ACID (CAS# 98-98-6); (M+H)+	PICOLINIC ACID (CAS# 98-98-6); (M+H)+	PICOLINIC ACID (CAS# 98-98-6); (M+H)+ [, tgt=59.10, over	98-98-6	(124.0399, 2026.178)(125.03835, 262.85797)	PICOLINIC ACID (CAS# 98-98-6); (M+H)+		FindByFormula	5	+	123.0331	1.0490007
PINITOL (CAS# 10284-63-6); (M+Na)+	PINITOL (CAS# 10284-63-6); (M+Na)+	PINITOL (CAS# 10284-63-6); (M+Na)+ [, tgt=38.98, overall	10284-63-6	(217.0688, 529.5)(218.067, 103.62)	PINITOL (CAS# 10284-63-6); (M+Na)+	C03844	FindByFormula	1	+	194.0787	0.8309938
PIPECOLATE (CAS# 535-75-1); (M+H)+	PIPECOLATE (CAS# 535-75-1); (M+H)+	PIPECOLATE (CAS# 535-75-1); (M+H)+ [, tgt=78.86, overal	535-75-1	(130.08641, 11601.022)(131.08778, 791.8501)(132.0865, 474	PIPECOLATE (CAS# 535-75-1); (M+H)+	C00408	FindByFormula	27	+	129.0786	0.70585334
PIPECOLATE (CAS# 535-75-1); (M+Na)+	PIPECOLATE (CAS# 535-75-1); (M+Na)+	PIPECOLATE (CAS# 535-75-1); (M+Na)+ [, tgt=58.23, overa	535-75-1	(152.0695, 16454.5)(153.0723, 1367.53)(154.0721, 2155.84)	PIPECOLATE (CAS# 535-75-1); (M+Na)+	C00408	FindByFormula	1	+	129.08	0.7929973
PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 11	PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 11	PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M	1190-94-9	(163.10785, 4278.035)(164.11044, 263.0)	PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M+H)+	C01211	FindByFormula	2	+	162.102	0.7499975
PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 11	PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 11	PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M	1190-94-9	(145.1008, 1039.02)(146.0949, 734.99)	PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M+H)+[-	C01211	FindByFormula	1	+	162.1005	0.8059941
PROGESTERONE (CAS# 57-83-0); (M+H)+	PROGESTERONE (CAS# 57-83-0); (M+H)+	PROGESTERONE (CAS# 57-83-0); (M+H)+ [, tgt=25.26, ove	57-83-0	(315.22974, 1545.0125)(316.2309, 416.7775)	PROGESTERONE (CAS# 57-83-0); (M+H)+		FindByFormula	4	+	314.2218	19.79762
PROLINE (CAS# 147-85-3); (M+H)+	PROLINE (CAS# 147-85-3); (M+H)+	PROLINE (CAS# 147-85-3); (M+H)+ [, tgt=87.97, overall=8	147-85-3	(116.07061, 65044.22)(117.07139, 4139.165)(118.0771, 29.8	PROLINE (CAS# 147-85-3); (M+H)+		FindByFormula	27	+	115.0629	0.617186
PROLINE (CAS# 147-85-3); (M+Na)+	PROLINE (CAS# 147-85-3); (M+Na)+	PROLINE (CAS# 147-85-3); (M+Na)+ [, tgt=84.53, overall=	147-85-3	(138.05319, 10546.97)(139.05533, 992.5633)	PROLINE (CAS# 147-85-3); (M+Na)+		FindByFormula	3	+	115.0644	0.7003324
PROMETRYN (CAS# 7287-19-6); (M+H)+	PROMETRYN (CAS# 7287-19-6); (M+H)+	PROMETRYN (CAS# 7287-19-6); (M+H)+ [, tgt=22.83, over	7287-19-6	(242.14467, 1047.5057)(243.14136, 196.12917)(244.1392, 37	PROMETRYN (CAS# 7287-19-6); (M+H)+		FindByFormula	12	+	241.1367	15.559841
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+ [, tgt=44.4	363-24-6	(353.2291, 4443.9424)(354.2313, 951.4055)(355.22986, 215.	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+		FindByFormula	9	+	352.2215	16.911491
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+[-H2O] [, tg	363-24-6	(335.21796, 1906.935)(336.21945, 354.065)(337.22034, 561.	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+[-H2O]		FindByFormula	2	+	352.2216	16.828516
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Na	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Na)	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Na)+ [, tgt=73.	363-24-6	(375.2135, 3383.215)(376.21536, 787.7322)(377.21082, 333.	PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Na)+		FindByFormula	18	+	352.2236	16.744904
PROTOPORPHYRIN (CAS# 553-12-8); (M+H)+	PROTOPORPHYRIN (CAS# 553-12-8); (M+H)+	PROTOPORPHYRIN (CAS# 553-12-8); (M+H)+ [, tgt=55.71,	553-12-8	(563.26636, 550.4125)(564.2729, 242.25125)(565.264, 247.1	PROTOPORPHYRIN (CAS# 553-12-8); (M+H)+	C02191	FindByFormula	8	+	562.2576	22.901775
PTERIN (CAS# 2236-60-4); (M+H)+	PTERIN (CAS# 2236-60-4); (M+H)+	PTERIN (CAS# 2236-60-4); (M+H)+ [, tgt=53.66, overall=5	2236-60-4	(164.05644, 2831.8408)(165.05597, 139.64888)	PTERIN (CAS# 2236-60-4); (M+H)+	C00715	FindByFormula	9	+	163.0491	1.7185721
PURINE (CAS# 120-73-0); (M+H)+	PURINE (CAS# 120-73-0); (M+H)+	PURINE (CAS# 120-73-0); (M+H)+ [, tgt=61.29, overall=61.	120-73-0	(121.050835, 2836.49)(122.05765, 280.19165)	PURINE (CAS# 120-73-0); (M+H)+	C00465	FindByFormula	6	+	120.044	1.3070091
PURINE (CAS# 120-73-0); (M+Na)+	PURINE (CAS# 120-73-0); (M+Na)+	PURINE (CAS# 120-73-0); (M+Na)+ [, tgt=55.00, overall=5	120-73-0	(143.03247, 1500.6967)(144.0332, 93.28333)	PURINE (CAS# 120-73-0); (M+Na)+	C00465	FindByFormula	3	+	120.0436	1.1013396
PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9)	PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9);	PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M+H)+[-H	89-00-9	(150.0187, 659.35)(151.0125, 49.75)	PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M+H)+[-H2O]		FindByFormula	1	+	167.0213	0.77500045
PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9)	PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9);	PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M+Na)+ [	89-00-9	(190.01201, 3738.6501)(191.01343, 287.42)(192.0116, 268.9	PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M+Na)+		FindByFormula	3	+	167.0233	0.92067
PYRIDOXAL (CAS# 66-72-8); (M+H)+	PYRIDOXAL (CAS# 66-72-8); (M+H)+	PYRIDOXAL (CAS# 66-72-8); (M+H)+ [, tgt=52.23, overall=	66-72-8	(168.06474, 1125.9484)(169.06549, 116.4275)	PYRIDOXAL (CAS# 66-72-8); (M+H)+	C00250	FindByFormula	12	+	167.0571	1.7787753
PYRIDOXAL (CAS# 66-72-8); (M+H)+[-H2O]	PYRIDOXAL (CAS# 66-72-8); (M+H)+[-H2O]	PYRIDOXAL (CAS# 66-72-8); (M+H)+[-H2O] [, tgt=50.37, o	66-72-8	(150.05548, 2794.15)(151.05753, 329.75)(152.0574, 6828.0)	PYRIDOXAL (CAS# 66-72-8); (M+H)+[-H2O]	C00250	FindByFormula	5	+	167.0595	1.6266029
PYRIDOXAL PHOSPHATE (CAS# 853645-22-4);	PYRIDOXAL PHOSPHATE (CAS# 853645-22-4); (	PYRIDOXAL PHOSPHATE (CAS# 853645-22-4); (2M+H)+ [,	853645-22-4	(495.06052, 726.6125)(496.05756, 321.39)(497.0531, 176.18	PYRIDOXAL PHOSPHATE (CAS# 853645-22-4); (2M+H)+		FindByFormula	4	+	247.0257	1.0135002
PYRIDOXINE (CAS# 65-23-6); (M+H)+	PYRIDOXINE (CAS# 65-23-6); (M+H)+	PYRIDOXINE (CAS# 65-23-6); (M+H)+ [, tgt=75.30, overall=	65-23-6	(170.0829, 1194.92)(171.085, 188.53)	PYRIDOXINE (CAS# 65-23-6); (M+H)+	C00314	FindByFormula	1	+	169.0754	1.1000023
QUINOLIN-2-OL (CAS# 59-31-4); (M+H)+	QUINOLIN-2-OL (CAS# 59-31-4); (M+H)+	QUINOLIN-2-OL (CAS# 59-31-4); (M+H)+ [, tgt=73.99, over	59-31-4	(146.06097, 1331.4535)(147.05814, 200.08601)	QUINOLIN-2-OL (CAS# 59-31-4); (M+H)+	C06338	FindByFormula	20	+	145.0528	7.6353836
QUINOLIN-2-OL (CAS# 59-31-4); (M+Na)+	QUINOLIN-2-OL (CAS# 59-31-4); (M+Na)+	QUINOLIN-2-OL (CAS# 59-31-4); (M+Na)+ [, tgt=60.55, ov	59-31-4	(168.04274, 1873.3732)(169.04207, 298.61282)(170.0426, 24	QUINOLIN-2-OL (CAS# 59-31-4); (M+Na)+	C06338	FindByFormula	25	+	145.0529	7.634779
RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-	RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-	RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-6); (M+Na)-	75685-84-6	(325.23547, 6151.9736)(326.23514, 1083.576)(327.22897, 72	RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-6); (M+Na)+		FindByFormula	26	+	302.244	22.181711
RAFFINOSE (CAS# 512-69-6); (M+K)+	RAFFINOSE (CAS# 512-69-6); (M+K)+	RAFFINOSE (CAS# 512-69-6); (M+K)+ [, tgt=70.60, overall=	512-69-6	(543.1347, 667.57623)(544.1355, 171.31749)(545.1315, 99.5	RAFFINOSE (CAS# 512-69-6); (M+K)+	C00492	FindByFormula	16	+	504.172	0.72343963
RAFFINOSE (CAS# 512-69-6); (M+Na)+	RAFFINOSE (CAS# 512-69-6); (M+Na)+	RAFFINOSE (CAS# 512-69-6); (M+Na)+ [, tgt=76.60, overal	512-69-6	(527.1605, 3406.7612)(528.1653, 772.09875)(529.1637, 244.	RAFFINOSE (CAS# 512-69-6); (M+Na)+	C00492	FindByFormula	16	+	504.1731	0.7233763
RIBOFLAVIN (CAS# 83-88-5); (M+H)+	RIBOFLAVIN (CAS# 83-88-5); (M+H)+	RIBOFLAVIN (CAS# 83-88-5); (M+H)+ [, tgt=56.78, overall=	83-88-5	(377.1478, 746.0178)(378.1467, 145.39444)(379.14288, 41.2	RIBOFLAVIN (CAS# 83-88-5); (M+H)+		FindByFormula	9	+	376.1418	7.581358
RIBOFLAVIN (CAS# 83-88-5); (M+Na)+	RIBOFLAVIN (CAS# 83-88-5); (M+Na)+	RIBOFLAVIN (CAS# 83-88-5); (M+Na)+ [, tgt=77.40, overal	83-88-5	(399.12918, 897.5406)(400.12997, 197.0311)(401.13168, 70.	RIBOFLAVIN (CAS# 83-88-5); (M+Na)+		FindByFormula	18	+	376.1417	7.5772915
RIBOSE (CAS# 50-69-1); (M+Na)+	RIBOSE (CAS# 50-69-1); (M+Na)+	RIBOSE (CAS# 50-69-1); (M+Na)+ [, tgt=72.74, overall=72.	50-69-1	(173.04222, 14187.223)(174.04117, 1619.8125)(175.0391, 69	RIBOSE (CAS# 50-69-1); (M+Na)+	C00121	FindByFormula	4	+	150.0531	0.91000307
S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-	S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-	S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-0); (M+H)+	979-92-0	(385.1297, 2344.0334)(386.1296, 421.25848)(387.12445, 207	S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-0); (M+H)+	C00021	FindByFormula	26	+	384.1224	1.5346624
SALICYLAMIDE (CAS# 65-45-2); (M+H)+	SALICYLAMIDE (CAS# 65-45-2); (M+H)+	SALICYLAMIDE (CAS# 65-45-2); (M+H)+ [, tgt=53.02, overa	65-45-2	(138.055, 780.89)(139.0641, 126.53)	SALICYLAMIDE (CAS# 65-45-2); (M+H)+		FindByFormula	1	+	137.0486	5.268
SALICYLURIC ACID (CAS# 487-54-7); (M+Na)+	SALICYLURIC ACID (CAS# 487-54-7); (M+Na)+	SALICYLURIC ACID (CAS# 487-54-7); (M+Na)+ [, tgt=63.86,	487-54-7	(218.04373, 1367.6521)(219.04337, 173.86398)	SALICYLURIC ACID (CAS# 487-54-7); (M+Na)+	C07588	FindByFormula	5	+	195.0548	6.1940846
SARCOSINE (CAS# 107-97-1); (M+H)+	SARCOSINE (CAS# 107-97-1); (M+H)+	SARCOSINE (CAS# 107-97-1); (M+H)+ [, tgt=88.46, overall	107-97-1	(90.05532, 2221.007)(91.05602, 66.617)	SARCOSINE (CAS# 107-97-1); (M+H)+	C00213	FindByFormula	10	+	89.048	0.67180026
SELENOCYSTAMINE (CAS# 2697-61-2); (M+H)	SELENOCYSTAMINE (CAS# 2697-61-2); (M+H)+	SELENOCYSTAMINE (CAS# 2697-61-2); (M+H)+ [, tgt=64.9	2697-61-2	(247.9401, 580.115)(248.93875, 181.83499)(249.93774, 948.	SELENOCYSTAMINE (CAS# 2697-61-2); (M+H)+		FindByFormula	2	+	247.9317	0.54850125
SERINE (CAS# 56-45-1); (M+H)+	SERINE (CAS# 56-45-1); (M+H)+	SERINE (CAS# 56-45-1); (M+H)+ [, tgt=80.04, overall=80.0	56-45-1	(106.0503, 1030.2699)(107.04927, 52.28643)	SERINE (CAS# 56-45-1); (M+H)+	C00065	FindByFormula	14	+	105.0434	1.0002174
SEROTONIN (CAS# 50-67-9); (M+H)+	SEROTONIN (CAS# 50-67-9); (M+H)+	SEROTONIN (CAS# 50-67-9); (M+H)+ [, tgt=80.84, overall=	50-67-9	(177.10342, 9302.439)(178.10648, 1224.0325)(179.1041, 70.	SEROTONIN (CAS# 50-67-9); (M+H)+	C00780	FindByFormula	4	+	176.0959	1.6822537
SEROTONIN (CAS# 50-67-9); (M+Na)+	SEROTONIN (CAS# 50-67-9); (M+Na)+	SEROTONIN (CAS# 50-67-9); (M+Na)+ [, tgt=49.19, overal	50-67-9	(199.08337, 1637.4473)(200.0836, 228.2443)	SEROTONIN (CAS# 50-67-9); (M+Na)+	C00780	FindByFormula	7	+	176.0936	1.6418661
SHIKIMATE (CAS# 138-59-0); (M+H)+[-H2O]	SHIKIMATE (CAS# 138-59-0); (M+H)+[-H2O]	SHIKIMATE (CAS# 138-59-0); (M+H)+[-H2O] [, tgt=51.10, c	138-59-0	(157.04985, 1123.615)(158.04971, 116.165)	SHIKIMATE (CAS# 138-59-0); (M+H)+[-H2O]	C00493	FindByFormula	2	+	174.0512	1.1549997
SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 2831	SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 2831	SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (M	28319-77-9	(258.11142, 23743.465)(259.11456, 2420.7312)(260.11386, 4	SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (M+H)+	C00670	FindByFormula	8	+	257.1041	0.64925
SPERMIDINE (CAS# 124-20-9); (M+H)+	SPERMIDINE (CAS# 124-20-9); (M+H)+	SPERMIDINE (CAS# 124-20-9); (M+H)+ [, tgt=88.54, overal	124-20-9	(146.1651, 56437.496)(147.16617, 5533.18)(148.16664, 241.	SPERMIDINE (CAS# 124-20-9); (M+H)+		FindByFormula	22	+	145.1577	0.52922845
SPERMINE (CAS# 71-44-3); (M+H)+	SPERMINE (CAS# 71-44-3); (M+H)+	SPERMINE (CAS# 71-44-3); (M+H)+ [, tgt=80.40, overall=8	71-44-3	(203.22305, 25630.225)(204.2253, 3238.8044)(205.229, 317.	SPERMINE (CAS# 71-44-3); (M+H)+		FindByFormula	19	+	202.216	0.5965285
SPHINGANINE (CAS# 764-22-7); (M+H)+	SPHINGANINE (CAS# 764-22-7); (M+H)+	SPHINGANINE (CAS# 764-22-7); (M+H)+ [, tgt=48.18, over	764-22-7	(302.3042, 2090.475)(303.30655, 462.94696)(304.3045, 111.	SPHINGANINE (CAS# 764-22-7); (M+H)+	C00836	FindByFormula	20	+	301.2968	21.003176
SPHINGANINE (CAS# 764-22-7); (M+Na)+	SPHINGANINE (CAS# 764-22-7); (M+Na)+	SPHINGANINE (CAS# 764-22-7); (M+Na)+ [, tgt=47.10, ov	764-22-7	(324.2862, 5572.0166)(325.2843, 1207.0353)(326.2838, 181.	SPHINGANINE (CAS# 764-22-7); (M+Na)+	C00836	FindByFormula	13	+	301.2958	21.054382
SQUALENE (CAS# 111-02-4); (M+K)+	SQUALENE (CAS# 111-02-4); (M+K)+	SQUALENE (CAS# 111-02-4); (M+K)+ [, tgt=31.51, overall=	111-02-4	(449.35703, 641.0375)(450.35944, 117.8875)(451.3471, 142.	SQUALENE (CAS# 111-02-4); (M+K)+		FindByFormula	4	+	410.3927	24.40785
STACHYOSE (CAS# 54261-98-2); (M+K)+	STACHYOSE (CAS# 54261-98-2); (M+K)+	STACHYOSE (CAS# 54261-98-2); (M+K)+ [, tgt=88.07, over	54261-98-2	(705.1857, 387.3663)(706.18634, 122.110535)(707.18115, 66	STACHYOSE (CAS# 54261-98-2); (M+K)+		FindByFormula	19	+	666.2214	0.7275285
STACHYOSE (CAS# 54261-98-2); (M+Na)+	STACHYOSE (CAS# 54261-98-2); (M+Na)+	STACHYOSE (CAS# 54261-98-2); (M+Na)+ [, tgt=54.47, ov	54261-98-2	(689.2122, 1556.6698)(690.21674, 480.5439)(691.21857, 177	STACHYOSE (CAS# 54261-98-2); (M+Na)+		FindByFormula	23	+	666.223	0.7260456
SUBERIC ACID (CAS# 505-48-6); (M+H)+[-H2O]	SUBERIC ACID (CAS# 505-48-6); (M+H)+[-H2O]	SUBERIC ACID (CAS# 505-48-6); (M+H)+[-H2O] [, tgt=76.1	505-48-6	(157.0854, 1282.27)(158.0789, 32.29)	SUBERIC ACID (CAS# 505-48-6); (M+H)+[-H2O]	C08278	FindByFormula	1	+	174.0885	8.193285
SUBERIC ACID (CAS# 505-48-6); (M+Na)+	SUBERIC ACID (CAS# 505-48-6); (M+Na)+	SUBERIC ACID (CAS# 505-48-6); (M+Na)+ [, tgt=81.61, ove	505-48-6	(197.0795, 4179.7544)(198.08083, 350.5741)(199.08119, 167	SUBERIC ACID (CAS# 505-48-6); (M+Na)+	C08278	FindByFormula	22	+	174.0908	8.212016
SUCROSE (CAS# 57-50-1); (M+Na)+	SUCROSE (CAS# 57-50-1); (M+Na)+	SUCROSE (CAS# 57-50-1); (M+Na)+ [, tgt=80.41, overall=8	57-50-1	(365.1071, 1436.5284)(366.10913, 190.30142)(367.11215, 64	SUCROSE (CAS# 57-50-1); (M+Na)+	C00089	FindByFormula	14	+	342.1189	0.716929
SULFADIMETHOXINE (CAS# 122-11-2); (M+Na	SULFADIMETHOXINE (CAS# 122-11-2); (M+Na	SULFADIMETHOXINE (CAS# 122-11-2); (M+Na)+ [, tgt=90.	122-11-2	(333.0641, 2382.22)(334.0684, 426.48)(335.0642, 200.26)(33	SULFADIMETHOXINE (CAS# 122-11-2); (M+Na)+		FindByFormula	1	+	310.0752	9.299706
TAURINE (CAS# 107-35-7); (M+H)+	TAURINE (CAS# 107-35-7); (M+H)+	TAURINE (CAS# 107-35-7); (M+H)+ [, tgt=40.13, overall=4	107-35-7	(126.022285, 20096.432)(127.025375, 730.7214)(128.02411,	TAURINE (CAS# 107-35-7); (M+H)+		FindByFormula	7	+	125.015	0.67314404
TAURINE (CAS# 107-35-7); (M+K)+	TAURINE (CAS# 107-35-7); (M+K)+	TAURINE (CAS# 107-35-7); (M+K)+ [, tgt=47.14, overall=4	107-35-7	(163.97743, 4516.4717)(164.97737, 256.21664)(165.97824, 6	TAURINE (CAS# 107-35-7); (M+K)+		FindByFormula	15	+	125.0137	0.57993394
TAURINE (CAS# 107-35-7); (M+Na)+	TAURINE (CAS# 107-35-7); (M+Na)+	TAURINE (CAS# 107-35-7); (M+Na)+ [, tgt=67.21, overall=	107-35-7	(148.0042, 18053.125)(149.0064, 686.58105)(150.00385, 203	TAURINE (CAS# 107-35-7); (M+Na)+		FindByFormula	19	+	125.0158	0.6321594
TAUROCHENODEOXYCHOLATE (CAS# 516-35-	TAUROCHENODEOXYCHOLATE (CAS# 516-35-	TAUROCHENODEOXYCHOLATE (CAS# 516-35-8); (M+Na)+	516-35-8	(522.2936, 400.62)(523.2877, 416.07)	TAUROCHENODEOXYCHOLATE (CAS# 516-35-8); (M+Na)+		FindByFormula	1	+	499.2997	19.941133
TAUROLITHOCHOLATE (CAS# 516-90-5); (M+	TAUROLITHOCHOLATE (CAS# 516-90-5); (M+H	TAUROLITHOCHOLATE (CAS# 516-90-5); (M+H)+[-H2O] [,	516-90-5	(466.3117, 303.63)(467.2992, 625.09)(468.3074, 146.78)	TAUROLITHOCHOLATE (CAS# 516-90-5); (M+H)+[-H2O]	C02592	FindByFormula	1	+	483.3051	22.093845
TERBINAFINE (CAS# 91161-71-6); (M+H)+	TERBINAFINE (CAS# 91161-71-6); (M+H)+	TERBINAFINE (CAS# 91161-71-6); (M+H)+ [, tgt=43.38, ov	91161-71-6	(292.20517, 5259.275)(293.20413, 1224.5917)(294.20743, 17	TERBINAFINE (CAS# 91161-71-6); (M+H)+	C08079	FindByFormula	6	+	291.1989	15.42543
THEOBROMINE (CAS# 83-67-0); (M+H)+	THEOBROMINE (CAS# 83-67-0); (M+H)+	THEOBROMINE (CAS# 83-67-0); (M+H)+ [, tgt=96.12, over	83-67-0	(181.07289, 29840.541)(182.07578, 2908.3743)(183.07701, 3	THEOBROMINE (CAS# 83-67-0); (M+H)+	C07480	FindByFormula	20	+	180.0655	3.483377
THEOBROMINE (CAS# 83-67-0); (M+Na)+	THEOBROMINE (CAS# 83-67-0); (M+Na)+	THEOBROMINE (CAS# 83-67-0); (M+Na)+ [, tgt=91.73, ov	83-67-0	(203.05315, 4060.324)(204.05615, 422.57303)(205.0562, 141	THEOBROMINE (CAS# 83-67-0); (M+Na)+	C07480	FindByFormula	13	+	180.0646	3.4573026
THEOPHYLLINE (CAS# 58-55-9); (M+H)+	THEOPHYLLINE (CAS# 58-55-9); (M+H)+	THEOPHYLLINE (CAS# 58-55-9); (M+H)+ [, tgt=76.17, over	58-55-9	(181.07288, 16258.382)(182.07664, 2008.4294)(183.08765, 1	THEOPHYLLINE (CAS# 58-55-9); (M+H)+	C07130	FindByFormula	19	+	180.066	4.2879405
THEOPHYLLINE (CAS# 58-55-9); (M+Na)+	THEOPHYLLINE (CAS# 58-55-9); (M+Na)+	THEOPHYLLINE (CAS# 58-55-9); (M+Na)+ [, tgt=86.25, ove	58-55-9	(203.0545, 5407.559)(204.05817, 643.0289)(205.06128, 55.5	THEOPHYLLINE (CAS# 58-55-9); (M+Na)+	C07130	FindByFormula	18	+	180.0655	4.420745
THREONINE (CAS# 72-19-5); (M+H)+[-H2O]	THREONINE (CAS# 72-19-5); (M+H)+[-H2O]	THREONINE (CAS# 72-19-5); (M+H)+[-H2O] [, tgt=74.88, o	72-19-5	(102.055305, 1418.679)(103.05322, 56.498005)	THREONINE (CAS# 72-19-5); (M+H)+[-H2O]	C00188	FindByFormula	20	+	119.0581	0.99815243
THROMBOXANE B2 (CAS# 54397-85-2); (M+H	THROMBOXANE B2 (CAS# 54397-85-2); (M+H)	THROMBOXANE B2 (CAS# 54397-85-2); (M+H)+[-H2O] [, t	54397-85-2	(353.22885, 3941.9739)(354.2312, 803.6364)(355.2318, 194.	THROMBOXANE B2 (CAS# 54397-85-2); (M+H)+[-H2O]	C05963	FindByFormula	14	+	370.2321	16.905521
THYMIDINE (CAS# 50-89-5); (M+Na)+	THYMIDINE (CAS# 50-89-5); (M+Na)+	THYMIDINE (CAS# 50-89-5); (M+Na)+ [, tgt=63.51, overall	50-89-5	(265.0807, 838.4533)(266.0782, 124.09333)(267.0779, 135.0	THYMIDINE (CAS# 50-89-5); (M+Na)+	C00214	FindByFormula	9	+	242.0917	2.747586
THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-(	THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-(	THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-07-1); (2M+	365-07-1	(645.1217, 234.62)(646.1154, 68.74)	THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-07-1); (2M+H)+	C00364	FindByFormula	1	+	322.0557	1.3119878
THYMINE (CAS# 65-71-4); (M+H)+	THYMINE (CAS# 65-71-4); (M+H)+	THYMINE (CAS# 65-71-4); (M+H)+ [, tgt=82.77, overall=82	65-71-4	(127.050575, 1225.1199)(128.05267, 114.2575)	THYMINE (CAS# 65-71-4); (M+H)+		FindByFormula	4	+	126.0437	1.723011
THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#)	THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#)	THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#); (M+H)+ [, tgt=89.37, overall=89.37]		(131.076, 120896.41)(132.0847, 2291.04)(133.0806, 504.97)	THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#); (M+H)+		FindByFormula	1	+	130.0688	1.6930073
THYROTROPIN RELEASING HORMONE (CAS# 2	THYROTROPIN RELEASING HORMONE (CAS# 2	THYROTROPIN RELEASING HORMONE (CAS# 24305-27-9);	24305-27-9	(385.162, 793.11)(386.1531, 323.36)	THYROTROPIN RELEASING HORMONE (CAS# 24305-27-9); (M+Na)+		FindByFormula	1	+	362.1694	1.6160349
THYROXINE (CAS# 51-48-9); (M+H)+	THYROXINE (CAS# 51-48-9); (M+H)+	THYROXINE (CAS# 51-48-9); (M+H)+ [, tgt=85.16, overall=	51-48-9	(777.6956, 1021.50665)(778.6922, 140.9)(779.6899, 58.6375)	THYROXINE (CAS# 51-48-9); (M+H)+	C01829	FindByFormula	6	+	776.6899	16.162603
TRANS-4-HYDROXYPROLINE (CAS# 51-35-4); (	TRANS-4-HYDROXYPROLINE (CAS# 51-35-4); (M	TRANS-4-HYDROXYPROLINE (CAS# 51-35-4); (M+H)+ [, tgt	51-35-4	(132.06696, 10858.069)(133.06458, 801.6425)(134.0635, 74.	TRANS-4-HYDROXYPROLINE (CAS# 51-35-4); (M+H)+	C01015	FindByFormula	4	+	131.0586	0.7009997
TRANS-ACONITATE (CAS# 4023-65-8); (M+Na	TRANS-ACONITATE (CAS# 4023-65-8); (M+Na)	TRANS-ACONITATE (CAS# 4023-65-8); (M+Na)+ [, tgt=80.	4023-65-8	(197.0053, 564.49)(198.0183, 37.47)	TRANS-ACONITATE (CAS# 4023-65-8); (M+Na)+	C02341	FindByFormula	1	+	174.0167	1.1500014
TRANS-CYCLOHEXANE-1,2-DIOL (CAS# 1460-5	TRANS-CYCLOHEXANE-1,2-DIOL (CAS# 1460-57	TRANS-CYCLOHEXANE-1,2-DIOL (CAS# 1460-57-7); (M+Na	1460-57-7	(139.0732, 117186.69)(140.07272, 17640.928)(141.06987, 71	TRANS-CYCLOHEXANE-1,2-DIOL (CAS# 1460-57-7); (M+Na)+	C03739	FindByFormula	6	+	116.0834	3.7495482
TRICARBALLYLIC ACID (CAS# 99-14-9); (M+H)+	TRICARBALLYLIC ACID (CAS# 99-14-9); (M+H)+	TRICARBALLYLIC ACID (CAS# 99-14-9); (M+H)+[-H2O] [, tg	99-14-9	(159.02881, 74990.17)(160.03096, 5201.3857)(161.031, 2322	TRICARBALLYLIC ACID (CAS# 99-14-9); (M+H)+[-H2O]		FindByFormula	19	+	176.0323	1.1144787
TRICARBALLYLIC ACID (CAS# 99-14-9); (M+Na	TRICARBALLYLIC ACID (CAS# 99-14-9); (M+Na)	TRICARBALLYLIC ACID (CAS# 99-14-9); (M+Na)+ [, tgt=48.	99-14-9	(199.02327, 896.3743)(200.02238, 208.40428)	TRICARBALLYLIC ACID (CAS# 99-14-9); (M+Na)+		FindByFormula	7	+	176.0337	1.0325733
TRYPTOPHAN (CAS# 73-22-3); (M+H)+	TRYPTOPHAN (CAS# 73-22-3); (M+H)+	TRYPTOPHAN (CAS# 73-22-3); (M+H)+ [, tgt=71.36, overal	73-22-3	(205.09746, 688093.94)(206.09999, 89091.81)(207.09303, 94	TRYPTOPHAN (CAS# 73-22-3); (M+H)+		FindByFormula	11	+	204.0895	3.6086106
TRYPTOPHAN (CAS# 73-22-3); (M+Na)+	TRYPTOPHAN (CAS# 73-22-3); (M+Na)+	TRYPTOPHAN (CAS# 73-22-3); (M+Na)+ [, tgt=71.66, overa	73-22-3	(227.07973, 53671.41)(228.08235, 7200.0664)(229.07516, 80	TRYPTOPHAN (CAS# 73-22-3); (M+Na)+		FindByFormula	12	+	204.0895	3.6104844
TYROSINE (CAS# 60-18-4); (M+H)+	TYROSINE (CAS# 60-18-4); (M+H)+	TYROSINE (CAS# 60-18-4); (M+H)+ [, tgt=95.90, overall=9	60-18-4	(182.08185, 424699.4)(183.0849, 43012.703)(184.08398, 575	TYROSINE (CAS# 60-18-4); (M+H)+		FindByFormula	25	+	181.0742	1.3355657
TYROSINE (CAS# 60-18-4); (M+Na)+	TYROSINE (CAS# 60-18-4); (M+Na)+	TYROSINE (CAS# 60-18-4); (M+Na)+ [, tgt=83.09, overall=	60-18-4	(204.06407, 6315.3496)(205.06682, 775.91394)(206.054, 878	TYROSINE (CAS# 60-18-4); (M+Na)+		FindByFormula	15	+	181.0749	1.333207
URACIL (CAS# 66-22-8); (M+H)+	URACIL (CAS# 66-22-8); (M+H)+	URACIL (CAS# 66-22-8); (M+H)+ [, tgt=72.23, overall=72.2	66-22-8	(113.03505, 6722.6772)(114.03825, 161.67714)(115.039665,	URACIL (CAS# 66-22-8); (M+H)+		FindByFormula	7	+	112.0281	0.9624282
URACIL 5-CARBOXYLATE (CAS# 23945-44-0); (	URACIL 5-CARBOXYLATE (CAS# 23945-44-0); (M	URACIL 5-CARBOXYLATE (CAS# 23945-44-0); (M+H)+ [, tgt	23945-44-0	(157.0249, 861.9133)(158.02417, 45.323334)	URACIL 5-CARBOXYLATE (CAS# 23945-44-0); (M+H)+	C03030	FindByFormula	6	+	156.0174	1.2935065
URATE (CAS# 69-93-2); (M+H)+	URATE (CAS# 69-93-2); (M+H)+	URATE (CAS# 69-93-2); (M+H)+ [, tgt=97.97, overall=97.9	69-93-2	(169.0362, 88822.03)(170.03964, 6514.674)(171.03983, 760.	URATE (CAS# 69-93-2); (M+H)+		FindByFormula	12	+	168.0288	1.0372494
URATE (CAS# 69-93-2); (M+Na)+	URATE (CAS# 69-93-2); (M+Na)+	URATE (CAS# 69-93-2); (M+Na)+ [, tgt=53.73, overall=53.	69-93-2	(191.0183, 1357.8684)(192.01945, 632.9817)	URATE (CAS# 69-93-2); (M+Na)+		FindByFormula	6	+	168.0296	1.0038338
URIDINE (CAS# 58-96-8); (M+H)+	URIDINE (CAS# 58-96-8); (M+H)+	URIDINE (CAS# 58-96-8); (M+H)+ [, tgt=73.62, overall=73.	58-96-8	(245.07812, 4572.151)(246.08212, 548.11145)(247.07953, 15	URIDINE (CAS# 58-96-8); (M+H)+		FindByFormula	14	+	244.0705	1.3495712
URIDINE (CAS# 58-96-8); (M+Na)+	URIDINE (CAS# 58-96-8); (M+Na)+	URIDINE (CAS# 58-96-8); (M+Na)+ [, tgt=84.71, overall=8	58-96-8	(267.05984, 36218.246)(268.06345, 3957.2458)(269.06122, 5	URIDINE (CAS# 58-96-8); (M+Na)+		FindByFormula	27	+	244.0706	1.3602282
URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9)	URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9);	URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (2M+Na)+	58-97-9	(671.0635, 1867.2666)(672.0648, 921.5817)(673.0681, 945.8	URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (2M+Na)+		FindByFormula	6	+	324.0382	0.74049944
URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9)	URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9);	URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (M+H)+ [,	58-97-9	(325.04382, 695.53)(326.046, 146.81999)	URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (M+H)+		FindByFormula	2	+	324.0348	0.9544985
UROCANATE (CAS# 104-98-3); (M+H)+	UROCANATE (CAS# 104-98-3); (M+H)+	UROCANATE (CAS# 104-98-3); (M+H)+ [, tgt=46.55, overa	104-98-3	(139.05049, 33484.875)(140.05496, 2168.7021)(141.05588, 4	UROCANATE (CAS# 104-98-3); (M+H)+	C00785	FindByFormula	13	+	138.0439	1.0178459
UROCANATE (CAS# 104-98-3); (M+Na)+	UROCANATE (CAS# 104-98-3); (M+Na)+	UROCANATE (CAS# 104-98-3); (M+Na)+ [, tgt=54.53, over	104-98-3	(161.0322, 3318.9438)(162.03384, 171.56769)(163.03902, 69	UROCANATE (CAS# 104-98-3); (M+Na)+	C00785	FindByFormula	13	+	138.0435	1.176696
URSODIOL (CAS# 128-13-2); (M+Na)+	URSODIOL (CAS# 128-13-2); (M+Na)+	URSODIOL (CAS# 128-13-2); (M+Na)+ [, tgt=87.49, overall	128-13-2	(415.281, 9671.675)(416.28537, 2732.861)(417.28592, 336.1	URSODIOL (CAS# 128-13-2); (M+Na)+		FindByFormula	8	+	392.2909	21.667603
VALINE (CAS# 72-18-4); (M+H)+	VALINE (CAS# 72-18-4); (M+H)+	VALINE (CAS# 72-18-4); (M+H)+ [, tgt=97.03, overall=97.0	72-18-4	(118.086586, 175130.17)(119.08914, 10872.538)(120.08798,	VALINE (CAS# 72-18-4); (M+H)+		FindByFormula	13	+	117.079	0.90300053
VALINE (CAS# 72-18-4); (M+Na)+	VALINE (CAS# 72-18-4); (M+Na)+	VALINE (CAS# 72-18-4); (M+Na)+ [, tgt=57.69, overall=57.	72-18-4	(140.06833, 6070.191)(141.06837, 799.793)(142.0683, 176.1	VALINE (CAS# 72-18-4); (M+Na)+		FindByFormula	20	+	117.0789	0.68065137
XANTHINE (CAS# 69-89-6); (M+H)+	XANTHINE (CAS# 69-89-6); (M+H)+	XANTHINE (CAS# 69-89-6); (M+H)+ [, tgt=66.91, overall=6	69-89-6	(153.04057, 29860.133)(154.04424, 2527.553)(155.04051, 26	XANTHINE (CAS# 69-89-6); (M+H)+		FindByFormula	25	+	152.0337	1.2730453
XANTHOSINE (CAS# 146-80-5); (M+H)+	XANTHOSINE (CAS# 146-80-5); (M+H)+	XANTHOSINE (CAS# 146-80-5); (M+H)+ [, tgt=64.37, overa	146-80-5	(285.08478, 1859.333)(286.08633, 266.49316)(287.08337, 45	XANTHOSINE (CAS# 146-80-5); (M+H)+	C01762	FindByFormula	25	+	284.0774	2.289024
XANTHOSINE (CAS# 146-80-5); (M+Na)+	XANTHOSINE (CAS# 146-80-5); (M+Na)+	XANTHOSINE (CAS# 146-80-5); (M+Na)+ [, tgt=67.07, ove	146-80-5	(307.06537, 2173.5596)(308.06665, 256.9638)(309.0667, 54.	XANTHOSINE (CAS# 146-80-5); (M+Na)+	C01762	FindByFormula	21	+	284.0765	2.2876015
XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8);	XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8);	XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8); (M+H)+ [, t	523-98-8	(365.0469, 610.29)(366.0469, 99.93)	XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8); (M+H)+	C00655	FindByFormula	1	+	364.0392	1.2250078
XANTHURENIC ACID (CAS# 59-00-7); (M+H)+	XANTHURENIC ACID (CAS# 59-00-7); (M+H)+	XANTHURENIC ACID (CAS# 59-00-7); (M+H)+ [, tgt=55.04,	59-00-7	(206.0436, 2692.1626)(207.04857, 263.12622)(208.04688, 14	XANTHURENIC ACID (CAS# 59-00-7); (M+H)+	C02470	FindByFormula	21	+	205.0358	4.6135798
XANTHURENIC ACID (CAS# 59-00-7); (M+Na)+	XANTHURENIC ACID (CAS# 59-00-7); (M+Na)+	XANTHURENIC ACID (CAS# 59-00-7); (M+Na)+ [, tgt=62.4	59-00-7	(228.02603, 597.8425)(229.02695, 85.51875)	XANTHURENIC ACID (CAS# 59-00-7); (M+Na)+	C02470	FindByFormula	8	+	205.0378	4.6090484
XYLOSE (CAS# 58-86-6); (2M+H)+[-H2O]	XYLOSE (CAS# 58-86-6); (2M+H)+[-H2O]	XYLOSE (CAS# 58-86-6); (2M+H)+[-H2O] [, tgt=34.59, over	58-86-6	(283.1059, 1117.82)(284.1039, 196.99)(285.0981, 256.6)	XYLOSE (CAS# 58-86-6); (2M+H)+[-H2O]	C00181	FindByFormula	1	+	150.0536	2.5680227
ZEATIN [ISTD] (CAS# 13114-27-7); (M+H)+	ZEATIN [ISTD] (CAS# 13114-27-7); (M+H)+	ZEATIN [ISTD] (CAS# 13114-27-7); (M+H)+ [, tgt=92.75, ov	13114-27-7	(220.1198, 741028.6)(221.12254, 91246.125)(222.1251, 7037	ZEATIN [ISTD] (CAS# 13114-27-7); (M+H)+		FindByFormula	28	+	219.1125	3.888838

Compound	Pos_Human Plasma Extraction_1	Pos_Human Plasma Extraction_2	Pos_Human Plasma Extraction_3	Pos_Human Plasma Extraction_4	Pos_Human Plasma Extraction_5	Pos_Human Plasma Extraction_6	Pos_Pool QC 1	Pos_Pool QC 2	Pos_Pool QC 3	Pos_Pool QC 4	Pos_S00015447_1	Pos_S00015448_2	Pos_S00015449_3	Pos_S00015450_4	Pos_S00015451_5	Pos_S00015452_6	Pos_S00015453_7	Pos_S00015454_8	Pos_S00015455_9	Pos_S00015456_10	Pos_S00015457_11	Pos_S00015458_12	Pos_S00015459_13	Pos_S00015460_14	Pos_S00015461_15	Pos_S00015462_16	Pos_S00015463_17	Pos_S00015464_18
C17 H10 N10 O3							245770	258748	260330	256998		124077		28606	9245	118389	201564			203100		100467	365691	522670	3045	431769	182133	
C22 H49 N5 O3 P2 S2	398265	400238	382854	319652	263192	227928	63114	21690	13697	58274	31836	23850	10482	23674	27036	8668	19033	17900	28546	65194	95071	5287	18884	19129	7509	19763	29627	70177
PROLINE (CAS# 147-85-3); (M+H)+	905004	1051452	971546	550515	515840	979468	6259	7117	6945	6615	733664	6746	252448	584831	868148	12591	5068	13416		2200	940795	33368	3700	15812	14395	14604	8844	5159
C15 H36 N8 O7			9983				52642	51828				49925				80806	37936			5952	50212		56183	97651	30367	45032	35626	49362
C25 H29 N3				3839	12709		133380	175157	163171	164643	531227	2437192	70979	380226	128631	4434	52026	50864	149411	54117	15861		39870	42979	35939	338674		14192
C38 H54 O11 S							89855	68688	65409	65689					5345				30777		1579		18484					
C26 H26 N10 S	11095	9392	13377		8747	12549	55464	70228	65197	64580	41635	110384	76831	125663	97072	47051	82890	19883	79664	10462	73811	22248	166975	33712	128162	54112	102775	32452
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Na)+	90950	97084	96328	101406			203812	206980	202473	199993	163496	180231	127193	201369	181933	156634	153290	186308	238951	154032	188935	204709	234061	207982	278997	279887	229280	219841
C17 H18 N10 O3							87404	83506	79696	79794									51684				30188					
C22 H36 N6 O11	6955	7321	6712	6886	5672	5355	306322	283054	294016	290435	5153	3780	4044	4841	22961	5050	3461	6517	116074		4791	4651	90761	4455	3035	3426	7445	6065
C7 H8 O				1271			70926	70108	72111	72202	55288	2694	10558	18538	14185	13087	143016	150768	191318	107072	153521	52997	46928	90436		121347		153668
C4 H14 N2 P2 S	88750	82114	68877	77630	65692	64992	220436	223936	218495	222263	168568	205792	137907	217679	188572	167499	162582	194096	250974	166577	207116	219328	116165	227151	297606	307524	254356	234351
C25 H33 N11	79267	80784	72957	79431	81359	83593	31105		34209			1048	44085	47901				49410			30313					34277	44942	36019
C22 H41 N3 O6				20119	7012		42785	49058	51657	44048	152319		244143	4195	26104	10031		11278	13467	8627	10383	2829				8960	17508	
C13 H30 N8 O S2							21866	24000	21081	42248						15008		43312	184375	23392	38556	26986					79444	90194
C26 H48 N3 O11 P	2724672	2594430	2723362	2740019	2522585	2497435	556284	589170	568196	543267	538677	516390	144197	425114	129039	221022	417255	747579	598049	1040835	832644	205765	616221	447701	19282	539170	427532	636420
C44 H41 N O3 S2	60928	59727	55684	56758	55259	49066	28160	25636	24047	27458	13810	4719	3464	12475	7537	1659	19608	11978	27300	7554	18989	6887	27465	19998		10571	3815	19420
THEOPHYLLINE (CAS# 58-55-9); (M+H)+	102616	109530	97570	99173	103109	95513	67373	66629	65618	64294		97493			24506		60709	293117		65035	216059		336229	125309				272669
C23 H25 N3							178453	249165	229172	229304	956458	4224080	100814	193809	42143	24108	73405	86054	79653	45854	14657		31378	45430		222279	6140	
C29 H50 N5 O2 P S3	117989	114748	116261	108749	102662	91471	7473	9075	6811	10399	5699			5975	11112		16866		15218	10662	16026		16183					21498
C22 H44 N2 P2	52903	25698	32346	38739	58617	57229	282206	282310	287397	266232	307729	238494	231202	114010	67115	160074	323009	279257	182354	241039	369669	128952	1211862	357636	153154	483601	276408	322809
C18 H33 O P3	33766	33278	30079	31975	30405	29135	36679	36126	36002	36098	34355	36722	32853	35640	34265	33768	32073	34650	34092	30828	39122	38064	37343	36041	42928	39729	41180	32670
C4 H9 N S	97375	107345	94187	97387	101639	94324	160941	2234	3864		200544	152678		96281	180183	163470	5721		30631		258707				5834			
GUANOSINE (CAS# 118-00-3); (M+H)+							825938	768938	690588	769363	344389	414545	160825	643101	729035	430089	1436946	1171804	1376791	760932	1047965	582558	1169406	1088933	191027	11850	1205541	979707
C16 H33 N O		2190		3067	3225	2300	323636	148940	131030	122402	12618	10755	20348	7709	101006	8118	13911	16583	117648	14765	14914	10320	134529	9804	18336	14446	12010	17884
C16 H24 O4 S	391335	400434	395552	423673	418522	420003	2733807	3084858	3068698	3006217	6910769	1688807	1.06E+07	1072774	2795654	1201011	1057124	706866	1509639	879431	713497	521328	2400886	592675	707308	1730986	1691272	908374
C31 H64 N2 O2 P2 S							52716	54755	56275	53872						30225						57227	87162			4763	5835	1336238
C17 H22 Cl N3 O3 P2 S2		1064					42636	43494	44393	45379		21114		12854	3055	32675	47395	27553	56329	42067	11773	42039	57457	65284	12495	51282	47125	48798
C15 H35 N7 O							44539	46706	44326	42187	10518	21846		9760		30807	128705	124106	164705	129098	94554	39469	78285	64547		8746	69349	154220
C28 H43 N O8 S2					2131	18710	48604	54312	53403	53237	7077	24156	41690	39070	8012	19345	146543	69304	153161	44406	40891	34887	79750	47967	35663	53017	77329	46050
C23 H41 N7 O2	54280	52801	53352	48086	42806	40387	40425	48674	41237	42688	97881	136971	15294	155852	124911	37834	8628	51082		12158	83168	5025	27297	15805		32710		36180
C28 H57 N4 O3 P S		67609	80365	27009	33235	50425	280906	293237	306984	286903	270840	356149	179621	202822	93826	87102	813635	325909	449898	241314	562753	87887	499887	322862	65074	353030	248726	635600
C12 H21 N4 O3 P	2613504	2637661	2594945	2585672	2451136	2440242	2963822	3192105	3086646	3051277	2844347	3040239	3445175	3156539	3133285	3025125	3621523	3115056	6880396	2971494	3372513	3112325	3740818	3337040	3354390	4014435	5283088	4782509
C7 H17 N5 S							1250216	1274691	1209308	1254691		3969				702100	204780			2476961		549868	1336286	1033646		903334		2625845
C15 H22 S2	10354	9935	5184	6114	6867	2033	61366	60706	55134	59607	42121	45079	47496	47822	45567	46472	56451	56845	65209	57300	55096	61035	59606	56434	51580	56247	61699	64196
C19 H29 N3 O P2	68449	71291	60980	60890	58074	52426	1532										2435		1199									14182
C41 H45 N3 O3 S	51108	31860	48157	54951	29717	51588	3231		5326	8778	35980			4373	24878		3054	7605	11737	3721	32066	2524	10965	5232				19377
C30 H64 N O2 P5 S3	176527	118020	175588	167713	223964	62862	26180	27522	28247	27872	19037				9735	16739	16759	25182	17132	40095	36834	16059	26130	19696		13695	11506	30410
C18 H31 N7	2960				6007		130890	145106	148406	142702	104608	257919			108008	62851		279267	74344	310243	290278		372614	209358		105598	350512	236235
C24 H33 N3 O2							303397	337152	334733	345795	178006	7783	34969	63942	73198	77838	870727	793336	1482545	1033441	1394898	291533	373052	449849	16606	617396	23301	1046912
C18 H22 N4 O	521345	547268	531622	553982	531210	532693	514937	536625	526993	519653	494735	522333	529838	522464	494095	518071	531583	503517	508053	506420	521960	535740	507520	540424	485576	590085	569727	542352
C29 H64 N12 O3 S2	7719		13845	24719	16738	13734	157482	158350	135639	166621	107956	151964	97929	101116	91832	41068	334280	159458	213740	130629	137011	44152	499103	136289	33075	190369	122083	316354
C12 H17 N5	200778	206899	183104	176074	155122	146052	266907	271577	256198	262011	623714	517649	123970	391020	450327	137134	202297	110074	736654	248359	303241	50486	350022	85776		162416	39070	211655
C25 H48 N2 O3 S	12090	17803	22145		33953		224867	215515	33730		4134	382472		2775	54928		845906	286194	29243	124678	429764		226432	150556	52093	219462	214593	390377
C7 H14 N6 O2	30363	32284	38209	44789	32885	39513	69361	66833	66122	61033		66021	28973	28322	44755	45272	25424	34555	31023	26418	35967	48799	73899	29951	38909	51424	58235	28350
TAURINE (CAS# 107-35-7); (M+Na)+				2773			15102	20202	15338		54926	71452	105463	101279	42643		12083		4413	2956	6676	21183	15855	7071		8916	44654	1919
MYO-INOSITOL (CAS# 87-89-8); (M+Na)+	364289	365594	293246	328859	322836	348341	34641	44043	34758	41463		18459	60080		59055	70703	19117	21588	24180		157899	53302	63782		45276	26694	52334	
C38 H35 N6 O5 P							426144	437384	427665	432859	8420	28411	5597	22746	83634	180507	212201	756549	3056828	505293	306610	505401	25741	70836	92207	58257	1505276	1624661
C38 H84 N7 O4 P							99172	31127	43901	41274					1162				18957				6083					
ADENINE (CAS# 73-24-5); (M+H)+	5929					4914	24585					49568	23446	23099			15192				8750	17811	18804		68674			
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4);	180317	180243	166244	172799	173175	173500	29439	29388	30173	29506	21645	3328	1486				15410						10622	353209				
C34 H59 N4 P5					1295		34473	24349	23096	22058									9329				5517					
C24 H50 N2 O2 P2 S	2626988		2459253			1565825	485927	302122	301386	296816	77642	509915	35400		2944024	162244	244137	246645	134075	366804	306687	105313	278271	195309	863611	87696	44216	133279
4-HYDROXYBENZALDEHYDE (CAS# 123-08-0); (M+H)+							20123	19501	23068	16422	1230	23135	7429	3758		12185	28309	20928		16061	3337	17277	30000	31404	14156	31972	20754	13391
C28 H44 N4 O7 S	42829	39111	35158	38235	37016	37161	85738	85577	82117	88034	64578	74186	60054	85204	72305	70969	65474	77872	94811	61941	70241	90730	101137	82286	122981	123420	91358	94382
C41 H50 N4 O S2			2602				7052	21093	1830	15742	25659	10781	20075	15524	17687	23632	14851	13870	10129			23185	17796	18531	23388	14435	8846	
C12 H18 N2 S3							71511	76266	71847	71476	82982		33423	53401	16669	58989	39715	89090	184864	57961	45414	55981	77331	169305	34392	177272	56927	88335
TRICARBALLYLIC ACID (CAS# 99-14-9); (M+H)+[-H2O]							1329921	1358452	1305647	1317317	706353	1066720	520660	376664	881317	878338	1492600			1761126	2412624	52671	1764829	1643341		1921645	957396	2173028
C22 H22 N12 O4							94351	66467	65400	63677									28385				25845					
C8 H17 N O2	292134	80807	80849	94767	77882	273934	32403	36068	30783	3864	99379	85677	21459	55512	93507	4533	50606		52080	13443	292113		157326	46119	4731	114858	29996	23963
C24 H19 N12 O4 P	24340	25102	36290		22977	20274	16618	9854	11256	10209	11618	20624		8149	11428		9423	20517	17009	13731	14666		15416	14396		16885	8503	22534
C26 H23 N6 O3 P	12072	11716	14078	12804	12774	13852	287547	318129	310956	308110	222001	229925	259415	279197	328308	219216	305670	303667	391642	337026	282661	305655	320626	303309	280639	284862	305438	347015
C13 H25 O P S	162416	161652	158424	164979	154988	151285	44488	45806	43998	44923	51055	48723		14652	58052	132388	19338	146511	104972	61510	88559	22852	27266	37153		68163	17725	99618
C17 H37 N							466229	386718	315310	275434					1733				5115		3883		4585			1734		4171
C25 H38 S		4733	6168	7183	5442	8740	91405	99507	95144	91934	124953	102581	223365	104083	37754	109357	127715	116512	163669	75170	133962	127929	175412	123926	170535	147591		166632
C19 H43 N3 O5	2611	2646	3014	6186	3127		73999	86528	82487	85374	36558	138002	45449	32397	38660		123801	126619	155103	85648	146880	41435	203658	166311	36071	85304	35972	73553
GLUCOSE (CAS# 50-99-7); (M+Na)+	364289	365594	293246	328859	322836	348341	34641	44043	34758	41463		18459	60080		59055	70703	19122	21588	24180		157899	36929	46675		12731	17518	52334	
C23 H53 N5 O P2 S2	3164685	3143035	3042779	2671440	2352359	2128073	277989	247292	223240	211656	322206	199204	114547	342060	128105	72652	457391	360358	373410	265114	491277	83004	257758	197438	22569	324297	142135	484843
N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3); (M+H)+				1985			39325		59561	68049	136717	100280		52712	71012	61477	77132	39667		35532	78435			108993		91922		109325
C17 H19 N O3	983436	955884	930729	933881	948385	936467	35549	41945	41064	38904					29709	12017	3417	38449	71741	122447	87278		42754	1094		92005	26436	212808
C21 H42 N5 O3 P3							5867																					
LAUROYLCARNITINE (CAS# 25518-54-1); (M+H)+	73003	76921	71820	10882	9825	52672	7152	7559	6378	6706	7928	10347	1356	2301	8474	1321	11195	7236	14147	6779	17983		10590	8394			3908	26944
C14 H31 N O	240116	237840	235032	234991	235187	221949	1569334	1377785	1311921	1272653	579232	668817	1423663	433230	1343671	297054	655050	2008037	766979	731532	583705	700874	479712	550107	2036505	838080	529418	1040018
C19 H20 N10	171221	185804	172800	178018	178402	186426	159612	167679	169283	167403	173674	163733	175693	179028	174087	166930	179025	171176	170976	165689	182895	183407	179413	188944	174021	183915	179833	172006
L-ORNITHINE (CAS# 70-26-8); (M+H)+	7362	6806	7361	7320	7412	7184	9650		9076		6767					16278		18685	8184			43576	4343		11875	21171		
C22 H24 N8 O P4							31803	30982	28170	30077		10179		2405	2373	16228	46811	39356	60803	34867		11514	48147	46852		49230	23168	49535
C14 H20 N2 O2							1751793	1359486	1702342	1678445	966165	208276	184492	194678	137690	139300	5776362	4868414	4140267	1872717	3035654	397844	583492	3825960	463700	1704478	436979	2772407
C31 H66 N8 O S3	83445	49901	95479	28019	88499	33325	167704	157557	139776	152642	181484	82717	109079	153442	287990	76656	175327	136355	269820	200429	247514	142595	343205	133910	114426	227108	60802	187323
C22 H50 N7 P S3	844076	831873	784655	672540	569964	502197	30896	65868	7915		9538	27638				6646		54201	54670	35986	40278	2166	36429	59417				29675
THROMBOXANE B2 (CAS# 54397-85-2); (M+H)+[-H2O]							116870	86386		90070		181997			50574	36187		147587		100527	98416		88201	82890		24887	37672	47830
C29 H46 N2 O2 S2	454334	481775	471340	464780	477070	453295	460750	471127	476965	460288	482099	455097	499724	492840	431862	475778	485211	475187	459443	460362	472737	386349	497795	444334	552990	511098	510179	478744
C20 H40 N6 O10	204873	199545	190642	194404	186862	185896	248810	245405	241623	239559	32549	89140	38598	50392	251623	51254	387437	458008	459769	287944	363253	74012	680039	333875	43141	482915	172072	442623
OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M+H)+							4552	5647	5167	4832	10451	1357		1298	14510	7019	5759	9461	34642		2410					8951	1365	2994
C22 H48 N2 O S3	68799	69772	62541	82857	63961	64000	12108	18357	15474			98452	21214		3426	26384		20776	45657	41989	15523	21401	31420	11084			32455	
C16 H29 N4 P3	16615	6180	7193	12563	8308	6194	39841	35483	35717	35891		6965	4021	4432	27045	4400	14267	17126	13926	15594	14292	4287	13512	16428	1180	18287	32844	18120
C36 H56 N6 O3 S	70165	31664	59336	99304	69429	72897	130876	125277	141951	146928	113791	2472	132067	116361	205489	89851	125502	116875	160202	125800	123391	93078	149687	176709	101774	264954	136873	145288
C15 H27 Cl3 N2 O3 S3							291145	153074	154337	149700									44382				21767					
C20 H32 N12	16076	13481	28160	12727	14628	12225	4830	310170	6563	298697						314731		459089	1048675	273536	8086	1682		326791		14155	320194	341806
DEOXYCORTICOSTERONE ACETATE (CAS# 56-47-3); (M+Na)+							6238	7583	7615	6954								13720	71220	9003	6011	9970					28391	30765
NICOTINE (CAS# 54-11-5); (M+H)+							42659	42635	40407	40312	60862	140441				4841	201345	89541				5487					22637	
C26 H33 O6 P S	10926	10071	6599		11412	10287	142880	154706	150198	148646	115869	121532	127117	144478	152573	114842	150377	159254	185468	167788	143786	147240	161706	151265	140131	153794	154562	168969
SPERMIDINE (CAS# 124-20-9); (M+H)+							270446	311797	300588	316030	64596	1095726	310504	41678	86587	70586	322883	168692	599877	258001	202071	23811	691187	651981	65421	394340	367170	185218
C33 H33 N3 O2	33781	36545	36127	35196	34027	32495	7122				3465								10461		4742					4685	7870	7505
C8 H10 O6	376436	368074	295231	331492	321950	351126	44512	44981		42266	58187	14990	61761	68834	114883	72247	26390	22104		54409	124415	75284	65206	40947	47629	46815		42149
C38 H62 O S2	146392	152298	142382		159452		44328	50515	7990		12114	58211		16396	20545	18178	49114	44762	16592	40013	15584		8381	43429	13225	71865	49650	123609
C34 H9 N5 O5 P4							131014	47076	52611	41192					3738				19911				8054					
C34 H52 N3 O6 P S	73246	60155	58555	77409	72055	56800	6372	7388							4895										1212			
L-ARGININE (CAS# 74-79-3); (M+Na)+	3868	3773	2502	2740	3130	2812	9313	9947		8917			10048					5325	9688				5636		18470	8981		7756
C16 H31 N7 O				8309			169201	188108	184202	180689	210932	130086	86401	120373	75811	97480	1145915	128635	106086	114760	105297		141360	190142		153818	129128	116268
C16 H31 N2 O4 P3	29838	31124	29252	29509	33556	30574	21670	21651	25635	25701	16217	18266	15367	19824	18034	15341	24259	27345	32800	24506	26284	18263	28292	26967	14603	38603	19327	30246
C42 H44 N O4 P3	15962	39277	65514	37638	42972	39985	12844	8417	6575	9159	11230		1724	5129	6550	3174	14332	12929	9068	9242	16372	3110	8582	4770		7463		20717
C40 H59 Cl N5 O3 P	25717	34784	29023	34192	27408	32038	78303	63698	70223	55252	88479	113379	96262	111504	142245	110674	131057	74476	104588	79305		29363		64195	55081		43080	
LAUROYLCARNITINE (CAS# 25518-54-1); (M+Na)+	44936	43866	43523	40820	36788	33326	3731								4174													14419
C18 H26 N6 O	37272	57547	44364		65626		251249	48514	252485	196838	236532	310685		59373	245008	133766	75112	228944	203799	251134	267450		498750	259269		256432	164865	294251
C16 H32 O2 P2	330349	334979	321210		330014	84220	249751	263560	266867	192757	61983	370251	259905	219166	204155	291089	168125	110650	316336	122039	355061	96087	367671	208378	184513	280044	376073	417412
C14 H9 N4 O P S2							83552	89724	81439	87756	73875	93973	31942	60393	65194	58673	124547	81059	82643	87386	114257	54069	115942	94642	21416	100649	93461	73634
C20 H37 N4 O3 P	2859456	2884245	2816563		2561437	382861	2145949	1795744			5004	1.41E+07		3441		907653	1703969	5315		350451	2161744		1984355	436497	846916	824929	1280087	1362578
C8 H4 N4 O3 S							982571	1001995	998046	1009502	881106	74663	282979	477764	364525	369342	1170858	1145387	356049	1075406	1187899	913360	838472	1063408	89506	1138861	135242	338702
C22 H39 N4 O4 P3	2082	2724			1626	2133	147787	142537	145261	140605	2146	1526	1467	3136	6070				67285		1864	5109	52157		2452		3661	
TERBINAFINE (CAS# 91161-71-6); (M+H)+					6673	6393	17385		18431	19291										253881								
C28 H19 N8 P3	1547					1465	29889	30987	30946	30509	19034	23444	23381	24731	23269	21125	27575	32770	39928	31835	26788	31502	31316	29497	29908	30523	34066	34690
C7 H14 N2 O	131969	121857	96406	127019	130071	121245	3904	8980	53489	17431	14747	24741	2237	9464	9414	7283	23918	103554	242067	101779	121434	14170	7688	36304	9479	11556	9660	455062
C38 H57 N O3 P2		829477					195522	196334		210446	220323	186378	191231	206969		166763	171685	199903	253517	180110	193529	220360	245699	196245	278341	336594	250333	216410
C6 H12 N4 O4	13503	14079	13368	13085	18007		21993	21842	18784	19089				4845	18877	5470	29154	35777	27573	17900	26250	14365	50881	24681		38454	16120	31924
C13 H23 N4 O3 P	334077	370465	360876	384870	379174	356457	244270	263878	290682	283569	356971	344978	366010	364931	332471	382372	347939	320090	311362	354593	328516	401229	316221	378387	363246	347907	365658	319290
C26 H31 N2 O3 P	55029	55482	53647	52365	53645	51285	24314	24401	23664	22265	6242	14872	7685	10640	60486	8431	15169	21454	29926	24446	17220	6931	26844	45591	9781	21305	19367	23635
C33 H50 N O10 P S2	76725	136340	258875	260444	257247	250859	26013	17686	13675	12660	11965	7122		3734	5730	10601	8129	16405	8578	31457	28992	8980	12234	13738		6285	8199	19441
XANTHINE (CAS# 69-89-6); (M+H)+	164374	159505	155801	155887		149510	524124	553755	535052	537816	1248215	1933926	258374	916589	1205077	721267	193984	241214	592140	317862	381636	92633			17838	303639	335694	403831
C25 H47 N O4	351923	350055	347062	338621	308019	297901	79079	138284		142916	336650	662065	62021	144348	448092	150587	133947	129770	164171	224155	397277	41777	103637	102052	3101	81260	67533	359466
C24 H46 N3 O11 P	2057271	1986102	1965262	1837200	1542034	1479204	169145	172822	191558	168626	349001	428047	68810	217065	252814	102708	68937	205363	118102	264626	179670	50670	177126	111264	2212	77766	76836	190631
THREONINE (CAS# 72-19-5); (M+H)+[-H2O]	8277	62235	59848	58322	54484	65647	11734	37209	15955	12817	16210	17170		5414	13874	14652	31852				20390		2221	18460			13104	
C16 H44 N14 O P4 S							248161	117905	104468	103321									41154				19123					
C35 H62 N7 O4 P S2	27951		46791	15402		33472	98514	94665	96945	49030	104561			78342	2390	278520	144373	93657	123500		173666		176441		24497	235895	71271	137852
C12 H10 N6 O2		11885	6815		19369	11473	104235	107865	105373	102468	31877	28798	6407	14163	22119	31268	112375	263738	351607	197546	275595	50401	168735	143912	2202	268444	41449	272257
ETHYLMALONIC ACID (CAS# 601-75-2); (M+Na)+							83096		87016	80264		75176				29391	123089	65014	111611	335338	65033		87941	107977		166023		73458
C25 H45 N14 P3							54165	44014	42638	41264									1538				8770	6280		1386		17619
C32 H45 P3	31812						28455	40206	40340	35848	28754	34434	34506	35710	36177	32803	33068	41920	48854	43480	34730	36613	37511	37445	36743	37930	35362	36472
C4 H7 N3 O2							64271	60600	62783	57972						140729	54052	140683		61618		64888	43865	56138	22762	97635		
C16 H26 N2 S3							77384	94189	96891	94435	56382	99226	76555	110300		74441	65108	49553	183111	61812	65663		178910	259211	59713	221974	58536	89519
C15 H30 N6 O2	46137	87303	56125	54476	46424	48323	82216	81901	84963	80570	75720	75715	70087	119228	77953	59368	77362	72960	87158	58028	71887		151737	75880	142140	105769	89657	84682
C26 H44 N23 P						3147	1416											1549	1325					1468		1927		
C27 H50 N O2 P S2	3156946	3080784	2911272	2482145	2092903	1838525	171228	189375	193040	186843	340268	499591	62364	217057	236564	103971	68796	214583	152936	287496	212181	56146	216077	133048		108123	70430	191882
C20 H35 N4 O3 P3							53650	49997	52317	48777									29628				21371					
C3 H12 N4 O4	28209	25107	27933	24809	24680	25368	49133		44170	46102	87706	25962	23430	48144		97332	43422	64823	57631	29933		73312	20905	48255	39057	61779	48500	68602
C14 H33 N4 P3	5452	1594	3488	7518	3865	4303	8405	6108	7060	11771	4532	5153	1509	3887	17256	3679	8756	9397		10156	7376	5715	7748	8551		9390		12176
C17 H40 N8 O8				16421			51433	49521			1940	46097	1963	12935	2604	92042		2084			56764	15027	54292	71190	28586	44811	40856	43584
C43 H85 P	26952	11023	1885	122280	175478	130808	20952	45590		45671	105102	56627		41947	57180	55198	90070	98522		119133	60420	14355				43784	6474	9499
D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (M+Na)+							1523	1255														1102					1833	
C24 H30 O6	1828769	1860907	1804817	1867224	1844229	1775453	2.39E+07	2.60E+07	2.55E+07	2.56E+07	2.05E+07	2.12E+07	2.25E+07	2.36E+07	2.64E+07	2.07E+07	2.51E+07	2.54E+07	2.91E+07	2.69E+07	2.36E+07	2.56E+07	2.58E+07	2.54E+07	2.40E+07	2.45E+07	2.55E+07	2.68E+07
C18 H24 O8 P2	60034	61212	58792	61577	59011	55046	111104	109097	107434	109356	92808	101718	68420	105702	98202	83382	84542	101229	122735	84763	100382	109419	125105	110759	147418	145841	120779	116167
C14 H17 N O8	271608	268485	251133	254334	252155	255611	42024	41826	39784	40699	27497	3568	2348				21865						15013	482298				
C28 H41 N5 S	102322	90679	96315	84653	76689	77618	22452	19871	22566		30090			22244	29231	17475	57231	37756			111289	61031	42182		6036	30448	40100	125289
C27 H54 N2 S3	228248	228939	223897	180449	150858	136996	650281	665939	647993	603588	626685	613319	301542		361601	208866	453570	894310	790136	1366722			838320		50978		466003	

C29 H47 O3 P S3			31328			29234	49269	56080	52051	56975	7841	20325	53329	41563	14516	14774	150855	65327	122602	34400	28547	30215	67047	46247	41920	49497	72598	40375
C37 H51 O3 P S2	24486	24753	24618	22809	24028	23042	54552	49999	44343	47689	35063	38733	31590	43458	37333	34284	33185	40874	49571	38799	41352	47213	48390	44429	60828	64466	51656	48746
C7 H3 N O6 S							344162	376989	362644	360616	69265	207766	33909	148238	100658	341101	393169	243407		312668	179313	144299	402107	436905	93039	385422	437602	287346
C33 H44 N O6 P			16069	16164			15438	22885	20514	21777	41304	93877	6402	27052	51571	19010	10169	28268	17638	10794	37279		11024			14053	22089	18429
C22 H42 N2 O3 S		10092		5151			67321	72132	67487	61353	53063	78588	64430	84690	39562	47603	83079	62869	81532	41399	61497	88524	99974	99816	162014	124447	73516	70931
C10 H11 N5	47389	42288	46440	43076	43478	39537	75149	77720	76151	74730	59629	63785	55531	74972	64546	57544	66404	65915	84023	57626	62570	81347	82142	75386	95570	98554	86085	75874
C15 H35 N2 O6 P S2	59567	76014	70737	49485	68126	57762	23552	31828	23863		26333	42004		17604	14975		20298	42907	43047	34143	37690		32810	28444		42073	16592	68781
C16 H35 N O	11593	12483	13964	11846	12501	5962	350083	216746	171692	151476	23579	49265	15749	13705	42376	138472	77784	47315	41979	28888	196242	83077	111222	55668	17114	125066	30151	176926
C18 H40 N5 P	10313	10427	13079		6107	12896	92569	73616	35202			172474		35540	225437	22716	279948	20168		14892	266434		214457	118890	20339	56911	68156	77500
C16 H25 P3	56451	56920	53193	54783	53667	51174	20725	16503	17257	18028	8384	12007		5299	15631	55011	5950	43304	43536	30068	22227	11709	10832	17298		30756		39670
C20 H37 N7			64529	71854	63868	62055	215034	252281	240952	233270	92109	384856	197303	235499	129831	83362	455542	285503	299407	332034	358562	170203	490476	460114	102197	458164	426260	345213
ELAIDIC ACID (CAS# 112-79-8); (M+Na)+	26136	65968	27434		7640	10795	6305	46845				22865		52365	60278		31293	1402			14433		17145	60012	10873	107804	33313	33419
C26 H35 O4 P3	13005	14459	9461	13284	13862	12920	41734	51725	48755	48200	79374	83974	90801	92939	74021	83146	74740	95003	54769	88378	104992	87387	68571	82507	86258	87964	96183	98309
C30 H63 N8 O P S2	38847	42900	17235		45040		42045	31405	25083	53552	26421	60069		33760	28634	9339	185882	81225	191690	56421	229075	23743	102289	56001		99595		176650
C27 H54 N2 O2 P4 S2							69770	54760	58882	51776					2055				31125				20431					
C30 H10 N3 O5 P5							107931	51320	47327	50445													6129					
C22 H24 N6 O4	171587	164062	168657	171383	180996	167764	2121445	2281290	2269407	2269582	1382840	1694607	1705070	1747966	2569308	1457310	1548929	2026930	2137396	1922690	2339225	1830944	2499631	1727244	1627881	2146124	2242198	2378855
C36 H74 N4				5015		1941	1751	55476		65831	7477	3850	22173	28703	61754	44478		49572				26301		4597	19627	50542		
C3 H9 N3 O2	1416						58004	51736	64430	40961						73700	46471		114063	45741		53212	46268	84279		109311	90719	93887
RIBOFLAVIN (CAS# 83-88-5); (M+Na)+							5916	5043	4523	5489	3797	1372		3476	1212	5407	5090	7836	8416	13789	5815		3864	5753		9496		10356
C18 H39 N O	3154	12414	11798	7961	8092	6416	593329	362481	349452	334824	7424		9653	8213	8806	21286	19303	114128	28178	8345	27359		34203	6829	7822	19023		29889
C15 H28 N6 O	194487	196306	186557	255424	276789	298519	117440	273266	220238	283463	169613	116262	121400	126978	262941	143388	239871	138576	132274	257910	75490	105570	134778	67118	132752	155194	249847	161067
C9 H7 N O	355516	341521	320963	329796	325573	313084	35311	37512	34547	36047		61105	12721	27211		26414	37049	245012	288240	23666	33339	31275	66959	48970	22324	53169	33228	36023
C35 H35 N5		26005		23675	68648	17155	15699	17854	24646				11056	12944			24002	25484			71485			25489				65138
C24 H52 N2 O8 P2 S							4262		2902		5217		1365				9308		3994		7421	3228		5601				
C21 H37 N8 P3	40453	38467	36052	42444	36002	39910	20332	12859	13778	13590	5707	12481	5766	7519	34260	5237		10871	17026	19874	12914	4311	17377	27958	5182	11237	11136	15521
C14 H12 N6	263784	259553	264031	262786	252091	248554	24843	23592	24410	25424	19736					4158	3538	5109			9828	3453	93734	19397		2973	10016	24279
C18 H43 Cl2 N13	47599		46287	40524	43836	40374	13611	35865		40287	23612		53558	49756	59519	19211		57168	31995	36246	39964		52447	48425	14225		46057	67912
C38 H43 N O S	2036029	2023107	1954312	1800277	1569889	296540	96071	238123	235966	205725	360908	477025	50234	75560	262595	43763	51059	211641	155887	272866	232246	61919	92085	139034	71008	34305	67071	195184
C21 H37 N4 O3 P3	8982	9802	10028	11804		15411	71466	90172	121413	147074	3242					3639	3571		53512				87091		2806	2968		1053
C24 H37 N7 O3	286152	284103	277375	293909	271552	269194	7011	3053	6407	14313			1510					7137	58661	18900	6099		27080	5468			1275	11723
C23 H47 N O4	242894	245793	228740	219933	204870	187165	156652	35353	31728	24977	45674	1243635	57065	223178	30726	24150	38179	30468	53372	70556	116266	19440	40129	48015	8656	67468	28528	68237
C6 H12 N6 O3	113476	144040	159193	169592	141948	137950	501409	497223	487109	522146	154549	267130	159955	158019	662576	249027	348236	616203	612040	342594	360657	171207	615944	328390	227082	503256	440403	1087481
C24 H33 N O6	232208	226822	237315	244445	237297	231584	841876	872021	846583	846025	736906	791030	792492	814872	783601	759605	859155	802521	813530	854515	828645	859515	893969	850963	829845	882693	812181	835449
C27 H51 O2 P3	94015	96929	94938	103432	110175	112732	621673	667326	687192	147232	142403	131746	135282	136922	126435	138653	121610	138582	143266	126776	128940	144389	127552	136883	1071630	151289	132117	133787
C25 H35 N O6	147931	154753	153490	159609	152276	146569	1264416	1377699	1343244	1342083	1185875	1195532	1279812	1309959	1393251	1219316	1360412	1358983	1437205	1408525	1256649	1398725	1370252	1355471	1324923	1312113	1368924	1354429
C16 H30 O2	24408	22774	24595	22396	19810	34320	34345	34482	32566	30736	22770	47661	29253	25451	8979	24228	30661	26476	39446	44267	29749	20628	29091	29221	31321	40394	31967	34355
C31 H47 N4 O P5	124642	143576	134081		10375	96148	24928	28496	27390	24587	16019	23179		10375	7369			7607	3770	11799	8180	2489						
C32 H64 N O2 P5 S3	166715	168662	163445	167383	143193	147474	17093	30635	17428	15996	17529	17780	4392	14300	12462	7243	16125	25337	16866	37000	31104		20651	15243		19654	15718	24527
3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M+H)+[-H2O]		4507			10562		2001													1094								
C21 H18 O5							25426	28979	25789	25324	4711		11923															
C38 H46 O12 S	38747	49362	26544	25634	22624	22292	41717	47230	42137	46554	95710	130011	122759	159573	202221	69862	152192	49790	111978	45217	18294	66398	12310	49073	70223	4037	24891	20055
C26 H44 N14 P4							222233	86361	97036	87095									44907				16657					
C16 H38 N6 O2 S	187097	178130	174132	26607	178432	30900	237312	238873	117962		172683	349632	93313	119645	852648	156289	340892	260391	185823	292385	423359	82709	181088	107663	41658	252631	136846	367395
C27 H41 N9 O12 S	86261	75235	82598	78832	69555	63356	26374	18243		12387	1665	7347	3403		7467	10078	8200	15932	9539	32873	9092	8898	12287	13932		6141	7670	5897
C13 H18 Cl N O2	112697	107595		109625	107848		41455	40898	40793	41692														517658				
C20 H43 N O							68944	47622	44301	39968		4603		3830				9291		11989			5625					15368
C33 H46 N10 P2							31073	30874	32909	34640	5791						36557	47667	52750	41554	47571	2073	17564	48544		56160		49256
C42 H87 O P		59709		874780	822140	788481	48574	287733		297390	344727	115637	301054	126828	320522	357647	104684	537127	523967	17634	11829	287244		53990	213439	391146	136015	
CAFFEINE (CAS# 58-08-2); (M+H)+	1315835	1275935	1239712	1307537	1240546	1197826	81189	84383	78773	78374		88726	2465		30678	26181	38713	291857	18912	30650	209290	29097	464454	203221				371997
C22 H46 N6 S2	3960	46194	22840			57383	44255	59084	61218	52116	106824	46339	212578	10124	55916	19472	88905	25668	79117	34711	72167	64524	181997	116793	125581	104090	35458	106711
C33 H47 N5 O5 S2	141116	143259	141187	126364	119600	114614	37548	49783	44177	26191	26705	33256		33248		5662	37333	24172	31388	61642	46402	16012	17458	41676		27973	7877	43652
C11 H25 Cl N8 S	69634	68299	61648		68527		20891	26572	8434			39156		12953		12432	21221	28779									28523	50947
C16 H33 N4 O3 P	14647		17627	14030			72833	73389	53622	70142	41288	36426	21877	16501	509492	14490	59718	75468	70056	89531	29411	15141	44703	31055	129342	42995	35207	37607
C11 H29 N6 P S2	36742	50432	48542			59672	31114	33968	28434	31303	25659	21573	22493	33596	33112	22634	33373	40623	36458	42130	47983	22776	36678	4820	14849	49242	31124	51389
C10 H18 N2 O5	104115	106911	89615	100008	96907	94924	95946	100032	98313	88250	161603	113387	15348	48092	60449	168615	5418	206155	216286	107238	66641	46059	47232	62297		109451	19383	138200
C4 H11 O3 P	815043		822949	869986			4025287	4199995	4019107	4104489	210526	1194080	706337	97815	290409	2780708	4400281	1.86E+07	898520	316368	1171296	1416521	9656459	1025205	411914	776579	5182790	1183292
C13 H20 Cl N O	68705	67504	63696	66358	66568	61094	54339	53647	55936	53428							2018							707790				
C21 H43 N5 O10 S	1370933	1366666	1330491	1214372	1047657	946553	61830	72020	54543		79099	102137	25222	47951	47275	37025	32708	60336	48395	70642	88834	21364	81248	48360	3706	43218	28561	77898
C18 H43 N7				1367			61877	66828	64738	60871	11143	15071		13369	13464	31822	116846	123440	162707	105207	142623	48991	86412	85428		118586	199796	220921
3-HYDROXYPHENYLACETATE (CAS# 621-37-4); (M+H)+							6292513	6481434	6609860	6742434	4862275	190688	837120	1621245	1145335	1148351	1.31E+07	1.39E+07		9758113	1.40E+07	4661780	4127420	8317110	241142	1.11E+07		1.37E+07
C7 H12 O4 P2							369166	379801	372862	377304	301745		42337	104159	64921	64855	528499	520315	564771	457194	544711	307898	280129	430609	4761	490371	11182	537085
ADIPIC ACID (CAS# 124-04-9); (M+Na)+		33046			24832		36637		37173	36645	19410				35562	20366			48388	20366	31340	5754				68255		
C33 H57 N O4 S4	192243	31653	52164	60954	163561	57381	5307	13519	11589	12051	21173			10443	7409		5018	13997	5973	3976	21452	6389	15569	13889				9871
C13 H13 N9 O	52860	49023	47635	49276	48687	46092	18503	19810	18107	22069	39007	67034	5769	22975	29162	28341	12454	14760	14228	15713	23129	5356	15413	10588		13693	7561	
C34 H73 N2 O2 P5 S							4800	5109	5567	4066	6355				2096	3658	1040	3571	74760	15430	33823	9620				4865		32156
C10 H14 O	22982	21574	25367	24394	20532	21982	44219	42329	41511	43718	34001	39319	27852	45205	34058	35649	34487	43612	55084	33909	44048	47950	52853	45206	56359	62920	52508	50771
C32 H70 N2 O10 S2			11465		16000	11397	37852	33973	34789	23999	34142	47651	22630	36886	17543	12822	139834	94213	169304	8575	158932	43044	41642	26918		44867	36461	128982
METHYLMALONATE (CAS# 516-05-2); (M+Na)+	27912	31872	32084	31816	30767	31175	15333	13314	13159	12587			14360	10679		6109	6994	9875							23644	9761		19667
C20 H36 O4				13519			183419	186994	180334	175731	227550	607794	104900	71926	133587	128314	499249	363738	203182	114493	178575	49238	149385	139810	70537	226559	185983	404838
C18 H40 N2 O2 S2	32823	150840	224994	158593	143291	145457	58049	33641	38271	61437		141018		5296	310812	7942	3958			46326	19951	10236	39672	9979	3236	77577	43259	42933
C27 H48 N3 O13 P	137003	256180	361730	366299	499787	490154	75357	78644	72286	73692	63195	29534	5406	27851		57618	51782	68451	50679	107937	98108	51809	66468	61149	13006		34738	30071
C9 H8 N6 O2	42562	48206	49560	52417	47365	42779	173227	177043	175044	172731	101636	79678	71334	69489	210730	104331	96612	133263	142291	109595	160893	106853	150861	106427	84769	149936	105683	155601
C18 H39 N							1607860	1345838	1125579	952016					6100	1983			8289				15271			5389	2714	17397
C36 H52 N3 O3 P S3	100710	242375	96306	88262	83439	76793	26841	22916	19853	16244	31577				13237	13358	44714	30922		29640	44850	9866	38426	22539			18992	33249
C27 H34 N2 O P2	24722	22262	22689	22625	22725	20918	57707	57421	54674	53188	38148	46077	27870	56072	46717	33037	33176	46462	77187	32034	44091	61213	72355	56686	102387	97691	77531	59877
C30 H41 N6 O3 P	133057	134511	138100	132775	127857	126567	234119	250517	255811	251385	216202	235655	193289	263781	236675	204030	199611	244297	293484	208678	237712	283245	294110	271983	385045	363483	303613	287665
C27 H51 N3 O6 S	1606603	1614396	1634467	729613	1.06E+07	1312598	400758	356033	94228	32375	78332	106583		49175	61835	150924	163969	128040	54332	260420	62115	42175	266369	54723	20421	191481	156392	54649
DEXTROMETHORPHAN (CAS# 125-69-9); (M+H)+						2293	4958		2232	2329	10840						50675											3049
C31 H43 Cl2 N	18691					11285	83671	83408	77118	76119	63599		20147	38143	69175		235362	167566	205053	142116	140000	20093	138525	68070		132728	87561	101417
C26 H48 N O7 P	2.20E+07	2.08E+07	2.19E+07	2.07E+07	1.92E+07	1.85E+07	1009258	931835	925735	865772	674889	389891	219576	254093	323349	584776	559612	978216	773859	1909993	1619329	104010	898446	799935	106043	518688	438348	1316295
C24 H52 N2 P2 S	62699	69853	63800	60793	67404	58449	113887	103780	129133	118021	110006	96146	86535	109525	100952	87806	80192	120042	146215	101233	114449	123281	157541	137599	174365	159497	130177	117306
C25 H47 N3 O S3	47254	43119	41447	44941	48148	44024	101181	89889	71338	63990	87933	52436	32670	78160	80083	44599	168713	137867	167323	78781	360201	36037	114782	62771		117441	49600	361960
C26 H58 N P3 S	1175619	1178528	1186572	1022527	908603	869337	5614		4837														31286					15652
C16 H20 N2 O3	102352	101401	98104	93673	98101	82989	1044295	1096524	1081468	1059221	145408	223764	180776	154020	279911	184042	236048	308531	266578	221715	265622	224263	234296	225869	228525	263491	302451	350217
C7 H18 Cl N5 O	31595	35696	39911	30139	29608	58336	47981	57016	19940	53327	63080	36386	27797	36307	32376	30877	23070				50658	30262	30819	48171	29000		27786	127499
C7 H4 O2							1405441	1446406	1454895	1442629			167120	355107	243496	239922	2605186	2700012	3286875	2038302	2766920	1062699	944273	1812874	42180	2277311	66072	2705138
C20 H41 N O	3361	2238	2131				258079	200592	165802	136832	1841												4546					
C22 H8 N2 O3	36094	35903	34990	32796	31771	32777	156841	154983	157491	151540	47403	1846810	39872	34281	123838	40583	53203	47285	101327	42242	40531	37837	54452	38234	33665	69378	39066	45513
C4 H8 N6 O2	120085	149455	157698	152987	144446	144166	432627	448813	433511	443136	216918	354750	222848	179781	414632	245967	261266	439340	503885	305367		210463	371304	246162	229906	384452	428836	475193
C16 H33 N O3	35790	37752		36863	37235	35484	670749	714726	707712	686635	1094186	461453	329340	406004	339778	445575	2140100	849009	659647	466630	440503	174076	613699	570854	169054	597587	470001	493062
C16 H33 N O2	2364		2380		1527	1635	2506726	1785655	1763878	1747957	44531	55573	42631	23526	62181	26366		31118	418091	26071	25062	42025	353676	20624	51204	52840		31363
C26 H26 N2 O3 P2	14680	14742	16007	14828	16721	16311	64412	68412	70064	65598	57537	58656	65955	66192	66597	60373	56620	69478	69166	65982	76297	66730	71772	63516	63209	68451	68422	69440
C19 H25 N15							20982	22883	22644	21946													11873					
C6 H12 N6 O	305759	306491	308377	318294	304583	293114	553255	574831	542764	522132	691924	361305	687877	561587	374380	319157	307728	338991	346889	291668	315804	415277	455813	411709	449300	2198531	1366109	631475
C10 H20 N2 O3	8616	10104	7585		9426	7385	45898	45617	44610	44213	102648	120469	11750	30265	41978	65304	33904	113367	108594	22147	37487	18827	28805	47310	1502	39158	10946	96607
C32 H63 O3 P S2			1199				32215	36557	35613	40060	72116	71957	142653	37581	26510	20200	10129	23478	34663	21878	24551	29322	125640	51384	93780	34946	12317	27607
C27 H36 N10	290584	297242	284344	287940	280278	279317	617663	536516	682274	542574	470114	630494	426124	540190	421909	450517	426817	500982	561042	411562	482741	67752	591920	564179	1069718	695343	599501	541620
ZEATIN [ISTD] (CAS# 13114-27-7); (M+H)+	5572818	5496355	5308931	5477671	5323081	5193972	9506954	9606771	9272271	9346710	7841025	8307701	7142254	9437523	8430501	7707158	7527556	8324285	1.02E+07	7392421	7658786	1.05E+07	1.06E+07	9305636	1.27E+07	1.16E+07	1.06E+07	9624313
C11 H20 N6 O3							41639	41770	41281	42280	18542	76769					78956	75308	111249	72614	108894		97067	104957				1419
C18 H46 N7 O2 P S2							77080	84777	81228	85103	142962	621033	26108	53450	288144	46500	22590	2187	17009	35440	44127		15120				18840	104480
C8 H17 O2 P	152529		149545	158998			6758	20258	8306	20696		69467					132653	24850		11092							59316	14407
C10 H13 N P2 S2	17824		20029	20299	22555	22910	54187	60548	59343	58313	19146	28431		27169	46254	62710	31914	41392	53876	65959	61058	33499	51115	42958	6848	37307	48963	63585
C21 H43 N O3							16311	15106	16731							4961	35422		55800		36216		30530	23635		30651		46379
C13 H14 N4 O3 P2	287636	276113	263466	159992	234490	250979	3521									1040					10230		1462					
C8 H14 N6 O	124799	113687	109918	113841	109076	100152	33391	38382	32879	31605						10003	14100	2651	2062	31961	29525		147437	91635	1475	2339	6802	41237
RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-6); (M+Na)+			6800	8564	12617	23980	69608	92985	88110	78644	63617	77026	81737	63082	261965	79753	68984	52582	74350	60178	47316	73067	72355	72494	78035	81303	86519	91877
C24 H48 N O7 P	2626505	2580869	2464598	2099067	1756484	1550225	146468	160326	157317	154262	284118	429557	58717	175378	40881	87196	61633	297316	208195	282281	239500	71222	178497	118867		131842	114273	181066
C19 H25 N5	28915	16258		14380	28074	13999	37249	40449	39144	36778	34229	30904	41407	34038	36209	33504	46942	38436	82461	34717	41938	36460	46471	42920	38990	55160	67415	60821
OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M+2H)+2							35444	39404	35453	32981	89300	18985	1300	20102	130177	59203	36298				14628	7422	10626			45849	13081	
C31 H44 N9 O4 P3	64581	80845	67422	76329	63257	57175	12608																1043	2648				1733
C16 H32 N6 O2	40750	59644	52019	12098	21644	45265	181526	177503	184339	181141	215508	597362	101860	102289	127404	118865	515222	372826	190974	111993	169113	73188	148094	133759	70054	228788	183653	396353
C18 H41 N7							154303	31899	55331	48604						7842	70647	64377		59320	45133	18024	48259	42773		63733	54201	69552
C21 H36 O9 P2 S						2539	40718	44825	42859	41212		16081	4713	38943	20468	34301	21466	65874	108233	48196	47465	37937	50514	67526	22476	93886	28242	49445
C31 H35 N5	48040	49879	49151	43489	196184	30471	92936	80637	77581	70140	49786		30339	24609		44870	141117	51035	74988	113758	103452	21656	65235	56210	60183	67530	63446	146865
SALICYLAMIDE (CAS# 65-45-2); (M+H)+							14772																					
PHENYLACETIC ACID (CAS# 103-82-2); (M+H)+							1096														2694							
C17 H35 N6 O P S2	4241	3345		4130		3506	79641	86604	83203	82565	268325	20680	603442		27955				35461	29250							30366	
C31 H62 N O7 P5 S	155224	157184	143361	129848	125723	117097	10360	19315	10787	8381	13947	7722		9111	15911	5950	4084	7608	2638	11335	9876	4594	11486	6750		3840		11158
C15 H28 N5 O P3							81767	74213	74594	78094					7657				31966				22651					
C13 H30 N2 O4 S							56475	48509	76106	57024						13570	23988	109911	455187	57782	61900	61787			7654		291544	213189
C26 H35 N11	24651	24306	19043	24723		22448	246505	264560	256047	262958	193949	219540	222647	231023	261671	200927	254407	260659	311947	281965	239502	251810	270117	261316	224263	242230	251708	277558
C12 H35 N14 O4 P3			5461				174842	93679	88460	86254									33734				19479					
C15 H20 N6 O	292624	321562	326545	354875	358339	345502	330835	368779	367125	358726	376997	351659	363521	386206	348107	368341	375023	367359	390031	366080	339723	392546	392115	357892	381273	368398	385604	323172
C12 H5 Cl N6 O3 S							122762	134351	130531	133103	6310	66006	7211	56501	22574	103683	144188	70849	146672	130045	49279	139061	160020	187315	59391	139249	149794	139877
C14 H28 N6 O	29357	14032		24414	24934	22579	187658	178698	225515	170207	180845	387776	87612	106550	128866	139020	334120	305764		177901	167778	121345	73717	238102	129471	257749	183375	247259
C24 H5 O11 P5 S2							13526	201566		206671	281926	417599	1565	182072	212866	371004		241750	288371	312988		125238	30348	88191		273886	37013	
C7 H8 N4 O2	757273	758257	728667	769229	736346	707881	77974	81021	77716	70726	4271	105116			25851	6307	71514	342521	286912	116547	245951		370656	139841	1634	32724	12323	532036
C15 H22 N2 O3	102072	93507	95853	92248	95538	91471	15230	11472	14519	15051	40468	38602	3165		14676	21966	5650	24171	25668	11788	29711			14422		11922		31888
C15 H22 O2	322172	318890	354257	345124	334355	358219	331835	355204	397382	374134	327712	343268	364953	350319	308409	354789	428895	388692	408018	410419	349296	362173	375193	423891	353641	359915	342865	346444
C10 H18 O3 P2	318026	309291	302199	305598	297652	289511	558692	559078	546157	548469	442576	496667	368931	538355	490382	425307	441389	508355	641394	432083	514956	596406	647418	561566	696281	732052	629476	605563
C24 H50 N O8 P	281975	262509	260668	199598	158973	132870	7290	9153	8434		5746	6586	3504		5689		6462	8485	12657	10318	24751	8898	21802	10301	15523	11474	10078	15289
C34 H65 N4 O P S3							34488	34333	34990	39172	9687	29139	30860	83122	21145	109418	4049	20530	23713	31523	20690	7489	21519			105366	58892	55257
C7 H10 N6 O		15403			3511		338867	327287	330913	332636	77001	371118	97195	358353	89235	78658	341766	491414	474424	294797	403556	67112	503654	476742		444876	308065	431019
C11 H6							772214	762518	3973508	708153						259430				397433		587520				9637207		1.18E+07
C32 H61 N O4 P6 S	100868	105017	100959	90090	77574	73850	2340	6312	12862	7166	6140	1919		7404	7023	3422		3199	8892	6240			8580	4486		6172	4810	9985
C30 H53 N4 O2 P S			51764				127712	133929	125673	118614	110838		128997	107770	229119	89732	114817	108210	200358	94811	132769	107273	131801	171468	102087	235652	125269	136685
C38 H75 N7 O2							105427	59636	41433	54253									15256				9265					
4-HYDROXY-3-METHOXY-BENZENEMETHANOL (CAS# 498-00-0); (M+H)+[-H2O]				3957			1096														2694							
C29 H42 N8 S2							44432	43010	40395	40613				2619	6342	3708	7550	8937	18313	5031	10645	6059	7405	7190	6086	10764	13670	19563
C30 H40 S	28647	18249	61818				83654	81925	92068	87042	49933	192371	48095	57099	125293	48154		85665	68129	56351		46213		94866	42858		76142	92981
C38 H46 N2 O6 P2 S	115638	11975		7508	148786	1453	17476	23695	20128	18730	33422		45829	59475	76892	27554	62634	19772	44388	20792	8150	23430	6177	19489	24308	2636	11439	9619
CHOLESTEROL (CAS# 57-88-5); (M+H)+[-H2O]	67336	66665	66864	67029	42589	57144	27537				12627	15524					39390		11616	47302	70553		11516	26928			19251	61438
C19 H24 O4	64154	53745	71960	71156	59808	77663	34528	41018	49736	40886	43233	47302	49013	51053	40485	44824	40723	46598	41665	47816	40927	53981	42106	45361	56892	44929	46828	44743
C6 H8 O3 P2							202738	206187	203462	201403	148459		12651	38240	23020	23787	365907	364198	423874	281594	377292	144336	132215	248078		318672	2836	379669
C25 H51 N2 O P S	17130	15200	34270	16624	24229	21126	165471	202471	198110	194612	53855	168194	75932	130109	155925	73392	199442	271788	517456	406465	416758	112926	585947	575058	60737	166282	132174	156268
C22 H50 Cl2 N8 O	76888	74545	62036	161013	75710	99481	24807	21799				10539		7097		18805	116297		1549	18645						109404	8703	177012
C20 H42 O11	367192	369646	358605	364129	351189	343842	456493	472780	418541	415193	52189	130783	59878	81692	357678	79832	716465	869899	870419	502350	659403	128736	1268856	580603	70439	915873	289816	
C20 H37 N4 O2 P3					4835		93549	86643	82381	82263			1230		9068				32046				90934					
GAMMA-LINOLENIC ACID (CAS# 506-26-3); (M+Na)+	33493	13055	21126	320054	8051	304055	52328	66846	18461	21911	9203	27179		6400	8776	2050	37810	38923	49033	45352	16639		10054	26527	61560	14313	47323	34567
C32 H44 O S			11759				89457	148080	136681	63756	120504	184986	67503	91085	154252	56984	87624	133308	148254	79660	127327	76517	132636	136012	67206	190945	96408	191697
C26 H50 N O7 P	1.42E+07	1.36E+07	1.36E+07	1.25E+07	1.21E+07	1.04E+07	942728	892578	807990	803936	690222	793233	151498	510783	436604	297302	580737	1278135	1112600	1928130	1541343	230530	1110575	658140	36184	875167	604497	1062113
C17 H38 N2 O2 S2	25921	32231	18262		30638		60421	75057	61910	59734	12239	51298			2893		3756		5901	630254	4899	19389	66150	19384	18213	51269	43339	
2'-DEOXYINOSINE (CAS# 890-38-0); (M+Na)+							26919	25243	25974	25167	58522	152713	10214	21853	29156	6984		24263				8637				16722	5622	

C20 H32 O3	222259	249830	254213	269200	257049	71886	288324	376162	295968	487655	401405	688712	235902	173413	341988	243171	232300	1061977	432842	453682	1126593	220973	912341	397141	587915	434990	573028	1057911
C31 H60 N8 O5 S2							1891	1708	2064	1561							4221		2467		4458		3106	4778		3278		8797
C46 H78 N O2 P S	17173	14315	17779	6324			21865				5310	1795					41007				235739			37640			1467	268104
C6 H13 Cl N6	9597526	9538664	9180479	9555067	9247353	9040986	3630419	3663625	3546237	3569400	2405034	2020843	753883	1937177	2635346	3513920	3342043	7753906	8964846	4500354	4866243	3236516	3937325	4518989		6430240	2663920	8074084
C13 H16 N6 O4	37530	40012	29026	44904	43366	33229	474395	512962	511776	505791	396711	467823	443706	560106	660738	375533	416282	556141	546635	520238	480658	489697	541953	420222	489656	495235	653960	518741
C27 H39 N5 O12	134614	128635	135357	120204	105405	98900	160443	138796	143811	155482		11000			61217				27189				16131					
C35 H45 N3 O2 P2							26348	28424	28512	24007	41341	48897	11905	34898	30164	14381	23824		23493	27247	28566	8167	29283	32976		27828	18311	24500
C17 H32 N6 O2	507346	505628	489445		504212	432299	1670079	1612741	1560355	1115500	657124	655714	92838	611598	9393612	689745	620629	681113	563952	2636565	755500	46958	624001	603588	671851	682050	685878	948202
C10 H26 N4			1040				63732	79878	75604	78322		227561	1871		3675	20312	25022	2763	100224	41505	5519		733128	278930	3666	53465	328247	20622
C24 H50 O13	134157	137720	137108	130860	131053	129263	191609	195654	189047	187224	31817	76750	36733	44153	244251	45126	279440	335706	364526	241381	279301	60555	474739	257356	36165	333365	133520	333297
C31 H27 N4 O P S3							43318	49247	57308	55929	8559	72291	6973	24596	17300	11421	53102	52270	534516	105308	14314	8121	141840	35328	16279	201191	19016	16751
C10 H22 O6	170894	177407	179643	174208	174237	160366	484695	489731	482899	469426	114841	257525	152806	147114	687497	169159	552538	1028034	518244	423387	477674	250737	981228	432032	208968	743756	482561	1145805
C15 H13 N O2	106653	106785	104835	105950	99221	97591	24300	25129	23880	24901	10294	20808			15595		22432	56609	71594	54389	77772		45496	30778		36983		70946
C26 H52 N2 O2 P2 S	106937	110761	107603	109730	106137	104578	102943	100458	102742	106388	117610	99929	89680	118388	98702	99179	102419	95253	122945	91831	88173	138460	113520	124820	197817	159616	123774	102098
C48 H59 N3 S2	20239	23611	23892	5432	29638	34385	23212	28660	16115	20271	12690	21918	6408	14091	7865	42361	36477	12000	50784	35523	79822	8609	73996	42163	5275	10913		27174
C15 H27 N O4	493341	490071	461084	409678	370023	328635	37980	40745	36941	38261	14167	8288		2524		3100	33066	30967	61079	169607	136272	2504	72321	39262		58914	30156	65159
QUINOLIN-2-OL (CAS# 59-31-4); (M+H)+	1782					2493	9243	12334	5391	11399		20278	1415	9088			11771	13143	27757	7182	13908	10358	24564	16669		15926	10263	12456
C21 H41 N2 O3 P S	19639	19580	22013	22251		22172	107543	124481	125592	122099	54410	614155	30851	34411	147975	127388	59488	280015	110444	89139	143336	50894	192760	70814	27329	87054	54664	549706
C5 H13 N O	224350	176552	229304	203144	175921	159124	3443	2848	3095	2314	2023	4590			2500		1697	2925	4526	10952	5585		6322	3542		2790	1483	4880
C19 H38 N2 O3	50077	50368	57455	47285	49372	44179	410535	445685	429696	432776	157482	2471078	83371	99905	452753	394532	190451	985468	395592	276151	489748	128083	692743	223998	74294	260291	161485	2341968
C8 H9 N O	1486552	1360839	1395961	1414518	1361847	1340170	1214008	1239732	1181555	1190443	797922	712734	85903	408055	868963	1177136	1213128	15470		1358305	1815899	760668	1276556	1715991		2394370	842281	28389
C20 H28 O2 P2	45490	45520	43259	45746	44605	46502	33377	34962	36481	31756	9077	22018	12250	17162	84470	11533	25402		43015	30861	26880	8288	36799	53453	13206	33033	25534	41124
C14 H12 O4			4843			5003	103453	102506	107180	105885		61214	55963	89320	28284	77171	75211	71040	87262	55066	82083	71196	105189	28435	77639	203987	253005	235659
C24 H4 N O11 P3							121652	54367	58838	55369					1836				29562				11482					6627
C14 H31 N4 O2 P	253925	229811	157858	272909	208445	205899	434350	660103	572342	539215	313271	766616	315088	342872	250022	184092	424274	775915	851974	812807	696382	224662	818679	758492	182829	840001	582796	510331
C14 H14 S							41269	40597	41617	41919	134774	465709			4626	3050												
C24 H49 N2 O P S							78459	87764	97441	92256		77173		36518		23641	72925	117929	286657	205645	227654	34939	317560	333446	19125	53950		
C6 H12 N6	91080	235895	307855	243202		228201	11078	14372	18793	28694		5822	14787	17144	4810	1188	4040	3635	12199	4542	5547		11593	6478		26714	50606	16119
C24 H49 N5 O6 P2	3468961	3556284	3335363	3022516	2905695	2525262	273600	300102	289829	283035	309255	228324	71760	200625	273934	151719	342988	271272	397975	369414	510779	112284	475331	243654	31098	300567	204018	395520
C16 H18 O2 P2	57180	50405	56813	55244	49735	51475	42493	41986	16094	16080	72297	160865	9887	63251	55598	52719	27996	31938	31349	26297	45356	10192	29402	13058		33362	16630	37467
C12 H23 N O2	76894	152815	136448	141678	134997	131350	201205	208707	206196	208542		335267			118972			105703	284480	254700	320056	239042	555069	295793	114014	89543		140868
C4 H4 N2 O2							502467		499505	510423	417979	520961	113340	253807	347781	264822	782852			567997	846072	194784	737018	577262	40542		434707	
C12 H23 N O3	9938	10611	9627	9945	9459	9085	84828	92556	90437	86082		112643	42032	32116	85433	31616	86409	127897	230251	157215	207584	32788	225376	227461	11224	77485	52169	102436
C12 H23 N O4	230417	227656	210814	223840	213414	203030	446522	451515	438897	434550	1371700	545380	288563	643115	709978	837784	498917	373244	834250	279842	614381	65277	136002	61537		269364	74504	162795
C8 H14 N6 O2	16807	20035	16741	24432	37574	22121	106526	100640	136186	122584	52293	182505	57172	87514	86925	112045	94418	123689	168618	121392	136130	55557	158300	123244	42850	176456	129794	180151
C8 H14 N6 O3							98042	104857	100099	100007	47717	217423			25901	21349	193007	197175	225379	179002	223903	33583	253174	237038			5407	9353
C19 H37 N O4	126262	125678	117992	113317	97648	88110	16127			12087	12455				17442		18829		24763		28843		16261				5302	44906
C22 H27 N3 S	41583	47815	44664	45423	44064	42105	414193	428553	410770	427466	272645	295027	311183	328182	307640	318237	381590	455334	649562	430071	377182	413765	393836	352268	349286	371862	500313	541889
C7 H20 N5 O2 P	3833		6057				61531	60130	58584	62762	19381	66488	24339	40871	62248	20085	53612	89054	113929	72145	95654	18916	115219			67392	51782	88173
CYTOSINE (CAS# 71-30-7); (M+H)+							12636				14746	40148	5351		9114								2547		2488			
L-HISTIDINE (CAS# 71-00-1); (M+Na)+		4283		2455			17391	17700	16807	15284		31956	2061	7578	11131	50227	12069	12196	16288	10076		25321	9784	32093		20443	12554	11609
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0); (M+	51840	53731	50174				32600	28226				10182				13436	5764			4696	12160	1498	4307	2523		7945	34662	16708
C24 H36 N6 O4 P6	31078	29918	32234	19986	29714	12536	25878	40900	31397			38101	17439			36416	43398	24321	30007		21604		55289	28117			35901	33101
C23 H49 N5 O9 S	418353	421260		353301	409557	385470	85188		32858	33937	161711					14868	37054			33967								
C24 H50 N6 S2	164208					113410	118762	115109	137831	106152	319384	198617	79829	136340	316699	172166	634051	91063	430195	71889	460369	3995	1105683	88267	49339	135953	255597	93835
C8 H16 N7 O P							100659	106818								139741	99250	189629	167394	257715		138689	107971	77281	8899	135045	28522	213194
STACHYOSE (CAS# 54261-98-2); (M+Na)+		2287					20825	22172	21720	21914	5109	7000	2548	18894	10482	18602	9367	32544	57600	23987	21195	17887	28762	36265	16597	51400	16354	24841
HYPOXANTHINE (CAS# 68-94-0); (M+H)+	1244959	1220877	1128955	1212671	1127630	1141635	8854164	9171860		8934224	7349395	1.02E+07	1762325	2224170	8162871	6139419	9008973				1.74E+07	3872628	1.18E+07		653867		6828042	
C34 H48 O2 S	4073255	3865085	3928105	3592397	3214132	2944680	151360	153493	128590	142541	213317	217363	123616	210215	216158	94727	152978	154815	196769	179467	195403	98208	134489	161493	135402	180754	107022	194950
C8 H21 N3 O4	31800	27795	34669	29836	32069	33561	2134			1965					1031	2060						1069	2627			2594		4053
C12 H8 P2	210866	215543	194607	204689	182065	178800	3461		4346	1753	20373			9634			3470				1018							
RIBOFLAVIN (CAS# 83-88-5); (M+H)+							2013	3808	2473	2852									8444	10005	3902	2284				3991		
C5 H5 N5	318358	294205	279875	304306	276283	279512	515523	525383	496041	503751	422911	417648	365061	508686	459242	403644	406415	475809	604880	393515	456603	548005	558251	507285	628850	674123	558591	563752
C28 H48 N3 O11 P	515906	533086	515435	500416	459930	441336	163544	148001	127033	126664	196639	49717	56890	134215	95405	61264	387612	219715	216382	223257	382207	53682	178879	104325	12443	166298	55097	400984
C32 H38 N10 O3 S2	66604	72647		46551	43254	40092	108438	117355	114267	113379	192894	168248	226174	248338	257286	162983	235784	125618	194122	101328	61076	159615	42830	125717	178034	21100	64861	59525
C13 H18 N2 O	4315	5642	4962		2869		1834339	2075343	2156679	2305420	58261	365985	339897	386617	108897	433981	2398183	2482808	7842151	4336306	3919497	517945	3846784	3918512	238394	3473462	367151	2828380
XANTHURENIC ACID (CAS# 59-00-7); (M+H)+	7880	5983	8211	7831	5727	6403	24006			23910		20633		7568	4583		5162	27626	82587		64646	24646	66710	43575		38431	21347	38852
C31 H58 N2 P2 S2			3753			6280	47693	24521		25008	5208	39129	18206		7380		34656	34549	44731	28844		12823	55935	50138	8588		8655	
C28 H57 N O5 P4	3532654	3594853	3524380	3298473	3122039	3013126	73384	61538	310999	51771	166048	67801	68245	180598	92909	53382	93668	85316	56648	90127	96747	42214	59166	60834	13383	57325	142619	111648
C30 H51 N O16	247781	244282	248539	49978	209279	45101	13665			5501	10524	17387	14626	4276		9075			36914	9405	18086					3401		
C39 H79 O P S4	9087	2688	8288	7405	2661	17873	13880		22409	10687	17435	20439	57250	14834		7002			1570				44812		26802	16341	9046	
C33 H54 N2 P2	60056	103665	22630	62175	57049	84770	102538	118648	115210	100584	159841	131227	172067				54758	77301	175269	89138	122534	11844	132827	189551	65629	92423		122429
C23 H43 N8 O P	269550	266916	268875	270960	253284	261955	28457	491929	602872	465341	426209	427017	389230	141486	420475	395515	378449	443838	616233	390222	426187	583656	674909	624523	807343	627555	531152	488499
C36 H47 N3 O5 S3	161921	134933	143222	132627	112370	130272	6775	17216	18455	10300	15153	72754		5436	8727	7391	9971	9754	34591	14347	12008	6195	10338	8598		3536		9245
C12 H25 N3 O3							65988	64109	62615	61557	204542	102543	25004	53772	92738	91716	50852	71000	91681	25639	57049	20349	25785	49997	2075	64471		66105
C16 H30 N6 O2	59149	58046	43388	44909	46135	36092	48737	111071	111945	113214	186627	57133	332712	29243	47487	61969	91422	168780	195491	117182	97610	29077	153246	105485	7722	184953	71681	151451
C11 H12 N6 O2	199571	132880	189215	170640	188152	169228	658109	678125	706616	694595	350148	219067	230089	226181	387271	309066	296153	391162	398759	303946	375643	360825	361560	311362	311911	466802	364802	370633
C23 H8 N2 O5 P6 S3							70862	165807		158285	67743	148789					53894			97968				89348			63192	
C27 H44	68453	68293	66865	66122	45976	55248	33411				5359	15724					42891		13934	48160	70541		13600	29372			18958	58507
C9 H23 N5 O P2 S			1397				20621		22967	22317			1536											296422				1505
C40 H61 N O4 P2						694728	237086	239582	242099	232283		224927	235024	260179		193258	217199	231731	309980	194893	218586		294083	233990	347237	323047	289740	266834
C17 H35 N O3							115664	115493	109073	109628	35365	72203		32712	32459	68811	273656	410221	297329	219817	165164	98174	185266	214723	20431	196210	119546	336716
C26 H51 N4 O2 P S						40694	55227	41548	39018	49362	26355	36180		14075	6989	9968	156208	86655	117572		163039	25124	129609			112099	32631	132749
C17 H35 N O2				21364		19003	615531	393293	397490	383510		72366			46020			30218					68547					
C39 H30 N6	183153	210536	212941	212225	197392	201346	67894																					
C37 H33 N10 P	35886	51659	41336	42946	93559	104847	31328	33466	30682	33391	22307	13771		6685	14485	21299	18852	33326	3138	49143	43426	18243	28362	27049		15001	15211	36962
C18 H37 N O2							1161257	714425	729159	720966									107108			1565	148724			18079		16942
C16 H36 N6 O2 S	12075	12698	15576	14700	146174	15082	38497	235252	236996	25150	87177	54519	27277	43862	29156	135769	122258	97620	58396	35170	45946	129455	313786	54460	64396	71216	226189	332677
C23 H20 N10	409599	420215	416755	415806	418767	412452	3462125	4217977	4253325	4295069	2984552	3311784	3774397	4029687	6713292	2817459	2603252	4189790	3963764	3878247	4493002	3558553	5079941	3542411	3433504	4133936	4492623	4845317
C17 H30 N6 O5	67547	66426	64160	66910	66286	66265	1460	2801	1749						2236	1995	2940	3539	7709		4500	1313	4068	7449		3635		5110
C16 H33 N4 O2 P3	52191	51050	51513	52010	50496	47927	29425	6226	25909	23578		16074	10395	12412	65189	9817	20424	24699	36468	25983	21291	6641		49173	12051	1021	18623	31435
C12 H24 N6	31653	10628	28612	34445	22114	23539	49086	42799	53799	54584	51874	54110	48736	49234	40955	36782	57744	42317	47917	34731	42511	44827	48081	54611	42954	54837	43400	58115
C32 H40 O6 S	5318	2757	1390	7118	5735	4896	42157	36337	32737	35021	26544	67465	33359	55800	229013	26879	47911	9942	34767	20050	51623	7770	92326	14364	96217	29368	69799	21248
C5 H9 N3					1291	1012	188355	192790	192232	185204	217474	74390	86948	114645	238179	81115	192555	222332	216924	245150	219563	131061		196860	29010	227018	158880	226337
C9 H23 Cl N8 O							2618317								2666338	1151788	58596		1408621								1631945	
C6 H6 O5							1337767	1365130	1310006	1315960	707877	1068222	525639	378377	884704	882880	1501036	961796		1774980	2431005	580282	1776207	1651906		1932695	961121	
C18 H43 N7 O				2215	4225		37129	37560	36403	41311	2289	13699	1527	6982		9887	84814	66838	95527	61504	91952	38775	76293	67067		69280	82050	119110
C20 H8 S2	6749	6460		7005	6194	4511	302989	331530	326230	326236		120062		49666		223007	306671	367460	546334	306455	102310	196218	467670	595618	15254	488323	303785	445793
C30 H44 N O2 P S2	9886		8661	9725	14551	10681	25301	21901	18721	16928	23303	40499		23165	19403	13156	45953	34955	39133	9785	86373	15584	25926	13941		25328	33870	82007
C35 H64 N6 S3			3155				23767	36305	40614		26005	55756	56850	39289	21404	39839	7127	13185	17935	22496	14407	5983			7296	49445	37561	16901
C23 H45 Cl N4 O3		14956	128725	59188	94292	66978	16633	26365		143536			6325	139765	263041		15268	34338		35688	35035		258978	33532		60263	41835	44560
C24 H29 N2 P3 S	39290	38014	40164	39696	37477	36381	549351	575853	557294	553152	387942	436378	451672	469252	440462	412415	528854	541718	678063	564129	507472	552825	595281	528108	507165	555807	568833	607644
C3 H10 N3 O2 P							547486	557446		551144	215998	216183	101488	137202	240928	245059	368457				1191607	559868	808116	825790	209410		583202	
5ALPHA-CHOLEST-7-EN-3BETA-OL (CAS# 80-99-9); (M+H)+[-H2O]	67336	66665	66864	67029	42589	57144	27417				12617	15498					39390		2871	47302	66948		11491	26928			19251	61438
C12 H14 N6 O	276227	291536	274271	261483	261103	265406	161761	180792	196878	194514	229251	204647	215681	193139	176914	219691	226034	184701	215655	188083	167780	209368	175525	220279	236423	197688	195532	188092
C9 H14 N4 O2 S				6943	5137		110092	121174	111945	110663	25127	142656	40256	101902	34032	26575	130835	156073	190437	136929	158773	22122	208677	188730	14575	152025	132344	162879
C18 H34 N8 O4 S	80584	56783	63403	70147	55912	45492	50841	17971	7011	13890	18573						5660			40790	36805	23868	23852	22331		11665		25478
C15 H27 Cl O S	100432	77954	94857	80616	96627	95998	78196	82216	72300	64595	70603	74622	74121	85886	70958	67424	77817	68667	72905	96865	75482	68406	88450	90117	65711	91366	69360	56461
C16 H28 N4 P2	51476	55259	48841	49471	49248	49256	23338	24872	23300	21717	26038	44916		13673	12648	11035	17106	33792	37283	31319	35321		30746	1973		31118	13569	58372
PHENYL ACETATE (CAS# 122-79-2); (M+H)+							1094														2694							
C15 H18 N6 O	21079	21953	20945	27024	9261	21277	65420	76047	61472	60834	61513	88544	60755	60950	82520	39005	71816	66971	94315	115204	57957	50386	83391	75200	55240	87089	92465	53159
C13 H19 N3 O7 S	37188	36768	34507	34727	34755	33909	51649	55052	48387	51578	26058	13289		4476	19602	4902	23890	20979	39379	154893	1935	2812	17375	236017		33715	45682	14226
C25 H24 N8 P2						1755	33453	43170	40838	39972	24935	28915	30555	36160	54461	25829	29953	37777	33813	37450	49905	31860	46029	36277	29278	35613	43815	48835
C20 H19 N2 P	33138	32499	34217	34135	32516	32282	49208	50093		51937		34113	17904	36789	80264	18744	61094	59704	28153	5474	58406			54591	27112	48972	32588	68582
C36 H43 N2 P	8857	11866	13911	16305	20854	23610	29167	34019	38273	33657	28622	32703	5467	35487	31937		24786	28040	38182		33479	32734	39437	29362	42419	42929	39283	33159
C28 H57 N4 O9 P S	24716	22727	22549	23157	27763	23291	45337	49574	46666	44466	10141	24509	11246	14604	91668	14791	54675	68656	83055	66238	60175	16862	85524	60722	9499	63665	31859	76838
C16 H35 N O3	105009	102786	103411	114333	127297	118367	866269	911418	894535	887291	841989	759862	714890	763859	1124222	731691	604105	1120478	731358	1121162	746288	943319	1182568	577202	667436	952286	1051124	1136916
C14 H14 O S	18036	19486	17631	5049	14414	17997	61679	62569	62857	4590	15820	52691	26467	38728	91824	23193	57106	61962	94007	61596	11547	17287	87204	75846	28712	69033	64143	109479
PALMITOYLCARNITINE (CAS# 2364-67-2); (M+Na)+	70376	73885	72915	70073	64379	61176	15583	19973	16600	20120	27745	29315	5909	10969		10988	30253	19536	39962	52523	110619	14763	25726	29912			14361	94595
C16 H35 N O2	688510	693678	669290	692219	680001	651482	4241310	4627624	4493189	4472456	2396159	2218640	4581898	1860418	4050571	1559634	3157792	4542449	3105154	3814002	3471626	3320367	2879056	2007852	4736581	3067890	2751433	4471785
C8 H10 N4 O2	1720148	1669872	1642277	1718852	1645662	1603841	104729	104530	102357	101648		123517			41777	39613	51510	338183	22891	36770	240693	35271	552306	240023	4971			427567
C12 H23 N7 O	72782	68948	70317	79455	76190	71045	1699884	1800896	1758773	1735780	820788	2793109	1289790	1033536	1238342	1546747	903697	1061524	2542702	2060147	2663416	1965462	4064966	2369873	993354	954735	913672	1571231
C21 H16 N10	4765884	4758901	4748128	4776485	4680134	4577328	2.85E+07	3659318	3562761	3602194	2232999	2781593	2744283	2808125	3016344	2.51E+07	2512327	3327699	3522560	2980270	3714918	2959039	3998894	2787035	2694321	3531087	3592910	3835753
C16 H22 N6 O2	39171	39440	49134	44918	48591	41935	28127	39039	43176	53448	47462	57177	37731	37380	55528	30773	47230	49277	67997	70684	59183	41066	108272	64812	32248	41657	89684	42168
C19 H25 N6 P3							67500	71373	68273	67093	42782	33277	6430	22132	29025	93766	97495	210027	58697	24733	61720	69965	89193	91318	7468	266833	118962	127387
C26 H51 N4 O3 P S			7533	5787		5730	71964	72612	74569	72921		27354	27982		39721	25795	349264	99376	250580		404662	14040	104404	35393	12211	90170		300737
C11 H9 N O2	6103946	6124230	5857046	5947306	5718049	5634792	20753	19355	20848	23524	19184				5577			4430391	5197045		60398					29691		4657196
C33 H59 N3 O3 P6			1391				53166	42812	40495	39708									16349				19047					
C18 H37 N O3				3497			398232	414458	418798	415273	359934	513984		165287	218407	397827	969756	1078247	1069947	900523	844485	318484	539604	632978	78560	736423	476072	1087256
C12 H22 N4 P2	38453	40856	39556	40169	39451	34890	50682	36985	37060	39997	15714	31736	12295	21748	23294	15290	47279	60459	70350	43377	51707	15801	56976	55806	8722	67617	32487	51924
C30 H62 N2 O5 P2 S	8069						412592	403648	409920	405673	93269	121183	28068	19305	3989585		180924	221130	173912			13611	29980	37615	733057	115593	79914	154247
C37 H74 N4 O4 S3	36354	43441	33320	5465	35237	9494	47457	45875	26713	40392	33087		15707			8469	105332	40371	124888	42690	94070	13341	57896			79546		105648
C14 H18 N2 O2	1436796	1434617	1378706	1425496	1387895	1335147	209948	208067	205106	196899	186022	44831	34190	33201	113885	39285	474308	230641	512389	594629	774375	37540	284694	392123	14202	358501	91849	1092092
C22 H28 O2	154157	149016	153028	157684	143249	138014	30790	40790	40277	30847	14996	46317		127448	31875	111950	6708	40044	47789	49937	63479		30559	189661		31934		62938
C16 H19 N O4							86004	82932	82126	83124	286320		49235			9553	679770										6729	
C8 H11 N	216720						77482	77477	73776	75859								108084	420824		135281	73066	58842	146307		164322		102026
C25 H46 N7 O2 P S2	351947	359114	365191	322019	294491	259538	28965		34944	35656	54041	57754	10680	27323	22467	34430	12539	51335		42228	47666	14079		35891				
C22 H46 O12	213350	212656	205647	207082	200826	197915	263911	262017	259242	254436	34379	93613	42383	53934	269604	54975	408430	488830	482325	309132	385542	79297	726876	354298	45799	511341	185865	470303
C10 H14 N2 O	1413						585171	574329	552313	558126	37273	36641	53095	55473	15418	67325	1370564	785605	2382677	924811	690829	170086	458133	1020362	22520	1151696	26969	648712
C27 H54 N5 P S	35071	33126	36190	37106	34257	35037	57753	61953	62879	63583	56428	58843	49939	68666	58241	56029	50769	59195	71348	52067	57794	77486	73218	64944	99683	81724	70686	63844
C14 H18 N6	127002	124591	136885	144939	135830	154137	126510	140305	152176	146420	130065	125783	155029	143120	145213	142498	134130	147022	160938	152153	126779	141785	137569	144540	153232	149217	157462	127513
C33 H57 N O P6	38312	39727	34915	27118	27191	23752	11357																					
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+H)+	277643	280047	269629	275885	300282	293574	554443	579517	561343	554485	436652		368581	538334	463426	405992	441738	505877	663722	438421	516562	589960	610402	575184	681892	773375	645313	617779
C12 H15 N6 O3 P	12147	12696	14296	14242	15006	12505	37757	37175	35827	37196	9993	20013	11899	12991	52823	13051	43714	74970	24996	33889	37175	20005	71427	34003	16194	55887	37195	81030
BENZOATE (CAS# 65-85-0); (M+H)+							20123	19833	23068	16450	1230	23135	7429	3758		12185	27118	20220		16402	3337	17277	28937	30076	14156	34317	20754	12675
C11 H15 N5	490739	456943	429239	352935	286829	259833	18311	112359	84786	112527	139525	99942	70791	91322	130724	36817	146859	54008	315470	35866	182850	25825	196389	22329	1262	99612	33561	85070
ANTHRANILATE (CAS# 118-92-3); (M+H)+							14772																					
C24 H47 N4 O6 P	1230757	1245531	1216790	1231168	1220053	1214859	1997886	2111592	2094192	2102034	1881039	1821941	1699804	2209958	1911352	1762605	1721898	1952225	2216708	1654751	1905608	2472470	2305649	2132732	3152973	2681454	2350358	2099360
C40 H53 N O2 P4	47330	19422	19522	42712	48944	15218	30603	7107		1126				2704	1511		5224	1564		5893	6999	47644	9773	4360				2926
C17 H7 N6 O P							183907	180290	172666	172253	120206		3437	16908	8522	7601	375768	377266	455001	277781	397079	109417	99120	229843		318342		393045
C8 H16 N6 O	276511	295878	272006	259296	232253	243127	193349	229086	221920	214354	337890	382211	732270	342277	338681	303295	729759	496623	500978	370623	426222	422692	592254	574062	467723	287189	989128	556414
C11 H22 O4 P2	79694	75095	74996	79243	77836	76213	130911	143714	137969	148118	117594	131636	101550	145109	122779	116541	113562	128645	159415	113629	128675	155683	153348	151967	185784	183432	168593	152400
C23 H40 O P2 S2	35173	32984	32463	32505	29949	27481	116272	118747	102797	112899	72244	85518	46262	100079	91864	67168	65482	93431	155293	73311	93621	115161	140039	116633	171821	181715	136099	129820
C12 H20 N6	65801	127673	174141	135784	139300	134957	184045	200070	203097	195888	100356	124449	133289	106944	189200	129532	173072	208039	207342	172242	152950	119942	140944	153320	111267	128748	160933	131510
HISTAMINE (CAS# 51-45-6); (M+Na)+						1012	13699	14967	15306	13841	15477			6330	12823	1087	15114	20326	17856	28074	23544		10746	13844		16384	9897	23154
C38 H65 O9 P S							5354	5109		4066	6355				2032	4671	1040	3571	77762	15300	33823	8049				4946		32170
C31 H39 N O S		21292			21774		128452	137613	129551	135017	109850	128210	121791	125256	117533	111389	136505	130866	132062	135538	126013	132587	143721	140595	127996	137067	128520	134864
C26 H48 N10 S3	26628	25654	27351	26473	27939	22469	40605	52099	48835	40789	37208	40928	38082	49837	42443	37606	41121	46329	49705	44340	49445	52539	55098	49987	70706	61055	49272	49449
C3 H13 N7 O S				2292			35636	34804	35192	36520		77622	18949	17706	10672	24190	25649	31308	36301			22794	65197	48225	33013	50399	67698	49118
C28 H49 N4 P3	34940	36090	34954	33450	36886	33973	55342	60359	56129	53243	52346	56087	47423	63745	50822	48504	48783	52354	39552	45698	48414	65432	61802	61733	97146	79799	59209	50609
C18 H38 O10	420435	429431	403479	425431	409519	403661	543319	543955	532741	531140	63164	171271	77830	107465	422541	95323	905998	1028121	915525	544453	850438	206666	1672896	685858	95464	1222485	396042	1031378
C14 H27 N4 O3 P	79837	82085	86493	79371	76579	70925	135862	171976	197839	213718	68804	169714	48817	47955	120387	60277	74405	107470	173377	750800	179321	59274	366019	147198	56224	120914	406795	151811
STACHYOSE (CAS# 54261-98-2); (M+K)+							2463	2141	2146	2462	1034	1850		3417	2466	3423		3611	9128	1454	1015	1501	2949	4234	1341	6862	3557	
LEUCINE (CAS# 328-39-2); (M+H)+	2.32E+07	2.32E+07	2.18E+07	2.39E+07	2.29E+07	2.27E+07	1.09E+07	285266	224943	6086566	1.03E+07	1.63E+07	3460135	5699008	8875961	1.40E+07	1.17E+07	513847	666204	1202318	458281	5831470	1.26E+07	1.31E+07	322695	1.50E+07	4170325	571147

C13 H24 N2 O	2614						28462	25702	39345	28217			24874	29339			23771	25598	32063	28122	29580	29505		30604	50089	40123	36738	
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+Na)+	236884	235808	231525	239019	226671	223291	7619	4925										8006	51459	16253	4888		20335	4994		9336	4169	9511
C34 H45 N4 O8 P S	40463	39873	38540	37872	39043	35818	57684	69099	64270	64038	57415	60050	51699	66201	59361	56313	51035	63393	69984	54298	60094	73250	71036	66318	94351	81179	74977	68640
C15 H14 N6 O	56069	58526	60300	60395	51936	50432	24987	20837	20653	20215	17957	20884		6466	20935	64457		60456		43803		12652	11918	17624		27122	7249	
C41 H80 N O P							230315	104565	93916	91033					2862				34389				19022					
RAFFINOSE (CAS# 512-69-6); (M+Na)+							34867	33144	34613	35960	7940	12822	4378	31428	16818	28460	18500			40409	39017	29327		54820	17171			
C22 H45 N O							75068	62610	65689	48063								2115	14194					2691				3113
C21 H43 N O							431574	339298	309083	273554													4426					
C23 H47 O P S2	7370	46694	47938	5213	44936	43808	3494	4512	39666	11527	25074	167920	15494	28934	4698	11694		7182		98195					3193	20062	135887	26261
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+H)+							9130	9071	10599	10007	10822	16179		4942	8531	9320	8169	14180	23898	7063	25925		11288	14775		14459		25401
C17 H11 N7 O6 S							211054	223290	222506	218086		63228		11695	5647	118818	193152	326344	546506	211962	39486	110567	372432	520988		418938	184445	392230
C19 H36 N2 O S2	62405	53898	66610	58926	84960	71857	4375		9510	14269							1438			178823								
C20 H47 N7 O2 S			40381	39232	35826	36873	366347	380070	371635	366789	1145687	126521	2015224	73327	238637	92152	33363	86279	138310	88202	87763	26954	77590	39265	15963	66603	106801	91334
C16 H35 N	1294	1278	1077	1029	2361		100658	65396	50728	40213	2624	5152	1701		6639	2118	4383		6579	2805			3446	3670		7504		12828
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+Na)+	180138	175693	167616	35378	169450	31308	240166	231331	109208		171843	337001	14285	116261	887088	164620	324433	256982	73084	285505	423144	12744	168135	107663		244190	138238	393182
C11 H14 N2 O5	149199	150726	142035	152250	146680	139859	266690	267624	257880	258698	208873	236196	177749	262480	234458	210650	205689	237524	292786	201293	239360	284520	305295	273199	337015	346330	320249	274424
C34 H61 N4 O5 P S	7337	6731	9133	20888	17584	11001	343896	345313	341641	338532	81537	119280	22205	42381	3473438	26703	131791	170431	117145	43282	19227	15697	28739	27676	505060	70692	43806	124556
C20 H37 O P S	56268	76258	62923	87932	104076	111429	9793	20178	11115	13595	38227		6757	1365		14735		4536		46481	18122	3713	9363	10453				13738
C38 H66 N2 O2 S4	4916	1634		1693			14443		10291		39112	15734	29224	30742	16185		15766		33125	13178	14869	24967	15557	14941	26890	23554	22024	19825
C16 H38 N2 O6	192582	46199	201193	54782	54109	193965	324023	311274	311616	426114	148102		198512	175254	355723	271887	530359	361230	110970			330032	1015621		284813	393123	97257	777157
C7 H12 N2 O2 S							1072461	1069639	1027815	1017581	964120	692935	461509	1001299	1052744	905577	757255			971525	1187627	1207407	1173484	1153007	902924	1520136	1037747	1499767
C23 H40 N4 O3	4404						37393	33878	33237	28055	23934	26796	21427	30816	23630	44471	44260	43677	54884	46140	28517	25693	31809	25224	23136	31063	22506	30752
C16 H24 N8 O4	162084	165033	157458		148109	52219	84585	75043	19962						42209	27618	66492	56519		66744	119972		131805	68034	3052	101676	82725	138209
C10 H19 N O3	31161	45094	43190	121907	44179	36540	9982	13201	36617	33692	10768	183012			15475		3775	81645	25112	130343	53549		26113	24242		58556	62008	127526
PROGESTERONE (CAS# 57-83-0); (M+H)+							2427						4882									6326	1064					
C29 H46 N6 O14	8823	8708	7364	7754	6256	6157	47635	56989	72161	90667	1932		3767	4719	7495		3048	2620	32711		9601	3497	54025					
C11 H31 Cl N10		3220	20133			9358	79263	87366	57786	43330	40196	52053	47945	48037	101982	42469	51933	61200	29979	50795	76965	43788	47841	40432	40516	51790		73642
C26 H54 N O7 P	1.25E+07	1.25E+07	1.23E+07	874729	1.10E+07	81590	406081	353006	93409	28634	94219			75256	94186	149347	179589	258762	45091	457920	696504		277919	253492	21582	197130	155376	664734
C28 H55 N4 O4 P S			17281				79655	73151	86522	83483	12962	28004	18797	17242	17496	28022	367277	98647	273026	25295	430839	18425	106334	34345	16067	84059	24779	313141
C38 H60 N6 O4 S	63702	52910	76326	83471	60612	1621	60958	119605	131423	141042	128460	145431	129995	117683	177756	80581	137109	115944	197071	131596	118915	96220	146419	161552	107365	212171	131803	130139
C31 H60 N O7 P5 S	51626	49989	48852	41783	38776	38500	17502	17103	17272	16209	6795	4819	4293	14306	12767	7120	12044	6724	7306	6610	11481		5010	14875		19650	3110	11653
C8 H9 N O2	473778	499182	454856	477867	472695	453382	396761	408548	401549	406854	676351	43290	162276		21711	23295	1273687	98632		22362		4277	273949	1552040	1623			
C23 H45 N O4	171911	180093	170439	162237	150122	141814	48877	58021	48200	57160	79909	71401	18633		39459	32715	88294	53067	107018	119161	274833	34696	58082	67915		59298	32872	243255
C22 H2 O S5			59913		60254	60619	16927	18474	15753	15244	16737	27028	10986	7683	1062	13612	18481	17453	21386	9180		9459	18808		5261		8668	18934
C28 H50 N O7 P	1.19E+07	1.19E+07	1.16E+07	1.04E+07	9385837	8728100	465100	462363	449297	437366	597031	497142	121221	317372	385313	290959	216814	555744	358996	846468	704401	200270	503041	395000	37437	314183	208423	669032
C23 H28 N2 O3 S	68161	74417	72568	52067	66294	58775	151463	160913	152523		28643	3396735			42424		36880	45603	45302		45774	1017	38853	30935		53759	21418	67518
PTERIN (CAS# 2236-60-4); (M+H)+							6254	10089	5089		29239								12466	13190	21591					5556		18290
C13 H22 N4 S	101250	109787	116061	125475	115196	126282	99503	101120	123334	120869	81596	106661	87015	100044	91026	70547	113864	129754	149274	125464	115045	86509	138557	121208	69545	175926	108930	140991
C21 H32 Cl N2 O P							65746	53866	70634	56887					20654	40495	54152	156470	98100	85634	39403	23866		3391		14830	66278	55120
C5 H11 N P2	20980	21027					158410					105874								569841			550587				151296	
C25 H14 N2 O3	63790	63191	75856	63157	61819	61918	129342	110432	97757	94070	63210	73978	57469	61102	61903	61322	59140	61204	69404	59958	58982	64225	82848	58937	79649	63027	66271	59449
C41 H66 N6 S2			15411		14803		123201	127703	145734	33112	128247	38657			231027		170594	39372	217411	138792	189607	39496	39328	52917	78869	130814	140835	192336
C13 H23 P S	17945	13299	14542	15229	18529	14179	62764	61290	59846	63673	42330	74379	3787	36792	34870	48783	56482	264994	228946	54033	54690	36746	99545	96519		144244	43365	201715
C7 H15 N O3	1449142	1828233	1650658	1170581	1151053	1797368	350189	350477	330283	332001	250969	169356	157580	217051	361276	148667	25970			590138	797691	5552	137571	357421		5661	202454	
C23 H40 N8 O9	106606	104632	100906	102157	101007	103974	1255		1967		3107				11481				18135	2929	10049		1148	4138				8885
C7 H15 N O2		28603			20499	18651	99642					56800	5347	91024		102591	31497				132182		45773	56485				
C16 H34 O9	441524	433096	421507	427058	414246	402445	625685	627924	605888	603217	73020	203975	95713	127265	484890	110689	1039110	1167351	971006	580547	940554	343159	1919772	750904	119663	1420664	451276	1169389
C24 H40 N5 O3 P	240711	238656	229862	195453	191384	151637	90617	63428	77019	64519	33694	51089		34181		30388	63824	51894	80432	112727	102666	14222	62572	25306	56187	78327	139590	151045
C27 H56 Cl3 N P2 S2							213261	179718	176002	212485											1528							4764
C28 H37 N4 O P S2			2555				36693	45819	42227	45188	31343	55894	53128	61478	58661	36021	41127	26951	53579	32916	62125	22936	91701	34354	52965	43938	61462	38888
C11 H19 N7 O	60476	62495	59268	59362	58487	58538	736267	769939	749845	732810	227537	818089	261006	390877	753567	257948	563716	860188	1501634	910908	1148799	233820	1445318	1250367	103095	604759	459205	909639
C28 H53 Cl O P2	20165	55125	18221	19640	54377	56801	34572	34314	36414	30643	25565	24656	26174	17437	37926	72857	32305	27643	35516	50169	26553	36422	33870	33766	50639	41673	31498	49467
C29 H30		14307	15521	19375	7276	5131	32328	32189	36000	35947		12232	28420		4873		13803	30581	9805	22476		31701		1166	31458	38288	28566	
3-METHYLHISTAMINE (CAS# 644-42-8); (M+H)+							19731	19687	16594	20266			6452	4576	39349			17770	6695	20113	13280	7778	18751	19438		11053	17222	11248
C26 H51 N3 O S2	1895				1499		72500	74317	73901	69374	212454		376504	6699	46991	16541	1091	22499		18314	15137	6969	13012		5066	8969	27609	24028
OLEIC ACID (CAS# 112-80-1); (M+Na)+	206314	252403	202446	276236	291242	282674	679557	948694	1196742	784101	615024	46940	1231402	381841	545583	550972	815006	485601	223895	372253	412631		275412	228673	838358	417846	412378	546630
CITRATE (CAS# 77-92-9); (M+Na)+	193468	20570	177253	185279	166559	163362	1741			2482	18493			11161	12861						1052							
C13 H10 N10	43524	50966	56052	65183	69516	66000	428929	368527	389824	438808	257379	336900	378121	298500	326090	291395	349119	316686	404157	365962	334622	437418	390457	291252	293213	403248	481346	417159
OPHTHALMIC ACID (CAS# 495-27-2); (M+H)+					5116		29348	27611	23072	26585	41527	3398		11829	48452	40421	29610	18051		8305	31240	7014	12660	20568	3569	48425	3937	
C26 H47 N4 O14 P							4650730	3650014	3557225	3552554					86325				1636329	1178			1198721			3489		
C29 H45 N3 O P2	252151	249958	232643	229762	229734	214069	148333	170468	187195	175970	352055	946502	62219	230828	454158	170422	88989	233218	159941	97370	317043		107260	73153		71936	156006	158369
C8 H8 O3							6354343	6543192	6678226	6851680	4919529	193979	853091	1645229	1165024	1175710	1.32E+07	1.40E+07	1.78E+07	9839101	1.41E+07	4713989	4173419	8395968	245788	1.12E+07	371327	1.38E+07
C8 H12 N6 O							85510	90247	85251	84253		116705		75194			115473	111639	147997	67319	96863		139718	108533	7239	101331	65784	96680
C18 H30 O2	454778	482286	470820	481877	461690	451781	40348	50596	31727	40736	22561	43439		13944	25428	11172	33010	83433	99233	80056	87887		53389	62545	64861	16348	49097	104378
C19 H37 P S		23617					37479	39571	35922	37692	7210	44695	34134	22737	17945	16486	33582	20623	36470	24884	32710	21634	31051	29956	17787	57958	72172	52406
C9 H24 N6 O2 S	85131	100864	103059	130166	77689	37612	113403	107421	64934	31034	40172	117451	48972		89110	59312	128639	50741	81454	77254	115225	98479	128538	128118	44609	91689	114330	142126
C19 H37 O P S2				1282	2872	3923	54785	65558	63529	57126	186640	16836	374733	11756	30512	18340	12370	21358	48866	19212	15648	13111	30864		6922	21738	24335	
C10 H15 N2 O P	42376	49080	43346	69100	48077	44815	41752	46777	43413	45619	29831	47931	23704	37810	29022	26696	53836	60416	92342	58584	60961	25525	62874	59423	18823	56162	41854	49681
C12 H14 N8					1180		229981	232208	227465	230937	45193	108717	139343	182515	27151	119134	528806	669199	681725	398099	347591	67155	234080	211369	40642	563917	168214	317552
C25 H52 N6 O7 S2	53417	57047	53464	52922	55369	53167	94661	94694	99141	94024	18270	42662	22348	25809	154701	26124	124330	152275	175391	127056	125683	33852	197868	127702	18757	143935	63106	157047
D-ORNITHINE (CAS# 348-66-3); (M+H)+	7362	6806	7361	7320	7412	7184	7056		9076		6767					17692		18685	8184			43576	4343		11875	21171		
C29 H50 N6 O7	1087171	558013	1073269	1109988	1080141	1074534	1896476	1916370	1891336	1884567	1411290	2010574	1429875	1503956	3897035	1085294	1558763	1551330	1994509	1477956	1821927	1385190	1944233	2364666	1565647	3348320	1776079	1846501
C18 H18 O3	12145	13245	12088	12194	18109	12311	28135		29318	22080	19584	21574	16620	22740	21178	19032	17029	21210	28938	16522	22757	24902	28209	23840	34095	31377	33029	25806
C20 H38 N6 O5			3327				31081	30200	28120	29356			21394	14224	4621	15024	122721	39560	93298	3841	146703		57601	18665		36440	10833	153228
5-OXOPROLINE (CAS# 4042-36-8); (M+H)+	1085793	1012923	1015277	1046038	956569	1042124	6808608	6974549		6721671	692808	3524401		1072637	1082405	4090315	6844720				3277663	1277015	9868229	1.19E+07	568875		5421973	
C17 H37 N4 O3 P	139481	128083	142361	147842	145973	143496	204685	235252	237784	232450	296142	384939	81358	118739	188213	133663	347064	604175	289996	374639	442319	124776	313786	370749	64083	411596	216302	343454
C12 H12 N8	876956	875965	850577	870360	847298	808030	190318	192392	184382	180266	169033	40513	31033	23048	74093	29151	314656	149239	328787	391946	505315	25576	191218	261604	9415	231602	61393	698343
C25 H34 N4	2940612	2997943	2922725	53042	2670148	590841	2198093	1844167		47273	43452	1.45E+07	42835			994612	1766893	61228		362058	2238072	39612	2023738	306648	921347		1393329	1408277
C22 H45 N4 P S		23240	26191	23080	24910		335733	328095	325419	319793	328849	683192	194322	216448	209054	136514	748374	469264	529948	272605	548807	87687	397357	361454	81784	395174	314060	669642
C33 H47 N7 S2	6686						15179	16728	20735	28164	11854	19180	23122	29155	16147	18622				15483	16349	9026	21665		19391	9377	22085	21282
C17 H4 N4 O4		9385	9798	21154	13587		53193	52349	47807	51269	45062	49492	22586	36240	41374	34280	73409	50837	49831	51765	62246	31129	68455	57017	8562	58376	50548	44671
C30 H57 N O2 S4	213224	120707	116709	206826	181490	74024	40902	28376	20558	8252	52903			27393	24283	20435	27558	41031	43845	34175	37611	10427		28477			78238	
C22 H34 N4	187665	186617	173849	187609	177348	175494	576864	321975	316939	300665	343236	606495	210795	196028	494101	321172	455633	729801	609124	623747	765873	205432	653337	873782	279257	399064	468486	761533
C11 H12 N5 O12 P3	2747	2095	2158				45903	45904				42014			1270		32263			25745	50438		43477	54404	21763	40472	36148	40131
C42 H38 N3 O2 P	73903	101309	70596	66620	67554	56798	1159		13412	13179		4660			5719		6340	11875			5649		4406	9153				4786
KYNURENINE (CAS# 343-65-7); (M+H)+	416731	401875	377539	394911	386425	368507	49433	50077		47452	28869	47622	3094		68358	31419	61106	101529	142733	62813	137739		60778	55689	3239	102999		115679
C24 H52 N O6 P	643231	642012	630749	564032	610407	581133	24348		22735					18079			21925	40111			48009	30251			7419	21054		43862
C9 H16 N2 O2	311611	310614	308378	310846	302224	299339	27317		25158	26240		7599					47250	36480	113551	41596	83587		49106	28498		47367		101147
C12 H25 N O2				14164	15195	13313	504832	533269	514251	510978	130620	674001	198897	208847	208144	199235	413412	405859	1203345	820776	990751	285457	1424339	1147581	99018	286801	202002	329163
C16 H38 N4 O4 S2							24769	19633					13910	3783	169997	12755	6166	13744	11292	42957	12681	9952	2504		5775		10794	
C38 H54 N O P S		14129		7807			6111	38842			6140	61066	36170				14665	8054		20975	9064	21135	73478				84201	22684
C17 H27 N5 O15 S							48129	52856	49678	48550	30761	31994	2346	16491	43713	40718	104823	67434	119533	8001	114141	15262	48656	81648	3745	142238	17563	78239
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4);	26684	25156	24555	25567	24020	24333	4113	5505		4266							2877							70628				
C24 H31 O4 P3	8072	6782	7665	8721	8152	7431	69460	69254	71046	65720	50026	52268	58304	60855	62001	52377	52541	62328	57763	57583	65442	62208	69281	56524	60920	62644	65801	63718
C6 H14 N5 O P S	63850	61309	61463	61120	60292	55331	185336	195206	186434	186241	152933	203471	166721	163068	126772	157683	197540	215431	241885	184625	215774	249627	215674	156235	207838	270666	242275	
C36 H69 N2 O3 P S3		2052		3841	3986		36525		8062	6923			50511	9322	17257	26004	15840	59121	13829		14155	5971	16941		10296		66683	76986
C13 H20 N2 O	6670	3503	3001			3136	85737	80077	87551	83252	24694		2529	1420	16517		127401	127270	170462	534551	419646			60813		83882		371159
C29 H47 N5 O3 P2 S	608815	569216	533358	490540	447803	401668	66956	27321		46028		48627			27676			19062	40992	37129	36575	3742		1297			8584	28062
C12 H14 N8 O							201098	206968	198145	202570							189635	480975	682344	223501	188361	81572	329615	258851		509853	188511	822442
C20 H42 N8 O4 P4							63894	31310	28558	29168									9141				7071					
C24 H45 P		29766	2588	232417	19061	203604	16643	23392	41389	235588	243696		2480	239800	2016	12898	16343	96837	209390	121055	2888	228901					30423	39066
C25 H44 N4 O3				1094			70791	70516	67422	66782	50270	64722	45820	58492	49945	90274	89092	96336	124224	106914	75158	59924	72708	57878	53571	67774	52449	70144
C47 H66 S	101607	27119	68499	31350	17606	39612	20340				1079	1815					6540		1039		80350		28134	7304			8824	24105
C28 H36 O4 P2							40010	37083	35633	34567									14834				13324					
C18 H20 P2		8698	7057				38836	39419	36391	35497	38017	30380	23214	36835	37378	33489	36763	62166	59232	38162	53402	42914	47212	45613	48139	50032	42751	49923
C32 H44 N13 P3	46117	18774	19694	15933	14741	13652	26753	7827		3289	3846				1531			1586	3407	8929	4185	47504	3209	3654				
C28 H52 N O2 P S2	136639	149055	158678	131041	106125	90265	9582	68097	21115	54039	29846	44915		37075	40433	48544		22049		49906						4571		
C32 H52 O6 S2	149765	147802	145839	150003	146184	143507	241033	252110	244285	241844	212206	218471	194866	237530	227663	205554	193978	233665	247500	208028	227229	263813	257318	243467	314979	293903	254031	241408
C7 H10 O2 S3							40074	42137	39497	38423	12833	27602		10377	40584	38101	27824	53351	59089	23836	70624	17120	101014	63720		49838	35666	96307
C16 H36 N2 O5	105064	98945	95214	134043	73591	41994	27714	58264	64675	21204	14401	219326	18942	74787	128191	7404	166947	72073	62008	90423	167270	17674	212760	83907	164227	157562	152801	214917
C13 H22 O3	40488	76027	77488		45053		89908	101739	59982	69427	95120	44010	126348	91019	68623	127005	93697	80463	69487	82848	93707	65425	87379	79583	63439	99174	154045	56553
C15 H14 P2							73125	77241	69674	72939	68679	78366	53485	83125	61125	64479	57569	68190	83864	53090	65077	84657	86862	84207	120696	108246	82269	81153
C36 H71 O P S4			6757		8522		28890	28449	42116	29603	33384	19278	44117	23655	110382	19992	33370		11841		5749	18072	59050	24667	37513	41391	45615	64960
3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CAS# 28822-73-3); (M+H)+[-H2O]				2096	2567		2621																					
C18 H48 N8 O2 S2	2368441	1815450	2312817	291210	1812927		395979	344481	381316	46013	47162	75016	216296	37811	81765	149973	771653	54281	26657	382109	76763	129722	78855	375477	71355	385048	294346	690197
C8 H16 N2 O3	10850		10547	12264	9702	12120	70266	79672	72546	75823	137374	105982	27102	61783	92183	66635	95921	187062	328611	27793	108158	40230	85707	116128	5678	129571	42497	222273
FERULATE (CAS# 1135-24-6); (M+H)+	13015	14654	13329	11310	14549	6944	18038	13217	31815	38703	27902		19340	33523	39993	39585	14991	23038	21968	10888	15206	33792	17557	26485	10416	40201	14839	34755
C13 H16 N6	246617	266129	268314	282788	315412	304829	222328	244948	262753		292057	268735	303670	299931	280083	294559	285462	255503		291549	238442	315709	260073	282537	279208	246518	255512	235517
C15 H18 N6 O S							131614	128020	127081	123881	112508	3522	22621	20935	13815	14482	579811	484746	221343	150789	190256	36059	56139	391143	16142	123181	4119	165466
C13 H31 N3 O3				7718		2455	54820	52783	60411	51399	29720	46636	75843	42269	20428	24629	46338		38825	45729		21179	64060	51511	70001	183070	90453	71980
C21 H46 N O P S			15573		48462	1878	74966	104773	117244	95990		151978	88216	105393	21040		134541	127443	122744	108712	162318	102618	221775	203348	130227	63210	108944	126795
C21 H37 N	47107	45894	45306	43870	43740	46575	506560	589506	566668	558593	62440	80840	85756	40071	1.10E+07	113480	106032	191550	150261	102951	220173	65204	135091	144402	94638	85959	74321	151565
C10 H18 N6 O3							147127	155180	149279	142291		280196			56665	54377	267735	259344	356894	246854	337707	78266	323931	344866				
C8 H15 N O4							16575	17002	16970	16277		5438					42632	37332	115025	47498	40785	5166	26655			1815	4665	37777
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+[-H2O]	12453	482502	397822	464450	12053	374586	12471	5491	6661965	6721671	76325		9550	50108	42369	38904	3212				3277663	15439		1.19E+07	4707		19924	
C10 H9 N O2	176313	176558	169731	85768	160773	64276	2206			3224		1208			2558			1900	3374				12915					2722
C8 H15 N O2	108361	100566	96000	91079	93494	92132	46820		1244		27635		5454	21233	24304					26592	12958	13039	20597	32318				
C13 H26 N6 O	44088	36419	45265	42292	41126	39940	81345	87931	86003	135950	95294	123272	136370	63235	82825	105411	125083	75784	83241	110058	64361	66913	201132	70212	76040	93096	73513	125226
C40 H76 O12	5421						46354	51773		5246	2915	41420	1534			96659	73441			2834	53849		61985	51005	25393	11124	43186	121677
C10 H9 N O3	127190	127965	117919	122362	117994	114127	15063	3413	14337	15621	8947	15376	1532	6481	19598	8751	16201	30480	42653	18902	40926	5712	18667	15529	1443	31685	7004	34207
C30 H57 N O4 P2 S3	179728	152237	180430	176279	164726	153527	75341	14205	13714	13049	18072	7296		9241		14831	18273	19695	18939	25914	35860	13916	66468	15488	13043		34782	30468
C15 H30 N6 O	179230	152749	171183	170929	165642	169143	424488	250419	420769		260975	485400	291659	298774	183261	314625	338499	360517	388870	482866	1167585	304628	912849	457836	316873	394362	413679	210583
C25 H49 N O4	34876	34514	38003	45552	34473	39841	12518	4249	16537	12218	29588	24615		11670	4287	21758	9376	26927	44007	32350	83838					9266	2389	67035
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Na)+							37189	29486	38556	33065	45643	67169	4572		48984		5282	162502	37438	117127	176930		16304	32870		30175	69041	60043
C12 H21 N3 O5		4519		4487		4178	50564	55686	54052	52519	1825	58450	21869	32051	51595	19756	39868	58893	96619	62643	77214	21200	97622	82998	10320	45056	33651	60790
C15 H26 N2 O4	97063	99852	95517	6146	96340	95919	35349	37029	34890	33184	35610	72523		24342	34819	14098	27407	58891	67072	47987	50265		43783	38667		57147	25087	105380
C16 H22 O4	2691785	2718465	2672945	2688626	2559549	2510124	3052671	3280815	3170530	3123960	2965819	3128019	3580238	3288272	3225447	3152184	3740763	3201501	7075624	3096811	3461197	3234668	3846602	3462992	3469058	4131481	5543126	4930099
ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+Na)+	33493	13055	21126	320054	8051	304055	52328	66846	18461	21911	9203	27179		6400	8776	2050	37810	38923	49033	45352	16639		10054	26527	61560	14313	47323	34567
C30 H36 O6 S		2939			5135		25546	31996	27698			63316	43242	72202	46216	28435	46575	6392	35245		43496		96141	14365	80702		56137	
C8 H16 N6 O4	158695	160592	171720	159949	166342	160570	454886	457133	439623	431037	103666	240209	136148	132428	631693	160580	509422	946303	472790	398022	436865	230540	903715	406809	192171	688551	444798	1049086
ASPARAGINE (CAS# 70-47-3); (M+H)+							2362						5144						2412							3900		
C8 H16 N6 O2	87769	88299	84919	78632	77067	76182	76444	88932	72751	85853	120073	97491	253355	128686	105208	97569	133692	108836	148525	109112	111223	99267	176984	153780	170070	111159	235462	181153
C12 H28 O2 S2	59171	62637	62281	60307	66039	59904	134159	137191	123876	136256	124701	79710	5230	31172	66802	107032	115704	240902	447807	123442	131506	55140	136990	150138		265259		444784
C12 H14 O5							56483	57300	56945	51736								40188	48653	40763	33045		41156	43062	45800	33096		46159
C28 H45 N7 O4 P2	275601	270985	267055	231398	203533	184085	6443	15061		10821		6040					5326	5345	7072	11409	15091							
C11 H14 N6 O2	25040	30403	27746	35275	31124	32319	67903	70603	70520	64474	24563	55041	55572	61060	32149	29726	53985			60102	54668		60604	58647	35636	148339		
L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M+H)+	711127	703632	677867	711245	682019	670630	1225134	1238710	1199773	1210194	1243376	830687	632182	1349502	1332420	1041621	821195	1147066	1350970	1022176	1269905	1501716	1351573	1258132	1250259	1658858	1309126	1361503
C48 H102 P2				14300		8748	2558	18967		204474	26379			208504	15761	85880			394164	12790		9051		8536	4077	259451	7764	
C7 H13 N7	98272	95612	97622	100432	99127	91880	13032	10631	8157	10424		6620			5515		5922	6536	14971	116899			14901	10768		28144		3793
DUMP (CAS# 964-26-1); (M+H)+	2351	40946	36919			40769	12089	10699	11047	11577		13042			31477					5915	16488		4126		3586		7824	
C28 H47 N4 O7 P3							179901	157022	148414	150505					19304	1507			78008				55985				7189	
1-METHYLADENOSINE (CAS# 15763-06-1); (M+H)+	10073	10017	10421	11568	10835	12770	1872										3279		3483				1039					
C6 H13 N O2	2.35E+07	2.34E+07	2.21E+07	2.41E+07	2.32E+07	2.29E+07	1.10E+07	282016	228637	6160438	1.05E+07	1.66E+07	3503454	5788939	8997067	1.42E+07	7152790	517961	653409	1217408	461479	5922618	1.28E+07	1.33E+07	325052	1.52E+07	4221309	497939
C17 H31 N2 O3 P			27326	29227	21137	27594	33238	28628	22589	36920		11469		14065			43828	34433			43919	6003		19946		10400	38629	

C27 H41 N8 O P3							32395	28936	28323	27323									14047									
C18 H28 O3	20028	21124		25731	20741	12346	63942	64003	61218	62929	38010	55613	70753	45785	31093	49559	87041	79449	103457	83231	80691	41091	106712	84196		130591	54503	61858
C14 H39 Cl N10 O	42642					15934	189676	113446	105231	391639	359807	427667	266857	174744	64736	190437	595236	131946	272680	268116	72997	7658	1247762	119336	205472	86168	173968	88584
C12 H21 N4 O4 P							153265	167180	162070	159038	12544	21496	20892	17810	10987	29178	29129	38623	52194	20287	30058	38629	40187	37679	38861	52832	57939	52862
C18 H28 O2	5072	116242	13219	12383	11928	12869	11436	12555	16514	15846	10460	25188	9734	15362	35327	30513	13781	12739	22891	12470	16867		20678	43638	12361	18842	16428	15109
METHYL JASMONATE (CAS# 1211-29-6); (M+Na)+	250752	247323	244907	246677	242594	293506	276272	290430	285429	280616	268937	265427	270439	279347	127833	262909		113454	118014	289673	113805	302443	270734	112160	138565	121515	293621	119602
C15 H29 N O4	303011	309732	286134	262597	241580	225046	16017	13967	13844	13866	4616	5143		1396	4181	3757	15726	5496	17246	37784	28619	3764	15746			10281	3909	90788
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+Na)+	1106242	1071034	1037023	1074322	1076252	1024860	2031404	2092096	2061244	2006634	1615004	1816197	1336185	2027385	1785077	1566501	1567463	1830902	2366856	1537659	1858374	2217223	2372229	2112117	2694445	2811722	2422420	2208573
C15 H14 N6							45829	48832	47180	40280	33837	86325	3577	12700	29229	54774	64110	52476	163539	54875	44118	11605	45635	60062		44341	25403	53930
C8 H12 P2 S2	74700	87213	74443	85424	103760	100463	79344	87860	89164	88213	123240	131743	26493	155222	302017	157118	38651		74409	81285	148346	53139		52696	29213	41102	67734	65510
C31 H43 N O7 P2							107684	94332	89394	89866					4087				40538				27179					
C21 H40 N2 O S				24523			183998	184541			6244	481982		75782	123419	132779		297459		89147	211597		169721	111598		145864	163410	261176
C32 H58 N2 O2 P6							48080	44204	41820	41312					36823				23589			1231	17243				1243	
C33 H39 N3							257606	331712	297725	284396	3155989	310865	190835	194131	268630	501925	468350	167221	553641	239024	238966	77477	1122550	669695	267298	292399	210862	2473740
C19 H24 N10 O5	32572	29508	29754	23186	22548	22237	706201	679486	672242	672211	19696	23987	22056	20379	182636	21521	28581	23138	268149	22562	24060	25958	262163	24350	20049	23110	29770	31118
C33 H44 O12	107525	106544	105196	106588	102667	102928	177649	159275	169775	168347	143622	148795	131040	160139	151616	144140	138664	152930	167581	137408	150783	177274	172163	162185	205401	185653	174760	163967
C9 H9 N	147379	140354	133622	135482	130473	128142	1972				21226			11136				100700										
C10 H22 N2 O3	75417	75598	73515	39129	50500	68415	2539	2522	1225	2007		2336					4137						8682	2912				2816
C27 H51 O3 P S2	244419	257839	241593	252874	252579	264183	233191	263359	261057	253443	323943	317911	309764	346274	289332	312094	311943	313113	286243	284776	323108	379072	290321	327043	414851	367779	347089	325468
C12 H6 N4 O2 P2 S4	6823	7528	6535	8804	7324	6381	2.55E+07	1.75E+07	1.60E+07	1.51E+07	15152	16295	14995	11266	3881657	14695	9628	10518	7614383		10405	10852	8790448	10460	12935	29922	28262	15364
C13 H10	62509	64209	60586	65047	61624	60970	5483	6348	5454	4726											7148			75584				12614
C11 H21 N7 O	8217	10264	10048	10357	10405	9321	389805	420316	403597	395165	177200	652994	315681	228944	240785	362655	214087	214224	577916	509273	624008	491377	1093591	601823	236986	183452	187728	283798
C26 H51 N7 O4	34806	33283	35306	34699	35421	32724	60623	61983	58142	57228	50304	51719	47603	58696	55457	50154	50070	52089	60704	57564	53483	66306	61442	57130	81557	67419	68072	63094
C31 H62 Cl2 N2 O2 P2			12354				45261		44277	40254	13346	41853	50447		20860	106193		31793	24081	30979	28576		30171			128792	87227	76928
C22 H47 N	72250	70683	70843	75527	67737	70630	133585	99706	101315	102756	13687	41414	15970	14982	23515	16103	16102	14084	8621	15519	18836	16048	21716	23892	14955	14569	12197	22901
DGMP (CAS# 902-04-5); (M+H)+	63324					54831	4155	2119			18495	6020									2854			2685				10227
C26 H44 N7 O5 P	1100043	1092089	1082346	938636	846266	787152	218926	193668	163755	161442	244546	86071	65897	167415	151333	72454	548964	290261	313247	319154	589754	63478	244744	126950	25470	224808	82163	651140
C8 H9 N	6722552	6538570	5974519	6385615	6019317	5907502	3656777	3687385	3569490	3539247	2989975	2866917	370957	1333319	2665163	2910264	3679545	7413039	6728671	4193191	6419718	1791367	3979433	4889433	120531	6206624	2236330	7368195
C19 H24 N10 P2	34344	37298	36219		33611	12379	94013	89000	26747	51521	11977	96172			69213		32761	29499		27462	41214		46132	35911	87615	44012	84608	38506
C26 H24 O2	22060	24973	29007	29830	28268	29108	1347								14323													
C18 H39 Cl N4 O3			44331	36058			128349	188601	179494	187467		209346	41971	13595	1782891	26571	23837	32510	33727	264444		38633	29916	33003		41932	14983	111715
2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M+Na)+		33046			24832		36637		37173	36749	19410				35562	20366			50137	20314	31340	5754				68121		
DEOXYCHOLIC ACID (CAS# 83-44-3); (2M+Na)+							8644	1269																				
C13 H17 P S	10305	12777	15907	10573		5848	68098	67961	72521	63940			6056	50561	22810	36418	91599	174448		65921		35728	66989	89037		151993	29638	117515
C21 H38 N6 O4 S2	2909				2031		130990	118958	114723	112504					7153				43756	3653	3080		43204					
PARAXANTHINE (CAS# 611-59-6); (M+H)+	102616	109530	97570	101894	103109	95513	70976	69886	69085	66542		100908			27854		64698	294461		66790	221219		339330	127336				275250
C41 H88 N6	6900	3466		11154	96960	9837	150651					99652					175387			227236	668881						66053	
3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (M+H)+							2362						5144													3900		
2-METHYLPROPANAL OXIME (CAS# 151-00-8); (M+H)+[-H2O]	141412	162624	4600	82085		154790	2695		1885		110350		40909	92069	131593					3902	50616		29963					
C23 H37 N3 O P2	56332	46366	45440	43326	33003	40502	15420		18865	7460	3927	5572			2319		5856	2870	4514		7386		11688					12005
C26 H28 N6 O S2	5014	8663	6713	6772	7996	3933	73294	77965	74960	75260	54479	59563	62831	65778	88935	57864	58409	68633	66505	66495	84984	67952	81921	60660	59558	71800	79725	91974
C16 H20 N4 O2 P2	23970	26153	24422	24859	20909	22062	32748	34066	31976	32039	29396	31598	36086	30679	27828	30187	36724	32107	73718	27612	34402	28386	40733	33106	27095	42921	56033	52590
C26 H52 N O7 P	1.25E+07	1.26E+07	1.23E+07	1.10E+07	9894455	9217362	481585	480817	467031	463291	625636	574904	137533	341526	418673	306168	241530	589323	386263	903085	736955	223205	539131	417391	87731	352126	233543	706400
C14 H19 P S							184865	181058	176391	175275	16246	112952	3640	23388	20986	131682	224605	494683	867706	177796	111651	98773	305197	321224	9152	598329	73757	447958
1,3-DIAMINOPROPANE (CAS# 109-76-2); (M+H)+							2201					8846							5615				5200	5489				
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+Na)+	6623	8021	8827	9315	10250	8228	37908	38611	38442	38607	38323	57546		20997	34672	35333	30047	59079	97049	30485	98767	10253	46149	56623		61367	22493	94981
C31 H53 N O9 P2 S	148221	149681	146801	142663	129906	126562	65937	26514	20940	21703	35434	20560	14808	40814	18344	7769	40665	31860	26592	23280	37709	10176	24397	20789	3693	28498	41611	34553
LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+				10391			31058	1048	29200	45160			29110		21731		59059	14619	64605	2888	7406		7421	11803		20071	33764	4211
C21 H23 N O2	36410	34283	32762	35267	33574	31462	19258	18930	19567	19106			3063							236606								
C15 H23 N5 O3	115313	119976	107670	108266	100240	101123	11526	17028	16726	17932	22028	16095		8842	19254	20779	17969	10044	34332	1495	20616		10529	21795		26915	3188	43852
C23 H30 O3	48939	54672	61402	65254	73930	66217	44674	55649	56239	56815	60224	59162	61242	64736	57796	60304	55895	75704	61118	57912	47392	59572	53585	57658	63621	66295	56041	57477
C14 H24 N6	27939	27280	35887	97613	107314	31830	38877	37836	55317	42666	32344	56844	38974	30739	31864	33959	43656	39295	54445	42806	47369	19543	45088	47333	34692	61716	44380	39808
C35 H70 O2 P4	32283	34161	25594	20357	16574	9008	343540	355991	353506	338153	82763	113885	15641		3493611		133200	165939	149465	3389			54062		508118	59901	64739	130194
C26 H53 N4 O P S	205136	209532	205930	192218	159505	253963	212101	202049	24651		45763	251505		54621	53669	104728	773111	209588		127261	510328		280470	145638	26118	240892	201876	360358
METHYL INDOLE-3-ACETATE (CAS# 1912-33-0); (M+Na)+	20821	21248	24482	25196	27032	26253	10137		10087	8830								14851	30722	19647	8379		25934	27067		16299		
C36 H64 S2	44844	48287	43589	44415	16185	33513	68116				45039	34650					17110		14202	178801	165836		21841	93378				373557
C16 H23 N5	86357	78963	75244	65241	55466	52215	4685		5176	6609	11731			1876		3015	34051	31240	12057	28849	135817	2327	7712	38315		57538		65008
C14 H26 N4 P2	59300	64605	65493	70423	62734	65564	62755	56724	69367	61920	56066	79759	54663	57980	50018	40110	61805	70385	80516	65396	64865	45840	66901	64397	47710	92054	62331	80951
C30 H43 N18 P3							212579	82256	53400	64350									18767				8328					
C23 H46 N O2 P3	34214		27890	27196	23487	23938	12613	13400	14618	16238	22790	45694		8401	14937	9125	18471	8703	27422	15395	49324		8004			18619	4462	46433
C28 H46 N3 O11 P	585348	601472	559166	513132	461214	416645	25308	14270	6764	80566	38560			41769	3215	12829	2617		51466	23901	21574		52901	37500				16715
C9 H5 N O4			6986	169462	203414		15350	14840	3492	14223	7102	2458	1660	5279	14925	2563		17173		7224	11369	9469	4583	3869	1834	17467	8402	12525
C7 H8 O2							1439			1033	1085													1440				
C13 H32 N2 O P2 S							57497	58738	52432	54512	19729	113146			17097		122723	109934	128665	101078	122937	13854	126501	122934				
C25 H29 N5 O2							66731	67052	67965	62161	64018	55791	60748	69036	74622	58315	66817	67982	81999	68216	40335	73496	70653	72764	68804	62788	69482	77400
C5 H10 N2 O S							75967	71716	69072	71232	59557	45312			73194	61858	45168	74985	94839	56761	71995	70070	71784	66963	53118	105893	65330	99841
C16 H31 O P3 S	95087	103160	97215	102589	89397	91927	399233	436919	424515	404201	368790	235294	225063	173107	1125083	267948	175061	218335	295875	190111	171472	209136	468953	143450	135427	459963	508444	258779
C12 H12 N6 O2	56211	56207	56917	68935	80406	78771	13981	36150	15622	14198	2447	5379		3425	20818			14469			19331		7575	22414			10357	12448
C5 H9 N O2	947803	1115046	1030768	505325	556852	1024303	5594		3135		735220	20039	248614	585057	913476	10957		15058	3660		970860			14404	5380	14314	6738	
C15 H34 N2 O5	132263		129817	145205	142787	146848	360344	374340	396704		87874	428759	346558	406432	299737		348566	361167	351902	242407	193939	306490	306637	24128	89774	357975	374716	256929
C23 H47 N5 S3		1396032			447124		40234	36836	42919	37701	72943	69776	17013		31602	32342	59799	47402	70173	81615	193618	28448	48905	47824	3227	44100	32654	151272
C19 H39 N4 O4 P	168861	154399	149047	164365	172218	172239	661676	704285	662433	665213	404013	2401029	418605	426634	1293971	280767	524514	414326	609695	385441	522054	323860	580206	836400	404891	776441	501439	562620
C25 H40 N10	1.14E+07	1.16E+07	1.13E+07	1.15E+07	1.13E+07	1.12E+07	1.49E+07	1.56E+07	1.54E+07	1.53E+07	1.40E+07	1.45E+07	1.34E+07	1.56E+07	1.36E+07	1.38E+07	1.39E+07	1.50E+07	1.66E+07	1.38E+07	1.47E+07	1.70E+07	1.69E+07	1.56E+07	1.99E+07	1.85E+07	1.67E+07	1.58E+07
C33 H5 O9 P5 S							4191	151019		161319		463308	5426	89816	183635	432742		263815		255445					1589	296720	310454	15422
C41 H53 N2 P S2	4888	1892	4887	4950		4544	43927	29730	22122	18089	21635	32821	49733	47350	39342		53337	16994	25640		29320	10948	59906		38271		41251	
C23 H34 O2 P2							15217	14319	13193	16576	20106	23347	5348	11133	33810	33895	4260	86225	158965		12866	12905	10355	30816	11849	27917	38665	21737
C21 H23 N2 O9 P S2		8514					43154	46651	49654	48662	31111	58545	4196	21785	25026	16677	95028	67955	89147	55313	92352	11445	90659	60919		83170	42833	61778
C28 H56 N2 O6 S2	16214	8973	11661	12899	11917		432943	435175	419678	412128	102599	107867	25588	16813	3978297	14199	197669	268997	180376	63182	17802	17695	33085	113334	914815	107211	47383	173245
C27 H38 N10	3042238	3081566	3002199	3115569	3038630	3039082	4381703	4647132	4652509	4624732	4217016	4411226	3937106	4780711	4256535	4108164	4132426	4506581	5018555	4023871	4410493	5312378	5139907	4876324	6221663	5642427	5101864	4767170
C9 H11 N							74210	85252	88739	94383		13031	13699	14823		15959	100557	103677	418077	193288	173137	20860	172593	171948	9429	145985	14491	
C31 H32 N O P							24044	26486	18860	24045	16643	19311	13687	18410	15944	28286	27133	31765	39384	30541	19798	17193	23018	16663	14285	19333	13229	18273
C9 H11 N O3	7616215	7436867	7314099	7644472	7374389	7296393	6781474	7014096	6744908	6776020	4627307	4089706	469088	2378985	5031092	6811840	6795039	79579	93908	7742689	1.01E+07	4478813	7158226	9647793	317108	1.33E+07	4885243	1.45E+07
C14 H38 N4 O6 P2	52536	53245	62167	50987	48325	52701	2896363	3140015	3091726	3068057	9498101	656872	1.65E+07	269393	1849517	710367	253059	645803	1000737	661015	550986	210214	535808	292322	142497	456739	936173	648857
C34 H49 Cl P2 S3	74176	69763	69324	66541	64493	64555	12437	12512	11847	10245		3443			3491	11507	13758	62989	73194	23069	24386		14023	19330		36068	4466	58611
C23 H46 N5 O3 P3	3635	30252			86230	16398	9387	12977			1947	16495	12245	6924	23094	7748	9621			2804	8745	5188	23945		21113		16141	
C6 H14 O4	131103	157361	160750	158512	149085	153409	464341	480749	470698	479668	227035	379413	234338	195835	446068	262903	286717	479870	544078	333492	327690	224930	394271	266971	248083	406794	458312	516634
C17 H32 N8 O	44199	43799	48653	42035	44742	44494	347153	383145	374894	371871	138247	2186992	74336	84836	395688	348273	162020	877441	343389	233240	430485	116145	604700	191489	63275	229077	144319	2070406
C14 H34 N2 O6			10341			41414	82216	78225	82339	82368	94854	77922	157212	119241	62591	87500	55724	65703	76629	110076	68173	96630	213001	53907	167584	159281	63124	97336
C34 H56 O2 P2				194429			65551	65203	64693	60310		76171				18783	194544	109153	136831		235361		149914	70121		128674	12692	200182
C9 H11 N O2	1.60E+07	1.58E+07	1.49E+07	1.61E+07	1.54E+07	1.52E+07	9364086	9520219	9298189	9353020	7974477	7487353	1031535	3529109	7032601	7656782	9476441	1.88E+07	1.88E+07	1.08E+07	1.62E+07	4753119	1.03E+07	1.26E+07	321614	1.59E+07	5920704	1.85E+07
C12 H25 N O	919777	971908	932320	958871	708720	898108	830619	880777	864824	855779	837084	911600	925077	920321	655515	688039	957504	911062	922629	936518	886217	991551	866805	946637	888191	879688	952629	895324
C23 H32 O4	40088	44302	52808	37394	40983	46079	32564	36106	41108	25515	21059		22033	44919	35043	36389	21588	27632		31924	22472	21476	25727	28641	22940	32005	28721	43275
C47 H34 N3 P	33796	53539	32411	57114	36308	112369	34693	27247	22328	24322		8143		7785	12981		18363	24764	21690	34345	36619	15397	21227	19174	1504	10727	6087	28215
C18 H23 N15							40709	37883	37279	36988							1165		22645				16630					
N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8); (M+H)+			1824				1234		2453			1975							2896			2738						
C16 H14 N2 P4	16496	29402	22945	30274	17233	19024	110134	110675	112778	116939		42549		20797	25144	81009	113385	115921	172129	109891	39323	76251	149536	183985	5684	167547	114297	145332
C33 H55 N P6	45498	53480	46661	42649	33444	33325	44529	33093	9929	27575	16483	54357	12115	15161	35471	14710	4497	28716	7408	34513	25032	7976	19380	12762		5254	6381	3728
C21 H43 N4 O5 P	313634	300986	334089	333409	337964	348314	919647	960514	956498	898252	619065	1836713	661888	675751	2234739	447481	755501	638980	929834	640920	813874	543039	879749	1268318	665059	1350705	787727	878272
C34 H62 N10 O S2	3419						38841	69925						62198	54354		154332	82387	184959		192662	21214	94866	15943	1711	101808		162409
C21 H25 N11	7837	11939	18827	10435	10907	10376	66935	72461	71018	66614	44256	56854	61425	62314	60232	49448	47935	66415	61408	61517	77139	54672	76271	56019	53223	64261	69256	75212
C24 H51 N O2							224445	226714	229920	230532	32168	55198		30137	42556	116673	377131	548165	398538	475810	1008754	261972	310760	322198		428000	1045071	744467
C22 H48 N2 O7 P2 S	2148	1360	2644				114564	102606	96432	98587		1536			7811		2186		39418				27777	5790				3304
C22 H23 N3							44170	60577	55657	56909	231863	1060230	31914	30451		6799	17134	21665	16930	13682			9702	9937		39238		
URIDINE (CAS# 58-96-8); (M+Na)+	48747	46797	45214	47937	43902	42490	803109	818891	813097	816646	554969	886539	206705	586486	518528	517378	1372637	1003005		928863	1484932	409662	1201314	947130	96692	1248161	858648	1146474
C23 H43 N3 O3 S2			19341	18207			136228	140556	136761	138554	122959	127170	123960	125683	143239	120885	140943	145001	157061	147585	133811	133275	149274	148331	130154	129338	139418	139692
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+H)+							4221	4760	4434	4749	10605	7175		10086	5792	3978	6336	4192	5196		10181			2419		4879	2843	6898
C15 H5 Cl3 N2 O3 P2							5793151	3495329	3139973	2920762					472936				1098081				1326411					
C26 H39 N3 O6	1823556	1806886	1733703	1439340	1202594	1062798	47314	61453	44071	55153	77891	104149	19422	40618	53017	35627	35728	64203	62902	70103	91949	26322	80698	47527	3002	46352	32587	78709
C18 H28 N4 O10	118726	128565	122938	20515	118229		77171	82180			12905	78333		38146	39981		57642	60505		48789	109615		112694	59348		114820	73907	107857
THYMINE (CAS# 65-71-4); (M+H)+							5834		1320					6908	5977													
C33 H64 N12 O3 S2	50658			51373	44727	65615	83673	88890	96188	104567	73970	96059	90958	90708	127145	8800	85127	79466	146349	79004	83959	74540	102007	118139	80713	144350	103284	107638
C34 H34 O7					4730		31725	37248	34803	38521	29586	56223	50759	57360	50158	33619	42390	17824	46843	28526	50759	18264	92194	29494	53249	37363	61506	34012
(-)-SALSOLINOL (CAS# 27740-96-1); (M+H)+							37386	39974	38850	41347	52576			24343	53250		127377	24029		25141	119624	12945				46791		69040
C16 H31 P3	37877	45796	47529	38064	35251	44334	28302	45693	46417	40079	36740	35857	39595	45907	45316	44454	35826	46195	35054	34378	49808	41705	34659	34519	45784	45065	39380	34012
C21 H44 N6 S2	109411	110805	117491	83317	73427	53752	44009	37860	40639	40060	63099	55152	121051	4254	59778	13699	24329	32761	41031	33425		6260		25866		41391	22563	49511
C24 H19 N6 O3 P	6072	6194	4626	4444	5202	4510	75780	83474	79384	80012	46145	55281	60772	63860	72002	48444	51672	72072	74340	66631	90831	58537	87000	58683	54991	74910	77615	87433
C36 H38 N2 O4	19052	9122	8913	9379	18880	7082	35126	32981	25204	10449	16235	14430	12245	21979	25855	13558	12725	28783	37790	25777	29741	21438	33861	12411	28830	22748	18260	27346
C21 H41 N O4	68669	73513	64761	62151	56458	54082	36853	38093	37570	37309	57366	116454	11228	26525	45326	18220	53128	29322	78062	46469	131911		24622	25639		48481		130713
C10 H12 N4 O5	53737	56345	59979	57666	54947	52263	1673260	1575451	1404887	1573166	1040560	1333852	983579	2004472	1640384	1088594	3394224	2219737	34314	2096884	1632710	1279797	2498672	2071233	393589		1851437	1776982
C3 H9 N2 O2 P	125561	1234227	1148948	125816	1173544	1159508	1.04E+07	1.08E+07	1.03E+07	1.05E+07	8175250	1.15E+07	945255	3186727	9110760	7031220	1.06E+07	5417712	6934891	1.21E+07	2.02E+07	4823442	1.38E+07	1.21E+07	891391	1.60E+07	7908045	1.57E+07
C19 H45 N7							24882	25975	27626	26331	5536				5714	20178	49487	74370	56357	41829	73065	26026	36335	38198		49477	88821	71349
C13 H20 N2	271982	34785	252412	256823	252897	237322	22669	16734	28650			25415		18817		17306	18467		86950	14626				32022		73959	12467	
C29 H61 N23	1112287	1103859	1079913	52389	857420	607754	665893	1077			68197	510664					747904	8324		495904	1401653		729609	526947				1877139
C30 H40 N13 P3	119553	111502	128505	102866	18542	68088	88307	18214	18440	48139		13737	2025	3813	3468			6755					2269					
HISTAMINE (CAS# 51-45-6); (M+H)+							173696	178986	175533	172065	203564	71042	82253	110153	225768	80776	177242	203241	198858	219946	195199	123271		186820	26823	211754	148497	204505
C3 H9 N2 O4 P	2003025	1954454	1835386	1926012	1845589	1842722	322273	331606		239565	629645			132968	629938	205688	394401	1708	1820	568611	519434	187908	180149	67017	23917		161508	
1,2-DIPALMITOYL-SN-GLYCEROL (CAS# 30334-71-5); (M+Na)+	115880	122615	181660				96941																32798	4961			22727	
C5 H10 N6 O	67554	104278	118655	102808	102469	113256	51279	51485	48044	57496		37598	57189		82485	43912	6761		41687	42672	47090	44300	49435	47483	55830	50662	126792	62637
C17 H26 O4	130063	135458	145421	143683	151749	137633	154765	142075	159465	153041	168869	162406	144261	160232	156528	153727	161734	147367	181989	160083	134825	146586	164080	156192	150086	162563	167717	147107
C18 H12 N10	95513	99402	102054	106138	108450	99054	213365	217515	212127	211654	172065	188163	133244	211283	190676	164381	161201	195216	250463	163906	198320	216216	245601	218227	293437	293238	240937	230138
C32 H59 N O4 P2 S3	380730	389882	381422	336630	323106	308030	24759	28887	31112	27914	42654	22504	11794	25905	29154	26327	12170	28040	10802	43492	31352	18132	31408	23384		14924	10354	33135
C23 H31 N O6	298125	301011	303321	306748	309398	297287	1072939	1131763	1108030	1112669	1003895	1050083	1067038	1087050	1046616	1035928	1129598	1092888	1075613	1115679	1078651	1144186	1132728	1118769	1095502	1152161	1078557	1092322
C18 H25 N4 O5 P	91170	71554	54628	59181	86702	50291	581354	806750	814164	611526	391294	680052	664062	841116	883410	469119	347924	732608	887812	805887	787289	440617	988009	513473	710832	551424	633880	776299
C29 H46 O4	21690	26403	23829	22671	21777	22486	29905	34368	32468	31480	27669	29787	27591	30721	29700	23985	31825	36162	39253	26008	31480	36451	42540	35307	53592	49148	35113	34216
PANTOTHENATE (CAS# 79-83-4); (M+Na)+	56143	56382	42937	56129	53184	54550	33873	32775	33305	32089	15749	18258		8633	24909	12308	22797	46810	93969	137233	63943	6054	33149	36677			12485	78730
TYROSINE (CAS# 60-18-4); (M+H)+	7527488	7086909	7225615	7555343	7293075	7214956	6684800	6910459	6647833	6673812	4563299	4038709	462310	2338214	4956498	6699394	6683338			7626629	9948751	4365362	7050568	9518401	313923	1.31E+07	4803369	
NAD (CAS# 53-84-9); (M+H)+			1957				8363	12480	10289	8828	25867	12237		5659	56745	12824	3325	12465	27626	1376	17039		2014	3090		9184	3517	11372
C26 H38 N10							7.88E+07	7.91E+07	7.79E+07	7.69E+07	4.64E+07	2023362	6412223	1.04E+07	1.41E+07	9280646				1.60E+08		4.38E+07	6.21E+07	1.03E+08	2233160	1.28E+08	3773794	
N1-ACETYLSPERMINE (CAS# 77928-70-2); (M+H)+							1427	1283	1645	1853		4371					1056					1400	1969	1937		1255		2348
C13 H23 N4 P	97299	85645	93636	81629	127697	75182	1104140	1136756	1124516	1104262	122172	218208	155841	153164	265566	139689	200090	323566	278090	186874	219209	235105	224074	240456	189461	250442	274041	325784
C27 H49 N4 O2 P5	55369	55397	55594	52348	53056	49967	4077	4438		3835	1725	1918		1488	3020		4089	8237	10614		9593	4455	6091	6465		8395		12565
C18 H40 N5 O2 P		18222				23162	28802	30305	29747	39060	18477		8941			52035	25412	20744	47550	28680	75917	23417	45683	42371	3998	26358		3391
C11 H12 N6 O	262041	260517	258361	263980	276233	257480	270579	254000	265623	257799	244952	249889	278906	269216	236451	252992	287174	272075	252118	236727	232528	268554	267259	263690	250712	293660	281767	259903
C24 H35 N O S2					1895	3413	61333	80095	68770	71644	52237	55619	61820	61236	53839	76477	61919	72545	60481	56295	74412	63771	81732	55538	51109	70490	79621	67147
C9 H19 N2 O3 P		3658	4960				1072814	1077271	1076791	1110521		272187		6593		178622	1727761	2746715	7279690	2029873	448823	437181	2266523	1607406	50459	1795055	394240	2834361
C9 H8 N5 O11 P3	3148	3315	2403		2341		53976	53822				50757			1180	95331	38108	2339		17449	54198		62053	95263	28988	45867	39799	54400
16:0-18:0 PC (CAS# 59403-51-9); (M+Na)+		48936	291967				6965														22689		9152				10541	43469
C13 H20 O4	17567	18552	18595	18501	10812	11655	51872	50518	49348	51462	55783	115243	25039	44030	52193	50650	61780	103644	73526	65827	73475	28218	76192	61726	40902	76478	61617	103636
C11 H11 N O3	53187	66473	62268	59717	57974	62878	1373		3987	1640		1981				1152	1525	2673	7661	2011	5105		7539	3581		5732		2395
C13 H20 O2	114430	103060	82615	67961	67083	92460	81077	60249	62696	76917	66237	62979	62872	63422	70714	64817	76986	117594	72620	60703	93388	73855	94457	61967	69572	69778	66168	61219
CHOLINE PHOSPHATE (CAS# 107-73-3); (M+H)+	3241	1732	6042	6553	7452	5990	82779					52412		59020	296344	98395	3022				173362	45291	5604				42229	
C21 H24 N4 O4	55017	47769	58758	70942	56807	62110	53980	45768	55467	61951	45067	59318	61082	62148	51300	42483	45986	42621	43247	44806	47065	53269		45837	61960	62984	55284	60198
S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-0); (M+H)+	3393	1726	2408	1093	3422	3530	56903	58917	54922	49330	62717	8740		30712	127469	58135	47435	153803	123277	53197	191842	27295	26549	37349		93881	13953	207574
C22 H26 O6	5281402	5292713	5275689	5289763	5175511	5077467	3.17E+07	3.31E+07	3.26E+07	3.27E+07	2.65E+07	2.88E+07	2.91E+07	3.01E+07	2.90E+07	2.80E+07	3.21E+07	3.19E+07	3.46E+07	3.31E+07	3.10E+07	3.28E+07	3.37E+07	3.22E+07	3.10E+07	3.33E+07	3.22E+07	3.31E+07

C30 H55 N O5 P4	513347	532607	668284	676711	457408	441531	173839	194025	127465	182320	234667	127988	53990	134009	164530	111409	225387	219715	230318	207076	286527	88334	266766	156827	15805	169161	118180	235903
C18 H20 N P	5203		2990	3335	4410		54687	58814	53811	53964		60843	19901	27289	54051	19778	43556	63892	113582	65501	81803	17834	104262	91296	8844	42669	34270	65481
BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7); (M+Na)+	2838541	2906889	2812278		2540504	766306	2145575	1792692				1.41E+07				906570	1702534	5315		351575	2147452		1984262	436497	845739	803630	1350317	1330197
C11 H12 N10 O		4657	4622			3505	98775	99149	97860	100836	2646		5019		8857	3392		4256	40979	4248		4502	48327	4385	3208		9697	9178
C21 H21 N5	4993				5131	4520	31200	36980	36029	35625	79607	21771	110355	15813	36147	15496			17193	12532	10948	6927	29029			22870	21483	11335
C26 H55 N12 O2 P	746954	702260	693983	506055	400898	330726	147781	9928	44013	39218		150449	5712	15092			27864	55120	30281			12754		55621	9278	73753		
C14 H24 N6 O	49558	223242	344994	238876	231212	705071	228140	224474	81926	91842	26882	726782	40812	43482	55708	28960	792950	59268	86582	818098	51364	27980	46187	51500	28010	75114	772379	665375
C14 H26 N6 O	14002	20023	25133		19233	38146	30073	70577	29856	29601	17721	35165		9208	56192		37278	72914	64302	45486	47501		54644	47397		67972	22100	39882
C23 H47 N4 O P S			25331	34760			63736	52635	71129	50995	32320	60550	217247	52806	60582	37440	52293	52973	68866	25437	87322	61080	182470	114379	125872	110020	61947	63366
C22 H49 N7							33263	33247	40454	32543	9037	24807		13682	27818	13243	62629	82667	33677	59771	91187	39583	35980	44739		59756	104242	52652
C9 H12 N6 P2							48008	47211	47238	45777	5233	32744		6411	5872	37239	61259	113961	174858	47208	31668	27833	77972	78850		140429	21030	103647
C17 H18 N12	41330	48200	52472	44171	40789	46885	2199										1337	7857		6213	10392			5263				
C11 H10 N8 O3							69824	61822	62878	60619					6609								21417					
C37 H77 N4 O P S3	26536		17658	8945	22268	17266	110877	88706			14948	88101	3283		25167	35091	194513	77632		67194	143561		650788	76163	24464	92405	64909	176340
C34 H52 N6 O2 S	63849		67200	60958	57970	62583	123647	136017	140241	126711	103609		127351	106352	215109	87823	110271	92900	160036	100319	139715	92128	149632	167552	124736	249079	115295	130414
C28 H24 N9 O P	35079	33783	32955	34286	32419	32152	16585	17197	17588	17316	11259	11223		1406	9224	11315	17413	79228	70771	29562	51245	3260	22100	28679		47512	5895	71752
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+H)+[-H2O]							2523			3793	1171	4685			3617													
C7 H19 N3							271053	312402	301524	316730	64831	1097112	311108	42026	86876	71202	324054	169322	601912	259506	203095	23942	693118	654301	65587	395365	367743	186465
C27 H48 N6 O S2		35025	42748		47310		413585	412569	416146	409753	81232	67090	28168	19721	3513553	72428	178739	247737	205784	44603	24006	19815	30196	47892	968905	76410	54759	204814
C11 H20 O3 P2 S							613501	630041	616066	615820	353189	527886	219557	169119	428640	432835	680087	622702	1179411	832308	1198015	312297	788304	744836	70521	901485	439145	972461
C15 H20 N6 O3	480627	497431	481393	488781	496627	477268	467765	492826	480218	471688	424704	481595	490977	490695	460470	459112	495112	463468	421412	475007	456966	502662	430139	499768	455774	494725	518203	507656
C23 H26 N3 P	11177	10650	12169	9195	9608	10011	21907	16595	25087	18823	27892		22854	9533	49868	16833		16392		8711	119141	12512	21768	12881	14644	12839	16386	
C15 H20 N6 O2	4385	145732	147449	146273	132857	153538	60737	60916	148910	58695	11065	46921	49433	49850	11743	13950	47002	52369	73004	45152	50763	157238	62387	55084	17633	195818	139023	180251
C13 H25 N7 O	6972	11813	10073	9800	10147	17462	110685	120291	133286	108081	53403	198085	79912	67823	71433	94351	62588	66152	172376	138398	175821	125789	297603	163076	61223	66108	61757	102657
C25 H51 N O4	30699	27701		32277	29577	30538	52040	44376	38588	40672	50663	59151	19363	19067	42259	56391	56130	34076	58590	106434	153855	44290	41297	31605	17987	39901	48458	115183
C17 H28 N2 O4	1302562	1336779	1289151	3194	1336514	567307	431853	424813	73862		78192	562635		126834	196313	113438	269159	482961	2208	289096	934591		980500	411360	2065	608464	458731	1034285
C19 H44 N2 P2 S	4401	42463	31838				77832	91144	103189	96683		39814		38891	697309	40437	24825	7877	13735	37312	34727	48297	14456	42493	12505	26366	36033	28928
C5 H4 N4 O2	164374	159505	155801	155887		149510	524124	553755	535052	537816	1248215	1941941	263331	920554	1205077	721267	369512	241214	592140	317862	381636	92633			17900	303639	331397	403831
C35 H50 N O10 P S2	191313	188785	201347	171622	162818	152152	17983	19535	11364	11809	12167	12424		9043	7095	4549	11369	20411	15846	30662	25470		12115	14972		18816	10088	14675
RAFFINOSE (CAS# 512-69-6); (M+K)+							5900	5292	6894	6114	1994	4802		6999	4313	6931				4940	6084	2414		7856	1114	13734		5226
C17 H36 N4 O10 S							71183	79817	81480	76684	239611	19706	414683	9570	51730	22754	11096	19692	26950	18429	15346		16009			14546	29214	17109
NICOTINAMIDE (CAS# 98-92-0); (M+H)+	120009	114097	105979	118009	109043	106190	1153554	1195240	1125611	1145077	970252	906776	256746	229340	1617502	477448	1330384			2187693	2458456	348180	1430661	1206666	106062			5709
C37 H49 N O8 S	114377	5133	118082	5050	21235	177155	12953			12465			18405										5303					
C32 H63 N4 O6 P S				17407			49035	45376	84373	49445			48733	35763	13378	43410	195257	82844	208361	14717	250922	18048	79286	18503	21276	35959		208581
CIS-VACCENIC ACID (CAS# 506-17-2); (M+H)+	19140	21193	21733				9936	10221				6403			2967		5520				11159		9207				7891	13213
C5 H15 N4 O3 P	93057	109624	105447	105950	101136	88079	324103	318626	329613	322189	201640	184390	103987	131847	462358	271747	199416	347399	383195	273867	386432	169174	281131	223145	137194	325344	185320	470265
C13 H27 N S2	64616	61360	57962	56588	53371	45238	95490	90666	89682	91047	26908	5134		21173	38954	16112	110692	630993	1213888	109976	165456	2143	71215	43342		66903	53669	124279
C33 H67 N4 O11 P	756782	559663	745679	772187	742044	730583	1341339	1337638	1336768	1297100	959671	1209037	975156	1073990	2619005	800361	1098379	1191786	1855981	1113729	1190372	1047010	1434895	1544952	1112250	2279234	1312565	1349007
C15 H28 N6 O2		18542	12145	14663	27348	35355	92056	93425	88110	78644	64404	75810	83502	63082	251459	80130	37440	44064	74350	80190	47316	74247	73116	73697	36299	81675	86519	98943
C31 H43 N5 O12	366480	346603	376838	367459	341637	338206	58382	59247	64441	61724	56644	52466	18174	52813	37664	29967	47933	88502	55853	109653	90942	25468	74646	51441	3543	58097	41984	67505
C22 H20 O5	12395	12779	13103	14751			50291	54604	55802	49805	43512	25686	25555	19555	87666	33684	21092	26015	33535	23429	22514	26313	57230	16281	16796	52069	46215	32625
C17 H34 N6 O6 S2							37567	38547	37271	36929	130336	7589	262793		21094	7623			11611		4656					1785		
C30 H51 O6 P S	57055	59891	55818	63398	57961	58849	82028	77335	80620	81044	88623	83471	80169	98840	82060	81137	84655	90512	93672	78379	90857	109844	90630	98062	131340	111726	97293	94923
THEOPHYLLINE (CAS# 58-55-9); (M+Na)+	106631	108422	100210	106745	101490	93345	18460	18025	18062		2378	16097						55081		7280	34267	7584	91024	19432				39845
MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M+Na)+		33046			24832		36637		37173	38287	19410				35562	20366			50137	21705	31340	5754				70349		
C20 H39 N O4	45968	44265	43206	46206	45113	42015	5692				6644	7728			1501	1148					9709		4043	16275				6146
C19 H34 N6 O2 S			7638		1583		20547	35384	31362	29034	3704	379856	6200													4342	11195	
C10 H13 N5	870412	778359	657872	396255	248330	176178	900306	909371	897043	874329	740813	346873	141601	261392	570146	239719	1720649	109268	257229	95292	2361805	196156	1712655	734708	49872	8345	282627	179751
C27 H43 N7 O16	87666	71785	79897	80569	73483	70654	26471	23744	19802	7464	6162	22184			8390	6953	6336	25356	17007	7968	10495	15819	30115			4225		9746
LYSINE (CAS# 56-87-1); (M+Na)+	4065	3783	4392	3841	4111	3754	15138	15566	15245	15296	28736						13394	20327	16744	8895	7221	23188		13359		20444		18614
C23 H20 N4 O						1265	34047	37018	35920	39057	26616	31620	29501	30136	30023	27053	34428	35775	45839	36929	34159	37524	37926	35122	30334	37553	38495	39176
C18 H33 N7	7748			68334			103286	124804	116765	104230	210555	370362	7656	62712	215603	87788		130992	34952	186391	174487	26057	185308	119660			182409	148887
C10 H28 N6 O S	37989	18879	52984	32408	55970	38136	30305	36621	33441	45154	52811	17825	79076	63017		47400	37604	31911		39051	48078	42311	18731	36499	72116		46221	58176
C28 H41 N O6	131691	131168	128159	137851	133865	129929	1596562	1732579	1640206	1645287	1256599	1367341	1395795	1516755	1680592	1266211	1646542	1671318	2029807	1733754	1546878	1611890	1768557	1696553	1513121	1580470	1658504	1798218
C34 H46 N3 O3 P	59189	22491			2319	1820	34580	31930	62983	27790	44035	64700	30382	80026	46749	10792	33430	55231	42267	19559	29052		67976	47829	49611		37121	85613
C14 H31 N6 O P S	1829						154922	165560	161101	157832		15479	1686	1546	57757	71554	99314	200969	1172329	134634	108739	204177			44974	17922	749749	511278
C14 H20 N2 O					2508		887229	917317	901986	889764	186288	7505	49981	80693	59752	79218	2671111	2140741	5012703	2728167	4390712	465532	927307	1716103	21868	2138567	6606	2627616
C40 H41 N7 O S2	84352	80757	79834	2354	20613		9198	4937	8612	7094		61880	18198	21125	33490	1022	25615		17288	5873	2592	9615	4515	3983	9519		2991	4272
C34 H55 N5 O11	107510	109404	106042	106256	97738	102503	188773	218399	204521	192474	362173	492248	407970	548354	687386	288739	543377	257097	476938	229141	121967	236821	97436	225498	234307	91803	142019	157846
C20 H39 Cl N10		37751	30984		10042	10755	35809	42892				101424		28367		28928	94974	55415	158190		76969			58365		121612		
C14 H27 N4 O2 P	437862	476995	469676	578843	649629	648353	189166	186896	329388	615863	643477	563438	704735	696371	632706	656190	586193	614326	573513	585010	520894	645389	565411	609923	736456	646127	642308	479880
C23 H44 N2 O2 S		20162			12067		137362	140919	31474			432498		30247	63201	69761	54002	327336	14331	79591	275892	8914	169174	110708	33493	111775	153266	184827
C26 H27 Cl O5		1777		1067	1688	3035	44279	55114	54546	55116	35105	55220	55013	58342	63254	40998	47876	36430	64230	46874	61700	31104	91301	41145	58360	58672	66040	53661
C10 H18 N6 O	219238	237241	236906	235513	235669	248877	212983	236428	224574	227264	229893	236350	369402	248242	295142	225880	270001	333117	285056	261548	274772	277597	326348	295231	295600	287757	457951	319510
C30 H56 N2 P6							52169	40443	45015	41092	1031								16011				15355					
C16 H24 N6 O	86438		71496	87111		69218	187476	195391	211335	278630	306660	604132	104136	237291	390455	154184	266999	194077	274224	736945	192652	97933	178809	126339	106614	219381	197227	156888
C18 H42 N5 P		232569	231034		43421	25192	3690084	3141238				5549240				966610	8368691	3923952		5675000	9242153		7899613	4603860	191133		3025876	4214297
C26 H50 N O2 P S2	142386	150294	142542	119499	103190	96166	13617	21086	49616	55499	31126	113672	11194	23292	21356	37683	27315	126877	47420	44753	31897	4206	31537				2447	29829
C16 H19 N8 O3 P	27730	25799	27218	26334	28699	25253	33322	29837	40035	43625	31608	30328	34560	29428	33647	31822	44832	47612	44394	45142	37201	31883	47080	7936	28921	47906	28190	35177
C29 H49 N3 P2 S	77066	157168					46931	49766	43201	50430	67049	103186	15938	56854	64311	20190	49995	62412	34518	61452	62368	12636	53468	58220	5072	64655	49899	49253
C23 H36 N17 O P	62387	55613	54762	50519	55616	48268	28318	10394			27736	23494		30895	18128	27365	8532	21648	6230		7837							3740
C41 H51 N3 O4 S				52935	41874	48657	38505	45136	38519	39632	72755	99196	83366	105622	142264	49949	100717	53463	95726	41154		49138		49238	52414			
C15 H31 N O2						8696	898851	890887	869869	880438	45203	113502		42686	198957	40246	60927	67086	200732	82967	52177	57091	384146	49436	60464	107181	61362	70161
C37 H56 N2 O2 P4	20954	3609	21972	3047	21222	17850	14905	26589	12061	10931	12654	15543	21001	35121	14933	21009	14172	11412	13797	9553	13744	9856	16930	17537	11523	17774	4100	11638
C24 H50 N O7 P	1.98E+07	1.86E+07	1.96E+07	1.84E+07	1.69E+07	1.61E+07	825680	780917	738067	690935	541195	314718	165140	196414	250203	469908	468560	818809	623086	1567334	1395695	419387	750500	656853	73000	434159	351505	1086377
C27 H46 N6 O6	1351140	1256074	1275975	1316837	1242086	1222758	1960005	1832286	1768528	1740750	1167509	2191344	1460684	1547564	4585793	1120552	1566628	1527677	1951002	1498304	1895770	1399008	1955985	2469878	1545848	3003229	1586108	1910455
IMIDAZOLE-4-ACETATE (CAS# 645-65-8); (M+H)+							4119																				7752	
C18 H37 N O							550157	273109	219864	183673									27367									
XANTHOSINE (CAS# 146-80-5); (M+Na)+	2526					5982	31068	32167	31870	33644	137351	52192	14417	38897	52862	45899	7400	17143	18910		44924		17059	17712		16429	29770	27513
C4 H11 O2 P	1760		3188	8764		1864	1133990	1192318	1126120	1138864			13947	235326			1325174	1040190		2182076	2394348	398887	1417657	1191440	64219	1500472		1479805
INOSINE (CAS# 58-63-9); (M+Na)+	16309	14467		16440	6363	16446	638872	536549	536448	601844	396881	751456	699655	1090714	807682	671506	1086695	640077	586011	638031	513542	717550	1098194	832794	292386	618204	949727	524263
C24 H29 O6 P S	22049	28154	21615	23300	21528	22399	138021	146429	144238	139491	105933	122665	125191	132974	120689	121400	139514	144230	165801	157480	139379	148202	154099	142099	135223	150201	155510	156648
C20 H41 N O3							141083	155896	137083	148850	20100	36048		15528	24086	39608	433854	344688	540405	447409	343736	105942	255482	209834	7769	283217	218012	538560
C16 H16 O4	101348	101579	38708	98862	92952	80477	84956	93777	83930	85882	79126	98673	77906	86043	83061	83560	129467	90349	85103	90927	105694	90385	95788	129839	78672	128897	97757	102226
C22 H44 N4 S2	28371	20660	25781	29011	30407	20738	84009	74010	80497	80318		148447			39701	33137		78046	67457	55385		50510	95724		7992	94557	90795	
C15 H11 N9	18735						56822	57860	54551	53247	68589	48088		17779	75286	48939	42439	45970	102391	62111	128309	17307	50561	55652		98070	36637	90733
C10 H13 N5 O	6270730	6193294	5962285	6156936	5983996	5829748	1.05E+07	1.06E+07	1.02E+07	1.03E+07	8691899	9219725	8092140	1.05E+07	9185992	8644021	8330223	9139480	1.10E+07	8167444	8386760	1.16E+07	1.16E+07	1.02E+07	1.39E+07	1.26E+07	1.17E+07	1.04E+07
LYSINE (CAS# 56-87-1); (M+H)+	11463	15756	14873	15224		15283	77216	75313	79115	81533	176337	75861	54710	121185	170468	222635	68215		84184		62221	136262	30961	65206	99213	103971	112994	98284
C12 H24 N6 O	90605	94085	58013	112654	86873	86313	57835	74839	70365	99563	145715	290619	206385	267272	170599	230248	278603	408580	395588	278758	322474	180442	348010	299927	188491	261334	302172	307698
C13 H14 O4 P2				1315			90751	71276	60666		4069				5894	45423	70168		88287	72778	2401		104493	139300	6055	92182	74040	79037
C27 H50 N7 P S2	1005725	671321	981419	904248	824698	779493	55955	50895	45837	52789	32075	36740	8913	29664	37015	21652	28722	44461	63758	95535	73339	27913	64149	29353	5619	61527		45594
C7 H18 O2 P2	13936	12758	7210	12332	13342	11299	166466	174039	168984	169726	36954	215243	49092	152185	47893	39302	192702	233207	297741	205080	243061	34163	306765	280335	19870	232459	202561	240114
C40 H51 N3 O4 S3	1959						22182	23387	21455	21739	1629	11432	30849	12647	3455	3317	60118	23106	29875	8971	10769	8972	31993	22634	20577	19305	37068	15481
PARAXANTHINE (CAS# 611-59-6); (M+Na)+	95799	108422	100210	106745	101490	93345	18460	18025	18062		2779	19551						55081		7561	40862	7584	91024	19432				39845
C16 H16 O3	103639	87681	86957	106074	102859	104980	83859	91245	84136	67983	80383			100741	98496		91925	85133		85391	74171		93011	89583	97856	85767		
C4 H8 N6 O	547501	564200	529036	591100	544822	522355	478771	487700	357901	373357	489425	263858	693650	152104	1062272	313265	180243	115510	265306	187735	1628255	358247	619341	446841	379153	250768	511413	167624
C17 H33 N O4	371383	354982	343659	314594	296946	262776	6217	5197	4258	5262				2740	3999	4876	5649	3028	11652		19743		12835			3118	2911	49646
C22 H32 N9 P3					1572		75110	64462	65238	64051					4886				24134				20930					
C27 H32 N6 O2 P4	32389	31102	30672	4312	31104		31106	20857	6663		25915	1944	12114	1157	15386	20556	19162				23041			7461	3588	33778	23667	7324
C26 H52 N2 O2 S2	150249	194717	215679		177888	11491	11678	17827	8759	66778		30185	32667		25745	23149			31470	7161	66598		23966	23056	6994		69372	53176
C20 H41 N O2							400682	192994	180573	182789	22338			14223	14064	45417	229309	175588	210129	147435	156201	54564	102584	105079		150030	118301	275265
C21 H26 S2	23746	86192	60841	55438	85323	58725	48558	52508	50491	50293	40933	43976	39626	50970	49176	49359	51026	51995	58092	37244	46805	82000	58964	56104	69516	68556	57037	52322
C10 H14 N6	18788		17797	21610	20596	19203	39567	36000	36175	32310	90481	65522		48255	9722	35906	35698	75617	84071	15178	38946		10834	20173			8265	79958
PHENYLALANINE (CAS# 63-91-2); (M+Na)+	433942	423952	395615	425132	390805	393284	229404	232734	227991	232022	200452	181539	21121	85388	177838	193944	234449	512830	478416	272929	418224	120306	258520	299698	4762	389868	148744	493157
C18 H41 N13 S	28616	20657	17807	20996	20365	13689	363362	371728	370690	359757	1135800	95037	2016398	48241	225149	81258		80999	123563	79667	73816	25917	68090	36802	18579	55827	115609	82155
ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M+Na)+	308761	311338	293536	309854	303447	291587	268175	274424	267312	269535	469672	31086	112490		13808		834132	65690		10147			182222	991228		17558		
C21 H40 N2 O3 S	1391	5570	3552	1101			43932	42662	42975	49000	67306	56253	134015	22773	42690		29963	37431		21076	28788	17876	27747	32226	34424	34688	35950	56391
C10 H18 N O6 P	119861	127669	80255	143254	153302	156102	4975	6669	4587		12340		5016	17045	7934	4539	8365	6188	11428		40508	7211	5753	1729	1047	3115		10962
C16 H28 N P S	1020	2611					43594	45221	44732	44377	24896	66773	36335	29817	35118	42279	25697	30712	55039	49680	60540	50916	86348	54871	28837		27077	40273
C30 H28 P2							43058	42104	40482	38818	24311	32683	36511	43432	42088	30022	25687	40016	46580	37772	60624	29989	48335	34197	30033	36326	35425	52250
NORMETANEPHRINE (CAS# 0); (M+H)+[-H2O]	1.56E+07	1.54E+07	1.45E+07	1.56E+07	1.49E+07	1.48E+07	9126915	9281787	9064085	9114624	7775118	7308179	1009688	3433790	6850878	7463582	9234501	1.83E+07	1.83E+07	1.05E+07	1.57E+07	4628126	9988971	1.23E+07	316889	1.55E+07	5764731	1.80E+07
C42 H41 N O3 S2	75616	54889	82175	83322	124545	116365	35389	27566	27801	26987	20605	8046	2773	8798	12478	14142	15861	28878	15307	34690	36737	14900	21806	19041	1500	13587	9133	28794
C22 H38 N10 O2	1780	4019	4084	4371	2704	2028	25520	26960	26406	26675	35284	11576	12240	9930	45489	16291	15569	12135	24387	10696	28648	18670	18710	13679	80143	16027	20941	34663
C21 H39 N3 O3 S2	33776	33845					119768	117837	121041	117982	101809	104410	109197	112402	107600	105877	113701	110302	109286	118765	106201	121255	125230	114568	114453	122062	119255	110556
C22 H38 N8 O			2185	7297		6421	39974	44298	53248	51873		55461	3616	34062	6870	10995	48067	77735	137485	93618	105586	22813	145156	141129		51880		
C36 H41 N3 O S	149972	918622	121882	115088	105319	94944	8084	71861		29983			27095	20430	31762		16970	7707	31850	18769	23609		48621	24527		11112		19422
FRUCTOSE (CAS# 57-48-7); (M+Na)+	364289	365594	293246	328859	322836	348341	34641	44043	34758	41463		18459	59063		59055	70703	19122	21588	24180		157899	36929	63782		45264	17518	52334	
C24 H27 N3							254444	359959	315211	327944	1285633	5600602	109795	490286	71480	28346	96006	104736	186025	71738	33531		45637	74082	15247	429724	18598	12020
C42 H65 N O5 P2			530045	543414		2267	220587	205547	199948	2584	307476	174563	185267	224125	1572	164000	189407	189186	248550	171242	185126	223691	229024	203056	276009	277562	247219	216914
C24 H46 N2 O3 S		14366	54362	35024	42914	40158	459225	480046	148894	420834	259030	660479	142387	93314	298127	126766	403392	100400	79681	276417	491058		103236	96982	55452	112242	226096	137491
C11 H8 O S3							81332	89095	90218	89443	78164	4749	19870	35924	24505	25483	128314	132004	144432	111240	123562	76538	66444	103036	5455	120009	8422	129887
C20 H43 N O4	3022	4393	3690	3201	3463	2545	51043	55924	50604	52154	33005	49530	56654	34809	38064	23133	33678	55698	49582	53731	45475	38123	46857	35864	60267	62051	44759	81708
C20 H43 N O3				2476			32977	40366	39582			19615			17795	13941	120746	64127	116347	97437	77679	32803	94376	63441		75503	84954	175728
C44 H86 N2	167761	87377		2298045	2812854	2294558	24850	1013916	1733	1097910		809048	38713	478986	596889	466393	2550603	1760139		842039	41937		2933909	819899	18737	1827190	2194383	279659
C4 H11 N3 O							394239	429566	399370	390598						361693	313752	4178482		402902		326523	282273	444283		329541	470983	264553
C14 H35 N7	32687	31467	32542	34612	32227	35603	112191	110423	103612		128032	51654	20998	45087	37331	73597	110034	69560	176956	84959	99882	31728	76386	107221	19743	113392	74262	195330
C31 H64 N2 O3 S4							25116	34475	32419	29068	9957	27166	33321	77400	23776	96683		25085	5663	23764	22751		20455	3801	5514	91868	59197	53137
C20 H35 N7	18867	3428	20262			21072	399057	435490	407881	397780	180949	681285	387360	408088	179877	145867	700513	468535	625970	619874	654506	197358	871250	819869	156729	427283	511838	329733
C12 H18 N2 O							8132561	8242538	8119127	7835089	2299591	432052	947265	1365157	909566	2302699	1.41E+07	1.43E+07	3.13E+07	1.55E+07	2.13E+07	5578973	7807550	1.07E+07	588067	1.38E+07	548981	1.32E+07
C32 H46 O8 S							90063	75731	71244	73439					2987			1277	28590	11416			19372			1774		
C18 H24 Cl N4 O4 P		4072			8103	4088	88830	104542	104882	105825	67449	89141	96669	95382	102485	74199	81634	92208	116529	97041	114912	78272	146257	82581	96313	104586	113244	111221
C25 H41 N7 O2 S	704234	692580	686758	578322	486723	447421	64633	52315	53069	55152	71036	120703	15842	49809	60829	36352		87940	43788	65196	145907	9195	81961	71168			38823	95667
C9 H16 N6 O2	23071	56439	23077	25101	25218	40300	112836	54363	56550	52557	23948	109042	67778	74030	33353	50319	46432	53310	76334	89685	84757	37744	95425	78935	55437	117838	184113	78620
C44 H86 O3					53885	95518	16131	76350			31137			22537		12003	4220	103816	72013	28423	11328		40173	49450		110767	1725	
THYMIDINE (CAS# 50-89-5); (M+Na)+							2801	3178	1920	2369		12785			8103			10382		2842			1241					
CHOLINE (CAS# 62-49-7); M+	91800	91957		88964			29250		30681	15440	81699	167873	32009	38265	62875		6952					4056	22659	15201		14922	49843	1216
C37 H69 N8 O P S	5471	7056	14998		19480		73295	62656				76726			8899		107843	7597		3547	73129		85326	30049	32027		46367	131514
C11 H9 N9 O							881534	820954	737399	823496	388052	491512	215964	743583	815567	527265	1520977	1231731	1463097	805796	1114544	673759	1286139	1167273	271896	1482673	1345850	1030277
C15 H35 N4 O3 P	404305	398037	399996	374550	380316	377013	317423	255069	327066	296977	278297	303168	244940	303823	250005	261432	316370	297086	331182	331633	303298	249103	312591	334835	285763	293052	303695	341649
C9 H19 N O	402347	396589	386014	400788	415792	403996	424649	448616	447406	443559	468592	424326	522339	434328	422289	413770	400325	403794	433221	412380	447269	424036	403587	449590	433516	419140	481557	451484
C14 H29 N O2							263457	208414	202036	199668					7601			1116	90523			2237	44140		4576			
C35 H40 N2 O4							358550	357109	349686	345201	186803		9512	22728	35266	18172	1017071	981217		838348		177779	260840	493722		637276	3543	
C54 H54 O2	11850	3474			2486		46092	47520	6568	28389	19289	61236		22998		30370	40892	32172			48823		56695		25595		45634	53223
C31 H55 N5 S4	25789	26539	34436	13034	27761		30141			3671			1280				1331			9020		3989						
C20 H32 O10		7450					9149411	8594746	8437348	8317010	3141	1252	4223		234624	1360	4513		3834434	2352			3316375			1257	9459	
C39 H83 N4 O P				49717	48736	61078	3855	20792		23099	40444	3323	27578	12065	22689	27914	19611	39470	32754	2683		25069			16258	22165	7324	
C18 H34 N6 O2		21827			88765		58022	57774	12774	6228	60697	67300		22501	135465	25627		34625					55605		33209			83019
C11 H18 N4 S	69596	71252	68775	73214	72723	67265	66697	66497	66294	65995	31796	54350	26438	39131	37759	30105	84317	99835	134878	80866	92883	28355	108535	107186	20935	131582	53538	95219
C19 H39 N7 O2	76837	75696	71831	73181	59473	67580	130558	145486	146544	149640	233453	1170452	38980	94065	501289	79494	62026	63103	48941	61132	81135	13225	40114	32163		36796	45474	193344
C17 H27 N O4	183854	181304	175418	161954	140795	123829	12318	7126		12157		4465					11373	23994	19700		62049		27269	5629		30102	11430	
C34 H69 N4 O5 P S		30634	1603	7554	11813		175689	169964	24797	4077	18314	89841	2783		37393		346250	125190		97273	261556		777464	118812	16846	16056	111223	263082
C29 H62 N8 O S3	9530		3982	1652			58999	56105	44262	57663	25951	60406	23809	8245	29632	40890	19617	12519	25574	20338	22904	15754	97399	21772	72908	29184	44129	29585
MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (M+Na)+							1523	1255														1102				1833		
C20 H27 N4 P							102674	103411	108047	103123					20784	35007	70847	207005	880858	125252	91666	120664	15162				417449	457510

C33 H50 Cl N O6	124277	140474	122975	292197	122834		54729	30638	40520	30427	65815	44607		44620	5092	28877	26442	36184	4056	64538	57892	33190		36322	23140	48448	100936	68009
C6 H4 O6 S	89144	100726	113424	121639	125803	111471	7634	8072	7868	10576	8306	3836	29488	4240	17516	5651	8381	4160	7985	19313	33043		6605	2777		8989		24399
C38 H58 N5 O2 P S							91734	63436	63157	69466					1610				15151				15416					
C18 H36 N6 O9	348082	350964	339558	340831	333553	326005	388189	388133	382959	381639	52527	122202	57150	75560	338089	76072	644615	737818	691251	420361	591112	120543	1154662	507334	65851	833256	274708	726473
C22 H27 N11	113832	126027	115594	125699	115388	114920	31930	49955	40045	41148	26643	31987	32606	47500	57278	29062	26719	35300	37249	44050	42353	33058	45887	33587	30954	45530	42709	50870
C18 H39 N9 S			12532	7469			85228	71467	71394	94035	15569	36238	8449		54809	52660	57188	93539	496185	60256	51029	92891		22668	25501	19616	343007	221570
C17 H35 N2 O P3 S	340381	339657	340134	349379	343564	338410	174441	146531	176204	116298	130078				289506	121844	72864	198435	216166	181891		86425		138342	123727		117411	132245
C32 H66 N8 S4	18362	18429	19513	18971	20185	20206	32660	32584	32088	31714	19051	32360	18955	27066	19314	18332		44511	50595	32061	40694	19295	48432	43178	20965	45093	32354	39056
C25 H42 N6 O5	858357	871611	856110	915712	860859	843072	1546015	1786740	1461531	1529631	1090976	2038566	1151039	1261863	3274695	837531	1213492	1078466	1703727	1086627	1656336	1039672	1735925	2233231	1320173	2791769	1616498	1524052
C5 H10 P2	370211	365416	335622	350965	336258	334551	556621	565450	546587	555187	650057	520300	49838	298588	596611	556574	486677			604650	875130	297944	485536	773071	40664	788532	445014	
HYPOXANTHINE (CAS# 68-94-0); (M+Na)+							1329921				707248	1066720	521435	289866	881317	878338	1492600				2412624	527835	1745220	1643341			957396	
GLUTATHIONE (CAS# 27025-41-8); (M+H2)+2							35444	39404	35453	32981	89300	18985	1300	20102	130177	59203	36298				14628	7422	10626			45849	13081	
C32 H30 O7	8559	10827	8651		7814		76935	84111	79019	76977	55055	85082	90271	100746	96159	60309	66060	53531	94007	71177	111735	50482	143447	65641	84198	79647	103994	80676
C14 H28 N6 O2					6777		44639	56486	57301	59675	66966	65411	78949	30124	39305	29362	40450	46956	66107	45486	38901	32523	71236	40108	38434	52569	56060	69594
C37 H47 N5 S			800303		151154		1430476	170799	769337	80676	290732		110461	76343	35076	61987	67550			1113450	436386	83656	100336	4491	341870			80630
C31 H41 N8 P							28020	15372	25630	18913		57935	9591		11563		49679	66624	66616	43185	65347	4584	71815	74236	9140			
SPERMINE (CAS# 71-44-3); (M+H)+							62012	78750	74501	77190		225991	1834		1149	24566	24959	2708	99569	41394	5519		727918	276954	3500	52891	326471	20448
C5 H13 N4 O5 P							78906	81987	74722	72854	7173		13775	8448	342749	4782					1316598	19955			15659		38193	1148261
C28 H34 O S	19918	23818	22760	30331	32637	31134	61254	70760	68452	73303	47673	57471	40238	50035	76655	43628	58961	48933	84563	71025	62825	55990	92896	58020	55618	70558	94309	55082
C15 H36 N2 O P2 S							58895	58873	61824	58120	22103	135027	1596		17507	15824	125486	127799	199979	119184	154428	20580	145310	172859			14513	29261
C34 H44 O S	67289	65310	59921	63510	64202	64066	42691	660711	60597	57135	75479	623887	72614	83786	78465	74676	81868	55848	80929	66830	70155	63177	78558	96997	152321	117751	92028	83511
C33 H67 N4 O5 P S				25528	22928	34769	157497	222543	210263	192587	114355	168793	45917		291758	76085	256999	66374	114034	172976	255592		67631	68292	93483	221654	57110	46537
C33 H44 O2 S3		5247					19891	25567	21280	22906	16684	30585	26441	32934	35361	16728	27888		23721	12947	31632	9326	61055	15466	33232	24966	33388	22036
C27 H33 N5 O2	174756	173945	166948	177489	65383	166109	52952	57984	92188	1299563	49855	69991	49318	57526	62797	50649	47187	59171	69180	53598	57546	47475	72746	54672	50550	61715	67039	65404
C19 H15 N2 O20 P3							88126	39679	37323	34839									12999				6291					
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)+							5183	5301	6471			11531			3693			6211					7665					
C11 H21 N O4	225111	218209	216741	208149	201707	191538	267788	265007	259877	266158	624996	519317	124464	395879	80136	136795	57028	97396	229653	65689	124153	50175	350022			49355	39919	211306
XANTHOSINE (CAS# 146-80-5); (M+H)+		4581	9516	6365	9922	4653	30199	30948	30798	30644	120022	52612	14178	32109	45680	40490	7102	8954	17326		37152	2724	15702	20661		13986	31770	21822
C22 H25 N4 O2 P3	33606	38779	36840	35625	37943	40268	45785	43233		51088		32922	2486	47944	33615	39143	41004	43084	68178	45610	41170				34704		41662	54755
C15 H20 O4	62196	59282	81657	74400	59586	65876	57171	82247	66645	86654	57858	57177	57723	54318	72272	55267	73995	54339	51457	66513	66896	64689	76386	71987	61055	58535	54106	72006
C19 H44 N4 S2	23931	30109	31371	35417	28888	26725	182082	204653	203943	193968	96300	1283794	54833	73031	250599	172271	128420	708133	166169	166797	343389	88712	226258	144109	49895	181683	105099	826212
C27 H50 N O4 P S	153777	146032	137240	128905	131179	109210	34329	63383		87957	182927	284954	45471	75029	227951	85340	69075	65572	73438	97702	184375	25549		50001	15870		32956	154172
C16 H14 N2 O4 S2							50289	50292	49022	49351		2444		2157	11364	25903	24926	88024	339158	56286	37964	65447	2918	8701	12420	8406	168278	185561
C31 H39 O2 P5 S		2507	2914	4157	11401	4650	56778	89804	91199	105415	6577	94539	4398	13113	22051	10743	31123	50415	371154	360989	20455	8422	458764	38986	10643	172647	91626	33013
C23 H28 O3							49861	42458	59852	85702						25949	54372	135918	868617	103084	67074	91129			22171	7595	427294	317944
C15 H20 O3	37788	36430	41724	33022	28963	31835	28860	27775	28370	26305	54790	49572	78777	39196	50820	46080	79918	66782	80909	61307	75237	60869	81238	62902	53066	61571	118200	78483
C18 H39 N O3	38965	40083	36047	39734	37839	35234	413839	443994	416144	419634	244604	367122	518616	221109	322229	157319	267501	440273	329005	382946	319620	306569	347346	267590	546341	421073	328185	506980
C31 H52 O2 P4	14970	17957	16250	17037	16103	13726	22761	42691	40589	35135	24439	27356	22662	31305	32083	23175	24415	31411	49563	26411	32430	38364	39720	49294	48250	46774	37504	45312
C11 H15 N O3	12752	1845	8934	9996	10394	11557	2371009	2448676	2432927	2425573	751388	222058	270844	528843	373599	850032	3086906	4192951	1.18E+07	6085535	8479839	1959602	3406186	3619192	226606	3945380	277019	4646468
C12 H24 N2 O3	76869	51749	71234	78378	73784	70840	12655	11775	13093	13846	67488	43774	8300	10600	21601	23826	7355	20217	33171		27878		12197	20987	1161	17246	3332	30559
C11 H33 Cl N10 O	3755				9393	16087	38796	34408	17847	53948	77089	66547	147705	47157	45736		57560		72476		93606	30766		68501	63903	49921		82650
C30 H48 N6 O15							134967	112999	110931	115070					3539		1047		56798				39102	23677		1352	4769	
C41 H69 Cl N O4 P S	1480			14413		4244	48965	45397	54752	50595	46089		44972	52541		33002	46907	54469	70202	44580	40922	52080	57315		55681	73904	25730	55270
C9 H17 N2 O3 P							346257	358139	347775	342472	1538477	82046	158777	307990	88137	188098	43410	111420	344251	237108	109748	211632	306295	465564	236609	539460	319433	286220
C24 H48 N3 O11 P	1695258	2249871	2975891	2990075	4197874	4186627	728534	740841	709112	687918	582552	268550	216018	233878	302948	531417	467161	681965	521278	1081360	940284	505777	634901	617099	110753	381604	340712	821752
C11 H20 N4 O3							103607	111108	104252	99435	64146			9906			367422	198570	548445	265523	481802	56229	68899	173094		230551		279509
C25 H26 N12	9915	9808	9990	11476	11594	9718	54648	48498	50315	54769	40940	43234	44010	46467	46971	41538	47715	43845	45784	45995	41504	45971	50389	50973	46906	56389	46011	46162
C32 H48 N2 O4 P2	17233	19183	18371	25941	19977		28607	33939	27097	34744	31478	31647	26839	34667	30292	33735	28909	34800	37889	25523	28254	39422	38501	34077	48934	47375	34180	41437
C30 H38 N6 O6	60581	56048	58920	53518	50333	49814	121674	119437	137198	86227	78931	82669	111614	89485	88086	90061	119444	86548	447762	79489	102662	79532	136318	95975	103075	156004	258826	217083
C14 H22 N2 O2							6119840	6305338	6303362	6318573	1196620	1217642	3173265	3489930	301040	2013080	1.57E+07	1.63E+07	2.19E+07	1.24E+07	1.34E+07	4221749	5438399	9675268	774046	1.93E+07	2882795	1.26E+07
C14 H22 N2 O3	37397	37511	36914	37727	35182	36701	18803	21665	19689	18093					30932	10268	45634	27992			40609		11731	34785		15422	11640	86489
C17 H25 N8 P3 S2		4495	4411		4493	3962	8350		9173			8041		9604	7661	6560			8606									
C24 H27 N5 O2			6345				55716	65578	61304	57119	38708	47162	50340	55240	59100	44472	41370	48096	82374	57064	66892	49181	60519	49046	47402	54580	59273	62237
C38 H45 N P2						10595	19273						25201	20477	25977	11005	13222	12173	15424	18155	23855		29861	14486	17853		18765	12385
C10 H10 N8							57546	61072	58261	54520	2852						203745	73202	270311	31227	35156	18149	46474	91774		292157		
C34 H40 N6 O S2					3408		38700	34160	33949	36040	28494	21781	68722		27071	12797			34529	11774			34424			27534	34824	13249
C39 H83 N9 O		3154		12074			13463	25326		23972			11236	31506	17512	27962		23714	40558						11064	44133	5249	
C9 H8 O3		1752070	1785985		1745883	1716350	1621101	1633712	1572237	1572252	1040363	947084	119103	539215	1142871	1532797	1594958			1907933	2355456	999548	1672253	2411520	84228		1172602	
DESMOSTEROL (CAS# 313-04-2); (M+H)+[-H2O]							2782					6517								1756	4745						1826	
C9 H8 O2	183425	176486	167633	179776	166224	159962	102488	101040	96706	100110	85282	82960	14981	41384	77272	82888	102830	208085	206332	116604	177541	52388	114865	138060		175677	65765	204914
C32 H67 O5 P S3			3820				29539	41053	38029	31832		25172	30980	79107	17669	75670		20155	19166	20393	18756					85991	53377	53033
C10 H19 N7 O	6526	5825		8828		7114	71528	80811	74471	69941	32529	114411	46016	46191	62885	57848	38897	68982	100815	82576	106617	77263	178875	106649	45376		47606	70465
C22 H26 N O P							204948	213042	206403	206954					47799	101437	111227	342591	995358	236887	157140	245811	12506	37933	49755	31453	601876	638598
C13 H31 N7			4149	4436	3281		35794	33515	32538	32952	44354	47116		20275	19915	44979	111844	124135	89207	52024	72018		38672	43079		63948	44051	93244
METHIONINE (CAS# 63-68-3); (M+H)+	1275667	1262042	1188487	1282374	1226182	1211138	2124896				2580750	2040613	364525	1222032	2406087	2135149			7900		3544422	1081566	1882967		102585		1718170	
NAD (CAS# 53-84-9); (M+2H)+2							4630	6942	4846		17046			4268	38764						7875						1730	2264
C5 H6 O3 P2							69946	76582	75340	73568	171611	37745	16826	12028			14403						166321	19812	64728		109059	
C28 H44 O4	67736	68490	66878	67560	67953	64406	127419	130926	131022	133912	103333	112425	89853	126291	114964	105341	99506	117100	152801	103477	115175	144616	152077	134276	192710	174228	142611	140151
C20 H39 N O2 P2	18033	17431	16983	17314	15336	15592	23544	23793	21908	21976	2787	7197	3388	6019	20022	4246	40530	42296	42991	20616	34266	13731	67491	30539	4466	50162	18270	42261
C12 H29 N4 O3 P	422892	431536	408741	412585	393337	393358	330512	358999	354571	341653	569946	611867	703611	607277	557337	467373	981669	694110	816801	646973	743668	688133	937899	853797	650842	614365	1045160	1147688
C24 H32 O3 P6	2002	1524	1724	2143		1431	31434	29123	29300	30488	22461	24381	23480	26984	25984	23068	27723	29786	34558	30381	26698	29266	31936	29607	28524	30107	31365	30788
C43 H82 O				2271687	2215891	2140472	8942					1065699		702102	1099119	811845	1477593		2468071	138101	4645			265643	21978		553614	2084
C38 H49 N5 P2 S2	100740	242702	98544	88220	82627	79293	31112	24561	12214	16278	26558				13163	13146	43777	30689	16592	29759	43831	8057	23415	7558			22245	46455
C11 H21 Cl N4 O3 S3							76232	78016	76481	77186	60043		7702	16944	11873	11933	120328	124532	137748	101142	123008	59298	51965	91169		111434		122671
ELAIDIC ACID (CAS# 112-79-8); (M+H)+	19140	21193	21733				9936	10221				6403			2967		5520				11159		9207				7891	13213
C39 H62 N O4 P S						15930	111305	69916		38308		80559	29032			198189	128988	29013		182223	112494		144851			269122	47321	106485
C16 H20 P2	31423	34400	32300	33822	31551	33429	39376		40928	40587	14262	39934	22153	26802	111779	19838	35809	32490	66795	35027	39332	12223	56002	44254	25415	35202	50112	73443
1-AMINOCYCLOPROPANE-1-CARBOXYLATE (CAS# 22059-21-8); (M	42601	62235	59848	58322	54484	65647	11734	37209	15955	12817	16210	17170		5414	13874	14652	31852			17278	20390	4023	2270	18460				
C26 H37 N12 O P	878543	892131	874761	870694	860964	845441	1497236	1497642	1467743	1482102	1260904	1339841	1146736	1462433	1346526	1210572	1235741	1391327	1573888	1229600	1365725	1610279	1631180	1500838	1960169	1794454	1601347	1523758
C24 H48 N3 O12 P	242039	238636	226914	179203	145344	112627	3750			1127		1661	1405							14231	17176	1221	6106		2906			5726
C26 H52 N2 S3				14680			39389	37551	29444	36659	61142	87705	113911	12839	41788	14713	21397	33123	71380	19894	29969	13821	33038	26844	29849	34600	37919	47633
C4 H4 N4 O3 S	173733	199798	192674	205034	196405	59467	17885	20677	13254	17333	21473	5752	22609	2178	30514	11460	22615	12509	21137	34749	68779	4242	17681	9369		18089	3208	48366
C11 H14 N6 O	254419	251229	252216	254807	233116	232963	251539	290534	286574	281158	271492	265614	272823	279961	186867	264818		183257	100045	290705	168381	303316	270734	294849	184108	172488	169173	179165
C41 H62 N5 O P S	37019	33644	54141	20685	52165	115815	122174	97158	97518	8063	79377	164128		16659		205719	99343	66175	104070	139987	108457	2681	110397	121193	19003	26808	65636	107159
C21 H40 N2 O2 S	25566	16335	21967	21989	23951	22501	51428	66663	307038	80060	59451	108326	66647	152331	182094	47876		73409	89467	51209	75643	43382	299785	63073	80270	68127	75663	
C18 H26 N6	793657	818864	781970	38335	817675	131419	753087	753346	415803		314474	822207	2095	165018	625642	312634	518919	1248465	19776	952267	2581408		2129116	407363	5741	763718	605909	2821483
C32 H40 Cl N3	172300	560270	545751	145630	100320	101548	86612	88769	89876	83554	64704	75092	37711	58540	60341	62798	107860	97455	143307	139944	143447	43772	137336	100907		118442	136803	134620
C34 H43 N4 O3 P	14492	11432	4543	11674	12099	10033	31140	27696	21408	28557	20120	19204	17074	21504	22936	22629	19536	25199	25241	18043	21717	24941	23729	21556	33720	26323	24711	20201
C18 H37 N9 O S		3342					35861	30624	26303	27083	7081	3886			36128	13064	45155	56316	223460	38307	25841	37806			7769	5845	117070	124195
C10 H16 Cl3 O10 P S4							126406	93265	104854	97862									31498				44945			3583	3630	
C20 H30 N8 O P4	49630	39912	39962		41499		37457	45859	23315			32597	56890	27976	27339	36187	37926	30170	54920	30930	42216		77265	29982	50952	53367	52675	48381
C30 H61 N4 O3 P S	52651	73500	77113	7451	69698		154838	170304	26935		17775	161002			52468	51393	554593	151237	39972	100987	414911		465245	132168	43091	159065	119990	316823
C21 H43 N4 P S		1485			5046		63552	73960	51863	65843	136044	53105	226627	78111	33077	52583	20808	35279	46119	40970	26252	88266	231891	80968	161682	131582	38709	49276
C17 H25 N12 P	17637	21120	21301				25390	24386				19088				16142	17851	2690		1083	18998		16321	15754	15258	17370	13701	18193
C15 H19 N7 O2 S3	1665	3471		2128	5412		208257	198468	188821	194227				14443		121155	192924	219775	396597	200611	52090	114590	301275	383796	5013	313508	174909	322176
C28 H41 N8 O2 P3				1694			23820	22755	26429	33168									22829				14613					
C24 H28 O3		4413				5231	15958	20091	20466	17509	20660	26259		3532	22568	5194	1763	71367	30659	26247	90904		52277	22803		15660	15891	64024
C24 H28 O2	37132	36317	36356	40542	37227	38686	293755	287361	138354		138297	349339		66623	204454	104467	190099	882762		411993			1003543	147672		328262	243768	
LEUCINE (CAS# 328-39-2); (M+Na)+	246008	240622	228942	235390	221391	220172	128720	220926	112970	136631		220177	41060	123417	162345	192298	114671	183174			78359	90964	182939	162555		217036	172453	181463
C12 H30 N2 O4 S2	14429	16309	12643	21758	24449	23065	7511	10145	13588	23657	24540		30294	27112	20973	26333	15902	22678			18593	25400	20120	22770	28583	23358	20230	14739
C9 H10		5995		7592	5951	3032	75699	76614		75268	56257	64731	65320	71277	77812	57769	72101	74298	90968	82967	70444	76394	76019	73964	70776	73630	78338	89548
C28 H52 N3 P S3	59275	68090	53861	56736	43054	39320	13986			29296	4529	30165	27303			14869	6267	27001	38008	47559	71468	29313		18141	5593	23084		72460
C29 H49 N4 O P S3	65330	60825	61594	67524	60593	55654	43694	41993	65271	46580	43646	46855	47499		48854	38797	51654	45816	40014	48547	48505	62563	39057	69526	70151		44315	46782
C26 H54 N6 O S2	258716		251474	235975			132678	146411	130226	101965	200965	285370	37955		317139	70658	586753	94838	406766			6752	941006		91952	140001	162592	
C30 H44 N4 O11	649485	661289	645462	612566	592909	563500	1470145	1700321	1639466	1599221	3067200	3826002	3789192	4681904	5864958	2259375	4479058	1869922	3701776	1667647	810324	2164016	536312	1847086	2364638	260873	937371	807301
C27 H47 N4 O P3 S2	1881						149156	132324	127848	129384					10731								42509					
C21 H30 O5	555525	523184	532961	545144	540784	521383	10649	9691	10254	11260	11303	3717					32297	26844	28655	15261	27735					8626		34562
C29 H58 N2 O S3							51908	55894	56468	55569	96969	44501	204337	53405	37539	25962	19192	35789	50098	29510	35536	59302	136909	51294	110365	81724	45301	58256
C21 H30 O3	72113	26746	23118	92554	33481	83599	39935	40211	50348	46882	85220	1390742	92512	33013	178098	83018	49427	100188	139210	163970	76095	31077	46693	160020	51561	157584	54700	97761
C8 H6	120218	118209	110948	116587	107435	109330	67291		61842		52449	50253	5745	23305	47001	53042	65510	134136	46492		114147	33927	73268	92269		110931	39981	131534
C7 H14 P2	9804	9469	9334	10337	10346	9140	14890	17304	15375	17218	3549	10328	4324	6372	21542	3322	19384	25801	16688	12255		13121	40837		7544	27268	18165	23677
C29 H61 N O P2 S3	251322	262189	254119	202019	253574		15283	19042	14125	2633	5076				51128	9047	32289	12263	30253	28277	25916	21407	21172		15416		9339	31504
C10 H17 N7 O							91773	99326	102095	96982	38171	162599	38918	38731	36426	68936	107992	72365	227822	134891	154451	99438	251061	160190	24466	59714	29518	50486
C16 H28 N6 O2	73929	300351	460561	307672	303846	287305	53681	49362	53558	51644	9761	251456	12734	11902	124650	14678	20804	27162	30937	19249	32140	11460	27714	20778	8322	26601	55495	48876
THEOBROMINE (CAS# 83-67-0); (M+H)+	583831	571100	546130	556543	543291	542586	55817	53201	52764	45674		23083						101063	243961	102492	118414		111674	30828		25213	7084	454594
C15 H30 N2 O							85356	102791	96493		63945		60979		18553	73898				31772	102274	93716		83959	93901		55296	
C30 H62 N6 O3 S2	38177		41334		7191	18936	240815	287284	261149	254356	220709	212975	41706		271464	159557	436797	259750	335494	244478	384382	4148	579285		111749		197740	320552
C24 H50 N O6 P	416317	425745	444952	418311	388727	416529	21472	35400						6693	13170					102489	82435	11627	4262					103375
(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-14-7); (M+Na)+							20623					23464				42481	12521			19259		16553						
C29 H42 N18	10174	51500	66439	55681		74666	43854		65619		73068	12943	17942								36962	22271	54307	58212				32273
C12 H22 O2 S3	126996	120632	119186	121943	119525	115660	223719	222366	218939	216980	174574	197197	148346	212348	193083	170731	175435	199455	249771	171215	206247	230056	249330	223380	263196	283142	266474	231388
C18 H15 O P	6687	1088		5048			2804950	2933509	2877452	2860564	60877	200930	33856	155257	621677	1449746	1540641	4975363	1.55E+07	3349948	2184182	3579281	163570	476100	672680	397357	9108625	9650609
(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-14-7); (M+H)+					14937	14738	48072		50464	51517		79387								4269								
C18 H33 N3 O3		8946	10967		17986	11725	100246	106668	99936	104628	16159	33787	19271	22315	29527	20039				20997	24473	22979	23822	24262	19576		26161	
C45 H61 N O3 S2	15810		6987	11200	14700	12005	31030			31168			52178	13994	15695	51688	6779	23751		38396		19303	37786	5029		67306	46730	66979
C31 H64 N6 O4 S2	11566	13368	25664	15016	24257	10373	212156	208292	207686	210490	158114	214033	133435	117879	84790	52939	514612	194836	260781	160332	242133	62330	581860	210783	45164	218892	167756	448603
C14 H30 O2 P2	105590	107948	107567	92683	109777	102651	48626	46021	49699	41687	50053	95636		30551	40332	21704	36831	68466	77390	55012	67031		61221		1005	65036	36629	115369
C20 H34 N2 S3	6040		2147		1830		31204	34878	24117	3625	124573	73251	19703	38877	13560	41335	33204	16721	21807	15885	36296		51649	48018	38125	37519	14728	34618
C22 H44 N6 O11	123982	128624	124885	120036	119436	117559	181496	185601	176242	176487	33034	72762	35805	41283	228267	42495	264431	317157	337518	228943	268940	61384	439902	243335	33071	315153	121905	326647
C21 H25 O P	30880	30725	29398	29415	32412	27268	349566	387651	391293	389542														4975202				
C12 H19 N O2 S2							161657	178610	170387	166350	52126	87297	166559	52282	52071	74369		88700	100794	217219	162851		252939	547304	65301	169182	47722	265942
C34 H52 O3 P4	17814	18999	19571	19227	19330	18960	41154	34979	36534	32099	29692	33248	25234	33197	33437	28570	28283	32916	39282	28351	32979	39489	37975	39518	50891	46511	39173	39357
C11 H22 N2 O3	226938	219562	212346	221670	215296	211232	42894	41334	42386	42665	47007	116679	6061	8700	16789	54640	18731	76852	28542	22950	15234	13606	20491	34197	1633	35981	10116	34943
C21 H34 O6		26436					69472	37921	73512	34958	64317	64398	36145				88385	78624	100902	100279	97648	80139	111935	152224				
C11 H28 N5 O3 P	46769	46787	46670	45829	42574	39449	27910	14693	12327			1725					23911		19700				17163	13966		29443	13822	19959
C25 H55 N5 O3 P2 S2	438319	433440	401309	392145	369734	350159	23407		26498	20803	22202	14586	5766		12117	16895	10332	33575	19071	43571	26974		19969		6487		82955	31979
C20 H26 O3 P2	44020	42920	42681	42510	40526	41688	10710	10225	11969	11102	1470	6859	2713	4836	2676	2171	6609	7890	11489	8403	9293		12567	69787		10301	6052	11885
DUMP (CAS# 964-26-1); (M+K)+							15457	15205		8170	3910			7242	3086	10737	18246					6903	9271	17231				
C12 H23 N7	7665	6038		4151			129363	136741	137132	134635		975912			101405	192054	1546	158956	371303				137740					109446
C37 H51 O11 P S							171239	97663	94326	95023					9162				44562				28470					
C16 H36 N2 O4 P2 S							60780	59211	57843	59004					14273	3161	6026	7884	22489	8447				7717		6336		10472
PALMITOYLCARNITINE (CAS# 2364-67-2); (M+H)+	96455	97790	96724	90389	82875	76670	29694	30097	26876	30275	47357	40707	10515		24865	19450	40514	28601	63813	66911	151957	20729	29091	35712		31063	18785	145354
C33 H38 N7 O P3		25192				25914	136247	134776	141246	152715									11541		1543		9451					
C10 H12 N2 O3	429626	416592	394976	409675	402555	390308	52137	56129	46350	48531	37974	59280	3208		70642	32053	65762	110588	150697	63502	136167		64689	59812		105349		116732
C15 H40 N8 S2			4503				94862	109023	107836	110361					829796			14929		136780		4212					8043	
C6 H10 N6 O	59069	59596	59582	58546	60005	59943	91073	93273	95298	87941	52360	51397	15916	41867	54910	45074	35923	33224	23535	2422	27495	28699	61753	37789	22946	20490	63620	36639
C6 H10 O4	2520454	2497435	2339499	2517011	2428235	2408168	4466			1840				2618	2434	3928	3393	7729		3427						4832		20234
CIS-ZEATIN (CAS# 1637-39-4); (M+H)+	5572818	5496355	5308931	5477671	5323081	5193972	9506954	9606771	9272271	9346710	7841025	8307701	7142254	9437523	8430501	7707158	7527556	8324285	1.02E+07	7392421	7658786	1.05E+07	1.06E+07	9305636	1.27E+07	1.16E+07	1.06E+07	9624313
GLUTATHIONE (CAS# 27025-41-8); (M+H)+							4552	5647	5167	4832	10451	1357		1298	14510	7019	5759	9461	34642		2410					8951	1365	2994
C29 H50 N7 P S2	92114	132021	133423	104753	122794		29434		31919	22282	50724			31301	50670	21902	38417	44847	56097	49155	41199	19062		28706				49104
AZELAIC ACID (CAS# 123-99-9); (M+Na)+		47239					139398	149836	138626	131704	87047	97942	30906	51054	255403	150679	103281	194058	250615	160828		65198	131001	107142	43739	171809	80006	308686
C17 H35 N4 O3 P	79957	88484	79845	66943	82908	96031	435331	454907	442104	454985	203662	3111983	198923	217673	583168	145079	328101	205906	373478	216307	249164	162374	328483	428947	206863	368759	270414	287971
C24 H33 N4 P	11773		16691	10364	10049	11853	29099	24749	23396	22115	23642	21541	15943	22078	16221	30413	17484	25951	32714	18550	14953		25096	25786	35802	40911	24549	23613
C23 H29 N11					2454	3924	51816	61326	55411	51533	47409	39546	41239	56423	75356	45751	39339	57165	65244	66375	69308	38647	52706	49997	36515	51034	6669	47563

C21 H20 N8 P4							4217	3249			4272	2950	3311		3099	2394	2021	4848		4549				4234	3767		4812	4387
NORLEUCINE (CAS# 327-57-1); (M+H)+	2.32E+07	2.32E+07	2.18E+07	2.39E+07	2.29E+07	2.27E+07	1372646	285266	224943	265893	1.03E+07	1.63E+07	3460135	5699008	8875961	1.40E+07	1.17E+07	513847	666204	308434	458281	5831470	1.26E+07	4425415	322695	1.50E+07	8238597	571147
4-ACETAMIDOBUTANOATE (CAS# 3025-96-5); (M+Na)+	6609	47265	42173	50873			21331	22054	19747	22850	1983	5347	2851			5529	12775	10857		14464	23255		25750	12778		19093	6339	13092
ANDROSTERONE (CAS# 53-41-8); (M+Na)+			2499				10803	12884	12735	14066		14300				1536					3475		15774	3904			92725	11707
C11 H12 N6	417174	424873	420057	430525	415189	406961	380179	392010	365800	372616	19322	135334		39020	25845	256647	491300	1032966	1788953	368882		217558	664239	686712	20489	1266260	158100	959081
C24 H49 N4 O P S	2384582	1811212	2356333	2060669	1821049	1666432	382737	344632	352878	352023	335260	490084	219153	225174	302750	116582	769904	424778	481060	273929	785098	133234	456256	393929	80646	378300	308907	689249
C20 H23 O P	10861		14709		9306		195965	234598	229701	236825														2707075				
C32 H45 N O8 S	102581	88384	96719	79688	71306	67145	24613		3060	41752	14001	30229					15718			12095	16516		10398	19627				12551
C14 H33 N4 O2 P	250388	225288	245334	213873	256041	210173	350441	370689	298178	322161	449668	689884	128966	189985	418697	218472	453121	1059646	695998	443491	1139049	299755	921724	485472	482429	668574	567762	1043116
C25 H54 N4 O2 S2	2021	2666					49179	42661	49229	47792	23492	47448	12972	33149	62783	20493	33089	43071	91763	69330	78582	15918	105441	111775	4256	25936	25595	42009
C12 H26 O7	207204	206554	213736	210048	205884	199923	532038	549681	515330	530149	94002	256648	121111	158677	578151	123774	776722	1083172	766524	494220	673094	351548	1359763	577344	168508	1056452	429319	970329
C17 H37 N O3							70898	72946	57987	51804		37091	2791	12755		23793	116557	153453	128916	80781	48950	63288	155844	177434		97151	139015	176780
C17 H37 N O2	56028	61941	58001	47613	46670	42372	349947	371688	357991	359372	192799	122463	243953	197437	230737	129994	140993	334015	202123	536358	131353	445747	224596	218711	211132	369710	113437	441717
C24 H36 N9 O P3							50459	45822	45917	43802									23082				13423					
C13 H18 O2	87069	60513	74016	82504	86708	73349	96367	78076	77345	88163	83626	66954	86027	84419	84879	78151	85223	76959	76559	87483	81107	85568	80603	80759	80417	84831	77163	84301
C12 H19 Cl3 O2 S3							401799	330896	320920	313172					70781				86114				132561					
UROCANATE (CAS# 104-98-3); (M+Na)+							35435	32836	34050	35340				1817		103115	37546			37682	70349	61774	50125	10525			19110	
C16 H22 N2 P2 S	84452	96692	91539	75842	71635	78141	185220	209300	198538	196585	81901	93820	70805	65568	1315630	105499	63970	208433	169408	146792	127897	166063	220111	87399	44083	230380	167537	218548
C25 H45 N O4	375172	400888	381260	350625	329053	312878	279156	312808	319359	301834	562216	2030678	106629	362415	765495	286437	103194	438203	211488	161263	538144	14770	193210	93618	4041	135852	286073	367371
C25 H45 N O8	57738	58408	58088	54600	56833	51667	21942	16960	42133		15710						41407	56861	66849	27517	17973	29732	2000	4387		7851		18787
C23 H25 N5 O2	29310	25025	25646	26025	23739	22636	153795	154973	147595	149905	119309	132421	135412	147779	138152	128264	151050	147682	157575	155933	149014	155702	163307	152289	144159	160785	145144	156232
C17 H18 N6 O3	39064	38797	35166	41904	39002	36366	38248	38582	37599	36913	48448	35376	36962	40537	35280	42203	39708	28701	33954	35682	37929	49206	35276	40093	34933	43458	37493	36837
1,3-DIELAIDIN (CAS# 98168-52-6); (M+Na)+	32038	12827	3644378				394182				15756										1608042		26844					119857
C21 H27 N O4	5972	6278	5666	7400	8254		45087	52736	50191	51211	107240		154983		49635	22726	18140					8747	42917					
C5 H4 O4 P2							183522	58755	198462		351009	279137		294182	594509	326611	154387			156732	259830	45626	98586	31456	182903	122057	227646	
C15 H16 N10 O3	2906			1236			60179	59275	59311	59903					16466								27183					
C30 H45 N5 O7 S2	216649	205739	202193	182065	170439	157178	26648	23108	20070	16347	42305	55494	16989	31176	34839	14627		34702	7274	27742	32795	3243	19624	17762		5254	6469	17239
ISOLEUCINE (CAS# 73-32-5); (M+H)+	2.32E+07	2.32E+07	2.18E+07	2.39E+07	2.29E+07	2.27E+07	1.09E+07	243281	224943	6086566	1.03E+07	1.63E+07	3460135	2437350	3787775	1.40E+07	7042923	513847	666204	1202318	458281	3595926	6790930	1.31E+07	322695	9480202	4170325	478344
C24 H36 O5	9975	18961	23782	31903	20164	17709	138460	165419	147332	119459	52945	21296	43098	20521	1015128	17459	110293	140498	93816	24977		26593		28877	281461	63735	25232	51810
GLUTAMATE (CAS# 56-86-0); (M+H)+[-H2O]	30543				12053		12471	5491			39401		41862	50108	42369	38904	3212					15439			8543		19924	
ASCORBATE (CAS# 50-81-7); (M+H)+[-H2O]							1329921	1358452	1305647	1317317	706353	1066720	520660	289866	881317	878338	1492600			1757359	2412624	578640	1742847	1643341		1921645	957396	2173028
C25 H39 N O6 S2		1186	1247				44472	45639	45766	44363	8294	16599	40893	33987	8747	17159	114076	63085	90144	34607	33857	28542	63848	36782	32185	39485	57763	38865
C18 H41 Cl N6 O S			42567			9058	94913	109788		93548		83817			69139	57597	27150	22391	69433	14439	16099	51843	138063	106295				
C34 H68 N2 S		5781	5356		246971	227853	3202	110213		102946	205796		16904	112490	85879	188780		103746	201667	13413	55103	54807		25002	11176	141956	43565	1917
C21 H30 S2	38143	47238	50791	42709	48345		65044	57915	58057	67114	50267	55547	44461	46487	48815	51466	63760	57874	60799	83907	63477	54750	62722	64906	54504	73730	88663	59907
INOSINE (CAS# 58-63-9); (M+H)+	27950	27060	28169	29554	28989	27288	996287	945400	842061	895199	613452		222437	797531	746901		2193363	1512788		1357570	1036567	490079	1297500	1151057	83521			1193926
C37 H45 O3 P S	2424		1983				41109	54380	47904	52377	14808		16171	2703	8697	2349					3146		6589	2466	2530	4866		
C10 H13 N							118395	125789	121815	117750	13815	2928	4860	10251	8713	9917	365551	289263	755438	367727	638246	60933	121079	239377		290818		371600
CYTOSINE (CAS# 71-30-7); (M+Na)+		2912	9978				13206			13592		11816							6202	18389				5758				
C31 H56 N2 O P6	622946	615472	592358	564990	550415	517832	1349465	1569041	1511550	1473358	2847698	3607473	3537909	4381869	5539281	2085663	4198742	1719468	3465708	1538546	741686	2014733	484428	1696534	2169849	244352	870298	737006
C19 H22 N6 O2	52929	57215	56752	47511	55414	50558	21961		25726		23406	41806		15712	23530		15510	36074	39786	26520	30198		27155	28590		31833		57459
C28 H59 N P2 S3	258229	869923	244923	222197	199597	177858	55303	22517	39178	48435	25085	49277		23260	32052	27072	28612	47370	58721	57675	69033	20175	63267	29264		23291	16246	53115
C23 H45 N2 O3 P S		11922	9274	10750			55128	75435	65101	61336	40274	351371	24768	21714	87089	63758	41873	202875	64676	54911	104036	27822	71879	40781	20651	58662	36448	232241
C30 H41 N14 O3 P3							33042	28649	25733	27290									13889				10279					
C29 H55 N3 O3 S3	3617520	3647107	3594286	3379855	3189232	3070788	428140	416176	417714	399981	174149	422964	102468	231505	125490	306448	122217	94096	299767	95095	123867	48185	445567	67031	116417	192104	233031	368824
C9 H17 N6 O P							489529	500949	489003	484740	51679	483430	563702	772837	29974	337945	1014188	1775433	637901	736799		38271	209698	101914	58439	988000	882819	640992
C11 H19 P3	76285	70269	67967	67803	68986	67413	1014773	1045838	1035038	1035197	745236	1119951	256947	706904	661870	615426	1711504	1284515		1176797	1869981	493990	1526346	1158989	119386	1536434	1045312	1429704
C26 H47 N6 O4 P S	238940	250945	232681	246942	231003	229051	416867	420572	406201	421092	336976	364277	303145	396632	336129	325190	334454	376372	456319	327710	379467	448762	459410	409835	563989	520654	433838	418506
C5 H10 N4 O2			3051				92408	90318	91099	84822		37220					97572		333373	88641		100418	65448		37099	174199	204879	185018
C12 H22 N8	1195						38771	36432	38069	34009		59730		16142	11040		63013	61202	83429	55890	69099	13907	81713	72625	5383	30064	20307	23361
C28 H47 N4 P S	70397	73646	69965	73559	69753	69098	130056	133497	131788	129315	103846	86135	98170	134880	110031	94209	94014	105308	130247	101373	106233	148491	142225	123203	209815	167045	141589	99144
CAFFEINE (CAS# 58-08-2); (M+Na)+	401450	390067	386723	407661	394558	368607	14277	17500	13414	14254		30475			6454	8186	4613	44568		1643	31403	4943	84239	36191	1292			50197
C17 H20 N10 O4	2381	1723					101748	93979	90573	91758									48324				40940				4051	
C26 H42 N6 O4	113872	119704	108684	112943	112679	112710	190267	201670	201752	200844	172431	182443	153205	208867	181616	163241	163159	178745	201105	150423	163018	235572	212134	199779	324995	266429	221624	182309
C24 H49 N5 O5 S3	421226	453878	439095	381946	338369	288849	72926	51522	57023	46935	141739	107869	52822	144298	61770	22381	36210	56426	35405	53752	48714	51366	39180	26027		81706	78273	75519
C32 H50 N10 O4	1124127	563928	1113413	1131441	1082564	1075429	1864406	1897677	1853833	1815692	1281459	1787171	1368458	1454797	4146425	1049116	1501412	1471606	2280937	1450121	1691257	1376836	1926117	2247438	1547209	3250851	1739700	1788248
C28 H47 N4 O15 P							66802	58104	56760	56673					6323				22878				19053					
C26 H42 N6 O5	880268	893471	857223	872705	862527	853599	1573832	1643507	1623566	1639458	1411257	1496890	1250944	1688689	1495365	1318978	1342946	1518503	1716118	1270746	1414093	1913184	1800344	1640451	2482787	2122219	1823255	1626442
C24 H47 N4 O2 P S			62356	66292			78185	73238	73114	66621	22544	37083	17461	26498	58942	27466	275737	133031	175577	38287	369259	21720	114719	42759	7740	90010	29580	327668
DEBRISOQUIN (CAS# 581-88-4); (M+H)+		9619			27948		349903	197817	77647	144925	254361	30059	162622	37831	76408	133481	43853		24946	26925			392221	397465	140336	140913	3045	13905
C17 H23 Cl O						46621	38103	44806	39251	31802	25246	19915	10752	24157	161243		31661		46173	31490	35209		51217	37260	6889	46954	45046	32094
C32 H36 N8 O3	6366	9030	9040	7869	7195	6984	24337	18024	21617	15773	12510	25107	14696	21928	17292	13733	11647	15210	23242	16985	18544	16603	20215	23188	28757	28450	18353	22227
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+Na)+							3496	4446	3914	3274	9077	6723		8950	5807	2528	5268	2881	3666	1252	9704		1573	2006		3837		4649
C19 H40 O2 S	26152	27923	17701	43925	24833	33855	30900	27188					36065	57987		23325	48802		25009	20014	23542	12535			11405			82349
C18 H32 N6 O3	14541	75138	108873	73292	65821	66067	20754	22524	30521	15144	4205	63411		6429	150115	5765				124861	8912	10722	28351	8053		13571	25216	37543
C41 H85 N2 P S2	4995	2012		24150	24208	24274	113162	70639	1029	71919			51609	104176	45684	92369	38256	77625	142235			60129		15418	27004	92555	9150	
C18 H39 O7 P	79403	57008	54721	64059	60363	51232	3014782	3271250	3209794	3198363	9863361	714319	1.72E+07	276359	1934078	723895	272563	679989	1095857	685286	588098	220959	558295	326013	151477	478129	980909	675149
C8 H12 O S3						1169	59865	62373	61263	67565	161859	35243		12722	76121	48209	9000		20723	60917	17004	82889	91132	19214	20229	13155	67247	46769
3-METHYLADENINE (CAS# 5142-23-4); (M+H)+							1177					1161																
C10 H17 N2 O2 P		10319					74572	78867	76572	76361	15844	92929	21350	66574	18703	14963	85763	108091	129914	93052	108392	11797	136623	124063	7736	110633	91346	104194
C21 H33 N3 O P2	76420	79160	76716	68681	63555	60783	3391	3445	4966	11835	7537		3063		3119	3952	6254		1354	4966	9982		16391				7801	20258
C10 H21 N6 P							1.64E+07	1.64E+07	1.61E+07	1.60E+07	9841607	811129	1813864	2709967	3512697	2455262		3.46E+07		3.18E+07		9620836	1.33E+07	2.11E+07	871422	2.60E+07	1261482	
PIPECOLATE (CAS# 535-75-1); (M+H)+	274025	320432	327322	342131	341852	332462	29171	28901	28857	28863	61704	26869	23897	72311	140574	75936	23230	30174	30126	14785		47893	12537	82116	3350	33841	37111	34178
C27 H57 N O2							22618		23784	25948	5834	1141	22249			16520	2321	82846	42358	70961	120972		23591	34747		55872	130840	88301
C11 H13 N4 O2 P	110521	111860	112844	106742	110871	105988	7695	9468	8153	7604											11866			125309				18658
C26 H37 N O6	173052	173693	168692	178895	173707	166486	1195172	1259380	1248596	1208890	1058196	1091427	1140727	1165322	1230305	1063845	1247559	1228720	1346440	1285312	1155658	1242213	1248647	1237859	1170147	1189711	1241444	1268723
C13 H24 N2 O4	25878	25303	27787	36235	31797	31753	27342	26726	25348	30965	21120	27067	10879	14028	14701	18881	26251	30300	39377	29326	31603	13014	29104	25757	12488	49677	28329	40883
C31 H63 N4 O10 P	997618	608019	992668	1010517	966465	962697	1686404	1710683	1673574	1645761	1158877	1513430	1235180	1349787	3564133	987150	1377342	1422889	2139105	1347913	1478748	1277553	1796541	1972727	1406666	2889277	1616617	1651142
C20 H42 O7 P4							217502	147659	145425	143421					12344				66431				48322					
C31 H54 N2 O P6							66001	46756	48124	43906									3676									
C23 H43 N O2	24579	19992	19600	20269	19386	16965	7810			18471	7382							10172	27362								29632	37373
C10 H25 N3 O3 P2 S2	82005	81465	79232	81121	79753	79444	228224	251038	240694	238681									22166							2211	44929	5091938
C32 H37 N20 P							24402	23317	23062	21666									21528		12441		60375	28712		1097	4651	43785
C22 H46 N O7 P	1583338	1564038	1497397	1242930	1039563	907805	42061	45740	38766	42754	60982	90152	12882	30866	34972	26810	24736	49305	44462	59529	76897	11606	63884	36483	1386	31920	21684	62248
C16 H36 N2 O2 S2							78797	100566	105447	99798	116424	151719	16554	30530	79019	62026	78988	134844	149072	351207	75055	12430	93162	97972		80791	66870	63950
C21 H42 Cl N	1942				25978		335307	261666	249803	247246		7797			14057				24899		23823		12626	16836				
3'-CMP (CAS# 63-37-6); (M+H)+		1273					29147	29062		27457	47745	19661		3100	45584	33374	8533			15648	32065	11909		29113	5735		47531	
C23 H30 N10 P6	24401	28146	28387	18254	23493	19782	14225	15671	11836	15989		21916	1726	12474		7347	19300		18618	16137	28816	4338	15516			25370	8877	24405
C22 H46 N8 O S3	15269	17429	19302	21492	17348	14428	38688	124835	34551	32639	26666	24826	27681	30105	26962	26747	26002	30542	103516	23453	26364	36492	31466	31320	48482	40938	30627	26728
C11 H20 N2 O3							195563	200604	202325	195182	192895	298634	25548	61752	194422	166338	159876	215569	471010	259597	267163	27672	148793	380075	6562	351731	162416	280790
C15 H18 N5 O2 P S3							79126	83623	82369	77811	24223	60910	3056	27830	32431	47893	113670	86524	128649	93724	75960	29556	119724	112942		114268	67850	100199
BETAINE (CAS# 107-43-7); (M+Na)+	20490	19673	27966	17214	19571	4247	3791	4227	3665		3881	4624	7242	5415	4167	8156	4305	304022	2663	4055		9131	5555	2666	17953		5388	
C15 H33 Cl N4 O	212872	208128	193741	233409	213829	219012	339923	233529	550527	531895	420110	95011	153886	356907	409253	310886	351789	314205	707388	304933	545301	268908	563899	407129		481021	378186	357325
3-METHYGLUTARIC ACID (CAS# 626-51-7); (M+Na)+		33046			24832		36637		37173	36645	19410				35562	20366			48388	20366	31340	5754				68255		
C7 H21 N3 O3 P2	367080	373002		434272	450936	481283	36239	26653	17908		83492		43833	138164	51145						184958		31757	9361		19907		
C6 H11 N O	193924	190774	183257	185548	186806	104378	2529747	2585249	2479079	2469104	3033226	1930522	1832682	1684778	2953164	1798913	1602077	1799434	3400591	3228473	1947267	2408230	2378232	1869948	2845906	2024275	3251085	4376001
C26 H48 N2 O2 S3	33078	48208	51142	46128	46438	49689	55648	96011	74395	65665	70292	68684	34253	85707	60705	70797	67856	72636	76264	52938	69931	95310	70663	77784	155890	93699	80003	76518
L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (CAS#); (M+H)+							18945	14922	17757	13278	42464	23612	109754	66919	37115	30405			7989			56977			257777		25831	4585
C14 H32 N2 S2	132477	100235	97006	92134	87359	73091	234520	250196	291532	208387	146753	267616		154024	119274	99824	210661	197908	306026	187886	242341	86601	319846	260210	111765	330756	240777	244240
C14 H35 N7 O2							57274	53724	44939	52350		15375		12790		11475	50032	89742	123171	73811	26068	32498	139377	201180	4846	76164	67072	88461
C21 H33 N3 O3	3415					2606	919383	965868	932335	915802	721266	871136	628550	873341	661532	1290694	1250138	1401057	1893307	1505041	1005921	799265	989701	788439	737401	861624	664546	898308
C21 H28 N10 P6	23528	28120	25256	27373	23239	28877	24108	31838		42978	29503			43360	29061	23317	27885			29887	30625	23582	26395	36551	35093	33185	23597	28029
C31 H38 O6 S							28296	28851	28922	24115	23227	54459	33982	66930	48877	23094	45964	9867	37630	12425	45998	5440	89592	15837	84416	19389	56152	18519
C22 H43 N7 O4 S2	149383	143192			130355		15830		14611		5399	21608	23913	39896	35983	13593					14062		35479		32504		25530	
C8 H19 N	9960	9005	9457	9858	10600	10095	185593	193400	186534	182389	604168	127355	610585	102676	115713	67283	101167	94728	268309	40205	59476	88302	68207	279519	113330	118120	59300	50545
C24 H53 N3 O P2 S3	331163				37955	41277	10929			2493		14217							2458		18188	10224			31702			5418
CMP (CAS# 63-37-6); (M+H)+		1273					29147	29062		27457	8468	27730		3100	12793	5089	8533			15648	32065	13906		29113	5735		47531	
C12 H18 O3	1611871	1550008	1508634	1628771	1597689	1488041	3020944	3096208	3076486	3013660	2429776	2690381	1966143	2883866	2514340	2317480	2228141	2623731	3507669	2204628	2781643	3198412	3547679	2983520	3882849	4096027	3425453	3269940
C8 H12 N6 O4	1156		1919		2308	1595	125445	121938	120984	118900		3148			138849	3933			45662			3160	48451		1582		7217	
C31 H47 N8 O5 P S							76529	65819	60732	60567					1118				25025				18162	1320	1408			
C24 H10 N2 O4	24167	24132	24085	24239	22771	23171	37628	36454	33021	38553	31470	33071	28139	38154	35191	31118	25823	33220	39484	28506	35827	39101	41130	36514	45824	46327	46633	42572
C16 H32 N8 S5	46331	49161	55573	42806	64454	51925	50428	42714	35149	24863	32031	44676	13046	41867	29434	27596	46045	47329	50627	39586	60818		66042	54281		56041	45627	68433
C20 H16 N4 O	10915	9846	9963	9065	9712	9507	19266	19831	18619	18463	16144	18336	10861	20637	17314	13962	15883	17569	25546	13752	17945	18049	22726	19411	25885	26080	22205	20681
ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M+H)+		170617		162633		156971	128207	126422	122136	127547	204403		42252	2493	6994		426015	33242						550609				
C30 H58 Cl N2 O3 P		27571	1531	30595		59210	400105	397965	54083	392880	34109	50182	212481	30889	329005	38830	905237	66615	55424	322248	41469	37888	50860	47895	68796	62710	40535	734717
C9 H17 N O2	154028	124810	143407	116174	191028	110106	21743		5664	127525	19451		7727			16956	214749			58273		28140	40217	32533	37422	57958	37803	
ISOLEUCINE (CAS# 73-32-5); (M+Na)+	246008	235474	228942	244412	228363	220172	128720	220926	112970	73871		220177	41060	123417	162345	192298	114671	183174			78359	90964	90229	162555		116243	172453	136859
ASPARTATE (CAS# 56-84-8); (M+Na)+							1100					1966			4421	5830						2260						
C9 H17 N O4	522656	522221	461489	396278	248265	176391	900596				1486315	677236	323895	688461	1202655	238085					1900661	196014	1229211		49550		228808	
C17 H19 P S2							105633				18975	69794			4739		83736	107501		89585	6169	44517	114367	155353		140244	71588	124472
C9 H18 N2 O3						3754	39585	36308	40738	39007	112122	91548	22215	40198	49915	47433	20890	102403	110178	25633	53381	14943	24400			33904	11226	90910
C20 H33 N4 O2 P3							9008522	8473377	8307477	8192691					219182				3769945				3256919					
C36 H78 N9 O P							121479	53238	54859	49389									22704				8894					
C22 H34 N2 O P2 S	71270	72026	70763	72566	73213	70966	790574	894129	840646	856719	563946	569943	714474	797906	1389754	613145	682103	907238	949941	806093	1039602	732438	887745	710620	555370	679739	741252	936942
C22 H45 N3 O3 S2	36960						42543		47386	44491		977050													46231			
C10 H31 N12 O3 P3							120547	66914	65311	71182				2175					22498			8936	17675					
C25 H34 O3 P2	10208	7897	9363	9730	7690	9576	16974	19025	21280	17793	16876	26799	19212	19654	18052	20747	16524	17211	14749	16890	18616	19857	14396	15379	24635	14955	16157	17908
C30 H61 N4 O4 P S	17053	17711	20976	25664	20892	25932	244370	253730	273238	267353	217035	297965	155631	167587	133877	75449	721606	261686	391675	175900	406626	69318	581767	274094	55783	292073	208364	562383
C29 H60 N11 O2 P3		12200				106113	233944	261163	284319	247305	25415		452227	585167	711031	419129	40132	323155		328477	202357	242039	183504	269529	7088		184175	257711
C19 H23 P				1896			27533	35431	30394	30009		64313	43932	30429		20765	32795	21199	61360	19879	18748	32947	50827	35547	30197	37116	25838	20567
C15 H29 P S	51753	61427	53533	54506	56924		39425	47252	43996	43981	68933	64936	77545	69112	55734	62643	73932	67324	63881	63248	67424	70720	64742	71796	74208	66050	84042	54889
C30 H50 N7 O2 P S2	138796	66683	138980	133265	126805	121091	34335	35387	27226	35314	57531	55029	7010	24599	45569		47787	26451	24837	48763	38665	18378	43155	21307		52124	18749	46473
C39 H37 N3 O2	684572	424719	677215	667297	623356	601978	40630			4578							17566		3943	66532	68927	16993						53720
C26 H52 N3 O11 P	2525650	2669629	2662873	400992	2334284	736473	317928	258540	60152	5841		1320050		43028		111502	126429	122973	12677	200400	235842	14161	111337	112748	26629	94249	79848	231119
C19 H35 O P S	56841	47779	63132	64839	51835	60448	201797	213609	39232	208008	236519	310150	42784	47669	235044	127508	84684		206224	268838	821187	33442		261693	4488	250564	170183	646600
ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 2255-14-3); (M+Na)+							1523	1255														1102					1833	
C10 H21 N4 O3 P	201478	207660	209048	246343	199086	200306	220132	179930	201149	200328		203251	208034	253130	234593	205015	250558	227012	178272	173894	190063	210162	240264	193731	237846	246730	255453	230336
C17 H34 N6 O S2							92029	97302	93722	94709	67781	135099	7034	40445	100392	193981	79442	148277	145189	45233	234991	28161	67963	180731	6807	288960	43928	291273
ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-19-8); (M+H)+	63324	8373				54831	4657	7728			36597	13073							6527		2854			2685				10227
N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M+H)+[-H2O]	7444	4760	5393		5289		6163	7418	4140	5741		6220					7756	6672	11390					9779		15536		
C21 H29 O4 P							83634	77108	82216	78351					25604	36392	62788	161924	718132	97973	82956	104254	8389			11126	338848	372207
C25 H52 O3 P2					102955	16937	26563				34636				8399		9596			15902	27092			14147			43396	13144
C37 H34 N O P							14276	8214	7119	2122	10535	4258		9061	6356		19213	17661	24760	27272	52681	3295	14489	5521		7422		41502
SUBERIC ACID (CAS# 505-48-6); (M+Na)+	19097		13416	16393			52233	53171	49192	53367		22848		15325	43950	36975	32669	61603	82161	44612	61045	12506	41247	35052		60502	21096	75872
C13 H24 N6 O2	12161	19623	17683	10661	15032	10972	26404	28714	25464	24957	14269	48811	14757	12567	54537	35654	29889	46536	33716	32332	42202	21931	21301	39004	24478	34731	36880	101479
C16 H39 N7						1099	43219	53033	50738	52593	27744	41261	1016	17286	12876	33053	97443	69946	157693	73922	69066	31559	62680	67135		90673	110654	193920
C10 H14 N2 O2	66961	70938	66312	71391	74637	68635	13326	13588	11917	13265	5137	14697		3597	6967	5935	20122	25576	28851	16687	39580	9325	17500	16997		13824	8363	27025
C13 H24 N6 O3							19272	18281	19017	20725	8692	38008					34767	34226	44190	32320	49130		42065	48637				
C22 H46 N2 O P2 S	22938	29356	36939	20941	37453	41172	249099	244198	251772	247163	82178	41912	31133	20948	1999107	29591	163473	208189	143819	54333	63087	39089	38498	69586	604171	100067	28016	109978
C11 H21 N7							80299	81710	82615	80178		70137		32379		11103	62572	64371	183156	154383	167191	20610	256339	226462		68369	44314	55396
C14 H33 N7	102569	103652	103674	106676	99782	100130	145673	140425	151732	143319	415039	371667	15155	118544	127929	276863	341477	361242	298598	216692	400207		156320	146414		227987	136436	389077
C17 H33 N2 O P S2							16484	14881	20102	36848							27427	73753	268784	47557	39282	46802					135734	143301
C9 H19 N4 O2 P	2364	3240			2792	4320	112199	115022	109621	106320		1635				21082					3988		1614	1111				1940
PANTOTHENATE (CAS# 79-83-4); (M+H)+	40273	40155	30911	38225	38176	37106	31732	31680	31140	30074				9058				43658	81102	121201	61217	7716	33930	35496		55199		72108

C26 H40 S	4969				24399	22238	281380	301594	300076	282714	324831	756604	157262	146348	188656	147234	689602	488375	472438	220218	368439	107923	300285	258945	82534	330054	265881	607223
N-ACETYL-DL-GLUTAMIC ACID (CAS# 5817-08-3); (M+H)+[-H2O]							1126						2679														1909	
C34 H46 N12	32959	35673	48333	44685	47863	31222	6571					16128		28902			9449	10784		24138	8875			43268		8081	29271	11816
C5 H7 N O3	1508935	1464110	1415897	1550969	1404236	1448504	8581064	8808021			803916	3911514		1333799	1404106	5111950	9046911				4489097	1630579	1.27E+07	1.51E+07	779938		6991759	
C4 H9 O2 P							158834	353229	153477	149193	42645	398501		31960	48275	1525589	161058	1.48E+07		246178	124957	1570492	378889	46645	6714	650032	193155	927506
QUINOLIN-2-OL (CAS# 59-31-4); (M+Na)+	7365		4645	9036	6589	6381	22333	25523	23522	23051		40357	9548	18748		17563	23345	25720	36842	14301	18652	21410	44828	32732	16861	33475	22247	21201
C20 H29 N4 O5 P	65490	33374			49657	50347	724880	839999	760187	829045	316941	427062	529961	644891	4809473	353272	397232	624403	650318	662573	675992	481007	737084	358938	546337	203930	608648	680803
C25 H26 N4 O2	231813	224879	219922	248582	241358	236338	2819952	3064534	3071510	3055087	1852589	2262851	2280208	2315282	3480921	1996015	2063343	2724388	2859603	2577651	3135261	2430564	3357174	2304611	2178933	2873287	3005483	3201103
C14 H27 N4 P3	10412	10153	12044	12002	13667	11667	196739	190452	187264	187059	10175	9810	10719	8400	56205	10906	12491	12457	96475	11659	9788	12850	75564	8904	18297	9890	15553	13228
C21 H17 N						1914	6202			73432	302906	18830											91367			122147		37846
C12 H11 N9 O			11153	24981	22833		53521	51787	53701	53150	103135	216909	15304	94727	94392	93951	65724	59971	104570	51894	106964	22375	43180	36326	2642	72424	38416	69348
C20 H35 N4 P3	60616	71965	63396	59759	59084	58152	109030	119229	116802	121924	76713	140491	102920	140061	85549	97980	102134	78548	100162	81215	115737	90971	126939	173300	95903	97174	108876	90816
C15 H31 N4 O2 P	72213	82800	81544	70562	89486	88911	159124	192803	186897	181585	89841	1390372	92512	93356	183894	83133	134346	100188	158325	64809	79058	64212	137005	159626	107034	157159	145838	104574
C15 H15 N3 O S	1558	2568	2787			1171	81029	84303	74058	75783	595326	73293	8484		154611	92885	69356			2152	169019	53331	62397	98848		91540	81027	124526
PHENYLALANINE (CAS# 63-91-2); (M+H)+	1.56E+07	1.54E+07	1.45E+07	1.56E+07	1.49E+07	1.48E+07	9126915	9281787	9064085	9114624	7775118	7308179	1009688	3440474	6850878	7463582	9234501	1.83E+07	1.83E+07	1.05E+07	1.57E+07	4628126	9988971	1.23E+07	316891	1.55E+07	5764731	1.80E+07
C14 H27 N7 O		13291		11939			75211	89615	75150	71461	29220	131297	53013	38086	52250	65886	35045	46569	139766	106049	129610	82989	238617	123073	36105		33790	67049
L-HISTIDINE (CAS# 71-00-1); (M+H)+	6617			15985	5895		36267	40082	38403	40366	23219	111091	4435	19534	6333	137779	29195	25708	21311	7161	3985	55787	22474	68525	34297	47753	16268	16355
C34 H68 N2 O9 S2	19928	15631	15056	16538		15005	254985	247580	264323	249080	77601	100353	12538	40338	2589935	31922	96811	100714	67294	37602	26376	36899	19666	25848	303434	87473	62587	100434
C36 H66 N O P	82614	89760	7917	12928	4273	236197	11320	13662	18660			19185	1543	17256	18411	14184		20183	21948	34533	32096	2285	24994	18792	4477	14604	16929	31236
C39 H48 O2 P4	131242	18331	131692	142477	117167	120991	28270	33971	30072	30694	28925	27319	6799	19139	20570	10557	6500	40364	31736	58889	45807	8892	35077	24600		31292	22450	36792
C27 H51 O4 P S2	109527	101594	108795	115547	99092	104158	153828	125934	131872	130419	124698	115153	113506	142616	123004	123906	126755	123895	120141	104117	115202	148190	122414	134489	188472	152261	145289	125861
C29 H32 N18 P2	50132	47230	48479	46509	48074	44243	74729	72036	66494	67317	62242	65502	58251	66588	71858	62399	60375	62935	68834	58021	62941	75329	69135	69247	80738	74109	70134	74243
C25 H53 N O2							108493	108171	105268	112398	15394	36954			24939	70227	141604	320373	197463	258248	491769	152425	152081	144517	5758	226546	532658	329154
C17 H29 N O S							18149	17642	21696	19811												2252		1581				
C32 H69 N4 P S4	24537	20853	4656	18437	11144	3826	20687	19526	1806		4454	42762			15998	10635	40990		27785	36989	67166		69586	28181			9062	41536
C50 H93 N3		27064		195198	171455	180673	316933	559489		552378	150563	50453	225482	688976	323907	586401		527402	975563			361854		41528	195530	1041431	183837	
C26 H44 O4		7095		33750			41582		36333		33035	216236	34457						8859	42843	57850	42677						
C30 H59 N O4 S5	198388	15070	193152	202738	188326	185258	58203	47896	49764	41558	41343	36799	8198	30499	26719	5644	36157	51118	35915	67961	60387	18021	56477	43095		43781	25795	50569
C16 H24 N6	520241	545424	543963	543482	522173	509934	21396	21127	31045	23763	15305	18759		10315	8865		17074	70566	80439	61354	85495	5572	37473	50645	49829	45734	13942	91917
16:0 LYSO PC (CAS# 17364-16-8); (M+Na)+	1.71E+07	1.62E+07	1.71E+07	1.62E+07	1.50E+07	1.44E+07	784305	707374	694836	639740	504810	288620	149226	185740	234786	445428	423725	753542	572071	1417201	1257295	395035	701468	611490	67947	394117	321508	1013916
C13 H11 O5 P	47809	46173	44649	49252	46022	44633	4417		4646									15587					21046	9602				14971
C26 H50 N3 O11 P	3546310	3597111	3515181	3298222	3121848	3005533	305535	308724	309710	289911	436692	282657	96764	245367	303015	233921	148903	329745	203347	468562	353705	157046	317153	257944	28237	175948	141147	343439
C17 H22 N10 P2	24316	25744	25356	20603	22867	24563	15495	1651	14099	13925	11665	65187		6633	10320	2612	8902	15209	21783	17115	17089		15831	15792		19505	9950	26805
C6 H4 O							102509	105930	105598	105754	74738		10003	21218	15173	14436	197490	210237	261521	150461	210170	72486	64901	133074		169076		212622
C23 H41 N	39319	39597	36714	44813	38655	39510	202768	213205	200578	189817	35502	47732	46321	17779	4738328	47969	49850	68556	76023	50989	111925	23070	63263	60010	40361	48645	43666	89095
C13 H25 N O2			38557			40106	847716	875428	855467	867975	388087	1374371	620939	497291	588286	729896	433922	504809	1279259	1008324	1334191	943609	2058298	1190853	470766	460369	437528	794836
C15 H19 N4 O3 P	360882	364521	362822	389245	385902	389392	2590443	2921888	2907114	2846185	6574129	1598718	1.01E+07	1003575	2641633	1125242	985799	661885	1423185	823113	667002	479199	2274848	553428	657667	1634453	1599049	847934
C24 H54 N12 S2	7533					1592	249186	282190	258895	284000	236929	123654	51088	92880	94720		489404	71922	266991	267683	354214	59888	721717	74840	116825	328030	126193	344113
C13 H25 N O4	76637	74641	64742	62380	56439	50452	21011	19309	20070	18761	15801	8806	2636		6013		36795	14448	35889	57462	39821	5454	17556	12433		19840	7669	103022
ALANINE (CAS# 56-41-7); (M+H)+		2449	4770			5825	3945																3677					
C13 H25 N O3	68827	71627	68122	67215	70916	63499	831233	871228	847731	835084	251780	923453	291066	434435	840701	285266	641568	979374	1710076	1037824	1300115	258624	1629328	1414689	115511	681456	517133	1031048
C25 H51 N5 O10 S	858057	920408	815778	401038	785877	715228	294486	286698	53498	5920	36597	1327214		43577		113352	122222	49413	31822	79534	45929	14385	111551	25363	25638	95038	79961	44434
C9 H20 N8 O2 S							164476	174177	171393	158467																		
C27 H41 N5	103122	104297	96739		95518	16022	88590	69668	3334			477210	4173	1742		47859					75400		98940		35661	5961	57987	83539
C9 H7 Cl2 N5	184287	186496	174482	186226	180191	172597	382964	396984	380967	371301		8120												3719618				
C19 H41 N3 O3	227090	613016	228050		22084	32581	3669679	3131445				5553692				533242	8384829		940463	9118	387418		8013788	94466	620075		3018668	4216482
C17 H33 O2 P S2		2448	2155	1641			44346	47367	45376	44600	121986	12209	270378	9727	29226	12273			25095	19658	18172	6628	22347			20964		17814
C13 H25 N7			9981			8629	821297	854057	825575	830472	44225	114736		46854	189119		66576	67061	203056	77581		53834	372573		59947	101709	63417	74039
C9 H24 N4 O2	3735	1669					227354	210782	230720	211947							203243	222147	228175	262124			393932	222952		186709	193353	170309
C22 H29 N3 O2							58729	61313	58034	59465	15366		1958	14510			66232	69127	353193	288368	90793	20070	13504	53218		148610		90918
C26 H58 N4 O2 S2		15947			3185		27103	26819	25203	25089	10235	28197	10542	12794	21196	15937		14530	43926	44496	56109	12163	88093	69400	4875	10660	16013	21835
C30 H53 N4 O P5	109225	104846	101388	102062	102930	103903	4445										1171											
C32 H65 N4 O4 P S	129558	24462	117961	51147	95206	21085	151405	166466	40658			177790		47829	48551	43026	442641	142739	75497	104856	391702		665534	132556	44394	150808	131200	301217
C21 H31 N3 O P2	47433	45271	40939	38830	34050	30674	3783		3837	2290										2863								
C29 H15 N8 O2 P	30580	50842	34798	34551	38974	37931	23887	27063	26443		3716	23748	34632	23608	18357	24474	29150	29357	34083	32490	26360	23268	38723		26718	33444	23728	20306
C31 H43 N3 O3 S	21389	21144	22196	23182	20417	18519	21352	21273	17059	22051	65160	60470	14966	98382	81014	27887	7063	24868	27658	8248	34130		12815	6893				15886
O-ACETYLCARNITINE (CAS# 461-77-8); (M+H)+	852479	757343	650892	378778	246803	163668	892893				751687	335193	139068	246781	556000	233145					2351848	192505	1226925		51432		217554	
C16 H37 N7			1557			4568	126557	70179	75686	79256	27000	31091	21159	13907	16636	38779	238628	180354	220073	142554	163376	55232	101492	108849	28847	151333	126088	273132
C36 H66 N6 O4 P2		1356					30901	19261	16063		18430	37745	36594	3063	19544	3273	11709	5097	4303		7313		11927		4132	1360		13333
C19 H41 N3 O5	5109	5658	4307	10230			38323	21417	36438		13745	83505	15892	15398	40504		71798	47544	93292	67285	87964	61103	73640	75116	19863	61136	50659	66640
C8 H14 N2 O3					3080		170034	184869	174744	175337	112383	308514		30349	110994	106353	178158	103017		64516	184871	1530	128648	348165	5616	267369	118641	186007
C30 H33 N7 O2	32820	25993	29558	24118	24973	23298	12500	78508	54869	8842	17792	23117		5151	34307	24981	74340	90228	119624	100162	142333	30750	19347		2052	110198	50562	42855
C35 H49 N17							28427	22458	20491	21248									6225				4166					
C28 H53 N5 O5 S3	293871	175650	347421	215295	224608	297139	35572	23998	22942	19558	57566	25711	7010	21287	51230		54905	23995	24989	56275	46929		43155	21307		24281	18749	54533
C6 H15 N3 O2							359179	362723	352330	355090		121599				438778	449140	699289		519154		701730	315083	439857	86768	484536		517179
C33 H27 N7 O2 P2							118145	139952	142613	128503	67920	87962	6258	32404	180216	943630	18456	132595	432298	131642	1887818	306744	311086	157828	4491	135218	76320	635426
C31 H37 N9 O6	105343	103171	95758	87095	458302	70769	12536		17375	24201	38560	46934		16817	2061	4027			48704	18453	13631		23573	17372				17994
C39 H31 N9	47948	241776	52010	184759	159460	150554	14177					6932		8228	13982	9084		13361				1723						5166
C19 H41 N	13491	16424	14762	18284	17025	15314	143317	102029	88162	79117	26586	31783	15109	22031	28127	21016	26512	19983	31417	34497	31717	13366	31599	17674	14958	39663	42486	55223
C34 H74 N7 P							224010	103312	106522	96270					3261				35251				21221					
THEOBROMINE (CAS# 83-67-0); (M+Na)+				29421	22553		5778	10227		4718		3647						21670	42143	12163		3817	25835			1268		82473
C26 H55 N O2				10953	13079	4235	321692	314599	326376	331988	40987	98110		39606	69437	146238	387372	934294	626341	1069985	1999123	490291	376781	447504	29438	682885	1876212	1371910
C12 H21 N7 O	7756	9909	5504	7740			32749	26208	26063			50908	35463	13810	18560				46529		35238	21299	61676	46079	27986		30960	
C19 H21 N9		1938				1243	23402	28259	25472	23940				2204			46187	30610	193067	19878	55938	3485	15629	50515		111944	1133	20707
C17 H38 N2 S2	217864	259927	218807	149321	155742	192560	456222	111373	95498	395356	356911		327147	309536	119043	127794	211990	130615		124391	123091		206244	139281			205720	353978
SERINE (CAS# 56-45-1); (M+H)+					5049		10919			10975	8351	15440		5246	8915	10588	6975			9782	13099		10487	14763			5566	
C21 H34 S5	38362	37726	35781	35181	34810	35066	7668	7861	9073	6675					3574	8282	8924	27229	29466	14196	14240	5608	8992	11315		17722	4327	26642
C28 H44 N6 O14							567662	493593	484497	484488					37045				182995			1231	151396				7520	
C35 H60 S3		3159			3390		28106	31975	24213	27389	42765	49276	86659		36093		12267	23882	17232	8785	20842	9535	18402		18102	11737		33832
C31 H68 N12 O4 S2	15414		5584		9067		91140	102821	94582	99660	67121	96029	58469	63455	53817	29063	184057	94234	131211	69442	117901	25074	343874	103684	20511	120399	84386	243658
C14 H30 O8	339289	328009	323681	333963	323444	313508	633791	643605	618743	621785	87221	243207	117089	154257	548091	122997	1029666	1205998	931755	568986	893529	468124	1865185	735610	145954	1428761	453676	1176478
C14 H34 N2 S2	177215	140092	146748	180948	243067	248285	375451	112963	96398	439075	277503	83764	82778	251550		205299	236633	68530	105789	801397	70021	132513	94824	253889	177518	81126	91522	272663
C25 H56 N12 P2 S		39293		12600		2350	53348	61921	60947	91711		15190	19661	6297	65655		291239	65466	268496	15231	388173		70479	15583	33530	71695	27219	291454
C13 H36 N8 O2								170530	173488	167068						113011			33632			86829	80909		321800		1827	
TAURINE (CAS# 107-35-7); (M+H)+								2551			36472	35052	130774	45444	15760												8835	
C19 H28 N6 O	60646	45168	64618	74867	76894	80899		15655	17473	21032				1385	2407	11502	6051	37062	41818	43532	10250	8556	8334	10453		16227	40403	39966
C20 H45 N3 S2	26616		9646	16845		9755		77706		98526	31146	100037	78733	87424		106071	158871	49391	52680					133342	11246	77371	61842	18256
C4 H11 N	35548	35809	34311	34033	32457	35808		304029	284640	289051	189840	214816	218017	220802	217927	222892	268472	304478	430387	302100	269578	296342	276555	254454	252728	247977	346653	377055
C42 H86 N2					219767	175707		306801			255531	277939		219922				247321			20984			285794	205149	289490	264906	5123
C7 H6 O4								60940					28148	39149	5687	30770		67860				43239	94953		24886		48450	
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+Na)+	26660	19398	20983	26562	24377	28082		34281	25283	29151	31547	47201	12911	39139	47038	19150	27854	25308	27231		55998		30113	23622	4272			21806
2,4-DIHYDROXYPTERIDINE (CAS# 487-21-8); (M+Na)+								2791				7897	5031	21016	8127									3657				
C14 H10 N4 O3 S	185624	186191	182904	184842	177703	174126		1304		2454					2081						44769							90901
SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (M+H)+	138605	155703	337801	168178	186402	202559		5310					36562															
C13 H32 N6 P2	81717	81435	78872	83661	80029	76586		11937	8504	17995										13932	9042					17363	20661	7338
C28 H49 N5 O2 S3								14040	8507	23863	17753	27689			24288		4796				18874				1309			24163
C20 H44 Cl N3								29385			1334								75900									
N-ACETYLNEURAMINATE (CAS# 131-48-6); (M+H)+								1614													1534							
C32 H8 N2 O P6 S3								113773		94917	189826	6250			224107	320812	96840	420571	274770	320847		276294		9040		245853		
ACETYLCHOLINE (CAS# 51-84-3); M+								7929		4457	9862	13942	3144	10540	17370		7152		14623			6706	3315		2401	7030	5020	
C19 H27 N3 O P2	68874	64788	58531	56927	52804	47150		1912	4112	2983	1389							2278	2859	17582	15315		4704	2240		6156	2427	2125
SEROTONIN (CAS# 50-67-9); (M+Na)+		37449	29660			27442		2280		4190							13212										11047	
CORTISOL (CAS# 50-23-7); (M+Na)+	484681	457178	453488	463576	456437	440270		15252	9955	8708	10656						36372	23790	27456	13105	25543					8438		38200
C27 H25 N6 O4 P	36518	30997	25030	3495	1743	2129		20004	4329		5972	23754	3962	9760			17806				26047	4886		7778		27962	25129	27946
C33 H50 N5 O3 P5	91720	50133	88573	79797	65794	57847		7154	14448		8843	12208		5324	8845	3993			9343			1313	9159					
C38 H82 N6 P2		54422		296688	292428	273244		943635		919365	328718	500305	469499	1291565	592649	1146976	366210	958508	1834551	1052135	13773			453172	324852	1519032	412117	
SQUALENE (CAS# 111-02-4); (M+K)+								4439		3847						4185						2259						
C23 H24 N8 P4								1085			2185		1670		1294					2428	1772		1666		2112		2164	2282
C21 H32 N6 O2	27755	17584	24716	41797	29075	43058		74277		77395	119201	97402		43615		48720	169940	183499	193442	70135	169811	57975	143858	96475		112903	49679	106769
2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Na)+								10393					1283							65152	37430							
L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M+H)+								146107		148036												1404650					1540429	
C30 H39 N5 P2	24346			3171				13125					5899	4247		2596	3832	11624					2566	6077				
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+H)+[-H2O]			7295	3121	2954	6650		60984	68605	58422	20760	90917	5415	19229	26709	85067	8243			63766	22676		16740	69622			5215	
C9 H15 O P S								121994	107212	95618						57817	77719	168353	205071	281029			206386	145841	36034	119025	155255	297716
C16 H20 O								42657	59981	43336					1355	19619	22669		62833	61132		69490	61866	83161	9842	81397		99061
C43 H83 P		17705	1886	136497	136025	125824		64808		76612	149099		1270	50615	72151	68897	72916	173773	175499	111768		20750		17314		76614	36665	
C3 H7 N	2943	28154	683298		29901	27214		112963				2944	11668		11144	29803	189434	188407	443090			71589				182619		173268
C27 H30 N6 O2 P4								3617	5261	1128					1260		20678	34845						24483		2165		2223
C16 H25 N O2	46163	32457	30556	31085	30934	30200		8569	12514			11951	1368		37062	6671	3841		16755	3616				7873			9318	
METHYLGUANIDINE (CAS# 471-29-4); (M+H)+								11386	12160	9914									19870	8972						17765	17379	16914
2-AMINOETHYL DIHYDROGEN PHOSPHATE (CAS# 1071-23-4); (M+H)+								6847			128649	18014			132910										3978			
C22 H37 N7 O2	40553	41313	39873	40589	40352	38019		1841				4189						3173	9973				2407					
C4 H7 N	141412	162624	152597	82085		154842		1194	1095				40651		131662	1930						6127	30037	2292			1312	
C9 H29 N6 O2 P3	21171	22796	21189	21661	23849	20131		1156				1773				1857			61967		27002	9235	46841	24891				
PHTHALATE (CAS# 88-99-3); (M+Na)+								9550		7971																	1495	
C8 H20 N8 O2	49885	50581	47716		51179	49327		1922	2322	1925	1977	1969		4583								1908	6244		1093		4174	
C20 H36 N2 S	165582	161924	164732	133137	198612	50453		32334	205478	21204	90449	20708			38545		173797	228876	61514	135499	220370	5679	216206	65190	231239	22959		194667
3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M+H)+	9064	11984	10410	10456	8436	10700		1376	2955							2886			8709	1758	4022		10301	1106				
3',5'-CYCLIC AMP (CAS# 60-92-4); (M+H)+								1135		1413				1521					3909		1694							
C5 H12 N3 O P								190151	183088	181903						215245	170649			371348				152221	73354	223021		96759
HIPPURATE (CAS# 495-69-2); (M+Na)+	352805	355729	347658	357901	354396	339281		19791	18245		31029	1886	5584				54233				72259			63510				
C12 H16 O4				68785	80026			139551	139925	136086					10709			66125			43700	32985	103377	116704		385443	252615	117124
C31 H64 N6 O2								21329	1764	79960	128469	98807	12041	60693					77799				5534	83101	10354	70740		
C13 H18 O3 S								63922	56686	60249	1178						36413		75595	146042		54762		74488	6356	139133	37632	98331
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+Na)+	7276	6449	5168	5162	7037			15628		20299	22144			12136	32320	14388	11144			47374	35460		4699					
C19 H36 S5	39384	41284	43255	41178	40966	39728		15614	35836	1853	12347		3773	10531	28477	26047	6088	8860		21103		19080			17409	4481	8352	9354
C41 H45 N7 S	20541				89419			26114	24824	24570	38684	52409	42355	54684	75863	33217	52705	26239	45166	28596	18921	26218	9481	23669	26060	8046		13503
BIURET (CAS# 108-19-0); (M+Na)+								27799				36001		104526		23136				17522		11211	17041	20131		22559	31871	
PURINE (CAS# 120-73-0); (M+Na)+								11522						5353		8374												
C8 H15 N4 O4 P	537968	540431	535063	540897	522292	507496		7945	8110	7101								10303	14258	38802				62336		1053		6413
C9 H5 N5	64982	62765	62525	66635	61328	50133		17357				9067					24541		57522	117225	2162		20785					
C23 H39 O7 P	280723	177598	251133	248992	223073	206871		18485	3861	16326	12544			4123		11128	8489	17842	6109	31387	26173	13905	16046	15370		10203		27371
PHENYLEPHRINE (CAS# 59-42-7); (M+H)+								3394	4039	5485							33843											
C9 H9 N O3	483106	485784	477970	499553	491733	457939		22641			45043	6631	6761			1020	84181		1932	1695	104421			90752	1735			
C31 H37 N9 O2 P2	24598	22960	24112	29406	24806	28103		1243																				
C16 H30 O2 P2	107680	109399	109925	113045	110373	106960		7797	3910		3389	7730		5377	8473	4085		17074			18408		13428				13871	20628
C15 H24 N2 O3								16869	16998	17249	16043	3435	3084	4592	4868	4031	58026	56247	50181	23255	41018	5343	9344	46451	1837	22399		31609
C9 H13 N8 O2 P3	69010	67528	55912	46334		58714		2053										3845										
C25 H37 N16 O2 P3								22222																				
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+								37437	38265														56991			55383	32024	
BETAINE (CAS# 107-43-7); (M+H)+	955416	908830	831624	879575	846845	839916		80854	132006	58969	231295	4524185	270217	2113765	2964739		116021	269114	76137		5023926	117509		68831	7653	90924		
OLEAMIDE (CAS# 301-02-0); (M+H)+				9154				4729		1967			2424	4598				3465	5078	4462			3948	6400		20141		
C21 H39 N3 S			19375					96309	92519	69056		115616	67704		75048	62980	212364	42213	68151	20521	46231	34172	91156	89812			78831	56869
C34 H45 N9 O S3								41781	43200														4928					

C39 H35 N9	37338	23272	32661	33483	28188	32476	52904																				
SPHINGANINE (CAS# 764-22-7); (M+H)+	7482		7773	9316		6964	14833	16415		37052	35159		13591		2110	29259	29921	50909	1912	1925	1883		26419		28339	23498	52550
C20 H46 N4 O P2				31570	37131	4295	48895		42828			6248	20907			34693		18673				34099	23934	26458	30410	42742	9845
C37 H52 S3				3245			39102	32552	33692	13740	20355	22180	81008	21740	66566	9691	28433	28100	27714	35257	8544	22475	13721		90770	59813	60225
C6 H14 O3	240266	345570	384036	339880	329728	332397	151773		166220	136305	127626	218964	155720	188849	149103	106192	122415	162100	121444	148159	177512	202100	154793	205295	162752	372594	
C7 H9 N O3 P2	79834	80640	77462	80805	73402	73342	5280	6576		8756				4381		17512				21986			19635		6173		6361
C28 H57 N3 P4 S4	8327	43761	45707	27812	5640	36885	3452			1712			3327		1162	3038		10704	3511	9262		7452			6929		
C38 H27 N15		204787			13752	25030	4394															3452	4272				
C46 H88		49088		3396450	160744		578265	9464		1311979	789156					1103762		1417529	1745586				1165803			583841	
C36 H54 N5 O4 P	1969	40360	6564	2164	7544		9925			23449	63042		38489		12325		59275	72641									
N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M+Na)+	7276	6449	5168	5162	7037		15628			22144	34414		12136		13075	6589				10162		4699					
C43 H84 N2				92213	93283	86309	101464		92129				90093	92873	55448	136526	209434	249857		32838		8779	12296		136094		
C13 H19 N O	116242	100788	106251	112628	103595	92706	2248								1097												1212
C8 H8 O							108801																				135980
C40 H86 N2 O4	3318	3798		131512	191706	136327	78226		88909	114231	86746		52444	63699	72241	231512	165453		163418	7420		236232	74093		131301	129889	39789
C16 H30 N6 O S	37642	37574	38308	61798	50568	61569	2259	4520				3763			9221	3006		43093	4726	1400						20734	
C28 H54 N2 O	1155			127184		109319	4088		110834	105959		121425	101401					138462			5851				136161	1389	
C27 H37 N11 P2			119733	85232		65714	6881				1826						3068										
C47 H37 N O3 S	85639	89302	89590	93927	85533	105832	25392	24336	23225	28092	23007	5567	16365	7158	1613	20643	31746	27130	40566	34665		27063	19822		25862	17516	27835
C39 H36 N5 O2 P S			110205	92653	84305	74310	7386	6293	5563	9579	13376		7077	3172			4652										
C21 H5 O8 P5 S4							95650		88138	166334			53377	65713	52769		169403	121374	282758	77036		18609	12584		94731	8130	
C33 H45 N O4 P2	100291	102370	48206	32433		29652	2698	4532			10609						3819			8928			4102		6040		
C18 H32 O2	3664		1792	32361	25014		53858	62010	10068		16532		131848				28666	27407	148771	54144	27932		112985		391366		62173
C22 H36 N P							49531				87456		58388		27415	104431	98359		58027	82591	36457	134109			104587		78248
C25 H51 O2 P3	6695		40356	35814	37736	24671	8527				12079	5602	2868		8409	17622		4813		8396			1016				
C19 H22 N10 P2	26259	20989	23633	25593	23207	22576	1037										1189	1453	3839	6419							1145
C17 H36 N6 O2 S	46728		62807	60809	44291	54275	93125	88289		32963	582420	25222	35953	73554	26375			53347				45234		28722	7209	65255	36813
EPINEPHRINE (CAS# 51-43-4); (M+H)+[-H2O]	8174	6942	1926		4942	6574	3033		4298	92076	2534	1721		3557		7230				5707		1919					
C27 H52 S2			6991			11508	39755		51017		38647		106341				38563		3205						60110		13922
4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-KRYNURENIC ACID (C	9194		6495		6920		1065				2341											1297					
C18 H39 N O4		9181	7198	10330	10061	9214	1653								79191					87056	96098	174495				116915	130954
C28 H48 N6 O S				5124			308783	293042		290879	429413	184814	209461	188140	92490	791064	35729	478845		651433	74307	441102	335435	70559	357729	270194	653875
C26 H55 N5 S5	29789	20111	19637	17546	11148	14676	5282	9409	28473	17711	8461	1361	32829	11613	5180	13849		6572			2195			7367			12812
C31 H66 N8 O2 S3				17741	7888	8190	66571	23211	19210	59212	34343	12421	33952	33432	13162	27597	18913	45943		8682	30595	62435	26059	38254	47029	7357	16002
C41 H82 O		8972		123702		127681	145089		151307	233820	150939	41203	142232	284731	143592	148738	173251		277660		80041		5421	30864	140102		
C37 H80 N4 O2				81712	38052	15936	94188	15511	91430	14612		27065	70058	134318	124395		250663	112767	30284		46056		2836	16916	83961	5913	
C30 H48 N7 P S	304466	282122	301294	210129	235013	212012	19861	33636	14965						20545			12009	27577				21475		21377		
C43 H91 N2 P	6376	10814	1728	54963	64612	53330	573607		582887	668509	270602	11765	280376	524294	607481	1513966	1195225		1475350		168186		49867	5838	767457	542378	
OLEIC ACID (CAS# 112-80-1); (M+H)+							5957	4338		2662		2947	6706							10072		4423			3002		
C4 H13 N3 S2	42527		41906	51061			26192	19799		2263		2904			5834	10156	7944		15138	12726			12675		15787	5996	10281
NICOTINAMIDE MONONUCLEOTIDE (CAS# 1094-61-7); (M+H)+							1297			9075				4323							2404						
C28 H38 O6 P6	30604	30112	30833	5276	26878	26701	3504	2278			3653		1954	1884	2207	2211	3112	14044	7252	7341	3637	6691				2584	5919
C23 H43 O2 P S	121871	122563	120969	121806	118910	114404	13013	2707		1220		6271		145808				7918	4207			27333	14881				30643
C32 H2 O5 P2 S5							69821		59015	329191	431350		62613	184601	221511											53934	
C43 H90 N5 P				23718	23465	24592	67555		59876	14661	45664	31116	86169	39310	73791		60074	103072	60796		46044		95022	26300	112173	7960	
HOMOGENTISATE (CAS# 451-13-8); (M+H)+							1009	3690														4635			4354		16429
C34 H64 N4 P2 S	122344	117876	110465	70595	53615	41382	10952	13947	20958	13605		8493	22607	11250	11475	17930	27209	63266		17496	18480		11158	1571		50171	
C6 H9 N O4 S	512219	666188	504814	659486	527624	708217	2550	1688			1410		5733	22120	2285	1381	8882	3471		26931	1753	12881	1167			1755	3022
C4 H13 N3							92818	116375	111017						27659	80996		158645	111910		10143	178725	119905			113180	
C7 H9 Cl N2 O3							71707										39087		1971			122609		26245		2057	52719
C30 H37 N13 O8 S	48582	49799	48157	40061	33751	32033	19120	11872	11961	4780	12448		7011	7236	4704	5982	5479	4922	6587	6082		3696	3363		18816	9936	14946
C13 H21 N O2	66279		54550	58638	60848	53528	3368		3370	6637	2984		2646	2769	3742		4806	6995			2956						7821
C49 H101 N							171498	58098	156014	184000	314835		175757	252304	497369	11312	250721	246376	10724				10158		209214	62731	
LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+[-H2O]			3262				9417			55616	21272								38677			9271		52730			
C32 H54 N2 O3 P2 S					26387		49809		39404		37417			87395	91810	16087	4495	10287	5266	751317	15872			3001	27849	23985	960648
L-CARNITINE (CAS# 541-15-1); (M+H)+	1434796	1812687	1633230	1156414	1137705	1784909	6200	328865	330664	250141	168126	156691	201854	358799	134070	25834			588745	795592		135381	364226			178223	
C27 H43 N3 P2	37256	36093	38290	34092	33638	30688		5123										6392	5826	1827							
C35 H52 N O P3	58685	48188	44140	40546		33784		26763	27996								29441				41445		7041				
ANDROSTERONE (CAS# 53-41-8); (M+H)+[-H2O]								2537																			
C14 H21 N O4	77021	76646	75572	73337	75919	75809		7337					1382	4032		5057			1079					1029	4350		
C21 H30 N2 O3	77650	87121	78287	85517	89640	50910		3016					5680	16579								5142			2779		
C25 H28 N6 O	58501	57605	54705			52962		1265		2378	9132	4646				2547					2755			1663	1956	10913	2057
C16 H14 N8	30874	30646	30953	32663	29149	32320		1773							4285	1191	1304						8910		4636		
O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5); (M+H)+								9002									37139	43042	3817						19821		45912
C32 H50 N O P S		75606	114713		89716			143285	25803	16370		21319		131105	124423		66859	24365	33557	93768		101841	5505			16102	
C20 H45 N3 O4 P2	63552	53262	58519	49317	50657	5484		47325	11276	38179	15912				18349	40233		52857		4064		39525			7905		
C5 H11 N	8721898	8784316	8221746	8953612	8548023	8572319		79441		1785742		351651	990729	1536017		2867026			120262	191978	1458635			125618	185192	1696891	
C33 H49 N O3 S3	456951	436094	424723	409553	352653	333284		3132	25485		30633		17163	9775	6210	15691			64341	49507	2366	10655	19627				11834
XANTHURENIC ACID (CAS# 59-00-7); (M+Na)+								1294	1304											4751	1856	5613	3210		2305		1013
C19 H28 N6 O2	24737	22284	29136	21245	26406	22228		14901	8844						2856												
D-ORNITHINE (CAS# 348-66-3); (M+H)+[-H2O]						2519		3079																			
C32 H51 N O4 P2 S2	78816	68037	49834	37989	53760	28866		11835					1657	7520			6151		6066		1901	6866	3952				4367
3-METHYLADIPIC ACID (CAS# 3058-01-3); (M+Na)+			6274					1773	1192		1579						1254	2279								1109	
DEOXYURIDINE (CAS# 951-78-0); (M+Na)+	2973							1478			25589										1161						
C11 H25 N3 O2 P2	158668	161230	157345	165886	158403	129751		2009																			
C20 H37 Cl N6 O3	43981	20623	18374	27716	18879	30999		9721		7528	12119		6424	66718			9752									9272	
C24 H37 N11 O5	128344	78232	73714	66126	113949	115205		8067	7773	18693	7488	10177	12085		14705		17266	40493	6997	17016	12890	10502	7382		12253		
D-GALACTOSAMINE (CAS# 7535-00-4); (M+H)+[-H2O]								131476		180830	173139	88297	101043	79123		3558				66508		80910					
C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12:0) (CAS# 41613-14-3); M+[-C6H11O6]								8221				2968						14184					5102				
5-METHYLCYTOSINE (CAS# 554-01-8); (M+H)+								4425		1550						3310				5607					6360		
C17 H33 N7 O2	88018	86802	77628	74732	66973	69599		1835		3566				1665		3642			3311	7689			1120				6520
C34 H43 N3 O6	266853	685202	259179	622502	204627	196719		41199		47796			32437		8154					53011		26122	33050				
GUANINE (CAS# 73-40-5); (2M+Na)+								59494	49041	55894		9345				33560				166996					68338		2321
C17 H40 Cl2 N17 O P	97278	94485	92546	83879	57082	74588		3482											4326	12447		3693	5677				9616
CALCIDIOL (CAS# 19356-17-3); (M+Na)+	9232		10149	9960		9460		1125					1438														
C18 H22 N6	217675	244411	233870	214185	214370	201579		4339	5206								23229	26682	17957	26204			11848		3131		35445
C25 H47 N3 O5 S	470754	475325	488163	469574	468080	452858		35323				21935				31251	91771	46894	137481	127181	18255	140416	29923				151249
DI-TERT-BUTYL DICARBONATE (CAS# 24424-99-5); (M+Na)+								3077		5149																	
C24 H36 N6 S2	69176	72641	60183	62242	68187	62054		71905				74418	124961			87476					25673	20592		133132		108956	
C39 H73 O P S3								2562	2285					4616		3522	1028	8494		6411		1462	5452			1292	5545
C39 H47 N P2					9375			6870			12096	18159	15491	12744	9095	8655			4419	13789		21968	18692	14936		38803	11845
C6 H11 N O2 S	234201	227616	214115		231461	59897		14184	8780	19680	11211			20293				1875		85865		53763	47884		34459	46792	
URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (M+H)+								1647		1371																	
C27 H51 N5 O3 S3	269286	684500	674912	620734	533949	201191		40315							11064				62508	53057		29044	32562				
4-AMINOBENZOATE (CAS# 150-13-0); (M+H)+		11531			4723			16173		21304				31137										4337			
C34 H33 N17 O4	31838	33159	31102	9817	28919			2777	2130				11199					5263			2951						
3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+Na)+								2289																			4086
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+Na)+								1219																	1060		
C32 H55 N3 O S3	138260	139036	138072	143829	113706	100356		12059	186309		247604											253895	150125	141898		235485	
C37 H39 N5 O P2								24814	77586										8913								
C4 H9 N3 O2	188762	141807	117919	125407	120072	120556		1654	1742	1032776		533724		1649469			2757	59836		844672			39940				2554
HOMOSERINE (CAS# 672-15-1); (M+Na)+		5106		5276				2048		6312		1405	3051	6212	5078			2964				2856					
D-MANNOSAMINE (CAS# 14307-02-9); (M+H)+[-H2O]								131476		180830	173139	88297	101043	79123		3558				66508		80910					
AHBA (CAS# 76045-71-1); (M+H)+								28294									15011		26907	56396							33778
C24 H35 N9 O P2	5044	4750		4182				2018						4782					4844								4806
N(PAI)-METHYL-L-HISTIDINE (CAS# 332-80-9); (M+H)+		3147	4848		2912	3919		1510	2054		8191	2254	4147	4026	8174						6565			4790	1334	4657	
C23 H48 N O7 P	566072	573545	531250	463898	385007	343125		11349	27192	50419	66783		27425	49751	31376		53894		56664	62313		9993	4995			24308	12124
6-CARBOXYHEXANOATE (CAS# 111-16-0); (M+Na)+			6274					1773									1254									1109	
C14 H14 O3	876429	871444	870840	868980	848007	817987		11921												195697							408824
TRICARBALLYLIC ACID (CAS# 99-14-9); (M+Na)+	11193		10004	11169	8877	9386		1057	1085																		
C5 H5 N5 O								561099		304728	369156	123519	500415	599976	340739	1135110		9994	610404	850061	14929	956110	14186				
C44 H58 O P2 S	4410	6100		5185	8034			6051	11315				34142	40391	13394					6471		27802	1101	25520			
URACIL 5-CARBOXYLATE (CAS# 23945-44-0); (M+H)+								2079	2398				2002	2694								2308				2752	
N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8); (M+Na)+	10464	8161	8588					14537	14586	15384		9474	9672	18932			13239	14606	13698	17699				18209	14532	20014	16688
C48 H86 N2				75472	20575	3347		10829	54931	85394	9877	73634	17629					128584	31410	9377	40111		16459		23415	5519	5396
C38 H47 N2 O8 P	92556	96759	96755	140776	153013	171861		9718		17644	20251	16465	17462	53645		21064	8273	20355	9228	1560			6892			5191	
C14 H22 N2 O	28459	31334	34257	346305	281349	249910		4.57E+08		3.23E+08	6.00E+07	1.18E+08	1.53E+08	1.79E+08	1.42E+08						3.21E+08	3.90E+08		6.24E+07		9.02E+07	
PROTOPORPHYRIN (CAS# 553-12-8); (M+H)+				1396				1851	4263	1620		2976	1389					4885			3408						
C33 H30	32602		37875	41003	38690	35909		67626	59005		170964													3436			
ERYTHRITOL (CAS# 149-32-6); (M+Na)+								9646	8440	2822	2053								1386			18171				6395	
MELANIN (CAS# 8049-97-6); (M+H)+								63870							36897	58536	79260		63329	4104	10569	87377	118506			52492	97439
DIPHENHYDRAMINE (CAS# 147-24-0); (M+H)+	9097	7791	9654	7365	7982	9223			8766														48624				
3-HYDROXYBENZALDEHYDE (CAS# 100-83-4); (M+H)+[-H2O]	23788	26355	25674	26862	25407	25440			1042	1125						2625				4467			6106				
BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7); (M+H)+	22538	23640	23981	52636	22016	17445			46609	43474	167013	40891	37350		6998		21513	36539			39448		16443		6169	7086	
C17 H31 N O4	215354	209341	205262	188640	168559	151210			3665										19306	15365		9536					19693
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+H)+									14402									36820			2581						
C33 H73 Cl N4 O3 P2 S2						1318			3051						13941	14489	7023				4935	4093				1579	
C9 H15 Cl									51744					21606	7974	29680								14163		12529	
C22 H22 N6 O2 P4	97198	96798	98366	111788	111452	111644			3391														3243				
C16 H42 N8 O S2				3476					11345	2992				53426		95034	23661						9101	37014		47814	
PROMETRYN (CAS# 7287-19-6); (M+H)+				1192					3907		14184			5624		7216	12962	9104	6864				2656		10101	7596	12136
LITHOCHOLIC ACID (CAS# 434-13-9); (M+Na)+				10261	25528				6559									5122									
LANTHIONINE (CAS# 3183-08-2); (M+H)+									1824	1805																	
GLUTARATE (CAS# 110-94-1); (M+Na)+									2559																		
2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M+H)+[-H2O]		2328							1217					1444				3097		1473					3133		
C21 H32 O3	23985	45375	29744	43723	49332	57187			25040		64314	1689	6218				52004		122669		12184				27876	43170	
C34 H70 N2 O9 S2	3665			3597		1515			21117	5794		7209	16663		67793				20579		12060			10827			51781
C4 H9 N	216862	530418	1743701	1917537	1809214	1847143			6641			450532						13210	5537			70998			8468		
C10 H19 N O2	79602	72895	71243	79004	74631	75013			3647	2531	1895			18102	17833		24997	3337	12104	1731							10546
C29 H48 N O8 P	139839	138992	151660	156960	160411	160256			21136	10028					12108	6859	59948		81626	69300		62223					78195
C10 H15 N4 P	2225	5325			1633	8238			56918			7829	6047			99800	134448	222340	48718			70414	77776	9276	123437	18318	116891
3-METHYLGLUTARIC ACID (CAS# 626-51-7); (M+H)+[-H2O]									1203					1443				3097		1389					3169		
N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M+Na)+			6089						9985									170672			4711	6200	23142				
11BETA-HYDROXYANDROST-4-ENE-3,17-DIONE (CAS# 382-44-5); (M+Na)+									4716									8292							17525		2832
C20 H53 Cl N13 O2 P S2	161044	184596	197678	129709	161825	138791			8220										146278				9572				
VALINE (CAS# 72-18-4); (M+Na)+	11983	20052	27966	18347	5228				34458	4577	4624	7359	5415	4167	8156		304022	177771	111608		9131	5555	111269	17662		5388	
PYRIDOXAL (CAS# 66-72-8); (M+H)+		4605	8249			1467			28260		6503	2689			3613			14779				17624	18308		16538		20640
C24 H35 N11 O5	30251	193183	159735	19920	50628	74015			2493											9969	8549	14013				6590	11658
C21 H38 N2 O S3	52973	41310	44207	46314	35772				3365													13144					
C16 H31 N O2 S	45736	34993	35815	38965	39516	34149			4733										4213								
CORTICOSTERONE (CAS# 50-22-6); (M+Na)+	24829		14069	14929	15288				4112																9834		
C24 H20 N8 O5 P4									2504																	1014	
C10 H18 N2 O	200917	199653	195184	200154	200134	187335			1272							3672	1569	4965	2443	5417					1904		
C27 H18 N4 O S3									1063							2991	3320		1322	2442			1216		1486		

C27 H34 N7 P	90364	95059	91265	94920	87824	90333	13594					1041				17747	1204								
TAURINE (CAS# 107-35-7); (M+K)+						23818	38647	47233	19602	6567	8619		3361	62702		28848		7663	32497	55764		95815	54710	4569	
C34 H45 N O3 S2	168518	182523	173853	162276	140107	125072	3385									4150			9960						
CALCIDIOL (CAS# 19356-17-3); (M+H)+				10148		8109	5072									4955			9109						
PURINE (CAS# 120-73-0); (M+H)+							3745	1673	2050		5630		7197			1903									
MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M+H)+[-H2O]							1203					1443				3171		1389					3149		
C26 H35 N19 O	65816	63153	82908	44353	60888	35349	1555				1254													3250	
C30 H58 Cl N O P4	43840	46174	34365	19593	138378	29278	8322		2803									6939							
C26 H56 N2 O9 P2 S							1356									2709							2714		19019
C18 H34 N8 O2 P2	58870	73413	50909	47055	41616	40605	3516	12604			8581		9223	4550	1596		3434		3407	7693		38385			5528
C7 H13 N O2	1897146	2145067	2025845	671934	829983	2085743		558288	62458	140885	234253	80952		32843	1890			135348	2447	800819	27226			9454	
5-OXOPROLINE (CAS# 4042-36-8); (M+Na)+				471502															345986	2775446		209038			
GLUTAMATE (CAS# 56-86-0); (M+H)+		2225						34726	103688		35222	37809		17516		8648		95301	7464	29363	3944		10356		
METHYL INDOLE-3-ACETATE (CAS# 1912-33-0); (M+H)+																2612				1641					
L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)+	11293	5438						10098	11561	11669	11157	8955						7449		4483					
HOMOSERINE (CAS# 672-15-1); (M+H)+	11293	5438						10098	11561	11669	11157	8955						7449		4483					
EPINEPHRINE (CAS# 51-43-4); (M+H)+			7733											4058		5571				3937					
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+								34726	103688		35222	18613		17516		6280		95301	7464	29363	3944		12346		9698
C40 H38 N5 P3	17428	18727	21561	18149	5582	15656		7685			5867		3074	22938	10550	9619	8402	27216		8575			6491	2991	31107
L-2,3-DIAMINOPROPANOATE (CAS# 4033-39-0); (M+Na)+																				7911		4528			
C37 H77 N9 O2 P2				38999	6857			4646									130460			136270					
GUANINE (CAS# 73-40-5); (M+H)+									167741	58769	104924	216283	179955					833573	390520	36126		170102			
C19 H35 N O4	114801	62784	108554	49215	56198	75040												2767		1883					
C15 H35 N7											8359			76472	62631	55610				58588				46985	69967
C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12:0) (CAS# 41613-14-3); (M+H)+														19929						1960					
CHOLATE (CAS# 81-25-4); (M+Na)+		35830	33937		33986	34540														35277					
C22 H34 N6 O2	34983	31008	33082	31740	29653	32117				1175		99608								37414					17404
ALLANTOIN (CAS# 97-59-6); (M+H)+																				1247					
3-DEHYDROXYCARNITINE (CAS# 407-64-7); (M+H)+				90300	85547			76986	22467			44579		27101						39862					
C21 H33 N2 P3	27948	31575	26856	29641	26507	28689														1307					
C10 H16 N6 O4	195159	198030	194143	192582	180226	173362					6791									3203		8546			
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+Na)+													1585							1058	1550				
GALACTITOL OR DULCITOL (CAS# 608-66-2); (M+Na)+																	1501			2787					2641
NORVALINE (CAS# 6600-40-4); M+[-CO2H]	1406165	1367899	1743520	1913848	1808945	1848763		1842952		450539	1211153	1735457								70928		203069			
NORADRENALINE (CAS# 51-41-2); (M+H)+[-H2O]														10935						40955					
C43 H84 O	295823	126389			2804107	2303291					563493	943107		1042874		347875	1714016	260371		177628	73234			98384	
C24 H38 N2 O6 S	194614	188827	175968	169911	149762	142062		6117		4883	10736				21899		35719	30695		18032			15918		20745
C25 H41 N9 O4 S	934630	906795				565963				28089	21575		88509				28956	26483		54075	71630				
N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M+H)+		2225						34726	103688		35222	37809		17516		8648		95301	7464	29363	3944		10279		
LUMICHROME (CAS# 1086-80-2); (M+Na)+				1003																2619					
GUANINE (CAS# 73-40-5); (2M+H)+																		4008		2802					
4-PYRIDOXATE (CAS# 82-82-6); (M+H)+	55345	53956	54061	52511	52142	41861			10126					25587		55461	96344			18963					
INDOLE-3-ACETATE (CAS# 87-51-4); (M+Na)+	119616	115909	111906	61700	85313	48878														6981					
PICOLINIC ACID (CAS# 98-98-6); (M+H)+	1666	2874										23506								1510				1594	
C9 H13 N O	239427	235278	229183	43121	227816	211523														1481					
C5 H11 N O2 S	1291589	1277785	1204111	1300246	1240472	1236365		2593487	2050337	366125	1228344	2417045	2155638			7900		3598332	1089864	1908694		102630		1728315	
C6 H15 N3 O																2792				1399			1804		
LOPERAMIDE (CAS# 34552-83-5); (M+H)+																	6552			11978					4655
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+									181997			50574	36187		147587		100527			88201	82890			37672	47830
C12 H18 N8	38141	40473	37828	23651	21471	41099		49005	11872		20795	1336	3284	1270	50441	1073	1648	8904	10803	58969					63733
C18 H33 N6 O2 P5	28638	25892	27164	27460	30464	27610		2171							3657	5888	5584	5582		2461	4085		3043	2806	6289
OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M+H)+[-H2O]																				1021					
MANNITOL (CAS# 69-65-8); (M+Na)+														1105			1501			2787					3494
10-HYDROXYDECANOATE (CAS# 1679-53-4); (M+Na)+																20018				33374	22507				
L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)+[-H2O]	8277			58322				2690			2815									1948					
URIDINE (CAS# 58-96-8); (M+H)+	4657	18183	12771	16633	11772	15751		159647		37475	98314		8391	302840					71459	272827		14525			
C10 H20 N6 O	18826	85835	121263	80918	79898	78286														2103			2309		
OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M+Na)+																36861				32450	24951				
PIPECOLATE (CAS# 535-75-1); (M+Na)+																				40955					
TYROSINE (CAS# 60-18-4); (M+Na)+		80740	80496			74449		54665	47430	5608	38911	69700		104712		146087		156750	74701	101283	122683		170697		
16:0 LYSO PC (CAS# 17364-16-8); (M+H)+	2387470	1923398	2318105	2012893	1788653	1626678							4657				87734	89585	18186	44794				3373	70583
PYRIDOXAL (CAS# 66-72-8); (M+H)+[-H2O]			9901			5010			3289											2409		101917			
C17 H35 O3 P S2	66653	65514	63404	67759	64734	62971		3807								3479		11374							9471
ADENOSINE 5'-DIPHOSPHATE (CAS# 58-64-0); (M+H)+								9590	34444		13674	14432						53211							
GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M+H)+								1367										8245							
C21 H42 N5 P3	73418	68356	63674	64782	64288	63097												2098							
SUCROSE (CAS# 57-50-1); (M+Na)+	4173	3430	3160	2418	2679	3429		26886	21121	25685		48881	23486	9027				13605				25104			
C23 H39 N4 O4 P	19191	19148	21778	12055	24785	20916		2227		7282				7261				1032	3889						
C10 H24 N8 O3	17085	18385	18160		17837	17234		4766			1489						3896	1486					2358		
N-ACETYLNEURAMINATE (CAS# 131-48-6); (M+Na)+																		3858							
NORVALINE (CAS# 6600-40-4); (M+H)+	2119751	2236309	1877293	2794091	2966336	2127501		3275075	4462186	814470	2115370	2972091						5168405				339053			
BETA-ALANINE (CAS# 107-95-9); (M+H)+	4135	2955			2809	3927		2091	5297	4473	4135	40558						9844							
C6 H6 N4 O2	58485	55007	54613	59497	52799	55382												5814							77530
O-PHOSPHOSERINE (CAS# 407-41-0); (M+Na)+																4383		1702							
CELLOBIOSE (CAS# 528-50-7); (M+Na)+	4173	2915	3160	2418	2144	3025		26886	21121	25685		48881	23486	9027				13605				25104			
C13 H15 N5 O2	182475							1200										1147			3995				
24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M+Na)+			8559															2317963							47241
O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (M+Na)+											4162					4383		1702							
CHOLINE PHOSPHATE (CAS# 107-73-3); (M+Na)+								5533				5748	2069				1458	6583							
N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-3); (M+Na)+	3641	1132	1466													3267	1687	1136							
C19 H29 O P3	58776	57593	57644	55296	52495	54135		36959			8985	52434	33129					93333							
LEUKOTRIENE B4 (CAS# 71160-24-2); (M+Na)+															15477	13153	22394	16819							
C13 H10 N2 O5	113316	119237	117640	119332	114376	109233												28645							56433
MELIBIOSE (CAS# 585-99-9); (M+Na)+	2679	2165	2115	2418	1836	3429		26886	21121	25685		48881	23486	9027				13605				25104			
NAPROXEN (CAS# 22204-53-1); (M+H)+	110941	114025	107868	113240	111297	106222						1540						24909							51704
C13 H21 N4 O P3	83194	81784	76276	74671	73850	68387										3522	1081	1406							7310
EPIANDROSTERONE (CAS# 481-29-8); (M+H)+[-H2O]									1032									1715							
C27 H40 N12 O4	18807	18154	18965	19153	19538	17842								2074		2918		2431			1521				5462
VALINE (CAS# 72-18-4); (M+H)+	2119751	2236309	1877293	2794091	2966026	2127501		3275075	4462186	824831	2115370	2972091						5168405				339053			
3-METHOXYTYROSINE (CAS# 4214-13-5); (M+H)+	21322	19120	20919		20452													8031							8170
C7 H10 N5 O2 P	187121	182325	177324	178673	164156	155556												1189					2217		
C23 H55 N10 O7 P S2															2818			9642							1259
C14 H14 N4 P2	55915	54389	55131	55886	53560	52613												13466							28456
BETA-MALTOSE (CAS# 69-79-4); (M+Na)+	4173	3430	3160	2418	2679	3429		26886	21121	25685		48881	23486	9027				13605				25104			
URATE (CAS# 69-93-2); (M+Na)+															1076		10727	2833	3636		1102			2827	
C29 H45 N4 O P5	67211	69704	66061	56998	50326	43873		2056	3246								2721	3571			1470				1713
URATE (CAS# 69-93-2); (M+H)+	1987267	1931806	1807831	1903847	1824205	1844858		316316			129097	621572		1212				501034	180250						
LACTOSE (CAS# 63-42-3); (M+Na)+	4173	3430	3160	2418	2679	2881		26886	21085	25685		48881	23486	9027				13605				25104			
C5 H11 N O2	2116322	2240409	2004487	3049415	2064812	2137339		3304109	2800184	814285	2115938	2766452			313049	177771	398529	5277255	141151		105973	280802			
20:0 LYSO PC (CAS# 108341-80-6); (M+Na)+	28880	29828	49794		25069						1801							8975							
CORTISONE (CAS# 53-06-5); (M+Na)+	52988	53529	50381	52935	51583	51277		2497						6171	8491	14890		8623							5691
PALATINOSE (CAS# 343336-76-5); (M+Na)+	4173	3430	3160	2418	2679	3429		26886	21121	25685		48881	23486	9027				13605				25104			
C25 H34 N19 P3	40405	40508	39634	40277	35810	32180			4807									2895							
SARCOSINE (CAS# 107-97-1); (M+H)+	4135	2965			2809	3927		2091	5297	4473	4135	40558						9844							
C35 H40 N5 O4 P3	35072	34611	31335	27373	23028	18298			3302						1182			1409			2498				
ALLOSE (CAS# 2595-97-3); (M+H)+[-H2O]	20905	21440		16556	16710													2132			1600				1554
C4 H7 N3 O						95760				16486		26600	1112				7715	39173							
GUANINE (CAS# 73-40-5); (M+Na)+								13453										231930				30178			
URACIL (CAS# 66-22-8); (M+H)+								129366	179853	35939	83402	115717						78216	15214						
SPHINGANINE (CAS# 764-22-7); (M+Na)+					16707			79316			28857		43861	62720		102484	44844	56730	18960		60315		61031	48442	118208
C4 H5 N O	126570	87755	34925	88402	27461			60800		16094	91147	92887						281339	116224			52993			
PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M+Na)+									12162			2449						133701							
C24 H32 N11 O P	40233	41091	10838	37415	34914	32000		2010						18568	7611		13680	26788			1459	1151			31300
C37 H36 N5 P3	38747	41938	35889	31667	29808	24372		2369							1116		1519	1308							2492
N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M+Na)+						5144												2868							
MALTOSE (CAS# 69-79-4); (M+Na)+	4173	3430	3160	1975	2679	3429		26886	21085	25685		48881	23486	9027				13605				25104			
5-AMINOPENTANOATE (CAS# 660-88-8); (M+H)+	955416	956326	899143	879575	846845	839974		231331	4524167	267514	2113765	2978204		116021	269114			5168405	117509		68831	121992	247780		
NAPROXEN (CAS# 22204-53-1); (M+Na)+	720432	713764	711493	714390	693153	669588												161253							332961
C13 H12 O	43958	48645	45495	46916	44314	43354												11998							21980
C17 H29 N O4	39892	40289	38638	37007	37873	36882										10355	2753	1590							
C18 H32 N2 O S2	188683	181485	176927	180103	174223	167681				1487		1240						61983			10148				2268
O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (2M+H)+	2127	3716		1810		1701		5144						1282				1580							
C25 H39 O7 P	38210	44684	43227	39054	35149	26850					11360				9478		35719	5468					15860		18425
C29 H46 N7 O P3	40360	39761	41777	38052	22488	27224												3045	1010						
C12 H25 N5 O3	43434	45459	43935	42632	40977	40485			1000						2211			4037			3630		7794		
GLYCOCHOLATE (CAS# 475-31-0); (M+Na)+	64441	69062	61372	63161	67218	56994			26225				28661					31020					35450		
C33 H46 N11 O P3		1079	1245			1122											1214	4003			1404				
CREATININE (CAS# 60-27-5); (M+Na)+			15197															14119							
ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-73-2); (M+H)+								9590	34444		13674	14432						54891							
C32 H69 O7 P3 S2												3679				1985		2386							2016
C20 H37 N O4	73240	70324	66141	65864	56659	57468												1750				1197			
C19 H9 P	43562	44477	46213	44565	43109	40667												10784							23353
C19 H30 O4 P2	31062	31606	34148	28679	31079	31423					5522		5318	6475		11338	3250	2525	5368		1707		7049	6210	
UROCANATE (CAS# 104-98-3); (M+H)+	14329	12195	17686	13729		18218		209472	1169108	13333	338173		2676048					299421	3797823			418975			
GAMMA-BUTYROLACTONE (CAS# 96-48-0); (M+H)+																		2297							
CYSTINE (CAS# 56-89-3); (M+Na)+		3623	3047	3125	3038	3713				2248								2747							
INDOLE-3-ACETATE (CAS# 87-51-4); (M+H)+	53706	50433	52142	22675	40884	26207											3274	2669							
HIPPURATE (CAS# 495-69-2); (M+H)+																		25671							
C21 H40 N17 P	71017	71151	70438	56220	50650	42099								1534				4147							
C8 H15 N O	966648	943594	875764	920135	910035	933867												1573				2302			
C38 H23 N17	28980	26977	26619	25284	25945	24451								1109											
C16 H29 Cl N6 O4	22097	25581	21586	22882	21003	23185					1341														
C13 H10 N4 O	60835	71042	67375	69200	68573	61537																			
C14 H22 O3	52461	52794	48154	48041	50451	43845																			
17ALPHA,20ALPHA-DIHYDROXYPREGN-4-EN-3-ONE (CAS# 652-69-7	1368	1226																							
C7 H6 O2	405447	364327		378939	368050	342074					26914	32241	295154						203377			1958			
C25 H32 O3	29229	32524	38198	53674	58949	56835																		3405	
C24 H42 N2 O3 P4	89394	92018	88065	88850	83335	83585																			
C21 H39 N O4	122054	117877	118574	106477	94440	83017			40385								5845								17085
INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+H)+	24543	24919	23786	22844	22515	21582		20429				13018													2236
DETHIOBIOTIN (CAS# 533-48-2); (M+H)+[-H2O]	10485	10802	9338	10817	12966	8268											7455								
C10 H21 N O2	125154	125974	130446	126326	124190	116714																			
C22 H17 N17 O	39349	36991	36597	35779	37096	34595						1473			10169	6815									
5-HYDROXYINDOLEACETATE (CAS# 54-16-0); (M+Na)+		1848																							

C22 H44 O6 P6 S	529156	511784	516013		459018	467267						1360												
C10 H9 N	218718	203836	193271	200926	196850	187333																		
C7 H16 N8 O S	90715	91274	91564	86131	82890	85578																		
EDTA (CAS# 60-00-4); (M+Na)+	3507625	3390991	3178967	3286224	3241117	3110888																		
C12 H21 N O	175949	166140	159460	170139	162267	165908																		
RIBOSE (CAS# 50-69-1); (M+Na)+		2212						213950	504399		92156													
C32 H33 N5 O4	81296	74930	72868	57242	48093	44598															4586			
4-AMINOBUTANOATE (CAS# 56-12-2); (M+H)+	2917	3837	4484	6133	6010	5765																		
C9 H19 N O2	516216	271487	480408	506582	462492	498167			15380		1844			4333	16800						6435		17979	
C21 H49 N2 P5	137240	123199	123877	113888	92487	86121		90538	1307												5286			
C6 H13 N O	1427423	1431703	1336578	1459286	1414913	1402367							2942							3006			1299	
EDTA (CAS# 60-00-4); (M+H)+	4.72E+07	4.74E+07	8.60E+07	9.06E+07	8.84E+07	9.46E+07																		
C7 H10 N6 O2	480835	490974	438890	493247	472474	452028					6409	4254												
C8 H11 N O		272942	251030	268385	250128	255517																		
CREATINE (CAS# 57-00-1); (M+H)+		138209	114035	140847	135065	117035	950939		524897		1628085													
2-HYDROXYBUTYRATE (CAS#); (M+Na)+	40851	41090	43389	43351	45146	40736			31000		5071		58980										1084	
C21 H41 P S	19078	29222	17016	18671	15373	18839			13493	4499		8269	11808								10956			
C8 H16 N2 O3 S	196028	169055	186960	190364	184634	179775		24627				18156	20137							33090			11511	
GUAIFENESIN (CAS# 93-14-1); (M+Na)+		25827			28759																			
4-HYDROXYPHENYLACETATE (CAS# 156-38-7); (M+H)+	8543	7204		8882	7262																			
DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Na)+	87991	90079	87529	89205	85734	83281					94582					4168								18598
C23 H10 O2	36760	36166	36179	41172	37378	35729			1659															
N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+Na)+	2125	2468	1928	1850	2185	2099						2160												
C13 H16 N6 O3	131077	122201	128303	139996	138355	130345																		
C39 H44	32793	18002	88723	18993	18792	36369			3809		15028					43059		60122						67475
C42 H19 N2 O P5	117162	110122	110826	114065	107653	109678										1058								3686
SALICYLURIC ACID (CAS# 487-54-7); (M+Na)+	15019	14471		12632	12335	14914																		
C27 H35 N23 P2	15428	13941	14067		12929	9247					1377			5098				3026						
IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M+Na)+	176757	167348	158026	166183	168395	160357																		
C23 H39 N4 P3	116101	105869	97766	93988	91429	89812																		
C20 H23 N S	28039	29016	28086	31769	27740	27318																		
C25 H33 N25 O	77835	75112	72260	74592	73881	73284									2222									
3-AMINOISOBUTANOATE (CAS# 144-90-1); (M+H)+[-H2O]	8991	10359	10838	8912	9456	5473							1161							1570				
4-PYRIDOXATE (CAS# 82-82-6); (M+Na)+		4908	7596	10013	7910	8272										19989								
C11 H28 N8 O9	189835	215528	196196	184952	183906	202320												2408						
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+H)+[-H2O]	22737	42232	21650	45361	20329	22763																		
GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (M+H)+	2768	3718	2391	3142	2794	2562	3381				5701													
C9 H17 N O	5951606	4714257	5511026	5878831	5611322	5419794										1480								
N,N-DIMETHYLGLYCINE (CAS# 1118-68-9); (M+H)+	2917	3837	4094	6133	6010	7471																		
C9 H14 N2 O3	42158	45748	42432	44950	50929	44193																		
BILIVERDIN (CAS# 114-25-0); (M+Na)+	41604	35382	38176	39592	38835	39450																		
OMEPRAZOLE SULFONE (CAS# 88546-55-8); (M+H)+	23047	22045	21756	20484	19646	20418																		
C18 H33 N O4	43528	43896	72925	41031	33538	28399										1510								
2-AMINOBUTANOATE (CAS# 2623-91-8); (M+H)+	2917	3837	5623	6133	6010	7471																		
C22 H34 N2 O15 P2	517407	533906	604277	161315	522074	441491																		
D-(-)-ARABINOSE (CAS# 10323-20-3); (M+Na)+		2212						215728	504399		92156													
CYSTATHIONINE (CAS# 56-88-2); (M+H)+[-H2O]	5245	5872	5611	5964	4959	5489																		
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+H)+		9508			10024	10370																		
3-HYDROXY-3-METHYLGLUTARATE (CAS# 503-49-1); (M+H)+	20905	21440		16556	16710															1600				1554
C25 H30 N10	19718	16250			16820	21454						1497												
NICOTINATE (CAS# 59-67-6); (M+H)+	1665	2874									23506												1595	
C4 H13 N2 O3 P S	87866	88860	84799	88997	88156	87356														1183				
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+Na)+		9764		2067							17354			13758		9529		2165						
C15 H16 N O3 P3	59804	58817	60316	61990	59182	55926																		
CITRAMALATE (CAS# 2306-22-1); (M+Na)+	2590	4815	5614	4443																				
ASPARTATE (CAS# 56-84-8); (M+H)+		1858		2620			5280		2313					6355										
TRYPTOPHAN (CAS# 73-22-3); (M+H)+	8066392	8033345	7742766	8077650	7818357	7634257			81951	469236				6106451	7054660									6167612
URSODIOL (CAS# 128-13-2); (M+Na)+	87991	90079	30557	89205	30932	83281					94582													18598
C21 H28 N11 P	6047	14211		14352	11942	6629					1122									1107				
C15 H30 N14 O5 P2 S3	260763	337570	260881	74833	284568	223590						1427												
C25 H18 O2	23133	22529	21594	22893	21448	23124																		
C30 H50 N2 P2	597128	170196	170181	126300	410510	359868							1838	16580		26758								
C8 H16 N2 O2	109723	97324	99473	96841	95023	102196																		1728
C12 H13 N2 P	66515	62478	62656	68854	60177	59948																		
C19 H30 N6 O	29945	30435	34386	7815	49708	45322		23547								12354								
C33 H36 N4 O6	87543	83527	82662	80828	79124	76859																		
CORTISONE (CAS# 53-06-5); (M+H)+	3462	3143	3466	3348	4188	3170																		
GLUCOSE (CAS# 50-99-7); (2M+Na)+[-H2O]	4173	3430		2418	2679	3429	26886		25685				9027											
C21 H19 N O3	33277	23525	20564	19917	21057	20871										8334								9864
TRYPTOPHAN (CAS# 73-22-3); (M+Na)+	711426	686882	658378	669319	652588	640606			5168	31021			155961	405496	445895									408477
C36 H54 N7 O4 P3	5756	5948	6177	5655	6062	5038										2171								3646
C25 H20 O	140687	142909	146123	154889	158413	152397															23114			
GLUCOSE (CAS# 50-99-7); (2M+Na)+	3249	3210	2581	3198	3099	2446																	2314	
C20 H9 N O2	55983	57457	55534	59801	57866	55544																		
C31 H30 N2	21383	30309	27166	22470	32504		19789				28985		2125											36872
C28 H57 Cl O P2	657613	313918		489113	346020	736523																	22128	
URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (2M+Na)+	95519	73349	62705	87689	100689	100176																		
C10 H11 N3 O3 S	317002	310359	307752	320624	307183	305568																		
C26 H50 P6	36937	35956	36682	32798	36282	34868																		
C28 H37 N15 O	4463	4447		2496	3948	4076									3400									
C31 H53 N P6	47782	50256	47339	39585	35468	29526		3243					5577											
N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+H)+	3361	2441		3005	2461	2806				16956	10561									3518				3084
C5 H12 O6 P2	93388	90157	97388	98506	94905	89847																		
C14 H9 N6 O2 P	71588	70972	72280	68684	70187	68269									1190	6985				8962				
N-METHYLNICOTINATE (CAS# 535-83-1); (M+H)+	61377	65065	63949	40850	39531	61043																		
THYROXINE (CAS# 51-48-9); (M+H)+	10245	11445	9950	11453	11913	10269																		
C11 H11 N O2	124946	126305	120268	124570	128773	120270																		
C13 H8 N8	116320	112682	111726	111957	116203	107263																		
BILIVERDIN (CAS# 114-25-0); (M+H)+	138695	127514	131103	141768	131596	123309																		
C33 H58 N5 O2 P5	66761	60197	62405	63876	62817	56851								2319	5754					1961				
C29 H43 O P	17528	13035	16123	15094	14433	16436	9820	54793						9016	15112			2823				9725		
C7 H9 N O	41780	40064				34720																		
KYNURENINE (CAS# 343-65-7); (M+Na)+	12250	16310				9155																		
CITRULLINE (CAS# 372-75-8); (M+Na)+	6352	4927	3107	4457	3604	3319																		
IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M+H)+[-H2O]	25796	21476	22349	24357	23446	23385																		
C10 H16 N2 O2	127022	125849	124380	124354	124557	117147		25518			15002	18432									17361		11938	4340
3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (CAS# 516-55-2); (M+Na)+		1446																						
C35 H37 N8 P3	33552	39277	31485	30575	26794	19635															40926		1091	
C14 H24 N3 O3 P	15688	14627	13142	14362	14242	13069																		
C6 H8 O3	68541	71828	62552	73008	62158	63922		2043																
C25 H15 N O2	53544	51190	50869	53765	53375	47845																		
GALACTURONIC ACID (CAS# 91510-62-2); (M+Na)+[-H2O]	11193	5016	6060	11742	4660	5192																		
TAUROCHENODEOXYCHOLATE (CAS# 516-35-8); (M+Na)+		3233																						
OMEPRAZOLE (CAS# 73590-58-6); (M+H)+		5666	3742	5370	5284	4860																		
C9 H19 Cl2 N5 O2 S	29211	28017	28159	27389	31487	26806																1631		
C11 H16 O4 P2	50785	48892	49002	49023	50931	45159																		
C4 H9 N O3 S	23007	19814	20651	21469	19936	19828																		
5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M+Na)+	30127	28649	29026	30711	30126	26984																		
C45 H15 N3 P2	159680	165752	152111	348324	324036	170312																		2301
C10 H16 N2 O	99314	100738	94432	100258	96050	95822																		
C14 H18 N4 O3	30296	30861	30380	29719	29499	29107																	50311	
ALPHA-TOCOPHEROL (CAS# 59-02-9); (M+H)+	4616	4046	4674	6334	5095	4565																		
C10 H16 N6 O	59998	64123	66619	63038	82558	64251	1666		4537															
C32 H55 N5 O6 P2	17763	18092	18061	16894	15652	16501																		
C12 H23 O2 P3	4.92E+07	1.10E+08	9.45E+07	9.62E+07	9.90E+07	1.07E+08																		
C13 H16 N4 P2	91458	99787	101995	99375	100847	90910																		
C4 H6 N6	1045262	1031890	1002585	1071843	1022599	1004345							1686											2366
C18 H15 N O3	229742	239161	228146	230958	230376	223244																		
C11 H21 N O2	224839	228220	220179	230177	207094	212862																		
C11 H19 N4 O4 P	44131	49141	49853	46245	46126	43173																		
C11 H10 N6 O2	182880	183307	174610	183640	185305	175398																		
C28 H40 O8	36688	35735	33732	36171	36066	33053								1037										
C9 H15 N O3	95834	77585	79416	102099	101083	83560		17402				11203	4264											
C9 H15 N O2	55240	57818	57005	58665	55786	55165																		
C12 H22 O3 P2	51137	58629	49303	45821	59536	58153																		
C13 H16 N4 O P2	46336	48498	48403	48277	47746	44047																		
TRANS-CYCLOHEXANE-1,2-DIOL (CAS# 1460-57-7); (M+Na)+	1049681	1034726	1001769	1066621	1025498	1008602																		
C7 H12 N6 O	360110	201366	343160	22182	342305	332200									1281									
D-PSICOSE (CAS# 551-68-8); (2M+Na)+[-H2O]	1578	3430				2159	26886		25685				9027											
C49 H71 N O4		21197		20159		15876		7256					73675		7874	61652				41495				125871
C14 H14 O6	93588	96826	89500	93290	91323	86205										3242				5390				
C6 H9 N O4	5472051	5944749	3087456	5876349	5743654	3189926				1103														
1-METHYLXANTHINE (CAS# 6136-37-4); (M+H)+		24815																						32922
C3 H9 N5 O	6516	6449		4554	5274	5135	18357	37909			7833	511398		1242588	1261309									
11-DEOXYCORTISOL (CAS# 152-58-9); (M+Na)+	24829	13525	21656	14929	15068																	9834		
C19 H22 Cl N5 O	45091	48023	45330	46032	47474	43053																		
C8 H10 N8 O6	1.09E+07	1.08E+07	1.03E+07	8912507	8302151	1.03E+07																		4456
C11 H16 N2 O	33013	33372				29108																		
C12 H22 N2 S2	129780	134435	136312	167215	177075	168057														5129			27482	
C26 H36 O5	23333	18980	19938	15795	24619	33428		100156		13014	10799	5724						6800			10558			
5-VALEROLACTONE (CAS# 542-28-9); (M+H)+		110026	104828	107976																				
C11 H17 N O2	97941	98721	99535	91800	94911	96504																		
GLYCOLITHOCHOLATE (CAS# 474-74-8); (M+Na)+	7414	6675		8016		8514																		
CORTISOL (CAS# 50-23-7); (M+H)+	22894	24285	21184	23020	21836	22344																		
C11 H29 N4 P S2	69238	50641	54759	54007	56899	52846									1876								2505	
PYRIDOXAL PHOSPHATE (CAS# 853645-22-4); (2M+H)+		7203		8800	8011	9121																		
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+H)+	3352	6270	15254																					
C10 H16 O5 P2	84789	86483	85786	85578	81532	82416										7344				8475				
C10 H19 N4 O4 P	308475	316053	298821	309777	313081	301555																		
C19 H21 N O3	55567	55472	55199	54284	80706	57965										6610								18359
ESTRONE (CAS# 53-16-7); (M+H)+		3646				2961																		
C17 H21 N2 O P	109169	109254	109328	102307	92222	91608		53515																
3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M+Na)+	28233	28757	26591	30951	27763	26732							1610	2580										1392
IBUPROFEN (CAS# 15687-27-1); (M+Na)+	307615	311611	306872	323344	310956	306782																	11170	10897

C12 H19 N O2	174876	176742	164948	166237	170589	146642																		
C26 H30 N14 O P2	29207	29640	26360	28951	27708	26946								1419	1779									
5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M+H)+	23047	22045	21756	21546	21907	20418																		
C9 H6 O2	187136	174730	171285	174238	155405	157674	91192		9331	46872								88328						
DIHYDRO-4,4-DIMETHYL-2,3-FURANDIONE (CAS# 13031-04-4); (M·	55911	57259		17066																				
ARABINOSE (CAS# 147-81-9); (M+Na)+		2212						214117	502813		92156													
C7 H8 N2 O2	672413	659258	614030	659294	626957	592582										387567				165181				
C37 H39 N2 P3	62735	60134	59324	65057	58372	58172	2139																	
C22 H12 N2 O3	46777	46053	45146	46926	42439	43966																		
C20 H50 N22 P4	118831	113123	110071	112379	111290	112857				1606														
N-ETHYLMALEIMIDE (CAS# 128-53-0); (M+H)+	5630	7686	7293	1849	3740	6741																		
2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 4026-18-0); (M+Na)+	54573				60639	56692																		
4-ACETAMINOPHEN SULFATE (CAS# 32113-41-0); (M+H)+	1855		4361		6113															11318				
SEROTONIN (CAS# 50-67-9); (M+H)+	125925			124464	138391	134718																		
DEOXYADENOSINE (CAS# 16373-93-6); (M+H)+	1566																							
GLYCERALDEHYDE (CAS# 367-47-5); (2M+H)+[-H2O]	20905				16710																			
PROLINE (CAS# 147-85-3); (M+Na)+	59649		63949		60120																			
SHIKIMATE (CAS# 138-59-0); (M+H)+[-H2O]	2294				2726																			
C18 H20 O3	17344						20120									23720								31056
3-HYDROXYPROPANOATE (CAS# 503-66-2); (M+Na)+	14234				4405																			
4-HYDROXY-L-PROLINE (CAS# 2584-71-6); (M+H)+	1418141			2528	2843	1914																		
(-)-COTININE (CAS# 486-56-6); (M+H)+	125925			124464	138391	134718																		
C31 H38 N7 O P3	7393			11732	9471	6868																		
GLYCOCHOLATE (CAS# 475-31-0); (M+H)+	3150		2869																					
C37 H77 N2 O P5	80562		69114	62515				3456						2015										41960
LANOSTEROL (CAS# 79-63-0); (M+Na)+	4780																							
C11 H11 N6 P	89256		87538	89414	85641	85052																		
MALATE (CAS# 636-61-3); (M+Na)+	1685																							
HOMOCYSTINE (CAS# 462-10-2); (M+Na)+	1185																							
1-METHYLXANTHINE (CAS# 6136-37-4); (M+Na)+	2693		3272	1695	4127																			
5-AMINOLEVULINATE (CAS# 106-60-5); (M+H)+	1418141			2528	2843	1914																		
4-METHYL-2-OXOVALERIC ACID (CAS# 816-66-0); (M+Na)+	4830				6080	5727																		
TRANS-4-HYDROXYPROLINE (CAS# 51-35-4); (M+H)+	1391280			2528	2843	1914																		
INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+Na)+					1499																			
C7 H3 P S3					603283							2544												
CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (2M+H)+					1762																			
CHOLESTEROL HYDROGEN SULFATE (CAS# 1256-86-6); M+[-HSO4]					1292																			
XYLOSE (CAS# 58-86-6); (2M+H)+[-H2O]					5008																			
1,3-DIMETHYLURIC ACID (CAS# 944-73-0); (M+Na)+					9462																			
DECANOATE (CAS# 334-48-5); (2M+Na)+					23268						149168			16959		60664							39426	
C22 H27 N2 O3 P					18823					1870	36003		42208	21537	33037	25756		59205				17228		
C39 H77 N2 O P5			36248	22438	23070	27773																		
3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+H)+				30074	24832			13432		7236					47132			8087			10765	65798		63410
BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (CAS# 584-85-0); (M+Na)+						2257																		
1-METHYLADENOSINE (CAS# 15763-06-1); (M+Na)+						1556																		
18:0 LYSO-PE (CAS# 69747-55-3); (M+H)+						4961										16110								
CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (2M+Na)+						2647																		
FERULATE (CAS# 1135-24-6); (M+Na)+				2967		1111																		
2-(DIPHENYLMETHOXY)-N-METHYLETHYLAMINE (CAS# 17471-10-2); (M+H)+			1860			1693																		
N-OLEOYLGLYCINE (CAS# 2601-90-3); (M+Na)+				1503		1656																		
CREATININE (CAS# 60-27-5); (M+H)+						79353																		
5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (M+H)+			26748																					
2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-5); (M+Na)+			1573																					
L-ARGININE (CAS# 74-79-3); (M+H)+			1141												40444									
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+[-H2O]			40643											56456										
DEHYDROASCORBATE (CAS# 490-83-5); (M+H)+[-H2O]							36497			12053	21781													
NORMETANEPHRINE (CAS# 0); (M+H)+											7865													
D-LYXOSE (CAS# 1114-34-7); (M+Na)+											92156													
N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8); (M+Na)+											1458													
ETHANOLAMINE PHOSPHATE (CAS# 1071-23-4); (M+H)+							128649	18014			132910							2224			3978		13603	
C5 H11 Cl O2										4844	18597		14510								5372			
5BETA-ANDROSTANE-3,17-DIONE (CAS# 1229-12-5); (M+Na)+							1099				2497													
CITRAMALATE (CAS# 2306-22-1); (2M+Na)+											1658													
ADP-RIBOSE (CAS#); (M+H)+[-H2O]											7738													
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+H)+							2412	16031		4546	11901													
3,3'-DITHIODIVALINE (PENICILLAMINE SS DIMER) (CAS# 20902-45-8); (M+H)+											6078													
3-HYDROXYKYNURENINE (CAS# 2147-61-7); (M+H)+											1862													
MEVALONIC ACID (CAS# 674-26-0); (M+Na)+											27636													
TRANS-ACONITATE (CAS# 4023-65-8); (M+Na)+				2810																				
NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE (CAS# 22052-73-9); (M+H)+				1342																				
GLYCOCHOLATE (CAS# 475-31-0); (M+H)+[-H2O]				5543																				
PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M+H)+				14274			1381																	
17ALPHA-HYDROXYPROGESTERONE (CAS# 68-96-2); (M+Na)+				4029																				
2'-DEOXYINOSINE (CAS# 890-38-0); (2M+Na)+							2590	13019							2987									
ABRINE (CAS# 526-31-8); (M+H)+													3112		3828									
INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M+Na)+														4438	11308									
DEOXYCHOLIC ACID (CAS# 83-44-3); (M+H)+									7273						10625									8703
2'-DEOXYCYTIDINE 5'-MONOPHOSPHATE (CAS# 1032-65-1); (M+H)+															7544							5391		
OCTACOSANOIC ACID (CAS# 506-48-9); (M+H)+							15107					15887			21911			14184				14739		
C22 H27 N4 O9 P S															1660									
C29 H56 S4															3171									
11-DEOXYCORTISOL (CAS# 152-58-9); (M+H)+															2954									
SUBERIC ACID (CAS# 505-48-6); (M+H)+[-H2O]															3303									
1-PHENYLETHANOL (CAS# 1445-91-6); (M+H)+[-H2O]															1736									
MANDELIC ACID (CAS# 611-71-2); (M+Na)+													3734		5984									
25-HYDROXYCHOLESTEROL (CAS# 2140-46-7); (M+Na)+								6258	6669						1888			1356						
C26 H20 N2 O4													31699		81233							62747	82170	55688
C39 H38 N11 O P										1307					7274									
C13 H14 N4 O P2										1039			2051			1302							1041	1443
C42 H51 N7 O S													1390	2288						3796				
MENAQUINONE (CAS# 11032-49-8); (M+Na)+													1236											
2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-5); (M+H)+[-H2O]													1774											
ASPARAGINE (CAS# 70-47-3); (M+Na)+								4402					1056											
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+H)+[-H2O]							1010	16673					89035											
SELENOCYSTAMINE (CAS# 2697-61-2); (M+H)+													10076	5444										
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+[-H2O]													1857											
PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M+H)+[-H2O]																								1969
C37 H47 N2 O P5																								2198
ARACHIDIC ACID (CAS# 506-30-9); (M+Na)+																							2380	1690
GULONO-1,4-LACTONE (CAS# 1128-23-0); (M+H)+[-H2O]																								3927
AZELAIC ACID (CAS# 123-99-9); (M+H)+[-H2O]																								9373
11-DEOXYCORTICOSTERONE (CAS# 64-85-7); (M+Na)+																								6046
DIETHYLSTILBESTROL (CAS# 56-53-1); (M+Na)+																								6156
4-PYRIDOXATE (CAS# 82-82-6); (M+H)+[-H2O]										2308						8665								
PYRIDOXINE (CAS# 65-23-6); (M+H)+																5353								
3-METHYLXANTHINE (CAS# 1076-22-8); (M+H)+										3058								23355		13291	54963		13999	
18:0 LYSO-PE (CAS# 69747-55-3); (2M+Na)+																				8209				
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (2M+H)+																				16012				
16:0-18:0 PC (CAS# 59403-51-9); (M+H)+																				1286				
THYROTROPIN RELEASING HORMONE (CAS# 24305-27-9); (M+Na)+																				1579				
3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-92-7); (M+H)+																				5113				
MELIBIOSE (CAS# 585-99-9); (M+K)+							6602	3919	2366												1569			
OLEAMIDE (CAS# 301-02-0); (M+Na)+								198815	88797													713935	317943	
(S)-2-AMINO-3-(3-HYDOXY-4-OXO-4H-PYRIDIN-1-YL)PROPANOATE OR L-MIMOSINE (CAS# 500-44-7); (M+Na)+								1630																
INDOLE (CAS# 120-72-9); (2M+Na)+								2078																
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)+[-H2O]							3912	12137																
LACTOSE (CAS# 63-42-3); (M+K)+							6602	3906	2366												1569			
CITRATE (CAS# 77-92-9); (M+H)+[-H2O]							1299	2611	1586															
MALEAMATE (CAS# 557-24-4); (M+H)+							1638	2051				2285												
CARNOSINE (CAS# 305-84-0); (M+H)+								1025																
DUMP (CAS# 964-26-1); (M+Na)+								1144																
THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-07-1); (2M+H)+							1401																	
18:0 LYSO-PE (CAS# 69747-55-3); (2M+H)+							2965																	
METHYL BETA-D-GALACTOSIDE (CAS# 1824-94-8); (M+Na)+							1318																	
PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M+H)+[-H2O]							1034																	
CYTIDINE (CAS# 65-46-3); (M+H)+							10291		1208	5026														
PINITOL (CAS# 10284-63-6); (M+Na)+							1318																	
4-GUANIDINOBUTANOATE (CAS# 463-00-3); (M+H)+							11331																	
18:0 LYSO-PE (CAS# 69747-55-3); (M+Na)+							9144																	
3-AMINO-4-HYDROXYBENZOIC ACID (CAS# 1571-72-8); (M+H)+														15011										
N-ACETYLSEROTONIN (CAS# 1210-83-9); (M+Na)+														4491										
BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (CAS# 584-85-0); (M+H)+														1191										
MELATONIN (CAS# 73-31-4); (M+Na)+														1006										
DEOXYCYTIDINE (CAS# 951-77-9); (2M+H)+												4644												
GUANOSINE (CAS# 118-00-3); (M+Na)+												86637									71638			
DEOXYCYTIDINE (CAS# 951-77-9); (M+H)+												2639												
C34 H19 Cl O																					2390	1595	1137	
GLUTAMINE (CAS# 56-85-9); (M+Na)+																							20942	
HOMOVANILLATE (CAS# 306-08-1); (M+H)+																							2469	
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M+Na)+																					1468	4686	1598	
XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8); (M+H)+																							1823	
NICOTINAMIDE MONONUCLEOTIDE (CAS# 1094-61-7); (M+Na)+																							1176	
3-HYDROXYANTHRANILATE (CAS# 548-93-6); (M+H)+																						2955		
5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+H)+																						1047		
SULFADIMETHOXINE (CAS# 122-11-2); (M+Na)+																						19553		
L-METHIONINE SULFOXIMINE (CAS# 15985-39-4); (M+H)+																						1497		
(S)-DIHYDROOROTATE (CAS# 5988-19-2); (M+H)+										37179														
GLYCINE (CAS# 56-40-6); (M+H)+										2330														
GUANIDINOACETATE (CAS# 352-97-6); (M+H)+										1193														
DETHIOBIOTIN (CAS# 533-48-2); (M+Na)+										2415											2042			
3-METHYL-2-BUTENAL (CAS# 107-86-8); (M+Na)+										5035								7469						
25-HYDROXYCHOLESTEROL (CAS# 2140-46-7); (M+H)+[-H2O]																		1144						
DIETHANOLAMINE (CAS# 111-42-2); (M+Na)+																		2699						
3,4-DICHLOROANILINE (CAS# 95-76-1); (M+H)+																		2077						

5-METHYLCYTOSINE (CAS# 554-01-8); (2M+H)+																					3658						
TAUROLITHOCHOLATE (CAS# 516-90-5); (M+H)+[-H2O]																					1402						
C7 H7 N O												1265															
2',3'-CYCLIC CMP (CAS# 0); (M+H)+												1110															
GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M+H)+[-H2O]												2403															
3-METHOXY-4-HYDROXYMANDELATE (CAS# 55-10-7); (M+Na)+																								2655			
N-ACETYLGLYCINE (CAS# 543-24-8); (M+Na)+																								16787			
THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#); (M+H)+																								1125432			
100.001@0.5352921	122078	123388	118004	133710	127172	133224	35301	36975	36785	29942	50015		66249	23308	13367		61612	39761	58542	30156	36995	20494		26267	50547		11064	29873
284.0765@2.291664		17922	17379	18811	17623	16031	66918	69129	67556	70495	292012	117450	33420	81498	114525	95709		30383	41146	11042	91857	6279	37267	44504		32519	72306	53741
226.0954@3.0594227	13250	11949	10560	11080	9410		22943	21852	21909	24043	9588	20999		6213		9206	30388	51394	85757	23789	34499	8909	35590	29894		45680	12940	55002
260.1374@3.1285338	27168	22262	21462		23830	23985	25087	23950	28009	26591	90187	37822		23412	54501	36985	11786	29542	52979	15907	35456		12559	22562		29360		47736
913.233@3.608588	37823	39017	37324	36388	36952	36123	7045	8017	6882	7378					2020	7642	9059	37353	37181	14979	13972			12003		21155		31610
987.5345@7.6266623							30334	34726	32677	29165	23561	4733		5864	71811	20266	9987	34292	32074		87752	19888	41542	61759	7074	23010	24814	188988
785.5006@8.232729							91112	94995	90645	90684	37017	12036	6108	13049	154408	48713	102373	86037	158138	43781	257263	40966	106851	205456	18601	212134	93294	311001
1039.5897@9.211685		2237				1437	250508	246723	240412	253734	242345	35606	7529	76507	417294	228422	354517	402696	662611	61780	934137	204824	177212	410117	15477	616352	113007	995510
520.0016@9.493141							1333537	739050	725517	710534									210126				108038					
1053.6014@10.078312							38109	37418	38720	35206	30368		2079	29230	33741	11279	157577	26883	115954		88674	53087	3913	30093		49539		189598
504.0074@10.469363							1037557	478023	454789	438998					128391				276464				65236					
939.5053@10.673127							58688	59176	60900	58432	34968		6131	15044		16059	70999	75442	162821	245529	138246	37422	38245	98810	18949	69690		123710
1005.4501@10.68129							17669	16222	17170	16537	11932		3395	5801		3916	20968	21198	32014	65417	30250	12222	10407	23966	7535	19013		24273
766.3968@12.524396	27010	27618	26705	27146	25051	24727	70474	70587	67651	66919	17362	45279	20693	27189	168493	30126	68540	83012	109456	101466	73100	28623	97446	84158	15638	76151	45141	102956
810.4211@12.899628	21883	23795	22384	23993	24099	21747	57808	58835	57495	61748	19181	58103	20279	24508	146083	29061	49183	64165	92776	81648	56733	24648	93154	65863	15723	62404	35996	86190
854.4479@13.245994	19838	18408	19556	20031	19113	19557	45577	46574	45794	45367	14617	34143	17462	21773	113403	25205	37953	48752	71553	67721	47188	17789	56242	48906	13472	50408	26179	66089
898.4725@13.568503	17838	18001	16274	18288	17588	15652	40739	38533	38276	37021	13220	27730	15302	18947	94077	23770	30253	38360	56383	56427	36633	16552	42969	36748	10616	39956	21839	51587
942.4985@13.866499	14811	16963	14547	14462	14590	13504	29754	31305	30971	31188	10861	24277	13745	15608	75521	20006	23084	29142	46343	42964	31418	14559	33419	29725		34298	18927	40143
1030.5504@14.407582	10975	12129		12138	10942	11189	20888	19791	20006	19533	8220	16110	9315	10197	50482	12220	13738	19022	30153	26397	20091	9285	20793	19266	7449	21450	11487	24414
775.324@15.16887							31907	25319	31724	25491									16621				7555					
754.3032@15.242076							76611	66995	64869	64335									31214				24883					
819.3509@15.503695							53684	42263	43939	42239					1566				20422				13115					
841.3327@15.513131							87520	69563	65002	68162					1297				31048				20160					
776.3455@15.591792	1864						194309	163488	152268	165044					6762				70346				51829					
798.3285@15.589261							233350	191517	198813	188290									77399				60063					
856.2961@16.427088							53511	57132	54622	56173	24922	32821	35299	37715	32865	29515	45342	52949	92960	57321	44328	49525	60073	48503	45890	52300	57487	65142
1196.4637@16.426586							67628	72550	71955	67626	24502	33942	35937	41374	36128	29643	55186	66593	127324	74340	53398	60195	78761	58756	53304	62537	71282	87559
810.295@16.42741	4108	1814		1524		5904	242778	260891	256016	248895	127496	158571	162917	180950	158376	142228	219976	244107	364854	260905	211106	236864	269559	221594	208664	237744	257059	292137
838.3228@16.71113							197584	146312	148417	150207					2826				33152				44255					
882.338@16.728094							136628	103675	102382	97098									50390				36297					
904.3297@16.73777							66662	55370	45456	47985									24781				16745					
860.3637@16.733767							56437	47166	42530	41196									27667				14551					
926.3723@16.754114							39320	27057	28272	26243									15687				9390					
794.3295@16.810375	8402	7550	7644	7653	7482	7589	609696	654308	638022	636705	268769	393738	377451	392095	469837	308619	320607	516821	592334	419956	673806	424038	725709	398252	385239	583149	617006	714194
969.383@16.880194							133176	85914	84844	84656									36544				23739					
1013.4035@16.89687							54087	36479	32644	35704									23835				11122					
762.3666@16.903872							72868	56898	55919	56616									20882				14669					
1016.3469@16.988739							72134	54289	53802	52524					2222				22716				16744					
926.3747@16.987732							969443	720286	709344	708448					19333				283666				214797				2331	
904.3903@16.992311							181677	129250	130038	126659					5426				48434				33508					
970.3987@16.999172							168989	127463	128109	125527					3389				63470				43007					
1057.4308@17.134548							127894	84524	86258	84208					4860				41308				23724					
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1190.5253@17.855618							128201	84555	81988	81140					2866				31784				20174					
1142.4716@18.042645							54403	35602	33017	33370									22129				11321					
1098.4341@18.046814							217540	158076	151244	157466									72185				43354					
1120.4318@18.050985							96845	59719	56309	60923									26417				16838					
1054.419@18.06434							388733	264004	251751	257210					15625			11318	85850			11559	74690					
1185.4822@18.109724							143044	83914	77365	79833									36856									
940.3933@18.134588		7654				6293	41758	42633	63121	67026			1711					3861	25534				33215		1484	1070		3285
1186.498@18.216084							228200	143569	166349	167037					6597				78621				55946					1270
1142.4731@18.225863							1234804	798357	774921	771087					15159				303104				194042				1925	
1273.5255@18.26263							126313	68873	69104	70113					6556				34632				17736					
1230.5209@18.384392							344689	203102	204119	201768									79102				52742					
866.3585@18.392859							73596	86434	84462	80898	41723	46622	57652	65224	85309	43359	75106	78649	130074	93234	71514	74405	88542	80085	70754	73221	81832	102638
950.3874@18.494951							65738	31890	29804	28758					2840				14122				9176					
908.3653@18.828564							583261	404770	386061	383000									194489				130765					
976.3546@18.827229							68449	47146	44401	45531									21067				13682					
886.3831@18.827066							1644385	1035087	1007765	1011276					41058				473990				309432					
1110.4423@18.905958							109186	52867	51852	49342									22979				14421					
1358.568@18.97668							44374	22356	23728	21341									11729				10048					
1314.5312@19.003178							213694	123596	126611	122739									59817									
1401.5758@19.0491							92776	44251	44279	45877					3049				16192				26980					
1270.5171@19.018045							365836	207636	208890	202373									60157				49653					
1402.5927@19.115122							266705	137076	148521	136296									63817				36773					
1489.6285@19.128792							111431	57604	55838	57831					5095				26235									
1358.5696@19.134098				1176			838275	464885	453735	442547					9111				186015				103157					
1156.4895@19.188068	5048						40641	32046	46249	53862					4694	3955	1230		23102				23975					
1446.6211@19.246643			1155				327679	175913	173510	170384					12526				72496			1079	39205					
445.2466@19.244831							36810	39659	45958			50187	51361	46733	93834	41500	35471	59079	44231	45430	59239	44636	54982	40661		55719	52192	61382
511.8361@19.314745							1404646	1001307	906176	840085					167791				382998				465764					
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1530.6337@19.741968							144347	74614	71353	69629									36566				16951					
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1486.6162@19.758654							334741	166815	159556	165176									51492				38941					
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925.573@25.266247	884510		696944	34709	45696	63032	26434				2860						23321			5183	182771		150553	10669				227994
1053.4802@7.6255107							17722	17564	18603	17814	17238	3368	2135	4080	47834	17079	6430	14939	4319		32769	14626	22316	26879	5561	11778	19814	70213
753.2803@15.102336							74040	57506	56128	56496									23640				15193					
868.2339@15.176519							32106	30162	30007	28488					2076				11310				8083					
800.2489@15.174374							45659	41417	40766	38785									15511				14856					
842.3543@15.861749							33701	27410	26638	28487									13524				6827					
886.3777@16.156132							38586	31903	31244	35386									27571				16658	2704		4969		
886.3806@16.197645							28822	20371	21070	56278									26994				16658	1917		4973		
1012.2439@16.705917							24698	19709	19623	18066									4468				6454					
816.3386@16.701916							75037	59605	58135	56340									15810				17385					
1018.4564@16.715847							101073	70998	69434	71412					2989				26076				21343					
904.3945@16.754278							22948	16036	17726	17411									10882				5633					
1084.3444@16.991095							26151	23235	21927	23327									10459				8435					
948.4163@17.00477							66087	53605	52725	56705									24208				15583					
1100.4362@17.020802							27498	17135	18435	15406									8339									
806.3896@17.155703							50259	37076	37580	35334									15245				13021					
970.4013@17.192896							38835	31305	29804	30295									13730				9237					
850.4168@17.390692							28886	21521	19438	19380									7967				4950					
784.3152@17.391024							31712	22263	20479	20784									11425				6801					
1058.4529@17.437723							53411	37961	34053	34072									24761				19078					
1058.4513@17.49708							41605	29270	28005	34139									25285				20545					
894.3493@17.671717							48548	29012	28252	28706									12478				9453					
872.3645@17.680222							44268	27469	29112	28852									12119				9220					
1146.5034@17.735426							116176	77308	76787	74483									32264				20133					
1188.4261@18.052319							24342	16788	16246	18826									6904				4581					
1296.3391@18.052319							22246	18481	17557	16028									4776				5475					
1166.3751@18.055323							30740	23790	24010	20775									5880				5409					
846.3861@18.078674							27260	19351	20343	20059									8021				6587					
1229.4987@18.098938							65444	36131	36428	36762					1692				20262				10103					
918.4083@18.132708	2359		2268	2887	1995		17985	18260	22997	29300			1421						11433				14269				1347	
1322.6031@18.199108							74887	44076	45908	45320													8465					
1232.4283@18.235004							94414	60455	60837	57916																		

890.4078@18.27498							37304	27774	24052	25811									12241				9149					
1186.4926@18.234165							39970	164580	191527	164522					6573				78617				55403					
934.4355@18.447943							36422	26007	23982	24523									9682				6617					
956.4175@18.450941							36161	25780	23892	21544									8511				7795					
972.3756@18.495142							54416	26663	24267	24625									11478				6268					
1000.4479@18.6169							44802	27118	25143	26449									10588				7807					
415.9055@18.622404							551277	366056	344368	340730									126940				156305					
1362.6011@18.73716							112951	63480	64144	64223									22712				14548					
842.3581@18.739824							31278	22416	23049	23143									12225				6885					
1044.4469@18.761848							40674	27016	28066	24842													6505					
1220.4956@18.800629							33274	15394	15114	14214									5152									
1406.6229@18.831232							114397	63897	63788	63976									22189				13254					
946.2066@18.899412							80450	69974	65439	59522					17165				32235				40242					
1088.493@18.905933							31303	19250	20449	20635													4798					
1450.6497@18.902102							93844	56993	52984	52592									18892									
1494.6759@18.967403							73429	48425	43208	42874																		
1336.5323@19.000364							78939	43131	41975	48068									17320				11333					
1445.5927@19.002205							54491	26209	27221	26488					2984								5729					
1382.4766@19.019548							29859	18393	17547	19354									3259				4953					
1448.5474@19.139809							40898	21596	19057	19621									7966				4658					
467.5116@19.133024							138339	73941	74130	74005					2780				25303				15485					
879.7467@19.318176							426284	251351	225849	190317					26949				71493				90087					
937.2088@19.411821							24450	20987	20356	19268					7921				12877				14138					
1534.6768@19.455566							63168	32839	30693	33203									12097				8192					
1578.6978@19.516186							71788	38211	36426	35118									13766									
801.6078@19.727795							38714	25434	26188	23303									2250				4868					
1216.546@19.763077				3437			62950	38631	37380	34350					6010				20828				14551					
1705.7194@19.802855							60245	27371	27368	26918									11534				3960					
532.5483@19.841719							147104	77979	74195	69868									28045				15788					
539.5427@19.849634							138691	69608	66447	68855					3667				22445				13346					
876.3051@19.871077							77978	66559	65308	63249					16162				19043				30759					
561.568@19.914976							147890	72200	67506	66173					4676				26525				14473					
1304.5859@19.938639							31674	15893	16738	14575									6679				4576					
589.5668@20.313803							93485	42548	40849	42441									15281				7544					
1702.7167@20.333158							120424	59692	58915	53592									19376				10849					
1834.7926@20.350834							124692		49933	44783									22361				8666					
604.5843@20.386108							213396	96938	95490	89562					4398				38670				20399					
1404.5671@20.50224							65671	36791															6851					
1388.6174@20.494795							67213	38018	31969	38384									18697				6391					
1432.636@20.576471							47025	23080	22212	20391													5267					
676.6165@20.836817							181060	76942	75941	72464					4657				30433				14472					
1025.4164@20.84796							58958	25254	25709	25608									6558				2278					
1036.4094@20.84011							88739	36829	36286	37251									10520									
1036.9066@20.835611							71657	29983	29104	29352									11104				5221					
1144.9528@21.155699							114376	48225	44942	43509					1489				15925				7231					
1144.4542@21.159016							146731	52566	50275	49333																		
748.6456@21.157753							128994	54335	56124	49658									20813				7378					
1133.4579@21.160587							98929	48912	41631	49133									16201				6586					
1133.9595@21.152266							93750	35027	36830	33669					1449				13313				4475					
755.6398@21.157751							84721	31088	28548	29071									10806				3004					
1177.9858@21.172935							99553	40225	39502	35699									16724				5254					
1624.6503@21.286255							48685	19899	24533	23448					1493				10228				5749					
790.996@21.349993							40573	18787	24695	15955									4721									
1252.9946@21.345747							117581	49150	48532	40655					1866				16106				7313					
1252.4971@21.35066							130545	47688	42738	51486													2782					
1242.0122@21.353111							113526	43957	46574	40140									13328				3604					
820.6785@21.350441							78710	32606	34069	29136									9153				2232					
1285.5272@21.354149							154388	72484	58493	66754																		
849.6965@21.359217							60643	39762		29694																		
1360.5453@21.476757							100353	19767	52587	60718													3134					
1361.0408@21.484573							52586	22821	21023	38914									8365				3215					
1350.0544@21.487574							71504	20613	24721	38237									13895				7906					
1394.0824@21.486767							92399	59270	36236	70262													6607					
1501.6198@21.599972					15361		54587	37157		23044																		
633.8683@21.74444							250290	178150	172167	156670					41978				71233				108634					
661.2191@21.898596							273137	259994	268110	305767					59298				26428				21498					
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888.5332@22.030827	7909		5994			2767	22490	30035	40394	47915	4753	24325	5673		243325		6423		6226	2087		11046	6087	11552	14104	7026		18798
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693.4089@22.273722							60855								73947										43322			
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962.62@22.774042	7295	7082					32881	33649	5226		7094	21372		2099			42311			22175	39228		49851			34763	33813	59622
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1190.7104@23.050585							23986	27406							1607	49442	20892	3008	1561	5234	28832		31119	49370	14970	18787	25506	28880
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968.6634@23.068396	3459	3583	6340				39472	41537				45195			5625	93467	37018	5882			43261		45321		18272	17251	34470	51522
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946.6215@23.066227							131701	123812				98744				294600	95707	25526		33708	111482		137812	207898	73323	37048	96753	166075
924.6419@23.040983	4088	4405	3045				37834	36842				34287				87822	31319				42322		44409	76819	17945	9862	31825	56784
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873.5456@24.969215						10056																						
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827.4638@1.3281665	109927	107470	106420	90049	96607	81464																						
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129.0578@3.6125422	78739	85974	73944	89051	86483	70971																						
780.4258@4.246074	48223	49645	46651	48454	48724	45915																						
1269.5417@4.962292	38910	34475	35151	35585	36806	42281																						
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838.3332@5.899891	126248	125366	124901	116702	122941	120514																						
906.3227@5.9000583	40460	39525	41607	41447	39775	39231																						
794.3422@6.6771693	29540	17176	24750	26800	24390	24167																						
906.2928@6.695007	50868	38913	51195	49604	51048	49669																						
890.3263@6.6908507	251351	236192	236463	242425	235302	232415															8002	1751				2117		
958.3127@6.69148	144758	136544	134482	145780	134223	131313															2982							
1211.5614@7.3494577	35985	37690	35279	35048	34287	30873			2482																			
1193.4915@8.418485	128497	125766	116542	105684	136083	81391																		2731				
1125.5085@8.435857	505279	498679	483264	427770	484699	338206																						3558
1059.5623@8.449423	1600607	1591309	1539148	1332478	1533004	1041934															4958							
1097.5607@8.660056	822260	774576	760565	799877	723247	709811									1882													

1163.5018@8.604081	305223	310648	295120	319819	318652	299526		2233					2371							4202							
1306.6158@8.93452	88392	97690	87752	85966	90338	80628																					
764.3666@9.155757	23183	22659	22001	23950	24901	23250																					
1535.682@9.172261	55452	54769	52788	52817	52361	53230																					
919.4562@9.677266	84033	92784	81818	88672	89231	84342																					
985.4018@9.678767	118681	120478	113035	117296	108418	109457																					
1053.388@9.672932	43865	46041	46285	45307	47805	43343																					
1172.5013@9.87934	33046	34093	32273	30846	33167	30355																					
961.3825@10.292669	41989	41273	37553	38830	36350	35366																					
1053.3593@10.285832	40970	42699	40193	41155	41233	41501																					
1105.3809@10.285832	114063	117811	109495	109849	107640	105750																					
1121.348@10.2873335	47968	47771	48347	48415	49338	47542																					
1037.3947@10.2885	218404	224043	214622	215222	217772	216425																					
969.4065@10.295565	575944	573391	542843	554463	556769	523171												4594	3936								
903.4606@10.295564	669033	671536	649679	643834	652231	604527												8795	5090								
1210.6443@10.313508	1325936	1280347	1262990	1196658	1231254	1149163																					
1248.5905@10.296051	115508	100355	103933	106934	102164	100069																					1106
941.4594@10.395044	241870	252521	238511	241742	234078	236654																					
1210.4646@11.948796	48912	51257	50955	50102	49731	47443																					
1142.472@11.969642	46401	46944	43169	45267	45112	43927																					
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1435.7126@12.813649	95423	85447	86338	87971	80644	88229																					
857.3804@13.576004	27344	26973	26214	26314	26054	25777																					
857.7144@13.581676	23466	22154	20066	22356	21766	21049																					
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763.2595@22.065031	20636	20804	19904	18153	16281	13824	5922	7162	7078	4704			3979	4663	2419	7990	6551	8442	3148	8259		7629	4026		5265	3594	9799
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1733.9208@22.305954	83595	62924	79795	84373	74867	70676																					
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992.6181@22.166582										6785							11315	15963								7762	
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1028.6116@22.4945							15771			46826			23021														
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875.5576@25.349667										39741																	
894.5349@22.419611			18184		15864		41144			37921	39253	37310	32664		31800	34361		82944	36515			47429	49391	28350	61117	46327	46618
874.5523@22.484612					6175			19107		16249		12510															
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830.5403@22.445963				6227				10557		7566		6161									2487		30702				
792.5548@22.774387										1503																	
857.8468@25.059256										27579																	
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875.8166@25.536413																115558											
925.8507@25.536413																8551											
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807.2472@21.983837			21753													1943											

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875.82@25.311146		151656																						458537				
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962.6126@22.455866										4900								3631	11383			2782		29968				
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1873.0225@24.628525												16324								33121								
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765.5647@24.971613												3168											107341					
852.5753@22.548275			1981									19262																
795.7901@25.479336																					3097							
832.9296@26.10271																					6791							
1185.4738@5.250163																					1474							
1210.6353@9.997115																					8436							
1052.6198@22.489832								4438													1357							
646.716@29.049877																					1532						1368	
260.136@2.8055449				6697																							1635	
1039.5977@8.992071				1053																								
802.5058@22.273735				1015																								
602.6712@25.634558				20251																								
1785.0562@24.577515				47303																								
1669.0471@24.240847				6195																						1808		
929.1763@0.6045015										1259																		3732
1029.376@5.4622707										2720																		
785.5877@24.955555										1565																		
1006.652@22.587593										52339																		
808.5483@22.446434										2137																		
1125.5096@8.545201																								2364				
1056.5461@22.146221																								2700				
1597.951@22.57967														2767										3379				
795.5113@24.243965																								137000			87142	
1603.0817@24.532478			55757																									
1110.685@22.736984			3661																									
1518.9471@23.276976			2019																									
861.5118@22.669655																							5813			3621		
633.8659@21.435715																										2114		
1138.7039@23.056713																										5213		
828.5102@22.623009																1854												
787.5016@22.77321																2902												
756.3915@6.384316																												5828
1210.6334@10.541441																												4646
1146.5872@21.792347																		12253										
1523.9374@22.582985																		14201				1974						
1270.505@18.84669	2378																											
1432.8774@22.841396	6003																											
1168.6298@22.010498																											8269	
823.5312@25.380026																											6191	
847.5656@23.07916														2358														
1366.7979@22.686644									6345					2833														
1595.9323@22.416012																							17296					
866.5028@21.646309									3594																			
1621.0645@24.825544								2566																				
833.825@25.63534													2023															

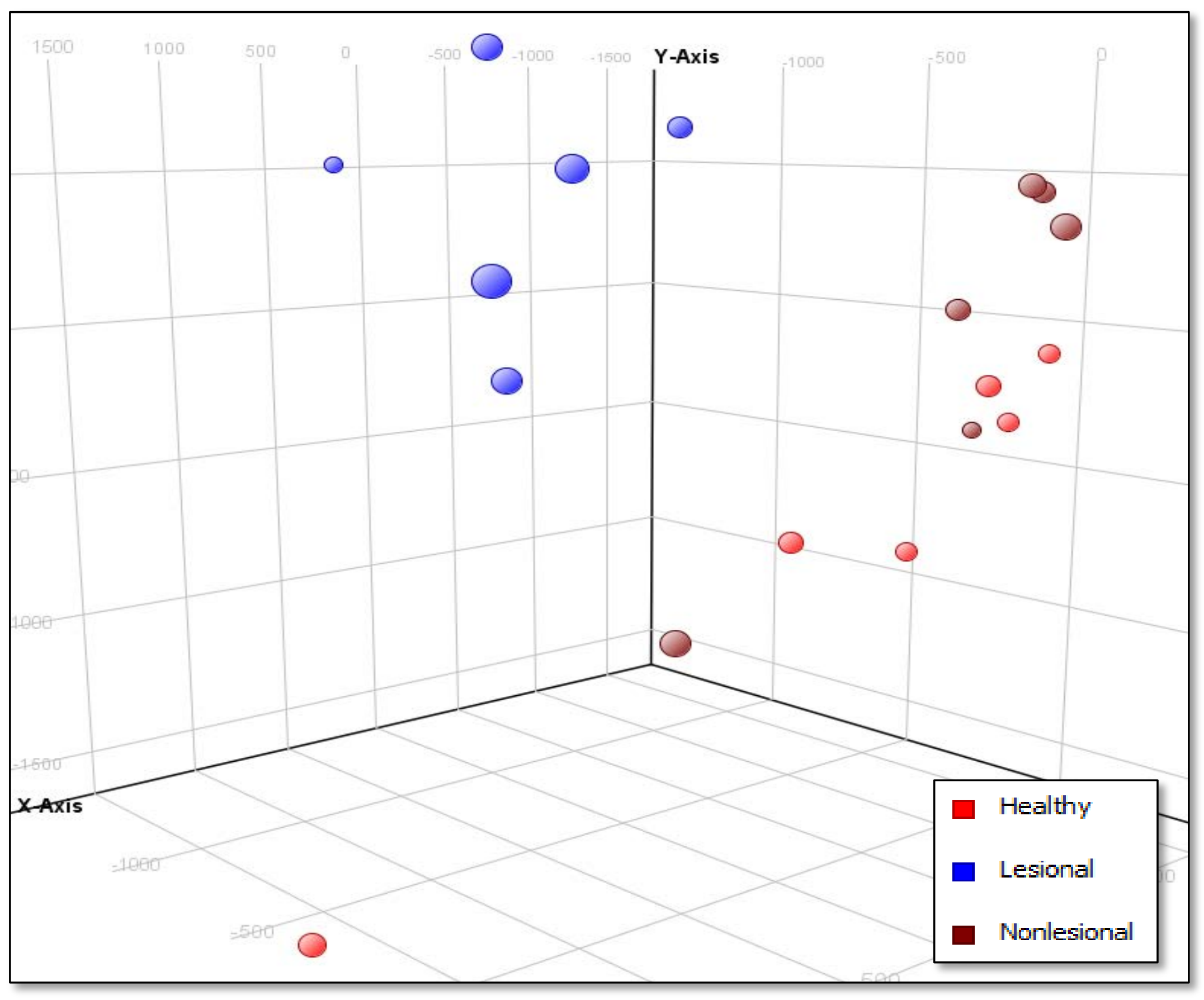
Compound	Pos_Human Plasma Extrac	Pos_Human Plasma Extrac	Pos_Human Plasma Extrac	Pos_Human Plasma Extrac	Pos_Human Plasma Extrac	Pos_Human Plasma Extrac	Pos_Pool QC 1	Pos_Pool QC 2	Pos_Pool QC 3	Pos_Pool QC 4	Pos_S00015447_1	Pos_S00015448_2	Pos_S00015449_3	Pos_S00015450_4	Pos_S00015451_5	Pos_S00015452_6	Pos_S00015453_7	Pos_S00015454_8	Pos_S00015455_9	Pos_S00015456_10	Pos_S00015457_11	Pos_S00015458_12	Pos_S00015459_13	Pos_S00015460_14	Pos_S00015461_15	Pos_S00015462_16	Pos_S00015463_17	Pos_S00015464_18
(-)-COTININE (CAS# 486-56-6); (M+H)+	125925			124464	138391	134718																						
(-)-SALSOLINOL (CAS# 27740-96-1); (M+H)+							37386	39974	38850	41347	52576			24343	53250		127377	24029		25141	119624	12945				46791		69040
(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-14-7); (M+H)+					14937	14738	48072		50464	51517		79387								4269								
(2-AMINOETHYL)PHOSPHONATE (CAS# 2041-14-7); (M+Na)+							20623					23464				42481	12521			19259		16553						
(S)-2-AMINO-3-(3-HYDOXY-4-OXO-4H-PYRIDIN-1-YL)PROPANOATE OR L-MIMOSINE (CAS# 500-44-7); (M+Na)+												1630																
(S)-DIHYDROOROTATE (CAS# 5988-19-2); (M+H)+														37179														
1,2-DIPALMITOYL-SN-GLYCEROL (CAS# 30334-71-5); (M+Na)+	115880	122615	181660				96941																32798	4961			22727	
1,3-DIAMINOPROPANE (CAS# 109-76-2); (M+H)+							2201					8846							5615				5200	5489				
1,3-DIELAIDIN (CAS# 98168-52-6); (M+Na)+	32038	12827	3644378				394182				15756										1608042		26844					119857
1,3-DIMETHYLURIC ACID (CAS# 944-73-0); (M+Na)+					9462																							
10-HYDROXYDECANOATE (CAS# 1679-53-4); (M+Na)+																			20018				33374	22507				
11BETA-HYDROXYANDROST-4-ENE-3,17-DIONE (CAS# 382-44-5); (M+Na)+										4716									8292							17525		2832
11-DEOXYCORTICOSTERONE (CAS# 64-85-7); (M+Na)+																												6046
11-DEOXYCORTISOL (CAS# 152-58-9); (M+H)+																			2954									
11-DEOXYCORTISOL (CAS# 152-58-9); (M+Na)+	24829	13525	21656	14929	15068																					9834		
16:0 LYSO PC (CAS# 17364-16-8); (M+H)+	2387470	1923398	2318105	2012893	1788653	1626678										4657				87734	89585	18186	44794				3373	70583
16:0 LYSO PC (CAS# 17364-16-8); (M+Na)+	1.71E+07	1.62E+07	1.71E+07	1.62E+07	1.50E+07	1.44E+07	784305	707374	694836	639740	504810	288620	149226	185740	234786	445428	423725	753542	572071	1417201	1257295	395035	701468	611490	67947	394117	321508	1013916
16:0-18:0 PC (CAS# 59403-51-9); (M+H)+																								1286				
16:0-18:0 PC (CAS# 59403-51-9); (M+Na)+		48936	291967				6965														22689		9152				10541	43469
17ALPHA,20ALPHA-DIHYDROXYPREGN-4-EN-3-ONE (CAS# 652-69-7); (M	1368	1226																										
17ALPHA-HYDROXYPROGESTERONE (CAS# 68-96-2); (M+Na)+				4029																								
18:0 LYSO-PE (CAS# 69747-55-3); (2M+H)+											2965																	
18:0 LYSO-PE (CAS# 69747-55-3); (2M+Na)+																								8209				
18:0 LYSO-PE (CAS# 69747-55-3); (M+H)+						4961														16110								
18:0 LYSO-PE (CAS# 69747-55-3); (M+Na)+											9144																	
1-AMINOCYCLOPROPANE-1-CARBOXYLATE (CAS# 22059-21-8); (M+H)+	42601	62235	59848	58322	54484	65647	11734	37209	15955	12817	16210	17170		5414	13874	14652	31852			17278	20390	4023	2270	18460				
1-METHYLADENOSINE (CAS# 15763-06-1); (M+H)+	10073	10017	10421	11568	10835	12770	1872										3279		3483				1039					
1-METHYLADENOSINE (CAS# 15763-06-1); (M+Na)+						1556																						
1-METHYLXANTHINE (CAS# 6136-37-4); (M+H)+		24815																										32922
1-METHYLXANTHINE (CAS# 6136-37-4); (M+Na)+	2693		3272	1695	4127																							
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+H)+										14402									36820			2581						
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+H)+[-H2O]											1010	16673					89035											
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+Na)+	180138	175693	167616	35378	169450	31308	240166	231331	109208		171843	337001	14285	116261	887088	164620	324433	256982	73084	285505	423144	12744	168135	107663		244190	138238	393182
1-PHENYLETHANOL (CAS# 1445-91-6); (M+H)+[-H2O]																			1736									
2-(DIPHENYLMETHOXY)-N-METHYLETHYLAMINE (CAS# 17471-10-2); (M+H)+			1860			1693																						
2',3'-CYCLIC CMP (CAS# 0); (M+H)+													1110															
2,4-DIHYDROXYPTERIDINE (CAS# 487-21-8); (M+Na)+								2791				7897	5031	21016	8127									3657				
20:0 LYSO PC (CAS# 108341-80-6); (M+Na)+	28880	29828	49794		25069									1801							8975							
24:0 SM (D18:1/24:0) (CAS# 60037-60-7); (M+Na)+			8559																		2317963							47241
25-HYDROXYCHOLESTEROL (CAS# 2140-46-7); (M+H)+[-H2O]																						1144						
25-HYDROXYCHOLESTEROL (CAS# 2140-46-7); (M+Na)+												6258	6669						1888			1356						
2-AMINOBUTANOATE (CAS# 2623-91-8); (M+H)+	2917	3837	5623	6133	6010	7471																						
2-AMINOETHYL DIHYDROGEN PHOSPHATE (CAS# 1071-23-4); (M+H)+								6847			128649	18014			132910										3978			
2'-DEOXYCYTIDINE 5'-MONOPHOSPHATE (CAS# 1032-65-1); (M+H)+																			7544							5391		
2-DEOXY-D-GLUCOSE (CAS# 154-17-6); (M+Na)+								10393					1283							65152	37430							
2'-DEOXYINOSINE (CAS# 890-38-0); (2M+Na)+											2590	13019							2987									
2'-DEOXYINOSINE (CAS# 890-38-0); (M+Na)+							26919	25243	25974	25167	58522	152713	10214	21853	29156	6984		24263				8637				16722	5622	
2-HYDROXY-3-METHYLBUTYRIC ACID (CAS# 4026-18-0); (M+Na)+	54573				60639	56692																						
2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-5); (M+H)+[-H2O]																	1774											
2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID (CAS# 583-91-5); (M+Na)+			1573																									
2-HYDROXYBUTYRATE (CAS#); (M+Na)+	40851	41090	43389	43351	45146	40736							31000		5071		58980										1084	
2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M+H)+[-H2O]		2328								1217					1444				3097		1473					3133		
2-METHYLGLUTARIC ACID (CAS# 18069-17-5); (M+Na)+		33046			24832		36637		37173	36749	19410				35562	20366			50137	20314	31340	5754				68121		
2-METHYLPROPANAL OXIME (CAS# 151-00-8); (M+H)+[-H2O]	141412	162624	4600	82085		154790	2695		1885		110350		40909	92069	131593					3902	50616		29963					
3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M+H)+	9064	11984	10410	10456	8436	10700		1376	2955							2886			8709	1758	4022		10301	1106				
3-(4-HYDROXYPHENYL)LACTATE (CAS# 6482-98-0); (M+Na)+	28233	28757	26591	30951	27763	26732											1610	2580										1392
3,3'-DITHIODIVALINE (PENICILLAMINE SS DIMER) (CAS# 20902-45-8); (M+H)+															6078													
3,4-DICHLOROANILINE (CAS# 95-76-1); (M+H)+																						2077						
3,4-DIHYDROXY-L-PHENYLALANINE (CAS# 59-92-7); (M+H)+																								5113				
3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+H)+				30074	24832							13432		7236					47132			8087			10765	65798		63410
3,4-DIHYDROXYPHENYLACETATE (CAS# 102-32-9); (M+Na)+									2289																			4086
3,4-DIHYDROXYPHENYLETHYLENEGLYCOL (CAS# 28822-73-3); (M+H)+[-H2O]				2096	2567		2621																					
3',5'-CYCLIC AMP (CAS# 60-92-4); (M+H)+								1135		1413				1521					3909		1694							
3-AMINO-4-HYDROXYBENZOIC ACID (CAS# 1571-72-8); (M+H)+																		15011										
3-AMINOISOBUTANOATE (CAS# 144-90-1); (M+H)+[-H2O]	8991	10359	10838	8912	9456	5473											1161							1570				
3BETA-HYDROXY-5ALPHA-PREGNAN-20-ONE (CAS# 516-55-2); (M+Na)+		1446																										
3'-CMP (CAS# 63-37-6); (M+H)+		1273					29147	29062		27457	47745	19661		3100	45584	33374	8533			15648	32065	11909		29113	5735		47531	
3-DEHYDROSHIKIMATE (CAS# 2922-42-1); (M+H)+[-H2O]		4507			10562		2001													1094								
3-DEHYDROXYCARNITINE (CAS# 407-64-7); (M+H)+				90300	85547						76986	22467			44579		27101						39862					
3-HYDROXY-3-METHYLGLUTARATE (CAS# 503-49-1); (M+H)+	20905	21440		16556	16710																			1600				1554
3-HYDROXYANTHRANILATE (CAS# 548-93-6); (M+H)+																										2955		
3-HYDROXYBENZALDEHYDE (CAS# 100-83-4); (M+H)+[-H2O]	23788	26355	25674	26862	25407	25440				1042	1125						2625				4467			6106				
3-HYDROXYKYNURENINE (CAS# 2147-61-7); (M+H)+															1862													
3-HYDROXYPHENYLACETATE (CAS# 621-37-4); (M+H)+							6292513	6481434	6609860	6742434	4862275	190688	837120	1621245	1145335	1148351	1.31E+07	1.39E+07		9758113	1.40E+07	4661780	4127420	8317110	241142	1.11E+07		1.37E+07
3-HYDROXYPROPANOATE (CAS# 503-66-2); (M+Na)+	14234				4405																							
3-METHOXY-4-HYDROXYMANDELATE (CAS# 55-10-7); (M+Na)+																									2655			
3-METHOXYTYROSINE (CAS# 4214-13-5); (M+H)+	21322	19120	20919		20452																8031							8170
3-METHYGLUTARIC ACID (CAS# 626-51-7); (M+H)+[-H2O]										1203					1443				3097		1389					3169		
3-METHYGLUTARIC ACID (CAS# 626-51-7); (M+Na)+		33046			24832		36637		37173	36645	19410				35562	20366			48388	20366	31340	5754				68255		
3-METHYL-2-BUTENAL (CAS# 107-86-8); (M+Na)+														5035								7469						
3-METHYLADENINE (CAS# 5142-23-4); (M+H)+							1177					1161																
3-METHYLADIPIC ACID (CAS# 3058-01-3); (M+Na)+			6274						1773	1192		1579						1254	2279								1109	
3-METHYLHISTAMINE (CAS# 644-42-8); (M+H)+							19731	19687	16594	20266			6452	4576	39349			17770	6695	20113	13280	7778	18751	19438		11053	17222	11248
3-METHYLXANTHINE (CAS# 1076-22-8); (M+H)+														3058								23355		13291	54963		13999	
3-UREIDOPROPIONIC ACID (CAS# 462-88-4); (M+H)+							2362						5144													3900		
4-ACETAMIDOBUTANOATE (CAS# 3025-96-5); (M+Na)+	6609	47265	42173	50873			21331	22054	19747	22850	1983	5347	2851			5529	12775	10857		14464	23255		25750	12778		19093	6339	13092
4-ACETAMINOPHEN SULFATE (CAS# 32113-41-0); (M+H)+	1855		4361		6113																			11318				
4-AMINOBENZOATE (CAS# 150-13-0); (M+H)+		11531			4723				16173		21304				31137										4337			
4-AMINOBUTANOATE (CAS# 56-12-2); (M+H)+	2917	3837	4484	6133	6010	5765																						
4-GUANIDINOBUTANOATE (CAS# 463-00-3); (M+H)+											11331																	
4-HYDROXY-2-QUINOLINECARBOXYLIC ACID-KRYNURENIC ACID (CAS# 4	9194		6495		6920			1065				2341											1297					
4-HYDROXY-3-METHOXY-BENZENEMETHANOL (CAS# 498-00-0); (M+H)+[-H2O]				3957			1096														2694							
4-HYDROXYBENZALDEHYDE (CAS# 123-08-0); (M+H)+							20123	19501	23068	16422	1230	23135	7429	3758		12185	28309	20928		16061	3337	17277	30000	31404	14156	31972	20754	13391
4-HYDROXY-L-PROLINE (CAS# 2584-71-6); (M+H)+	1418141			2528	2843	1914																						
4-HYDROXYPHENYLACETATE (CAS# 156-38-7); (M+H)+	8543	7204		8882	7262																							
4-METHYL-2-OXOVALERIC ACID (CAS# 816-66-0); (M+Na)+	4830				6080	5727																						
4-PYRIDOXATE (CAS# 82-82-6); (M+H)+	55345	53956	54061	52511	52142	41861						10126					25587		55461	96344			18963					
4-PYRIDOXATE (CAS# 82-82-6); (M+H)+[-H2O]														2308						8665								
4-PYRIDOXATE (CAS# 82-82-6); (M+Na)+		4908	7596	10013	7910	8272														19989								
5ALPHA-CHOLEST-7-EN-3BETA-OL (CAS# 80-99-9); (M+H)+[-H2O]	67336	66665	66864	67029	42589	57144	27417				12617	15498					39390		2871	47302	66948		11491	26928			19251	61438
5-AMINOLEVULINATE (CAS# 106-60-5); (M+H)+	1418141			2528	2843	1914																						
5-AMINOPENTANOATE (CAS# 660-88-8); (M+H)+	955416	956326	899143	879575	846845	839974					231331	4524167	267514	2113765	2978204		116021	269114			5168405	117509		68831	121992	247780		
5BETA-ANDROSTANE-3,17-DIONE (CAS# 1229-12-5); (M+Na)+											1099				2497													
5'-DEOXYADENOSINE (CAS# 4754-39-6); (M+H)+																										1047		
5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M+H)+	23047	22045	21756	21546	21907	20418																						
5-HYDROXY OMEPRAZOLE (CAS# 92340-57-3); (M+Na)+	30127	28649	29026	30711	30126	26984																						
5-HYDROXYINDOLEACETATE (CAS# 54-16-0); (M+Na)+		1848																										
5-HYDROXYTRYPTOPHAN (CAS# 4350-09-8); (M+H)+			26748																									
5-METHYLCYTOSINE (CAS# 554-01-8); (2M+H)+																						3658						
5-METHYLCYTOSINE (CAS# 554-01-8); (M+H)+									4425		1550						3310				5607					6360		
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+H)+							4221	4760	4434	4749	10605	7175		10086	5792	3978	6336	4192	5196		10181			2419		4879	2843	6898
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+Na)+							3496	4446	3914	3274	9077	6723		8950	5807	2528	5268	2881	3666	1252	9704		1573	2006		3837		4649
5-OXOPROLINE (CAS# 4042-36-8); (M+H)+	1085793	1012923	1015277	1046038	956569	1042124	6808608	6974549		6721671	692808	3524401		1072637	1082405	4090315	6844720				3277663	1277015	9868229	1.19E+07	568875		5421973	
5-OXOPROLINE (CAS# 4042-36-8); (M+Na)+				471502																		345986	2775446		209038			
5-VALEROLACTONE (CAS# 542-28-9); (M+H)+		110026	104828	107976																								
6-CARBOXYHEXANOATE (CAS# 111-16-0); (M+Na)+			6274						1773									1254									1109	
ABRINE (CAS# 526-31-8); (M+H)+																	3112		3828									
ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M+H)+		170617		162633		156971	128207	126422	122136	127547	204403		42252	2493	6994		426015	33242						550609				
ACETAMINOPHEN (TN TYLENOL) (CAS# 103-90-2); (M+Na)+	308761	311338	293536	309854	303447	291587	268175	274424	267312	269535	469672	31086	112490		13808		834132	65690		10147			182222	991228			17558	
ACETYLCHOLINE (CAS# 51-84-3); M+								7929		4457	9862	13942	3144	10540	17370		7152		14623			6706	3315		2401	7030	5020	
ADENINE (CAS# 73-24-5); (M+H)+	5929					4914	24585					49568	23446	23099			15192				8750	17811	18804		68674			
ADENOSINE 3',5'-BISPHOSPHATE (CAS# 1053-73-2); (M+H)+											9590	34444		13674	14432						54891							
ADENOSINE 5'-DIPHOSPHATE (CAS# 58-64-0); (M+H)+											9590	34444		13674	14432						53211							
ADENOSINE 5'-MONOPHOSPHATE (CAS# 61-19-8); (M+H)+	63324	8373				54831	4657	7728			36597	13073							6527		2854			2685				10227
ADIPIC ACID (CAS# 124-04-9); (M+Na)+		33046			24832		36637		37173	36645	19410				35562	20366			48388	20366	31340	5754				68255		
ADP-RIBOSE (CAS#); (M+H)+[-H2O]															7738													
AHBA (CAS# 76045-71-1); (M+H)+									28294									15011		26907	56396							33778
ALANINE (CAS# 56-41-7); (M+H)+		2449	4770			5825	3945																3677					
ALLANTOIN (CAS# 97-59-6); (M+H)+																							1247					
ALLOSE (CAS# 2595-97-3); (M+H)+[-H2O]	20905	21440		16556	16710																2132			1600				1554
ALPHA-D-GALACTOSE 1-PHOSPHATE (CAS# 2255-14-3); (M+Na)+							1523	1255														1102					1833	
ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+Na)+	33493	13055	21126	320054	8051	304055	52328	66846	18461	21911	9203	27179		6400	8776	2050	37810	38923	49033	45352	16639		10054	26527	61560	14313	47323	34567
ALPHA-TOCOPHEROL (CAS# 59-02-9); (M+H)+	4616	4046	4674	6334	5095	4565																						
ANDROSTERONE (CAS# 53-41-8); (M+H)+[-H2O]									2537																			
ANDROSTERONE (CAS# 53-41-8); (M+Na)+			2499				10803	12884	12735	14066		14300				1536					3475		15774	3904			92725	11707
ANTHRANILATE (CAS# 118-92-3); (M+H)+							14772																					
ARABINOSE (CAS# 147-81-9); (M+Na)+		2212										214117	502813		92156													
ARACHIDIC ACID (CAS# 506-30-9); (M+Na)+																											2380	1690
ASCORBATE (CAS# 50-81-7); (M+H)+[-H2O]							1329921	1358452	1305647	1317317	706353	1066720	520660	289866	881317	878338	1492600			1757359	2412624	578640	1742847	1643341		1921645	957396	2173028
ASPARAGINE (CAS# 70-47-3); (M+H)+							2362						5144						2412							3900		
ASPARAGINE (CAS# 70-47-3); (M+Na)+												4402					1056											
ASPARTATE (CAS# 56-84-8); (M+H)+		1858		2620							5280		2313					6355										
ASPARTATE (CAS# 56-84-8); (M+Na)+							1100					1966			4421	5830						2260						
AZELAIC ACID (CAS# 123-99-9); (M+H)+[-H2O]																												9373
AZELAIC ACID (CAS# 123-99-9); (M+Na)+		47239					139398	149836	138626	131704	87047	97942	30906	51054	255403	150679	103281	194058	250615	160828		65198	131001	107142	43739	171809	80006	308686
BENZOATE (CAS# 65-85-0); (M+H)+							20123	19833	23068	16450	1230	23135	7429	3758		12185	27118	20220		16402	3337	17277	28937	30076	14156	34317	20754	12675

BETA-ALANINE (CAS# 107-95-9); (M+H)+	4135	2955			2809	3927					2091	5297	4473	4135	40558						9844							
BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (CAS# 584-85-0); (M+H)+																		1191										
BETA-ALANYL-N(PAI)-METHYL-L-HISTIDINE (CAS# 584-85-0); (M+Na)+						2257																						
BETAINE (CAS# 107-43-7); (M+H)+	955416	908830	831624	879575	846845	839916		80854	132006	58969	231295	4524185	270217	2113765	2964739		116021	269114	76137		5023926	117509		68831	7653	90924		
BETAINE (CAS# 107-43-7); (M+Na)+	20490	19673	27966	17214	19571	4247	3791	4227	3665		3881	4624	7242	5415	4167	8156	4305	304022	2663	4055		9131	5555	2666	17953		5388	
BETA-MALTOSE (CAS# 69-79-4); (M+Na)+	4173	3430	3160	2418	2679	3429					26886	21121	25685		48881	23486	9027				13605				25104			
BILIVERDIN (CAS# 114-25-0); (M+H)+	138695	127514	131103	141768	131596	123309																						
BILIVERDIN (CAS# 114-25-0); (M+Na)+	41604	35382	38176	39592	38835	39450																						
BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7); (M+H)+	22538	23640	23981	52636	22016	17445				46609	43474	167013	40891	37350		6998		21513	36539			39448		16443		6169	7086	
BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7); (M+Na)+	2838541	2906889	2812278		2540504	766306	2145575	1792692				1.41E+07				906570	1702534	5315		351575	2147452		1984262	436497	845739	803630	1350317	1330197
BIURET (CAS# 108-19-0); (M+Na)+								27799				36001		104526		23136				17522		11211	17041	20131		22559	31871	
C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12:0) (CAS# 41613-14-3); (M+H)+																	19929						1960					
C12 GALACTOSYL(BETA) CERAMIDE (D18:1/12:0) (CAS# 41613-14-3); M+[-C6H11O6]									8221				2968						14184					5102				
CAFFEINE (CAS# 58-08-2); (M+H)+	1315835	1275935	1239712	1307537	1240546	1197826	81189	84383	78773	78374		88726	2465		30678	26181	38713	291857	18912	30650	209290	29097	464454	203221				371997
CAFFEINE (CAS# 58-08-2); (M+Na)+	401450	390067	386723	407661	394558	368607	14277	17500	13414	14254		30475			6454	8186	4613	44568		1643	31403	4943	84239	36191	1292			50197
CALCIDIOL (CAS# 19356-17-3); (M+H)+				10148		8109				5072									4955			9109						
CALCIDIOL (CAS# 19356-17-3); (M+Na)+	9232		10149	9960		9460			1125					1438														
CARNOSINE (CAS# 305-84-0); (M+H)+												1025																
CELLOBIOSE (CAS# 528-50-7); (M+Na)+	4173	2915	3160	2418	2144	3025					26886	21121	25685		48881	23486	9027				13605				25104			
CHOLATE (CAS# 81-25-4); (M+Na)+		35830	33937		33986	34540																	35277					
CHOLESTEROL (CAS# 57-88-5); (M+H)+[-H2O]	67336	66665	66864	67029	42589	57144	27537				12627	15524					39390		11616	47302	70553		11516	26928			19251	61438
CHOLESTEROL HYDROGEN SULFATE (CAS# 1256-86-6); M+[-HSO4]					1292																							
CHOLINE (CAS# 62-49-7); M+	91800	91957		88964			29250		30681	15440	81699	167873	32009	38265	62875		6952					4056	22659	15201		14922	49843	1216
CHOLINE PHOSPHATE (CAS# 107-73-3); (M+H)+	3241	1732	6042	6553	7452	5990	82779					52412		59020	296344	98395	3022				173362	45291	5604				42229	
CHOLINE PHOSPHATE (CAS# 107-73-3); (M+Na)+											5533				5748	2069				1458	6583							
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0); (M+Na)+	51840	53731	50174				32600	28226				10182				13436	5764			4696	12160	1498	4307	2523		7945	34662	16708
CIS-VACCENIC ACID (CAS# 506-17-2); (M+H)+	19140	21193	21733				9936	10221				6403			2967		5520				11159		9207				7891	13213
CIS-ZEATIN (CAS# 1637-39-4); (M+H)+	5572818	5496355	5308931	5477671	5323081	5193972	9506954	9606771	9272271	9346710	7841025	8307701	7142254	9437523	8430501	7707158	7527556	8324285	1.02E+07	7392421	7658786	1.05E+07	1.06E+07	9305636	1.27E+07	1.16E+07	1.06E+07	9624313
CITRAMALATE (CAS# 2306-22-1); (2M+Na)+															1658													
CITRAMALATE (CAS# 2306-22-1); (M+Na)+	2590	4815	5614	4443																								
CITRATE (CAS# 77-92-9); (M+H)+[-H2O]											1299	2611	1586															
CITRATE (CAS# 77-92-9); (M+Na)+	193468	20570	177253	185279	166559	163362	1741			2482	18493			11161	12861						1052							
CITRULLINE (CAS# 372-75-8); (M+Na)+	6352	4927	3107	4457	3604	3319																						
CMP (CAS# 63-37-6); (M+H)+		1273					29147	29062		27457	8468	27730		3100	12793	5089	8533			15648	32065	13906		29113	5735		47531	
CORTICOSTERONE (CAS# 50-22-6); (M+Na)+	24829		14069	14929	15288					4112																9834		
CORTISOL (CAS# 50-23-7); (M+H)+	22894	24285	21184	23020	21836	22344																						
CORTISOL (CAS# 50-23-7); (M+Na)+	484681	457178	453488	463576	456437	440270		15252	9955	8708	10656						36372	23790	27456	13105	25543					8438		38200
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)+							5183	5301	6471			11531			3693			6211					7665					
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+H)+[-H2O]											3912	12137																
CORTISOL 21-ACETATE (CAS# 50-03-3); (M+Na)+		9764		2067											17354			13758		9529		2165						
CORTISONE (CAS# 53-06-5); (M+H)+	3462	3143	3466	3348	4188	3170																						
CORTISONE (CAS# 53-06-5); (M+Na)+	52988	53529	50381	52935	51583	51277					2497						6171	8491	14890		8623							5691
CREATINE (CAS# 57-00-1); (M+H)+		138209	114035	140847	135065	117035					950939		524897		1628085													
CREATININE (CAS# 60-27-5); (M+H)+						79353																						
CREATININE (CAS# 60-27-5); (M+Na)+			15197																		14119							
CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (2M+H)+					1762																							
CREATININE-(GUANIDINO-13C) [ISTD] (CAS#); (2M+Na)+						2647																						
CYSTATHIONINE (CAS# 56-88-2); (M+H)+[-H2O]	5245	5872	5611	5964	4959	5489																						
CYSTINE (CAS# 56-89-3); (M+Na)+		3623	3047	3125	3038	3713							2248								2747							
CYTIDINE (CAS# 65-46-3); (M+H)+											10291		1208	5026														
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+H)+											2412	16031		4546	11901													
CYTIDINE 5'-DIPHOSPHOCHOLINE (CAS# 987-78-0); (M+Na)+																1585							1058	1550				
CYTOSINE (CAS# 71-30-7); (M+H)+							12636				14746	40148	5351		9114								2547		2488			
CYTOSINE (CAS# 71-30-7); (M+Na)+		2912	9978				13206			13592		11816							6202	18389				5758				
D-(-)-ARABINOSE (CAS# 10323-20-3); (M+Na)+		2212										215728	504399		92156													
DEBRISOQUIN (CAS# 581-88-4); (M+H)+		9619			27948		349903	197817	77647	144925	254361	30059	162622	37831	76408	133481	43853		24946	26925			392221	397465	140336	140913	3045	13905
DECANOATE (CAS# 334-48-5); (2M+Na)+					23268										149168			16959		60664							39426	
DEHYDROASCORBATE (CAS# 490-83-5); (M+H)+[-H2O]											36497			12053	21781													
DEOXYADENOSINE (CAS# 16373-93-6); (M+H)+	1566																											
DEOXYCHOLIC ACID (CAS# 83-44-3); (2M+Na)+							8644	1269																				
DEOXYCHOLIC ACID (CAS# 83-44-3); (M+H)+													7273						10625									8703
DEOXYCHOLIC ACID (CAS# 83-44-3); (M+Na)+	87991	90079	87529	89205	85734	83281									94582					4168								18598
DEOXYCORTICOSTERONE ACETATE (CAS# 56-47-3); (M+Na)+							6238	7583	7615	6954								13720	71220	9003	6011	9970					28391	30765
DEOXYCYTIDINE (CAS# 951-77-9); (2M+H)+																4644												
DEOXYCYTIDINE (CAS# 951-77-9); (M+H)+																2639												
DEOXYURIDINE (CAS# 951-78-0); (M+Na)+	2973								1478			25589										1161						
DESMOSTEROL (CAS# 313-04-2); (M+H)+[-H2O]							2782					6517								1756	4745						1826	
DETHIOBIOTIN (CAS# 533-48-2); (M+H)+[-H2O]	10485	10802	9338	10817	12966	8268														7455								
DETHIOBIOTIN (CAS# 533-48-2); (M+Na)+														2415											2042			
DEXTROMETHORPHAN (CAS# 125-69-9); (M+H)+						2293	4958		2232	2329	10840						50675											3049
D-GALACTOSAMINE (CAS# 7535-00-4); (M+H)+[-H2O]									131476		180830	173139	88297	101043	79123		3558				66508		80910					
D-GLUCOSE 6-PHOSPHATE (CAS# 56-73-5); (M+Na)+							1523	1255														1102					1833	
DGMP (CAS# 902-04-5); (M+H)+	63324					54831	4155	2119			18495	6020									2854			2685				10227
DIETHANOLAMINE (CAS# 111-42-2); (M+Na)+																						2699						
DIETHYLSTILBESTROL (CAS# 56-53-1); (M+Na)+																												6156
DIHYDRO-4,4-DIMETHYL-2,3-FURANDIONE (CAS# 13031-04-4); (M+Na)	55911	57259		17066																								
DIPHENHYDRAMINE (CAS# 147-24-0); (M+H)+	9097	7791	9654	7365	7982	9223				8766														48624				
DI-TERT-BUTYL DICARBONATE (CAS# 24424-99-5); (M+Na)+									3077		5149																	
D-LYXOSE (CAS# 1114-34-7); (M+Na)+															92156													
D-MANNOSAMINE (CAS# 14307-02-9); (M+H)+[-H2O]									131476		180830	173139	88297	101043	79123		3558				66508		80910					
D-ORNITHINE (CAS# 348-66-3); (M+H)+	7362	6806	7361	7320	7412	7184	7056		9076		6767					17692		18685	8184			43576	4343		11875	21171		
D-ORNITHINE (CAS# 348-66-3); (M+H)+[-H2O]						2519			3079																			
D-PSICOSE (CAS# 551-68-8); (2M+Na)+[-H2O]	1578	3430				2159					26886		25685				9027											
DUMP (CAS# 964-26-1); (M+H)+	2351	40946	36919			40769	12089	10699	11047	11577		13042			31477					5915	16488		4126		3586		7824	
DUMP (CAS# 964-26-1); (M+K)+							15457	15205		8170	3910			7242	3086	10737	18246					6903	9271	17231				
DUMP (CAS# 964-26-1); (M+Na)+												1144																
EDTA (CAS# 60-00-4); (M+H)+	4.72E+07	4.74E+07	8.60E+07	9.06E+07	8.84E+07	9.46E+07																						
EDTA (CAS# 60-00-4); (M+Na)+	3507625	3390991	3178967	3286224	3241117	3110888																						
ELAIDIC ACID (CAS# 112-79-8); (M+H)+	19140	21193	21733				9936	10221				6403			2967		5520				11159		9207				7891	13213
ELAIDIC ACID (CAS# 112-79-8); (M+Na)+	26136	65968	27434		7640	10795	6305	46845				22865		52365	60278		31293	1402			14433		17145	60012	10873	107804	33313	33419
EPIANDROSTERONE (CAS# 481-29-8); (M+H)+[-H2O]												1032									1715							
EPINEPHRINE (CAS# 51-43-4); (M+H)+			7733														4058		5571				3937					
EPINEPHRINE (CAS# 51-43-4); (M+H)+[-H2O]	8174	6942	1926		4942	6574		3033		4298	92076	2534	1721		3557		7230				5707		1919					
ERYTHRITOL (CAS# 149-32-6); (M+Na)+									9646	8440	2822	2053								1386			18171				6395	
ESTRONE (CAS# 53-16-7); (M+H)+		3646				2961																						
ETHANOLAMINE PHOSPHATE (CAS# 1071-23-4); (M+H)+											128649	18014			132910							2224			3978		13603	
ETHYLMALONIC ACID (CAS# 601-75-2); (M+Na)+							83096		87016	80264		75176				29391	123089	65014	111611	335338	65033		87941	107977		166023		73458
FERULATE (CAS# 1135-24-6); (M+H)+	13015	14654	13329	11310	14549	6944	18038	13217	31815	38703	27902		19340	33523	39993	39585	14991	23038	21968	10888	15206	33792	17557	26485	10416	40201	14839	34755
FERULATE (CAS# 1135-24-6); (M+Na)+				2967		1111																						
FRUCTOSE (CAS# 57-48-7); (M+Na)+	364289	365594	293246	328859	322836	348341	34641	44043	34758	41463		18459	59063		59055	70703	19122	21588	24180		157899	36929	63782		45264	17518	52334	
GALACTITOL OR DULCITOL (CAS# 608-66-2); (M+Na)+																				1501			2787					2641
GALACTURONIC ACID (CAS# 91510-62-2); (M+Na)+[-H2O]	11193	5016	6060	11742	4660	5192																						
GAMMA-BUTYROLACTONE (CAS# 96-48-0); (M+H)+																					2297							
GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M+H)+											1367										8245							
GAMMA-L-GLUTAMYL-L-CYSTEINE (CAS# 686-58-8); (M+H)+[-H2O]													2403															
GAMMA-LINOLENIC ACID (CAS# 506-26-3); (M+Na)+	33493	13055	21126	320054	8051	304055	52328	66846	18461	21911	9203	27179		6400	8776	2050	37810	38923	49033	45352	16639		10054	26527	61560	14313	47323	34567
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (2M+Na)+																									1468	4686	1598	
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Na)+	90950	97084	96328	101406			203812	206980	202473	199993	163496	180231	127193	201369	181933	156634	153290	186308	238951	154032	188935	204709	234061	207982	278997	279887	229280	219841
GLUCOSE (CAS# 50-99-7); (2M+Na)+	3249	3210	2581	3198	3099	2446																					2314	
GLUCOSE (CAS# 50-99-7); (2M+Na)+[-H2O]	4173	3430		2418	2679	3429					26886		25685				9027											
GLUCOSE (CAS# 50-99-7); (M+Na)+	364289	365594	293246	328859	322836	348341	34641	44043	34758	41463		18459	60080		59055	70703	19122	21588	24180		157899	36929	46675		12731	17518	52334	
GLUTAMATE (CAS# 56-86-0); (M+H)+		2225									34726	103688		35222	37809		17516		8648		95301	7464	29363	3944		10356		
GLUTAMATE (CAS# 56-86-0); (M+H)+[-H2O]	30543				12053		12471	5491			39401		41862	50108	42369	38904	3212					15439			8543		19924	
GLUTAMINE (CAS# 56-85-9); (M+Na)+																											20942	
GLUTARATE (CAS# 110-94-1); (M+Na)+										2559																		
GLUTATHIONE (CAS# 27025-41-8); (M+H)+							4552	5647	5167	4832	10451	1357		1298	14510	7019	5759	9461	34642		2410					8951	1365	2994
GLUTATHIONE (CAS# 27025-41-8); (M+H2)+2							35444	39404	35453	32981	89300	18985	1300	20102	130177	59203	36298				14628	7422	10626			45849	13081	
GLYCERALDEHYDE (CAS# 367-47-5); (2M+H)+[-H2O]	20905				16710																							
GLYCINE (CAS# 56-40-6); (M+H)+														2330														
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+H)+		9508			10024	10370																						
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+H)+[-H2O]	22737	42232	21650	45361	20329	22763																						
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+Na)+	236884	235808	231525	239019	226671	223291	7619	4925										8006	51459	16253	4888		20335	4994		9336	4169	9511
GLYCOCHOLATE (CAS# 475-31-0); (M+H)+	3150		2869																									
GLYCOCHOLATE (CAS# 475-31-0); (M+H)+[-H2O]				5543																								
GLYCOCHOLATE (CAS# 475-31-0); (M+Na)+	64441	69062	61372	63161	67218	56994						26225				28661					31020					35450		
GLYCOLITHOCHOLATE (CAS# 474-74-8); (M+Na)+	7414	6675		8016		8514																						
GUAIFENESIN (CAS# 93-14-1); (M+Na)+		25827			28759																							
GUANIDINOACETATE (CAS# 352-97-6); (M+H)+														1193														
GUANINE (CAS# 73-40-5); (2M+H)+																					4008		2802					
GUANINE (CAS# 73-40-5); (2M+Na)+									59494	49041	55894		9345				33560				166996					68338		2321
GUANINE (CAS# 73-40-5); (M+H)+												167741	58769	104924	216283	179955					833573	390520	36126		170102			
GUANINE (CAS# 73-40-5); (M+Na)+											13453										231930				30178			
GUANOSINE (CAS# 118-00-3); (M+H)+							825938	768938	690588	769363	344389	414545	160825	643101	729035	430089	1436946	1171804	1376791	760932	1047965	582558	1169406	1088933	191027	11850	1205541	979707
GUANOSINE (CAS# 118-00-3); (M+Na)+																86637									71638			
GUANOSINE 5'-PHOSPHATE (CAS# 85-32-5); (M+H)+	2768	3718	2391	3142	2794	2562					3381				5701													
GULONO-1,4-LACTONE (CAS# 1128-23-0); (M+H)+[-H2O]																												3927
HIPPURATE (CAS# 495-69-2); (M+H)+																					25671							
HIPPURATE (CAS# 495-69-2); (M+Na)+	352805	355729	347658	357901	354396	339281		19791	18245		31029	1886	5584				54233				72259			63510				
HISTAMINE (CAS# 51-45-6); (M+H)+							173696	178986	175533	172065	203564	71042	82253	110153	225768	80776	177242	203241	198858	219946	195199	123271		186820	26823	211754	148497	204505
HISTAMINE (CAS# 51-45-6); (M+Na)+						1012	13699	14967	15306	13841	15477			6330	12823	1087	15114	20326	17856	28074	23544		10746	13844		16384	9897	23154
HOMOCYSTINE (CAS# 462-10-2); (M+Na)+	1185																											
HOMOGENTISATE (CAS# 451-13-8); (M+H)+								1009	3690														4635			4354		16429
HOMOSERINE (CAS# 672-15-1); (M+H)+	11293	5438									10098	11561	11669	11157	8955						7449		4483					
HOMOSERINE (CAS# 672-15-1); (M+Na)+		5106		5276					2048		6312		1405	3051	6212	5078			2964				2856					
HOMOVANILLATE (CAS# 306-08-1); (M+H)+																											2469	
HYPOXANTHINE (CAS# 68-94-0); (M+H)+	1244959	1220877	1128955	1212671	1127630	1141635	8854164	9171860		8934224	7349395	1.02E+07	1762325	2224170	8162871	6139419	9008973				1.74E+07	3872628	1.18E+07		653867		6828042	
HYPOXANTHINE (CAS# 68-94-0); (M+Na)+							1329921				707248	1066720	521435	289866	881317	878338	1492600				2412624	527835	1745220	1643341			957396	
IBUPROFEN (CAS# 15687-27-1); (M+Na)+	307615	311611	306872	323344	310956	306782																					11170	10897
IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M+H)+[-H2O]	25796	21476	22349	24357	23446	23385																						
IBUPROFEN CARBOXYLIC ACID (CAS# 15935-54-3); (M+Na)+	176757	167348	158026	166183	168395	160357																						
IMIDAZOLE-4-ACETATE (CAS# 645-65-8); (M+H)+							4119																				7752	
INDOLE (CAS# 120-72-9); (2M+Na)+												2078																
INDOLE-3-ACETATE (CAS# 87-51-4); (M+H)+	53706	50433	52142	22675	40884	26207														3274	2669							
INDOLE-3-ACETATE (CAS# 87-51-4); (M+Na)+	119616	115909	111906	61700	85313	48878																	6981					

INDOLE-3-PYRUVIC ACID (CAS# 392-12-1); (M+Na)+																		4438	11308									
INOSINE (CAS# 58-63-9); (M+H)+	27950	27060	28169	29554	28989	27288	996287	945400	842061	895199	613452		222437	797531	746901		2193363	1512788		1357570	1036567	490079	1297500	1151057	83521			1193926
INOSINE (CAS# 58-63-9); (M+Na)+	16309	14467		16440	6363	16446	638872	536549	536448	601844	396881	751456	699655	1090714	807682	671506	1086695	640077	586011	638031	513542	717550	1098194	832794	292386	618204	949727	524263
INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+H)+	24543	24919	23786	22844	22515	21582					20429				13018													2236
INOSINE 5'-PHOSPHATE (CAS# 131-99-7); (M+Na)+					1499																							
ISOLEUCINE (CAS# 73-32-5); (M+H)+	2.32E+07	2.32E+07	2.18E+07	2.39E+07	2.29E+07	2.27E+07	1.09E+07	243281	224943	6086566	1.03E+07	1.63E+07	3460135	2437350	3787775	1.40E+07	7042923	513847	666204	1202318	458281	3595926	6790930	1.31E+07	322695	9480202	4170325	478344
ISOLEUCINE (CAS# 73-32-5); (M+Na)+	246008	235474	228942	244412	228363	220172	128720	220926	112970	73871		220177	41060	123417	162345	192298	114671	183174			78359	90964	90229	162555		116243	172453	136859
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+H)+	277643	280047	269629	275885	300282	293574	554443	579517	561343	554485	436652		368581	538334	463426	405992	441738	505877	663722	438421	516562	589960	610402	575184	681892	773375	645313	617779
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+Na)+	1106242	1071034	1037023	1074322	1076252	1024860	2031404	2092096	2061244	2006634	1615004	1816197	1336185	2027385	1785077	1566501	1567463	1830902	2366856	1537659	1858374	2217223	2372229	2112117	2694445	2811722	2422420	2208573
KYNURENINE (CAS# 343-65-7); (M+H)+	416731	401875	377539	394911	386425	368507	49433	50077		47452	28869	47622	3094		68358	31419	61106	101529	142733	62813	137739		60778	55689	3239	102999		115679
KYNURENINE (CAS# 343-65-7); (M+Na)+	12250	16310				9155																						
L-[15N]ANTHRANILIC ACID [ISTD] (CAS#); (M+H)+								146107		148036												1404650					1540429	
L-2,3-DIAMINOPROPANOATE (CAS# 4033-39-0); (M+Na)+																							7911		4528			
LACTOSE (CAS# 63-42-3); (M+K)+											6602	3906	2366												1569			
LACTOSE (CAS# 63-42-3); (M+Na)+	4173	3430	3160	2418	2679	2881					26886	21085	25685		48881	23486	9027				13605				25104			
L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)+	11293	5438									10098	11561	11669	11157	8955						7449		4483					
L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)+[-H2O]	8277			58322							2690			2815									1948					
LANOSTEROL (CAS# 79-63-0); (M+Na)+	4780																											
LANTHIONINE (CAS# 3183-08-2); (M+H)+										1824	1805																	
L-ARGININE (CAS# 74-79-3); (M+H)+			1141																40444									
L-ARGININE (CAS# 74-79-3); (M+Na)+	3868	3773	2502	2740	3130	2812	9313	9947		8917			10048					5325	9688				5636		18470	8981		7756
L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (CAS#); (M+H)+							18945	14922	17757	13278	42464	23612	109754	66919	37115	30405			7989			56977			257777		25831	4585
LAUROYLCARNITINE (CAS# 25518-54-1); (M+H)+	73003	76921	71820	10882	9825	52672	7152	7559	6378	6706	7928	10347	1356	2301	8474	1321	11195	7236	14147	6779	17983		10590	8394			3908	26944
LAUROYLCARNITINE (CAS# 25518-54-1); (M+Na)+	44936	43866	43523	40820	36788	33326	3731								4174													14419
L-CARNITINE (CAS# 541-15-1); (M+H)+	1434796	1812687	1633230	1156414	1137705	1784909		6200	328865	330664	250141	168126	156691	201854	358799	134070	25834			588745	795592		135381	364226			178223	
LEUCINE (CAS# 328-39-2); (M+H)+	2.32E+07	2.32E+07	2.18E+07	2.39E+07	2.29E+07	2.27E+07	1.09E+07	285266	224943	6086566	1.03E+07	1.63E+07	3460135	5699008	8875961	1.40E+07	1.17E+07	513847	666204	1202318	458281	5831470	1.26E+07	1.31E+07	322695	1.50E+07	4170325	571147
LEUCINE (CAS# 328-39-2); (M+Na)+	246008	240622	228942	235390	221391	220172	128720	220926	112970	136631		220177	41060	123417	162345	192298	114671	183174			78359	90964	182939	162555		217036	172453	181463
LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+				10391			31058	1048	29200	45160			29110		21731		59059	14619	64605	2888	7406		7421	11803		20071	33764	4211
LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+[-H2O]			3262					9417			55616	21272								38677			9271		52730			
LEUKOTRIENE B4 (CAS# 71160-24-2); (M+Na)+																		15477	13153	22394	16819							
L-HISTIDINE (CAS# 71-00-1); (M+H)+	6617			15985	5895		36267	40082	38403	40366	23219	111091	4435	19534	6333	137779	29195	25708	21311	7161	3985	55787	22474	68525	34297	47753	16268	16355
L-HISTIDINE (CAS# 71-00-1); (M+Na)+		4283		2455			17391	17700	16807	15284		31956	2061	7578	11131	50227	12069	12196	16288	10076		25321	9784	32093		20443	12554	11609
LITHOCHOLIC ACID (CAS# 434-13-9); (M+Na)+				10261	25528					6559									5122									
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+H)+	3352	6270	15254																									
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+H)+[-H2O]			7295	3121	2954	6650		60984	68605	58422	20760	90917	5415	19229	26709	85067	8243			63766	22676		16740	69622			5215	
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+Na)+									1219																	1060		
L-METHIONINE SULFOXIMINE (CAS# 15985-39-4); (M+H)+																										1497		
LOPERAMIDE (CAS# 34552-83-5); (M+H)+																				6552			11978					4655
L-ORNITHINE (CAS# 70-26-8); (M+H)+	7362	6806	7361	7320	7412	7184	9650		9076		6767					16278		18685	8184			43576	4343		11875	21171		
L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M+H)+	711127	703632	677867	711245	682019	670630	1225134	1238710	1199773	1210194	1243376	830687	632182	1349502	1332420	1041621	821195	1147066	1350970	1022176	1269905	1501716	1351573	1258132	1250259	1658858	1309126	1361503
LUMICHROME (CAS# 1086-80-2); (M+Na)+				1003																			2619					
LYSINE (CAS# 56-87-1); (M+H)+	11463	15756	14873	15224		15283	77216	75313	79115	81533	176337	75861	54710	121185	170468	222635	68215		84184		62221	136262	30961	65206	99213	103971	112994	98284
LYSINE (CAS# 56-87-1); (M+Na)+	4065	3783	4392	3841	4111	3754	15138	15566	15245	15296	28736						13394	20327	16744	8895	7221	23188		13359		20444		18614
MALATE (CAS# 636-61-3); (M+Na)+	1685																											
MALEAMATE (CAS# 557-24-4); (M+H)+											1638	2051				2285												
MALTOSE (CAS# 69-79-4); (M+Na)+	4173	3430	3160	1975	2679	3429					26886	21085	25685		48881	23486	9027				13605				25104			
MANDELIC ACID (CAS# 611-71-2); (M+Na)+																	3734		5984									
MANNITOL (CAS# 69-65-8); (M+Na)+																	1105			1501			2787					3494
MANNOSE-6-PHOSPHATE (CAS# 3672-15-9); (M+Na)+							1523	1255														1102					1833	
MELANIN (CAS# 8049-97-6); (M+H)+									63870							36897	58536	79260		63329	4104	10569	87377	118506			52492	97439
MELATONIN (CAS# 73-31-4); (M+Na)+																		1006										
MELIBIOSE (CAS# 585-99-9); (M+K)+											6602	3919	2366												1569			
MELIBIOSE (CAS# 585-99-9); (M+Na)+	2679	2165	2115	2418	1836	3429					26886	21121	25685		48881	23486	9027				13605				25104			
MENAQUINONE (CAS# 11032-49-8); (M+Na)+																	1236											
METHIONINE (CAS# 63-68-3); (M+H)+	1275667	1262042	1188487	1282374	1226182	1211138	2124896				2580750	2040613	364525	1222032	2406087	2135149			7900		3544422	1081566	1882967		102585		1718170	
METHYL BETA-D-GALACTOSIDE (CAS# 1824-94-8); (M+Na)+											1318																	
METHYL INDOLE-3-ACETATE (CAS# 1912-33-0); (M+H)+																			2612				1641					
METHYL INDOLE-3-ACETATE (CAS# 1912-33-0); (M+Na)+	20821	21248	24482	25196	27032	26253	10137		10087	8830								14851	30722	19647	8379		25934	27067		16299		
METHYL JASMONATE (CAS# 1211-29-6); (M+Na)+	250752	247323	244907	246677	242594	293506	276272	290430	285429	280616	268937	265427	270439	279347	127833	262909		113454	118014	289673	113805	302443	270734	112160	138565	121515	293621	119602
METHYLGUANIDINE (CAS# 471-29-4); (M+H)+								11386	12160	9914									19870	8972						17765	17379	16914
METHYLMALONATE (CAS# 516-05-2); (M+Na)+	27912	31872	32084	31816	30767	31175	15333	13314	13159	12587			14360	10679		6109	6994	9875							23644	9761		19667
MEVALONIC ACID (CAS# 674-26-0); (M+Na)+															27636													
MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M+H)+[-H2O]										1203					1443				3171		1389					3149		
MONO-METHYL GLUTARATE (CAS# 1501-27-5); (M+Na)+		33046			24832		36637		37173	38287	19410				35562	20366			50137	21705	31340	5754				70349		
MYO-INOSITOL (CAS# 87-89-8); (M+Na)+	364289	365594	293246	328859	322836	348341	34641	44043	34758	41463		18459	60080		59055	70703	19117	21588	24180		157899	53302	63782		45276	26694	52334	
N(PAI)-METHYL-L-HISTIDINE (CAS# 332-80-9); (M+H)+		3147	4848		2912	3919			1510	2054		8191	2254	4147	4026	8174						6565			4790	1334	4657	
N,N-DIMETHYLGLYCINE (CAS# 1118-68-9); (M+H)+	2917	3837	4094	6133	6010	7471																						
N1-ACETYLSPERMINE (CAS# 77928-70-2); (M+H)+							1427	1283	1645	1853		4371					1056					1400	1969	1937		1255		2348
N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+H)+	3361	2441		3005	2461	2806								16956	10561									3518				3084
N6,N6,N6-TRIMETHYL-L-LYSINE (CAS#); (M+Na)+	2125	2468	1928	1850	2185	2099										2160												
N-ACETYL-DL-GLUTAMIC ACID (CAS# 5817-08-3); (M+H)+[-H2O]							1126						2679														1909	
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+H)+							9130	9071	10599	10007	10822	16179		4942	8531	9320	8169	14180	23898	7063	25925		11288	14775		14459		25401
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+H)+[-H2O]							2523			3793	1171	4685			3617													
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+Na)+	6623	8021	8827	9315	10250	8228	37908	38611	38442	38607	38323	57546		20997	34672	35333	30047	59079	97049	30485	98767	10253	46149	56623		61367	22493	94981
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+											34726	103688		35222	18613		17516		6280		95301	7464	29363	3944		12346		9698
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+[-H2O]	12453	482502	397822	464450	12053	374586	12471	5491	6661965	6721671	76325		9550	50108	42369	38904	3212				3277663	15439		1.19E+07	4707		19924	
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+Na)+	7276	6449	5168	5162	7037			15628		20299	22144			12136	32320	14388	11144			47374	35460		4699					
N-ACETYLGLYCINE (CAS# 543-24-8); (M+Na)+																									16787			
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+								37437	38265														56991			55383	32024	
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+H)+[-H2O]																	1857											
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+Na)+	26660	19398	20983	26562	24377	28082		34281	25283	29151	31547	47201	12911	39139	47038	19150	27854	25308	27231		55998		30113	23622	4272			21806
N-ACETYL-L-LEUCINE (CAS# 1188-21-2); (M+Na)+			6089							9985									170672			4711	6200	23142				
N-ACETYL-L-PHENYLALANINE (CAS# 2018-61-3); (M+Na)+	3641	1132	1466																3267	1687	1136							
N-ACETYLNEURAMINATE (CAS# 131-48-6); (M+H)+								1614													1534							
N-ACETYLNEURAMINATE (CAS# 131-48-6); (M+Na)+																					3858							
N-ACETYLSEROTONIN (CAS# 1210-83-9); (M+Na)+																		4491										
NAD (CAS# 53-84-9); (M+2H)+2							4630	6942	4846		17046			4268	38764						7875						1730	2264
NAD (CAS# 53-84-9); (M+H)+			1957				8363	12480	10289	8828	25867	12237		5659	56745	12824	3325	12465	27626	1376	17039		2014	3090		9184	3517	11372
N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3); (M+H)+				1985			39325		59561	68049	136717	100280		52712	71012	61477	77132	39667		35532	78435			108993		91922		109325
NAPROXEN (CAS# 22204-53-1); (M+H)+	110941	114025	107868	113240	111297	106222									1540						24909							51704
NAPROXEN (CAS# 22204-53-1); (M+Na)+	720432	713764	711493	714390	693153	669588															161253							332961
N-BOC-D-GLUCOSAMINE (CAS# 75251-80-8); (M+Na)+															1458													
N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8); (M+H)+			1824				1234		2453			1975							2896			2738						
N-CYCLOHEXYLFORMAMIDE (CAS# 766-93-8); (M+Na)+	10464	8161	8588						14537	14586	15384		9474	9672	18932			13239	14606	13698	17699				18209	14532	20014	16688
N-ETHYLMALEIMIDE (CAS# 128-53-0); (M+H)+	5630	7686	7293	1849	3740	6741																						
NICOTINAMIDE (CAS# 98-92-0); (M+H)+	120009	114097	105979	118009	109043	106190	1153554	1195240	1125611	1145077	970252	906776	256746	229340	1617502	477448	1330384			2187693	2458456	348180	1430661	1206666	106062			5709
NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE (CAS# 22052-73-9); (M+H)+				1342																								
NICOTINAMIDE MONONUCLEOTIDE (CAS# 1094-61-7); (M+H)+								1297			9075				4323							2404						
NICOTINAMIDE MONONUCLEOTIDE (CAS# 1094-61-7); (M+Na)+																											1176	
NICOTINATE (CAS# 59-67-6); (M+H)+	1665	2874													23506												1595	
NICOTINE (CAS# 54-11-5); (M+H)+							42659	42635	40407	40312	60862	140441				4841	201345	89541				5487					22637	
N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M+H)+		2225									34726	103688		35222	37809		17516		8648		95301	7464	29363	3944		10279		
N-METHYL-D-ASPARTIC ACID (CAS# 6384-92-5); (M+Na)+	7276	6449	5168	5162	7037			15628			22144	34414		12136		13075	6589				10162		4699					
N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M+H)+[-H2O]	7444	4760	5393		5289		6163	7418	4140	5741		6220					7756	6672	11390					9779		15536		
N-METHYL-L-GLUTAMATE (CAS# 6753-62-4); (M+Na)+						5144															2868							
N-METHYLNICOTINATE (CAS# 535-83-1); (M+H)+	61377	65065	63949	40850	39531	61043																						
N-OLEOYLGLYCINE (CAS# 2601-90-3); (M+Na)+				1503		1656																						
NORADRENALINE (CAS# 51-41-2); (M+H)+[-H2O]																	10935						40955					
NORLEUCINE (CAS# 327-57-1); (M+H)+	2.32E+07	2.32E+07	2.18E+07	2.39E+07	2.29E+07	2.27E+07	1372646	285266	224943	265893	1.03E+07	1.63E+07	3460135	5699008	8875961	1.40E+07	1.17E+07	513847	666204	308434	458281	5831470	1.26E+07	4425415	322695	1.50E+07	8238597	571147
NORMETANEPHRINE (CAS# 0); (M+H)+															7865													
NORMETANEPHRINE (CAS# 0); (M+H)+[-H2O]	1.56E+07	1.54E+07	1.45E+07	1.56E+07	1.49E+07	1.48E+07	9126915	9281787	9064085	9114624	7775118	7308179	1009688	3433790	6850878	7463582	9234501	1.83E+07	1.83E+07	1.05E+07	1.57E+07	4628126	9988971	1.23E+07	316889	1.55E+07	5764731	1.80E+07
NORVALINE (CAS# 6600-40-4); (M+H)+	2119751	2236309	1877293	2794091	2966336	2127501					3275075	4462186	814470	2115370	2972091						5168405				339053			
NORVALINE (CAS# 6600-40-4); M+[-CO2H]	1406165	1367899	1743520	1913848	1808945	1848763					1842952		450539	1211153	1735457								70928		203069			
O-ACETYLCARNITINE (CAS# 461-77-8); (M+H)+	852479	757343	650892	378778	246803	163668	892893				751687	335193	139068	246781	556000	233145					2351848	192505	1226925		51432		217554	
OCTACOSANOIC ACID (CAS# 506-48-9); (M+H)+											15107					15887			21911			14184				14739		
OLEAMIDE (CAS# 301-02-0); (M+H)+				9154				4729		1967			2424	4598				3465	5078	4462			3948	6400		20141		
OLEAMIDE (CAS# 301-02-0); (M+Na)+												198815	88797													713935	317943	
OLEIC ACID (CAS# 112-80-1); (M+H)+								5957	4338		2662		2947	6706							10072		4423			3002		
OLEIC ACID (CAS# 112-80-1); (M+Na)+	206314	252403	202446	276236	291242	282674	679557	948694	1196742	784101	615024	46940	1231402	381841	545583	550972	815006	485601	223895	372253	412631		275412	228673	838358	417846	412378	546630
OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M+H)+[-H2O]																							1021					
OMEGA-HYDROXYDODECANOIC ACID (CAS# 505-95-3); (M+Na)+																			36861				32450	24951				
OMEPRAZOLE (CAS# 73590-58-6); (M+H)+		5666	3742	5370	5284	4860																						
OMEPRAZOLE SULFONE (CAS# 88546-55-8); (M+H)+	23047	22045	21756	20484	19646	20418																						
O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (2M+H)+	2127	3716		1810		1701					5144						1282				1580							
O-PHOSPHO-DL-SERINE (CAS# 17885-08-4); (M+Na)+														4162					4383		1702							
O-PHOSPHOSERINE (CAS# 407-41-0); (M+Na)+																			4383		1702							
OPHTHALMIC ACID (CAS# 495-27-2); (M+H)+					5116		29348	27611	23072	26585	41527	3398		11829	48452	40421	29610	18051		8305	31240	7014	12660	20568	3569	48425	3937	
O-SUCCINYL-L-HOMOSERINE (CAS# 1492-23-5); (M+H)+									9002									37139	43042	3817						19821		45912
OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M+2H)+2							35444	39404	35453	32981	89300	18985	1300	20102	130177	59203	36298				14628	7422	10626			45849	13081	
OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M+H)+							4552	5647	5167	4832	10451	1357		1298	14510	7019	5759	9461	34642		2410					8951	1365	2994
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (2M+H)+																								16012				
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (M	26684	25156	24555	25567	24020	24333	4113	5505		4266							2877							70628				
P-ACETAMIDOPHENYL BETA-D-GLUCURONIDE (CAS# 120595-80-4); (M	180317	180243	166244	172799	173175	173500	29439	29388	30173	29506	21645	3328	1486				15410						10622	353209				
PALATINOSE (CAS# 343336-76-5); (M+Na)+	4173	3430	3160	2418	2679	3429					26886	21121	25685		48881	23486	9027				13605				25104			
PALMITOYLCARNITINE (CAS# 2364-67-2); (M+H)+	96455	97790	96724	90389	82875	76670	29694	30097	26876	30275	47357	40707	10515		24865	19450	40514	28601	63813	66911	151957	20729	29091	35712		31063	18785	145354
PALMITOYLCARNITINE (CAS# 2364-67-2); (M+Na)+	70376	73885	72915	70073	64379	61176	15583	19973	16600	20120	27745	29315	5909	10969		10988	30253	19536	39962	52523	110619	14763	25726	29912			14361	94595
PANTOTHENATE (CAS# 79-83-4); (M+H)+	40273	40155	30911	38225	38176	37106	31732	31680	31140	30074				9058				43658	81102	121201	61217	7716	33930	35496		55199		72108
PANTOTHENATE (CAS# 79-83-4); (M+Na)+	56143	56382	42937	56129	53184	54550	33873	32775	33305	32089	15749	18258		8633	24909	12308	22797	46810	93969	137233	63943	6054	33149	36677			12485	78730
PARAXANTHINE (CAS# 611-59-6); (M+H)+	102616	109530	97570	101894	103109	95513	70976	69886	69085	66542		100908			27854		64698	294461		66790	221219		339330	127336				275250
PARAXANTHINE (CAS# 611-59-6); (M+Na)+	95799	108422	100210	106745	101490	93345	18460	18025	18062		2779	19551						55081		7561	40862	7584	91024	19432				39845
PHENYL ACETATE (CAS# 122-79-2); (M+H)+							1094														2694							
PHENYLACETIC ACID (CAS# 103-82-2); (M+H)+							1096														2694							
PHENYLALANINE (CAS# 63-91-2); (M+H)+	1.56E+07	1.54E+07	1.45E+07	1.56E+07	1.49E+07	1.48E+07	9126915	9281787	9064085	9114624	7775118	7308179	1009688	3440474	6850878	7463582	9234501	1.83E+07	1.83E+07	1.05E+07	1.57E+07	4628126	9988971	1.23E+07	316891	1.55E+07	5764731	1.80E+07
PHENYLALANINE (CAS# 63-91-2); (M+Na)+	433942	423952	395615	425132	390805	393284	229404	232734	227991	232022	200452	181539	21121	85388	177838	193944	234449	512830	478416	272929	418224	120306	258520	299698	4762	389868	148744	493157
PHENYLEPHRINE (CAS# 59-42-7); (M+H)+								3394	4039	5485							33843											
PHTHALATE (CAS# 88-99-3); (M+Na)+								9550		7971																	1495	
PICOLINIC ACID (CAS# 98-98-6); (M+H)+	1666	2874													23506								1510				1594	
PINITOL (CAS# 10284-63-6); (M+Na)+											1318																	
PIPECOLATE (CAS# 535-75-1); (M+H)+	274025	320432	327322	342131	341852	332462	29171	28901	28857	28863	61704	26869	23897	72311	140574	75936	23230	30174	30126	14785		47893	12537	82116	3350	33841	37111	34178
PIPECOLATE (CAS# 535-75-1); (M+Na)+																							40955					
PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M+H)+				14274							1381																	
PROCOLLAGEN 5-HYDROXY-L-LYSINE (CAS# 1190-94-9); (M+H)+[-H2O]											1034																	
PROGESTERONE (CAS# 57-83-0); (M+H)+							2427						4882									6326	1064					
PROLINE (CAS# 147-85-3); (M+H)+	905004	1051452	971546	550515	515840	979468	6259	7117	6945	6615	733664	6746	252448	584831	868148	12591	5068	13416		2200	940795	33368	3700	15812	14395	14604	8844	5159

PROLINE (CAS# 147-85-3); (M+Na)+	59649		63949		60120																							
PROMETRYN (CAS# 7287-19-6); (M+H)+				1192						3907		14184			5624		7216	12962	9104	6864				2656		10101	7596	12136
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+												181997			50574	36187		147587		100527			88201	82890			37672	47830
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+H)+[-H2O]			40643															56456										
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Na)+							37189	29486	38556	33065	45643	67169	4572		48984		5282	162502	37438	117127	176930		16304	32870		30175	69041	60043
PROTOPORPHYRIN (CAS# 553-12-8); (M+H)+				1396					1851	4263	1620		2976	1389					4885			3408						
PTERIN (CAS# 2236-60-4); (M+H)+							6254	10089	5089		29239								12466	13190	21591					5556		18290
PURINE (CAS# 120-73-0); (M+H)+										3745	1673	2050		5630		7197			1903									
PURINE (CAS# 120-73-0); (M+Na)+								11522						5353		8374												
PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M+H)+[-H2O]																												1969
PYRIDINE-2,3-DICARBOXYLATE (CAS# 89-00-9); (M+Na)+												12162			2449						133701							
PYRIDOXAL (CAS# 66-72-8); (M+H)+		4605	8249			1467				28260		6503	2689			3613			14779				17624	18308		16538		20640
PYRIDOXAL (CAS# 66-72-8); (M+H)+[-H2O]			9901			5010						3289											2409		101917			
PYRIDOXAL PHOSPHATE (CAS# 853645-22-4); (2M+H)+		7203		8800	8011	9121																						
PYRIDOXINE (CAS# 65-23-6); (M+H)+																				5353								
QUINOLIN-2-OL (CAS# 59-31-4); (M+H)+	1782					2493	9243	12334	5391	11399		20278	1415	9088			11771	13143	27757	7182	13908	10358	24564	16669		15926	10263	12456
QUINOLIN-2-OL (CAS# 59-31-4); (M+Na)+	7365		4645	9036	6589	6381	22333	25523	23522	23051		40357	9548	18748		17563	23345	25720	36842	14301	18652	21410	44828	32732	16861	33475	22247	21201
RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-6); (M+Na)+			6800	8564	12617	23980	69608	92985	88110	78644	63617	77026	81737	63082	261965	79753	68984	52582	74350	60178	47316	73067	72355	72494	78035	81303	86519	91877
RAFFINOSE (CAS# 512-69-6); (M+K)+							5900	5292	6894	6114	1994	4802		6999	4313	6931				4940	6084	2414		7856	1114	13734		5226
RAFFINOSE (CAS# 512-69-6); (M+Na)+							34867	33144	34613	35960	7940	12822	4378	31428	16818	28460	18500			40409	39017	29327		54820	17171			
RIBOFLAVIN (CAS# 83-88-5); (M+H)+							2013	3808	2473	2852									8444	10005	3902	2284				3991		
RIBOFLAVIN (CAS# 83-88-5); (M+Na)+							5916	5043	4523	5489	3797	1372		3476	1212	5407	5090	7836	8416	13789	5815		3864	5753		9496		10356
RIBOSE (CAS# 50-69-1); (M+Na)+		2212										213950	504399		92156													
S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-0); (M+H)+	3393	1726	2408	1093	3422	3530	56903	58917	54922	49330	62717	8740		30712	127469	58135	47435	153803	123277	53197	191842	27295	26549	37349		93881	13953	207574
SALICYLAMIDE (CAS# 65-45-2); (M+H)+							14772																					
SALICYLURIC ACID (CAS# 487-54-7); (M+Na)+	15019	14471		12632	12335	14914																						
SARCOSINE (CAS# 107-97-1); (M+H)+	4135	2965			2809	3927					2091	5297	4473	4135	40558						9844							
SELENOCYSTAMINE (CAS# 2697-61-2); (M+H)+																	10076	5444										
SERINE (CAS# 56-45-1); (M+H)+					5049		10919			10975	8351	15440		5246	8915	10588	6975			9782	13099		10487	14763			5566	
SEROTONIN (CAS# 50-67-9); (M+H)+	125925			124464	138391	134718																						
SEROTONIN (CAS# 50-67-9); (M+Na)+		37449	29660			27442		2280		4190							13212										11047	
SHIKIMATE (CAS# 138-59-0); (M+H)+[-H2O]	2294				2726																							
SN-GLYCERO-3-PHOSPHOCHOLINE (CAS# 28319-77-9); (M+H)+	138605	155703	337801	168178	186402	202559		5310					36562															
SPERMIDINE (CAS# 124-20-9); (M+H)+							270446	311797	300588	316030	64596	1095726	310504	41678	86587	70586	322883	168692	599877	258001	202071	23811	691187	651981	65421	394340	367170	185218
SPERMINE (CAS# 71-44-3); (M+H)+							62012	78750	74501	77190		225991	1834		1149	24566	24959	2708	99569	41394	5519		727918	276954	3500	52891	326471	20448
SPHINGANINE (CAS# 764-22-7); (M+H)+	7482		7773	9316		6964		14833	16415		37052	35159		13591		2110	29259	29921	50909	1912	1925	1883		26419		28339	23498	52550
SPHINGANINE (CAS# 764-22-7); (M+Na)+					16707						79316			28857		43861	62720		102484	44844	56730	18960		60315		61031	48442	118208
SQUALENE (CAS# 111-02-4); (M+K)+								4439		3847						4185						2259						
STACHYOSE (CAS# 54261-98-2); (M+K)+							2463	2141	2146	2462	1034	1850		3417	2466	3423		3611	9128	1454	1015	1501	2949	4234	1341	6862	3557	
STACHYOSE (CAS# 54261-98-2); (M+Na)+		2287					20825	22172	21720	21914	5109	7000	2548	18894	10482	18602	9367	32544	57600	23987	21195	17887	28762	36265	16597	51400	16354	24841
SUBERIC ACID (CAS# 505-48-6); (M+H)+[-H2O]																			3303									
SUBERIC ACID (CAS# 505-48-6); (M+Na)+	19097		13416	16393			52233	53171	49192	53367		22848		15325	43950	36975	32669	61603	82161	44612	61045	12506	41247	35052		60502	21096	75872
SUCROSE (CAS# 57-50-1); (M+Na)+	4173	3430	3160	2418	2679	3429					26886	21121	25685		48881	23486	9027				13605				25104			
SULFADIMETHOXINE (CAS# 122-11-2); (M+Na)+																										19553		
TAURINE (CAS# 107-35-7); (M+H)+								2551			36472	35052	130774	45444	15760												8835	
TAURINE (CAS# 107-35-7); (M+K)+						23818				38647	47233	19602	6567	8619		3361	62702		28848		7663	32497	55764		95815	54710	4569	
TAURINE (CAS# 107-35-7); (M+Na)+				2773			15102	20202	15338		54926	71452	105463	101279	42643		12083		4413	2956	6676	21183	15855	7071		8916	44654	1919
TAUROCHENODEOXYCHOLATE (CAS# 516-35-8); (M+Na)+		3233																										
TAUROLITHOCHOLATE (CAS# 516-90-5); (M+H)+[-H2O]																						1402						
TERBINAFINE (CAS# 91161-71-6); (M+H)+					6673	6393	17385		18431	19291										253881								
THEOBROMINE (CAS# 83-67-0); (M+H)+	583831	571100	546130	556543	543291	542586	55817	53201	52764	45674		23083						101063	243961	102492	118414		111674	30828		25213	7084	454594
THEOBROMINE (CAS# 83-67-0); (M+Na)+				29421	22553		5778	10227		4718		3647						21670	42143	12163		3817	25835			1268		82473
THEOPHYLLINE (CAS# 58-55-9); (M+H)+	102616	109530	97570	99173	103109	95513	67373	66629	65618	64294		97493			24506		60709	293117		65035	216059		336229	125309				272669
THEOPHYLLINE (CAS# 58-55-9); (M+Na)+	106631	108422	100210	106745	101490	93345	18460	18025	18062		2378	16097						55081		7280	34267	7584	91024	19432				39845
THREONINE (CAS# 72-19-5); (M+H)+[-H2O]	8277	62235	59848	58322	54484	65647	11734	37209	15955	12817	16210	17170		5414	13874	14652	31852				20390		2221	18460			13104	
THROMBOXANE B2 (CAS# 54397-85-2); (M+H)+[-H2O]							116870	86386		90070		181997			50574	36187		147587		100527	98416		88201	82890		24887	37672	47830
THYMIDINE (CAS# 50-89-5); (M+Na)+							2801	3178	1920	2369		12785			8103			10382		2842			1241					
THYMIDINE 5'-MONOPHOSPHATE (CAS# 365-07-1); (2M+H)+											1401																	
THYMINE (CAS# 65-71-4); (M+H)+							5834		1320					6908	5977													
THYMINE-D4(METHYL-D3,6-D1) [ISTD] (CAS#); (M+H)+																									1125432			
THYROTROPIN RELEASING HORMONE (CAS# 24305-27-9); (M+Na)+																								1579				
THYROXINE (CAS# 51-48-9); (M+H)+	10245	11445	9950	11453	11913	10269																						
TRANS-4-HYDROXYPROLINE (CAS# 51-35-4); (M+H)+	1391280			2528	2843	1914																						
TRANS-ACONITATE (CAS# 4023-65-8); (M+Na)+				2810																								
TRANS-CYCLOHEXANE-1,2-DIOL (CAS# 1460-57-7); (M+Na)+	1049681	1034726	1001769	1066621	1025498	1008602																						
TRICARBALLYLIC ACID (CAS# 99-14-9); (M+H)+[-H2O]							1329921	1358452	1305647	1317317	706353	1066720	520660	376664	881317	878338	1492600			1761126	2412624	52671	1764829	1643341		1921645	957396	2173028
TRICARBALLYLIC ACID (CAS# 99-14-9); (M+Na)+	11193		10004	11169	8877	9386			1057	1085																		
TRYPTOPHAN (CAS# 73-22-3); (M+H)+	8066392	8033345	7742766	8077650	7818357	7634257							81951	469236				6106451	7054660									6167612
TRYPTOPHAN (CAS# 73-22-3); (M+Na)+	711426	686882	658378	669319	652588	640606							5168	31021			155961	405496	445895									408477
TYROSINE (CAS# 60-18-4); (M+H)+	7527488	7086909	7225615	7555343	7293075	7214956	6684800	6910459	6647833	6673812	4563299	4038709	462310	2338214	4956498	6699394	6683338			7626629	9948751	4365362	7050568	9518401	313923	1.31E+07	4803369	
TYROSINE (CAS# 60-18-4); (M+Na)+		80740	80496			74449					54665	47430	5608	38911	69700		104712		146087		156750	74701	101283	122683		170697		
URACIL (CAS# 66-22-8); (M+H)+											129366	179853	35939	83402	115717						78216	15214						
URACIL 5-CARBOXYLATE (CAS# 23945-44-0); (M+H)+									2079	2398				2002	2694								2308				2752	
URATE (CAS# 69-93-2); (M+H)+	1987267	1931806	1807831	1903847	1824205	1844858					316316			129097	621572		1212				501034	180250						
URATE (CAS# 69-93-2); (M+Na)+																		1076		10727	2833	3636		1102			2827	
URIDINE (CAS# 58-96-8); (M+H)+	4657	18183	12771	16633	11772	15751					159647		37475	98314		8391	302840					71459	272827		14525			
URIDINE (CAS# 58-96-8); (M+Na)+	48747	46797	45214	47937	43902	42490	803109	818891	813097	816646	554969	886539	206705	586486	518528	517378	1372637	1003005		928863	1484932	409662	1201314	947130	96692	1248161	858648	1146474
URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (2M+Na)+	95519	73349	62705	87689	100689	100176																						
URIDINE-5-MONOPHOSPHATE (CAS# 58-97-9); (M+H)+									1647		1371																	
UROCANATE (CAS# 104-98-3); (M+H)+	14329	12195	17686	13729		18218					209472	1169108	13333	338173		2676048					299421	3797823			418975			
UROCANATE (CAS# 104-98-3); (M+Na)+							35435	32836	34050	35340				1817		103115	37546			37682	70349	61774	50125	10525			19110	
URSODIOL (CAS# 128-13-2); (M+Na)+	87991	90079	30557	89205	30932	83281									94582													18598
VALINE (CAS# 72-18-4); (M+H)+	2119751	2236309	1877293	2794091	2966026	2127501					3275075	4462186	824831	2115370	2972091						5168405				339053			
VALINE (CAS# 72-18-4); (M+Na)+	11983	20052	27966	18347	5228					34458	4577	4624	7359	5415	4167	8156		304022	177771	111608		9131	5555	111269	17662		5388	
XANTHINE (CAS# 69-89-6); (M+H)+	164374	159505	155801	155887		149510	524124	553755	535052	537816	1248215	1933926	258374	916589	1205077	721267	193984	241214	592140	317862	381636	92633			17838	303639	335694	403831
XANTHOSINE (CAS# 146-80-5); (M+H)+		4581	9516	6365	9922	4653	30199	30948	30798	30644	120022	52612	14178	32109	45680	40490	7102	8954	17326		37152	2724	15702	20661		13986	31770	21822
XANTHOSINE (CAS# 146-80-5); (M+Na)+	2526					5982	31068	32167	31870	33644	137351	52192	14417	38897	52862	45899	7400	17143	18910		44924		17059	17712		16429	29770	27513
XANTHOSINE 5'-PHOSPHATE (CAS# 523-98-8); (M+H)+																											1823	
XANTHURENIC ACID (CAS# 59-00-7); (M+H)+	7880	5983	8211	7831	5727	6403	24006			23910		20633		7568	4583		5162	27626	82587		64646	24646	66710	43575		38431	21347	38852
XANTHURENIC ACID (CAS# 59-00-7); (M+Na)+									1294	1304											4751	1856	5613	3210		2305		1013
XYLOSE (CAS# 58-86-6); (2M+H)+[-H2O]					5008																							
ZEATIN [ISTD] (CAS# 13114-27-7); (M+H)+	5572818	5496355	5308931	5477671	5323081	5193972	9506954	9606771	9272271	9346710	7841025	8307701	7142254	9437523	8430501	7707158	7527556	8324285	1.02E+07	7392421	7658786	1.05E+07	1.06E+07	9305636	1.27E+07	1.16E+07	1.06E+07	9624313

Compound	Component 1 (23.82%)	Component 2 (12.43%)	Component 3 (8.52%)	Component 4 (6.71%)
C17 H10 N10 O3	-1.8110192	0.7861337	1.9194349	0.58030605
C22 H49 N5 O3 P2 S2	-2.6638293	1.7023263	-0.47409153	0.3951305
PROLINE (CAS# 147-85-3); (M+H)+	1.5461737	1.2296405	-1.606269	-0.32374325
C15 H36 N8 O7	0.030021474	-0.04865852	-0.24292046	0.9486955
C25 H29 N3	0.4297526	0.43352222	-1.3420265	1.2718039
C26 H26 N10 S	0.6824951	-0.8423137	-1.537645	2.801491
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Na)+	-1.4155821	-3.4872868	-1.1676011	0.3857476
C22 H36 N6 O11	-1.9609218	-0.23847057	-1.5264182	-0.07132915
C7 H8 O	-2.4644833	-1.1968178	1.1872263	-1.7965921
C4 H14 N2 P2 S	-0.39388472	-2.6071248	-0.9278337	-0.60992527
C22 H41 N3 O6	0.9510055	1.2147033	-0.35062182	1.1829151
C13 H30 N8 O S2	-1.2823722	-0.84280276	-0.76720685	0.6288872
C26 H48 N3 O11 P	-3.0007622	1.9824305	1.1690322	-0.106442854
C44 H41 N O3 S2	-2.5529857	-0.68545777	0.011455998	0.1466165
C23 H25 N3	0.82194006	0.9446682	-0.48041186	0.9904418
C22 H44 N2 P2	-2.2916527	-0.1927312	1.8713794	1.9100627
C18 H33 O P3	0.51306915	-2.9044178	-0.66216534	1.2006066
C4 H9 N S	-0.08192217	1.7333279	-0.80622786	0.068882585
GUANOSINE (CAS# 118-00-3); (M+H)+	-1.2382023	1.1255282	0.3809381	-0.5463847
C16 H33 N O	-1.6909117	-0.46898982	-2.2381592	0.25658423
C16 H24 O4 S	1.2576525	1.5295047	-1.0450273	1.5487266
C17 H22 Cl N3 O3 P2 S2	-1.5164626	-0.7786907	2.781347	0.21699974
C15 H35 N7 O	-2.0265143	-0.16898553	0.7455468	-0.7502855
C28 H43 N O8 S2	-2.2495723	-1.7589899	2.123714	0.27056715
C23 H41 N7 O2	0.14805102	1.14441	-2.4623098	0.90637463
C28 H57 N4 O3 P S	-3.2666388	1.0389394	1.2862134	1.3088032
C12 H21 N4 O3 P	-2.2541168	-1.7985982	-0.2408275	0.34161794
C15 H22 S2	-2.8952246	-2.221283	1.3586001	-0.80099213
C41 H45 N3 O3 S	-0.4897147	0.89593077	-1.8331461	0.60409623
C30 H64 N O2 P5 S3	-1.1910554	0.7458955	1.8579415	0.063218005
C18 H31 N7	-0.96965015	-0.3082778	1.09371	1.3356507
C24 H33 N3 O2	-3.0455503	0.3333711	1.2400312	-1.9823217
C18 H22 N4 O	-1.0998708	-0.9801987	1.2725432	0.8943161
C29 H64 N12 O3 S2	-3.36718	0.74886703	0.41376477	1.4529076
C12 H17 N5	-0.61754954	1.5389912	-1.823723	0.71186006
C25 H48 N2 O3 S	-1.885852	-0.08919026	1.1418288	0.70024145
C7 H14 N6 O2	0.04723926	-0.7725452	-1.3154808	1.538207
TAURINE (CAS# 107-35-7); (M+Na)+	2.7394686	0.689175	-0.90353596	1.2402995
MYO-INOSITOL (CAS# 87-89-8); (M+Na)+	0.654366	0.2164067	-0.022376895	0.06789872
C38 H35 N6 O5 P	-2.30281	-1.1333663	0.31780237	-2.204831
C24 H50 N2 O2 P2 S	-0.19141752	0.31640458	-2.4619372	-0.23466586
4-HYDROXYBENZALDEHYDE (CAS# 123-08-0); (M+H)+	-1.5554693	-1.5842661	0.31342906	0.4268636
C28 H44 N4 O7 S	-0.84486014	-3.7732503	-0.8158323	0.43745494
C41 H50 N4 O S2	2.1632419	0.26030955	0.45482844	-0.89646804
C12 H18 N2 S3	-2.2167416	-0.8472885	1.1870003	-0.06760684
TRICARBALLYLIC ACID (CAS# 99-14-9); (M+H)+[-H2O]	-2.3224525	0.62762636	-0.18938357	1.311617
C8 H17 N O2	-1.8927789	1.0182205	-0.9106842	1.0758228
C24 H19 N12 O4 P	-1.6184932	-0.14214608	0.020974783	0.06133406
C26 H23 N6 O3 P	-2.7459729	-1.5730429	-0.5418917	-1.1211721
C13 H25 O P S	-1.1311178	0.81015587	-0.6123555	-1.4264674
C25 H38 S	-0.12846988	-1.7339305	2.463483	1.3381757
C19 H43 N3 O5	-3.0220273	0.67651784	1.1120775	0.79487425
GLUCOSE (CAS# 50-99-7); (M+Na)+	-0.001271532	1.547341	0.0521734	-0.012799507
C23 H53 N5 O P2 S2	-3.0138788	1.8746523	0.6142985	0.043679506
N-ALPHA-ACETYL-L-LYSINE (CAS# 1946-82-3); (M+H)+	-0.015916223	-0.02796764	-0.40819594	1.6707612
C17 H19 N O3	-0.9127244	-0.33957005	-0.7385104	-0.42057478
LAUROYLCARNITINE (CAS# 25518-54-1); (M+H)+	-2.7716444	-0.25842315	-0.6343872	0.12542051
C14 H31 N O	0.22648849	-1.2894652	-1.2561339	-0.7130051
C19 H20 N10	-0.41540715	-1.6286497	0.75168777	0.4588017
C22 H24 N8 O P4	-2.1008692	-0.8336065	2.0023148	0.07633144
C14 H20 N2 O2	-3.030766	-0.2538384	1.5594546	-1.0590303
C31 H66 N8 O S3	-2.254258	0.1958552	-1.193163	-0.61126274
C22 H50 N7 P S3	-2.0082614	0.05124879	-0.35185117	1.0198436
THROMBOXANE B2 (CAS# 54397-85-2); (M+H)+[-H2O]	-0.29975468	1.0485346	0.4947127	0.49457735
C29 H46 N2 O2 S2	0.42273664	-1.3132164	0.33037204	1.6874317
C20 H40 N6 O10	-4.0140123	-0.3338561	-0.14895475	-0.22072428
OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M+H)+	-0.5793206	-0.05154653	-0.95783395	-1.8208103
C22 H48 N2 O S3	-0.33079976	-0.17139511	1.5475966	1.0310913
C16 H29 N4 P3	-3.1109798	1.1744331	-0.83983964	-0.24933541
C36 H56 N6 O3 S	-0.7496492	-1.1942801	0.019276388	-1.8386773
C20 H32 N12	-0.61831236	0.48122352	-0.32457703	0.119059086
DEOXYCORTICOSTERONE ACETATE (CAS# 56-47-3); (M+Na)+	-0.54320145	-0.67997056	-0.67900586	0.29179448
C26 H33 O6 P S	-3.130391	-1.7117157	-0.30382884	-1.0376647
SPERMIDINE (CAS# 124-20-9); (M+H)+	-2.592518	0.33635157	0.43699178	2.5060382
C8 H10 O6	0.6781336	-0.026660219	-0.96410215	-0.920998
C38 H62 O S2	-1.3646892	0.022837713	0.73524064	0.048461035
C16 H31 N7 O	-0.34119427	0.18319727	1.6903077	0.2131108
C16 H31 N2 O4 P3	-3.8821588	-0.6767182	0.43313837	-0.2442143
C42 H44 N O4 P3	-2.5773184	0.30687386	-0.32623687	-0.23521051
C40 H59 Cl N5 O3 P	-0.37003624	2.3017497	-1.1966269	0.6571088
C18 H26 N6 O	-1.5491207	-0.21390632	-0.81100196	0.95189714
C16 H32 O2 P2	-1.5708963	-0.6448884	-0.45727867	2.479775
C14 H9 N4 O P S2	-3.244692	1.5651591	0.4714679	0.41928625
C20 H37 N4 O3 P	-0.96882164	-0.49063703	0.16157795	1.8097152
C8 H4 N4 O3 S	-1.606489	1.0161108	1.4541523	-1.881242
C22 H39 N4 O4 P3	-1.8356285	-0.8602085	-0.44783336	-0.4848067
C28 H19 N8 P3	-2.7385006	-2.6528292	0.65479803	-0.76081717
C7 H14 N2 O	-3.0826845	0.3552745	0.37687132	-1.3347032
C38 H57 N O3 P2	-0.6651954	-3.127215	-1.4126284	0.3911884
C6 H12 N4 O4	-2.4300582	-0.6518424	-0.04960506	0.7893544
C13 H23 N4 O3 P	3.0713246	-0.43308932	1.4376446	-0.3967173
C26 H31 N2 O3 P	-3.0293875	-0.055663645	-1.9037333	0.14251241
C33 H50 N O10 P S2	-1.44333	0.7498543	1.6593784	-0.7201575
XANTHINE (CAS# 69-89-6); (M+H)+	-0.74701273	2.9741054	-1.3644147	0.7518645
C25 H47 N O4	-1.8143421	3.492704	-0.8614134	0.19416009
C24 H46 N3 O11 P	-1.6870466	3.3043547	-0.546248	0.12997808
THREONINE (CAS# 72-19-5); (M+H)+[-H2O]	0.1892515	0.87379897	0.38805324	-0.7359475
C35 H62 N7 O4 P S2	-1.0092036	0.14086005	2.800027	0.35012192
C12 H10 N6 O2	-3.888624	0.59151286	0.8838733	-0.9932523
ETHYLMALONIC ACID (CAS# 601-75-2); (M+Na)+	-0.78258574	-0.49367204	0.21291262	-0.13000944
C32 H45 P3	-2.3083754	-1.5429554	-0.25483906	-1.3590018
C16 H26 N2 S3	-1.5683964	-1.0607796	-0.45312935	1.1837602
C15 H30 N6 O2	0.014421865	-2.9275486	-0.83081675	1.5219032
C27 H50 N O2 P S2	-0.8677006	1.6469728	-1.7129443	0.7054461
C3 H12 N4 O4	0.16100293	0.02755645	-0.17708081	-2.6694257
C14 H33 N4 P3	-2.516133	-0.49042457	-1.5677638	-1.037795
C17 H40 N8 O8	-1.2981651	-1.1543643	1.0587137	1.263429
C43 H85 P	0.18858445	1.8356044	-0.005602211	-0.56479
C24 H30 O6	-2.7043667	-1.7350681	-0.5390655	-1.2536925
C18 H24 O8 P2	-1.3930186	-3.3822794	-1.2232151	0.4827523
C28 H41 N5 S	-2.2007232	1.2359959	0.93230975	0.043127865
C27 H54 N2 S3	-2.1286583	1.6021094	0.45655394	-0.37128454
C29 H47 O3 P S3	-1.8777238	-1.9204859	1.5567329	0.3370874
C37 H51 O3 P S2	-1.253616	-3.7160714	-0.6393652	0.25012988
C7 H3 N O6 S	-2.6941957	-0.5108939	1.0252237	-0.007244095
C33 H44 N O6 P	0.22941677	1.0258303	-2.1793153	0.24175638
C22 H42 N2 O3 S	-0.043815292	-3.4121687	0.77167416	1.5548468
C10 H11 N5	-0.960321	-3.853217	-0.5808439	0.42435938
C15 H35 N2 O6 P S2	-1.7231547	-0.34270155	1.0050409	-0.015969729
C16 H35 N O	-2.4720356	0.31064928	0.60955375	-0.25165737
C18 H40 N5 P	-1.1715808	0.9735458	-0.70693105	1.8354924
C16 H25 P3	-1.3719358	-0.42861283	-0.06024237	-1.469666
C20 H37 N7	-3.1941073	-0.37520754	1.2295494	1.663382
ELAIDIC ACID (CAS# 112-79-8); (M+Na)+	0.09923578	-0.003800951	-0.6592643	0.9269416
C26 H35 O4 P3	0.8187348	0.102336615	1.1958869	0.07019805
C30 H63 N8 O P S2	-2.7484014	-0.7432753	0.6372396	1.012951
C22 H24 N6 O4	-2.8268127	-0.8996017	-1.791262	0.18380857
C36 H74 N4	-0.050408833	-0.6222052	-0.7763956	-1.8530756



C3 H9 N3 O2	-0.6129747	-0.8282217	-1.0129027	0.11748785
RIBOFLAVIN (CAS# 83-88-5); (M+Na)+	-1.4348856	-1.0805701	2.237447	-1.514881
C18 H39 N O	-2.2043471	-0.1264525	0.5492704	-0.8182727
C15 H28 N6 O	-0.035653055	0.5333473	-1.2336273	-0.92974555
C9 H7 N O	-2.461869	-0.1991852	-0.91401863	-0.923063
C21 H37 N8 P3	-2.9402735	0.7600409	-1.6375077	0.5269356
C14 H12 N6	-0.8146719	0.14573279	-0.41921398	1.7042925
C18 H43 Cl2 N13	-1.7713125	0.77618295	-0.33318937	0.5551579
C38 H43 N O S	-1.2041482	2.1571612	-1.5114666	0.087273136
C23 H47 N O4	-0.83816	2.0152125	-0.08318332	2.1441298
C6 H12 N6 O3	-3.525665	-0.4974774	-1.3877429	-0.27024162
C24 H33 N O6	-2.1051772	-2.2312462	1.3420029	0.52924573
C27 H51 O2 P3	1.7600093	-2.801207	-0.4842854	0.118399434
C25 H35 N O6	-1.8518777	-1.9378976	-0.3200803	-1.5709543
C16 H30 O2	-1.4322007	-0.76784414	2.4000301	1.4512357
C31 H47 N4 O P5	0.33760104	1.4758443	-0.20582466	1.6222947
C32 H64 N O2 P5 S3	-2.590787	-0.34134564	0.11569515	-0.71527696
C38 H46 O12 S	2.2574935	1.5927544	-0.8181315	-0.5598436
C16 H38 N6 O2 S	-2.3950763	2.5482414	-1.7065572	-0.2533914
C27 H41 N9 O12 S	-1.6215476	-0.5526788	0.7157018	-1.0854635
C33 H46 N10 P2	-1.7369746	0.06736314	-0.17072213	0.5322056
C42 H87 O P	0.9967271	-0.9399774	-1.3187528	-0.8810526
CAFFEINE (CAS# 58-08-2); (M+H)+	-2.020741	-0.3900073	-0.066599935	0.52173495
C22 H46 N6 S2	-0.5791972	-0.95956373	0.27005416	1.6531515
C33 H47 N5 O5 S2	-1.4017001	0.6601058	0.118363395	0.31675428
C16 H33 N4 O3 P	-0.84889454	-0.19188544	-2.9457715	-0.68692786
C11 H29 N6 P S2	-1.7081144	0.55415666	-0.51959956	-0.91614646
C10 H18 N2 O5	-0.9591618	0.2588809	-1.1809723	-1.3641424
C4 H11 O3 P	-1.7090849	-0.38792142	1.3731614	0.038580764
C21 H43 N5 O10 S	-2.4585555	2.9583356	-0.122428924	0.49939185
C18 H43 N7	-2.549827	-1.6567835	1.7297195	-0.3452018
3-HYDROXYPHENYLACETATE (CAS# 621-37-4); (M+H)+	-2.6201513	0.38920516	1.5030679	-1.5957241
C7 H12 O4 P2	-2.7614117	1.5740829	1.0684202	-0.95909876
C33 H57 N O4 S4	0.046093196	0.37339106	-0.13284284	1.1320927
C13 H13 N9 O	0.012458891	2.0376399	-1.7950423	0.75195634
C34 H73 N2 O2 P5 S	-1.213471	-0.64136916	0.32017845	0.1569298
C10 H14 O	-1.7902223	-3.4154239	-0.3419975	0.24331696
C32 H70 N2 O10 S2	-2.0816286	-0.7875426	0.47030407	0.15178882
C20 H36 O4	-2.2776933	1.646414	-0.013751239	1.0563571
C18 H40 N2 O2 S2	-1.3946412	1.0868418	-2.2737768	0.709316
C27 H48 N3 O13 P	-2.2516942	1.17626	0.29786807	-1.6432809
C9 H8 N6 O2	-2.8789682	0.021343503	-2.0146418	-1.218037
C36 H52 N3 O3 P S3	-1.603536	0.6070125	1.0983881	1.1856382
C27 H34 N2 O P2	-1.0469767	-3.6677184	-1.2199157	0.54493666
C30 H41 N6 O3 P	-0.84655255	-3.8144474	-0.9967992	0.45892662
C27 H51 N3 O6 S	-1.4837523	1.4656483	1.0436583	0.4379838
C31 H43 Cl2 N	-2.7845397	0.11141145	-0.06447366	-0.25444734
C26 H48 N O7 P	-3.2085686	1.9461291	0.74841946	-0.2530142
C24 H52 N2 P2 S	-1.2340915	-3.4305565	-0.72461873	0.2830431
C25 H47 N3 O S3	-2.8539422	-0.005094439	-0.16616595	-0.32378817
C16 H20 N2 O3	-2.956608	-1.332033	-0.89204717	-0.46277907
C7 H18 Cl N5 O	-1.4234776	0.6693722	-0.17108908	-0.10357334
C7 H4 O2	-2.9793098	1.1195394	1.0937942	-0.965667
C22 H8 N2 O3	-0.5598179	1.251503	-1.644833	1.8216293
C4 H8 N6 O2	-3.1785717	-0.3139683	-1.602894	-0.02822563
C16 H33 N O3	-1.9028535	1.9528356	0.9249439	0.07114661
C16 H33 N O2	-1.3420157	-1.0587993	-1.1260084	0.8251769
C26 H26 N2 O3 P2	-2.1427462	-1.3628907	-0.4285949	-0.34937462
C6 H12 N6 O	0.090699136	-1.6242691	-0.338017	1.115976
C10 H20 N2 O3	-2.079581	2.6463537	-0.40932003	-0.5606792
C32 H63 O3 P S2	1.3189942	-0.554193	-0.39574474	2.2601066
C27 H36 N10	-0.73991287	-0.4727239	-0.9803268	2.0202143
ZEATIN [ISTD] (CAS# 13114-27-7); (M+H)+	-0.41960472	-3.9008493	-0.91059935	0.42690715
C11 H20 N6 O3	0.037064627	-0.032357395	0.21818477	0.14329195
C18 H46 N7 O2 P S2	0.94115394	1.2150999	-1.721572	1.318211
C10 H13 N P2 S2	-2.5137856	1.693509	0.46958476	-0.63968635
C8 H14 N6 O	-0.86626863	1.3647116	0.83859915	1.2097605
RAC-GLYCEROL 1-MYRISTATE (CAS# 75685-84-6); (M+Na)+	0.5095395	0.008328799	-3.3250427	0.09685048
C24 H48 N O7 P	-1.4321856	0.5025517	0.52108395	0.5768461
C19 H25 N5	-2.5213764	-1.8891839	0.06092664	0.20766598
OXIDIZED GLUTATHIONE (CAS# 27025-41-8); (M+2H)+2	-0.42786938	0.7958617	-1.8007054	-1.1201842
C16 H32 N6 O2	-2.194741	1.5481482	0.14208099	0.9357928
C18 H41 N7	-1.6931152	-0.2997868	-0.23282918	0.8580241
C21 H36 O9 P2 S	-2.7573092	-1.0268861	0.041866183	-1.6206478
C31 H35 N5	-2.7059038	0.50238115	0.1220738	0.33269346
C31 H62 N O7 P5 S	0.5283102	1.5547525	-1.3342835	0.67513543
C13 H30 N2 O4 S	-1.8544204	0.0945655	-0.44874245	-0.007353831
C26 H35 N11	-3.1854641	-1.1297741	-0.26931074	-0.88401324
C15 H20 N6 O	1.2167463	-1.7266268	0.7271414	-0.5364442
C12 H5 Cl N6 O3 S	-2.4226677	-1.8386059	1.1605008	-0.37583724
C14 H28 N6 O	-1.6839077	0.79706323	0.40107873	-0.15951738
C24 H5 O11 P5 S2	-0.8694008	0.47392827	-1.0217435	-1.5961022
C7 H8 N4 O2	-2.9328523	0.69814265	0.76238894	0.22843519
C15 H22 N2 O3	-0.88740426	0.2871713	-1.0460308	-0.29992938
C15 H22 O2	-1.6132677	-0.4111204	2.6990094	-0.5880548
C10 H18 O3 P2	-1.6005579	-3.527548	-0.91915816	0.3972981
C24 H50 N O8 P	-2.0895953	-1.7568185	0.38118082	0.17060885
C34 H65 N4 O P S3	-0.017082393	-0.694564	-0.5595753	0.6183233
C7 H10 N6 O	-3.0245047	-1.078264	0.61050844	1.2767832
C32 H61 N O4 P6 S	-0.9604204	-0.9556467	-0.4941495	-0.50464535
C30 H53 N4 O2 P S	-1.9158691	-0.54559356	-2.3650923	0.66469836
C29 H42 N8 S2	-2.486317	-0.75823975	-0.23349816	0.4360846
C30 H40 S	-1.7456176	1.1092402	-1.6846038	1.4064023
C38 H46 N2 O6 P2 S	2.062737	1.4378054	-0.7512784	-1.0049976
C19 H24 O4	2.5838225	-2.2435539	0.93881285	-0.20717156
C6 H8 O3 P2	-2.2564778	-0.025899082	0.9103808	-0.93385637
C25 H51 N2 O P S	-3.493145	0.1389477	0.4203813	0.2306096
C20 H42 O11	-3.699928	-0.40232652	0.006213367	-0.30984336
GAMMA-LINOLENIC ACID (CAS# 506-26-3); (M+Na)+	-1.3317596	-1.6304352	0.66926885	0.13086995
C32 H44 O S	-2.9816675	0.33904195	-1.8699532	1.059677
C26 H50 N O7 P	-3.4308968	1.9321854	0.27183297	-0.24671924
C17 H38 N2 O2 S2	-0.22962637	-0.3433057	1.1665725	0.48234397
2'-DEOXYINOSINE (CAS# 890-38-0); (M+Na)+	-0.32432556	1.2626354	-1.0954539	1.0364583
C20 H32 O3	-2.585979	-0.41184458	-0.4268613	0.8642461
C6 H13 Cl N6	-3.1234236	-1.1663479	-0.024309129	-1.7842351
C13 H16 N6 O4	-1.3213587	-1.3351054	-2.3703916	-0.2749966
C35 H45 N3 O2 P2	-1.2410378	1.1592038	-1.4614979	1.5625234
C17 H32 N6 O2	-1.376452	1.1789831	-2.6448689	-0.2944237
C10 H26 N4	-1.5182264	-0.41845366	0.52488697	1.6498927
C24 H50 O13	-4.0064316	-0.16102879	-0.33294636	-0.2676929
C31 H27 N4 O P S3	-2.9126465	-0.72754425	-0.25426883	0.29767448
C10 H22 O6	-3.645227	-0.7319036	-0.68109024	-0.2886305
C15 H13 N O2	-1.8057715	-1.1677386	1.1978132	-0.5795674
C26 H52 N2 O2 P2 S	0.9090315	-3.5958297	-0.46843985	0.072289646
C48 H59 N3 S2	-2.6745698	1.1814549	1.3348281	0.6285976
C15 H27 N O4	-2.7156	-0.17937812	0.07835108	0.4403262
QUINOLIN-2-OL (CAS# 59-31-4); (M+H)+	-2.1579435	-0.6558381	-0.9901736	0.020036608
C21 H41 N2 O3 P S	-2.5779712	1.4219954	-0.9266729	0.4961825
C5 H13 N O	-1.0544282	0.24704719	0.5984796	0.14049482
C19 H38 N2 O3	-2.671622	1.4031583	-0.8666874	0.5918561
C8 H9 N O	0.047961764	-0.043207347	-0.14805602	0.7161529
C20 H28 O2 P2	-3.0113032	0.104013234	-1.8966099	0.47287536
C14 H12 O4	-1.1503232	-1.5960568	0.7612329	0.49734432
C14 H31 N4 O2 P	-3.547164	0.26413003	0.63887286	1.0661994
C24 H49 N2 O P S	-2.5883193	0.94549686	0.18276913	0.6306132
C6 H12 N6	-0.5335025	-1.9604905	-0.2779467	1.476427
C24 H49 N5 O6 P2	-3.4486275	1.9756382	-0.1736241	-0.11213213
C16 H18 O2 P2	-0.08400455	1.7440577	-1.8755966	0.7607584
C12 H23 N O2	-0.6314309	0.91588837	1.1339604	1.4837229

C4 H4 N2 O2	-2.557703	2.038757	0.4305456	0.4452058
C12 H23 N O3	-3.4442046	1.5991731	0.059304208	0.42961445
C12 H23 N O4	0.70305187	2.1393158	-1.3441573	-0.5952557
C8 H14 N6 O2	-3.5553784	0.50920546	-0.09929907	0.9343488
C8 H14 N6 O3	-1.0559283	0.5302934	0.8484343	0.5620718
C22 H27 N3 S	-2.8123558	-1.7342755	0.656439	-1.2831258
C7 H20 N5 O2 P	-3.324263	-0.67595875	-0.8635602	0.7348014
L-HISTIDINE (CAS# 71-00-1); (M+Na)+	-0.53454506	-0.17396542	-0.10731281	-0.6736531
CIS-7,10,13,16-DOCOSATETRAENOIC ACID (CAS# 28874-58-0); (M+Na)+	-0.29517204	0.33230558	-0.66266394	0.76793975
C24 H50 N6 S2	-1.7227273	1.5252552	-0.9723884	1.7086477
C8 H16 N7 O P	-1.6012398	1.9312695	0.5291655	-1.2125872
STACHYOSE (CAS# 54261-98-2); (M+Na)+	-2.8203487	-1.9802258	0.027828721	-1.364197
HYPOXANTHINE (CAS# 68-94-0); (M+H)+	-2.1064136	1.9689856	-0.19064218	0.32878083
C34 H48 O2 S	-1.528486	1.4962565	-1.9073944	0.59773564
C5 H5 N5	-1.3804045	-3.6267197	-0.9644028	-0.047020346
C28 H48 N3 O11 P	-3.0339074	1.8940784	0.75637305	-0.81739104
C32 H38 N10 O3 S2	2.51545	1.3395578	-0.5538242	-0.8526995
C13 H18 N2 O	-3.4786198	-0.67821586	1.7435861	-0.28819364
XANTHURENIC ACID (CAS# 59-00-7); (M+H)+	-1.6328268	-0.976271	1.042801	0.40375108
C31 H58 N2 P2 S2	-2.0942154	0.27427027	1.4297799	0.7547298
C28 H57 N O5 P4	-0.9135726	2.6472225	-0.0849804	0.019420117
C30 H51 N O16	-0.6329665	0.4561404	-0.079994254	0.17938891
C39 H79 O P S4	1.0750953	0.10105556	0.41198066	1.5111954
C33 H54 N2 P2	-0.9571959	1.266038	-0.6544272	1.8301767
C23 H43 N8 O P	-1.1660886	-2.2836988	-0.18202838	0.25237307
C36 H47 N3 O5 S3	-0.5269438	1.176951	-0.43279833	1.3099062
C12 H25 N3 O3	-1.3350897	2.8977523	-0.7999803	-0.3150881
C16 H30 N6 O2	-2.1280298	1.8195024	0.95107293	0.276086
C11 H12 N6 O2	-2.3427134	-1.3397735	-1.0902243	-1.9119565
C40 H61 N O4 P2	-0.3062867	-3.121337	-1.387301	0.7692593
C17 H35 N O3	-3.269943	0.15952127	1.932386	-0.5092676
C26 H51 N4 O2 P S	-2.5352912	-0.8382777	1.6429727	0.7186745
C37 H33 N10 P	-0.4730512	0.9261138	1.3750365	-0.1388776
C16 H36 N6 O2 S	-1.2617824	-1.1202041	1.0794013	0.21711221
C23 H20 N10	-1.6795253	-0.5565544	-2.6607964	0.16468744
C17 H30 N6 O5	-1.8375367	-0.27344692	0.1873396	1.1748016
C16 H33 N4 O2 P3	-0.94302607	1.3992387	-0.9948313	-0.23837814
C12 H24 N6	-0.9069268	-0.24601977	0.46239105	2.092834
C32 H40 O6 S	0.42833224	-0.05897829	-2.6799235	2.113511
C5 H9 N3	-2.879429	1.5302732	-0.2361941	-1.3665009
C6 H6 O5	-2.68171	-0.14731872	0.46873868	0.59034574
C18 H43 N7 O	-3.1789649	-1.5568995	0.053403318	-0.6727695
C20 H8 S2	-2.5126476	0.9158701	0.5204826	-0.4695596
C30 H44 N O2 P S2	-1.6385255	-0.065847546	-0.01912731	1.2086604
C35 H64 N6 S3	0.37540707	1.3511277	-0.602083	1.8560952
C23 H45 Cl N4 O3	-0.567095	-0.42438853	-2.27869	0.029445956
C24 H29 N2 P3 S	-3.037068	-2.368517	0.8510951	-0.515206
C3 H10 N3 O2 P	-2.2562091	-0.57704383	0.762924	-0.041431665
C12 H14 N6 O	2.2686536	-0.7397944	1.1746154	-0.051007755
C9 H14 N4 O2 S	-3.6308432	0.38013658	0.8106497	1.1666074
C15 H27 Cl O S	-0.86584795	0.3482622	0.7862782	0.84950393
C16 H28 N4 P2	-1.0857748	0.09530035	-0.17126498	-0.022718381
C15 H18 N6 O	-2.1433852	0.022448301	-0.95564127	0.9227145
C13 H19 N3 O7 S	-1.1569183	-0.24486014	0.018981874	0.30177385
C25 H24 N8 P2	-2.488781	-0.30593038	-1.6154324	0.19768512
C20 H19 N2 P	-1.1169033	-0.2329594	-1.3568861	0.31962866
C36 H43 N2 P	-1.5469201	-1.4645189	-1.1889714	-0.58075196
C28 H57 N4 O9 P S	-3.8942442	0.24469426	-0.8323957	-0.39841068
C16 H35 N O3	-1.4652175	-0.06844614	-1.3659254	-0.931805
C14 H14 O S	-2.5581489	-0.68772614	-1.3132188	0.5493528
PALMITOYLCARNITINE (CAS# 2364-67-2); (M+Na)+	-2.684665	0.33893973	-0.25004846	-0.09972918
C16 H35 N O2	-0.6481234	-1.1737231	-0.53861386	-0.81408036
C8 H10 N4 O2	-1.9488537	1.2251433	0.6225436	1.1125948
C12 H23 N7 O	-1.8572614	0.40037942	0.42102522	1.1762774
C21 H16 N10	0.25344712	0.539888	0.42322946	-0.8836698
C16 H22 N6 O2	-2.6220307	0.23070404	-0.33521435	1.241884
C19 H25 N6 P3	-2.7942939	-0.09601774	0.5769035	-0.97458386
C26 H51 N4 O3 P S	-2.8235388	0.85831904	0.49761856	-0.09545168
C18 H37 N O3	-3.2064939	1.3829465	1.5978804	-0.36756277
C12 H22 N4 P2	-4.0838957	0.24028268	0.36579198	0.08243111
C30 H62 N2 O5 P2 S	-0.34689862	0.11067003	-2.744165	-0.7697966
C37 H74 N4 O4 S3	-2.579517	-0.5039576	-0.550817	0.68749577
C14 H18 N2 O2	-3.731638	0.9802223	0.56477815	-0.51057005
C22 H28 O2	0.20655318	-0.4699707	0.15913627	0.071746856
C25 H46 N7 O2 P S2	-1.0284488	0.781335	-0.5773204	0.105566174
C22 H46 O12	-4.007866	-0.33419925	-0.14339525	-0.22220826
C10 H14 N2 O	-3.2916117	-0.2070967	1.9244423	-0.9755474
C27 H54 N5 P S	0.09708911	-3.8981972	-0.8306422	0.2124446
C14 H18 N6	0.57104033	-2.0983245	-0.29761642	-1.1784627
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+H)+	-1.7107263	-3.307788	-0.70424694	0.55899495
C12 H15 N6 O3 P	-3.4474993	-0.5759835	-0.60114205	-0.19865663
BENZOATE (CAS# 65-85-0); (M+H)+	-1.5320184	-1.6089373	0.29550135	0.41920418
C11 H15 N5	-2.167644	2.4226515	-0.5242731	0.42785615
C24 H47 N4 O6 P	0.14453319	-3.9625347	-0.7581564	0.21630043
C40 H53 N O2 P4	0.40022555	-0.8453919	1.5072305	-0.013352454
C17 H7 N6 O P	-2.8005326	-0.8657101	1.043972	-0.53067
C8 H16 N6 O	-0.6783592	-0.954904	1.4839137	1.3601494
C11 H22 O4 P2	-0.99979645	-3.7017832	-0.7077645	0.46457282
C23 H40 O P2 S2	-1.7297742	-3.415017	-1.1551683	0.17939346
C12 H20 N6	-2.5714715	0.50198895	-0.60143226	-1.3975856
HISTAMINE (CAS# 51-45-6); (M+Na)+	-1.8810128	-0.30957943	-0.07717003	0.023000155
C38 H65 O9 P S	-1.2056212	-0.58225614	0.33320653	0.17556705
C31 H39 N O S	-2.6891353	-1.964104	1.3619943	0.82208014
C26 H48 N10 S3	-0.8579906	-3.8328736	-0.28590912	0.23170212
C3 H13 N7 O S	-1.8866587	-0.9050912	1.0134718	1.9999418
C28 H49 N4 P3	1.3342322	-3.0592012	-0.34552115	0.9307182
C18 H38 O10	-3.9778159	-0.6050532	0.08459178	-0.20902477
C14 H27 N4 O3 P	-2.8440723	0.1805251	-0.0732275	0.6456424
STACHYOSE (CAS# 54261-98-2); (M+K)+	-1.5335232	-1.049953	-0.3563915	-0.107705325
LEUCINE (CAS# 328-39-2); (M+H)+	0.88537276	1.2880313	-0.21365419	1.3761312
C13 H24 N2 O	0.42880347	-2.4620988	-1.233915	0.5465057
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+Na)+	-0.5683355	-0.16634735	-0.4004168	-0.44382983
C34 H45 N4 O8 P S	-0.27193832	-3.8982384	-0.8821032	0.23758033
C15 H14 N6 O	-0.38461667	1.0685048	0.3024841	-1.5729955
RAFFINOSE (CAS# 512-69-6); (M+Na)+	-1.4057988	-0.56657183	0.5772118	-1.0769364
C23 H47 O P S2	-0.8752514	0.89896584	1.0860094	1.2857876
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+H)+	-1.9224414	-0.6746156	0.07670759	0.51278424
C17 H11 N7 O6 S	-1.7468479	-1.2691876	2.0909042	5.56E-04
C20 H47 N7 O2 S	0.90099406	2.4352386	-0.75739825	0.69892323
C16 H35 N	-2.0189774	-1.0876995	-1.4810696	-0.09909929
1-OLEOYL-RAC-GLYCEROL (CAS# 111-03-5); (M+Na)+	-1.792089	1.2368438	-1.851403	0.20630306
C11 H14 N2 O5	-1.2179183	-3.6101239	-0.93018675	0.51599395
C34 H61 N4 O5 P S	0.009749591	-0.19679263	-3.3793855	-0.54893523
C38 H66 N2 O2 S4	1.8431304	-1.0065193	-0.23286545	-0.70218384
C16 H38 N2 O6	-1.3156747	-0.0588565	0.27304298	0.44120318
C7 H12 N2 O2 S	-2.204101	-1.3750087	-0.6883463	-1.1189032
C23 H40 N4 O3	-2.0118096	0.6951542	1.103343	-1.9926896
C16 H24 N8 O4	-2.2317088	1.3673209	0.6574846	0.48511377
C10 H19 N O3	-0.61875165	-0.3761592	0.15877387	0.37049183
C29 H46 N6 O14	-1.627816	-0.83979154	-0.6588407	0.97500294
C11 H31 Cl N10	-0.9116694	1.2907778	-1.775228	-0.06281473
C26 H54 N O7 P	-2.1078525	1.5582509	1.5103111	0.17331493
C28 H55 N4 O4 P S	-3.3354588	0.053930968	0.97087216	-0.03747478
C38 H60 N6 O4 S	-2.3722646	-0.29773143	-1.795211	1.1511779
C31 H60 N O7 P5 S	-0.805899	-0.29627728	-0.5971516	-0.97616446
C8 H9 N O2	-1.1893934	1.549257	0.96985865	1.0523889
C23 H45 N O4	-2.4202366	0.45193142	0.3345098	-0.048963368
C22 H2 O S5	-1.2882074	0.47627386	2.5243783	0.86566
C28 H50 N O7 P	-2.6854377	2.6778955	-0.12679207	-0.44266382

C23 H28 N2 O3 S	-0.5983506	1.2488241	-0.8375437	2.1116085
C13 H22 N4 S	-3.837069	-0.45618522	0.29980755	0.37232342
C21 H32 Cl N2 O P	-0.4620298	0.36516324	0.3208124	-0.98919666
C25 H14 N2 O3	0.018762631	-2.0661705	-1.0645568	1.7131431
C41 H66 N6 S2	-0.7393994	0.6663743	-1.0455828	-0.74139875
C13 H23 P S	-3.006574	-1.0221837	-0.4098743	-0.89568526
C7 H15 N O3	-0.13875034	1.6872091	-0.7262174	0.6755185
C16 H34 O9	-3.9015882	-0.75326556	0.13870107	-0.28130963
C24 H40 N5 O3 P	-2.2217698	-0.16285712	-0.37648436	0.83057004
C28 H37 N4 O P S2	-0.52781326	-0.48832348	-1.482877	2.9296737
C11 H19 N7 O	-3.806268	1.0667577	-0.34944502	0.5516082
C28 H53 Cl O P2	-0.2724341	-1.0073507	0.03266443	-1.4391776
C29 H30	0.73006797	-1.0074127	0.82491195	-0.552251
3-METHYLHISTAMINE (CAS# 644-42-8); (M+H)+	-0.9963517	0.6899124	-1.4900931	-0.15721908
C26 H51 N3 O S2	0.8513994	1.5209352	-0.8398854	0.42883265
OLEIC ACID (CAS# 112-80-1); (M+Na)+	1.486107	-0.5062395	0.58140105	-1.5466195
C13 H10 N10	-1.7523265	-1.6030536	0.5174086	0.2761181
OPHTHALMIC ACID (CAS# 495-27-2); (M+H)+	-0.68598044	1.7098026	-0.57633805	-1.1948482
C29 H45 N3 O P2	0.47865322	1.4377685	-2.2030776	0.20910539
C8 H8 O3	-2.8482122	0.5381946	1.2812766	-1.9603312
C8 H12 N6 O	-2.0477405	1.9469728	0.38856634	0.10897944
C18 H30 O2	-2.1092556	-0.8320708	0.6466523	0.020696227
C19 H37 P S	-2.24126	-1.2741507	0.6311614	1.8270042
C9 H24 N6 O2 S	-2.545555	-0.10405266	0.2605688	1.431413
C19 H37 O P S2	0.5646168	1.5282812	-0.0652404	0.62753576
C10 H15 N2 O P	-3.8941584	0.4615011	0.61939067	0.2072291
C12 H14 N8	-3.1017	-0.050714105	2.0404558	-0.38391095
C25 H52 N6 O7 S2	-3.9436479	0.037387967	-0.5670347	-0.36669162
C29 H50 N6 O7	-1.8767904	-0.5504375	-2.8927968	0.87038934
C18 H18 O3	-0.981238	-3.5560863	-1.1220775	0.7482836
C20 H38 N6 O5	-1.6409062	-0.48842895	1.1819241	0.5725369
5-OXOPROLINE (CAS# 4042-36-8); (M+H)+	-1.8990902	0.46441057	1.4690636	1.2454655
C17 H37 N4 O3 P	-3.5073888	1.4843628	0.30292135	-0.10596073
C12 H12 N8	-3.6438644	1.2214867	0.62184364	-0.35758942
C25 H34 N4	-1.292741	0.026212394	-0.5418974	2.0855284
C22 H45 N4 P S	-3.2421446	1.6193696	0.3220579	1.289182
C33 H47 N7 S2	0.30061534	0.27440965	0.0228692	1.6837595
C17 H4 N4 O4	-3.1260989	1.9819947	0.48383692	0.21892966
C30 H57 N O2 S4	-1.0039228	0.16967604	-0.29789978	0.95427036
C22 H34 N4	-3.568965	0.83671916	-0.30198583	0.43984705
C11 H12 N5 O12 P3	-0.78432	-0.51563686	2.655273	1.0493503
KYNURENINE (CAS# 343-65-7); (M+H)+	-3.1842337	0.8371433	-0.42316607	-1.0112402
C9 H16 N2 O2	-0.95383245	-0.74892473	0.12656352	-1.3072805
C12 H25 N O2	-3.2098935	0.65779966	0.91713554	0.75643194
C16 H38 N4 O4 S2	-0.11578165	1.411642	-1.9650513	-1.361313
C38 H54 N O P S	-0.037738502	-0.98401624	-0.2845663	2.05981
C17 H27 N5 O15 S	-3.1720316	0.70318556	-0.45109868	-0.44988108
C24 H31 O4 P3	-1.5541413	-2.262147	-0.68170977	0.19745924
C6 H14 N5 O P S	-1.6958358	-2.4573169	1.3038672	0.016175568
C36 H69 N2 O3 P S3	-0.8688624	0.7440169	0.27659562	0.47567546
C13 H20 N2 O	-2.3697796	-0.19255581	0.71169984	-0.88776803
C29 H47 N5 O3 P2 S	-0.63861775	1.0088459	-0.97372144	0.15445969
C12 H14 N8 O	-1.4391114	-0.14428788	-0.9568284	0.2512659
C24 H45 P	-0.23104815	-0.858065	0.79502517	-1.1209384
C25 H44 N4 O3	-2.4907143	0.4876861	1.1970344	-1.7949463
C18 H20 P2	-2.7684937	-1.9843507	-0.34605002	-1.5470408
C32 H44 N13 P3	0.7578278	-0.7113665	1.4599562	-0.58766985
C28 H52 N O2 P S2	0.8152689	1.2693583	-0.0461964	-0.02344215
C32 H52 O6 S2	-0.46261254	-3.8200407	-1.0364127	0.08882958
C7 H10 O2 S3	-2.6531847	-0.8373215	-0.2247502	0.8183775
C16 H36 N2 O5	-2.463318	-1.1642834	-1.0118464	1.8769995
C13 H22 O3	0.8249457	0.3313735	1.3484138	-0.19006279
C15 H14 P2	-0.20710087	-3.509773	-0.68946564	0.8719148
C36 H71 O P S4	0.35045058	-0.42051938	-1.6533626	0.5299125
C18 H48 N8 O2 S2	-0.8388306	-0.055755522	1.7692661	0.36622527
C8 H16 N2 O3	-2.8827982	1.6768484	-0.5566831	-0.3969028
FERULATE (CAS# 1135-24-6); (M+H)+	0.18329042	0.74892056	-1.4050504	-0.88105965
C13 H16 N6	2.9642324	0.59634984	0.61558604	-0.9716052
C15 H18 N6 O S	-2.3789008	0.38592222	1.577905	-1.6373224
C13 H31 N3 O3	-1.2056282	-1.839304	0.8591075	1.8758631
C21 H46 N O P S	-0.8949916	-0.41283822	2.8344157	1.2972097
C21 H37 N	-0.7868902	0.92449373	-3.22057	-0.8064803
C10 H18 N6 O3	-1.7416226	-0.25317606	1.2008743	1.4179223
C8 H15 N O4	-0.9955815	0.9047992	0.34301296	-0.88091373
N-ACETYL-DL-SERINE (CAS# 97-14-3); (M+H)+[-H2O]	-1.3434834	0.7818122	0.0813066	0.3240615
C13 H26 N6 O	-0.6748641	1.0656413	0.64067674	1.9410596
C40 H76 O12	-1.3165092	-0.6071454	-0.09742066	0.37908825
C10 H9 N O3	-3.7955844	1.1768328	-0.6227312	-0.7814392
C30 H57 N O4 P2 S3	-2.1183305	-0.24727291	0.3524888	0.24635275
C15 H30 N6 O	-1.8386497	-0.035384625	1.4706063	1.526237
C25 H49 N O4	-0.96916264	0.74424684	1.1975647	-0.3862605
PROSTAGLANDIN E2 (CAS# 363-24-6); (M+Na)+	-1.057416	0.20742206	-0.8643784	-1.291334
C12 H21 N3 O5	-3.1377301	-0.22655863	-0.06458884	0.5556354
C15 H26 N2 O4	-2.1785462	-0.5409069	-0.3899839	0.50768995
C16 H22 O4	-2.1941526	-1.801065	-0.20474404	0.3300118
ALPHA-LINOLENIC ACID (CAS# 463-40-1); (M+Na)+	-1.3317596	-1.6304352	0.66926885	0.13086995
C30 H36 O6 S	0.84348094	-0.70580053	-0.63163656	1.9340677
C8 H16 N6 O4	-3.6480403	-0.7253966	-0.6675352	-0.29859534
C8 H16 N6 O2	0.1240489	-1.5539788	0.7453752	1.9532802
C12 H28 O2 S2	-2.942992	-0.7840021	-0.37931484	-1.0546898
C12 H14 O5	0.29046708	-0.6118406	-0.2633012	-0.16762048
C28 H45 N7 O4 P2	-0.22478154	0.19407108	0.15094668	-0.066190615
C11 H14 N6 O2	-1.6977525	-1.1438372	0.92469364	0.8447863
L-TRYPTOPHAN-15N2 [ISTD] (CAS#); (M+H)+	-1.4129399	-2.119947	-1.4432677	-1.279818
C6 H13 N O2	0.9571188	1.2422783	-0.328742	1.3841684
C18 H28 O3	-2.5467653	-1.2306739	1.7175896	0.7827469
C14 H39 Cl N10 O	-0.4272654	1.0368086	0.44320965	2.2305093
C12 H21 N4 O4 P	-2.0690746	-2.9101777	1.4982846	0.042711362
C18 H28 O2	-0.9783491	0.23612046	-1.5764129	0.35208607
METHYL JASMONATE (CAS# 1211-29-6); (M+Na)+	2.1247923	0.9073864	1.2088023	0.7607207
C15 H29 N O4	-2.4811547	-0.034050435	0.9604906	0.20969684
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+Na)+	-1.3333988	-3.605035	-0.9280966	0.45793965
C15 H14 N6	-2.68001	0.19918884	-0.46115172	-0.28609776
C8 H12 P2 S2	-0.2348295	2.3174767	-2.2211218	-0.54335207
C21 H40 N2 O S	-1.3684893	-0.7809839	0.058613148	0.76206744
C33 H39 N3	-1.168969	1.0472331	-0.19384512	1.0016146
C19 H24 N10 O5	-1.8789372	-0.33890897	-2.1788828	0.22878043
C33 H44 O12	-0.37446105	-3.8893852	-0.9037441	0.17749396
C27 H51 O3 P S2	1.8378421	-2.9053972	0.48399764	0.06675321
C12 H6 N4 O2 P2 S4	-1.5973027	-0.2918124	-2.309619	0.21888162
C11 H21 N7 O	-1.4377849	0.352964	0.7802347	1.2264699
C26 H51 N7 O4	-0.2328046	-3.8841336	-0.6787214	-0.053887427
C31 H62 Cl2 N2 O2 P2	0.014689431	-1.2589974	1.0264157	0.48606613
C22 H47 N	-0.15663928	1.4038491	-0.7464515	2.2943811
C26 H44 N7 O5 P	-3.2179546	1.7112396	0.4692979	-0.6463922
C8 H9 N	-3.4836438	1.6258802	0.12129421	-0.9203101
C19 H24 N10 P2	0.3378684	-1.5889173	-1.314361	1.4895552
C18 H39 Cl N4 O3	-0.26156563	1.3064289	-2.529562	-0.22399637
C13 H17 P S	-2.2195508	-0.58278626	0.45313329	-0.7071752
C26 H28 N6 O S2	-2.3008924	-0.5496447	-1.6244138	0.11511711
C16 H20 N4 O2 P2	-2.5514488	-1.1571907	0.118986845	0.6851344
C26 H52 N O7 P	-2.722033	2.4432104	-0.30748862	-0.37696946
C14 H19 P S	-3.6244783	-0.3377337	0.8360598	-0.8332908
N-ACETYL-DL-METHIONINE (CAS# 1115-47-5); (M+Na)+	-2.3723052	0.3880761	-0.5027405	0.9602256
C31 H53 N O9 P2 S	-2.4912858	1.654848	0.27985123	0.43337333
LEUKOTRIENE B4 (CAS# 71160-24-2); (M+H)+	0.6732704	-0.46714255	-0.46478832	0.033953212
C15 H23 N5 O3	-0.44029203	-0.02797804	-0.7873759	0.2510338
C23 H30 O3	0.9975152	-0.9851292	-0.37811267	-1.5577122
C14 H24 N6	-2.6350932	0.14731318	0.093862355	2.0670946

C35 H70 O2 P4	0.27911067	-0.56471336	-2.6221297	-0.3693717
C26 H53 N4 O P S	-2.5401177	0.69916975	1.77561	0.76350236
C16 H23 N5	-2.0915666	0.24697253	0.11248317	0.54632974
C14 H26 N4 P2	-3.3063567	-0.2093288	0.0299232	1.257437
C23 H46 N O2 P3	-0.9408423	0.8785209	-0.12574802	0.5672213
C9 H5 N O4	-2.3110569	0.115735605	-1.0341995	-1.9708568
C13 H32 N2 O P2 S	-1.6721852	-0.09505564	1.3696065	1.2264802
C25 H29 N5 O2	-0.41844994	-1.6274889	-0.9199759	-1.0961945
C5 H10 N2 O S	-1.9703293	-1.206024	-0.8658367	-0.96177363
C16 H31 O P3 S	-0.6819438	0.4584741	-3.0215716	0.09952554
C5 H9 N O2	0.7783901	2.0439384	-0.76184493	0.12372125
C15 H34 N2 O5	-0.49500063	0.33408463	-0.41874987	-0.1490111
C23 H47 N5 S3	-2.8141212	2.4013622	0.5666471	-0.088118955
C19 H39 N4 O4 P	-1.2973654	0.7431546	-2.2988377	2.2898479
C25 H40 N10	-0.48622626	-4.013825	-0.15321806	0.34591642
C33 H5 O9 P5 S	-1.1563135	1.442202	-0.32357526	-0.59401613
C41 H53 N2 P S2	0.006936431	0.16335848	-0.24427676	2.3355722
C23 H34 O2 P2	-1.7117599	-0.27597845	-1.5702329	-1.6223966
C21 H23 N2 O9 P S2	-3.3154047	-0.4462774	-0.11125556	0.39834684
C28 H56 N2 O6 S2	-0.4907223	-0.5787221	-2.8995137	-0.5115645
C27 H38 N10	-0.33637512	-3.9749305	-0.51640075	0.3629254
C9 H11 N	-3.1607258	0.44684738	0.20453696	-0.845454
C31 H32 N O P	-2.133883	0.9557488	0.85302603	-1.8891648
C9 H11 N O3	-0.6451698	1.0930635	0.36333093	1.0531056
C14 H38 N4 O6 P2	0.92503834	2.211652	-0.7024074	0.48408383
C34 H49 Cl P2 S3	-1.5139349	-0.8473667	1.3099754	-1.5352638
C23 H46 N5 O3 P3	-0.35408485	-1.3747739	-1.4619274	1.7878395
C6 H14 O4	-3.3032238	-0.33257142	-1.6184118	-0.08928284
C17 H32 N8 O	-2.6536386	1.3973045	-0.86513317	0.58493733
C14 H34 N2 O6	1.0201678	-1.6787924	0.31678203	1.167074
C34 H56 O2 P2	-1.3997166	0.119522266	0.08198981	0.0476294
C9 H11 N O2	-3.475202	1.6352051	0.10573781	-0.93291396
C12 H25 N O	-0.79872674	-1.4480178	2.7266896	0.68432635
C23 H32 O4	-0.7876915	0.24237227	-1.2589808	-0.3347191
C47 H34 N3 P	-2.4026256	2.1525257	1.0582318	-1.0768117
C16 H14 N2 P4	-2.5350754	0.6817584	1.5508347	-0.33742657
C33 H55 N P6	0.6062651	1.9165235	-1.3426484	0.34697413
C21 H43 N4 O5 P	-1.5275222	0.32373205	-2.8185031	1.7794255
C34 H62 N10 O S2	-2.1412222	1.8101802	0.24228145	-0.058830738
C21 H25 N11	-2.5600443	-0.85910296	-0.3287924	0.9293349
C24 H51 N O2	-2.3390393	-1.5149329	1.8192888	-0.37755492
C22 H23 N3	0.71830237	0.8888848	-0.90388817	1.3691064
URIDINE (CAS# 58-96-8); (M+Na)+	-3.337608	1.4968606	0.63917315	0.19937573
C23 H43 N3 O3 S2	-3.151598	-0.73476535	-0.39902008	-0.73213106
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+H)+	0.5187355	1.2371997	-0.38853636	0.2664074
C26 H39 N3 O6	-2.7090073	2.7618566	-0.2417179	0.19701724
C18 H28 N4 O10	-1.8639069	-1.4094297	0.6612856	1.1100347
C33 H64 N12 O3 S2	-1.8422446	-1.2129576	-1.201676	1.1851974
C34 H34 O7	-0.08377248	-0.44385302	-1.1896963	3.1859322
(-)-SALSOLINOL (CAS# 27740-96-1); (M+H)+	-0.9303589	0.84444636	-0.121444374	1.1776818
C16 H31 P3	1.45409	-0.6820437	-1.0952138	-1.2632142
C21 H44 N6 S2	-0.7173506	1.0139636	-1.0139425	1.2084687
C24 H19 N6 O3 P	-3.020796	-0.9762962	-0.7990893	0.39975184
C36 H38 N2 O4	-2.0538673	-1.6803122	-1.4916426	-1.1507511
C21 H41 N O4	-1.8918039	0.17958337	-0.78468484	0.1715483
C10 H12 N4 O5	0.0779763	1.3228431	0.89268434	0.63092625
C3 H9 N2 O2 P	-3.2232912	1.5068239	-0.15810895	0.098381236
C19 H45 N7	-1.8921871	-1.4352933	1.9418081	0.49913687
HISTAMINE (CAS# 51-45-6); (M+H)+	-2.8192756	1.5860589	-0.2706797	-1.3639263
C3 H9 N2 O4 P	0.8716119	1.5958061	0.017834403	0.77206445
C5 H10 N6 O	0.31144547	-0.9996286	-1.7575706	0.23180282
C17 H26 O4	-0.8099831	-0.15693319	-0.9477377	0.44559354
C18 H12 N10	-1.4110717	-3.5011985	-1.1434186	0.3483774
C32 H59 N O4 P2 S3	-0.14834033	1.6379851	-0.5982574	-0.629639
C23 H31 N O6	-1.6392821	-2.379481	1.6513839	-0.17731547
C18 H25 N4 O5 P	-1.4662533	-0.62250876	-1.8304433	0.73771447
C29 H46 O4	-1.0545561	-3.7499475	-0.4940603	0.5176574
PANTOTHENATE (CAS# 79-83-4); (M+Na)+	-2.5931046	0.28602707	0.09570083	-0.28899282
TYROSINE (CAS# 60-18-4); (M+H)+	-2.546705	1.2996312	0.180734	-0.6370119
NAD (CAS# 53-84-9); (M+H)+	0.46440828	0.77522814	-2.4924366	-0.958249
C26 H38 N10	-1.6424911	0.32634795	0.78751045	-1.1960614
C13 H23 N4 P	-3.021763	-1.5210049	-1.0222526	-0.453725
C27 H49 N4 O2 P5	-2.3409967	-1.303094	0.7799925	-0.73264706
C18 H40 N5 O2 P	-1.216688	1.2504787	0.34847152	-0.35703975
C11 H12 N6 O	-0.0434165	-1.611689	1.6104758	0.65363276
C24 H35 N O S2	-1.6081812	-0.418997	1.2427925	0.114243455
C9 H19 N2 O3 P	-2.810835	0.40706152	0.3565895	-0.6139711
C9 H8 N5 O11 P3	-0.10903058	-0.4970411	2.1700907	1.7174007
C13 H20 O4	-3.2540736	0.7873666	-0.55641246	0.65270984
C11 H11 N O3	-1.3927623	-1.4080682	-0.76707405	0.63989896
C13 H20 O2	-1.5531888	-0.24955577	0.11848647	-0.9482984
C21 H24 N4 O4	1.1624027	-1.8361392	-0.7054998	2.163001
S-ADENOSYL-L-HOMOCYSTEINE (CAS# 979-92-0); (M+H)+	-1.3930523	0.27375588	-0.72545934	-2.0499868
C22 H26 O6	-2.9378746	-2.4299026	1.0294114	-0.49207193
C30 H55 N O5 P4	-3.143554	2.2944813	0.080285296	-0.4995067
C18 H20 N P	-3.56117	1.4881521	-0.4189207	0.48777837
BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7); (M+Na)+	0.29441693	0.26293138	-0.27852386	2.2934747
C11 H12 N10 O	-2.2030475	-0.67148364	-0.785097	1.0573977
C21 H21 N5	1.3246123	1.0368407	-0.7789979	1.369925
C14 H24 N6 O	-1.8375827	0.7136058	0.62384593	0.92211616
C14 H26 N6 O	-1.9916086	-0.5320938	-0.36841777	-0.7258844
C23 H47 N4 O P S	-0.062287726	-1.9913726	0.062489294	2.4112506
C22 H49 N7	-2.1964662	-1.3178734	0.9794999	-0.11866776
C9 H12 N6 P2	-2.4978676	-1.417713	1.5853488	-0.05373214
C37 H77 N4 O P S3	-2.8408024	-0.5043814	0.6036434	0.512692
C34 H52 N6 O2 S	-1.6631095	-0.88720953	-2.2695282	1.3411736
C28 H24 N9 O P	-2.7288408	-0.07032862	0.3719665	-0.32635212
C7 H19 N3	-2.594733	0.3385852	0.43932837	2.504736
C27 H48 N6 O S2	-0.08485809	-0.52320886	-2.9643157	-1.0076337
C11 H20 O3 P2 S	-3.79427	1.3782586	0.4589143	-0.25616407
C15 H20 N6 O3	0.30418497	-0.67084515	1.2623825	0.4647657
C23 H26 N3 P	-0.58682114	1.373982	-1.245364	0.50251126
C15 H20 N6 O2	-2.1774423	-1.8226835	1.5169814	0.40243298
C13 H25 N7 O	-2.0219238	0.34090114	0.5942794	1.3724834
C25 H51 N O4	-2.549553	1.7206575	0.4703652	-0.6271171
C17 H28 N2 O4	-1.413315	1.6007912	0.77730435	0.98279464
C19 H44 N2 P2 S	0.8184459	1.4941815	-2.406882	-0.18710016
C5 H4 N4 O2	-0.8045942	3.1011634	-1.183265	0.78429824
C35 H50 N O10 P S2	-1.9671538	-0.42434978	1.2231797	-0.29898006
RAFFINOSE (CAS# 512-69-6); (M+K)+	-1.6844046	0.8469633	0.34711856	0.41335484
C17 H36 N4 O10 S	1.9506555	0.9650649	-0.4227391	0.28606868
NICOTINAMIDE (CAS# 98-92-0); (M+H)+	-0.33425203	1.4665644	-0.1566468	0.029289491
C32 H63 N4 O6 P S	-2.0079856	0.57612836	1.0119458	0.5375158
C5 H15 N4 O3 P	-3.2375026	0.722772	-1.6091368	-1.4133008
C13 H27 N S2	-2.4487584	-0.28318727	-0.001753181	-0.8258197
C33 H67 N4 O11 P	-2.282196	-0.9927593	-2.861115	0.19018449
C15 H28 N6 O2	-0.24735357	0.98031026	-2.7466145	-0.017516177
C31 H43 N5 O12	-3.0320117	2.2974217	0.44149986	-0.3559481
C22 H20 O5	-0.87684965	0.4589346	-2.6973872	-0.012257889
C17 H34 N6 O6 S2	1.4118364	0.79099107	0.19977903	0.1807589
C30 H51 O6 P S	0.48212135	-3.7905126	-0.101022035	-0.13517699
C10 H13 N5	-0.6011265	2.0919893	0.2129242	0.99724925
C27 H43 N7 O16	-0.697048	-0.50239456	-0.006752558	0.72844803
LYSINE (CAS# 56-87-1); (M+Na)+	0.8565466	-0.60583484	-0.625834	-0.47107795
C23 H20 N4 O	-3.3330393	-1.8335449	0.6150744	-0.4425868
C18 H33 N7	-1.4163085	0.8956879	-1.2872088	0.6788082
C10 H28 N6 O S	1.8742523	-0.7782141	0.19121788	-1.0781043
C28 H41 N O6	-3.1205096	-1.6268837	-0.41023397	-0.7784794
C34 H46 N3 O3 P	-0.8971503	-1.1497995	-1.24172	1.4168925

C14 H31 N6 O P S	-2.179431	-0.6678458	-0.006038189	-1.5983853
C14 H20 N2 O	-2.9765277	0.19555348	1.3711474	-1.6826026
C40 H41 N7 O S2	0.57698673	0.42319083	-1.464516	0.7719332
C34 H55 N5 O11	1.7895309	1.8090847	-1.2311745	-0.5681226
C14 H27 N4 O2 P	3.4212785	-1.2863847	-0.33984	-0.4477488
C23 H44 N2 O2 S	-1.4549971	1.4889709	0.013958603	1.8278941
C26 H27 Cl O5	-1.3818434	-1.0116944	-1.4894403	2.5248098
C10 H18 N6 O	-0.82154906	-1.8163897	0.020863034	0.76211566
C16 H24 N6 O	-1.1799576	2.2797146	-1.3427334	0.10932675
C18 H42 N5 P	-1.9774412	1.7729076	0.6010467	0.52662337
C26 H50 N O2 P S2	-1.2152525	1.4566998	-0.36627242	-0.027483642
C16 H19 N8 O3 P	-0.91831076	0.22202273	-0.21801805	-0.96303874
C29 H49 N3 P2 S	-2.4957068	2.447485	-0.746608	0.80663514
C23 H36 N17 O P	1.934663	0.7851167	-0.49641567	-0.018218003
C41 H51 N3 O4 S	-0.1365713	0.9487623	-2.0693111	1.2244427
C15 H31 N O2	-1.8990791	-0.4398917	-1.9410796	1.1056299
C37 H56 N2 O2 P4	0.87752753	1.0859064	-0.118912324	0.7511898
C24 H50 N O7 P	-3.187512	1.6661218	1.2988892	-1.0906082
C27 H46 N6 O6	-1.7529426	-0.28354144	-2.947007	0.8713429
XANTHOSINE (CAS# 146-80-5); (M+Na)+	1.3178105	1.4454154	-1.6789218	-0.15018973
C4 H11 O2 P	-2.6744719	0.7945962	0.099191986	-0.6618179
INOSINE (CAS# 58-63-9); (M+Na)+	-0.7928662	0.9005589	0.4277577	0.9627808
C24 H29 O6 P S	-2.8928735	-2.2909963	1.1365883	-0.55561805
C20 H41 N O3	-3.3486717	0.075364724	1.7783133	-0.48853528
C16 H16 O4	-2.4234247	-0.26294878	1.307554	0.922678
C15 H11 N9	-2.0896447	0.601145	-1.0208343	0.3224817
C10 H13 N5 O	-0.19186951	-3.9258687	-0.8144287	0.48616758
LYSINE (CAS# 56-87-1); (M+H)+	1.7208912	0.49590546	-1.3599594	-2.3655195
C12 H24 N6 O	-3.2682366	-0.31778073	1.1211922	0.47359636
C13 H14 O4 P2	-1.4799974	-0.7355219	1.3989365	0.37457895
C27 H50 N7 P S2	-3.3488908	1.2309847	-0.19664553	-0.6512173
C7 H18 O2 P2	-3.6692696	0.35740626	0.79786706	1.060679
C40 H51 N3 O4 S3	-1.5501273	-2.0396678	1.6301292	1.3773642
C4 H8 N6 O	0.54897374	0.42919147	-1.282306	1.2576783
C27 H32 N6 O2 P4	-1.4108886	0.07381738	1.6212491	0.117373936
C26 H52 N2 O2 S2	-1.1010486	0.70340705	-0.042864725	0.7562456
C20 H41 N O2	-2.5332134	-0.9478686	1.9209479	0.23878138
C21 H26 S2	-0.2494868	-3.5499218	-0.17343098	-0.67273164
C10 H14 N6	0.021141317	0.6053931	0.6751953	-0.6287955
PHENYLALANINE (CAS# 63-91-2); (M+Na)+	-3.3943985	1.725188	0.10723989	-0.96528393
C18 H41 N13 S	0.9178934	2.400365	-0.429247	0.60870045
C21 H40 N2 O3 S	0.959175	1.2449143	-0.5767095	1.5278773
C10 H18 N O6 P	-1.057164	2.0523863	-0.07628386	-0.44931805
C16 H28 N P S	-1.872255	0.14047562	0.28471267	1.2501595
C30 H28 P2	-2.5311677	-0.1663066	-0.8619591	0.40824974
NORMETANEPHRINE (CAS# 0); (M+H)+[-H2O]	-3.4768162	1.6336782	0.105398856	-0.9313097
C42 H41 N O3 S2	-2.976767	1.8772143	0.6133791	-1.5053883
C22 H38 N10 O2	0.44429946	-1.4722084	-2.1419895	-0.30557746
C21 H39 N3 O3 S2	-1.0294995	-2.7108278	1.0689812	0.091822565
C22 H38 N8 O	-2.584483	-0.73459363	0.88656634	0.2906121
C36 H41 N3 O S	0.16620329	0.12904067	-0.7994133	1.4692539
FRUCTOSE (CAS# 57-48-7); (M+Na)+	0.62752813	0.49657622	-0.11321928	0.26126263
C24 H27 N3	0.5143176	1.5730917	-0.5334772	0.93903023
C42 H65 N O5 P2	-0.18906955	-1.2329373	3.3165383	0.6736731
C24 H46 N2 O3 S	-0.34366626	2.7419562	-0.15276214	0.804878
C11 H8 O S3	-2.5961952	0.68180436	1.2880679	-2.0200512
C20 H43 N O4	-1.6650671	-1.7191294	-0.20606238	0.7920922
C20 H43 N O3	-2.0749602	-1.0581517	1.4669526	0.22319864
C44 H86 N2	-1.7757478	0.5462092	0.024454072	-0.25669938
C4 H11 N3 O	-0.16478236	0.2525591	-0.1598764	-1.169029
C14 H35 N7	-3.2280962	0.991594	0.63845587	-0.43778947
C31 H64 N2 O3 S4	0.2397959	0.66952616	0.24532297	-0.03524429
C20 H35 N7	-2.8537922	0.40233982	1.4518205	1.8268226
C12 H18 N2 O	-3.141184	0.09596422	1.5607386	-1.7203114
C18 H24 Cl N4 O4 P	-2.46888	-1.4701505	-0.94768727	1.4629153
C25 H41 N7 O2 S	-2.081546	1.1131183	-0.8617533	1.1295877
C9 H16 N6 O2	-1.8751132	-1.2677754	0.7819985	2.1530013
C44 H86 O3	-0.82405996	-0.3999859	-0.62328094	-0.65445197
CHOLINE (CAS# 62-49-7); M+	1.1054405	1.1545273	-1.4431905	1.1899222
C37 H69 N8 O P S	-0.38370454	-0.37028226	0.80927044	1.9503996
C11 H9 N9 O	-3.5972872	-0.38881463	0.08815856	-0.67520726
C15 H35 N4 O3 P	-3.0747097	-0.34977302	1.0646961	0.7665492
C9 H19 N O	1.4369434	0.10731107	0.30858237	1.3942978
C35 H40 N2 O4	-1.7198716	0.013036888	0.8610764	-0.8700451
C20 H32 O10	-1.337029	-0.8649652	-1.2380102	-0.001063943
C39 H83 N4 O P	0.3837369	-0.31290197	-0.28252026	-1.4425733
C18 H34 N6 O2	-0.9997245	0.7329143	-1.6243795	0.51311886
C11 H18 N4 S	-4.060697	0.012310207	0.5527016	0.19040355
C19 H39 N7 O2	0.22965598	2.100902	-2.4336417	1.208274
C34 H69 N4 O5 P S	-2.4088316	0.32563886	0.71342814	0.10262379
C29 H62 N8 O S3	-0.10653184	-1.0392276	-0.93665695	2.3816285
C20 H27 N4 P	-0.8686928	-0.90859175	0.66199243	-0.567844
C33 H50 Cl N O6	0.17425802	0.29823408	2.2149363	1.0070224
C6 H4 O6 S	-0.21822317	0.42043018	-0.18909878	-0.27727124
C18 H36 N6 O9	-4.01029	-0.42210126	-0.012967959	-0.23133004
C22 H27 N11	-1.922956	-0.5243874	-2.0952306	0.11792205
C18 H39 N9 S	-2.0766897	-0.84315515	-0.36145002	-1.2458003
C17 H35 N2 O P3 S	-0.93431896	0.613497	-2.3893356	-0.580998
C32 H66 N8 S4	-3.7172291	-0.74611366	0.567598	0.7309977
C25 H42 N6 O5	-1.8127514	-0.57999504	-2.7492557	1.6323388
C5 H10 P2	-2.3211322	1.755446	-0.32519838	-0.5061576
HYPOXANTHINE (CAS# 68-94-0); (M+Na)+	-2.1142962	0.22089863	0.3198531	0.84797144
GLUTATHIONE (CAS# 27025-41-8); (M+H2)+2	-0.42786938	0.7958617	-1.8007054	-1.1201842
C32 H30 O7	-1.1188438	-0.6955401	-1.3051231	2.627499
C14 H28 N6 O2	-1.3548312	0.3270161	-0.15176137	2.067302
C37 H47 N5 S	0.2241396	0.102959126	0.45331317	-0.48361325
C31 H41 N8 P	-2.405971	1.1174704	0.6383574	0.76455563
SPERMINE (CAS# 71-44-3); (M+H)+	-1.4724699	-0.48232645	0.98494756	1.6386261
C5 H13 N4 O5 P	-2.0830278	0.2587247	-0.8396586	0.18973774
C28 H34 O S	-2.5565796	-1.3313075	-1.414851	0.61599433
C15 H36 N2 O P2 S	-2.5265934	-0.15423894	0.29181325	-0.013741657
C34 H44 O S	0.3786145	-0.14090577	-0.8828739	2.7217443
C33 H67 N4 O5 P S	-0.54813707	1.0159677	-1.2902151	-0.52247804
C33 H44 O2 S3	-0.69098973	-0.5295145	-1.5647521	2.4806046
C27 H33 N5 O2	-2.6873767	-0.43004328	-1.9420924	1.6762724
C11 H21 N O4	0.35463363	1.2372783	-0.56311464	1.6644078
XANTHOSINE (CAS# 146-80-5); (M+H)+	0.5693944	1.8235838	-1.7599267	1.2719653
C22 H25 N4 O2 P3	-1.7845329	-0.47684512	-0.60096556	-1.2278816
C15 H20 O4	-1.2848021	0.34222728	0.051127367	0.6478447
C19 H44 N4 S2	-2.5818446	1.5095164	-0.80024195	0.41746026
C27 H50 N O4 P S	-1.3634415	3.07518	-1.5152714	0.6247584
C16 H14 N2 O4 S2	-1.2160589	-0.4010983	0.69945896	-2.236611
C31 H39 O2 P5 S	-3.2798429	-0.6123199	-0.23776561	0.5728971
C23 H28 O3	-1.1875893	0.32382485	-0.181075	-0.2032182
C15 H20 O3	-2.1084585	-0.8934052	1.2067223	0.6846894
C18 H39 N O3	-0.79396	-1.7999752	-0.34364468	0.81750447
C31 H52 O2 P4	-1.872562	-3.3209677	-0.8438075	0.14631023
C11 H15 N O3	-3.3402073	0.05524803	1.3920562	-1.6038486
C12 H24 N2 O3	-1.4156773	2.6835446	-0.50119513	-0.5210086
C11 H33 Cl N10 O	-0.14473605	1.0667293	0.88681495	1.449045
C41 H69 Cl N O4 P S	-1.2173558	-1.245638	-0.7123915	-0.24698922
C9 H17 N2 O3 P	0.1527536	-0.9756197	0.05625136	-0.04384329
C24 H48 N3 O11 P	-2.8135076	1.7517741	1.3918991	-1.4843936
C11 H20 N4 O3	-1.9097579	0.15401979	0.2433273	-0.3505216
C25 H26 N12	-1.4895638	-2.3532188	-0.3146832	0.72809356
C32 H48 N2 O4 P2	-0.3152967	-3.4775326	-0.6716405	-0.05226709
C30 H38 N6 O6	-2.217404	-1.6959329	-0.26365936	0.42705804
C14 H22 N2 O2	-2.9781218	-0.40678203	2.5125046	-0.8289071
C14 H22 N2 O3	-0.7763522	0.5676595	0.083179474	-0.29929233

C24 H27 N5 O2	-2.569183	-1.0259805	-1.1560919	0.02097787
C38 H45 N P2	0.41074485	-0.0741137	-1.2635521	1.6554695
C10 H10 N8	-1.3801056	-1.0778587	-0.030124873	0.2659476
C34 H40 N6 O S2	0.6212681	-0.6253468	-0.26243016	1.2133362
C9 H8 O3	-2.3081973	1.6398762	0.3316581	-0.60779923
C9 H8 O2	-3.2516687	-0.48286426	-0.33203435	-1.0087023
C32 H67 O5 P S3	0.8403674	-0.96592367	0.7793864	0.49936825
C10 H19 N7 O	-2.5631657	-0.19270962	-0.077308714	1.0182031
C22 H26 N O P	-0.6273321	0.27898994	0.601552	-1.4613223
C13 H31 N7	-1.7861114	-0.37457713	1.9300246	-0.91676635
METHIONINE (CAS# 63-68-3); (M+H)+	0.39339742	1.7002417	-0.014037641	0.5661249
C28 H44 O4	-0.9457129	-3.8322854	-0.88295823	0.22819833
C20 H39 N O2 P2	-3.8927822	-0.7983079	0.056466836	-0.37344325
C12 H29 N4 O3 P	-2.4048326	-1.201638	1.2923999	1.1738257
C24 H32 O3 P6	-2.9286754	-2.6074295	0.2311258	-0.60867316
C38 H49 N5 P2 S2	-1.1910388	0.7905516	0.6776308	0.49557638
C11 H21 Cl N4 O3 S3	-2.78245	-0.87357944	1.1033089	-0.5571558
C16 H20 P2	-2.8303294	-0.02361992	-2.2925568	0.93575746
1-AMINOCYCLOPROPANE-1-CARBOXYLATE (CAS# 22059-21-8); (M+H)+	-0.18683308	1.4025908	0.17046556	-0.23272222
C26 H37 N12 O P	-0.7709343	-3.8845398	-0.8397014	0.3643939
C26 H52 N2 S3	-0.46155572	0.6959591	-1.194835	1.9812045
C4 H4 N4 O3 S	-1.6650536	1.1359941	-0.29450256	-0.4357684
C11 H14 N6 O	2.0374207	1.3794377	1.4729135	0.70738274
C41 H62 N5 O P S	-1.620256	2.3118987	0.058413923	1.1651245
C21 H40 N2 O2 S	-0.915529	-0.08301538	-2.0771165	1.9053531
C18 H26 N6	-2.4745262	1.3081623	-0.096214674	-0.2244426
C32 H40 Cl N3	-3.4147706	-0.8438026	0.36777842	0.33062238
C34 H43 N4 O3 P	0.08314637	-3.4359403	-1.2496223	-0.948853
C18 H37 N9 O S	-1.7449074	-0.4141979	0.26848263	-1.2678397
C20 H30 N8 O P4	-0.65903413	-1.9273384	0.69745815	1.4735435
C30 H61 N4 O3 P S	-1.9585905	0.022175506	1.5755622	1.335317
C21 H43 N4 P S	1.6904793	-1.552038	0.28185385	1.5812641
C17 H25 N12 P	0.29292172	-0.62832433	-0.4267869	1.8672929
C15 H19 N7 O2 S3	-2.4536922	1.0608481	0.41788608	-0.17857379
C24 H28 O3	-1.788072	-0.28276846	-0.6920932	0.14021924
C24 H28 O2	-1.7322998	-0.59460455	0.09009376	0.2725147
LEUCINE (CAS# 328-39-2); (M+Na)+	-1.4444165	-0.38930625	-1.2948031	0.02162695
C12 H30 N2 O4 S2	2.8624387	-0.69142425	-0.056247517	-0.27241585
C9 H10	-2.8066947	-1.7445331	-0.54219306	-0.815472
C28 H52 N3 P S3	-2.0458956	0.33511603	0.07217221	-0.11774642
C29 H49 N4 O P S3	1.1482825	-1.7873992	0.43348235	-0.15745291
C26 H54 N6 O S2	-1.8639265	0.78943545	-1.0771527	1.4792682
C30 H44 N4 O11	2.207239	1.5924603	-0.8796319	-0.619435
C21 H30 O5	-0.8647858	-0.37023312	0.64123833	-1.3708183
C29 H58 N2 O S3	1.2313832	-1.5761112	-0.18502611	1.8582547
C21 H30 O3	-0.966231	1.6194232	-1.3435256	1.34384
C8 H6	-2.7115002	-0.30883497	-0.22211505	-0.7482686
C7 H14 P2	-3.161009	-1.2522731	-0.74292105	0.06797283
C29 H61 N O P2 S3	-1.5305443	-0.09472809	-0.9041861	-0.023290493
C10 H17 N7 O	-2.603875	0.81531596	1.2503074	0.430794
C16 H28 N6 O2	-1.8889366	1.1345959	-2.2213817	1.4976355
THEOBROMINE (CAS# 83-67-0); (M+H)+	-0.9467404	0.35950112	0.10052814	-1.0745842
C30 H62 N6 O3 S2	-2.2078123	1.1161628	-0.8375847	1.010348
C12 H22 O2 S3	-1.6233032	-3.4761684	-0.8761188	0.5072347
C18 H15 O P	-2.2272055	-1.0909793	0.3069124	-2.279276
C18 H33 N3 O3	-1.3898236	0.18224819	-1.4697437	1.2023038
C45 H61 N O3 S2	-0.16637176	-0.4294921	-0.074697554	0.22208619
C31 H64 N6 O4 S2	-3.2963057	0.805253	0.96840274	1.6004059
C14 H30 O2 P2	-2.4089208	2.089634	0.21851227	0.12945601
C20 H34 N2 S3	0.6951906	0.64246607	0.67265195	1.6268091
C22 H44 N6 O11	-4.0175004	-0.10673125	-0.3018859	-0.30213764
C12 H19 N O2 S2	-2.0526128	-0.14322022	1.7974864	0.80446297
C34 H52 O3 P4	-0.9692929	-3.6680236	-1.0741669	0.3207746
C11 H22 N2 O3	-1.9285351	2.3921406	0.008385062	-0.354084
C21 H34 O6	-1.879443	-0.76146907	0.021656195	-0.48260945
C11 H28 N5 O3 P	-0.63308096	-0.9155462	0.4153787	-1.248221
C25 H55 N5 O3 P2 S2	-1.9203286	0.21114072	0.4140254	-0.84157413
C20 H26 O3 P2	-2.4961576	-1.536549	1.0134574	0.711536
PALMITOYLCARNITINE (CAS# 2364-67-2); (M+H)+	-2.3083832	0.49806675	0.105006814	-0.18443897
C10 H12 N2 O3	-2.5707867	-0.846345	-0.8782654	-1.0373552
C6 H10 N6 O	0.2754684	0.05525829	-1.4007286	1.331529
CIS-ZEATIN (CAS# 1637-39-4); (M+H)+	-0.4201027	-3.9006648	-0.9105878	0.42689693
GLUTATHIONE (CAS# 27025-41-8); (M+H)+	-0.5793206	-0.05154653	-0.95783395	-1.8208103
C29 H50 N7 P S2	-1.5561215	0.6503134	-1.3932365	0.22404402
AZELAIC ACID (CAS# 123-99-9); (M+Na)+	-3.1299403	0.81008613	-1.4422836	-1.4165155
C17 H35 N4 O3 P	-1.1180226	0.88309586	-1.7002059	2.4426382
C24 H33 N4 P	-0.25362027	-2.6761765	-0.12945026	-0.45344973
C23 H29 N11	-0.826315	1.3887455	-0.7382666	-1.1302816
C21 H20 N8 P4	-0.81995714	-0.9678023	-0.11490905	-0.4439449
NORLEUCINE (CAS# 327-57-1); (M+H)+	1.0404081	0.9623961	-0.5133288	1.5111212
4-ACETAMIDOBUTANOATE (CAS# 3025-96-5); (M+Na)+	-2.4631655	-1.1882318	0.21306837	-0.13937147
C11 H12 N6	-2.9822955	-0.40019894	1.7200354	-0.34629804
C24 H49 N4 O P S	-3.3523226	1.6320684	0.17529792	1.0687658
C14 H33 N4 O2 P	-3.4017413	-0.53856635	-0.57567555	0.27728158
C25 H54 N4 O2 S2	-3.271101	1.7340217	-0.4549206	0.32021484
C12 H26 O7	-3.8268924	-0.8478243	-0.21607164	-0.3024776
C17 H37 N O3	-2.732467	-1.0837011	-0.32149985	-0.74921656
C17 H37 N O2	-0.80330515	-0.9402544	0.29374582	-1.9303854
C13 H18 O2	0.52069646	-0.19092578	0.59810627	-1.5705454
C16 H22 N2 P2 S	-1.8350623	0.40450373	-2.8569293	-1.1447672
C25 H45 N O4	-1.4635088	3.1497617	-1.3230102	0.8263296
C25 H45 N O8	0.18014513	0.41581666	0.13475657	-2.0159664
C23 H25 N5 O2	-2.7797492	-2.2771661	0.85691583	-0.3147609
C17 H18 N6 O3	1.6009111	0.21947986	0.9603101	-0.3057463
C5 H4 O4 P2	0.8226571	1.6412295	-2.0452955	-0.002666593
C30 H45 N5 O7 S2	0.2809836	2.5823164	-0.9093129	0.966123
ISOLEUCINE (CAS# 73-32-5); (M+H)+	0.9349172	1.4446275	0.14903757	1.4926987
C24 H36 O5	-0.27926755	-0.64663804	-2.6511507	-0.82587695
GLUTAMATE (CAS# 56-86-0); (M+H)+[-H2O]	0.56274635	1.0588931	-1.0864909	0.001961008
ASCORBATE (CAS# 50-81-7); (M+H)+[-H2O]	-2.9173715	-0.21005988	0.4337232	0.43063426
C25 H39 N O6 S2	-2.059012	-1.7253608	2.1965508	0.1383245
C18 H41 Cl N6 O S	0.22006708	-0.69259465	-1.0952579	1.5801868
C34 H68 N2 S	0.33676127	0.8299302	-0.85166854	-0.9744285
C21 H30 S2	-2.5498548	-1.0395691	1.0600046	0.001785696
INOSINE (CAS# 58-63-9); (M+H)+	-2.5350058	1.755865	0.6250512	-0.47881138
C37 H45 O3 P S	0.35526836	1.120194	-0.6102664	0.35236308
C10 H13 N	-3.0214548	-1.3294933	1.2575492	-1.2440262
C31 H56 N2 O P6	2.2066207	1.5929185	-0.8946528	-0.6174226
C19 H22 N6 O2	-1.5113672	-0.5802331	-0.27376142	0.2257811
C28 H59 N P2 S3	-2.1608481	0.8317865	-0.015097857	0.5091136
C23 H45 N2 O3 P S	-2.4579387	1.6133301	-0.95880544	0.40847474
C29 H55 N3 O3 S3	-1.1232305	0.39993262	-0.95062006	2.0266302
C9 H17 N6 O P	-1.7250009	0.3625476	1.6732081	0.2988295
C11 H19 P3	-3.3454404	1.558203	0.5880763	0.20506614
C26 H47 N6 O4 P S	-0.9153549	-3.875309	-0.431529	0.39789674
C5 H10 N4 O2	-1.4204123	-0.15839247	-0.02418144	-1.1528546
C12 H22 N8	-2.4051878	1.8015163	1.5759989	0.61454135
C28 H47 N4 P S	0.45753914	-3.8859985	-0.6023104	-0.054563403
CAFFEINE (CAS# 58-08-2); (M+Na)+	-1.7747911	0.72083783	0.068304434	1.366834
C26 H42 N6 O4	0.52323896	-3.8589365	-0.91144186	0.3780163
C24 H49 N5 O5 S3	0.85156685	0.28283107	-1.2518072	0.838803
C32 H50 N10 O4	-1.9256002	-0.77536416	-2.9935637	0.55131745
C26 H42 N6 O5	-0.022092357	-3.9160583	-0.92101604	0.35505745
C24 H47 N4 O2 P S	-3.6115005	0.9015045	0.23518114	-0.26053602
DEBRISOQUIN (CAS# 581-88-4); (M+H)+	0.9159082	0.2123944	0.13889118	0.3559305
C17 H23 Cl O	-2.1015012	0.9003232	-1.9405293	-0.92224526
C32 H36 N8 O3	-1.0326775	-2.6388087	-1.2173208	1.5747638
5'-METHYLTHIOADENOSINE (CAS# 2457-80-9); (M+Na)+	0.9873009	0.78674877	-1.0767608	0.5151356
C19 H40 O2 S	-0.9320564	1.1703225	0.1166603	0.83229536

C18 H32 N6 O3	-1.0421462	0.27779284	-1.5605522	0.33721638
C18 H39 O7 P	0.9000418	2.2117705	-0.70227	0.50629723
C8 H12 O S3	0.63958657	0.9185847	-0.91437536	-0.46819395
C10 H17 N2 O2 P	-3.6344306	0.38425463	0.8077787	1.1033921
C10 H21 N6 P	-1.9915897	0.31568348	0.86835396	-1.7025832
PIPECOLATE (CAS# 535-75-1); (M+H)+	0.020870104	2.0813816	-1.1817509	-0.9992457
C27 H57 N O2	-1.3305688	-1.4377587	-0.023987733	-1.33011
C26 H37 N O6	-2.688886	-1.6709335	-0.02198276	-1.1029866
C13 H24 N2 O4	-3.7947245	0.05881849	0.40113842	0.17862675
C31 H63 N4 O10 P	-2.0524595	-0.9271771	-2.9519703	0.33988956
C32 H37 N20 P	-0.31341884	0.51340747	0.21848918	0.28110808
C22 H46 N O7 P	-2.6760228	2.87958	-0.15487677	0.38421327
C16 H36 N2 O2 S2	-2.1878152	0.97456753	-0.6659534	-0.072297096
3'-CMP (CAS# 63-37-6); (M+H)+	-0.800255	1.3853083	-0.91564757	0.013159439
C23 H30 N10 P6	-2.465314	0.08979222	-0.75536466	0.30899203
C22 H46 N8 O S3	-0.8032601	-2.6048622	-0.67647016	-0.77277
C11 H20 N2 O3	-3.2444563	2.0066342	-0.44166505	-0.065648854
C15 H18 N5 O2 P S3	-3.1555371	-0.94203424	0.10304649	-0.3633859
BETAINE (CAS# 107-43-7); (M+Na)+	0.17615424	-0.69782907	0.3230062	-1.4677306
C15 H33 Cl N4 O	-1.9816093	-1.1635113	-0.6120607	-1.290493
C6 H11 N O	-1.0402366	-0.96091	-1.4753895	-0.64407456
C26 H48 N2 O2 S3	0.18221232	-3.0800796	-0.52345765	-0.5109757
L-ARGININE-(GUANIDINEIMINO-15N2) [ISTD] (CAS#); (M+H)+	2.455324	-0.8164439	0.23420995	0.23392113
C14 H32 N2 S2	-3.1535602	-0.066664726	0.4863919	2.1262956
C14 H35 N7 O2	-2.7975955	0.2591924	0.3843004	-0.17077656
C21 H33 N3 O3	-2.1613255	0.6126399	1.1801457	-1.8766453
C21 H28 N10 P6	0.24761665	-0.46458918	-0.453092	0.683571
C31 H38 O6 S	0.40431857	-0.37620574	-1.4180899	2.7914858
C22 H43 N7 O4 S2	-0.22204679	-1.5132259	-0.79459643	0.6443212
C8 H19 N	1.5068749	0.63243365	-0.27610946	0.7370734
CMP (CAS# 63-37-6); (M+H)+	-1.6521672	0.16065486	0.10496664	1.009805
C12 H18 O3	-1.3902559	-3.511129	-0.87153786	0.57382864
C24 H10 N2 O4	-0.8926612	-3.3410938	-1.3214732	0.5922127
C16 H32 N8 S5	-2.9509618	-1.3447529	0.17114234	0.20781523
C20 H16 N4 O	-1.6660924	-3.0784311	-1.321156	0.57912016
C30 H58 Cl N2 O3 P	-0.899711	0.8736598	-0.03450544	-0.3017166
C9 H17 N O2	-1.5948788	-0.42260742	0.25795537	-0.22345376
ISOLEUCINE (CAS# 73-32-5); (M+Na)+	-0.6322275	0.2908464	-1.2654359	-0.54647386
C9 H17 N O4	-1.4700621	2.240821	-0.7529726	0.5174755
C17 H19 P S2	-0.8496146	-1.2875836	1.933502	0.5831768
C9 H18 N2 O3	-0.88311327	1.2579893	-1.3701508	-0.41679347
C22 H34 N2 O P2 S	-2.1804414	0.55784124	-1.9876138	-1.1000556
C25 H34 O3 P2	2.6306808	0.16653825	-0.38697064	0.73470086
C30 H61 N4 O4 P S	-3.3451693	1.0727993	0.65575397	1.4803919
C29 H60 N11 O2 P3	-0.81063306	1.3885523	-0.4517434	-0.48169512
C19 H23 P	-0.004701974	-0.50477993	-0.7715693	2.1119483
C15 H29 P S	1.672865	-1.3149023	2.0235431	0.9704685
C30 H50 N7 O2 P S2	-1.5262157	0.9418884	-1.1678815	0.011010855
C39 H37 N3 O2	-0.003377281	0.66429037	0.357515	0.32037103
C26 H52 N3 O11 P	-0.89842176	2.3310246	0.13046044	1.8557563
C19 H35 O P S	-2.812059	2.246336	-0.40005866	0.2544191
C10 H21 N4 O3 P	0.70400697	-1.344861	-0.8492375	0.8301645
C17 H34 N6 O S2	-3.0119808	1.3759003	-0.5132402	-0.4653518
C21 H29 O4 P	-0.46729064	-0.24698038	0.5301953	-0.8735655
C37 H34 N O P	-1.7595633	0.44970414	0.9144659	-0.48334116
SUBERIC ACID (CAS# 505-48-6); (M+Na)+	-2.3372936	0.24483895	-0.60351133	-0.54602313
C13 H24 N6 O2	-2.565735	0.2345376	-1.0955749	-0.36115986
C16 H39 N7	-2.977581	-1.1020622	0.3820385	-0.6685385
C10 H14 N2 O2	-2.8630767	-0.41943976	1.0489948	0.21649265
C13 H24 N6 O3	-1.2227757	-0.8956388	0.26569265	0.50700444
C22 H46 N2 O P2 S	-0.37526888	-0.6224128	-2.8084404	-1.2218671
C11 H21 N7	-2.1817799	-0.038139343	-0.19885612	1.260706
C14 H33 N7	-1.7741457	0.3726176	-0.094569504	-1.1385244
C17 H33 N2 O P S2	-0.66518176	-0.8270929	-0.99747974	0.1718282
PANTOTHENATE (CAS# 79-83-4); (M+H)+	-1.6983728	0.5888702	-0.14895846	0.060058296
C26 H40 S	-3.0164807	1.6316212	0.25449747	0.95056695
C5 H7 N O3	-1.9166262	0.36456174	1.4787228	1.1904776
C4 H9 O2 P	-1.4160053	0.56677324	1.1411588	-1.3797493
QUINOLIN-2-OL (CAS# 59-31-4); (M+Na)+	-2.3281374	-0.5223669	-1.0092891	1.0219636
C20 H29 N4 O5 P	-0.28090334	0.59043944	-2.9899757	-0.57850087
C25 H26 N4 O2	-2.8149436	-0.84862053	-1.832703	0.14682889
C14 H27 N4 P3	-1.449138	-0.9307176	-2.184616	-0.07811267
C12 H11 N9 O	-1.8634112	2.9373853	-0.8023087	0.001104772
C20 H35 N4 P3	-0.3360408	-0.29040676	0.66372657	2.8554215
C15 H31 N4 O2 P	-0.6221055	0.5516157	-1.5241657	2.5978038
C15 H15 N3 O S	-0.18015173	0.11000836	-1.4114119	0.200831
PHENYLALANINE (CAS# 63-91-2); (M+H)+	-3.47659	1.6337947	0.1053538	-0.93130374
C14 H27 N7 O	-2.283327	0.1419703	0.33421814	1.0528297
L-HISTIDINE (CAS# 71-00-1); (M+H)+	0.535075	-0.79187787	0.6550308	0.14525077
C34 H68 N2 O9 S2	0.14085308	-0.3079712	-3.4921167	-0.87787634
C36 H66 N O P	-2.9102216	1.2615827	-0.7432839	0.049583733
C39 H48 O2 P4	-2.5140915	-0.07350227	-0.98119676	-0.015322149
C27 H51 O4 P S2	1.4660705	-3.5059004	-0.4183405	-0.08587012
C29 H32 N18 P2	-0.17558366	-3.3436742	-1.7797967	0.13272539
C25 H53 N O2	-2.6074934	0.1025264	1.7483596	-0.4909326
C50 H93 N3	-0.51051056	-0.74196273	-0.29819965	-1.9893136
C30 H59 N O4 S5	-2.8096802	-0.28160182	-0.3038973	0.31222567
C16 H24 N6	-2.291918	-0.44818506	0.90627927	0.023580372
16:0 LYSO PC (CAS# 17364-16-8); (M+Na)+	-3.1719608	1.6643655	1.2767842	-1.114255
C26 H50 N3 O11 P	-2.145818	2.9821892	-0.26768672	-0.6194793
C17 H22 N10 P2	-1.7350199	-0.32104635	-0.38529387	1.5623258
C6 H4 O	-2.862411	-0.84616905	1.0480105	-0.559262
C23 H41 N	-0.9276067	1.0527897	-3.3050396	-0.47811922
C13 H25 N O2	-1.9377297	0.37788555	0.4373712	1.2103382
C15 H19 N4 O3 P	1.2445924	1.5317042	-1.0503185	1.5571406
C24 H54 N12 S2	-2.4477189	0.3108641	0.47011635	0.6990042
C13 H25 N O4	-2.3848212	0.13015506	0.80546355	-0.72080135
C13 H25 N O3	-3.8153675	1.0531999	-0.335806	0.55016166
C25 H51 N5 O10 S	-0.4125616	1.6652141	-0.32186195	2.2270908
C27 H41 N5	-1.0765033	0.50431097	-0.2588837	0.7250476
C19 H41 N3 O3	-0.21193415	-0.310225	-0.45329502	1.4201757
C17 H33 O2 P S2	0.8623839	0.9109814	-0.04936862	0.7632493
C13 H25 N7	-1.8187919	0.01670222	-1.4561292	1.1435982
C9 H24 N4 O2	-0.14215603	0.1888665	0.07217372	0.6151617
C22 H29 N3 O2	-2.384029	-0.40573943	-0.35983124	-1.3595994
C26 H58 N4 O2 S2	-2.8838975	1.2346417	0.3855582	0.91291225
C32 H65 N4 O4 P S	-2.1897807	0.5465899	1.5819854	1.4987729
C29 H15 N8 O2 P	-1.3228158	-1.5502125	0.93104404	0.44416627
C31 H43 N3 O3 S	1.2703378	0.6481671	-2.4226532	-0.06282191
O-ACETYLCARNITINE (CAS# 461-77-8); (M+H)+	-1.9016253	1.7323239	-0.34413695	0.32612163
C16 H37 N7	-3.5521493	-0.65984666	1.6952922	-0.75136405
C36 H66 N6 O4 P2	0.5407739	1.9235818	-0.34100312	1.5942875
C19 H41 N3 O5	-3.2433107	-0.021940462	0.49688154	-0.017239347
C8 H14 N2 O3	-2.1494737	2.0360065	-0.27266398	1.6424339
C30 H33 N7 O2	-2.7778862	1.2456592	0.6974162	-1.0813364
C28 H53 N5 O5 S3	-1.3092748	0.91677123	-0.6819412	-1.0493118
C6 H15 N3 O2	-1.1118852	0.79566646	0.9538605	-1.9947717
C33 H27 N7 O2 P2	-2.4883726	1.0062563	-0.26818478	-1.1441529
C31 H37 N9 O6	-0.77764595	-0.42948803	1.2877584	1.1042563
C19 H41 N	-2.909659	0.654234	-0.8644799	0.8841508
C26 H55 N O2	-2.907174	-0.24001545	1.689203	-0.57549775
C19 H21 N9	-1.6176797	0.38296217	-0.12459368	-0.22165361
C17 H38 N2 S2	0.90069944	-0.25480807	0.5686795	1.2617636
SERINE (CAS# 56-45-1); (M+H)+	-0.7678914	0.63687336	0.11695189	0.73615736
C21 H34 S5	-1.7127398	-0.16253382	0.97692555	-0.41466036
C35 H60 S3	1.18297	1.5417689	-1.0611129	1.7368314
C31 H68 N12 O4 S2	-3.45781	0.7120056	0.4453294	1.6488909
C14 H30 O8	-3.8241472	-0.84312403	0.09045547	-0.32810897
C14 H34 N2 S2	0.534711	0.87463343	0.68519163	-1.1509943

C25 H56 N12 P2 S	-2.1143537	0.02245161	-0.021685451	-0.90621895
TAURINE (CAS# 107-35-7); (M+H)+	0.76844406	0.47388414	1.0040014	0.39297175
C19 H28 N6 O	-1.6187874	-0.6070419	1.1022297	-0.5827672
C20 H45 N3 S2	-0.2822333	1.5939156	0.9308505	0.48558742
C4 H11 N	-2.780722	-1.7659676	0.72089547	-1.1499754
C42 H86 N2	1.1800228	-0.3466407	-0.26359123	0.14799711
N-ACETYL-L-ALANINE (CAS# 97-69-8); (M+Na)+	-1.6347704	2.2952836	-0.79736954	0.14185011
C32 H8 N2 O P6 S3	0.06538431	-0.4090121	-0.18010804	-2.3882694
ACETYLCHOLINE (CAS# 51-84-3); M+	-0.8655904	1.7714357	-1.6501684	-0.85534865
C19 H27 N3 O P2	-0.5269767	0.2573803	0.49181807	-0.07394842
CORTISOL (CAS# 50-23-7); (M+Na)+	-0.6662936	0.044468783	0.3758621	0.047200523
C33 H50 N5 O3 P5	-0.92209965	0.81498045	-1.1711361	1.4879258
C38 H82 N6 P2	0.122279406	-0.62248033	-0.48856646	-0.9578908
C21 H32 N6 O2	-2.1526122	0.29305547	-0.19093189	0.17249721
LL-2,6-DIAMINOHEPTANEDIOATE (CAS# 583-93-7); (M+H)+[-H2O]	-0.31178278	0.8098593	-0.38024768	-0.48301673
C9 H15 O P S	-2.1166484	0.84750724	0.018924996	-0.044335186
C16 H20 O	-1.371158	-0.52811515	2.311214	0.34410638
C43 H83 P	-1.5291489	0.2537691	-1.0262668	-1.5384846
C20 H36 N2 S	-0.8420156	0.2553447	0.6973457	0.2990107
C12 H16 O4	-0.69368345	-1.0567733	1.3245394	1.0393218
C13 H18 O3 S	-1.7595942	-0.33174354	0.47004682	-0.23983082
C19 H36 S5	0.6685475	0.36934212	-1.3506957	-1.4899983
C41 H45 N7 S	1.9303429	1.8148142	-1.1541102	-0.5197281
C23 H39 O7 P	-1.0706313	0.5452222	0.5277791	-0.12613921
C16 H30 O2 P2	-2.01192	-1.015799	0.32191992	0.24304107
C15 H24 N2 O3	-3.2572901	0.60805315	1.1614771	-1.1466576
BETAINE (CAS# 107-43-7); (M+H)+	-0.37598276	2.4193182	-1.0862541	0.7661112
C21 H39 N3 S	-2.04E-04	0.21904132	-0.33056733	2.1596715
SPHINGANINE (CAS# 764-22-7); (M+H)+	-1.003644	-0.422272	-0.97796655	1.2873054
C20 H46 N4 O P2	-0.6178836	-0.81665003	-0.23142417	-0.011427254
C37 H52 S3	-0.53668475	-0.7697058	-0.5922158	0.1915589
C6 H14 O3	0.76897144	-2.1254287	-0.9142275	1.1650923
C40 H86 N2 O4	0.08853406	-0.5266889	0.45573092	-0.09168099
C47 H37 N O3 S	-2.357916	-0.70370317	0.4800816	0.22379391
C18 H32 O2	-0.13532886	-0.48710632	0.20809129	0.029394746
C22 H36 N P	-1.7811922	-0.27337602	-0.4113684	1.6251421
C17 H36 N6 O2 S	-0.1828109	1.1894494	-0.8047407	1.2260027
C28 H48 N6 O S	-2.2257326	1.035175	0.24311101	2.141442
C26 H55 N5 S5	-0.7487448	0.59391177	-0.9878284	0.14912829
C31 H66 N8 O2 S3	-0.09545933	-0.6142831	-1.2322397	0.16917491
C41 H82 O	-0.3428986	1.5428442	-1.08895	-1.1072782
C37 H80 N4 O2	-0.47074848	0.59376884	-1.0756961	-1.6648291
C43 H91 N2 P	-1.7499524	1.7508134	-0.12637375	-1.3998361
C28 H38 O6 P6	-2.017348	-0.5381319	0.62650526	0.151021
C32 H2 O5 P2 S5	0.08294627	1.0633451	-0.24891165	0.1991936
C43 H90 N5 P	-1.3191514	0.03184442	0.32445377	-0.8037986
C34 H64 N4 P2 S	-1.9763083	0.78502464	0.24885064	-0.64804304
C6 H9 N O4 S	-0.6582972	0.479218	-1.6867607	-0.38556182
C30 H37 N13 O8 S	-0.4048864	-0.732766	-0.7602055	0.6703085
C13 H21 N O2	-1.3177867	-0.12827902	0.5718017	-0.32219037
C49 H101 N	0.6738378	0.09538162	-1.734575	-0.18994945
C32 H54 N2 O3 P2 S	-0.8700016	1.3289783	-0.40891945	0.83614457
L-CARNITINE (CAS# 541-15-1); (M+H)+	-0.48420376	0.19912083	-0.921164	-0.5743407
C24 H37 N11 O5	-0.63058674	-0.4168931	-0.68541354	-1.5609187
D-GALACTOSAMINE (CAS# 7535-00-4); (M+H)+[-H2O]	0.56483096	0.14363825	-1.0266951	0.48380283
C25 H47 N3 O5 S	-1.6242768	0.39577955	-0.5330588	0.1585083
C39 H47 N P2	0.18893452	-1.4997265	-0.5121084	1.6046941
HOMOSERINE (CAS# 672-15-1); (M+Na)+	-0.009428233	0.6503602	-1.2359178	-1.0011944
D-MANNOSAMINE (CAS# 14307-02-9); (M+H)+[-H2O]	0.56483096	0.14363825	-1.0266951	0.48380283
N(PAI)-METHYL-L-HISTIDINE (CAS# 332-80-9); (M+H)+	0.56839526	0.6502844	0.12715934	-0.25883344
C23 H48 N O7 P	0.7589052	1.337892	-0.79690266	-0.998718
C5 H5 N5 O	0.069346935	1.4159623	-0.3799913	0.86852956
C38 H47 N2 O8 P	0.9607913	0.44412968	-1.7561116	-0.09910061
C14 H22 N2 O	-0.56243527	0.56866944	0.21965945	-1.0004283
MELANIN (CAS# 8049-97-6); (M+H)+	-0.5513027	-0.15168649	-0.14979348	0.5496983
BIS(2-ETHYLHEXYL)PHTHALATE (CAS# 117-81-7); (M+H)+	0.53341085	1.0396384	-0.2806837	0.9324283
C10 H15 N4 P	-2.7237012	0.41507423	-0.017599922	-1.0249571
VALINE (CAS# 72-18-4); (M+Na)+	-1.8509051	-0.5131101	0.98530877	-1.7584146
C10 H18 N2 O	-0.1903761	0.27304414	0.042691447	0.4995675
TAURINE (CAS# 107-35-7); (M+K)+	-0.6062918	-1.3427849	-0.38771334	-0.01004532
C7 H13 N O2	0.25909254	1.0302854	-0.6323632	1.8298174
L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)+	1.3134838	0.6000143	-0.07406078	-0.22656216
HOMOSERINE (CAS# 672-15-1); (M+H)+	1.3134838	0.6000143	-0.07406078	-0.22656216
C40 H38 N5 P3	-1.4764123	0.46536747	0.42611203	0.09916575
GUANINE (CAS# 73-40-5); (M+H)+	-0.2487285	0.2070626	-0.14342019	-1.299055
C5 H11 N O2 S	0.39013368	1.6998246	-0.011307837	0.5661986
C12 H18 N8	-0.022234444	-0.34453958	0.5037062	0.9398397
C18 H33 N6 O2 P5	-1.0346354	0.13746454	0.30472612	-0.8208366
TYROSINE (CAS# 60-18-4); (M+Na)+	-2.2257247	-0.851846	-0.33259523	-0.83227634
SUCROSE (CAS# 57-50-1); (M+Na)+	0.85790384	-0.09594981	-2.0631404	-0.29919556
NORVALINE (CAS# 6600-40-4); (M+H)+	-1.170278	1.73229	-0.38000676	0.03255901
BETA-ALANINE (CAS# 107-95-9); (M+H)+	-0.5941436	-0.059084453	-1.5174391	-0.4500078
CELLOBIOSE (CAS# 528-50-7); (M+Na)+	0.85790384	-0.09594981	-2.0631404	-0.29919556
MELIBIOSE (CAS# 585-99-9); (M+Na)+	0.85790384	-0.09594981	-2.0631404	-0.29919556
VALINE (CAS# 72-18-4); (M+H)+	-1.1694851	1.7363962	-0.37619135	0.034828518
BETA-MALTOSE (CAS# 69-79-4); (M+Na)+	0.85790384	-0.09594981	-2.0631404	-0.29919556
LACTOSE (CAS# 63-42-3); (M+Na)+	0.8582601	-0.096490055	-2.062766	-0.3008445
C5 H11 N O2	0.41108897	1.9850076	-1.2280855	1.1903361
PALATINOSE (CAS# 343336-76-5); (M+Na)+	0.85790384	-0.09594981	-2.0631404	-0.29919556
SARCOSINE (CAS# 107-97-1); (M+H)+	-0.5941436	-0.059084453	-1.5174391	-0.4500078
URACIL (CAS# 66-22-8); (M+H)+	-0.49581882	1.0910883	-1.2493235	0.96567726
SPHINGANINE (CAS# 764-22-7); (M+Na)+	-1.7665622	0.42062566	-0.6012409	0.6995569
MALTOSE (CAS# 69-79-4); (M+Na)+	0.8582601	-0.096490055	-2.062766	-0.3008445
5-AMINOPENTANOATE (CAS# 660-88-8); (M+H)+	-0.4155491	1.5047652	-1.6625125	0.87145287
C19 H30 O4 P2	0.025088236	-0.80140036	-0.6536106	-0.46980318
UROCANATE (CAS# 104-98-3); (M+H)+	-0.31037295	-0.3818244	-0.12329705	-0.96736974
C22 H27 N2 O3 P	-0.5312381	-0.010013178	0.04940693	-0.6584667
100.001@0.5352921	0.16412914	0.3495564	1.5191069	0.21195203
284.0765@2.291664	0.61268085	1.6767333	-1.7048345	1.4425174
226.0954@3.0594227	-2.965444	-0.66347253	-0.28079778	0.1498254
260.1374@3.1285338	0.6586319	0.6347213	-1.9348218	-0.68691593
913.233@3.608588	-1.2571018	-1.0077349	1.4767283	-0.16466562
987.5345@7.6266623	-2.2357683	0.48103446	-0.52235234	-0.75561684
785.5006@8.232729	-3.3811388	-0.36604983	-0.60161185	-0.9833654
1039.5897@9.211685	-2.9704952	0.4780026	-0.5416486	-1.6201197
1053.6014@10.078312	-1.6771326	-0.3559702	-0.22722168	-1.2355721
939.5053@10.673127	-3.2486427	0.27962577	-0.002281278	-0.97655517
1005.4501@10.68129	-3.0068686	0.24528679	0.086904116	-0.95831954
766.3968@12.524396	-3.6357691	0.5967283	-1.2316749	-0.49425656
810.4211@12.899628	-3.524336	0.8156637	-1.5854195	-0.10295531
854.4479@13.245994	-3.436826	0.8213225	-1.5884084	-0.47098106
898.4725@13.568503	-3.2934394	1.0110323	-1.6458393	-0.6694556
942.4985@13.866499	-2.6954756	-0.26289642	-2.1467936	-0.50219166
1030.5504@14.407582	-3.118217	0.88869303	-2.0793436	-0.5690428
856.2961@16.427088	-3.015727	-2.3159213	0.69787276	-0.56994987
1196.4637@16.426586	-3.114346	-2.2405977	0.6917736	-0.64135313
810.295@16.42741	-3.080004	-2.270409	0.8272909	-0.64661527
794.3295@16.810375	-3.121972	-1.5414342	-0.6859598	0.5808411
794.326@17.455503	-2.8074403	-1.0101734	-0.7901785	0.5737963
822.3579@17.51095	-2.1449137	0.21224381	-2.4849718	-0.525661
866.3585@18.392859	-2.9016666	-1.8014011	-0.48186633	-0.9293755
445.2466@19.244831	-0.5296072	0.21577355	-3.1368089	0.021820083
982.6736@19.445652	0.48032218	-3.715164	-0.26398352	0.16855511
1484.9976@19.447369	0.8294047	-3.5186996	0.011755079	0.06499675
828.3997@19.74982	-0.39976084	0.7023258	-1.6332053	1.5834197
1614.941@19.78335	-0.5769902	-3.7234483	-0.95336163	0.39338467
1608.9333@19.784367	-0.5638368	-3.8360445	-0.9435173	0.3029771
1546.945@19.785664	-0.75003904	-3.8333268	-0.98309267	0.323585
1478.96@19.788363	-1.0699009	-3.8123696	-0.62493956	0.47000355

1066.6136@19.785637	-4.55E-04	-3.851453	-0.59747845	0.8789802
1134.606@19.783178	-0.6634289	-3.7631912	-0.9938318	0.0082075
1959.3063@19.789024	1.0602012	-1.843538	-0.83862895	0.030881375
1484.9901@19.787737	-0.77564615	-3.9231732	-0.224803	0.2770639
796.4833@19.792416	-0.4672908	-0.6141853	-3.122058	-0.09503983
359.3533@21.494558	-1.097992	0.58036906	-3.560374	-0.3714043
359.3371@21.756748	-1.4537189	0.47858936	-0.5948731	0.80843896
988.3911@21.79887	-0.41267532	-1.8841902	2.972952	0.8612528
778.4451@21.968401	0.6257381	0.16757329	-2.778667	-0.16278602
756.4574@21.98579	-0.06415888	-0.40934306	-3.5022597	-0.015260607
822.4739@21.999432	0.5668273	-0.40014803	-3.1677854	-0.22778423
1018.4765@21.967066	2.828886	-1.5884718	-1.6188385	-0.034849927
866.4949@22.026224	-0.25587797	0.7876873	-3.229449	-0.25260866
764.412@22.092783	-1.299006	-0.44963726	-0.82381636	-1.2496815
954.5524@22.05358	-0.7026156	0.42912236	-2.603876	0.3481785
808.4348@22.107382	-1.2976373	0.47841227	-0.98295164	-0.95509166
1138.606@22.160442	-1.4454733	-0.50520927	-1.6396536	-0.35560942
1182.6368@22.152647	-2.1714933	1.4615786	-0.7937895	0.22143173
750.4164@22.246555	-0.73968196	-1.5062995	-2.7196357	0.12021892
748.44@22.25464	-1.6927853	-1.3720008	-2.8986127	0.10146748
794.4457@22.256075	-1.8493072	-0.8668705	-2.361962	0.35113037
854.4511@22.263014	-2.4082384	-0.574216	-2.9453168	-0.17284527
792.4642@22.26437	-1.9998589	-1.4633468	-2.7938497	-0.03741055
838.4701@22.265482	-2.3424723	-1.4172603	-1.5788046	-0.86439484
770.4795@22.26616	-2.5268018	-1.0230439	-2.7195923	-0.25649822
898.4602@22.272749	-2.76495	-0.7793151	-2.1214411	-0.8236143
836.4918@22.271847	-2.4311512	-1.038885	-2.5021164	-0.9517447
814.5071@22.272953	-2.7230067	-1.0140438	-2.4287324	-0.68591535
942.4895@22.279886	-2.5765831	-0.9320904	-0.6893071	-1.2812144
880.5145@22.278997	-2.5452716	-0.4362031	-2.0072927	-1.4894061
858.5306@22.280897	-2.8018057	-0.471175	-2.0297613	-1.1694361
902.5615@22.287943	-2.704971	0.07564606	-1.5250709	-1.4924477
924.5438@22.285477	-2.5220652	0.25688428	-1.3772837	-1.6549523
946.5839@22.293484	-2.5434048	0.3770061	-1.0708764	-1.7440593
968.5668@22.29198	-2.309438	0.43737683	-1.0141076	-1.8870124
990.6147@22.29418	-2.4984605	0.5434772	-0.77680105	-1.6467692
1012.5953@22.298977	-1.2082728	-1.0322262	-1.346019	-1.8083262
1080.592@22.3007	-2.8425608	0.6910039	-0.20789067	-1.3051335
1056.6182@22.300308	-2.0162976	0.47606778	-0.48484522	-2.0162644
1124.6028@22.293247	-1.0520512	-0.54988027	-1.2749617	-1.3056477
1168.6357@22.313885	-1.3579533	0.48737502	-0.5531902	-1.6028947
1144.6743@22.311687	-1.9125451	0.5053896	-0.4402694	-1.8459238
1232.7281@22.32031	-2.0435483	0.5162121	-0.38941255	-1.4822232
367.417@22.331345	-2.2632394	2.1664658	-1.1032573	0.2623653
781.4594@22.326466	-2.1317627	-2.60799	-0.5548234	0.7286661
825.4897@22.337337	-1.1370274	-2.6883116	-0.86262196	0.49544305
806.4853@22.410055	-0.70123243	-1.7241931	-2.5481207	0.63226753
850.5065@22.444714	0.116760895	-0.2944993	-1.9587244	1.9890904
784.4937@22.412384	-2.9630787	-0.704131	-1.8688354	0.67195445
828.5144@22.427803	-3.0833902	-0.22040573	-1.2846974	0.057210803
758.4818@22.426146	-3.2933521	1.0410728	0.637151	1.5150822
872.544@22.427355	-3.273843	0.08884093	-1.4593308	0.23286214
802.5088@22.430168	-3.1748803	1.6627078	0.6831033	0.85701954
780.5207@22.436514	-3.509741	0.8486444	0.15303475	1.5863944
824.546@22.43388	-3.0996475	0.95889306	0.42513475	0.2742019
934.5858@22.438871	-3.2703366	0.57413447	0.2910257	1.1043471
868.572@22.445438	-3.4628239	0.7000948	0.20803207	0.49025682
912.5968@22.448559	-3.1726594	-0.5597121	-0.5351518	1.2457788
1066.6592@22.45198	-2.8568704	0.22600812	-0.11193704	0.73618686
904.5756@22.50441	-2.826008	0.9944166	-0.29817784	2.113467
1036.6488@22.501652	-1.4711394	0.9902615	0.58783233	2.0646303
1168.7233@22.505514	-0.81396306	0.76747656	0.8946537	2.3730135
763.4031@22.503992	-2.905166	1.0057354	1.9542351	-0.04063937
948.6022@22.490602	-2.0088577	1.2325108	-0.32170075	2.6593182
1080.6711@22.493565	-1.8897781	1.1581717	-0.5398027	1.6270409
1344.8298@22.509373	-0.94737625	0.413022	0.98968947	2.6877642
1432.8842@22.508942	-1.5021545	0.76250124	0.6787473	2.2903562
1212.753@22.50781	-1.1422384	0.20075254	0.47492087	2.4207077
1124.6996@22.511711	-0.5750532	0.5846409	0.70231044	2.55178
1256.7773@22.507423	-0.6171715	0.9925729	-0.37830678	2.3089542
1300.8066@22.50717	-0.47405547	0.58459175	1.0488569	2.326171
862.2494@22.540915	2.0332382	1.126893	-0.9471235	-0.7404379
794.2594@22.54076	2.4909315	0.58574396	-1.1090535	-0.66278636
750.5114@22.61297	-1.7202623	-0.4194867	-1.0606234	0.7909405
757.5616@24.534454	-0.25068274	0.52565956	0.8346377	0.052632615
829.5609@24.580767	-0.16320789	0.48330402	0.4135195	0.7893194
983.5043@24.547352	-0.64234746	0.11587797	1.0127871	0.51181066
873.5459@24.643751	-0.1281141	0.15246436	0.46694762	1.2388698
959.4948@24.635881	-0.35725328	0.20188706	0.7057124	0.9069576
849.7948@25.00409	-0.24859564	0.5815352	-0.66942275	-2.253247
899.8317@25.102629	-0.54616076	-0.11961137	-0.90866524	-2.3863087
831.8173@25.115229	-1.3181657	1.0213486	-0.39928073	-2.8248353
807.8118@25.191593	-1.3649106	0.8886391	-0.8423552	-1.4598292
875.8232@25.200348	-1.6474032	0.6054729	-0.5794347	-1.5863667
925.8544@25.280811	-1.0179827	-0.5978279	-0.36822262	-1.8399799
588.6146@25.369286	-1.1985176	1.8494838	-1.2035127	-1.9102168
767.7954@25.46408	-0.3301623	-0.4999879	-0.77204525	-2.0919895
851.8118@25.594587	0.45719063	-0.5248392	-1.1666756	-0.8889386
1185.4827@5.0349865	0.36276293	1.3490485	-1.7445568	-0.91546583
756.3904@6.6820736	-1.212087	0.023725867	-0.5999614	0.076318204
822.3443@6.673502	-0.9882525	-0.8720015	-0.19076703	0.7571432
980.6528@19.790384	1.4399601	-3.450898	-0.09484346	-0.017360002
1054.6086@22.301497	-2.0957096	0.5524047	-0.44374782	-1.8896326
764.5205@22.788843	-2.597632	-0.22326759	0.5051686	1.1981924
1342.8453@23.021261	-0.03754004	-0.38746583	1.7533503	1.8471206
1298.8292@23.027048	-0.40511116	-0.31166935	2.5575845	0.934256
1210.7787@23.040709	-0.003026098	-0.54005885	1.3802359	1.9753644
1166.7499@23.045338	0.2821926	-0.1518658	-0.109127715	1.8421941
1122.7275@23.046068	0.26409256	-0.15079154	-0.14114834	1.622332
1078.6967@23.051666	0.25740358	0.021866016	-0.0620273	1.6097625
871.5331@24.445992	-0.23041794	0.3984509	0.7881726	1.2395511
803.5482@24.449387	-0.06605914	0.60979086	0.7183601	0.87436324
795.5152@24.516008	0.15458573	0.4668205	0.5461925	0.97059137
925.4703@24.515404	-0.03724107	0.6494166	0.71075016	0.6089351
1819.008@24.514679	-0.014913574	0.659459	0.5843771	0.87668854
1825.0208@24.524853	0.012680426	0.3536985	0.34289718	0.78906167
779.5456@24.53104	-0.51656795	0.36505646	0.9657357	0.002262257
915.5211@24.535116	0.14078175	0.65420365	0.68221414	0.8546211
847.5322@24.538563	-0.116289586	0.53604496	0.90813977	0.29463938
783.5801@24.648405	-0.18144883	0.16921979	0.46569952	1.0501392
1053.4802@7.6255107	-1.7537252	0.3572247	-0.96805173	-1.0007141
844.5074@22.009975	0.6337739	0.18939619	-3.153501	-0.609717
888.5332@22.030827	0.30238402	0.15047115	-2.86988	0.13642639
769.46@22.165522	-0.7104667	-3.6980329	-1.2123183	0.67987525
1074.5717@22.300463	-1.3095697	1.8890297	0.47037515	-1.5623145
890.5538@22.44111	-3.4580703	0.9800283	-0.3817491	1.1800768
1388.8752@22.508917	-0.7268254	1.3142902	-0.29394308	2.2970953
521.5911@22.722954	-0.25890252	1.437565	0.543279	1.4091403
1006.6558@22.773655	-2.5751688	0.39584634	0.73855776	0.41691765
918.5902@22.784018	-2.7482407	-0.6831187	1.3379585	1.1394196
852.5821@22.78476	-2.2125044	0.13212608	1.6248322	0.8256672
808.5553@22.77996	-2.6582105	-0.3071209	1.616416	1.3752242
786.5182@22.788322	-2.012808	0.24925832	1.247339	1.3302791
830.5392@22.788803	-1.8733913	0.13729185	1.0571501	1.3270203
788.5265@22.951626	-1.1584473	-0.32701015	0.54578865	0.45447728
1474.927@23.01443	-0.23659551	-0.1324678	2.167883	1.6936723
1430.9071@23.017159	-0.16865402	-0.15124543	2.0625093	1.5095196
1454.8632@23.030483	-0.91223276	0.6185347	0.080804236	0.34541225
1386.8802@23.00639	0.014213324	-0.1463407	1.1603017	0.7234416

1410.8372@23.022943	-0.5843329	1.370288	0.4190223	-0.03366426
1366.8147@23.031672	0.19167826	0.034984946	0.07920424	1.6478257
1254.8029@23.033033	0.22378314	-0.04377941	-0.05440586	1.8241614
1278.7646@23.037779	-0.27884975	-0.08038813	0.007164996	1.6708889
1234.7437@23.039314	-0.6254495	-0.017898895	0.14381535	1.3402479
1190.7104@23.050585	0.4011259	-0.2771787	1.9813964	1.6403872
1102.6552@23.055687	0.63566816	0.40672785	0.19617064	0.9673574
1034.6707@23.058197	0.30744165	0.73283553	0.20588782	0.9532256
968.6634@23.068396	0.007600963	0.46482086	1.8179661	1.2568288
990.6445@23.054432	0.083702564	-0.39270943	1.7334217	1.5368601
946.6215@23.066227	0.45765305	0.51337117	0.22082183	1.1394573
924.6419@23.040983	-0.105006695	1.5552266	0.6335422	-0.21194051
902.5975@23.068104	0.27043056	0.16216555	0.0642433	1.1528131
792.5564@23.077744	0.28790012	0.4847381	0.13310328	1.3627756
580.276@19.786844	-1.7687696	-3.5725284	-0.6850851	0.19814743
968.5658@22.031195	-1.0293839	-0.6583518	-2.3330114	0.62307954
796.3903@21.512106	-1.1981789	-0.9945609	0.45411915	0.08566591
813.488@22.168575	-0.344835	-3.332937	-1.0688767	1.2139883
1320.7703@22.341627	-2.20808	0.7721035	-0.44742143	-0.033212632
938.564@22.436773	-0.7535994	0.76874286	0.6810486	0.7061027
846.533@22.45591	-3.1896753	1.4119911	-0.33094817	1.4442244
749.7589@25.361473	-0.56598157	0.062352262	-0.79821104	-1.3753767
113.9797@0.5336199	0.7590653	-0.69577014	1.3736111	0.47318026
762.242@19.776638	-0.027886383	-3.5981152	-1.6728379	0.81320393
763.2595@22.065031	-2.030754	-0.5510601	0.017154321	0.5579724
769.2738@22.124748	-1.1572421	1.3249271	-0.26858985	0.46515694
789.2611@22.251148	-0.5382751	-0.42299145	-0.44695988	0.029075932
789.2642@22.332657	-0.54382384	0.6216276	-0.10265769	-0.57954633
1110.6819@22.456293	-2.6151953	-1.3377303	-0.5283869	0.5311138
644.697@27.795586	-1.0705788	2.2092388	-0.81762815	0.3758279
1066.6133@19.442995	-1.3860914	-2.2540905	-0.21002571	0.45281813
1198.6483@22.548525	-1.1031477	-0.30919892	-0.5145377	-0.57893884
894.5349@22.419611	-2.6662657	-0.7736501	-0.6523726	-0.07638407
719.4407@22.357714	0.37796888	1.3684976	0.9710736	-0.13884753
629.7354@26.437578	0.41156536	1.3952956	-0.6918311	1.2668812
808.8757@26.516602	-0.2398255	0.8261973	0.087129265	-1.0408125
765.7811@25.317173	-0.3902478	-0.72350514	-1.1854254	-0.84860766

Compound	p	p (Corr)	FC ([Healthy] vs [Lesional])	Log FC ([Healthy] vs [Lesional])	FC (abs) ([Healthy] vs [Lesional])	Regulation ([Healthy] vs [Lesional])	FC ([Healthy] vs [Nonlesional])	Log FC ([Healthy] vs [Nonlesional])	FC (abs) ([Healthy] vs [Nonlesional])	Regulation ([Healthy] vs [Nonlesional])	FC ([Lesional] vs [Nonlesional])	Log FC ([Lesional] vs [Nonlesional])	FC (abs) ([Lesional] vs [Nonlesional])	Regulation ([Lesional] vs [Nonlesional])
C13 H30 N8 O S2	0	0	8.840688	3.1441586	8.840688	up	-173.33847	-7.437448	173.33847	down	-1532.4315	-10.581607	1532.4315	down
C4 H9 N S	0	0	-4959.664	-12.276027	4959.664	down	-44.505363	-5.4759073	44.505363	down	111.43966	6.800119	111.43966	up
C20 H32 N12	0	0	342.2992	8.419114	342.2992	up	-3.9035184	-1.9647751	3.9035184	down	-1336.1713	-10.383889	1336.1713	down
DEOXYCORTICOSTERONE ACETATE (CAS# 56-47-3); (M+Na)+	0	0	30.917631	4.950358	30.917631	up	-91.93015	-6.522466	91.93015	down	-2842.2625	-11.472824	2842.2625	down
C3 H9 N3 O2	0	0	1914.624	10.902845	1914.624	up	8.095078	3.017045	8.095078	up	-236.51704	-7.8858004	236.51704	down
C31 H47 N4 O P5	0	0	-552.31604	-9.10935	552.31604	down	-1379.4188	-10.429845	1379.4188	down	-2.4975173	-1.3204947	2.4975173	down
C33 H46 N10 P2	0	0	272.2588	8.088835	272.2588	up	-23.292688	-4.5418053	23.292688	down	-6341.639	-12.63064	6341.639	down
C8 H14 N6 O	0	0	3306.5928	11.69113	3306.5928	up	7.512436	2.9092808	7.512436	up	-440.14923	-8.781849	440.14923	down
C18 H41 N7	0	0	1996.0295	10.962917	1996.0295	up	1.1455369	0.19602394	1.1455369	up	-1742.4402	-10.766893	1742.4402	down
C13 H30 N2 O4 S	0	0	57.208805	5.8381653	57.208805	up	-286.88498	-8.164329	286.88498	down	-16412.346	-14.002494	16412.346	down
C8 H16 N7 O P	0	0	8709.0625	13.088302	8709.0625	up	2.8549564	1.5134687	2.8549564	up	-3050.506	-11.574833	3050.506	down
C30 H51 N O16	0	0	-559.07196	-9.12689	559.07196	down	-35.025238	-5.130323	35.025238	down	15.96198	3.9965677	15.96198	up
C39 H79 O P S4	0	0	-4.780502	-2.257162	4.780502	down	219.90396	7.78073	219.90396	up	1051.2516	10.037892	1051.2516	up
C25 H46 N7 O2 P S2	0	0	-5193.781	-12.342569	5193.781	down	-893.32983	-9.803049	893.32983	down	5.8139563	2.5395203	5.8139563	up
GLYCOCHENODEOXYCHOLATE (CAS# 640-79-9); (M+Na)+	0	0	1830.2837	10.837852	1830.2837	up	3.2361462	1.6942768	3.2361462	up	-565.5751	-9.143575	565.5751	down
C29 H46 N6 O14	0	0	-41.020863	-5.358286	41.020863	down	-233.56319	-7.867669	233.56319	down	-5.693764	-2.5093827	5.693764	down
C9 H16 N2 O2	0	0	309.697	8.2747135	309.697	up	-6.8298345	-2.7718506	6.8298345	down	-2115.1792	-11.046564	2115.1792	down
C12 H14 N8 O	0	0	43466.797	15.407626	43466.797	up	-5.625378	-2.49195	5.625378	down	-244517.16	-17.899576	244517.16	down
C28 H52 N O2 P S2	0	0	-1665.4698	-10.701714	1665.4698	down	-7.887179	-2.9795094	7.887179	down	211.16168	7.722204	211.16168	up
C8 H15 N O4	0	0	107.7828	6.751983	107.7828	up	-77.39283	-6.274128	77.39283	down	-8341.618	-13.026112	8341.618	down
C12 H14 O5	0	0	7061.6167	12.785783	7061.6167	up	6.009079	2.587144	6.009079	up	-1175.158	-10.198639	1175.158	down
C28 H45 N7 O4 P2	0	0	-4.2674932	-2.0933888	4.2674932	down	-1805.6877	-10.818333	1805.6877	down	-423.12616	-8.724944	423.12616	down
C17 H34 N6 O6 S2	0	0	-1691.4209	-10.72402	1691.4209	down	-5.5830827	-2.481062	5.5830827	down	302.95465	8.242958	302.95465	up
LYSINE (CAS# 56-87-1); (M+Na)+	0	0	23.6933	4.566407	23.6933	up	-104.9409	-6.7134333	104.9409	down	-2486.3962	-11.27984	2486.3962	down
C23 H36 N17 O P	0	0	-1177.8597	-10.201952	1177.8597	down	-115.79925	-6.855482	115.79925	down	10.171566	3.3464699	10.171566	up
C4 H11 N3 O	0	0	4923.071	12.265343	4923.071	up	5.569805	2.4776268	5.569805	up	-883.8856	-9.787716	883.8856	down
C18 H34 N6 O2	0	0	-35.73226	-5.1591554	35.73226	down	40.522186	5.34064	40.522186	up	1447.9498	10.499796	1447.9498	up
C23 H28 O3	0	0	309.6552	8.274519	309.6552	up	-74.91731	-6.227227	74.91731	down	-23198.537	-14.501746	23198.537	down
C10 H10 N8	0	0	87.109604	6.44476	87.109604	up	-200.24048	-7.64559	200.24048	down	-17442.863	-14.090349	17442.863	down
THEOBROMINE (CAS# 83-67-0); (M+H)+	0	0	1515.3821	10.565466	1515.3821	up	3.1265824	1.6445866	3.1265824	up	-484.67685	-8.920879	484.67685	down
C11 H28 N5 O3 P	0	0	1020.37823	9.994888	1020.37823	up	126.682175	6.9850698	126.682175	up	-8.054634	-3.009819	8.054634	down
C25 H45 N O8	0	0	65.96303	6.043586	65.96303	up	-110.172905	-6.7836256	110.172905	down	-7267.3384	-12.827211	7267.3384	down
C37 H45 O3 P S	0	0	-6.3587456	-2.6687422	6.3587456	down	63.176792	5.981323	63.176792	up	401.725	8.650064	401.725	up
C5 H10 N4 O2	0	0	2748.148	11.424244	2748.148	up	6.1738	2.6261587	6.1738	up	-445.1307	-8.798085	445.1307	down
C32 H37 N20 P	0	0	2699.8108	11.398643	2699.8108	up	106.33839	6.7325187	106.33839	up	-25.388863	-4.666124	25.388863	down
C22 H43 N7 O4 S2	0	0	-110.7875	-6.7916512	110.7875	down	35.767227	5.1605663	35.767227	up	3962.56	11.952217	3962.56	up
C39 H37 N3 O2	0	0	6.142653	2.618862	6.142653	up	-681.82904	-9.413266	681.82904	down	-4188.2397	-12.032128	4188.2397	down
C17 H33 N2 O P S2	0	0	51.858852	5.6965184	51.858852	up	-1160.6011	-10.180656	1160.6011	down	-60187.42	-15.877174	60187.42	down
PANTOTHENATE (CAS# 79-83-4); (M+H)+	0	0	284.40744	8.151815	284.40744	up	-5.902441	-2.5613117	5.902441	down	-1678.6981	-10.713127	1678.6981	down
C27 H41 N5	0	0	9.218407	3.2045174	9.218407	up	1051.4504	10.038165	1051.4504	up	114.05989	6.8336477	114.05989	up
C9 H24 N4 O2	0	0	28536.275	14.800509	28536.275	up	7.6470237	2.9348984	7.6470237	up	-3731.6838	-11.865611	3731.6838	down
C19 H21 N9	0	0	989.87744	9.951106	989.87744	up	-8.938792	-3.16008	8.938792	down	-8848.309	-13.111186	8848.309	down
TAURINE (CAS# 107-35-7); (M+H)+	0	0	-1544.0804	-10.592532	1544.0804	down	4.54675	2.1848357	4.54675	up	7020.5464	12.777368	7020.5464	up
C19 H27 N3 O P2	0	0	249.43451	7.9625173	249.43451	up	2.3992836	1.2626038	2.3992836	up	-103.962074	-6.6999135	103.962074	down
CORTISOL (CAS# 50-23-7); (M+Na)+	0	0	5.581934	2.480765	5.581934	up	-170.62178	-7.414658	170.62178	down	-952.3994	-9.895423	952.3994	down
C33 H50 N5 O3 P5	0	0	-361.0817	-8.4961815	361.0817	down	-3.320095	-1.7312245	3.320095	down	108.75647	6.7649574	108.75647	up
C9 H15 O P S	0	0	21657.904	14.402606	21657.904	up	44.640102	5.4802685	44.640102	up	-485.16696	-8.922338	485.16696	down
C12 H16 O4	0	0	4839.5425	12.240655	4839.5425	up	106.308655	6.7321153	106.308655	up	-45.523518	-5.50854	45.523518	down
C13 H18 O3 S	0	0	2432.0227	11.247941	2432.0227	up	4.7210727	2.2391148	4.7210727	up	-515.14197	-9.008826	515.14197	down
C17 H36 N6 O2 S	0	0	-10.700421	-3.4195957	10.700421	down	865.98474	9.758198	865.98474	up	9266.401	13.1777935	9266.401	up
C32 H2 O5 P2 S5	0	0	-4346.283	-12.0855665	4346.283	down	6.146725	2.619818	6.146725	up	26715.404	14.705384	26715.404	up
C13 H21 N O2	0	0	-202.73122	-7.6634245	202.73122	down	-15.275737	-3.93317	15.275737	down	13.271455	3.7302547	13.271455	up
D-GALACTOSAMINE (CAS# 7535-00-4); (M+H)+[-H2O]	0	0	-2547.24	-11.314719	2547.24	down	-3.781635	-1.9190102	3.781635	down	673.58167	9.395709	673.58167	up
C25 H47 N3 O5 S	0	0	55.419514	5.792322	55.419514	up	-201.80743	-7.6568356	201.80743	down	-11184.07	-13.449158	11184.07	down
HOMOSERINE (CAS# 672-15-1); (M+Na)+	0	0	-258.56808	-8.0144005	258.56808	down	-1.0062054	-0.008924961	1.0062054	down	256.97354	8.005476	256.97354	up
D-MANNOSAMINE (CAS# 14307-02-9); (M+H)+[-H2O]	0	0	-2547.24	-11.314719	2547.24	down	-3.781635	-1.9190102	3.781635	down	673.58167	9.395709	673.58167	up
N(PAI)-METHYL-L-HISTIDINE (CAS# 332-80-9); (M+H)+	0	0	-20.955084	-4.3892283	20.955084	down	12.864526	3.6853263	12.864526	up	269.57715	8.074554	269.57715	up
C14 H22 N2 O	0	0	-12617.024	-13.623084	12617.024	down	435.5415	8.766666	435.5415	up	5495234	22.38975	5495234	up
MELANIN (CAS# 8049-97-6); (M+H)+	0	0	335.86285	8.391728	335.86285	up	-2.4939818	-1.3184509	2.4939818	down	-837.6358	-9.710179	837.6358	down
C10 H18 N2 O	0	0	3.520555	1.8158029	3.520555	up	-241.58884	-7.91641	241.58884	down	-850.52686	-9.732213	850.52686	down
L-ALLOTHREONINE (CAS# 28954-12-3); (M+H)+	0	0	-558.5363	-9.125507	558.5363	down	-1.0883156	-0.122097015	1.0883156	down	513.21173	9.00341	513.21173	up
HOMOSERINE (CAS# 672-15-1); (M+H)+	0	0	-558.5363	-9.125507	558.5363	down	-1.0883156	-0.122097015	1.0883156	down	513.21173	9.00341	513.21173	up
C18 H33 N6 O2 P5	0	0	250.76637	7.9702	250.76637	up	3.0495892	1.6086149	3.0495892	up	-82.22955	-6.361585	82.22955	down
SUCROSE (CAS# 57-50-1); (M+Na)+	0	0	-934.73334	-9.868411	934.73334	down	-4.1201835	-2.0427086	4.1201835	down	226.86688	7.825702	226.86688	up
NORVALINE (CAS# 6600-40-4); (M+H)+	0	0	-24583.139	-14.5853815	24583.139	down	-1.5746406	-0.6550226	1.5746406	down	15611.904	13.930359	15611.904	up
BETA-ALANINE (CAS# 107-95-9); (M+H)+	0	0	-1423.1665	-10.474889	1423.1665	down	-4.6294413	-2.210838	4.6294413	down	307.41644	8.2640505	307.41644	up
CELLOBIOSE (CAS# 528-50-7); (M+Na)+	0	0	-934.73334	-9.868411	934.73334	down	-4.1201835	-2.0427086	4.1201835	down	226.86688	7.825702	226.86688	up
MELIBIOSE (CAS# 585-99-9); (M+Na)+	0	0	-934.73334	-9.868411	934.73334	down	-4.1201835	-2.0427086	4.1201835	down	226.86688	7.825702	226.86688	up
VALINE (CAS# 72-18-4); (M+H)+	0	0	-24635.031	-14.588424	24635.031	down	-1.5746406	-0.6550226	1.5746406	down	15644.859	13.933401	15644.859	up
BETA-MALTOSE (CAS# 69-79-4); (M+Na)+	0	0	-934.73334	-9.868411	934.73334	down	-4.1201835	-2.0427086	4.1201835	down	226.86688	7.825702	226.86688	up
LACTOSE (CAS# 63-42-3); (M+Na)+	0	0	-934.4683	-9.868002	934.4683	down	-4.1201835	-2.0427086	4.1201835	down	226.80255	7.825293	226.80255	up
PALATINOSE (CAS# 343336-76-5); (M+Na)+	0	0	-934.73334	-9.868411	934.73334	down	-4.1201835	-2.0427086	4.1201835	down	226.86688	7.825702	226.86688	up
SARCOSINE (CAS# 107-97-1); (M+H)+	0	0	-1423.1665	-10.474889	1423.1665	down	-4.6294413	-2.210838	4.6294413	down	307.41644	8.2640505	307.41644	up
URACIL (CAS# 66-22-8); (M+H)+	0	0	-14162.705	-13.789809	14162.705	down	-32.552906	-5.0247145	32.552906	down	435.0673	8.765095	435.0673	up
MALTOSE (CAS# 69-79-4); (M+Na)+	0	0	-934.4683	-9.868002	934.4683	down	-4.1201835	-2.0427086	4.1201835	down	226.80255	7.825293	226.80255	up
UROCANATE (CAS# 104-98-3); (M+H)+	0	0	-4379.1714	-12.096442	4379.1714	down	-11.810586	-3.5620086	11.810586	down	370.78354	8.534433	370.78354	up
C22 H27 N2 O3 P	0	0	-3.9687853	-1.9886975	3.9687853	down	-1176.9655	-10.200856	1176.9655	down	-296.55548	-8.212158	296.55548	down
1959.3063@19.789024	0	0	12457.482	13.604725	12457.482	up	48.379692	5.5963297	48.379692	up	-257.49405	-8.008395	257.49405	down
359.3371@21.756748	0	0	6022.4873	12.556144	6022.4873	up	-4.9783254	-2.3156605	4.9783254	down	-29981.9	-14.871804	29981.9	down
757.5616@24.534454	0	0	2304.1292	11.170006	2304.1292	up	-12.123564	-3.599742	12.123564	down	-27934.256	-14.769748	27934.256	down
829.5609@24.580767	0	0	6191.1763	12.595998	6191.1763	up	-6.889959	-2.7844954	6.889959	down	-42656.95	-15.380493	42656.95	down
1185.4827@5.0349865	0	0	-5.701159	-2.5112553	5.701159	down	248.67422	7.958113	248.67422	up	1417.7318	10.469369	1417.7318	up
756.3904@6.6820736	0	0	4.9842687	2.3173819	4.9842687	up	-96.78763	-6.5967507	96.78763	down	-482.41537	-8.914132	482.41537	down
803.5482@24.449387	0	0	1189.5914	10.21625	1189.5914	up	-5.9734826	-2.5785723	5.9734826	down	-7106.0034	-12.794823	7106.0034	down
795.5152@24.516008	0	0	59.206566	5.8876853	59.206566	up	-197.2464	-7.623855	197.2464	down	-11678.282	-13.51154	11678.282	down
925.4703@24.515404	0	0	95.250084	6.5736485	95.250084	up	-3.7672935	-1.9135284	3.7672935	down	-358.83502	-8.487177	358.83502	down
1819.008@24.514679	0	0	206.68944	7.691321	206.68944	up	-25.8059	-4.689629	25.8059	down	-5333.807	-12.38095	5333.807	down
1825.0208@24.524853	0	0	5.8223896	2.5416114	5.8223896	up	-335.63425	-8.390746	335.63425	down	-1954.1937	-10.932358	1954.1937	down
915.5211@24.535116	0	0	411.22046	8.683768	411.22046	up	-38.655098	-5.272587	38.655098	down	-15895.768	-13.956355	15895.768	down
847.5322@24.538563	0	0	1971.4412	10.945035	1971.4412	up	-9.8361435	-3.2980928	9.8361435	down	-19391.379	-14.243128	19391.379	down
1102.6552@23.055687	0	0	494.1525	8.9488125	494.1525	up	3884.9731	11.923689	3884.9731	up	7.8618913	2.9748764	7.8618913	up
789.2611@22.251148	0	0	328.16147	8.358262	328.16147	up	-3.1343591	-1.6481705	3.1343591	down	-1028.5759	-10.006433	1028.5759	down
789.2642@22.332657	0	0	331.80182	8.374178	331.80182	up	-5.392495	-2.430953	5.392495	down	-1789.2397	-10.805131	1789.2397	down
629.7354@26.437578	0	0	-1503.4806	-10.5540905	1503.4806	down	-20.888008	-4.384603	20.888008	down	71.978165	6.1694875	71.978165	up
C10 H13 N	6.68E-07	8.23E-04	-1.953605	-0.96613884	1.953605	down	-84.52639	-6.40133	84.52639	down	-43.26688	-5.435191	43.26688	down
C15 H22 S2	6.38E-06	0.001572385	1.2718408	0.3469181	1.2718408	up	-1.0070583	-0.010147095	1.0070583	down	-1.2808177	-0.3570652	1.2808177	down
C18 H43 N7	3.35E-06	0.001572385	5.8521333	2.5489626	5.8521333	up	-5.956157	-2.5743818	5.956157	down	-34.856224	-5.1233444	34.856224	down
C18 H43 N7 O	4.28E-06	0.001572385	10.078633	3.333228	10.078633	up	-5.699471	-2.510828	5.699471	down	-57.44288	-5.844056	57.44288	down
C24 H51 N O2	5.57E-06	0.001572385	7.0756636	2.8228655	7.0756636	up	-8.229903	-3.0408754	8.229903	down	-58.232025	-5.863741	58.232025	down

C22 H26 O6	1.91E-05	0.003912708	1.1402967	0.18940926	1.1402967	up	1.0001758	2.54E-04	1.0001758	up	-1.1400962	-0.18915558	1.1400962	down
C28 H19 N8 P3	5.11E-05	0.007912692	1.4099609	0.49565506	1.4099609	up	1.0046287	0.006662369	1.0046287	up	-1.4034647	-0.4889927	1.4034647	down
C24 H29 N2 P3 S	5.21E-05	0.007912692	1.2942225	0.37208557	1.2942225	up	-1.000615	-8.87E-04	1.000615	down	-1.2950183	-0.3729725	1.2950183	down
810.295@16.42741	5.78E-05	0.007912692	1.5967796	0.6751652	1.5967796	up	-1.0233587	-0.033311844	1.0233587	down	-1.6340781	-0.708477	1.6340781	down
C24 H29 O6 P S	9.87E-05	0.009192768	1.2273555	0.2955532	1.2273555	up	-1.000283	-4.08E-04	1.000283	down	-1.2277029	-0.29596138	1.2277029	down
C20 H41 N O2	8.45E-05	0.009192768	25.255663	4.658535	25.255663	up	-7.659135	-2.9371815	7.659135	down	-193.43654	-7.5957165	193.43654	down
C24 H32 O3 P6	1.04E-04	0.009192768	1.2475631	0.31911278	1.2475631	up	1.024682	0.035176277	1.024682	up	-1.2175125	-0.2839365	1.2175125	down
C16 H37 N7	9.30E-05	0.009192768	4.673698	2.2245646	4.673698	up	-1.3939266	-0.4791546	1.3939266	down	-6.514792	-2.7037191	6.514792	down
1196.4637@16.426586	9.00E-05	0.009192768	2.0429664	1.0306654	2.0429664	up	-1.0252329	-0.035951614	1.0252329	down	-2.094516	-1.066617	2.094516	down
C11 H21 Cl N4 O3 S3	1.60E-04	0.01263669	-1.6057535	-0.6832504	1.6057535	down	-53.52464	-5.742131	53.52464	down	-33.333035	-5.058881	33.333035	down
C6 H4 O	1.64E-04	0.01263669	-1.4955806	-0.58070564	1.4955806	down	-65.66424	-6.037036	65.66424	down	-43.905518	-5.4563303	43.905518	down
C7 H8 O	2.35E-04	0.013794394	-6.394786	-2.676896	6.394786	down	-59.730125	-5.900387	59.730125	down	-9.340442	-3.2234907	9.340442	down
C17 H7 N6 O P	2.08E-04	0.013794394	1.3590013	0.44254684	1.3590013	up	-80.54767	-6.331771	80.54767	down	-109.464386	-6.7743177	109.464386	down
C12 H21 N4 O4 P	2.31E-04	0.013794394	2.5816045	1.368268	2.5816045	up	1.379234	0.4638672	1.379234	up	-1.8717669	-0.9044008	1.8717669	down
C20 H43 N O3	2.34E-04	0.013794394	105.6023	6.7224975	105.6023	up	-5.6675925	-2.502736	5.6675925	down	-598.5106	-9.225233	598.5106	down
856.2961@16.427088	2.30E-04	0.013794394	1.7075974	0.7719679	1.7075974	up	-1.0117236	-0.016815186	1.0117236	down	-1.7276165	-0.7887831	1.7276165	down
C19 H45 N7	3.16E-04	0.01735956	93.81588	6.55176	93.81588	up	-5.795971	-2.5350504	5.795971	down	-543.7543	-9.086811	543.7543	down
C17 H37 N O3	3.24E-04	0.01735956	35.789196	5.1614523	35.789196	up	-4.538605	-2.182249	4.538605	down	-162.43304	-7.3437014	162.43304	down
C22 H49 N7	3.88E-04	0.019924572	2.785615	1.4779959	2.785615	up	-6.4386916	-2.6867676	6.4386916	down	-17.935717	-4.1647635	17.935717	down
580.276@19.786844	4.27E-04	0.021037083	1.3268285	0.40798187	1.3268285	up	1.1562991	0.20951462	1.1562991	up	-1.1474786	-0.19846725	1.1474786	down
C23 H25 N5 O2	4.49E-04	0.021287674	1.1516702	0.20372772	1.1516702	up	1.0045902	0.006607056	1.0045902	up	-1.1464081	-0.19712067	1.1464081	down
C27 H49 N4 O2 P5	5.36E-04	0.023572594	2.5568116	1.3543458	2.5568116	up	-3.9289012	-1.9741259	3.9289012	down	-10.04546	-3.3284717	10.04546	down
C23 H20 N4 O	5.17E-04	0.023572594	1.2472967	0.31880474	1.2472967	up	-1.0261997	-0.037311554	1.0261997	down	-1.2799755	-0.3561163	1.2799755	down
C31 H39 N O S	6.37E-04	0.02708072	1.1390898	0.18788147	1.1390898	up	1.0235901	0.033638	1.0235901	up	-1.1128379	-0.15424347	1.1128379	down
C31 H52 O2 P4	8.87E-04	0.035254396	1.6648515	0.7353935	1.6648515	up	1.3484678	0.43132114	1.3484678	up	-1.2346245	-0.30407238	1.2346245	down
C41 H45 N7 S	8.69E-04	0.035254396	-16.280941	-4.025112	16.280941	down	-10.5699625	-3.4018984	10.5699625	down	1.5403025	0.62321377	1.5403025	up
C37 H51 O3 P S2	9.42E-04	0.03625557	1.4394517	0.5255194	1.4394517	up	1.2685871	0.34322262	1.2685871	up	-1.1346889	-0.18229675	1.1346889	down
C14 H20 N2 O2	0.001079289	0.04029345	4.988992	2.3187485	4.988992	up	-2.2306514	-1.157465	2.2306514	down	-11.128702	-3.4762135	11.128702	down
TAURINE (CAS# 107-35-7); (M+Na)+	0.002006192	0.040899575	-5.2470765	-2.3915138	5.2470765	down	1.2515237	0.32368565	1.2515237	up	6.5668406	2.7151995	6.5668406	up
C22 H24 N8 O P4	0.001854072	0.040899575	22.654655	4.5017357	22.654655	up	1.1895987	0.25047493	1.1895987	up	-19.04395	-4.2512608	19.04395	down
C10 H11 N5	0.001948791	0.040899575	1.3653125	0.44923115	1.3653125	up	1.2340362	0.30338478	1.2340362	up	-1.1063795	-0.14584637	1.1063795	down
C24 H33 N O6	0.001214501	0.040899575	1.0911236	0.12581444	1.0911236	up	1.0171754	0.024568558	1.0171754	up	-1.0726994	-0.10124588	1.0726994	down
C10 H14 O	0.001902117	0.040899575	1.4924824	0.57771397	1.4924824	up	1.2495605	0.32142067	1.2495605	up	-1.194406	-0.2562933	1.194406	down
C30 H41 N6 O3 P	0.001562281	0.040899575	1.4081092	0.49375916	1.4081092	up	1.3016044	0.380291	1.3016044	up	-1.0818257	-0.11346817	1.0818257	down
C24 H52 N2 P2 S	0.002174182	0.040899575	1.4764904	0.56217194	1.4764904	up	1.2886393	0.36584854	1.2886393	up	-1.1457747	-0.1963234	1.1457747	down
C10 H18 O3 P2	0.001519089	0.040899575	1.4069926	0.49261475	1.4069926	up	1.2435862	0.31450653	1.2435862	up	-1.1313993	-0.17810822	1.1313993	down
C13 H18 N2 O	0.002100437	0.040899575	6.7886577	2.7631264	6.7886577	up	-1.7791219	-0.8311653	1.7791219	down	-12.077849	-3.5942917	12.077849	down
C10 H14 N2 O	0.002155893	0.040899575	6.085707	2.605425	6.085707	up	-3.3096461	-1.726677	3.3096461	down	-20.141537	-4.332102	20.141537	down
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+H)+	0.001322842	0.040899575	12.8623085	3.6850777	12.8623085	up	1.2450421	0.31619453	1.2450421	up	-10.330822	-3.3688831	10.330822	down
C11 H22 O4 P2	0.001770443	0.040899575	1.3572704	0.44070816	1.3572704	up	1.2518687	0.32408333	1.2518687	up	-1.0841954	-0.11662483	1.0841954	down
C23 H40 O P2 S2	0.00196233	0.040899575	1.926049	0.9456444	1.926049	up	1.5130521	0.5974617	1.5130521	up	-1.2729561	-0.34818268	1.2729561	down
C26 H48 N10 S3	0.001600862	0.040899575	1.3582783	0.44177914	1.3582783	up	1.1767968	0.23486519	1.1767968	up	-1.1542165	-0.20691395	1.1542165	down
C11 H14 N2 O5	0.001532536	0.040899575	1.3998919	0.48531532	1.3998919	up	1.2782955	0.35422134	1.2782955	up	-1.0951238	-0.13109398	1.0951238	down
C16 H34 O9	0.002289758	0.040899575	4.8663845	2.2828503	4.8663845	up	-1.0931666	-0.12851334	1.0931666	down	-5.319769	-2.4113636	5.319769	down
C13 H20 N2 O	0.001475415	0.040899575	1.0437044	0.06171322	1.0437044	up	-83.02242	-6.375429	83.02242	down	-86.65087	-6.4371424	86.65087	down
JASMONIC ACID [ISTD] (CAS# 77026-92-7); (M+Na)+	0.001673901	0.040899575	1.4459662	0.5320339	1.4459662	up	1.2951107	0.3730755	1.2951107	up	-1.1164808	-0.15895844	1.1164808	down
C23 H31 N O6	0.002144916	0.040899575	1.0603632	0.08455849	1.0603632	up	1.0050445	0.007259369	1.0050445	up	-1.0550411	-0.07729912	1.0550411	down
C29 H46 O4	0.002076582	0.040899575	1.4566016	0.54260635	1.4566016	up	1.2336806	0.30296898	1.2336806	up	-1.1806959	-0.23963737	1.1806959	down
C34 H55 N5 O11	0.001777541	0.040899575	-3.0123253	-1.5908775	3.0123253	down	-1.8616177	-0.89655685	1.8616177	down	1.6181223	0.6943207	1.6181223	up
C20 H41 N O3	0.002384401	0.040899575	32.99508	5.044179	32.99508	up	-2.1363642	-1.0951576	2.1363642	down	-70.48951	-6.1393366	70.48951	down
C12 H18 N2 O	0.002343498	0.040899575	3.4940474	1.8048992	3.4940474	up	-3.6546128	-1.8697186	3.6546128	down	-12.76939	-3.6746178	12.76939	down
C11 H15 N O3	0.002076821	0.040899575	3.509747	1.811367	3.509747	up	-3.2092702	-1.6822453	3.2092702	down	-11.263726	-3.4936123	11.263726	down
C28 H44 O4	0.002111477	0.040899575	1.4309068	0.5169296	1.4309068	up	1.2832568	0.35980988	1.2832568	up	-1.1150588	-0.15711975	1.1150588	down
C26 H37 N12 O P	0.002030677	0.040899575	1.2872533	0.36429596	1.2872533	up	1.192206	0.2536335	1.192206	up	-1.079724	-0.11066246	1.079724	down
C12 H22 O2 S3	0.001248244	0.040899575	1.3882676	0.47328568	1.3882676	up	1.2382412	0.3082924	1.2382412	up	-1.1211609	-0.16499329	1.1211609	down
C34 H52 O3 P4	0.001549289	0.040899575	1.3808469	0.46555328	1.3808469	up	1.2628407	0.33667278	1.2628407	up	-1.0934448	-0.1288805	1.0934448	down
4-ACETAMIDOBUTANOATE (CAS# 3025-96-5); (M+Na)+	0.002140249	0.040899575	12.087709	3.595469	12.087709	up	4.7283654	2.2413416	4.7283654	up	-2.5564244	-1.3541274	2.5564244	down
C26 H47 N6 O4 P S	0.00215928	0.040899575	1.3562031	0.4395733	1.3562031	up	1.2095572	0.2744789	1.2095572	up	-1.1212394	-0.16509438	1.1212394	down
C12 H18 O3	0.002239034	0.040899575	1.434957	0.52100754	1.434957	up	1.2936956	0.3714981	1.2936956	up	-1.1091923	-0.14950943	1.1091923	down
C35 H60 S3	0.001792084	0.040899575	-1.9182893	-0.9398203	1.9182893	down	-20.134693	-4.3316116	20.134693	down	-10.496172	-3.3917913	10.496172	down
C14 H30 O8	0.002354058	0.040899575	4.25234	2.0882568	4.25234	up	-1.1032516	-0.14176178	1.1032516	down	-4.6914005	-2.2300186	4.6914005	down
C4 H11 N	0.001554156	0.040899575	1.3496888	0.43262672	1.3496888	up	-1.0666735	-0.09311867	1.0666735	down	-1.4396772	-0.5257454	1.4396772	down
C16 H30 O2 P2	0.002390235	0.040899575	-10.404966	-3.3792005	10.404966	down	4.799605	2.2629156	4.799605	up	49.939728	5.642116	49.939728	up
C23 H48 N O7 P	0.001489625	0.040899575	-14.628388	-3.870699	14.628388	down	2.0639536	1.0454106	2.0639536	up	30.192316	4.9161096	30.192316	up
1614.941@19.78335	0.002362363	0.040899575	-3.272813	-1.7105312	3.272813	down	-3.773694	-1.9159775	3.773694	down	-1.1530429	-0.20544624	1.1530429	down
1478.96@19.788363	0.001396195	0.040899575	1.9829614	0.9876566	1.9829614	up	1.5812318	0.6610489	1.5812318	up	-1.2540611	-0.3266077	1.2540611	down
1484.9901@19.787737	0.001819664	0.040899575	1.4925998	0.57782745	1.4925998	up	1.2860626	0.36296082	1.2860626	up	-1.1605966	-0.21486664	1.1605966	down
GIBBERELLIC ACID [ISTD] (CAS# 77-06-5); (M+Na)+	0.002631209	0.04103354	1.4398048	0.5258732	1.4398048	up	1.2948402	0.37277412	1.2948402	up	-1.1119555	-0.15309906	1.1119555	down
C28 H44 N4 O7 S	0.002551557	0.04103354	1.4329835	0.519022	1.4329835	up	1.3368315	0.41881752	1.3368315	up	-1.0719254	-0.10020447	1.0719254	down
C18 H20 P2	0.002597424	0.04103354	1.4410301	0.52710056	1.4410301	up	-1.0112596	-0.016153336	1.0112596	down	-1.4572556	-0.5432539	1.4572556	down
C25 H40 N10	0.002627568	0.04103354	1.2176839	0.28413963	1.2176839	up	1.1361599	0.18416595	1.1361599	up	-1.0717539	-0.09997368	1.0717539	down
C18 H12 N10	0.002499499	0.04103354	1.4409416	0.5270119	1.4409416	up	1.2903714	0.3677864	1.2903714	up	-1.1166874	-0.15922546	1.1166874	down
C20 H39 N O2 P2	0.00257929	0.04103354	4.660916	2.2206135	4.660916	up	-1.1229447	-0.16728687	1.1229447	down	-5.2339506	-2.3879004	5.2339506	down
1546.945@19.785664	0.002548934	0.04103354	2.0171623	1.0123272	2.0171623	up	1.674954	0.74412155	1.674954	up	-1.204309	-0.26820564	1.204309	down
1005.4501@10.68129	0.002704689	0.04165221	9.901779	3.3076878	9.901779	up	-8.572263	-3.0996761	8.572263	down	-84.88065	-6.407364	84.88065	down
C18 H18 O3	0.002766195	0.042073477	1.4560106	0.5420208	1.4560106	up	1.3577926	0.4412632	1.3577926	up	-1.0723364	-0.1007576	1.0723364	down
862.2494@22.540915	0.002817032	0.042324185	-19.791256	-4.3067913	19.791256	down	-2.544282	-1.3472586	2.544282	down	7.77872	2.9595327	7.77872	up
C22 H27 N3 S	0.002902899	0.043088816	1.3507884	0.43380165	1.3507884	up	-1.0758411	-0.105464935	1.0758411	down	-1.4532336	-0.5392666	1.4532336	down
C18 H24 O8 P2	0.002964078	0.04347314	1.3983583	0.48373413	1.3983583	up	1.2739208	0.3492756	1.2739208	up	-1.0976808	-0.13445854	1.0976808	down
C32 H40 Cl N3	0.003130361	0.045371823	-3.3222454	-1.7321587	3.3222454	down	-5.9369116	-2.5697126	5.9369116	down	-1.7870178	-0.837554	1.7870178	down
C26 H33 O6 P S	0.003186803	0.0456528	1.2034687	0.26719856	1.2034687	up	-1.0229772	-0.03277397	1.0229772	down	-1.231121	-0.29997253	1.231121	down
C5 H5 N5	0.00352547	0.045964718	1.35604	0.43939972	1.35604	up	1.2190804	0.2857933	1.2190804	up	-1.1123466	-0.15360641	1.1123466	down
C26 H51 N4 O2 P S	0.003544357	0.045964718	-1.5678966	-0.6488304	1.5678966	down	-6.8529935	-2.7767344	6.8529935	down	-4.37082	-2.127904	4.37082	down
C14 H22 N2 O2	0.003419785	0.045964718	3.781145	1.9188232	3.781145	up	-2.2732213	-1.1847382	2.2732213	down	-8.59538	-3.1035614	8.59538	down
C30 H44 N4 O11	0.003489468	0.045964718	-4.258697	-2.0904121	4.258697	down	-2.4102714	-1.2691956	2.4102714	down	1.7668953	0.8212166	1.7668953	up
C21 H34 O6	0.003257551	0.045964718	-4.5425496	-2.1835022	4.5425496	down	-1784.502	-10.801306	1784.502	down	-392.84152	-8.617804	392.84152	down
C20 H26 O3 P2	0.003440881	0.045964718	-1.0283619	-0.040348053	1.0283619	down	1.550422	0.63266087	1.550422	up	1.5943948	0.6730089	1.5943948	up
C31 H56 N2 O P6	0.003315874	0.045964718	-4.3291683	-2.11409	4.3291683	down	-2.4298522	-1.2808685	2.4298522	down	1.7816592	0.83322144	1.7816592	up
C24 H10 N2 O4	0.003412637	0.045964718	1.3150866	0.3951578	1.3150866	up	1.293303	0.37106037	1.293303	up	-1.0168433	-0.024097443	1.0168433	down
C26 H55 N O2	0.003482125	0.045964718	41.87897	5.388154	41.87897	up	-1.7346967	-0.79468346	1.7346967	down	-72.64731	-6.1828375	72.64731	down
ZEATIN [ISTD] (CAS# 13114-27-7); (M+H)+	0.003711702	0.04619007	1.3168429	0.39708328	1.3168429	up	1.2556164	0.32839584	1.2556164	up	-1.0487621	-0.06868744	1.0487621	down
C18 H38 O10	0.003668969	0.04619007	4.9665117	2.312233	4.9665117	up	-1.0689605	-0.09620857	1.0689605	down	-5.3090053	-2.4084415	5.3090053	down
CIS-ZEATIN (CAS# 1637-39-4); (M+H)+	0.003711209	0.04619007	1.3168012	0.3970375	1.3168012	up	1.2555766	0.32835007	1.2555766	up	-1.0487621	-0.06868744	1.0487621	down
C26 H37 N O6	0.003710698	0.04619007	1.091024	0.12568283	1.091024	up	-1.0196272	-0.02804184	1.0196272	down	-1.1124378	-0.15372467	1.1124378	down
C38 H46 O12 S	0.003984956	0.048465367	-5.854888	-2.5496416	5.854888	down	-2.8581684	-1.515091	2.8581684	down	2.0484755	1.0345507	2.0484755	up
C27 H34 N2 O P2	0.00398117	0.048465367	1.8854294	0.91489315	1.8854294	up	1.6264892	0.70176125	1.6264892	up	-1.159202	-0.2131319	1.159202	down
C24 H50 N O8 P	0.004128518	0.048465367	44.87852	5.487953	44.87852	up	1.2550621	0.3277588	1.2550621	up	-35.758007	-5.1601944	35.758007	down
C26 H51 N7 O4	0.004027428	0.048465367	1.2651126	0.33926582	1.2651126	up	1.1699811	0.22648525	1.1699811	up	-1.0813103	-0.11278057	1.0813103	down
C12 H26 O7	0.004084519	0.048465367	3.4729915	1.7961788	3.4729915	up	-1.0440805	-0.06223297	1.0440805	down	-3.6260827	-1.8584118	3.6260827	down
C10 H14 N2 O2	0.004130571	0.048465367	2.0875523	1.0618124	2.0875523	up	-6.7946377	-2.7643967	6.7946377	down	-14.184162	-3.826209	14.184162	down
C17 H11 N7 O6 S	0.004299512	0.04859632	47.749683	5.5774193	47.749683	up	-4.1912484	-2.06738	4.1912484	down	-200.13078	-7.644799	200.13078	down
C21 H30 S2	0.004275768	0.04859632	1.3477567	0.4305601	1.3477567	up	1.0484425	0.068247795	1.0484425	up	-1.2854846	-0.36231232	1.2854846	down
939.5053@10.673127	0.004288544	0.04859632	15.113867	3.917801	15.113867	up	-11.023498	-3.46251	11.023498	down	-166.60767	-7.380311	166.60767	down
1066.6133@19.442995	0.004223931	0.04859632	-2.3591669	-1.2382774	2.3591669	down	37.137924	5.2148213	37.137924	up	87.61456	6.453099	87.61456	up
1608.9333@19.784367	0.004382304	0.0490818	1.7702109	0.8239212	1.7702109	up	1.5343201	0.6175995	1.5343201	up	-1.1537429	-0.20632172	1.1537429	down