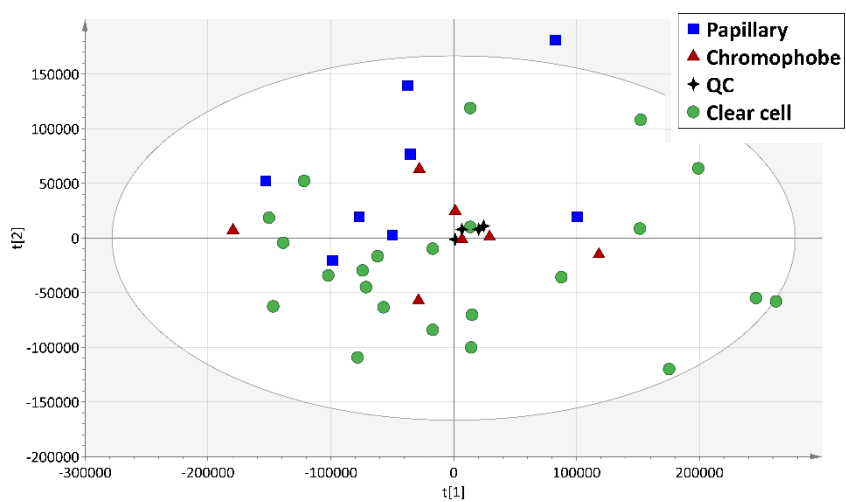


## **LC-MS based metabolomic profiling for renal cell carcinoma histologic subtypes**

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Damien Ambrosetti

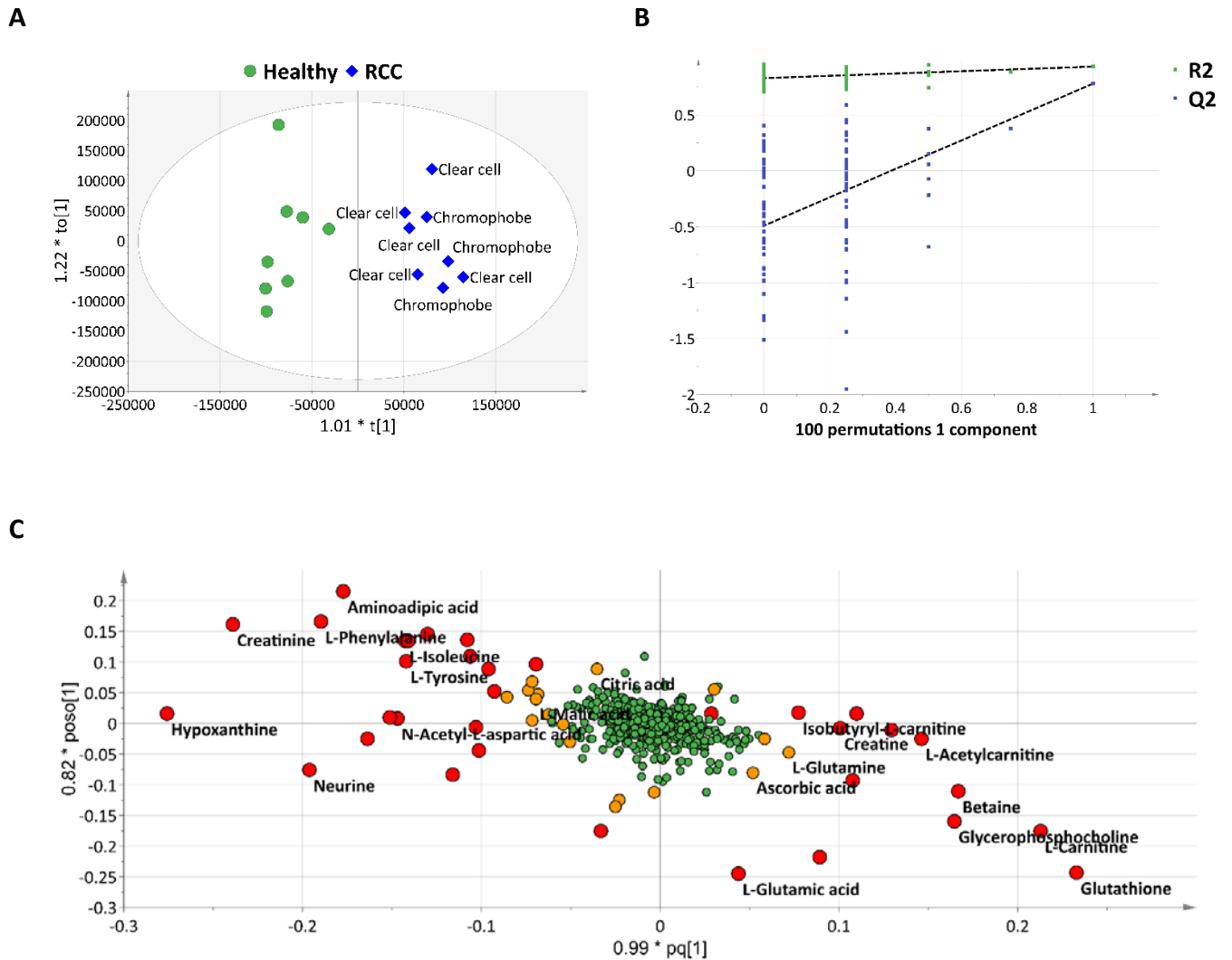
**Supplementary information**

# Supplementary Figure 1



**Supplementary Figure 1. Principal component analysis (PCA) of RCC subtype based on untargeted metabolomics data.**

## Supplementary Figure 2



**Supplementary Figure 2. Discrimination between healthy controls and renal cell carcinomas based on untargeted metabolomics data. A. OPLS-DA analysis showing the discrimination between healthy control and carcinoma samples (8 matched pairs including 5 clear cell and 3 chromophobe). The model presents 1 predictive component, 2 orthogonal components,  $R^2X_{(cum)}$  of 55.5%, a goodness-of-fit  $R^2$  of 93.2%, a goodness-of-prediction  $Q^2$  of 78.0% and CV-ANOVA p-value of 0.015. B. Validation plot obtained from 100 permutation tests. C. Loading plot showing the most discriminative metabolites in normal and RCC tissue discrimination. The metabolites with VIP (Variable Importance for the Projection)  $> 3$  are highlighted with red circles; with  $VIP > 2$  are highlighted with orange circles.**

**Supplementary Table 1.** Variable influence on projection (VIP) for RCC subtype classification.

Var ID (Primary)	Var ID (row m/z)	Var ID (ID)	M3.VIP[2+1+0]
Creatine	132.077	HMDB00064	10,5111
L-Acetylcarnitine	204.123	HMDB00201	10,4271
L-Carnitine	162.113	HMDB00062	6,84946
L-Proline	116.071	HMDB00162	6,45495
L-Phenylalanine	166.086	HMDB00159	6,07172
Dihydrothymine	129.066	HMDB00079	5,16308
Betaine	118.087	HMDB00043	5,1483
Hypoxanthine	137.046	HMDB00157	5,10661
L-Lactic acid	89.0229	HMDB00190	4,99924
L-Isoleucine	132.102	HMDB00172	4,65421
5-Aminoimidazole ribonucleotide	296.066	HMDB01235	4,03263
L-Methionine	150.058	HMDB00696	3,89251
Humulinic acid A	265.148	HMDB30104	3,77026
L-Tyrosine	182.081	HMDB00158	3,69869
L-Palmitoylcarnitine	400.343	HMDB00222	3,6649
Dimethylglycine	104.071	HMDB00092	3,62773
L-Tryptophan	205.097	HMDB00929	3,40488
Hydroxybutyrylcarnitine	248.149	HMDB13127	3,2158
N-Acetyl-L-aspartic acid	174.04	HMDB00812	3,2133
Adenosine	268.104	HMDB00050	3,19064
L-Malic acid	133.013	HMDB00156	3,18659
Isobutyryl-L-carnitine	232.154	HMDB00736	3,14472
L-Glutamic acid	148.061	HMDB00148	3,0703
Glutathione	308.091	HMDB00125	2,9841
Glycerophosphocholine	258.11	HMDB00086	2,96531
trans-Hexadec-2-enoyl carnitine	398.327	HMDB06317	2,94701
Tetradecanoylcarnitine	372.311	HMDB05066	2,89112
Nalbuphine	358.201	HMDB14982	2,82291
Beta-Alanine	90.0555	HMDB00056	2,76142
Oleoylecarnitine	426.358	HMDB05065	2,64926
Neurine	104.107	HMDB31259	2,56708
Linoelaidyl carnitine	424.342	HMDB06461	2,50077
Amino adipic acid	162.076	HMDB00510	2,47727
Methylmalonic acid	117.018	HMDB00202	2,42256
Isoplumbagin	187.041	HMDB35291	2,40383
N-Desmethylvenlafaxine	264.196	HMDB13892	2,37449
Cysteineglutathione disulfide	214.051	HMDB00656	2,36515
Guanidoacetic acid	118.061	HMDB00128	2,28672
Indoleacrylic acid	188.071	HMDB00734	2,27785
Adenine	136.062	HMDB00034	2,24758
2-Octenoylcarnitine	286.201	HMDB13324	2,24301
Adenosine monophosphate	348.07	HMDB00045	2,23197
LysoPC(16:0)	496.34	HMDB10382	2,19013
Pyrrolidine	72.0814	HMDB31641	2,13555
Hexanoylcarnitine	260.186	HMDB00705	2,06003
N-a-Acetyl-L-arginine	217.129	HMDB04620	2,03322
L-1,2,3,4-Tetrahydro-beta-carboline-3-carboxylic acid	217.097	HMDB35665	1,97511
Acetaminophen	152.071	HMDB01859	1,95179
Citramalic acid	147.029	HMDB00426	1,92319
cis-5-Tetradecenoylcarnitine	370.295	HMDB02014	1,88553
Tyrosol 4-sulfate	110.02	HMDB41785	1,85842
N-Methylethanolaminium phosphate	156.042	HMDB60173	1,85049
Niacinamide	123.056	HMDB01406	1,83226
Valganciclovir	353.161	HMDB15548	1,80062

3-Hydroxy-11Z-octadecenoylcarnitine	442.353	HMDB13339	1,79403
Galactonic acid	195.05	HMDB00565	1,74207
Spermidine	146.165	HMDB01257	1,71571
Imidazole acetol-phosphate	111.021	HMDB12236	1,70828
Alnustone	263.146	HMDB31664	1,67864
Xanthine	151.025	HMDB00292	1,65658
Pyridine N-oxide glucuronide	273.084	HMDB61177	1,65468
PC-M6	420.251	HMDB38568	1,64902
3-Methyl sulfolene	133.032	HMDB59667	1,64129
p-Cresol sulfate	187.006	HMDB11635	1,63924
N6-Acetyl-L-lysine	189.124	HMDB00206	1,61829
Methoxsalen	215.032	HMDB14693	1,61131
Lidocaine	235.181	HMDB14426	1,59592
Dihydrouracil	115.051	HMDB00076	1,59318
Proline betaine	144.102	HMDB04827	1,59157
Taurine	124.006	HMDB00251	1,58823
L-Lysine	147.113	HMDB00182	1,57718
Dichloromethane	84.9603	HMDB31548	1,56566
Dodecanoylcarnitine	344.279	HMDB02250	1,53279
2-O-Galloyl-1,4-galactarolactone	343.026	HMDB37199	1,51337
N-Methylnicotinamide	137.071	HMDB03152	1,46751
Triethanolamine	150.113	HMDB32538	1,43795
N-Heptanoylglycine	188.128	HMDB13010	1,43557
Uric acid	167.02	HMDB00289	1,43158
3-Hydroxyhexadecanoylcarnitine	416.337	HMDB13336	1,43105
Piperidine	86.097	HMDB34301	1,42661
Glycerolphosphorylethanolamine	214.048	HMDB00114	1,41495
PC(14:0/20:1(11Z))	760.584	HMDB07879	1,41027
Ribose-1-arsenate	272.959	HMDB12285	1,40237
3(S)-hydroxy-13-cis-docosenoyl-CoA	130.017	HMDB62200	1,39011
DL-2-Aminooctanoic acid	160.133	HMDB00991	1,37792
hydroxyisovaleroyl carnitine	262.165	HMDB62555	1,3641
Isoleucyl-Isoleucine	245.186	HMDB28910	1,35068
LysoPE(0:0/18:1(11Z))	480.309	HMDB11475	1,34772
Diphenyl disulfide	219.027	HMDB31823	1,34432
Dehydroxizyleuton	111.039	HMDB13970	1,32777
Isoleucyl-Valine	231.17	HMDB28920	1,32402
Phenylpyruvic acid	165.055	HMDB00205	1,29824
Ascorbic acid	175.024	HMDB00044	1,28794
3,5,3-triiodothyronine-4-sulfate	129.02	HMDB62205	1,28414
5'-Methylthioadenosine	298.097	HMDB01173	1,27028
Amoxapine	312.095	HMDB14683	1,27022
Diisopropyl sulfide	119.09	HMDB29579	1,26252
Selenium Sulfide	112.896	HMDB15106	1,25687
N2-Succinyl-L-ornithine	233.113	HMDB01199	1,22232
L-Kynurenine	209.092	HMDB00684	1,21881
N-Acetylarlyamine	136.076	HMDB01250	1,19761
1-Oxo-1H-2-benzopyran-3-carboxaldehyde	88.0237	HMDB30577	1,19331
1-Pyrroline	70.0658	HMDB12497	1,19245
Hippuric acid	178.05	HMDB00714	1,18142
Dibenzyl disulfide	245.043	HMDB32077	1,15664
3-hydroxyoctanoyl carnitine	304.212	HMDB61634	1,1535
(2S,4R)-4-(9H-Pyrido[3,4-b]indol-1-yl)-1,2,4-butanetriol	273.121	HMDB35191	1,13778
1-(Isothiocyanatomethyl)-4-methoxybenzene	90.5264	HMDB32581	1,12798
Trigonelline	138.055	HMDB00875	1,1251
Ophthalmic acid	290.135	HMDB05765	1,12354
Gamma-Butyrolactone	87.0446	HMDB00549	1,10032
Thiolutin	226.996	HMDB34228	1,09423
5-Hydroxyisourate	185.032	HMDB30097	1,09399

9,12-Hexadecadienoylcarnitine	396.311	HMDB13334	1,09208
Lenticin	247.144	HMDB61115	1,08828
Aniline	94.0656	HMDB03012	1,08206
L-argininium(1+)	176.128	HMDB62762	1,08044
Ethyl aconitate	203.053	HMDB40275	1,07958
1-(4-Hydroxy-3-methoxyphenyl)-3-decanone	279.192	HMDB30801	1,07098
LysoPC(18:1(9Z))	522.355	HMDB02815	1,06414
Inosine	267.073	HMDB00195	1,06232
2-Hydroxyadipic acid	161.044	HMDB00321	1,0502
Ureidopropionic acid	133.061	HMDB00026	1,04489
Pseudoecgonine	186.113	HMDB06348	1,03703
3-Hydroxy-2-methyl-[R-(R,S)]-butanoic acid	117.054	HMDB00351	1,03695
Phosphodimethylethanolamine	168.042	HMDB60244	1,02397
3,4-Dihydroxymandelic acid	185.042	HMDB01866	1,02144
Caffeine	195.088	HMDB01847	1,01403
3-Hydroxy-9-hexadecenoylcarnitine	414.321	HMDB13333	1,01221
Valerenic acid	235.166	HMDB30016	1,0086
Creatinine	114.067	HMDB00562	1,00418
Uridine 5'-monophosphate	323.029	HMDB00288	0,999177
N-(4-hydroxyphenyl)ethoxycarbothioamide	99.5316	HMDB33179	0,966969
2,5-Dichloro-4-oxohex-2-enedioate	226.952	HMDB60363	0,955923
3-Hexenedioic acid	145.05	HMDB00393	0,945752
Propionylcarnitine	218.139	HMDB00824	0,939206
2-Methyl-3-ketovaleric acid	129.054	HMDB00408	0,937506
Pseudoephedrine	166.123	HMDB01943	0,933523
2,5-Furandicarboxylic acid	157.011	HMDB04812	0,929247
Salsoline-1-carboxylate	236.092	HMDB13067	0,927692
L-Arginine	175.119	HMDB00517	0,900684
3-hydroxydecanoyl carnitine	332.243	HMDB61636	0,89175
Phosphoric acid	96.9682	HMDB02142	0,888322
Fenamiphos	302.101	HMDB31787	0,863479
Spermine	203.223	HMDB01256	0,85868
2-Hydroxy-lauroylcarnitine	360.275	HMDB13164	0,858169
Gravelliferone	297.153	HMDB30729	0,845069
L-Glutamine	147.077	HMDB00641	0,842453
L-Octanoylcarnitine	288.217	HMDB00791	0,842017
Cytidine	242.08	HMDB00089	0,836793
Erythronic acid	135.029	HMDB00613	0,836236
2-Methylbutyrylcarnitine	246.17	HMDB00378	0,831544
12-Hydroxy-12-octadecanoylcarnitine	444.369	HMDB13154	0,830441
Taurocholic acid	516.296	HMDB00036	0,820824
Isoelemicin	207.102	HMDB29867	0,820639
Dihydrolipoate	207.05	HMDB12210	0,820224
(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform B (protein)	234.961	HMDB62252	0,817224
Phosphoserine	186.016	HMDB00272	0,811223
3-(3,4,5-Trimethoxyphenyl)propanoic acid	239.092	HMDB30254	0,808955
Glutamylalanine	219.098	HMDB03764	0,80435
N-Methylcalystegine B2	188.092	HMDB36604	0,77938
Histidinyl-Isoleucine	267.144	HMDB28888	0,778403
Pipecolic acid	130.086	HMDB00070	0,77376
L-Threonine	120.066	HMDB00167	0,773686
Decanoylcarnitine	316.248	HMDB00651	0,770765
Ornithine	133.097	HMDB00214	0,758882
Citric acid	191.019	HMDB00094	0,75466
6-Methylquinoline	144.081	HMDB33115	0,752539
Durupcoside B	464.254	HMDB30976	0,748659
Succinyladenosine	384.115	HMDB00912	0,746469
N1-Acetylspermidine	188.176	HMDB01276	0,74626

Cinitapride	403.233	HMDB15698	0,745467
3-(Acetylthio)-2-methylfuran	79.0185	HMDB32160	0,741323
2-Pyrrolidinone	86.0606	HMDB02039	0,739414
D-Glucose	181.072	HMDB00122	0,739399
Isobutyrylglycine	146.081	HMDB00730	0,735231
Glucosamine-1P	260.053	HMDB01109	0,727695
Gamma Glutamylglutamic acid	277.103	HMDB11737	0,725478
Phosphohydroxypyruvic acid	184.986	HMDB01024	0,724684
2-Hydroxymyristoylcarnitine	388.306	HMDB13166	0,720521
Pyroglutamic acid	130.05	HMDB00267	0,71765
Flupenthixol	437.193	HMDB15013	0,704809
L-Aspartic acid	132.029	HMDB00191	0,699801
Hexanoylglycine	172.097	HMDB00701	0,698426
cis-Aconitic acid	173.008	HMDB00072	0,695489
Homovanillic acid	181.05	HMDB00118	0,6926
Pentadecanoylcarnitine	386.326	HMDB62517	0,689707
4-Guanidinobutanoic acid	146.093	HMDB03464	0,689601
Benzothiazole	136.023	HMDB32930	0,687216
Glycine	76.04	HMDB00123	0,681152
3-Methylglutarylcarnitine	290.16	HMDB00552	0,679099
Ammonium peroxydisulfate	226.965	HMDB37638	0,678327
O-Demethylfonsecin	275.054	HMDB33649	0,676863
Deoxycytidine	228.098	HMDB00014	0,676779
Indolelactic acid	204.066	HMDB00671	0,676476
LysoPC(18:3(6Z,9Z,12Z))	518.322	HMDB10387	0,673194
Zapotin	343.115	HMDB29461	0,669919
2-Hydroxybutyric acid	103.039	HMDB00008	0,669885
4-Thialysine	83.0381	HMDB29178	0,663878
Isoacitretin	325.184	HMDB03039	0,662896
(S)-Isowillardiine	200.068	HMDB30376	0,660535
Norphthalmic acid	276.119	HMDB05766	0,651114
5-Acetylamino-6-formylamino-3-methyluracil	225.061	HMDB11105	0,650626
3-Hydroxy-cis-5-tetradecenoylcarnitine	386.29	HMDB13330	0,650235
Pantothenic acid	220.118	HMDB00210	0,64752
Meprobamate	219.134	HMDB14515	0,64715
Methyl (9Z)-10'-oxo-6,10'-diapo-6-carotenoate	311.169	HMDB31976	0,644891
3, 5-Tetradecadiencarnitine	368.28	HMDB13331	0,641433
Benzoic acid	123.044	HMDB01870	0,638064
2-Hexenoylcarnitine	258.17	HMDB13161	0,63459
1,3,5-Trihydroxy-10-methylacridone	256.059	HMDB41468	0,633363
(S)-Metalaxyl	280.154	HMDB31802	0,626213
3-(3-Hydroxyphenyl)propanoic acid	165.055	HMDB00375	0,623728
D-Erythrose 4-phosphate	201.016	HMDB01321	0,622294
L-isoleucyl-L-proline	229.155	HMDB11174	0,621977
1-Butylamine	74.0971	HMDB31321	0,621876
3-Hydroxy-6,8-dimethoxy-7(11)-eremophilin-12,8-olide	309.174	HMDB40756	0,619669
LysoPC(18:0)	524.371	HMDB10384	0,618178
L-Histidine	154.061	HMDB00177	0,612274
Fumaric acid	115.002	HMDB00134	0,612105
L-2-Amino-5-hydroxypentanoic acid	134.081	HMDB31658	0,608407
Spermic acid 2	233.15	HMDB13075	0,607225
Zymonic acid	159.028	HMDB31210	0,601689
Homo-L-arginine	189.135	HMDB00670	0,601499
3,5,6-Trihydroxy-5-(hydroxymethyl)-2-methoxy-2-cyclohexen-1-one	205.068	HMDB41031	0,600432
Pyridoxamine	169.095	HMDB01431	0,599498
2,3-Diaminosalicylic acid	169.059	HMDB13159	0,594786
2-Furoylglycine	170.042	HMDB00439	0,590499
Tetrahydropentoxylene	367.15	HMDB29992	0,586858

N-Acetylneuraminic acid	308.099	HMDB00230	0,583551
Trifluoroacetic acid	112.984	HMDB14118	0,581749
4-Aminobiphenyl	170.097	HMDB13195	0,579898
Dracunculin	221.042	HMDB30789	0,579183
Fexofenadine	500.279	HMDB05030	0,576125
4-Methoxyphenylethanol sulfate	249.046	HMDB29229	0,574918
Pyruvic acid	87.0073	HMDB00243	0,573194
3'-Hydroxyhexobarbital	253.118	HMDB13940	0,571425
2-Furancarboxaldehyde	97.0289	HMDB32914	0,570307
Erinapyrone C	187.058	HMDB41026	0,568303
Thiomorpholine 3-carboxylate	148.043	HMDB59611	0,567885
Phloretin	273.08	HMDB03306	0,567562
Cedryl acetate	265.212	HMDB35910	0,567103
Asymmetric dimethylarginine	203.15	HMDB01539	0,564187
Gamma-linolenyl carnitine	422.327	HMDB06318	0,564083
4-Hydroxy-2-butenic acid gamma-lactone	85.029	HMDB32330	0,552483
Sphingosine	300.29	HMDB00252	0,549955
Fomepizole	83.061	HMDB15344	0,539807
Histamine	112.087	HMDB00870	0,533286
Mitotane	316.948	HMDB14786	0,532122
Xanthosine	283.068	HMDB00299	0,529921
Arginyl-Proline	272.172	HMDB28717	0,529196
Glyoxylic acid	72.9916	HMDB00119	0,526732
1-Arachidonoylglycerophosphoinositol	619.289	HMDB61690	0,523828
5-Hydroxymethyl-4-methyluracil	157.061	HMDB00544	0,521406
3-Methylene-indolenine	130.063	HMDB11664	0,520481
Octadecanamide	284.295	HMDB34146	0,519262
Oxoglutaric acid	147.031	HMDB00208	0,510612
Quinone	109.029	HMDB03364	0,510298
Arabinonic acid	165.039	HMDB00539	0,510254
Monoisobutyl phthalic acid	223.097	HMDB02056	0,509122
Sphinganine	302.305	HMDB00269	0,504593
L-beta-aspartyl-L-leucine	247.129	HMDB11166	0,504166
Acetyl-N-formyl-5-methoxykynurenamine	263.104	HMDB04259	0,502465
Aspartyl-Histidine	269.088	HMDB28755	0,499879
Erythro-5-hydroxy-L-lysiniun(1+)	164.117	HMDB62570	0,499849
Deoxyinosine	251.077	HMDB00071	0,498243
trans-2-Dodecenoylcarnitine	342.264	HMDB13326	0,496868
(ent-2b,4S,9a)-2,4,9-Trihydroxy-10(14)-oplopen-3-one 2-(2-methylbutanoate) 9-(3-methyl-2E-pentenoate)	449.287	HMDB40993	0,496129
Cinnamic acid	149.06	HMDB00567	0,495998
(S)-3,4-Dihydroxybutyric acid	119.034	HMDB00337	0,495077
Thorium	233.042	HMDB29215	0,495014
S-Acetyldihydrolipoamide	250.094	HMDB01526	0,494141
Asparaginyln-Isoleucine	246.145	HMDB28734	0,493467
5,6,7,8-Tetrahydro-4-methylquinoline	148.112	HMDB29709	0,491869
4-Pyridoxic acid	184.058	HMDB00017	0,48913
Tiglylcarnitine	244.154	HMDB02366	0,483509
Formiminoglutamic acid	173.056	HMDB00854	0,482806
Orotidine	287.052	HMDB00788	0,478949
N-(3-Methylbutyl)acetamide	116.107	HMDB31651	0,478408
(1R,3R,4R,5S,6S,8x)-1-Acetoxy-8-angeloyloxy-3,4-epoxy-5-hydroxy-7(14),10-bisaboladien-2-one	405.192	HMDB39971	0,475249
N-Acetylvanilalanine	252.088	HMDB11716	0,474226
Methocarbamol	242.1	HMDB14567	0,472488
Methionyl-Threonine	251.103	HMDB28983	0,47117
2-Aminomuconic acid	158.045	HMDB01241	0,469803
Uracil	113.035	HMDB00300	0,468658
N'-Formylkynurenine	237.087	HMDB01200	0,462608



2,4,6-Octatriyn-1-ol	119.049	HMDB30968	0,459115
Chlorohydrin	109.023	HMDB35190	0,458711
2,8-Dihydroxyadenine	166.038	HMDB00401	0,458449
Isoprothiolane	291.07	HMDB31779	0,457873
Glutaryl glycine	188.056	HMDB00590	0,457184
3-Dehydroxycarnitine	146.118	HMDB06831	0,454728
1-Methylhistidine	170.093	HMDB00001	0,452375
5-Aminopentanal	102.092	HMDB12815	0,45122
Dihydro-4-mercapto-3(2H)-furanone	119.016	HMDB39786	0,45094
N-Ornithyl-L-aurine	240.102	HMDB33519	0,449861
6-Feruloylglucose 2,3,4-trihydroxy-3-methylbutylglycoside	238.091	HMDB36214	0,447969
Aspartyl-L-proline	231.098	HMDB02335	0,446086
3-Sulfinoalanine	152.001	HMDB00996	0,445549
Glycerol 3-phosphate	171.005	HMDB00126	0,440815
Coumarin	147.044	HMDB01218	0,438759
Prostaglandin F1a	357.262	HMDB02685	0,438351
Glycyl-Phenylalanine	223.108	HMDB28848	0,438265
N-Acetylornithine	175.108	HMDB03357	0,437715
Succinic anhydride	101.024	HMDB32523	0,436918
Lofexidine	257.028	HMDB15606	0,43447
Trifluoromethyl-bismethyl ketone	71.0298	HMDB61928	0,43216
Pyridine	80.0501	HMDB00926	0,431432
Kamahine C	267.124	HMDB38935	0,426584
Vorinostat	265.155	HMDB15568	0,42391
(S)C(S)S-Methylcysteine sulfoxide	152.036	HMDB29432	0,419726
Trimethylamine N-oxide	76.0764	HMDB00925	0,418566
Glycylprolylhydroxyproline	286.144	HMDB02171	0,418389
2-Hydroxy-3-methylpentanoic acid	131.07	HMDB00317	0,415475
3-Hydroxyhexadecadienoylcarnitine	412.306	HMDB13335	0,41402
2,2-dichloro-1,1-ethanediol	130.965	HMDB62193	0,411393
13-L-Hydroperoxylinoleic acid	313.237	HMDB03871	0,410271
1-(2,3-Dihydro-1H-pyrrolizin-5-yl)-1,4-pentanedione	206.117	HMDB40046	0,409167
Glutaconic acid	129.018	HMDB00620	0,406239
Canrenone	339.2	HMDB03033	0,405598
Glycylproline	173.092	HMDB00721	0,40499
2-Ketobutyric acid	101.023	HMDB00005	0,40331
5-Hydroxylysine	163.11	HMDB00450	0,401736
Magnesium Sulfate	118.929	HMDB14791	0,400846
Toxin T2 tetrol	299.148	HMDB36159	0,397572
L-Agaridoxin	255.098	HMDB29445	0,397471
Indoxyl sulfate	212.002	HMDB00682	0,396788
1-Isothiocyanatobutane	116.053	HMDB31328	0,394638
Alanyl-Proline	187.108	HMDB28695	0,39459
N-Acetylhistidine	196.074	HMDB32055	0,392507
L-gamma-glutamyl-L-isooleucine	261.145	HMDB11170	0,391282
1-Methyladenosine	282.119	HMDB03331	0,391124
Liqcoumarin	217.048	HMDB29518	0,389805
(1'R)-Nepetalic acid	185.115	HMDB36117	0,388907
1,3,11-Tridecatriene-5,7,9-triyne	167.084	HMDB34294	0,38854
N-Stearoyl tyrosine	448.342	HMDB62343	0,386684
Hexylamine	102.128	HMDB32323	0,38591
Arachidonic acid	305.247	HMDB01043	0,383897
Benzaldehyde	107.05	HMDB06115	0,381844
3a,7a,12b-Trihydroxy-5b-cholanoic acid	407.284	HMDB00312	0,379739
2-Diethylaminoethanol	118.123	HMDB33971	0,379062
Castavinol	549.168	HMDB29808	0,378224
Allixin	227.126	HMDB40705	0,375349
L-Serine	104.034	HMDB00187	0,374837
Aldosterone	361.201	HMDB00037	0,374241

1-Isothiocyanato-3-phenylpropane	176.055	HMDB38444	0,373976
(2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid	148.097	HMDB29449	0,37193
Glyceric acid	105.018	HMDB00139	0,368375
S-(Allylthio)-L-cysteine	194.033	HMDB38669	0,367234
5-Hydroxyindoleacetic acid	192.065	HMDB00763	0,365973
3-Hydroxycapric acid	187.133	HMDB02203	0,364507
Putrescine	89.1079	HMDB01414	0,362615
4'-Hydroxyclobazam	315.059	HMDB60771	0,362492
Urocanic acid	139.05	HMDB00301	0,360576
S-Cysteinosuccinic acid	236.023	HMDB29418	0,360406
N-lactoyl-Tryptophan	275.104	HMDB62178	0,36011
Lucidenic acid M	463.303	HMDB35973	0,359889
Wasalexin A	293.043	HMDB34765	0,359524
Emtricitabine	246.038	HMDB15017	0,359008
Phenylalanylphenylalanine	313.154	HMDB13302	0,358407
8-Hydroxy-5,6-octadienoic acid	157.084	HMDB31101	0,355539
N-Acetylputrescine	131.118	HMDB02064	0,352938
Sinapyl alcohol	211.097	HMDB13070	0,352875
5-Hydroxy-2-furoic acid	127.002	HMDB59784	0,35205
Oxalosuccinic acid	189.002	HMDB03974	0,35019
(-)-erythro-Anethole glycol 1-glucoside	343.14	HMDB33066	0,349764
Lysyl-Tryptophan	331.176	HMDB28962	0,348595
Cytosine	112.051	HMDB00630	0,348285
1,3,7-Trimethyluric acid	209.066	HMDB02123	0,347447
Dihydrovaltrate	425.215	HMDB34492	0,346613
Indole	118.065	HMDB00738	0,346375
7-Hydroxyoctanoic acid	159.102	HMDB00486	0,34637
Gerberinol	365.105	HMDB33304	0,345033
Pirbuterol	241.155	HMDB15407	0,34433
Prazepam	325.113	HMDB15527	0,342993
4-Hydroxyproline	132.066	HMDB00725	0,342562
LysoPC(20:4(5Z,8Z,11Z,14Z))	544.339	HMDB10395	0,340499
Phthalic acid	167.032	HMDB02107	0,338523
2-Acetylthiazole	126.002	HMDB32964	0,336651
Carissanol	377.157	HMDB30081	0,336136
Dimethylallylpyrophosphate	247.013	HMDB01120	0,335953
3-Dehydroquinate	189.04	HMDB12710	0,335825
Uridine	245.077	HMDB00296	0,335794
Finasteride	187.144	HMDB01984	0,335347
2-phosphonato-D-glycerate(3-)	181.965	HMDB62707	0,335038
Deoxycholic acid glycine conjugate	448.307	HMDB00631	0,334603
(S)-Reticuline	330.17	HMDB03601	0,333141
Vanillactic acid	213.075	HMDB00913	0,331174
3-Hydroxy-2-methylpyridine-4,5-dicarboxylate	196.028	HMDB06955	0,329989
GlutaminyI-Isoleucine	260.161	HMDB28800	0,328322
1-Isothiocyanato-7-(methylthio)heptane	204.087	HMDB38440	0,326609
S-(2-carboxypropyl)-Cysteamine	164.074	HMDB02169	0,322331
Palmitoyl glucuronide	419.301	HMDB10331	0,321019
N-Acetylserotonin	219.113	HMDB01238	0,320448
Norfuraneol	113.023	HMDB31859	0,320244
Cyanidin-3-galactoside	243.045	HMDB29195	0,319348
AsparaginyI-Proline	230.114	HMDB28739	0,317168
Heptanoylcarnitine	274.201	HMDB13238	0,317044
(+)-2,3-Dihydro-3-methyl-1H-pyrrole	84.0814	HMDB33529	0,316943
Androsterone sulfate	369.174	HMDB02759	0,316472
Modafinil	274.092	HMDB14883	0,314921
Indane	119.086	HMDB59837	0,312361
3',4'-Dihydrodiol	287.1	HMDB13895	0,312263
Dezocine	246.182	HMDB15340	0,311838

2,6-Dimethoxy-4-methylphenol	169.086	HMDB29680	0,311386
Loxapine	326.109	HMDB14552	0,311283
N-acetyltryptophan	245.093	HMDB13713	0,308575
Vinylacetylglycine	144.066	HMDB00894	0,30738
Serinyl-Valine	205.119	HMDB29052	0,306301
Dicumarol	335.061	HMDB14411	0,306187
Epinephrine	184.095	HMDB00068	0,306155
Tranexamic Acid	158.118	HMDB14447	0,305513
L-cysteine Hydrochloride	158.003	HMDB62799	0,305171
Stearyl citrate	445.314	HMDB32521	0,305126
2-Methylbutyrylglycine	158.081	HMDB00339	0,304747
Phenol	95.0497	HMDB00228	0,304618
Amyl 2-furoate	183.102	HMDB29456	0,303357
2-Methylcitric acid	207.051	HMDB00379	0,303316
Prolyl-Threonine	217.118	HMDB29027	0,301516
N-Acetylgalactosamine	220.082	HMDB00212	0,299517
Amidosulfonic acid	97.9918	HMDB34830	0,298202
2-Hydroxyethanesulfonate	124.99	HMDB03903	0,296578
Pravastatin	425.25	HMDB05022	0,296109
Dehydroepiandrosterone sulfate	367.158	HMDB01032	0,296044
2,4-Hexadienyl acetate	141.091	HMDB32311	0,294837
Ascorbigen	304.08	HMDB29839	0,294199
Ornithinium(1+)	134.106	HMDB62718	0,292581
L,L-Cyclo(leucylprolyl)	211.144	HMDB34276	0,291363
5-hydroxy-2-oxo-4-ureido-2,5-dihydro-1H-imidazole-5-carboxylate	203.04	HMDB59663	0,289736
Casimiroin	232.059	HMDB33349	0,289574
p-Cresol glucuronide	285.1	HMDB11686	0,289249
LysoPE(0:0/20:1(11Z))	508.34	HMDB11482	0,288256
Diflubenzuron	311.04	HMDB31778	0,286856
Isepamicin	570.306	HMDB41911	0,286776
Monoethyl malonic acid	131.034	HMDB00576	0,28644
N,N-Dimethylaniline	122.097	HMDB01020	0,285125
2-Isopropyl-3,5-dimethoxy-6-methylpyrazine	197.129	HMDB29741	0,284175
3-Ethylpyridine	108.081	HMDB29734	0,283244
Acetylcarnosine	269.126	HMDB12881	0,281354
5,8-Dihydro-6-(4-methyl-3-pentenyl)-1,2,3,4-tetrathiocin	265.023	HMDB38142	0,281278
1,3-Dimethyluracil	141.066	HMDB02144	0,280609
3-Methoxybenzenepropanoic acid	181.086	HMDB11751	0,280179
Hexobarbital	237.123	HMDB15444	0,279731
Cadmium	112.895	HMDB03638	0,279502
N-Acetyl-L-phenylalanine	206.082	HMDB00512	0,279186
Arachidyl carnitine	456.406	HMDB06460	0,278713
Phenol sulphate	172.99	HMDB60015	0,278286
Diethanolamine	106.087	HMDB04437	0,277395
3-Hydroxydodecanoic acid	215.165	HMDB00387	0,27675
L-Aspartyl-L-phenylalanine	281.113	HMDB00706	0,276261
3-Methylindole	132.081	HMDB00466	0,275242
Diaminopimelic acid	191.103	HMDB01370	0,274496
Hydroxyprolyl-Isoleucine	243.135	HMDB28866	0,274441
p-Mentha-1,3,5,8-tetraene	133.099	HMDB29641	0,274131
N-Acetylgalactosamine 4-sulphate	300.04	HMDB00781	0,273081
Ribothymidine	259.093	HMDB00884	0,272365
3-Methyladipic acid	159.065	HMDB00555	0,271209
(9E)-10-nitrooctadecenoic Acid	328.248	HMDB62737	0,271009
9-Decenoylcarnitine	314.233	HMDB13205	0,27079
Leucyl-phenylalanine	277.156	HMDB13243	0,270493
Acrylamide	72.0451	HMDB04296	0,268104
Homocysteine	136.043	HMDB00742	0,267061

D-Alanyl-D-alanine	161.092	HMDB03459	0,265271
4-Ethylphenol	123.081	HMDB29306	0,262775
Nadolol	310.201	HMDB15334	0,261697
Isoleucyl-Tyrosine	295.165	HMDB28919	0,260683
Alanyl-Hydroxyproline	203.103	HMDB28688	0,260491
Dethiobiotin	215.139	HMDB03581	0,259775
Cubebinone	429.154	HMDB33259	0,259438
Homoarecoline	170.118	HMDB38321	0,259189
Propionic acid	75.0447	HMDB00237	0,259055
Progabide	335.095	HMDB14975	0,258801
2-Piperidinone	100.076	HMDB11749	0,257056
Carbidopa	245.113	HMDB14336	0,256853
N(6)-Methyllysine	161.129	HMDB02038	0,256725
Oleamide	282.279	HMDB02117	0,256174
N-Acetyl-L-tyrosine	222.077	HMDB00866	0,255833
4-Methyl-1-phenyl-2-pentanone	177.128	HMDB31569	0,254456
Glutarylcarntine	276.144	HMDB13130	0,25366
Cytidine monophosphate	322.045	HMDB00095	0,253618
2-Octenedioic acid	173.079	HMDB00341	0,252851
Carbenicillin	377.086	HMDB14717	0,251365
5-Methylthioribose 1-phosphate	259.001	HMDB00963	0,250569
Garcinia acid	207.012	HMDB31159	0,250457
2-[(5-Methylsulfinyl)-4-penten-2-ynylidene]-1,6-dioxaspiro[4.4]non-3-ene	249.062	HMDB32670	0,24969
Phenylglyoxylic acid	151.039	HMDB01587	0,249049
Methyl methanethiosulfonate	126.99	HMDB31832	0,248106
Bergaptol	203.032	HMDB13679	0,246743
Pyrocatechol	111.044	HMDB00957	0,246244
2-Methylglutaric acid	145.049	HMDB00422	0,245382
1,2,3-Trihydroxybenzene	125.023	HMDB13674	0,244881
7-Hydroxy-5-(4-hydroxy-2-oxopentyl)-2-methylchromone 7-glucoside	437.143	HMDB34698	0,244154
2,6-Diamino-4-hydroxy-5-N-methylformamidopyrimidine	184.085	HMDB11657	0,24338
Phenmetrazine	178.123	HMDB14968	0,243214
Citrulline	176.103	HMDB00904	0,242819
2-Propanoylthiazole	142.034	HMDB37168	0,242759
Losartan	421.156	HMDB14816	0,242277
Allantoic acid	177.061	HMDB01209	0,241871
Quinic acid	191.055	HMDB03072	0,241834
N6,N6,N6-Trimethyl-L-lysine	189.16	HMDB01325	0,241787
D-Xylose	149.044	HMDB00098	0,241732
2-Hydroxymyristic acid	243.196	HMDB02261	0,241378
6-Keto-decanoylcarnitine	330.227	HMDB13202	0,240373
Lead	206.972	HMDB04628	0,240216
Cyclohexylamine	100.112	HMDB31404	0,239036
D-1-Piperideine-2-carboxylic acid	128.071	HMDB01084	0,238865
N1-Methyl-2-pyridone-5-carboxamide	153.066	HMDB04193	0,238556
1,2-Diacylglycerol-LD-PI-pool	120.045	HMDB62270	0,2381
7a,12a-Dihydroxy-3-oxo-4-cholenoic acid	405.261	HMDB00447	0,237956
Dexfenfluramine	232.129	HMDB15322	0,237587
6,7-Dimethyl-8-(1-D-ribityl)lumazine	164.067	HMDB03826	0,236985
Shikimic acid	175.058	HMDB03070	0,236885
Mukonidine	242.079	HMDB30214	0,236556
Isosakuranin	447.135	HMDB29481	0,235884
Ethyl trans-p-methoxycinnamate	205.086	HMDB30762	0,235821
3-Hydroxy-5, 8-tetradecadiencarnitine	384.274	HMDB13332	0,235552
Androsterone glucuronide	234.132	HMDB02829	0,234673
Cotinine methonium ion	192.123	HMDB01365	0,234654
2-Phosphoglyceric acid	184.985	HMDB00362	0,234443

Alpha-CEHC	279.159	HMDB01518	0,2343
2,3,5-Trimethylfuran	111.081	HMDB29721	0,234157
beta-D-3-[5-Deoxy-5-(dimethylarsinyl)ribofuranosyloxy]-2-hydroxy-1-propanesulfonic acid	391.001	HMDB32686	0,233566
Choline	105.114	HMDB00097	0,233535
1,7-Dimethylguanosine	310.115	HMDB01961	0,23321
Sulfinpyrazone sulfide	387.115	HMDB60943	0,232496
3-(1,1-Dimethylallyl)scopoletin 7-glucoside	421.148	HMDB32853	0,232088
Citicoline	245.061	HMDB01413	0,231374
1-Methylguanosine	298.115	HMDB01563	0,231232
LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	526.293	HMDB11496	0,230299
3-Oxo-octadecanoic acid	297.243	HMDB10736	0,229843
3-Oxohexadecanoic acid	269.212	HMDB10733	0,22926
Cymorcin monoglucoside	329.159	HMDB29777	0,228514
Cascarillin	407.207	HMDB36836	0,228151
Galactitol	181.071	HMDB00107	0,227881
Methyl bisnorbiotinyl ketone	215.088	HMDB04822	0,227033
Miglitol	206.103	HMDB14634	0,226827
Sorbitan oleate	429.319	HMDB29886	0,226617
Diplosporin	223.097	HMDB30680	0,226478
2(N)-Methyl-norsalsolinol	180.102	HMDB01189	0,225745
1H-Indole-3-carboxaldehyde	144.044	HMDB29737	0,225592
3-Furoic acid	111.007	HMDB00444	0,225584
PI(16:0/22:3(10Z,13Z,16Z))	445.288	HMDB09792	0,225522
2,2,4,4,-Tetramethyl-6-(1-oxopropyl)-1,3,5-cyclohexanetrione	237.116	HMDB33191	0,224723
L-beta-aspartyl-L-alanine	205.082	HMDB11162	0,224683
Malonylcarnitine	248.113	HMDB02095	0,22428
Cadaverine	103.123	HMDB02322	0,221904
Methyl 2-octynoate	155.107	HMDB31302	0,220412
trans-3,3',4',5,5',7-Hexahydroxyflavanone	321.06	HMDB30835	0,219917
D-Glucuronic acid	193.035	HMDB00127	0,219592
9,12,13-TriHOME	329.234	HMDB04708	0,219242
2,3-diketogulonate	192.024	HMDB62803	0,21648
2-Octenoic acid	141.091	HMDB00392	0,215812
1-(1-Propenylthio)propyl propyl disulfide	223.064	HMDB33041	0,215371
cis-4-Decenedioic acid	199.097	HMDB00603	0,215316
3-Aminopropionaldehyde	74.0607	HMDB01106	0,214759
7-Methylguanine	166.073	HMDB00897	0,214208
Docosanamide	340.358	HMDB00583	0,213605
Azelaic acid	187.097	HMDB00784	0,213455
Homocitrulline	190.119	HMDB00679	0,213147
Stearidonyl carnitine	420.31	HMDB06463	0,213042
3-Hydroxyisoheptanoic acid	145.086	HMDB02207	0,212542
N-Acetyl-S-(N-methylcarbamoyl)cysteine	219.045	HMDB41942	0,212115
6-Dimethylaminopurine	162.076	HMDB00473	0,211978
5'-(3',4'-Dihydroxyphenyl)-gamma-valerolactone sulfate	289.033	HMDB29191	0,210825
Carboxyphosphamide	291.008	HMDB60449	0,210804
Glycerol tripropanoate	261.131	HMDB32857	0,210443
Acetylphosphate	140.996	HMDB01494	0,210335
Guanidinosuccinic acid	176.066	HMDB03157	0,209922
Ecgonine methyl ester	200.128	HMDB06406	0,20991
3-Bromosulfolane	198.94	HMDB40457	0,209435
3,4,5-Trimethoxycinnamic acid	239.09	HMDB02511	0,20898
Alpha-ketoisovaleric acid	115.039	HMDB00019	0,208811
2-Methyl-2-cyclopenten-1-one	97.0653	HMDB31545	0,208213
alpha-Hydroxymetoprolol	284.186	HMDB60994	0,207985
Suberic acid	173.081	HMDB00893	0,206208
Potassium 2-(1'-ethoxy) ethoxypropanoate	199.037	HMDB37192	0,205702

Allantoin	157.036	HMDB00462	0,205391
(R)-N-Methylsalsolinol	194.118	HMDB03626	0,205235
2-Amino-3,4-dimethylimidazo[4,5-f]quinoline	213.112	HMDB29707	0,204682
Cortisol	363.217	HMDB00063	0,203878
Metenamine	141.114	HMDB29598	0,203834
(S)-9-Hydroxy-10-undecenoic acid	201.148	HMDB32662	0,203571
1-Cyano-2-hydroxy-3-butene	98.0606	HMDB31339	0,20316
Sertraline	304.071	HMDB05010	0,203085
Osmundalactone	129.055	HMDB31303	0,202332
alpha-(1,2-Dihydroxyethyl)-1,2,3,4-tetrahydro-7-hydroxy-9-methoxy-3,4-dioxocyclopenta[c][1]benzopyran-6-acetaldehyde	347.075	HMDB62442	0,201546
Methyl (7Z,9Z,9'Z)-6'-apo-y-caroten-6'-oate	473.345	HMDB31381	0,201432
Pregnanetriol	337.274	HMDB06070	0,201374
Scopolamine	302.135	HMDB03573	0,201111
Phosphoglycolic acid	156.991	HMDB00816	0,200671
Docosa-4,7,10,13,16-pentaenoyl carnitine	474.358	HMDB06321	0,200487
PC(14:0/18:1(11Z))	732.548	HMDB07872	0,199924
Plastoquinone 3	341.251	HMDB33786	0,199015
Citranaxanthin	457.35	HMDB36883	0,197356
Methoxybrassinin	267.059	HMDB33351	0,197003
Ciclopirox	208.133	HMDB15319	0,196955
Oleic acid	281.249	HMDB00207	0,195361
Dihydro-2,4,6-tris(2-methylpropyl)-4h-1,3,5-dithiazine	290.196	HMDB32221	0,194704
Capryloylglycine	200.129	HMDB00832	0,19306
Zalcitabine	212.103	HMDB15078	0,192929
Chlorphenesin	201.034	HMDB14994	0,19243
Tetraphyllin B	286.091	HMDB29914	0,189763
3-Indolebutyric acid	204.102	HMDB02096	0,189663
Indoleacetic acid	176.071	HMDB00197	0,189621
Flumequine	262.084	HMDB41895	0,188507
Prolylhydroxyproline	229.118	HMDB06695	0,188281
Acidissiminin	660.49	HMDB38619	0,18803
Succinylacetone	159.063	HMDB00635	0,187944
2-Isopropyl-1,4-benzenediol	153.091	HMDB32132	0,187594
MG(0:0/16:0/0:0)	331.284	HMDB11533	0,186804
2,4-Dimethylthiazole	114.038	HMDB32974	0,186354
L-3-Aminodihydro-2(3H)-furanone	102.055	HMDB29387	0,18623
Vanylglycol	185.081	HMDB01490	0,185819
3-Oxodecanoic acid	185.117	HMDB10724	0,185661
Santalyl acetate	263.197	HMDB32501	0,185545
Toluene	93.0704	HMDB34168	0,183753
Daucic acid	203.02	HMDB31665	0,183569
3-Butyn-1-al	69.0342	HMDB06853	0,183442
3-Amino-2-piperidone	115.087	HMDB00323	0,182882
Fluvoxamine	319.165	HMDB14322	0,182291
L-Fucose	165.076	HMDB00174	0,181782
3-Oxododecanoic acid	213.149	HMDB10727	0,179982
(4-Methylphenyl)acetaldehyde	135.081	HMDB29639	0,179811
Homocysteine thiolactone	118.032	HMDB02287	0,179723
Simvastatin	419.277	HMDB05007	0,179365
Nor-psi-tropine	128.107	HMDB31667	0,178957
Histidinyl-Proline	253.127	HMDB28893	0,177674
PE(18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	392.748	HMDB09210	0,177591
Linoleic acid	281.248	HMDB00673	0,177341
Genipinic acid	243.087	HMDB38126	0,177149
Cyclohexanone	97.0645	HMDB03315	0,177077
LysoSM(d18:1)	466.352	HMDB06482	0,176675
Isoleucyl-Tryptophan	318.181	HMDB28918	0,17623

Jasmonic acid	211.133	HMDB32797	0,176058
Cibulins	93.0372	HMDB30299	0,175881
Vanilpyruvic acid	211.058	HMDB11714	0,175763
Erythrityl Tetranitrate	300.991	HMDB15551	0,175639
3-carboxy-2,3-dihydroxypropanoate	150.014	HMDB62642	0,175458
Delta-Hexanolactone	115.076	HMDB00453	0,17531
Nabam	254.917	HMDB31224	0,175069
3b,12a-Dihydroxy-5a-cholanoic acid	391.289	HMDB00348	0,174884
LysoPC(20:3(5Z,8Z,11Z))	546.355	HMDB10393	0,174594
Marmesin rhamnoside	393.152	HMDB39564	0,173562
Nookatone	219.175	HMDB13687	0,172998
2-(2-Thienylmethylene)-1,6-dioxaspiro[4.4]non-3-ene	219.051	HMDB34857	0,171869
5-Dodecenoic acid	199.169	HMDB00529	0,171459
Propofol	177.127	HMDB14956	0,171242
(R)-3-Hydroxy-5-phenylpentanoic acid	193.086	HMDB31517	0,171234
L-Menthyl acetoacetate	239.165	HMDB32369	0,170495
Octadecylamine	270.315	HMDB29586	0,169947
Dehydrophytosphingosine	316.285	HMDB38057	0,169417
(3R,7R)-1,3,7-Octanetriol	163.133	HMDB33625	0,169251
Varenicline	212.118	HMDB15398	0,168032
(Z)-1,3-Octadiene	109.102	HMDB61897	0,167738
Mesuagin	389.137	HMDB35876	0,167574
Arecoline	156.102	HMDB30353	0,167573
Ribitol	151.06	HMDB00508	0,167428
lysoPC(6:0)	356.185	HMDB29207	0,166807
Pyruvaldehyde	71.0124	HMDB01167	0,166434
5-Hydroxy-L-tryptophan	221.092	HMDB00472	0,166423
1-Methylinosine	283.104	HMDB02721	0,165728
Niazirin	280.122	HMDB32807	0,165696
Guanosine	284.099	HMDB00133	0,164486
Alclometasone	409.175	HMDB14385	0,164172
(S,E)-Zearalenone	319.153	HMDB31752	0,162668
3-Methylcyclopentadecanone	239.237	HMDB34181	0,162249
2-Hydroxyfluorene	92.0433	HMDB13163	0,16084
4-Methylcatechol	125.06	HMDB00873	0,160452
N-Carboxyethyl-g-aminobutyric acid	174.076	HMDB02201	0,159822
Cortolone-3-glucuronide	541.266	HMDB10320	0,159756
Quinolinic acid	166.017	HMDB00232	0,159728
4-Ketocyclophosphamide	275.008	HMDB60686	0,159391
L-phenylalanyl-L-proline	263.139	HMDB11177	0,158454
Alosetron	295.152	HMDB15104	0,158075
Methylarsonate	140.951	HMDB12258	0,157761
Mizoribine	258.075	HMDB41934	0,15774
Guaifenesin	197.081	HMDB04998	0,157291
Tetrahydrofuran	73.0655	HMDB00246	0,156877
Pipericyclobutanamide B	595.289	HMDB36361	0,156858
LysoPE(0:0/20:5(5Z,8Z,11Z,14Z,17Z))	498.263	HMDB11489	0,156857
Glucosamine	180.087	HMDB01514	0,155956
Citronellyl anthranilate	276.199	HMDB32208	0,155703
D-glycero-L-galacto-Octulose	239.077	HMDB29954	0,155432
5-Methoxytryptophol	192.102	HMDB01896	0,155366
2,6 Dimethylheptanoyl carnitine	302.233	HMDB06320	0,154887
Glycerol	93.0552	HMDB00131	0,154758
Diethylthiophosphate	171.026	HMDB01460	0,153305
3-hydroxynonanoyl carnitine	318.228	HMDB61635	0,152824
4-Hydroxybenzoic acid	137.023	HMDB00500	0,15197
Homogentisic acid	169.047	HMDB00130	0,151555
Bissulfine	179.022	HMDB30000	0,151553
2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]nona-3,8-diene	181.122	HMDB30007	0,151378

3-Methylcyclopentene	83.0861	HMDB31544	0,151348
3,4-Dihydroxybenzylamine	138.055	HMDB12153	0,151127
5-Hydroxytryptophol	178.086	HMDB01855	0,150989
2-Bromophenol	170.943	HMDB32059	0,150333
2-Furanmethanol	99.0445	HMDB13742	0,150251
3,4-Dihydroxyphenylglycol	169.05	HMDB00318	0,150158
Arbutamine	318.166	HMDB15234	0,150005
Meperidine	248.168	HMDB14597	0,149162
5-O-Feruloylnigrumin	226.583	HMDB38735	0,148292
Selenomethionine	198.001	HMDB03966	0,148238
2-trans,4-cis-Decadienoylcarnitine	312.217	HMDB13325	0,14799
N4-Acetylcytidine	286.103	HMDB05923	0,14793
N-Methylcalystegine C1	206.102	HMDB36394	0,14686
1,3-Diacetylpropane	127.075	HMDB29165	0,146285
Silicic acid	94.9794	HMDB31436	0,146095
4-Heptenal diethyl acetal	201.076	HMDB32306	0,145984
Foeniculoside VIII	349.183	HMDB33009	0,145359
Glycolic acid	75.0073	HMDB00115	0,144319
L-beta-aspartyl-L-threonine	233.078	HMDB11169	0,143914
Undecanedioic acid	215.128	HMDB00888	0,143765
Butyric acid	87.0438	HMDB00039	0,143758
(S)-5-Diphosphomevalonic acid	306.999	HMDB01090	0,143197
(9Z,11E,13E,15Z)-4-Oxo-9,11,13,15-octadecatetraenoic acid	291.194	HMDB31098	0,143178
Dodecanedioic acid	229.144	HMDB00623	0,143031
O-Phosphoethanolamine	142.026	HMDB00224	0,142718
Imiquimod	241.144	HMDB14862	0,142122
Methylmalonylcarnitine	262.129	HMDB13133	0,142016
Cervonyl carnitine	472.342	HMDB06510	0,141059
Azosemide	368.999	HMDB41831	0,140887
Methyl sorbate	127.076	HMDB29582	0,140853
Polyethylene, oxidized	243.124	HMDB32472	0,140559
Hydroxylated lecithin	147.042	HMDB32332	0,140258
5-Methyl-2-thiophenecarboxaldehyde	125.006	HMDB32431	0,140015
2-Oxo-3-hydroxy-4-phosphobutanoic acid	212.979	HMDB06801	0,139443
alpha-hydroxysalmeterol	432.28	HMDB61045	0,138889
Propenoylcarnitine	216.123	HMDB13124	0,138344
l(-)	126.904	HMDB59634	0,138317
Riboflavin	377.144	HMDB00244	0,138213
6-Dehydrotestosterone glucuronide	463.232	HMDB10337	0,137973
Tocainide	193.132	HMDB15189	0,13731
2,3,6-Trimethylphenol	137.098	HMDB29667	0,136851
S-2-Propenyl 1-propenesulfinothioate	163.026	HMDB32750	0,135255
(S)-Spirobrassinin	251.034	HMDB35974	0,135138
Oxprenolol	266.173	HMDB15520	0,135128
p-Cresol	109.065	HMDB01858	0,135118
Porphobilinogen	227.103	HMDB00245	0,135038
11-Hydroxy-12-methoxydihydrokawain	279.12	HMDB30766	0,134992
7-Ketodeoxycholic acid	405.268	HMDB00391	0,134506
(S)-3-Hydroxynonanoic acid	173.117	HMDB31513	0,134425
Cassiachromone	233.079	HMDB30813	0,13426
LysoPC(18:2(9Z,12Z))	520.333	HMDB10386	0,133747
2,4-Dihydroxy-6,7-dimethoxy-2H-1,4-benzoxazin-3(4H)-one	240.049	HMDB37548	0,132866
(-)-trans-Carveol glucoside	313.164	HMDB29848	0,132694
1,1'-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-ethanone	257.103	HMDB32527	0,132654
trans-trans-Muconic acid	141.018	HMDB02349	0,132647
Tetradecanedioic acid	257.176	HMDB00872	0,132498
8-O-Methylolongine	327.18	HMDB34579	0,132354
Fenthion	279.029	HMDB33209	0,132124



4-Aminophenol	110.06	HMDB01169	0,132065
1-Methyl-1,3-cyclohexadiene	95.0861	HMDB31532	0,131971
3-hydroxyundecanoyl carnitine	346.259	HMDB61637	0,131762
Alpha-Linolenic acid	279.232	HMDB01388	0,130933
Vitamin K1 2,3-epoxide	467.358	HMDB02972	0,130763
(2xi,6xi)-7-Methyl-3-methylene-1,2,6,7-octanetetrol	203.128	HMDB33217	0,130526
Avenic acid A	323.147	HMDB30416	0,130201
Melibiose	341.109	HMDB00048	0,130116
2-Propene-1-thiol	75.0267	HMDB31635	0,130014
Dityrosine	359.125	HMDB06045	0,129805
Chondrillasterol 3-[glucosyl-(1->2)-glucosyl-(1->2)-glucoside]	450.274	HMDB33887	0,129442
Cordeauxione	293.063	HMDB34310	0,129189
Glutaminy-Glutamate	275.11	HMDB28796	0,128527
Sertindole	441.189	HMDB15618	0,127675
(E)-2-octenal	127.112	HMDB13809	0,127577
Ethyl glucuronide	223.085	HMDB10325	0,127427
Menadiol dibutyrate	315.157	HMDB32726	0,127052
Glycyl-Tryptophan	262.119	HMDB28852	0,126906
Flurandrenolide	437.236	HMDB14984	0,126137
Desflurane	166.992	HMDB15320	0,125997
Propyl propane thiosulfonate	227.091	HMDB32496	0,125682
Hydrocortamate	476.307	HMDB14907	0,125264
(10S,11S)-Pterosin C	235.132	HMDB30763	0,125155
3-Hydroxysebacic acid	217.108	HMDB00350	0,124702
2,6-Dimethoxy-4-propylphenol	195.102	HMDB36226	0,124646
PI(16:0/20:2(11Z,14Z))	863.557	HMDB09786	0,124614
Benzene	79.0547	HMDB01505	0,123817
Pregnenolone sulfate	397.2	HMDB00774	0,123761
Metyrosine	194.081	HMDB14903	0,121544
Betamethasone	393.21	HMDB14586	0,121014
Coriandrone D	353.158	HMDB29972	0,120967
Pteroside B	381.188	HMDB30760	0,120581
2-(3-carboxy-3-(trimethylammonio)propyl)-L-histidine	300.181	HMDB59617	0,120055
Melphalan	305.086	HMDB15176	0,119978
2,3-Dihydroxyvaleric acid	133.049	HMDB00421	0,119737
Clenbuterol	275.076	HMDB15477	0,119713
8-Acetylegelolide	309.131	HMDB37772	0,119021
Indole-3-carbinol	148.076	HMDB05785	0,118909
Berberine	337.126	HMDB03409	0,118683
Cysteinyl-Cysteine	225.035	HMDB28772	0,118673
Citronellyl beta-sophoroside	481.262	HMDB32839	0,118648
Asparaginy-Hydroxyproline	246.108	HMDB28732	0,11857
(R)-3-Hydroxy-Octadecanoic acid	299.259	HMDB10737	0,118406
Gentisic acid	153.018	HMDB00152	0,118262
6,11-Dihydroxy-2,2-dimethylpyrano[3,2-c]xanthen-7(2H)-one	311.089	HMDB40357	0,118099
2-Aminoacrylic acid	88.0399	HMDB03609	0,116965
Tungsten	184.96	HMDB01989	0,116644
Gabapentin	172.133	HMDB05015	0,116553
Fluorouracil	131.024	HMDB14684	0,116546
S-Carboxymethyl-L-cysteine	178.017	HMDB29415	0,116308
N-Desmethylpromazine	269.113	HMDB13939	0,116227
Eplerenone	413.2	HMDB14838	0,116164
(E)-2-Butenal	71.0498	HMDB34233	0,116132
3'-Hydroxy-HT2 toxin	441.21	HMDB36162	0,115243
Dimethyl sulfone	95.0166	HMDB04983	0,114925
3-Indolepropionic acid	190.086	HMDB02302	0,114497
Acetylglycine	116.034	HMDB00532	0,114155

5-Hexyltetrahydro-2-oxo-3-furancarboxylic acid	215.126	HMDB30984	0,114121
3-Hydroxy-4-aminopyridine sulfate	188.997	HMDB61120	0,113939
1-(beta-D-Ribofuranosyl)-1,4-dihyronicotinamide	257.113	HMDB11648	0,113779
Corchorifatty acid F	329.231	HMDB35919	0,113331
(R)-2-Benzylsuccinate	209.078	HMDB12127	0,112923
2-Hydroxypyridine	96.0449	HMDB13751	0,112871
Gluconolactone	177.04	HMDB00150	0,111834
Ethambutol	205.193	HMDB14474	0,111246
Lorazepam	319.002	HMDB14332	0,11057
N-Undecanoylglycine	244.191	HMDB13286	0,110256
5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid	185.081	HMDB30988	0,109882
1-(alpha-Methyl-4-(2-methylpropyl)benzeneacetate)-beta-D-Glucopyranuronic acid	383.168	HMDB10343	0,109545
D-Glyceraldehyde 3-phosphate	171.006	HMDB01112	0,109378
Hydroxyphenylacetyl glycine	208.06	HMDB00735	0,108777
4-Hydroxypropofol	195.138	HMDB14018	0,108555
7(14)-Bisabolene-2,3,10,11-tetrol	271.192	HMDB35918	0,108163
Methionyl-Methionine	281.1	HMDB28979	0,107804
L-beta-aspartyl-L-glutamic acid	263.087	HMDB11164	0,107235
Forasartan	209.128	HMDB15434	0,107212
Dolichosterone	463.342	HMDB34336	0,107122
Hydralazine pyruvate hydrazone	231.084	HMDB61143	0,107094
Benzamide	122.06	HMDB04461	0,106965
Methylimidazole acetaldehyde	125.071	HMDB04181	0,106745
Santene	123.117	HMDB38140	0,106193
3-Chloro-1-(4-hydroxy-3-methoxyphenyl)-1,2-propanediol	233.059	HMDB34633	0,105833
Schidigeragenin B	429.302	HMDB35506	0,105654
N-(1-Deoxy-1-fructosyl)phenylalanine	326.125	HMDB37846	0,104784
Fructose 6-phosphate	259.022	HMDB00124	0,104755
1,2-Benzisothiazol-3(2H)-one	152.017	HMDB34413	0,104086
2,3,6,7-Tetrahydro-7-methylcyclopent[b]azepin-8(1H)-one	164.107	HMDB39661	0,104064
Gibberellin A55	365.157	HMDB33420	0,103741
2-Keto-glutaramic acid	144.029	HMDB01552	0,103707
Pyridoxal	168.066	HMDB01545	0,103419
Chlorhexidine	253.109	HMDB15016	0,102984
2-Phenylethyl beta-D-glucopyranoside	283.119	HMDB29819	0,102591
1-Stearoylglycerophosphoserine	522.284	HMDB61698	0,10256
Polypropylene glycol (m w 1,200-3,000)	135.102	HMDB32478	0,102247
Glutamyl-Lysine	275.147	HMDB28824	0,102026
Cycloserine	103.051	HMDB14405	0,101399
1-(2,4,6-Trimethoxyphenyl)-1,3-butanedione	251.092	HMDB30668	0,101363
Cerulein	224.13	HMDB15168	0,101103
Debrisoquine	176.117	HMDB06543	0,100561
Sebacic acid	201.113	HMDB00792	0,10046
beta-D-Glucopyranosyl-11-hydroxyjasmonic acid	387.166	HMDB39964	0,100325
Hexadecanedioic acid	285.207	HMDB00672	0,0993983
1,11-Undecanedicarboxylic acid	243.16	HMDB02327	0,099126
Triamcinolone	393.172	HMDB14758	0,0983637
(3beta,22E)-26,27-Dinorergosta-5,22-dien-3-ol	371.327	HMDB29863	0,0981042
5-Phenylvaleric acid	179.107	HMDB02043	0,0974069
4,4'-Thiobis-2-butanone	175.079	HMDB37155	0,0967678
9-Hydroxycalabaxanthone	409.162	HMDB31920	0,0959451
5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	143.07	HMDB33551	0,0958729
Bethanidine	178.134	HMDB14362	0,0957617
1-Methoxy-1-(2,4,5-trimethoxyphenyl)-2-propanol	255.122	HMDB31772	0,0956969
12(13)Ep-9-KODE	309.207	HMDB13623	0,0954374
Isovalerylglutamic acid	232.118	HMDB00726	0,0954082
Corchoionoside B	399.165	HMDB30975	0,0953589
Galactosylhydroxylysine	325.162	HMDB00600	0,0949313

Sunitinib	397.205	HMDB15397	0,0949266
epsilon-Viniferin	228.08	HMDB30604	0,0949212
trans-4,5-epoxy-2(E)-decenal	169.122	HMDB13105	0,0948911
(R)-Pelletierine	142.123	HMDB30324	0,0948115
Otobanone	339.12	HMDB30618	0,0947246
Nevirapine	267.121	HMDB14383	0,0943626
Porson	387.18	HMDB30810	0,0938045
N-Nonanoylglycine	214.144	HMDB13279	0,0937379
Carbendazim	192.075	HMDB31769	0,0937373
Parabanic Acid	112.998	HMDB62802	0,0934994
Decitabine	227.077	HMDB15391	0,0932818
Salicyluric acid	194.045	HMDB00840	0,0928555
Guanine	152.057	HMDB00132	0,0922906
Methylphosphate	110.984	HMDB61711	0,0915161
1-Propenyl 1-(1-propenylthio)propyl disulfide	219.033	HMDB38967	0,0913672
Dihydro-2-methoxy-2-methyl-3(2H)-thiophenone	147.047	HMDB40237	0,0911947
Polyporusterone B	477.319	HMDB38496	0,0893446
S-2-Propenyl 1-propanesulfinothioate	163.024	HMDB32741	0,0888471
Neuroprotectin D1	361.235	HMDB03689	0,0883374
4-Hydroxy-2-oxoglutaric acid	161.008	HMDB02070	0,0882962
16-Oxoestrone	283.137	HMDB00372	0,0881417
Norcotinine	163.086	HMDB01297	0,0881024
Distichonic acid A	295.115	HMDB38752	0,0880972
Penmacric acid	201.052	HMDB29436	0,08809
Hydroxytyrosol	155.07	HMDB05784	0,088026
Phthalide	135.044	HMDB32469	0,0879617
Boviquinone 4	413.266	HMDB30057	0,0874027
Desglucocoroloside	505.314	HMDB33709	0,0864361
2,3-Dehydrosalvipisone	309.153	HMDB40742	0,0864201
N-Succinyl-L,L-2,6-diaminopimelate	291.12	HMDB12267	0,0861827
1b-Hydroxycholic acid	425.289	HMDB00307	0,0856382
p-Hydroxyphenylacetic acid	151.039	HMDB00020	0,0852118
trans-Ferulic acid	193.05	HMDB00954	0,0849677
Chloral hydrate	162.911	HMDB60451	0,0847882
2,3-Dinor-6-keto-prostaglandin F1 a	341.196	HMDB02277	0,0845584
5-[(4-Hydroxyphenyl)ethenyl]-2-(3-methyl-1-butenyl)-1,3-benzenediol	295.137	HMDB30599	0,0844419
3-Methyluric acid	181.038	HMDB01970	0,0838787
Chloroxine	213.983	HMDB15373	0,0835698
2-Chloro-5-methylmaleylacetate	207.008	HMDB60346	0,0834839
Lipoyllysine	335.147	HMDB12996	0,0832959
N-Desalkyl flurazepam	289.05	HMDB61161	0,0831391
p-Anisidine	124.076	HMDB29300	0,0829851
Hydrocinnamic acid	151.075	HMDB00764	0,0829497
Gentian Violet	373.256	HMDB14550	0,0826514
1-Pyrroline-5-carboxylic acid	114.055	HMDB01301	0,0825673
3-Hydroxydodecanedioic acid	245.139	HMDB00413	0,0824737
Leukotriene A4	319.225	HMDB01337	0,0813787
Arbutin	273.097	HMDB29943	0,081259
Methyl 2-(10-heptadecenyl)-6-hydroxybenzoate	387.286	HMDB38523	0,081212
MG(0:0/16:1(9Z)/0:0)	327.254	HMDB11534	0,0811735
Gemfibrozil	251.161	HMDB15371	0,0808314
13'-Carboxy-gamma-tocopherol	447.346	HMDB12557	0,0807315
13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid	343.248	HMDB40901	0,0804823
4-Nitrophenol	138.018	HMDB01232	0,0804275
2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrione	251.132	HMDB33197	0,07979
(-)-trans-Carveol	153.128	HMDB03450	0,0796106
Dodecamethylpentasiloxane	383.135	HMDB62731	0,0795961

4-Hydroxy-3-prenylbenzoic acid glucoside	367.139	HMDB39891	0,0795733
Isopentenyladenine-9-N-glucoside	364.197	HMDB12240	0,0791677
O-methoxycatechol-O-sulphate	205.017	HMDB60013	0,079141
Phaseolic acid	261.134	HMDB31897	0,0785469
(R)-Dihydromaleimide	98.0233	HMDB30276	0,0778666
3-Methylcrotonylglycine	158.081	HMDB00459	0,0776371
alpha-Fluoro-beta-alanine	108.045	HMDB60434	0,0776099
Traumatic acid	229.141	HMDB00933	0,0758664
6-Gingesulfonic acid	359.156	HMDB38999	0,0758278
Allolithocholic acid	375.294	HMDB00381	0,0758195
Indoleacetaldehyde	160.076	HMDB01190	0,0751403
Neryl glucoside	315.181	HMDB29346	0,0743013
Aspartyl-Glutamine	262.103	HMDB28751	0,0738087
Sumatriptan	296.146	HMDB05037	0,073654
Oxalic acid	88.9866	HMDB02329	0,0731684
Glaucarubin	497.236	HMDB35626	0,0730867
threo-Syringoylglycerol	243.086	HMDB31237	0,0730468
Chloropentafluoroethane	154.967	HMDB31333	0,0721315
Oxymorphone	302.135	HMDB15323	0,0721031
Methyl 3-(2,3-dihydroxy-3-methylbutyl)-4-hydroxybenzoate	253.108	HMDB32796	0,0717016
3,4,5-Trimethoxyphenyl acetate	225.075	HMDB31722	0,0715307
Nicotinic acid	124.04	HMDB01488	0,0712056
Atenolol	267.172	HMDB01924	0,0711442
N-Methylphenylethanolamine	152.107	HMDB01387	0,0708852
4-Hydroxyphenylpyruvic acid	179.034	HMDB00707	0,0704858
Fucose 1-phosphate	243.027	HMDB01265	0,0704778
Lomustine	234.097	HMDB15337	0,0704106
Valproic acid glucuronide	319.14	HMDB00901	0,0703511
7-Acetoxy-2-methylisoflavone	295.094	HMDB29364	0,0703281
Phenyl vinyl sulfide	137.041	HMDB31825	0,070179
Tetrahydrofurfuryl butyrate	171.102	HMDB36188	0,0693923
Cuminaldehyde	149.096	HMDB02214	0,0687087
5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	255.16	HMDB30993	0,0686841
11-nitro-1-undecene	200.165	HMDB62669	0,0682814
2-Dodecylbenzenesulfonic acid	327.201	HMDB31031	0,0681098
15-Deacetylneosalinol	341.157	HMDB36157	0,0676934
p-Cymene	135.117	HMDB05805	0,0675947
Anileridine	353.222	HMDB15049	0,0673208
Caproic acid	117.091	HMDB00535	0,0665534
2-(4-Methyl-5-thiazolyl)ethyl octanoate	270.155	HMDB32423	0,0659651
Cucurbitic acid	211.133	HMDB29388	0,0659273
Levocabastine	421.234	HMDB15238	0,0654754
Prostaglandin E2	353.231	HMDB01220	0,0652796
Dimethylethanolamine	90.0919	HMDB32231	0,065246
3-Methyl-4-phenyl-3-buten-2-one	161.096	HMDB31567	0,0650726
Trifluridine	297.074	HMDB14576	0,0643098
Norepinephrine	170.081	HMDB00216	0,0637832
2-Phenylbutyric acid	165.091	HMDB00329	0,0637657
Hexaethylene glycol	283.175	HMDB61822	0,0635475
N-Decanoylglycine	228.16	HMDB13267	0,0633085
D-Limonene	137.133	HMDB03375	0,0620937
N-Deschlorobenzoyl indomethacin	220.097	HMDB13988	0,06194
3-Propylidene-1(3H)-isobenzofuranone	175.075	HMDB31845	0,0616228
Malonic acid	103.002	HMDB00691	0,0606631
3,6-Dihydro-4-(4-methyl-3-pentenyl)-1,2-dithiin	199.061	HMDB30009	0,0606573
Corchoionol C 9-glucoside	385.186	HMDB29772	0,0602567
Clozapine	327.142	HMDB14507	0,0597853
Dimethicone	161.081	HMDB33532	0,0597408

Jasmolone glucoside	343.174	HMDB32870	0,0593304
cis-Methylbixin	409.236	HMDB32021	0,058687
PE(P-16:0e/0:0)	436.283	HMDB11152	0,0576932
L-Cysteine	122.027	HMDB00574	0,0568922
Spirolactone	415.197	HMDB14565	0,0563162
4-Hydroxycyclohexylcarboxylic acid	143.07	HMDB01988	0,0555263
Armillane	421.22	HMDB35779	0,0549709
Octanal	129.128	HMDB01140	0,0549198
Senecioic acid	101.06	HMDB00509	0,0548396
Morellin	273.134	HMDB30794	0,054526
Oxoadipic acid	159.029	HMDB00225	0,0543651
Paxilline	436.254	HMDB30323	0,0538385
trans-3-Hydroxycotinine glucuronide	369.131	HMDB01204	0,0526173
beta-Damascenone	191.143	HMDB13804	0,0525836
2-Isopropylmalic acid	175.06	HMDB00402	0,0517888
Caprylic acid	143.107	HMDB00482	0,0515803
Dicyclohexyl disulfide	231.121	HMDB41448	0,0515567
3-Hydroxy-9-(4-hydroxyphenyl)-1H,3H-naphtho[1,8-cd]pyran-1-one	293.078	HMDB39404	0,0514536
3-Methyl-1-butylamine	88.1126	HMDB31659	0,0514471
4-Fumarylacetoacetic acid	199.022	HMDB01268	0,051298
Mevalonic acid	147.065	HMDB00227	0,0499493
Latanoprost	433.293	HMDB14792	0,0498631
1,4-Ipomeadiol	169.086	HMDB30471	0,0490004
Rishitin	223.169	HMDB35593	0,0479272
Histidylproline diketopiperazine	247.118	HMDB02053	0,0478659
Octadecanedioic acid	313.239	HMDB00782	0,0470027
3,4-DHPEA-EA	379.137	HMDB29304	0,0468817
Crotamiton	204.138	HMDB14410	0,0467148
p-Toluenesulfonic acid	171.01	HMDB59933	0,0452802
2,3-Dimethyl-2-cyclohexen-1-one	125.096	HMDB31414	0,0452144
Methylgingerol	309.206	HMDB29852	0,0441857
Tridecanoylglycine	272.222	HMDB13317	0,0435835
6-Acetyl-1,2,3,4-tetrahydropyridine	126.092	HMDB30345	0,0431619
N-Acetyl-2,3-dihydro-1H-pyrrole	112.076	HMDB31163	0,0425068
Lucidenic acid A	459.28	HMDB37611	0,0424766
12-Oxo-20-carboxy-leukotriene B4	365.193	HMDB12550	0,0419289
3-Hydroxyanthranilic acid	152.034	HMDB01476	0,0417897
(Z)-5-[(5-Methyl-2-thienyl)methylene]-2(5H)-furanone	193.029	HMDB33845	0,0410083
13-HDoHE	315.264	HMDB60043	0,0407911
Trigoforin	189.091	HMDB29495	0,0407383
Verimol B	317.139	HMDB38323	0,0406362
Glycerol 1-propanoate diacetate	231.087	HMDB31640	0,0389345
(Z)-[3-(Methylsulfinyl)-1-propenyl] 2-propenyl disulfide	209.013	HMDB32653	0,0382957
(2R*,3R*)-1,2,3-Butanetriol	107.071	HMDB34778	0,0378536
Metaxalone	222.113	HMDB14798	0,0368016
Cinnassiol D2 glucoside	531.275	HMDB34679	0,0365703
1-(4-Methoxyphenyl)-1-penten-3-one	191.107	HMDB30905	0,0346418
Dimethylbenzyl carbonyl hexanoate	249.185	HMDB32228	0,03309
Vanilloside	315.109	HMDB32013	0,0327461
Elenolide	223.061	HMDB30018	0,0327129
Barbituric acid	127.014	HMDB41833	0,0318121
Galactosylglycerol	253.093	HMDB06790	0,0313474
(1R,3S,4S,6R)-6,9-Dihydroxyfenchone 6-O-b-D-glucoside	345.156	HMDB33222	0,0304542
Pyruvatoxime	102.018	HMDB02455	0,0271757
12S-HHT	281.209	HMDB12535	0,0269099
Phenylacetic acid	137.06	HMDB00209	0,021672
(Z)-1-(Methylthio)-5-phenyl-1-penten-3-yne	189.073	HMDB32688	0,0215873
Linocinnamarin	341.119	HMDB30678	0,0207849

<b>3-[[5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]-1,2-propanediol</b>	229.18	HMDB36133	0,0198932
<b>5-Aminopentanamide</b>	117.103	HMDB12176	0,0175487
<b>Methyl 7-epi-12-hydroxyjasmonate glucoside</b>	401.182	HMDB31763	0,0130457
<b>Homoveratric acid</b>	195.066	HMDB00434	0,00734863