

Metabolite content profiling of bottlenose dolphin exhaled breath.

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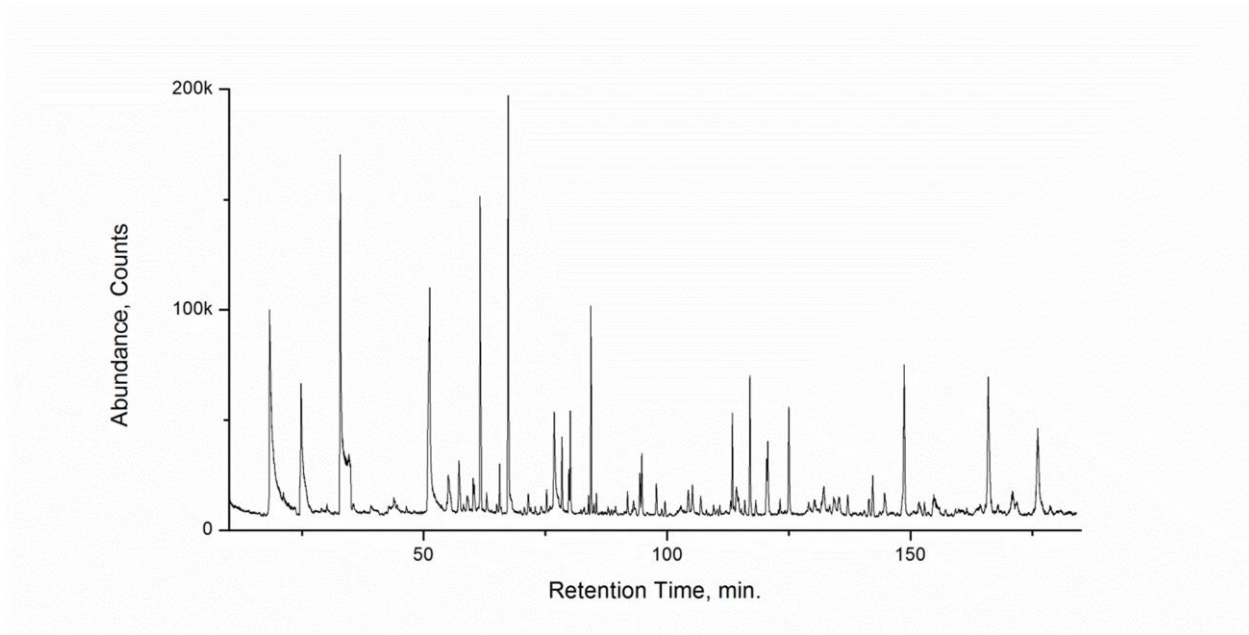
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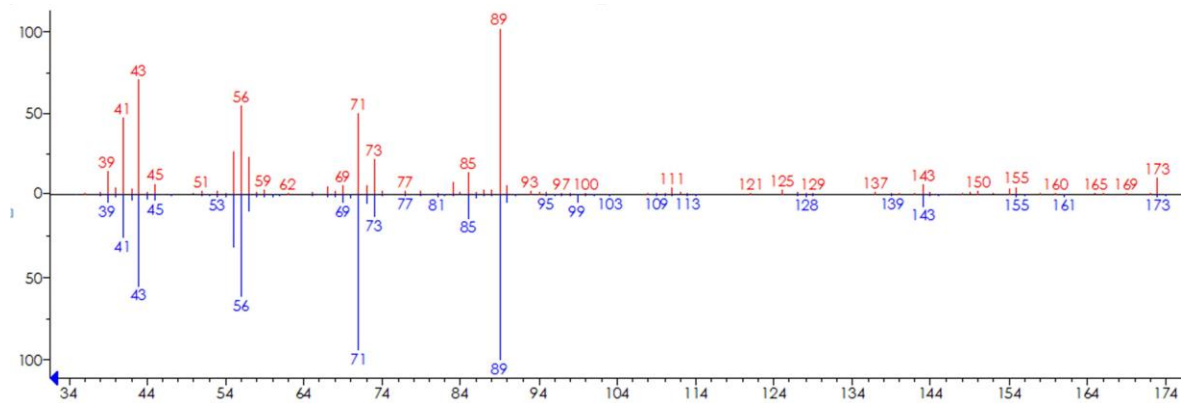
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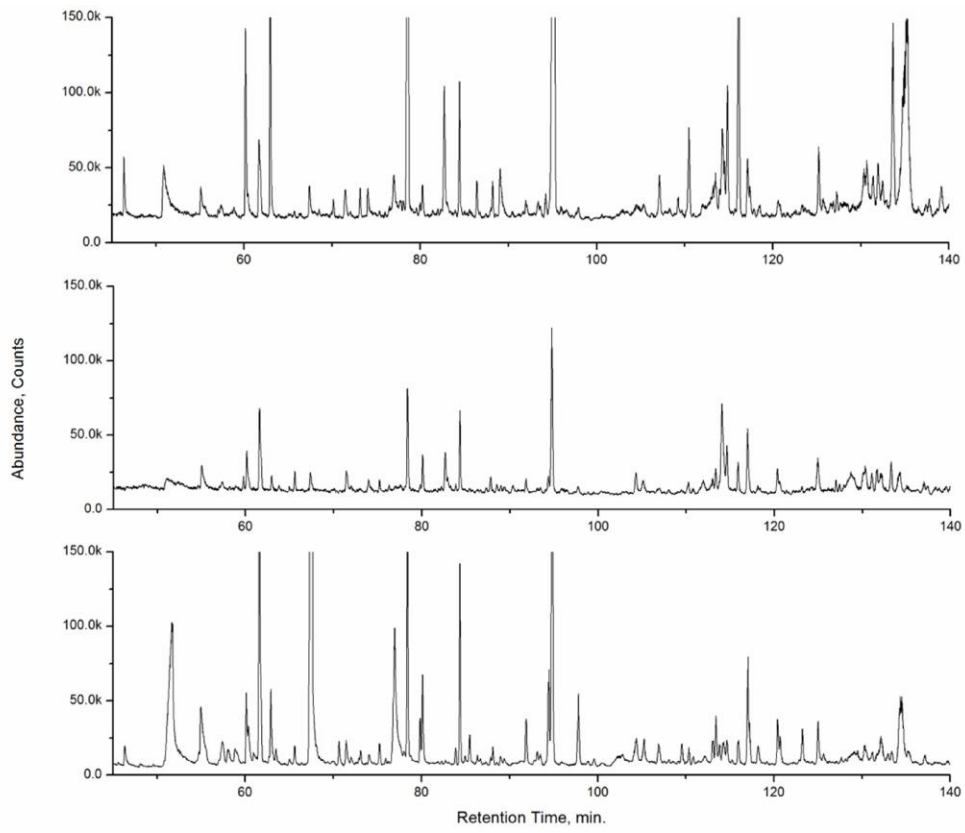
a)



b)



c)



d)

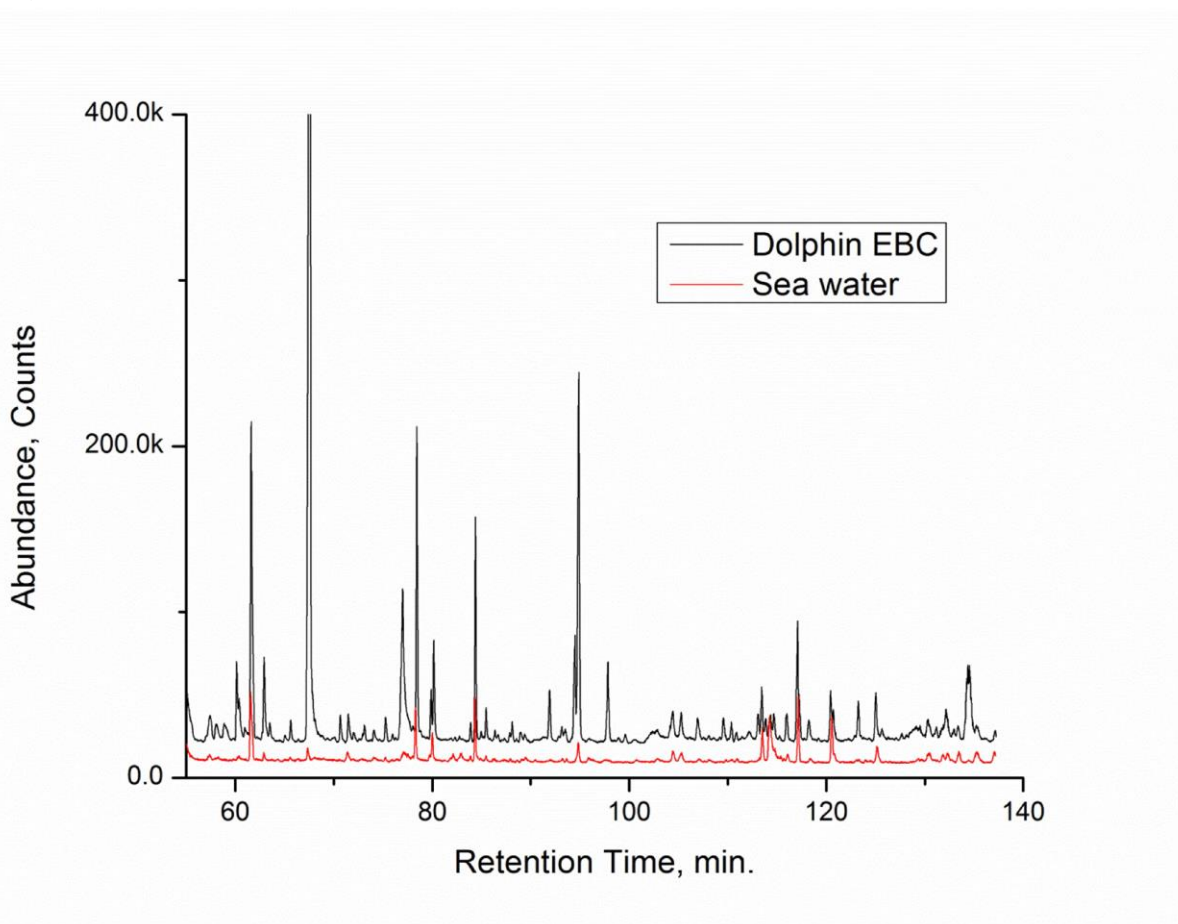


Figure A1. GC/MS analysis. a) Typical GC profile for EBC of dolphin. A large number of peaks indicates high chemical information content. b) Example of chemical identification for the compound tentatively identified as Propanoic acid, 2-methyl-, 2-ethyl-3-hydroxyhexyl ester. Head-to-tail comparison of an experimental mass spectrum (top) with a NIST database search hit (bottom) is shown as well as the NIST database entry. The x-axis is m/z in Th, the y-axis is relative abundance in %, with the most abundant peak at 100%. c) A fragment of chromatograms for EBC samples from three animals side-by-side. This example demonstrates that many peaks are similar between samples, while some are different in either presence or abundance. d) A fragment of chromatogram of EBC from an animal side-by-side with sea water blank; chromatograms are offset for clarity. The majority of the compounds in the breath are not present in the sea water.

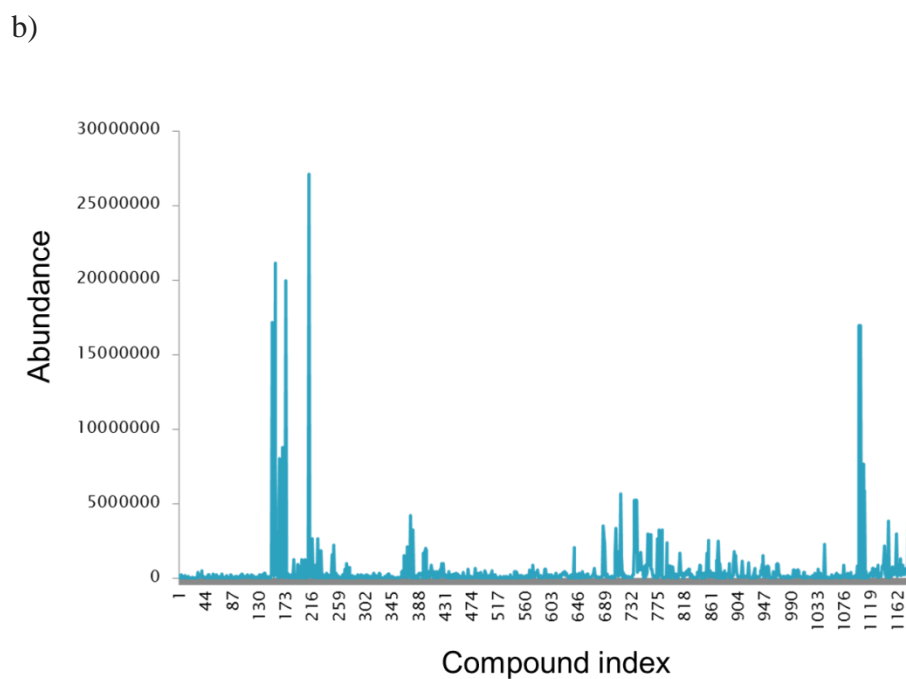
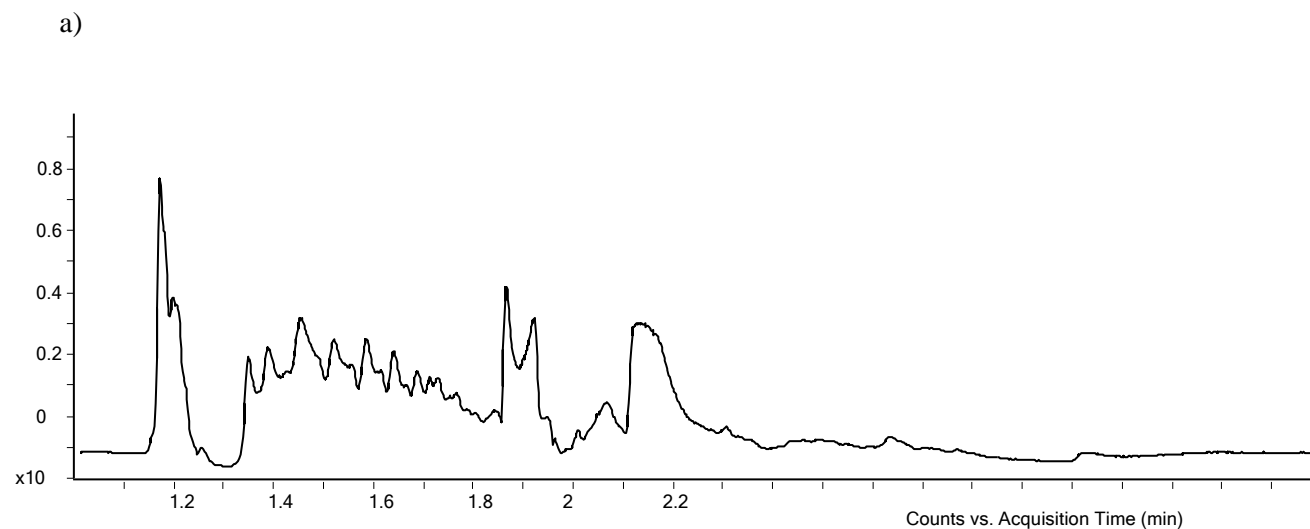


Figure A2. Typical results from μ HPLC-MS. a) Total Ion Current LC profile. The x-axis is retention time in minutes, the y-axis is relative abundance in a.u. b) Abundances of indexed compounds in the LC/MS experiments. The x-axis is compound index number (a number given to a species identified as a unique compound in order of elution time), the y-axis is relative abundance in a.u.

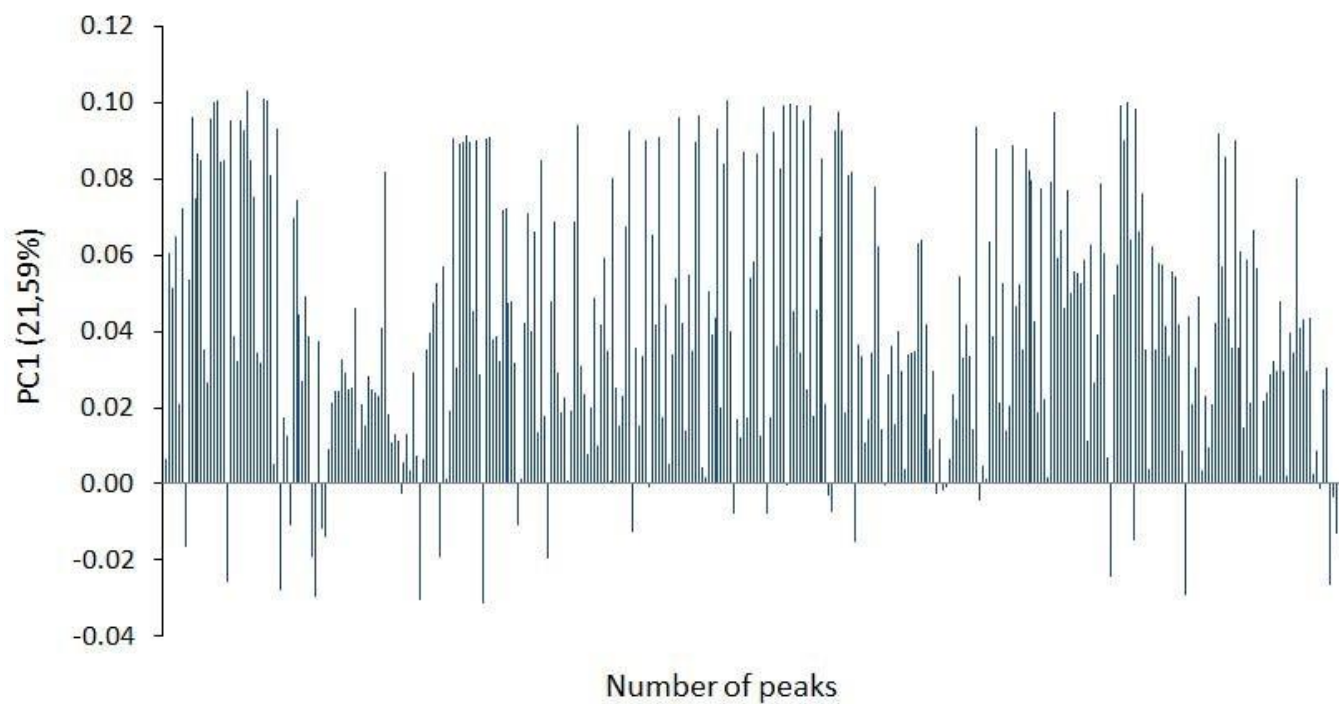


Figure A3. Loading plot of Figure 2 in main text. PC1 vs. number of peaks/chemicals.

Table A1. Compounds in dolphin breath identified with GC/MS using chemical derivatization.

1-Hexadecanol	Valine
Alanine	Urocanic Acid
Aspartic Acid	Tyrosine
Benzoic Acid	Tryptophan
C18:0	Threonine
C18:1 Cis6	Succinic Acid
C9:0	Succinate Semialdehyde
Capric Acid	Stearic Acid
Conduritol B Expoxide	Serine
Glycerol	Salicylaldehyde
Glycine	Phosphoric Acid
Lactic Acid	Phenylalanine
Lauric Acid	Pelargonic Acid
Malonic Acid	Palmitoleic Acid
Methylmalonic Acid	Oxoproline
N-Methyltryptophane	Oxalic Acid
Octadecanol	Ornithine
Oxoproline	Oleic Acid
Palmitic Acid	Octadecanol
Pentadecanoic Acid	Nonadecanoic Acid
Proline	Myristic Acid
Serine	Urea
Sorbose	Methylhexadecanoic Acid
Sucrose	Mannitol
Tagatose	Maltose
Talose	Malic Acid

Table A2. Compounds in dolphin breath identified with GC/MS using head space SPME extraction.

Column bleed compounds are excluded. The most likely chemical match is given; alternative structures such as isomers or homologues are possible in some cases, especially for high molecular weight compounds such as those with long chain; some of the compounds that could not be identified are not listed.

* Compound is likely of exogenous origin

1,1-Ethandiol, Diacetate	Tetradecanal
Octane, 2-Chloro-	Heptanoic Acid, 1-Methylethyl Ester
1,3-Butanediol, (R)-	Benzene, 1,3-Diisocyanato-2-Methyl-
1-Pentanamine	Benzene, 2,4-Diisocyanato-1-Methyl-
Oxime-, Methoxy-Phenyl-	Phenol, 2-(1,1-Dimethylethyl)-4-Methyl-
Propanoic Acid, 2-Hydroxyethyl Ester	Propanoic Acid, 2-Methyl-, 3-Hydroxy-2,4,4-Trimethylpentyl Ester
Thiazole, Tetrahydro-	1,3-Dioxolane-2-Butanol, 2-Methyl-
2-Butene-1,4-Diol, Diformate	Dodecanal
1-Octene, 6-Methyl-	Nalidixic Acid
Octanal	2,5-Cyclohexadiene-1,4-Dione, 2,6-Bis(1,1-Dimethylethyl)-
Ethanol, 2-[2-(2-Ethoxyethoxy)Ethoxy]-	5-Methoxy-2,2,6-Trimethyl-1-(3-Methyl-Buta-1,3-Dienyl)-7-Oxa-Bicyclo[4.1.0]Heptane
Butane, 2-Methoxy-2-Methyl-	1-Hepten-4-Ol
1-Hexanol, 2-Ethyl-	Diphenylmethane
Butanoic Acid, Propyl Ester	Butylated Hydroxytoluene
1-Butanol, 4-(1-Methylethoxy)-	Bibenzyl
2(3H)-Furanone, Dihydro-3-Methyl-	Phenol, 3,5-Bis(1,1-Dimethylethyl)-

Benzene, 1-Isocyanato-4-Methyl-	7-Hexadecyn-1-ol
4-Dodecene, (E)-	1-Butanol, 4-(1-Methylethoxy)-
Benzoic Acid, Methyl Ester	Benzene, 1-Methyl-3-(Phenylmethyl)-
5-Tridecene, (Z)-	Phenol, 4,6-Di(1,1-Dimethylethyl)-2-Methyl-
2-Nonen-1-ol	9H-Pyrido[3,4-B]Indol-7-ol, 1-Methyl-
Glutamine	Octadecane, 6-Methyl-
2-Pyrrolidinone, 5-(Cyclohexylmethyl)-	Benzene, 1-Methyl-2-(2-Phenylethenyl)-
1-Butanol, 4-Butoxy-	Dodecane, 1-Isocyanato-
2,2-Dimethyl-N-Ethylpyrrolidine	Diethyl Phthalate*
2-O-Methyl-D-Mannopyranosa	1-Dodecanol, 3,7,11-Trimethyl-
Cyclohexaneacetic Acid	1-(3-(Cyclohexylamino)Propyl)Guanidine
Benzoic Acid	3-Ethyl-5-Methylindolizidine
Ethanol, 2-(2-Ethoxyethoxy)-, Acetate	Benzophenone
1-Tridecanol	2,6-Bis(1,1-Dimethylethyl)-4-(1-Oxopropyl)Phenol
2h-Pyran, Tetrahydro-2-(1-Methylethoxy)-	Phenol, 2,4,6-Tris(1-Methylethyl)-
2-Hexenoic Acid, 3,4,4-Trimethyl-5-Oxo-, (Z)-	5-Methyl-4,5-Dihydro-1h-Pyrrolo[3,2-c]Quinolin-4-One
1,10-Decanediol	Undecane
2(3H)-Furanone, Dihydro-5-Pentyl-	1H-Indazole, 4,5,6,7-Tetrahydro-
Mequinol	7-Ethoxy-8-Methoxy-2,2-Dimethyl-2H-Chromene
Cyclohexanone, 2-Propyl-	Benzyl Benzoate
Cyclohexanol, 1r-4cis-Acetamido-5,6cis-Epoxy-2trans,3cis-Dimethoxy-	Benzoic Acid, 2-Hydroxy-, Pentyl Ester
Methyl Pyrrole-2-Carboxylate	4-Heptenal, 6-(Acetyloxy)-4-Methyl-, (E)-
Ethanol, 2-(Octadecyloxy)-	4-(2-Propen-1-yloxy)Benzeneamine
2-Propenoic Acid, Oxybis(2,1-Ethanedioxy-2,1-Ethanediyloxy-2,1-Ethanediyloxy) Ester	Homosalate
1-Penten-3-ol, 3-Methyl-	1,1-Dimethyldihydrobenzofuran-5-ol
Acetic Acid, Ethyl Ester	2,4-Hexadiene
2-Pentanone, 4-Methyl-	Hexanal
Benzene, 1,2-Dimethyl-	Styrene*
1-Formylcyclopentene	2-Hexanone, 5-Methyl-
Heptanal	Oxime-, Methoxy-Phenyl-
Benzaldehyde	2-Propanol, 1,1,1-Trichloro-2-Methyl-
Benzonitrile	6-Methyl-5-Hepten-2-One
1,8-Cineole	Octanal
3-Cyclohexene-1-Carboxaldehyde	Benzene, 1-Methyl-2-(1-Methylethyl)-
Cyclohexene, 1-Methyl-4-(1-Methylethenyl)-	1-Hexanol, 2-Ethyl-*
Cyclohexanol, 3,3,5-Trimethyl-	1,2-Diphenylpropanone
Benzaldehyde, 3-Methyl-	1-Tridecyne
1-Octanol	Benzene, 1-Methyl-4-(1-Methylethenyl)-
3-Cyclohexen-1-ol, 4-Methyl-1-(1-Methylethyl)-	Pyridine, 4-Methoxy-
2-Nonen-1-ol	1,1-Dimethyl-3-Methylidene-2-Vinylcyclohexane
Benzene, 1-Isocyano-2-Methyl-	Acetic Acid, 2-Ethylhexyl Ester
Nonenal	Naphthalene
3,4-Dimethylcyclohexanol	Nonanol
Glyoxal, 4-Methylphenyl-	Cycloocta-1,3,6-Triene, 2,3,5,5,8,8-Hexamethyl-
Hydroxylamine, O-Decyl-	7-Decen-1-Al
3,9-Dodecadiyne	1,10-Decanediol

6-Methyl-1,2,3,5,8,8a-Hexahydronaphthalene	Cyclohexane, 1-Bromo-3-Methyl-
2-Decenal	Nonanoic Acid
1-Heptadecyne	1-Octadecyne
Alpha-Ionol	Oxalic Acid, Isobutyl Nonyl Ester
1,3-Isobenzofurandione*	Pentadecanal
(1rs,2rs,7rs)-1,2,6,6-Tetramethyl-10-Oxatricyclo[5.2.1.0(2,7)]Decan-3-One	Propanoic Acid, 2-Methyl-, 3-Hydroxy-2,4,4-Trimethylpentyl Ester
10-Undecenal	Docosane
Tetradecane	Pentadecanal
2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol	Decanoic Acid, Ethyl Ester
5,9-Undecadien-2-One, 6,10-Dimethyl-	2,5-Cyclohexadiene-1,4-Dione, 2,6-Bis(1,1-Dimethylethyl)-*
4-Tridecen-6-Yne	Nonanoic Acid, 9-Oxo-, Methyl Ester
Butyl Hydroxy Anisole	1-Heptanol, 2-Propyl-*
9-Octadecenal	5-Hydroxy-8-Methyl-1,2,3,4-Tetrahydro-2-Quinolinone
Cyclotetradecane	Hydroxylamine, O-Decyl-
1,15-Pentadecanediol	1,2-Benzenedicarboxylic Acid, Diethyl Ester*
Ethyl 1,4,5,6-Tetrahydro-5-Hydroxy-5-Methyl-6-Oxo-2-Pyridinecarboxylate	3-Octyn-2-One
5-Octen-2-Yn-4-Ol	Bicyclo[3.1.1]Heptan-3-Ol, 2,6,6-Trimethyl-
1,4,4-Trimethylcyclohexa-2-En-1-Ol	1-Decanol
Benzeneacetonitrile	1-Cyclohexanol, 1-Vinyl-
Decanal	1-Pentadecyne
Trans-2-Tridecenal	Dodecen-1-Al
Dodecane	Dodecane
Dipentene Oxide	Tetradecanal
8-Hexadecenal, 14-Methyl-,	Heptanoic Acid, 1-Methylethyl Ester
2,6-Di-t-Butyl-4-Methylene-2,5-Cyclohexadiene-1-One*	Benzene, 1,3-Diisocyanato-2-Methyl-
1,1-Ethanediol, Diacetate	Benzene, 2,4-Diisocyanato-1-Methyl-
Octane, 2-Chloro-	Phenol, 2-(1,1-Dimethylethyl)-4-Methyl-
1,3-Butanediol, (R)-	Propanoic Acid, 2-Methyl-, 3-Hydroxy-2,4,4-Trimethylpentyl Ester
1-Pentanamine	1,3-Dioxolane-2-Butanol, 2-Methyl-
Oxime-, Methoxy-Phenyl-	Dodecanal
Propanoic Acid, 2-Hydroxyethyl Ester	Nalidixic Acid
Thiazole, Tetrahydro-	2,5-Cyclohexadiene-1,4-Dione, 2,6-Bis(1,1-Dimethylethyl)-
2-Butene-1,4-Diol, Diformate	5-Methoxy-2,2,6-Trimethyl-1-(3-Methyl-Buta-1,3-Dienyl)-7-Oxa-Bicyclo[4.1.0]Heptane
1-Octene, 6-Methyl-	1-Hepten-4-Ol
Octanal	Diphenylmethane
Ethanol, 2-[2-(2-Ethoxyethoxy)Ethoxy]-	Butylated Hydroxytoluene
Butane, 2-Methoxy-2-Methyl-	Bibenzyl
1-Hexanol, 2-Ethyl-	Phenol, 3,5-Bis(1,1-Dimethylethyl)-
Butanoic Acid, Propyl Ester	7-Hexadecyn-1-Ol
1-Butanol, 4-(1-Methylethoxy)-	1-Butanol, 4-(1-Methylethoxy)-
2(3H)-Furanone, Dihydro-3-Methyl-	Benzene, 1-Methyl-3-(Phenylmethyl)-
Benzene, 1-Isocyanato-4-Methyl-	Phenol, 4,6-Di(1,1-Dimethylethyl)-2-Methyl-
4-Dodecene, (E)-	9H-Pyrido[3,4-B]Indol-7-Ol, 1-Methyl-

Benzoic Acid, Methyl Ester	Octadecane, 6-Methyl-
5-Tridecene, (Z)-	Benzene, 1-Methyl-2-(2-Phenylethenyl)-
2-Nonen-1-Ol	Dodecane, 1-Isocyanato-
Glutamine	Diethyl Phthalate*
2-Pyrrolidinone, 5-(Cyclohexylmethyl)-	1-Dodecanol, 3,7,11-Trimethyl-
1-Butanol, 4-Butoxy-	1-(3-(Cyclohexylamino)Propyl)Guanidine
2,2-Dimethyl-N-Ethylpyrrolidine	3-Ethyl-5-Methylindolizidine
2-O-Methyl-D-Mannopyranosa	Benzophenone
1-Cyclohexaneacetic Acid	Benzophenone
Benzoic Acid	Ethanol, 2-(2-Ethoxyethoxy)-, Acetate

Table A3. List of volatile metabolites (GC/MS) detected in sea water (column bleed compounds excluded). The most likely chemical match is given; alternative structures such as isomers or homologues are possible in some cases, especially for long-chain compounds.

Oxime-, Methoxy-Phenyl-	Benzaldehyde
3-Nonen-1-Ol	1-Hexanol, 2-Ethyl-
Ethanone, 2,2-Dihydroxy-1-Phenyl-	Benzene, (2-Methyl-1-Propenyl)-
Dodecanal	Decanol
Undecanol	Octane
Tetradecanal	Benzothiazole
Isooctanol	1-Phenoxypropan-2-Ol
Phthalic Anhydride	Pentadecanal
Selinan	2-Hexanone, 6-Hydroxy-
Propanoic Acid, 2-Methyl-, 3-Hydroxy-2,4,4-Trimethylpentyl Ester	Pentadecane
Cyclodecanol	Phenol, 3,4-Dimethoxy-, Acetate
4-Ethylbenzoic Acid, Phenyl Ester	5,9-Undecadien-2-One, 6,10-Dimethyl-
2,5-Cyclohexadiene-1,4-Dione, 2,6-Bis(1,1-Dimethylethyl)-	Oleic Acid
(3-Ethoxy-Hexa-1,5-Dienyl)-Benzene	Tridecane
2-Allyl-5-t-Butylhydroquinone	Diethyl Phthalate
Decane, 6-Ethyl-2-Methyl-	

Table A4. List of volatile metabolites (GC/MS) in air condensate (column bleed compounds excluded and blank peaks excluded). The most likely chemical match is given; alternative structures such as isomers or homologues may be possible in some cases.

Hexanal	Alpha-Methylstyrene
5-Hepten-2-One, 6-Methyl-	Octanal
2,6-Dimethyl-1,3,5,7-Octatetraene	Benzene, 1-Methyl-3-(1-Methylethyl)-
Linalool	Camphene
Carvone	Dodecanal

Table A5. List of non-volatile metabolites (LC/MS) for managed population animals. Sample was pooled from multiple animals (collection in May 2011). Experiment was conducted using HILIC column in positive ion mode (refer to Materials and Methods section). Only top match is given for each compound.

Parent m/z	Mass	Delta (m/z)	Library Precursor m/z	Match Score	Probability (%)	Chem ID
170.1278	187.121	-0.0102	170.1176	417	76	7-Keto-8-Aminopelargonic Acid
472.2733	471.314	0.048	472.321	99	61.1	Terfenadine
516.3059	515.292	-0.007	516.2989	105	100	Taurocholic Acid
170.1278	187.121	-0.0102	170.1176	451	72.6	7-Keto-8-Aminopelargonic Acid
370.2514	369.288	0.0438	370.2952	191	35	N-Oleoyl-L-Serine
170.1278	187.121	-0.0102	170.1176	383	75.9	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	94	12.6	Palmitoyl-L-Carnitine Cation
472.2733	471.314	0.048	472.321	134	80.3	Terfenadine
170.1278	187.121	-0.0102	170.1176	405	73.6	7-Keto-8-Aminopelargonic Acid
370.2514	369.288	0.0438	370.2952	248	27.8	N-Oleoyl-L-Serine
461.2907	460.28	-0.0036	461.2871	33	100	Trp-Lys-Lys
655.4719	654.492	0.0272	655.4991	194	51.2	Deca(Propylene Glycol) Monobutyl Ether
474.2957	473.275	-0.0134	474.2823	56	20.6	Leu-Trp-Arg
458.3162	435.281	-0.0463	458.2699	63	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
472.2733	471.314	0.048	472.321	86	100	Terfenadine
170.116	187.121	0.0016	170.1176	408	78.4	7-Keto-8-Aminopelargonic Acid
472.2733	471.223	-0.043	472.2303	83	100	Pyroglu-Trp-Arg
414.278	449.314	0.0223	414.3003	241	97.3	Glycodeoxycholic Acid
472.2733	471.314	0.048	472.321	139	89.1	Terfenadine
170.1278	187.121	-0.0102	170.1176	439	77	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	197	19.9	Palmitoyl-L-Carnitine Cation
414.278	449.314	0.0223	414.3003	306	99	Glycodeoxycholic Acid
472.3027	471.314	0.018	472.321	148	100	Terfenadine
391.2842	390.277	0.0001	391.2843	115	54.1	Bis(2-Ethylhexyl) Phthalate
170.1278	169.074	-0.0466	170.0812	244	39.5	DL-Norepinephrine
419.3154	418.308	0.0002	419.3156	205	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
149.0229	166.027	0.0004	149.0233	440	98.6	1,2-Benzenedicarboxylic Acid
343.2918	342.256	-0.0286	343.2632	301	95.4	Retinyl Propionate
170.1383	169.085	-0.0459	170.0924	248	31.8	L-Histidine, 3-Methyl-
391.2842	390.277	0.0001	391.2843	103	52.2	Bis(2-Ethylhexyl) Phthalate
399.251	398.243	-0.0004	399.2506	174	100	Tris(Butoxyethyl) Phosphate
472.3317	471.314	-0.011	472.321	164	100	Terfenadine
516.3458	515.292	-0.0469	516.2989	282	100	Taurocholic Acid

516.3458	515.292	-0.0469	516.2989	212	100	Taurocholic Acid
387.1816	193.074	-0.0265	387.1551	172	26.2	Hippuric Acid, Methyl Ester
404.2057	403.254	0.0559	404.2616	6	26.3	Arg-Thr-Lys
474.2957	473.275	-0.0134	474.2823	76	100	Leu-Trp-Arg
472.3317	471.314	-0.011	472.321	164	100	Terfenadine
170.1278	169.085	-0.0354	170.0924	376	38.1	L-Histidine, 3-Methyl-
655.4719	654.492	0.0272	655.4991	252	19.9	Deca(Propylene Glycol) Monobutyl Ether
170.1278	169.085	-0.0354	170.0924	423	56	L-Histidine, 3-Methyl-
279.0936	278.086	-0.0002	279.0933	11	100	Triphenylphosphine Oxide
516.3458	515.292	-0.0469	516.2989	161	100	Taurocholic Acid
655.4533	654.492	0.0458	655.4991	304	22.1	Deca(Propylene Glycol) Monobutyl Ether
288.2533	287.196	-0.05	288.203	105	26.1	Leu-Arg
472.3317	471.314	-0.011	472.321	118	100	Terfenadine
170.1278	169.085	-0.0354	170.0924	294	43	L-Histidine, 1-Methyl-
496.4192	495.369	-0.043	496.3762	167	100	2-O-Methyl PAF C-16
655.5042	654.492	-0.0051	655.4991	289	19.2	Deca(Propylene Glycol) Monobutyl Ether
695.4768	695	0.04	695.52	85	50	DG 42:10; [M+Li] ⁺ ; DG(20:5/22:5/0:0)
516.3458	515.292	-0.0469	516.2989	197	100	Taurocholic Acid
472.3317	471.314	-0.011	472.321	190	100	Terfenadine
414.278	413.239	-0.0321	414.2459	176	69.2	Pyroglu-Arg-Lys
516.3458	515.292	-0.0469	516.2989	169	100	Taurocholic Acid
170.116	187.121	0.0016	170.1176	386	45.1	7-Keto-8-Aminopelargonic Acid
472.3317	471.314	-0.011	472.321	216	100	Terfenadine
461.2907	460.243	-0.04	461.2507	87	80.4	Trp-Gln-Lys
516.3458	515.292	-0.0469	516.2989	282	100	Taurocholic Acid
170.116	169.085	-0.0236	170.0924	420	38.9	L-Histidine, 1-Methyl-
370.2514	369.288	0.0438	370.2952	302	26.5	N-Oleoyl-L-Serine
516.3458	515.292	-0.0469	516.2989	229	100	Taurocholic Acid
170.1132	187.121	0.0044	170.1176	403	54.8	7-Keto-8-Aminopelargonic Acid
414.278	449.314	0.0223	414.3003	238	88.8	Glycodeoxycholic Acid
370.2514	369.288	0.0438	370.2952	93	9.3	N-Oleoyl-L-Serine
461.2907	460.243	-0.04	461.2507	108	85.2	Trp-Gln-Lys
516.3458	515.292	-0.0469	516.2989	240	100	Taurocholic Acid
474.2738	473.275	0.0085	474.2823	19	57.9	Leu-Trp-Arg
151.0962	150.089	0.0003	151.0965	238	100	Triethylene Glycol
414.278	449.314	0.0223	414.3003	291	92.4	Glycodeoxycholic Acid
370.2514	369.288	0.0438	370.2952	204	18	N-Oleoyl-L-Serine
516.3458	515.292	-0.0469	516.2989	191	100	Taurocholic Acid
474.2738	473.275	0.0085	474.2823	33	20.6	Ile-Trp-Arg
461.2907	460.243	-0.04	461.2507	124	23.9	Trp-Gln-Lys
474.2957	473.275	-0.0134	474.2823	70	33.4	Leu-Trp-Arg
370.2514	369.288	0.0438	370.2952	121	10.1	N-Oleoyl-L-Serine

461.2907	460.243	-0.04	461.2507	91	22.7	Trp-Gln-Lys
474.2738	473.275	0.0085	474.2823	106	35.6	Leu-Trp-Arg
458.2953	457.244	-0.044	458.251	54	32.9	Pro-Trp-Arg
244.1905	226.193	0.0366	244.2271	483	98.5	2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol
472.3027	471.314	0.018	472.321	174	100	Terfenadine
370.238	370	-0.03	370.21	121	50	MGDG 7:0; [M+NH ₄ -CO] ⁺ ; MGDG(2:0/5:0)
422.2569	421.233	-0.0171	422.2398	56	53.1	Phe-Gln-Lys
474.2957	473.275	-0.0134	474.2823	28	35	Leu-Trp-Arg
370.2514	370	-0.04	370.21	70	21.8	MGDG 7:0; [M+NH ₄ -CO] ⁺ ; MGDG(2:0/5:0)
414.278	413.239	-0.0321	414.2459	75	54.2	Pyroglu-Lys-Arg
370.2514	369.288	0.0438	370.2952	115	13.5	N-Oleoyl-L-Serine
170.116	187.121	0.0016	170.1176	273	59.3	7-Keto-8-Aminopelargonic Acid
239.1485	238.099	-0.042	239.106	58	100	4-(2-Hydroxyethyl)Piperazine-1-Ethanesulfonic Acid
370.2514	369.288	0.0438	370.2952	176	21.2	N-Oleoyl-L-Serine
414.278	449.314	0.0223	414.3003	52	100	Glycodeoxycholic Acid
139.0499	138.043	0.0003	139.0502	548	83.8	4-Imidazoleacrylic Acid
638.6063	638	-0.04	638.57	133	29.3	DG 36:2; [M+NH ₄] ⁺ ; DG(14:1/22:1/0:0)
239.1485	238.099	-0.042	239.106	43	100	4-(2-Hydroxyethyl)Piperazine-1-Ethanesulfonic Acid
472.2733	471.314	0.048	472.321	160	93.1	Terfenadine
370.2514	369.288	0.0438	370.2952	290	23	N-Oleoyl-L-Serine
474.2957	473.275	-0.0134	474.2823	69	44.6	Ile-Trp-Arg
516.3059	515.292	-0.007	516.2989	87	100	Taurocholic Acid
458.3162	435.281	-0.0463	458.2699	50	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
474.2957	473.275	-0.0134	474.2823	35	100	Ile-Trp-Arg
400.319	400.343	0.0231	400.3421	76	26.1	Palmitoyl-L-Carnitine Cation
787.6526	786.661	0.0162	787.6688	102	100	N-Docosanoyl-4-Sphinganyl-1-O-Phosphorylcholine
170.1132	187.121	0.0044	170.1176	255	62.8	7-Keto-8-Aminopelargonic Acid
655.4719	654.492	0.0272	655.4991	281	27.4	Deca(Propylene Glycol) Monobutyl Ether
548.3399	548	0.04	548.38	149	8.3	MGDG 20:2; [M+NH ₄ -CO] ⁺ ; MGDG(2:0/18:2(2E,4E))
170.116	187.121	0.0016	170.1176	15	100	7-Keto-8-Aminopelargonic Acid
170.116	169.085	-0.0236	170.0924	35	59.3	L-Histidine, 1-Methyl-
170.116	169.074	-0.0348	170.0812	147	49.1	DL-Norepinephrine
343.31	342.256	-0.0468	343.2632	174	100	Retinyl Propionate

170.116	187.121	0.0016	170.1176	93	47.9	7-Keto-8-Aminopelargonic Acid
655.4533	654.492	0.0458	655.4991	250	29.8	Deca(Propylene Glycol) Monobutyl Ether
170.116	187.121	0.0016	170.1176	84	45.7	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	72	41.1	Palmitoyl-L-Carnitine Cation
655.4719	654.492	0.0272	655.4991	224	24.9	Deca(Propylene Glycol) Monobutyl Ether
170.116	187.121	0.0016	170.1176	148	52.6	7-Keto-8-Aminopelargonic Acid
461.2907	460.243	-0.04	461.2507	42	57.3	Gln-Trp-Lys
400.319	400.343	0.0231	400.3421	51	15.8	Palmitoyl-L-Carnitine Cation
461.2907	460.28	-0.0036	461.2871	41	100	Trp-Lys-Lys
170.1446	187.121	-0.027	170.1176	285	56.5	7-Keto-8-Aminopelargonic Acid
461.2907	230.163	0.0427	461.3334	295	59.8	Val-Leu
461.2907	230.163	0.0427	461.3334	269	59.8	Val-Leu
170.1278	187.121	-0.0102	170.1176	192	47.6	7-Keto-8-Aminopelargonic Acid
655.4533	654.492	0.0458	655.4991	109	37	Deca(Propylene Glycol) Monobutyl Ether
343.2918	342.256	-0.0286	343.2632	110	100	Retinyl Propionate
461.2907	230.163	0.0427	461.3334	274	58.4	Val-Leu
787.6804	786.661	-0.0116	787.6688	70	39.7	N-Docosanoyl-4-Sphingeny-1-O-Phosphorylcholine
170.1278	169	-0.04	170.09	275	36	3-Methyl-L-Histidine
655.4719	654.492	0.0272	655.4991	105	38.5	Deca(Propylene Glycol) Monobutyl Ether
343.2918	342.256	-0.0286	343.2632	53	77.9	Retinyl Propionate
787.6377	786.661	0.0311	787.6688	73	100	N-Docosanoyl-4-Sphingeny-1-O-Phosphorylcholine
170.1278	187.121	-0.0102	170.1176	163	54	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	187	9.1	Palmitoyl-L-Carnitine Cation
787.6526	786.661	0.0162	787.6688	37	38.7	N-Docosanoyl-4-Sphingeny-1-O-Phosphorylcholine
170.1278	169.085	-0.0354	170.0924	229	32.7	L-Histidine, 1-Methyl-
474.2957	473.275	-0.0134	474.2823	31	100	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	64	54	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	47	53.1	Leu-Trp-Arg
458.3162	435.281	-0.0463	458.2699	78	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
474.2957	473.275	-0.0134	474.2823	66	45.2	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	54	59.7	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	74	30.4	Trp-Ile-Arg

474.2957	473.275	-0.0134	474.2823	52	20.6	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	54	28.9	Trp-Ile-Arg
518.3145	495.332	0.0072	518.3217	91	100	1-Hexadecanoyl-Sn-Glycero-3-Phosphocholine
474.2957	473.275	-0.0134	474.2823	52	31.8	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	81	27.4	Leu-Trp-Arg
400.319	400.343	0.0231	400.3421	65	47.4	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	31	38.4	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	45	21.2	Leu-Trp-Arg
400.319	400.343	0.0231	400.3421	58	47	Palmitoyl-L-Carnitine Cation
474.2957	473.275	-0.0134	474.2823	60	40.9	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	31	22.9	Trp-Ile-Arg
170.1278	187.121	-0.0102	170.1176	141	43.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	128	45.7	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	95	39.8	7-Keto-8-Aminopelargonic Acid
414.278	449.314	0.0223	414.3003	66	100	Glycodeoxycholic Acid
474.2738	473.275	0.0085	474.2823	34	57.3	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	77	76.9	Trp-Ile-Arg
170.1278	187.121	-0.0102	170.1176	151	72	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	136	46.6	7-Keto-8-Aminopelargonic Acid
474.2738	473.275	0.0085	474.2823	110	71.5	Trp-Ile-Arg
170.1278	187.121	-0.0102	170.1176	173	51	7-Keto-8-Aminopelargonic Acid
458.3162	435.281	-0.0463	458.2699	102	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	142	45.7	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	44	57.9	Ile-Trp-Arg
458.2757	435.281	-0.0058	458.2699	101	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
400.319	400.343	0.0231	400.3421	55	80.2	Palmitoyl-L-Carnitine Cation
170.1278	169.085	-0.0354	170.0924	130	31.6	L-Histidine, 1-Methyl-
458.3162	435.281	-0.0463	458.2699	78	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
343.2759	342.256	-0.0127	343.2632	161	93.2	Retinyl Propionate
170.1278	187.121	-0.0102	170.1176	143	32.3	7-Keto-8-Aminopelargonic Acid
458.3162	435.281	-0.0463	458.2699	62	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	151	30.3	7-Keto-8-Aminopelargonic

						Acid
474.2957	473.275	-0.0134	474.2823	72	100	Leu-Trp-Arg
458.3162	435.281	-0.0463	458.2699	32	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	162	45.6	7-Keto-8-Aminopelargonic Acid
400.319	401.278	-0.0485	400.2705	103	100	Myriocin
170.1278	187.121	-0.0102	170.1176	148	44.6	7-Keto-8-Aminopelargonic Acid
458.2549	435.281	0.015	458.2699	69	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	143	40.2	7-Keto-8-Aminopelargonic Acid
518.3145	495.332	0.0072	518.3217	66	100	1-Hexadecanoyl-Sn-Glycero-3-Phosphocholine
170.1278	187.121	-0.0102	170.1176	161	37.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	140	42	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	52	63.5	Leu-Trp-Arg
170.1278	169.085	-0.0354	170.0924	160	35.9	L-Histidine, 3-Methyl-
458.3162	435.281	-0.0463	458.2699	40	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	156	45.2	7-Keto-8-Aminopelargonic Acid
458.3162	435.281	-0.0463	458.2699	37	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
400.36	400.343	-0.0179	400.3421	25	56.6	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	170	50.5	7-Keto-8-Aminopelargonic Acid
400.319	401.278	-0.0485	400.2705	16	100	Myriocin
343.2918	342.256	-0.0286	343.2632	81	100	Retinyl Propionate
170.1278	187.121	-0.0102	170.1176	190	66.2	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	47	100	Ile-Trp-Arg
170.1278	187.121	-0.0102	170.1176	165	48.8	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	72	26.5	Palmitoyl-L-Carnitine Cation
474.2957	473.275	-0.0134	474.2823	43	38.5	Leu-Trp-Arg
170.1278	187.121	-0.0102	170.1176	235	73.6	7-Keto-8-Aminopelargonic Acid
518.3145	495.332	0.0072	518.3217	104	100	1-Hexadecanoyl-Sn-Glycero-3-Phosphocholine
400.319	400.343	0.0231	400.3421	119	30.9	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	185	52.3	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	96	36.3	Palmitoyl-L-Carnitine Cation

170.1278	187.121	-0.0102	170.1176	165	49.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	202	40	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	159	84.5	Palmitoyl-L-Carnitine Cation
655.4719	654.492	0.0272	655.4991	151	51.2	Deca(Propylene Glycol) Monobutyl Ether
170.1278	187.121	-0.0102	170.1176	189	48.1	7-Keto-8-Aminopelargonic Acid
414.278	413.239	-0.0321	414.2459	70	100	Pyroglu-Lys-Arg
370.2514	370	-0.04	370.21	88	39.3	MGDG 7:0; [M+NH4-CO]++; MGDG(2:0/5:0)
400.319	400.343	0.0231	400.3421	39	28.8	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	194	41.3	7-Keto-8-Aminopelargonic Acid
414.278	413.239	-0.0321	414.2459	59	55.4	Pyroglu-Lys-Arg
458.2953	457.244	-0.044	458.251	59	67.1	Pro-Trp-Arg
343.2918	342.256	-0.0286	343.2632	156	93.4	Retinyl Propionate
458.2953	457.244	-0.044	458.251	90	31.9	Pro-Trp-Arg
170.1278	187.121	-0.0102	170.1176	198	50.9	7-Keto-8-Aminopelargonic Acid
370.2514	370	-0.04	370.21	182	37	MGDG 7:0; [M+NH4-CO]++; MGDG(2:0/5:0)
474.2957	473.275	-0.0134	474.2823	47	35.6	Ile-Trp-Arg
458.2953	457.244	-0.044	458.251	130	23	Pro-Trp-Arg
170.1278	169.085	-0.0354	170.0924	208	32.3	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	155	49.3	7-Keto-8-Aminopelargonic Acid
458.2953	435.281	-0.0254	458.2699	80	81.9	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	174	51	7-Keto-8-Aminopelargonic Acid
458.2953	435.281	-0.0254	458.2699	70	83.8	N-Acetyl-S-Geranylgeranyl-L-Cysteine
474.2957	473.275	-0.0134	474.2823	23	56.6	Ile-Trp-Arg
170.1278	169.085	-0.0354	170.0924	218	47.4	L-Histidine, 1-Methyl-
474.2957	473.275	-0.0134	474.2823	36	100	Ile-Trp-Arg
370.2244	370	-0.01	370.21	200	50	MGDG 7:0; [M+NH4-CO]++; MGDG(2:0/5:0)
170.1278	187.121	-0.0102	170.1176	223	57.4	7-Keto-8-Aminopelargonic Acid
518.3145	495.332	0.0072	518.3217	94	100	1-Hexadecanoyl-Sn-Glycero-3-Phosphocholine
170.1278	169.085	-0.0354	170.0924	193	36	L-Histidine, 3-Methyl-
458.3162	435.281	-0.0463	458.2699	13	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	192	36.9	7-Keto-8-Aminopelargonic

						Acid
474.2957	473.275	-0.0134	474.2823	33	100	Leu-Trp-Arg
170.1278	187.121	-0.0102	170.1176	189	45	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	37	25.7	Ile-Trp-Arg
170.1278	187.121	-0.0102	170.1176	146	44.1	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	181	38.4	7-Keto-8-Aminopelargonic Acid
458.2953	435.281	-0.0254	458.2699	50	77.3	N-Acetyl-S-Geranylgeranyl-L-Cysteine
474.2957	473.275	-0.0134	474.2823	36	100	Leu-Trp-Arg
170.1278	169.085	-0.0354	170.0924	250	37.9	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	221	44.7	7-Keto-8-Aminopelargonic Acid
458.3162	435.281	-0.0463	458.2699	21	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	241	41.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	177	48.1	7-Keto-8-Aminopelargonic Acid
370.2514	370	-0.04	370.21	152	38.1	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)
170.1278	187.121	-0.0102	170.1176	163	51.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	288	67.7	7-Keto-8-Aminopelargonic Acid
414.2587	413.239	-0.0128	414.2459	77	100	Pyroglu-Lys-Arg
170.1278	187.121	-0.0102	170.1176	216	47.7	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	209	47.1	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	185	44	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	189	68.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	180	41.1	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	73	42.6	Leu-Trp-Arg
370.2244	370	-0.01	370.21	150	38.5	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)
170.1278	187.121	-0.0102	170.1176	191	29.9	7-Keto-8-Aminopelargonic Acid
472.2733	471.223	-0.043	472.2303	39	100	Pyroglu-Trp-Arg
170.1278	169.085	-0.0354	170.0924	211	31.1	L-Histidine, 3-Methyl-
655.5145	654.492	-0.0154	655.4991	243	27.8	Deca(Propylene Glycol) Monobutyl Ether
370.2514	370	-0.04	370.21	169	24.2	MGDG 7:0; [M+NH4-CO] ⁺ ;

						MGDG(2:0/5:0)
170.1278	187.121	-0.0102	170.1176	189	48.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	232	51.4	7-Keto-8-Aminopelargonic Acid
370.2244	370	-0.01	370.21	150	48.6	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
472.3027	471.314	0.018	472.321	106	100	Terfenadine
170.1278	187.121	-0.0102	170.1176	210	51.6	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	25	54.2	Leu-Trp-Arg
370.2514	370	-0.04	370.21	135	36.8	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
170.1278	187.121	-0.0102	170.1176	196	43.5	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	238	48.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	183	50.5	7-Keto-8-Aminopelargonic Acid
458.3162	435.281	-0.0463	458.2699	38	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	181	60.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	301	34.6	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	32	62.3	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	198	38.8	7-Keto-8-Aminopelargonic Acid
370.2244	370	-0.01	370.21	95	50	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
170.1278	169.085	-0.0354	170.0924	394	46.7	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	385	74.8	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	119	24	Palmitoyl-L-Carnitine Cation
102.1273	102.092	-0.036	102.0913	214	11.4	Betaine Aldehyde Cation
276.1948	319.133	-0.0441	276.1507	107	77.8	Norfloxacin
170.1278	187.121	-0.0102	170.1176	372	58.3	7-Keto-8-Aminopelargonic Acid
472.2733	471.223	-0.043	472.2303	131	100	Pyroglu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	59	100	Leu-Trp-Arg
170.1278	187.121	-0.0102	170.1176	358	55.9	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	83	40.7	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	353	72.6	7-Keto-8-Aminopelargonic Acid
518.3145	495.332	0.0072	518.3217	62	100	1-Hexadecanoyl-Sn-Glycero-3-Phosphocholine

474.2957	473.275	-0.0134	474.2823	99	68.4	Leu-Trp-Arg
170.1278	187.121	-0.0102	170.1176	437	77.3	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	67	66.1	Leu-Trp-Arg
474.2738	473.275	0.0085	474.2823	51	100	Leu-Trp-Arg
472.2733	471.314	0.048	472.321	190	100	Terfenadine
474.2957	473.275	-0.0134	474.2823	93	44.3	Ile-Trp-Arg
170.1278	187.121	-0.0102	170.1176	449	76.2	7-Keto-8-Aminopelargonic Acid

Table A6. List of non-volatile metabolites (LC/MS) for managed population animals. Samples collected in May 2011 from two animals were pooled. Experiment was conducted using HILIC column (refer to Materials and Methods section) in positive ion mode. Top three matches are given for each compound.

Parent m/z	Mass	Delta (m/z)	Library Precursor m/z	Match Score	Probability (%)	Chem ID
170.1278	187.121	-0.0102	170.1176	417	76	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	363	14.9	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	310	2.9	L-Histidine, 3-Methyl-
472.2733	471.314	0.048	472.321	99	61.1	Terfenadine
472.2733	471.314	0.048	472.321	86	61.1	Terfenadine
472.2733	471.223	-0.043	472.2303	72	18	Pyroglu-Trp-Arg
516.3059	515.292	-0.007	516.2989	105	100	Taurocholic Acid
170.1278	187.121	-0.0102	170.1176	451	72.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	427	24.3	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	338	2.1	7-Keto-8-Aminopelargonic Acid
370.2514	369.288	0.0438	370.2952	191	35	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	174	19.1	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	172	17.6	N-Oleoyl-L-Serine
170.1278	187.121	-0.0102	170.1176	383	75.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	335	15.7	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	300	3.9	L-Histidine, 1-Methyl-
400.319	400.343	0.0231	400.3421	94	12.6	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	93	12.1	Palmitoyl-L-Carnitine

						Cation
400.319	400.343	0.0231	400.3421	93	12.1	Palmitoyl-L-Carnitine Cation
472.2733	471.314	0.048	472.321	134	80.3	Terfenadine
472.2733	471.314	0.048	472.321	115	80.3	Terfenadine
472.2733	471.314	0.048	472.321	79	80.3	Terfenadine
170.1278	187.121	-0.0102	170.1176	405	73.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	374	20.1	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	315	3.6	L-Histidine, 1-Methyl-
370.2514	369.288	0.0438	370.2952	248	27.8	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	237	19.1	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	221	11	N-Oleoyl-L-Serine
461.2907	460.28	-0.0036	461.2871	33	100	Trp-Lys-Lys
655.4719	654.492	0.0272	655.4991	194	51.2	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	177	27.9	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	169	20.8	Deca(Propylene Glycol) Monobutyl Ether
474.2957	473.275	-0.0134	474.2823	56	20.6	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	53	18.2	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	35	9.4	Leu-Trp-Arg
458.3162	435.281	-0.0463	458.2699	63	100	N-Acetyl-S-Geranylgeranyl- L-Cysteine
472.2733	471.314	0.048	472.321	86	100	Terfenadine
472.2733	471.314	0.048	472.321	75	100	Terfenadine
170.116	187.121	0.0016	170.1176	408	78.4	7-Keto-8-Aminopelargonic Acid
170.116	187.121	0.0016	170.1176	366	17.6	7-Keto-8-Aminopelargonic Acid
170.116	169.085	-0.0236	170.0924	302	2.9	L-Histidine, 1-Methyl-
472.2733	471.223	-0.043	472.2303	83	100	Pyroglu-Trp-Arg
414.278	449.314	0.0223	414.3003	241	97.3	Glycodeoxycholic Acid
414.278	449.314	0.0223	414.3003	214	97.3	Glycodeoxycholic Acid
414.278	449.314	0.0223	414.3003	170	97.3	Glycodeoxycholic Acid
472.2733	471.314	0.048	472.321	139	89.1	Terfenadine
472.2733	471.314	0.048	472.321	125	89.1	Terfenadine
472.2733	471.314	0.048	472.321	97	89.1	Terfenadine
170.1278	187.121	-0.0102	170.1176	439	77	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	400	18.1	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	335	2.9	7-Keto-8-Aminopelargonic

						Acid
400.319	400.343	0.0231	400.3421	197	19.9	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	195	18.3	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	187	13.7	Palmitoyl-L-Carnitine Cation
414.278	449.314	0.0223	414.3003	306	99	Glycodeoxycholic Acid
414.278	449.314	0.0223	414.3003	260	99	Glycodeoxycholic Acid
414.278	413.239	-0.0321	414.2459	64	1	Pyroglu-Arg-Lys
472.3027	471.314	0.018	472.321	148	100	Terfenadine
472.3027	471.314	0.018	472.321	135	100	Terfenadine
391.2842	390.277	0.0001	391.2843	115	54.1	Bis(2-Ethylhexyl) Phthalate
391.2842	390.277	0.0001	391.2843	109	42.5	Diethyl Phthalate
391.2842	390.277	0.0001	391.2843	100	42.5	Diethyl Phthalate
170.1278	169.074	-0.0466	170.0812	244	39.5	DL-Norepinephrine
170.1278	169.074	-0.0466	170.0812	237	39.5	DL-Norepinephrine
170.1278	169.074	-0.0466	170.0812	233	39.5	DL-Norepinephrine
419.3154	418.308	0.0002	419.3156	205	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
149.0229	166.027	0.0004	149.0233	440	98.6	1,2-Benzenedicarboxylic Acid
149.0229	166.027	0.0004	149.0233	429	98.6	1,2-Benzenedicarboxylic Acid
149.0229	166.027	0.0004	149.0233	425	98.6	1,2-Benzenedicarboxylic Acid
343.2918	342.256	-0.0286	343.2632	301	95.4	Retinyl Propionate
343.2918	342.256	-0.0286	343.2632	297	95.4	Retinyl Propionate
343.2918	342.256	-0.0286	343.2632	288	95.4	Retinyl Propionate
170.1383	169.085	-0.0459	170.0924	248	31.8	L-Histidine, 3-Methyl-
170.1383	187.121	-0.0207	170.1176	240	23.7	7-Keto-8-Aminopelargonic Acid
170.1383	169.085	-0.0459	170.0924	232	31.8	L-Histidine, 3-Methyl-
391.2842	390.277	0.0001	391.2843	103	52.2	Bis(2-Ethylhexyl) Phthalate
391.2842	390.277	0.0001	391.2843	99	44.1	Diethyl Phthalate
391.2842	390.277	0.0001	391.2843	89	44.1	Diethyl Phthalate
399.251	398.243	-0.0004	399.2506	174	100	Tris(Butoxyethyl) Phosphate
399.251	398.243	-0.0004	399.2506	73	100	Tris(Butoxyethyl) Phosphate
399.251	398.243	-0.0004	399.2506	72	100	Tris(Butoxyethyl) Phosphate
472.3317	471.314	-0.011	472.321	164	100	Terfenadine
472.3317	471.314	-0.011	472.321	132	100	Terfenadine
516.3458	515.292	-0.0469	516.2989	282	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	280	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	212	100	Taurocholic Acid

516.3458	515.292	-0.0469	516.2989	203	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	193	100	Taurocholic Acid
387.1816	193.074	-0.0265	387.1551	172	26.2	Hippuric Acid, Methyl Ester
387.1816	193.074	-0.0265	387.1551	169	26.2	Hippuric Acid, Methyl Ester
387.1816	193.074	-0.0265	387.1551	166	26.2	Hippuric Acid, Methyl Ester
404.2057	403.254	0.0559	404.2616	6	26.3	Arg-Thr-Lys
404.2057	403.254	0.0559	404.2616	5	25.2	Arg-Thr-Lys
404.2057	403.254	0.0559	404.2616	4	24.3	Arg-Thr-Lys
474.2957	473.275	-0.0134	474.2823	76	100	Leu-Trp-Arg
472.3317	471.314	-0.011	472.321	164	100	Terfenadine
472.3317	471.314	-0.011	472.321	129	100	Terfenadine
170.1278	169.085	-0.0354	170.0924	376	38.1	L-Histidine, 3-Methyl-
170.1278	169.085	-0.0354	170.0924	372	32.2	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	370	32.2	L-Histidine, 1-Methyl-
655.4719	654.492	0.0272	655.4991	252	19.9	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	251	19.1	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	239	12.8	Deca(Propylene Glycol) Monobutyl Ether
170.1278	169.085	-0.0354	170.0924	423	56	L-Histidine, 3-Methyl-
170.1278	169.085	-0.0354	170.0924	405	28.9	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	404	56	L-Histidine, 3-Methyl-
279.0936	278.086	-0.0002	279.0933	11	100	Triphenylphosphine Oxide
279.0936	278.086	-0.0002	279.0933	9	100	Triphenylphosphine Oxide
279.0936	278.086	-0.0002	279.0933	8	100	Triphenylphosphine Oxide
516.3458	515.292	-0.0469	516.2989	161	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	156	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	154	100	Taurocholic Acid
655.4533	654.492	0.0458	655.4991	304	22.1	Deca(Propylene Glycol) Monobutyl Ether
655.4533	654.492	0.0458	655.4991	299	17.8	Deca(Propylene Glycol) Monobutyl Ether
655.4533	654.492	0.0458	655.4991	293	14	Deca(Propylene Glycol) Monobutyl Ether
288.2533	287.196	-0.05	288.203	105	26.1	Leu-Arg
288.2533	287.196	-0.05	288.203	101	22.1	Arg-Leu
288.2533	287.196	-0.05	288.203	91	15.6	Arg-Ile
472.3317	471.314	-0.011	472.321	118	100	Terfenadine
472.3317	471.314	-0.011	472.321	99	100	Terfenadine
170.1278	169.085	-0.0354	170.0924	294	43	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	291	43	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	285	43	L-Histidine, 1-Methyl-

496.4192	495.369	-0.043	496.3762	167	100	2-O-Methyl PAF C-16
496.4192	495.369	-0.043	496.3762	167	100	2-O-Methyl PAF C-16
496.4192	495.369	-0.043	496.3762	163	100	2-O-Methyl PAF C-16
655.5042	654.492	-0.0051	655.4991	289	19.2	Deca(Propylene Glycol) Monobutyl Ether
655.5042	654.492	-0.0051	655.4991	287	17.7	Deca(Propylene Glycol) Monobutyl Ether
655.5042	654.492	-0.0051	655.4991	283	14.9	Deca(Propylene Glycol) Monobutyl Ether
695.4768	695	0.04	695.52	85	50	DG 42:10; [M+Li]+; DG(20:5/22:5/0:0)
695.4768	695	0.04	695.52	85	50	DG 42:10; [M+Li]+; DG(22:5/20:5/0:0)
516.3458	515.292	-0.0469	516.2989	197	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	196	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	195	100	Taurocholic Acid
472.3317	471.314	-0.011	472.321	190	100	Terfenadine
472.3317	471.314	-0.011	472.321	167	100	Terfenadine
414.278	413.239	-0.0321	414.2459	176	69.2	Pyroglu-Arg-Lys
414.278	413.239	-0.0321	414.2459	132	15	Pyroglu-Arg-Lys
414.278	413.239	-0.0321	414.2459	110	5.9	Pyroglu-Lys-Arg
516.3458	515.292	-0.0469	516.2989	169	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	167	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	160	100	Taurocholic Acid
170.116	187.121	0.0016	170.1176	386	45.1	7-Keto-8-Aminopelargonic Acid
170.116	169.085	-0.0236	170.0924	364	17.9	L-Histidine, 1-Methyl-
170.116	169.085	-0.0236	170.0924	362	17.9	L-Histidine, 1-Methyl-
472.3317	471.314	-0.011	472.321	216	100	Terfenadine
472.3317	471.314	-0.011	472.321	194	100	Terfenadine
472.3317	471.314	-0.011	472.321	151	100	Terfenadine
461.2907	460.243	-0.04	461.2507	87	80.4	Trp-Gln-Lys
461.2907	460.28	-0.0036	461.2871	50	19.6	Trp-Lys-Lys
516.3458	515.292	-0.0469	516.2989	282	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	264	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	263	100	Taurocholic Acid
170.116	169.085	-0.0236	170.0924	420	38.9	L-Histidine, 1-Methyl-
170.116	187.121	0.0016	170.1176	419	37.4	7-Keto-8-Aminopelargonic Acid
170.116	169.085	-0.0236	170.0924	416	38.9	L-Histidine, 1-Methyl-
370.2514	369.288	0.0438	370.2952	302	26.5	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	297	21.3	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	279	11	N-Oleoyl-L-Serine
516.3458	515.292	-0.0469	516.2989	229	100	Taurocholic Acid

516.3458	515.292	-0.0469	516.2989	226	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	218	100	Taurocholic Acid
170.1132	187.121	0.0044	170.1176	403	54.8	7-Keto-8-Aminopelargonic Acid
170.1132	169.085	-0.0208	170.0924	379	18.4	L-Histidine, 1-Methyl-
170.1132	169.085	-0.0208	170.0924	376	18.4	L-Histidine, 1-Methyl-
414.278	449.314	0.0223	414.3003	238	88.8	Glycodeoxycholic Acid
414.278	449.314	0.0223	414.3003	191	88.8	Glycodeoxycholic Acid
414.278	413.239	-0.0321	414.2459	151	7.8	Pyroglu-Arg-Lys
370.2514	369.288	0.0438	370.2952	93	9.3	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	93	9.3	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	92	9	N-Oleoyl-L-Serine
461.2907	460.243	-0.04	461.2507	108	85.2	Trp-Gln-Lys
461.2907	460.28	-0.0036	461.2871	47	14.8	Trp-Lys-Lys
516.3458	515.292	-0.0469	516.2989	240	100	Taurocholic Acid
516.3458	515.292	-0.0469	516.2989	204	100	Taurocholic Acid
474.2738	473.275	0.0085	474.2823	19	57.9	Leu-Trp-Arg
474.2738	473.275	0.0085	474.2823	10	42.1	Leu-Trp-Arg
151.0962	150.089	0.0003	151.0965	238	100	Triethylene Glycol
151.0962	150.089	0.0003	151.0965	236	100	Triethylene Glycol
151.0962	150.089	0.0003	151.0965	232	100	Triethylene Glycol
414.278	449.314	0.0223	414.3003	291	92.4	Glycodeoxycholic Acid
414.278	413.239	-0.0321	414.2459	145	2.7	Pyroglu-Arg-Lys
414.278	413.239	-0.0321	414.2459	134	1.9	Pyroglu-Arg-Lys
370.2514	369.288	0.0438	370.2952	204	18	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	200	15.2	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	196	12.8	N-Oleoyl-L-Serine
516.3458	515.292	-0.0469	516.2989	191	100	Taurocholic Acid
474.2738	473.275	0.0085	474.2823	33	20.6	Ile-Trp-Arg
474.2738	473.275	0.0085	474.2823	28	16.6	Leu-Trp-Arg
474.2738	473.275	0.0085	474.2823	26	15.4	Trp-Ile-Arg
461.2907	460.243	-0.04	461.2507	124	23.9	Trp-Gln-Lys
461.2907	460.243	-0.04	461.2507	121	21.1	Trp-Gln-Lys
461.2907	460.243	-0.04	461.2507	103	10.9	Trp-Gln-Lys
474.2957	473.275	-0.0134	474.2823	70	33.4	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	59	22.9	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	48	15.7	Trp-Ile-Arg
370.2514	369.288	0.0438	370.2952	121	10.1	N-Oleoyl-L-Serine
370.2514	370	-0.04	370.21	121	10.1	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)
370.2514	370	-0.04	370.21	121	10.1	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(5:0/2:0)

461.2907	460.243	-0.04	461.2507	91	22.7	Trp-Gln-Lys
461.2907	460.243	-0.04	461.2507	85	17.8	Trp-Gln-Lys
461.2907	460.28	-0.0036	461.2871	83	16.4	Lys-Trp-Lys
474.2738	473.275	0.0085	474.2823	106	35.6	Leu-Trp-Arg
474.2738	473.275	0.0085	474.2823	89	19.4	Ile-Trp-Arg
474.2738	473.275	0.0085	474.2823	84	15.7	Trp-Ile-Arg
458.2953	457.244	-0.044	458.251	54	32.9	Pro-Trp-Arg
458.2953	435.281	-0.0254	458.2699	53	31.6	N-Acetyl-S-Geranylgeranyl-L-Cysteine
458.2953	457.244	-0.044	458.251	36	17.2	Pro-Trp-Arg
244.1905	226.193	0.0366	244.2271	483	98.5	2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol
244.1905	243.158	-0.0249	244.1656	202	1	Pro-Lys
244.1905	243.158	-0.0249	244.1656	99	0.1	Lys-Pro
472.3027	471.314	0.018	472.321	174	100	Terfenadine
472.3027	471.314	0.018	472.321	159	100	Terfenadine
370.238	370	-0.03	370.21	121	50	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)
370.238	370	-0.03	370.21	121	50	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(5:0/2:0)
422.2569	421.233	-0.0171	422.2398	56	53.1	Phe-Gln-Lys
422.2569	421.233	-0.0171	422.2398	53	46.9	Phe-Gln-Lys
474.2957	473.275	-0.0134	474.2823	28	35	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	26	32.2	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	10	18.6	Trp-Ile-Arg
370.2514	370	-0.04	370.21	70	21.8	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)
370.2514	370	-0.04	370.21	70	21.8	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(5:0/2:0)
370.2514	369.288	0.0438	370.2952	69	20.9	N-Oleoyl-L-Serine
414.278	413.239	-0.0321	414.2459	75	54.2	Pyroglu-Lys-Arg
414.278	413.239	-0.0321	414.2459	71	45.8	Pyroglu-Lys-Arg
370.2514	369.288	0.0438	370.2952	115	13.5	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	106	9.8	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	106	9.8	N-Oleoyl-L-Serine
170.116	187.121	0.0016	170.1176	273	59.3	7-Keto-8-Aminopelargonic Acid
170.116	187.121	0.0016	170.1176	255	30.6	7-Keto-8-Aminopelargonic Acid
170.116	169.085	-0.0236	170.0924	204	6.2	L-Histidine, 1-Methyl-
239.1485	238.099	-0.042	239.106	58	100	4-(2-Hydroxyethyl)Piperazine-1-Ethanesulfonic Acid
370.2514	369.288	0.0438	370.2952	176	21.2	N-Oleoyl-L-Serine

370.2514	369.288	0.0438	370.2952	169	16.3	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	167	15	N-Oleoyl-L-Serine
414.278	449.314	0.0223	414.3003	52	100	Glycodeoxycholic Acid
414.278	449.314	0.0223	414.3003	43	100	Glycodeoxycholic Acid
414.278	449.314	0.0223	414.3003	35	100	Glycodeoxycholic Acid
139.0499	138.043	0.0003	139.0502	548	83.8	4-Imidazoleacrylic Acid
139.0499	138.043	0.0003	139.0502	546	83.8	4-Imidazoleacrylic Acid
139.0499	138.043	0.0003	139.0502	536	83.8	4-Imidazoleacrylic Acid
638.6063	638	-0.04	638.57	133	29.3	DG 36:2; [M+NH4]+; DG(14:1/22:1/0:0)
638.6063	638	-0.04	638.57	133	29.3	DG 36:2; [M+NH4]+; DG(22:1/14:1/0:0)
638.6063	638	-0.04	638.57	123	20.7	DG 36:2; [M+NH4]+; DG(16:1/20:1/0:0)
239.1485	238.099	-0.042	239.106	43	100	4-(2-Hydroxyethyl)Piperazine-1-Ethanesulfonic Acid
239.1485	238.099	-0.042	239.106	37	100	4-(2-Hydroxyethyl)Piperazine-1-Ethanesulfonic Acid
239.1485	238.099	-0.042	239.106	28	100	4-(2-Hydroxyethyl)Piperazine-1-Ethanesulfonic Acid
472.2733	471.314	0.048	472.321	160	93.1	Terfenadine
472.2733	471.223	-0.043	472.2303	60	6.9	Pyroglu-Trp-Arg
370.2514	369.288	0.0438	370.2952	290	23	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	283	17.6	N-Oleoyl-L-Serine
370.2514	369.288	0.0438	370.2952	280	15.6	N-Oleoyl-L-Serine
474.2957	473.275	-0.0134	474.2823	69	44.6	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	61	33.3	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	49	22.1	Trp-Ile-Arg
516.3059	515.292	-0.007	516.2989	87	100	Taurocholic Acid
516.3059	515.292	-0.007	516.2989	85	100	Taurocholic Acid
516.3059	515.292	-0.007	516.2989	74	100	Taurocholic Acid
458.3162	435.281	-0.0463	458.2699	50	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
458.3162	435.281	-0.0463	458.2699	29	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
474.2957	473.275	-0.0134	474.2823	35	100	Ile-Trp-Arg
400.319	400.343	0.0231	400.3421	76	26.1	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	68	19.4	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	56	12.9	Palmitoyl-L-Carnitine Cation
787.6526	786.661	0.0162	787.6688	102	100	N-Docosanoyl-4-

						Sphingeny-1-O-Phosphorylcholine
170.1132	187.121	0.0044	170.1176	255	62.8	7-Keto-8-Aminopelargonic Acid
170.1132	169.085	-0.0208	170.0924	227	18.1	L-Histidine, 3-Methyl-
170.1132	187.121	0.0044	170.1176	224	16	7-Keto-8-Aminopelargonic Acid
655.4719	654.492	0.0272	655.4991	281	27.4	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	271	19.3	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	271	19.3	Deca(Propylene Glycol) Monobutyl Ether
548.3399	548	0.04	548.38	149	8.3	MGDG 20:2; [M+NH4-CO] ⁺ ; MGDG(2:0/18:2(2E,4E))
548.3399	548	0.04	548.38	149	8.3	MGDG 20:2; [M+NH4-CO] ⁺ ; MGDG(2:0/18:2(6Z,9Z))
548.3399	548	0.04	548.38	149	8.3	MGDG 20:2; [M+NH4-CO] ⁺ ; MGDG(2:0/18:2(9E,10E))
170.116	187.121	0.0016	170.1176	15	100	7-Keto-8-Aminopelargonic Acid
170.116	169.085	-0.0236	170.0924	35	59.3	L-Histidine, 1-Methyl-
170.116	169.085	-0.0236	170.0924	35	59.3	L-Histidine, 1-Methyl-
170.116	169.085	-0.0236	170.0924	34	59.3	L-Histidine, 1-Methyl-
170.116	169.074	-0.0348	170.0812	147	49.1	DL-Norepinephrine
170.116	169.085	-0.0236	170.0924	143	41.5	L-Histidine, 1-Methyl-
170.116	169.085	-0.0236	170.0924	142	41.5	L-Histidine, 1-Methyl-
343.31	342.256	-0.0468	343.2632	174	100	Retinyl Propionate
343.31	342.256	-0.0468	343.2632	170	100	Retinyl Propionate
343.31	342.256	-0.0468	343.2632	165	100	Retinyl Propionate
170.116	187.121	0.0016	170.1176	93	47.9	7-Keto-8-Aminopelargonic Acid
170.116	187.121	0.0016	170.1176	80	30.9	7-Keto-8-Aminopelargonic Acid
170.116	169.085	-0.0236	170.0924	69	21.2	L-Histidine, 1-Methyl-
655.4533	654.492	0.0458	655.4991	250	29.8	Deca(Propylene Glycol) Monobutyl Ether
655.4533	654.492	0.0458	655.4991	246	25.1	Deca(Propylene Glycol) Monobutyl Ether
655.4533	654.492	0.0458	655.4991	234	16.7	Deca(Propylene Glycol) Monobutyl Ether
170.116	187.121	0.0016	170.1176	84	45.7	7-Keto-8-Aminopelargonic Acid
170.116	187.121	0.0016	170.1176	82	42.1	7-Keto-8-Aminopelargonic Acid

170.116	187.121	0.0016	170.1176	54	12.2	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	72	41.1	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	64	30.6	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	62	28.3	Palmitoyl-L-Carnitine Cation
655.4719	654.492	0.0272	655.4991	224	24.9	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	220	21	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	217	18.6	Deca(Propylene Glycol) Monobutyl Ether
170.116	187.121	0.0016	170.1176	148	52.6	7-Keto-8-Aminopelargonic Acid
170.116	187.121	0.0016	170.1176	140	39.2	7-Keto-8-Aminopelargonic Acid
170.116	169.085	-0.0236	170.0924	92	8.1	L-Histidine, 1-Methyl-
461.2907	460.243	-0.04	461.2507	42	57.3	Gln-Trp-Lys
461.2907	460.243	-0.04	461.2507	34	42.7	Gln-Trp-Lys
400.319	400.343	0.0231	400.3421	51	15.8	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	48	14	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	46	12.9	Palmitoyl-L-Carnitine Cation
461.2907	460.28	-0.0036	461.2871	41	100	Trp-Lys-Lys
170.1446	187.121	-0.027	170.1176	285	56.5	7-Keto-8-Aminopelargonic Acid
170.1446	187.121	-0.027	170.1176	262	20.6	7-Keto-8-Aminopelargonic Acid
170.1446	169.085	-0.0522	170.0924	245	11.3	L-Histidine, 3-Methyl-
461.2907	230.163	0.0427	461.3334	295	59.8	Val-Leu
461.2907	230.163	0.0427	461.3334	283	39.8	Leu-Val
461.2907	230.152	0.0202	461.3109	40	0.4	Dodecanedioic Acid
461.2907	230.163	0.0427	461.3334	269	59.8	Val-Leu
461.2907	230.163	0.0427	461.3334	257	39.8	Leu-Val
461.2907	230.152	0.0202	461.3109	33	0.4	Dodecanedioic Acid
170.1278	187.121	-0.0102	170.1176	192	47.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	179	30.7	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	162	16.8	L-Histidine, 1-Methyl-
655.4533	654.492	0.0458	655.4991	109	37	Deca(Propylene Glycol) Monobutyl Ether
655.4533	654.492	0.0458	655.4991	106	32.7	Deca(Propylene Glycol)

						Monobutyl Ether
655.4533	654.492	0.0458	655.4991	104	30.2	Deca(Propylene Glycol) Monobutyl Ether
343.2918	342.256	-0.0286	343.2632	110	100	Retinyl Propionate
461.2907	230.163	0.0427	461.3334	274	58.4	Val-Leu
461.2907	230.163	0.0427	461.3334	264	41.2	Leu-Val
461.2907	230.152	0.0202	461.3109	45	0.4	Dodecanedioic Acid
787.6804	786.661	-0.0116	787.6688	70	39.7	N-Docosanoyl-4- Sphingenyl-1-O- Phosphorylcholine
787.6804	786.661	-0.0116	787.6688	68	36.6	N-Docosanoyl-4- Sphingenyl-1-O- Phosphorylcholine
787.6804	786.661	-0.0116	787.6688	45	13.4	N-Docosanoyl-4- Sphingenyl-1-O- Phosphorylcholine
170.1278	169	-0.04	170.09	275	36	3-Methyl-L-Histidine
170.1278	169.085	-0.0354	170.0924	270	29	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	265	23.4	L-Histidine, 3-Methyl-
655.4719	654.492	0.0272	655.4991	105	38.5	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	102	34	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	97	27.4	Deca(Propylene Glycol) Monobutyl Ether
343.2918	342.256	-0.0286	343.2632	53	77.9	Retinyl Propionate
343.2918	342.256	-0.0286	343.2632	50	77.9	Retinyl Propionate
343.2918	342.256	-0.0286	343.2632	47	77.9	Retinyl Propionate
787.6377	786.661	0.0311	787.6688	73	100	N-Docosanoyl-4- Sphingenyl-1-O- Phosphorylcholine
170.1278	187.121	-0.0102	170.1176	163	54	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	142	23	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	129	14.8	L-Histidine, 1-Methyl-
400.319	400.343	0.0231	400.3421	187	9.1	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	186	8.7	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	185	8.4	Palmitoyl-L-Carnitine Cation
787.6526	786.661	0.0162	787.6688	37	38.7	N-Docosanoyl-4- Sphingenyl-1-O- Phosphorylcholine
787.6526	786.661	0.0162	787.6688	25	25.8	N-Docosanoyl-4- Sphingenyl-1-O-

						Phosphorylcholine
787.6526	786.661	0.0162	787.6688	20	20.8	N-Docosanoyl-4-Sphinganyl-1-O-Phosphorylcholine
170.1278	169.085	-0.0354	170.0924	229	32.7	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	227	32.7	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	226	28.9	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	31	100	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	64	54	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	43	23	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	43	23	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	47	53.1	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	44	46.9	Ile-Trp-Arg
458.3162	435.281	-0.0463	458.2699	78	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
474.2957	473.275	-0.0134	474.2823	66	45.2	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	51	27.4	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	51	27.4	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	54	59.7	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	31	21.8	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	27	18.4	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	74	30.4	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	60	19	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	52	14.2	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	52	20.6	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	41	14.1	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	39	13	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	54	28.9	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	42	19.3	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	38	16.3	Ile-Trp-Arg
518.3145	495.332	0.0072	518.3217	91	100	1-Hexadecanoyl-Sn-Glycero-3-Phosphocholine
474.2957	473.275	-0.0134	474.2823	52	31.8	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	50	29.3	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	40	20.7	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	81	27.4	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	71	19.4	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	68	17.1	Ile-Trp-Arg
400.319	400.343	0.0231	400.3421	65	47.4	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	63	43.7	Palmitoyl-L-Carnitine Cation

400.319	401.278	-0.0485	400.2705	12	8.8	Myriocin
170.1278	187.121	-0.0102	170.1176	31	38.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	30	36.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	18	24.6	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	45	21.2	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	43	19.6	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	38	15.8	Leu-Trp-Arg
400.319	400.343	0.0231	400.3421	58	47	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	56	43.3	Palmitoyl-L-Carnitine Cation
400.319	401.278	-0.0485	400.2705	14	9.7	Myriocin
474.2957	473.275	-0.0134	474.2823	60	40.9	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	53	31.4	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	50	27.7	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	31	22.9	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	30	22.1	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	24	17.3	Ile-Trp-Arg
170.1278	187.121	-0.0102	170.1176	141	43.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	137	36.5	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	111	10.9	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	128	45.7	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	123	36.9	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	94	10.4	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	95	39.8	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	93	36.7	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	61	9.8	7-Keto-8-Aminopelargonic Acid
414.278	449.314	0.0223	414.3003	66	100	Glycodeoxycholic Acid
474.2738	473.275	0.0085	474.2823	34	57.3	Trp-Ile-Arg
474.2738	473.275	0.0085	474.2823	26	42.7	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	77	76.9	Trp-Ile-Arg
474.2957	473.275	-0.0134	474.2823	51	23.1	Ile-Trp-Arg
170.1278	187.121	-0.0102	170.1176	151	72	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	126	22	7-Keto-8-Aminopelargonic Acid

170.1278	187.121	-0.0102	170.1176	95	6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	136	46.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	131	37.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	99	10	7-Keto-8-Aminopelargonic Acid
474.2738	473.275	0.0085	474.2823	110	71.5	Trp-Ile-Arg
474.2738	473.275	0.0085	474.2823	67	15.8	Ile-Trp-Arg
474.2738	473.275	0.0085	474.2823	62	12.7	Leu-Trp-Arg
170.1278	187.121	-0.0102	170.1176	173	51	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	159	31.9	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	130	9	L-Histidine, 3-Methyl-
458.3162	435.281	-0.0463	458.2699	102	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	142	45.7	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	137	36.9	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	111	11	L-Histidine, 1-Methyl-
474.2957	473.275	-0.0134	474.2823	44	57.9	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	35	42.1	Trp-Ile-Arg
458.2757	435.281	-0.0058	458.2699	101	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
400.319	400.343	0.0231	400.3421	55	80.2	Palmitoyl-L-Carnitine Cation
400.319	401.278	-0.0485	400.2705	19	19.8	Myriocin
400.319	401.278	-0.0485	400.2705	16	19.8	Myriocin
170.1278	169.085	-0.0354	170.0924	130	31.6	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	128	31.6	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	126	31.6	L-Histidine, 1-Methyl-
458.3162	435.281	-0.0463	458.2699	78	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
458.3162	435.281	-0.0463	458.2699	72	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
458.3162	435.281	-0.0463	458.2699	39	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
343.2759	342.256	-0.0127	343.2632	161	93.2	Retinyl Propionate
343.2759	342.256	-0.0127	343.2632	155	93.2	Retinyl Propionate
343.2759	342.256	-0.0127	343.2632	127	93.2	Retinyl Propionate
170.1278	187.121	-0.0102	170.1176	143	32.3	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	141	29.8	7-Keto-8-Aminopelargonic Acid

170.1278	169.085	-0.0354	170.0924	133	22.2	L-Histidine, 1-Methyl-
458.3162	435.281	-0.0463	458.2699	62	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
458.3162	435.281	-0.0463	458.2699	61	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
458.3162	435.281	-0.0463	458.2699	54	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	151	30.3	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	148	26.8	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	144	22.6	L-Histidine, 3-Methyl-
474.2957	473.275	-0.0134	474.2823	72	100	Leu-Trp-Arg
458.3162	435.281	-0.0463	458.2699	32	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
458.3162	435.281	-0.0463	458.2699	25	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
458.3162	435.281	-0.0463	458.2699	18	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	162	45.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	150	30.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	104	6.4	7-Keto-8-Aminopelargonic Acid
400.319	401.278	-0.0485	400.2705	103	100	Myriocin
400.319	401.278	-0.0485	400.2705	102	100	Myriocin
170.1278	187.121	-0.0102	170.1176	148	44.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	142	35.1	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	87	6.8	7-Keto-8-Aminopelargonic Acid
458.2549	435.281	0.015	458.2699	69	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	143	40.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	141	37	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	100	8.4	7-Keto-8-Aminopelargonic Acid
518.3145	495.332	0.0072	518.3217	66	100	1-Hexadecanoyl-Sn-Glycero-3-Phosphocholine
170.1278	187.121	-0.0102	170.1176	161	37.6	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	146	22.8	L-Histidine, 3-Methyl-
170.1278	187.121	-0.0102	170.1176	141	18.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	140	42	7-Keto-8-Aminopelargonic

						Acid
170.1278	187.121	-0.0102	170.1176	137	37.1	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	99	8.9	L-Histidine, 1-Methyl-
474.2957	473.275	-0.0134	474.2823	52	63.5	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	36	36.5	Ile-Trp-Arg
170.1278	169.085	-0.0354	170.0924	160	35.9	L-Histidine, 3-Methyl-
170.1278	169.085	-0.0354	170.0924	160	35.9	L-Histidine, 3-Methyl-
170.1278	169.085	-0.0354	170.0924	158	35.9	L-Histidine, 3-Methyl-
458.3162	435.281	-0.0463	458.2699	40	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	156	45.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	156	45.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	111	9.6	7-Keto-8-Aminopelargonic Acid
458.3162	435.281	-0.0463	458.2699	37	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
400.36	400.343	-0.0179	400.3421	25	56.6	Palmitoyl-L-Carnitine Cation
400.36	400.343	-0.0179	400.3421	18	43.4	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	170	50.5	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	161	36.7	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	113	7.6	7-Keto-8-Aminopelargonic Acid
400.319	401.278	-0.0485	400.2705	16	100	Myriocin
343.2918	342.256	-0.0286	343.2632	81	100	Retinyl Propionate
170.1278	187.121	-0.0102	170.1176	190	66.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	169	28.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	117	5.6	7-Keto-8-Aminopelargonic Acid
474.2957	473.275	-0.0134	474.2823	47	100	Ile-Trp-Arg
170.1278	187.121	-0.0102	170.1176	165	48.8	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	160	39.3	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	116	8.5	L-Histidine, 1-Methyl-
400.319	400.343	0.0231	400.3421	72	26.5	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	68	22.4	Palmitoyl-L-Carnitine Cation

400.319	400.343	0.0231	400.3421	66	20.6	Palmitoyl-L-Carnitine Cation
474.2957	473.275	-0.0134	474.2823	43	38.5	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	40	34	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	35	27.4	Ile-Trp-Arg
170.1278	187.121	-0.0102	170.1176	235	73.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	200	18.5	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	154	3.9	L-Histidine, 1-Methyl-
518.3145	495.332	0.0072	518.3217	104	100	1-Hexadecanoyl-Sn-Glycero-3-Phosphocholine
400.319	400.343	0.0231	400.3421	119	30.9	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	117	28.5	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	111	22.4	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	185	52.3	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	175	36.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	129	7.8	7-Keto-8-Aminopelargonic Acid
400.319	400.343	0.0231	400.3421	96	36.3	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	92	30.7	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	91	29.5	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	165	49.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	155	34.9	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	106	7.2	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	202	40	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	201	38.4	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	149	7.7	L-Histidine, 3-Methyl-
400.319	400.343	0.0231	400.3421	159	84.5	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	60	6.4	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	54	5	Palmitoyl-L-Carnitine Cation
655.4719	654.492	0.0272	655.4991	151	51.2	Deca(Propylene Glycol) Monobutyl Ether

655.4719	654.492	0.0272	655.4991	134	27.9	Deca(Propylene Glycol) Monobutyl Ether
655.4719	654.492	0.0272	655.4991	126	20.8	Deca(Propylene Glycol) Monobutyl Ether
170.1278	187.121	-0.0102	170.1176	189	48.1	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	184	38.8	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	120	6.4	L-Histidine, 1-Methyl-
414.278	413.239	-0.0321	414.2459	70	100	Pyroglu-Lys-Arg
370.2514	370	-0.04	370.21	88	39.3	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)
370.2514	370	-0.04	370.21	88	39.3	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(5:0/2:0)
370.2514	370	-0.04	370.21	57	10.7	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(3:0/4:0)
400.319	400.343	0.0231	400.3421	39	28.8	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	38	27.7	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	32	21.8	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	194	41.3	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	189	33.3	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	137	6.6	7-Keto-8-Aminopelargonic Acid
414.278	413.239	-0.0321	414.2459	59	55.4	Pyroglu-Lys-Arg
414.278	413.239	-0.0321	414.2459	54	44.6	Pyroglu-Lys-Arg
458.2953	457.244	-0.044	458.251	59	67.1	Pro-Trp-Arg
458.2953	457.244	-0.044	458.251	34	20.5	Pro-Trp-Arg
458.2953	457.244	-0.044	458.251	19	12.4	Trp-Pro-Arg
343.2918	342.256	-0.0286	343.2632	156	93.4	Retinyl Propionate
343.2918	408.288	-0.0275	343.2643	53	6.6	Cholic Acid
343.2918	408.288	-0.0275	343.2643	53	6.6	Cholic Acid
458.2953	457.244	-0.044	458.251	90	31.9	Pro-Trp-Arg
458.2953	435.281	-0.0254	458.2699	77	20.6	N-Acetyl-S-Geranylgeranyl-L-Cysteine
458.2953	457.244	-0.044	458.251	69	15.4	Pro-Trp-Arg
170.1278	187.121	-0.0102	170.1176	198	50.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	188	35.9	7-Keto-8-Aminopelargonic Acid
170.1278	169.074	-0.0466	170.0812	124	5.9	Pyridoxine
370.2514	370	-0.04	370.21	182	37	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)

370.2514	370	-0.04	370.21	182	37	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(5:0/2:0)
370.2514	369.288	0.0438	370.2952	124	6.8	N-Oleoyl-L-Serine
474.2957	473.275	-0.0134	474.2823	47	35.6	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	47	35.6	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	42	28.7	Trp-Ile-Arg
458.2953	457.244	-0.044	458.251	130	23	Pro-Trp-Arg
458.2953	457.244	-0.044	458.251	126	19.5	Trp-Pro-Arg
458.2953	457.244	-0.044	458.251	122	16.4	Trp-Pro-Arg
170.1278	169.085	-0.0354	170.0924	208	32.3	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	207	31.1	L-Histidine, 3-Methyl-
170.1278	169.085	-0.0354	170.0924	207	31.1	L-Histidine, 3-Methyl-
170.1278	187.121	-0.0102	170.1176	155	49.3	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	151	41.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	92	7.5	7-Keto-8-Aminopelargonic Acid
458.2953	435.281	-0.0254	458.2699	80	81.9	N-Acetyl-S-Geranylgeranyl- L-Cysteine
458.2953	435.281	-0.0254	458.2699	75	81.9	N-Acetyl-S-Geranylgeranyl- L-Cysteine
458.2953	435.281	-0.0254	458.2699	57	81.9	N-Acetyl-S-Geranylgeranyl- L-Cysteine
170.1278	187.121	-0.0102	170.1176	174	51	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	163	35	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	137	10.5	7-Keto-8-Aminopelargonic Acid
458.2953	435.281	-0.0254	458.2699	70	83.8	N-Acetyl-S-Geranylgeranyl- L-Cysteine
458.2953	457.244	-0.044	458.251	15	16.2	Trp-Pro-Arg
474.2957	473.275	-0.0134	474.2823	23	56.6	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	16	43.4	Ile-Trp-Arg
170.1278	169.085	-0.0354	170.0924	218	47.4	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	217	47.4	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	208	33.5	L-Histidine, 3-Methyl-
474.2957	473.275	-0.0134	474.2823	36	100	Ile-Trp-Arg
370.2244	370	-0.01	370.21	200	50	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)
370.2244	370	-0.01	370.21	200	50	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(5:0/2:0)
170.1278	187.121	-0.0102	170.1176	223	57.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	207	33.1	7-Keto-8-Aminopelargonic

						Acid
170.1278	187.121	-0.0102	170.1176	160	6.9	7-Keto-8-Aminopelargonic Acid
518.3145	495.332	0.0072	518.3217	94	100	1-Hexadecanoyl-Sn-Glycero-3-Phosphocholine
170.1278	169.085	-0.0354	170.0924	193	36	L-Histidine, 3-Methyl-
170.1278	169.085	-0.0354	170.0924	182	24.7	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	179	21.8	7-Keto-8-Aminopelargonic Acid
458.3162	435.281	-0.0463	458.2699	13	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	192	36.9	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	190	34	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	186	34	L-Histidine, 1-Methyl-
474.2957	473.275	-0.0134	474.2823	33	100	Leu-Trp-Arg
170.1278	187.121	-0.0102	170.1176	189	45	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	174	27.3	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	158	15.7	L-Histidine, 1-Methyl-
474.2957	473.275	-0.0134	474.2823	37	25.7	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	34	22.7	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	30	19.2	Ile-Trp-Arg
170.1278	187.121	-0.0102	170.1176	146	44.1	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	141	35.5	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	95	7.5	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	181	38.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	178	34	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	146	9.1	L-Histidine, 1-Methyl-
458.2953	435.281	-0.0254	458.2699	50	77.3	N-Acetyl-S-Geranylgeranyl-L-Cysteine
458.2953	457.244	-0.044	458.251	23	22.7	Trp-Pro-Arg
474.2957	473.275	-0.0134	474.2823	36	100	Leu-Trp-Arg
170.1278	169.085	-0.0354	170.0924	250	37.9	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	245	30.5	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	243	37.9	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	221	44.7	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	218	39.5	7-Keto-8-Aminopelargonic Acid

170.1278	169.085	-0.0354	170.0924	152	6.2	L-Histidine, 1-Methyl-
458.3162	435.281	-0.0463	458.2699	21	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	241	41.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	237	35.4	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	218	17.2	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	177	48.1	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	172	38.8	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	122	7.9	L-Histidine, 1-Methyl-
370.2514	370	-0.04	370.21	152	38.1	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)
370.2514	370	-0.04	370.21	152	38.1	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(5:0/2:0)
370.2514	369.288	0.0438	370.2952	66	3.4	N-Oleoyl-L-Serine
170.1278	187.121	-0.0102	170.1176	163	51.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	138	15.8	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	138	15.8	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	288	67.7	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	265	24.7	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	223	5.5	7-Keto-8-Aminopelargonic Acid
414.2587	413.239	-0.0128	414.2459	77	100	Pyroglu-Lys-Arg
170.1278	187.121	-0.0102	170.1176	216	47.7	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	207	34.6	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	184	12.6	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	209	47.1	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	206	41.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	149	7.8	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	185	44	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	183	40.6	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	145	9.7	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	189	68.4	7-Keto-8-Aminopelargonic Acid

170.1278	187.121	-0.0102	170.1176	160	19.4	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	136	6.5	L-Histidine, 3-Methyl-
170.1278	187.121	-0.0102	170.1176	180	41.1	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	171	29.8	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	162	21.6	L-Histidine, 3-Methyl-
474.2957	473.275	-0.0134	474.2823	73	42.6	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	58	25.8	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	44	16.1	Ile-Trp-Arg
370.2244	370	-0.01	370.21	150	38.5	MGDG 7:0; [M+NH ₄ -CO] ⁺ ; MGDG(2:0/5:0)
370.2244	370	-0.01	370.21	150	38.5	MGDG 7:0; [M+NH ₄ -CO] ⁺ ; MGDG(5:0/2:0)
370.2244	370	-0.05	370.17	124	11.5	MGDG 5:0; [M+NH ₄] ⁺ ; MGDG(2:0/3:0)
170.1278	187.121	-0.0102	170.1176	191	29.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	188	26.4	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	187	25.4	L-Histidine, 1-Methyl-
472.2733	471.223	-0.043	472.2303	39	100	Pyroglu-Trp-Arg
170.1278	169.085	-0.0354	170.0924	211	31.1	L-Histidine, 3-Methyl-
170.1278	187.121	-0.0102	170.1176	204	23.8	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	194	16.8	7-Keto-8-Aminopelargonic Acid
655.5145	654.492	-0.0154	655.4991	243	27.8	Deca(Propylene Glycol) Monobutyl Ether
655.5145	654.492	-0.0154	655.4991	233	19.6	Deca(Propylene Glycol) Monobutyl Ether
655.5145	654.492	-0.0154	655.4991	230	17.3	Deca(Propylene Glycol) Monobutyl Ether
370.2514	370	-0.04	370.21	169	24.2	MGDG 7:0; [M+NH ₄ -CO] ⁺ ; MGDG(2:0/5:0)
370.2514	370	-0.04	370.21	169	24.2	MGDG 7:0; [M+NH ₄ -CO] ⁺ ; MGDG(5:0/2:0)
370.2514	369.288	0.0438	370.2952	141	7	N-Oleoyl-L-Serine
170.1278	187.121	-0.0102	170.1176	189	48.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	183	37.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	129	7.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	232	51.4	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	225	39.4	7-Keto-8-Aminopelargonic

						Acid
170.1278	187.121	-0.0102	170.1176	162	6.6	7-Keto-8-Aminopelargonic Acid
370.2244	370	-0.01	370.21	150	48.6	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)
370.2244	370	-0.01	370.21	150	48.6	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(5:0/2:0)
370.2244	369.172	-0.0449	370.1795	32	2.7	Amisulpride
472.3027	471.314	0.018	472.321	106	100	Terfenadine
170.1278	187.121	-0.0102	170.1176	210	51.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	200	36.5	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	166	9.3	L-Histidine, 1-Methyl-
474.2957	473.275	-0.0134	474.2823	25	54.2	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	21	45.8	Trp-Ile-Arg
370.2514	370	-0.04	370.21	135	36.8	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(2:0/5:0)
370.2514	370	-0.04	370.21	135	36.8	MGDG 7:0; [M+NH4-CO] ⁺ ; MGDG(5:0/2:0)
370.2514	369.288	0.0438	370.2952	67	5.6	N-Oleoyl-L-Serine
170.1278	187.121	-0.0102	170.1176	196	43.5	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	195	41.8	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	146	8.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	238	48.4	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	217	20.6	L-Histidine, 3-Methyl-
170.1278	169.085	-0.0354	170.0924	216	20.6	L-Histidine, 3-Methyl-
170.1278	187.121	-0.0102	170.1176	183	50.5	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	171	33.7	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	120	6.8	L-Histidine, 3-Methyl-
458.3162	435.281	-0.0463	458.2699	38	100	N-Acetyl-S-Geranylgeranyl-L-Cysteine
170.1278	187.121	-0.0102	170.1176	181	60.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	161	27.4	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	112	5.6	L-Histidine, 3-Methyl-
170.1278	187.121	-0.0102	170.1176	301	34.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	300	33.3	7-Keto-8-Aminopelargonic Acid

170.1278	169.085	-0.0354	170.0924	284	19.2	L-Histidine, 3-Methyl-
400.319	400.343	0.0231	400.3421	32	62.3	Palmitoyl-L-Carnitine Cation
400.319	401.278	-0.0485	400.2705	17	37.7	Myriocin
400.319	401.278	-0.0485	400.2705	17	37.7	Myriocin
170.1278	187.121	-0.0102	170.1176	198	38.8	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	191	29.7	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	188	29.7	L-Histidine, 1-Methyl-
370.2244	370	-0.01	370.21	95	50	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2244	370	-0.01	370.21	95	50	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
170.1278	169.085	-0.0354	170.0924	394	46.7	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	388	46.7	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	388	46.7	L-Histidine, 1-Methyl-
170.1278	187.121	-0.0102	170.1176	385	74.8	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	338	15.6	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	295	3.5	L-Histidine, 1-Methyl-
400.319	400.343	0.0231	400.3421	119	24	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	117	22.1	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	107	15.6	Palmitoyl-L-Carnitine Cation
102.1273	102.092	-0.036	102.0913	214	11.4	Betaine Aldehyde Cation
102.1273	102.092	-0.036	102.0913	213	10.9	Betaine Aldehyde Cation
102.1273	102.092	-0.036	102.0913	213	10.9	Betaine Aldehyde Cation
276.1948	319.133	-0.0441	276.1507	107	77.8	Norfloxacin
276.1948	319.133	-0.0441	276.1507	98	77.8	Norfloxacin
276.1948	319.133	-0.0441	276.1507	86	77.8	Norfloxacin
170.1278	187.121	-0.0102	170.1176	372	58.3	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	348	19.5	L-Histidine, 1-Methyl-
170.1278	169.085	-0.0354	170.0924	347	19.5	L-Histidine, 1-Methyl-
472.2733	471.223	-0.043	472.2303	131	100	Pyroglu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	59	100	Leu-Trp-Arg
170.1278	187.121	-0.0102	170.1176	358	55.9	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	341	30.5	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	314	9	L-Histidine, 1-Methyl-
400.319	400.343	0.0231	400.3421	83	40.7	Palmitoyl-L-Carnitine Cation

400.319	400.343	0.0231	400.3421	78	32.8	Palmitoyl-L-Carnitine Cation
400.319	400.343	0.0231	400.3421	73	26.4	Palmitoyl-L-Carnitine Cation
170.1278	187.121	-0.0102	170.1176	353	72.6	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	322	19.8	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	256	3.1	7-Keto-8-Aminopelargonic Acid
518.3145	495.332	0.0072	518.3217	62	100	1-Hexadecanoyl-Sn-Glycero-3-Phosphocholine
474.2957	473.275	-0.0134	474.2823	99	68.4	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	72	20.1	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	48	6.7	Leu-Trp-Arg
170.1278	187.121	-0.0102	170.1176	437	77.3	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	387	15.7	7-Keto-8-Aminopelargonic Acid
170.1278	169.085	-0.0354	170.0924	317	2.3	L-Histidine, 1-Methyl-
474.2957	473.275	-0.0134	474.2823	67	66.1	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	38	18.7	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	33	15.1	Ile-Trp-Arg
474.2738	473.275	0.0085	474.2823	51	100	Leu-Trp-Arg
472.2733	471.314	0.048	472.321	190	100	Terfenadine
472.2733	471.314	0.048	472.321	162	100	Terfenadine
474.2957	473.275	-0.0134	474.2823	93	44.3	Ile-Trp-Arg
474.2957	473.275	-0.0134	474.2823	89	37.5	Leu-Trp-Arg
474.2957	473.275	-0.0134	474.2823	70	18.2	Ile-Trp-Arg
170.1278	187.121	-0.0102	170.1176	449	76.2	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	415	19.5	7-Keto-8-Aminopelargonic Acid
170.1278	187.121	-0.0102	170.1176	328	1.7	7-Keto-8-Aminopelargonic Acid

Table A7. List of non-volatile metabolites (LC/MS) for managed population animals. Sample was pooled from multiple animals (sample collected in Dec 2011). Experiment was conducted using specialized lipids fraction protocol on RP column (refer to Materials and Methods section) in positive ion mode. Top four matches are given for each compound.

Parent m/z	Mass	Delta (m/z)	Library Precursor m/z	Match Score	Probability (%)	Chem ID
118.0873	117.079	-0.001	118.0863	220	67.5	Betaine
118.0873	117.079	-0.001	118.0863	452	58.8	Betaine

118.0873	117.079	-0.001	118.0863	340	82.5	Betaine
118.0873	117.079	-0.001	118.0863	352	65.8	Betaine
224.1293	223.106	-0.0164	224.1129	65	56.6	N-Acetyl-D-Galactosaminitol
224.1293	223.084	-0.0376	224.0917	159	47	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	202	89.1	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	218	79.4	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	382	100	Betaine
118.0873	117.079	-0.001	118.0863	460	45.1	Betaine
118.0873	117.079	-0.001	118.0863	322	81.8	Betaine
118.0873	117.079	-0.001	118.0863	207	66.5	Betaine
186.0588	370.196	0.0467	186.1055	52	100	Ser-His-Lys
224.1293	223.084	-0.0376	224.0917	307	90.4	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	205	76.2	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	318	32.2	Betaine
118.0873	117.079	-0.001	118.0863	472	64.4	Betaine
118.0873	117.079	-0.001	118.0863	275	67.5	Betaine
118.0873	117.079	-0.001	118.0863	368	68.7	Betaine
186.0588	163.084	0.0149	186.0737	117	80.1	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	223.106	-0.0164	224.1129	42	58.6	N-Acetyl-D-Galactosaminitol
224.1293	446.228	-0.0081	224.1212	120	49.7	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	249	55.6	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	205	77.6	N-Acetyl-L-Tyrosine
224.1293	223.106	-0.0164	224.1129	93	100	N-Acetyl-D-Galactosaminitol
224.1293	223.106	-0.0164	224.1129	86	100	N-Acetyl-D-Galactosaminitol
243.1858	220.183	-0.0139	243.1719	64	100	Butylated Hydroxytoluene
118.0959	117.079	-0.0096	118.0863	295	100	Betaine
118.0959	117.079	-0.0096	118.0863	268	96.4	Betaine
118.0959	117.079	-0.0096	118.0863	332	31.6	Betaine
139.0603	138.032	-0.021	139.039	120	37.2	Salicylic Acid
139.0603	138.043	-0.0101	139.0502	163	28.4	4-Imidazoleacrylic Acid
139.0603	138.043	-0.0101	139.0502	163	72.5	4-Imidazoleacrylic Acid
273.1777	290.225	0.0436	273.2213	67	73.2	5-Androsten-3.Beta.,17.Beta.-Diol
273.1777	290.225	0.0436	273.2213	102	42	5-Androsten-3.Beta.,17.Beta.-Diol
195.1333	194.115	-0.0106	195.1227	209	100	Tetraethylene Glycol
432.2891	449.314	0.0217	432.3108	66	100	Glycodeoxycholic Acid
387.1819	386	-0.05	387.13	258	28.5	1-O-B-D-Glucopyranosyl Sinapate
387.1819	193.074	-0.0268	387.1551	252	31.3	Hippuric Acid, Methyl Ester
387.1819	193.074	-0.0268	387.1551	301	54.5	Hippuric Acid, Methyl Ester

387.1819	193.074	-0.0268	387.1551	237	28.3	Hippuric Acid, Methyl Ester
404.2081	403.207	0.006	404.214	79	12.7	Gln-Glu-Lys
404.2081	403.222	0.0211	404.2292	16	11.4	Trp-Ala-Lys
404.2081	403.207	0.006	404.214	49	42.5	Gln-Glu-Lys
404.2081	403.207	0.006	404.214	64	17.2	Gln-Glu-Lys
409.1633	386.17	-0.0038	409.1595	113	81.2	N6-2-(4-Aminophenyl)Ethyladenosine
343.291	408.288	-0.0267	343.2643	88	100	Cholic Acid
387.176	193.074	-0.0209	387.1551	237	100	Hippuric Acid, Methyl Ester
387.176	193.074	-0.0209	387.1551	264	69	Hippuric Acid, Methyl Ester
387.176	193.074	-0.0209	387.1551	266	100	Hippuric Acid, Methyl Ester
387.176	193.074	-0.0209	387.1551	308	49.2	Hippuric Acid, Methyl Ester
118.0821	117.079	0.0042	118.0863	392	68.2	Betaine
118.0821	117.079	0.0042	118.0863	547	97.5	Betaine
118.0821	117.079	0.0042	118.0863	345	76.5	Betaine
118.0821	117.079	0.0042	118.0863	376	35.4	Betaine
118.0873	117.079	-0.001	118.0863	344	100	Betaine
118.0873	117.079	-0.001	118.0863	365	31.3	Betaine
118.0873	117.079	-0.001	118.0863	294	66.7	Betaine
118.0873	117	0	118.09	317	27.8	Betaine
118.0873	117.079	-0.001	118.0863	424	62.4	Betaine
118.0873	117.079	-0.001	118.0863	295	68.2	Betaine
118.0873	117.079	-0.001	118.0863	321	70.2	Betaine
288.2597	270.219	-0.0064	288.2533	61	100	Surfynol PSA-336
288.2547	287.196	-0.052	288.203	89	20.4	Leu-Arg
288.2547	287.196	-0.052	288.203	271	67.2	Leu-Arg
288.2547	287.196	-0.052	288.203	116	32.9	Leu-Arg
118.0873	117.079	-0.001	118.0863	449	66.5	Betaine
118.0873	117.079	-0.001	118.0863	309	68.9	Betaine
118.0873	117.079	-0.001	118.0863	299	73.6	Betaine
244.2278	226.193	-0.0007	244.2271	146	100	2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol
244.2278	226.193	-0.0007	244.2271	135	100	2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol
304.3018	304.3	-0.0019	304.2999	183	12.9	Benzyl Dodecyl Dimethylammonium Cation
304.3018	304.3	-0.0019	304.2999	301	46	Benzyl Dodecyl Dimethylammonium Cation
304.3018	304.3	-0.0019	304.2999	170	15.6	Benzyl Dodecyl Dimethylammonium Cation
304.3018	304.3	-0.0019	304.2999	182	10.4	Benzyl Dodecyl Dimethylammonium Cation
118.0873	117.079	-0.001	118.0863	378	34.6	Betaine
118.0873	117.079	-0.001	118.0863	333	81.7	Betaine

118.0873	117.079	-0.001	118.0863	376	62.6	Betaine
186.0588	370.196	0.0467	186.1055	65	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	62	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	302	68.4	Betaine
118.0873	117.079	-0.001	118.0863	391	39.1	Betaine
118.0873	117.079	-0.001	118.0863	320	100	Betaine
118.0873	117.079	-0.001	118.0863	346	60.5	Betaine
267.1739	266.165	-0.002	267.172	266	100	Tributyl Phosphate
118.0873	117.079	-0.001	118.0863	331	98.4	Betaine
118.0873	117.079	-0.001	118.0863	437	72	Betaine
118.0873	117.079	-0.001	118.0863	317	74.1	Betaine
118.0873	117.079	-0.001	118.0863	312	55.2	Betaine
118.0873	117.079	-0.001	118.0863	409	52.8	Betaine
118.0873	117.079	-0.001	118.0863	350	59.1	Betaine
118.0873	117.079	-0.001	118.0863	347	58.6	Betaine
279.1625	278.152	-0.0035	279.1591	251	81.2	Dibutyl Phthalate
279.1625	278.152	-0.0035	279.1591	250	96.5	Dibutyl Phthalate
279.1625	278.152	-0.0035	279.1591	308	96	Dibutyl Phthalate
279.1625	278.152	-0.0035	279.1591	284	97	Dibutyl Phthalate
399.2537	398.243	-0.0031	399.2506	165	100	Tris(Butoxyethyl) Phosphate
399.2537	398.243	-0.0031	399.2506	113	100	Tris(Butoxyethyl) Phosphate
444.3346	443.297	-0.0305	444.3041	62	27.4	Arg-Ile-Arg
532.3865	514.318	-0.0351	532.3514	207	100	3,6,9,12,15-Pentaoxonacosan-1-Ol, Hydrogen Sulfate
532.3865	514.318	-0.0351	532.3514	129	100	3,6,9,12,15-Pentaoxonacosan-1-Ol, Hydrogen Sulfate
400.3098	399.259	-0.0431	400.2667	17	18.5	Arg-Pro-Lys
186.0588	163.084	0.0149	186.0737	128	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	448	48.6	Betaine
118.0873	117.079	-0.001	118.0863	319	74	Betaine
118.0873	117.079	-0.001	118.0863	343	65.7	Betaine
97.0774	114.104	0.0238	97.1012	23	62.3	Cyclohexanemethanol
332.332	332.332	-0.0009	332.3312	225	11.3	Benzyl Tetradecyl Dimethylammonium Cation
332.332	332.332	-0.0009	332.3312	237	26.7	Benzyl Tetradecyl Dimethylammonium Cation
332.332	332.332	-0.0009	332.3312	170	12.8	Benzyl Tetradecyl Dimethylammonium Cation
332.332	332.332	-0.0009	332.3312	213	18.3	Benzyl Tetradecyl Dimethylammonium Cation
118.0873	117.079	-0.001	118.0863	385	71.1	Betaine
118.0873	117.079	-0.001	118.0863	295	64.3	Betaine
118.0873	117.079	-0.001	118.0863	324	30.8	Betaine

118.0873	117.079	-0.001	118.0863	383	52.7	Betaine
118.0873	117.079	-0.001	118.0863	370	89.7	Betaine
118.0873	117.079	-0.001	118.0863	316	76.1	Betaine
332.332	332.332	-0.0009	332.3312	97	42	Benzyl Tetradecyl Dimethylammonium Cation
332.332	332.332	-0.0009	332.3312	150	21.2	Benzyl Tetradecyl Dimethylammonium Cation
186.0588	370.196	0.0467	186.1055	65	100	Ser-His-Lys
284.3311	284.332	0	284.3312	25	100	Hexadecyltrimethylammonium Cation
284.3311	284.332	0	284.3312	202	84.5	Hexadecyltrimethylammonium Cation
284.3311	284.332	0	284.3312	160	73.4	Hexadecyltrimethylammonium Cation
284.3311	284.332	0	284.3312	163	78.8	Hexadecyltrimethylammonium Cation
118.0873	117.079	-0.001	118.0863	234	100	Betaine
118.0873	117.079	-0.001	118.0863	430	60.3	Betaine
118.0873	117.079	-0.001	118.0863	337	80.8	Betaine
118.0873	117.079	-0.001	118.0863	392	63.6	Betaine
546.3998	523.364	-0.047	546.353	115	100	PAF C-16
546.3998	523.364	-0.047	546.353	95	100	PAF C-16
118.0873	117.079	-0.001	118.0863	358	48	Betaine
118.0873	117.079	-0.001	118.0863	419	100	Betaine
118.0873	117.079	-0.001	118.0863	386	98.4	Betaine
118.0873	117.079	-0.001	118.0863	310	66.3	Betaine
284.3311	284.332	0	284.3312	160	77.5	Hexadecyltrimethylammonium Cation
186.0588	370.196	0.0467	186.1055	76	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	413	63.5	Betaine
118.0873	117.079	-0.001	118.0863	360	91.2	Betaine
118.0873	117.079	-0.001	118.0863	336	74.1	Betaine
140.0692	139.1	0.038	140.107	98	100	Tropinone
118.0873	117.079	-0.001	118.0863	421	62.4	Betaine
118.0873	117.079	-0.001	118.0863	320	63.9	Betaine
118.0873	117.079	-0.001	118.0863	282	64.4	Betaine
118.0873	117.079	-0.001	118.0863	286	41.8	Betaine
118.0873	117	0	118.09	431	31.7	Betaine
118.0873	117.079	-0.001	118.0863	287	70.3	Betaine
118.0873	117.079	-0.001	118.0863	383	75.4	Betaine
428.3751	427	0.03	428.41	233	51.5	N-Octanoylsphinganine,D-Erythro
186.0588	163.084	0.0149	186.0737	151	89.1	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	333	100	Betaine
118.0873	117.079	-0.001	118.0863	370	66.4	Betaine

118.0873	117.079	-0.001	118.0863	314	74.1	Betaine
118.0873	117.079	-0.001	118.0863	256	65.4	Betaine
186.0588	370.196	0.0467	186.1055	70	100	Ser-His-Lys
224.1293	446.228	-0.0081	224.1212	124	55.4	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	328	93.2	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	303	92.7	N-Acetyl-L-Tyrosine
195.1236	194.115	-0.0009	195.1227	248	100	Tetraethylene Glycol
118.0873	117.079	-0.001	118.0863	325	100	Betaine
118.0873	117.079	-0.001	118.0863	488	66.2	Betaine
118.0873	117.079	-0.001	118.0863	382	97.3	Betaine
118.0873	117.079	-0.001	118.0863	389	62.7	Betaine
360.3626	360.363	-0.0002	360.3625	283	40.4	Benzyl Hexadecyl Dimethylammonium Cation
360.3626	360.363	-0.0002	360.3625	299	41.1	Benzyl Hexadecyl Dimethylammonium Cation
360.3626	360.363	-0.0002	360.3625	350	87.6	Benzyl Hexadecyl Dimethylammonium Cation
360.3626	360.363	-0.0002	360.3625	309	72.3	Benzyl Hexadecyl Dimethylammonium Cation
97.0774	114.104	0.0238	97.1012	24	23.1	Cyclohexanol, 1-Methyl-
118.0873	117.079	-0.001	118.0863	256	55.8	Betaine
118.0873	117.079	-0.001	118.0863	381	45	Betaine
118.0873	117.079	-0.001	118.0863	304	76.5	Betaine
118.0873	117.079	-0.001	118.0863	276	61.5	Betaine
360.3626	360.363	-0.0002	360.3625	285	56.7	Benzyl Hexadecyl Dimethylammonium Cation
118.0873	117.079	-0.001	118.0863	424	59.2	Betaine
118.0873	117.079	-0.001	118.0863	261	65.9	Betaine
118.0873	117.079	-0.001	118.0863	398	41.3	Betaine
369.3861	386.355	-0.0345	369.3516	260	55.4	Cholesterol
97.0774	114.104	0.0238	97.1012	71	100	Cyclopentanemethanol, .Alpha.- Methyl-
186.0588	370.196	0.0467	186.1055	50	100	Ser-His-Lys
385.3803	384.339	-0.0338	385.3465	21	53.1	Cholesta-5,7-Dien-3-Ol, (3.Beta.)-
385.3803	384.339	-0.0338	385.3465	102	100	Cholecalciferol
385.3803	402.35	-0.0338	385.3465	3	100	25-Hydroxycholesterol
195.1236	194.115	-0.0009	195.1227	272	100	Tetraethylene Glycol
118.0873	117.079	-0.001	118.0863	225	100	Betaine
118.0873	117.079	-0.001	118.0863	424	44.4	Betaine
118.0873	117.079	-0.001	118.0863	299	68.2	Betaine
118.0873	117.079	-0.001	118.0863	340	60.9	Betaine
224.1293	223.084	-0.0376	224.0917	222	76.2	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	265	83.2	N-Acetyl-L-Tyrosine

224.1293	223.084	-0.0376	224.0917	251	89.1	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	353	32.5	Betaine
118.0873	117.079	-0.001	118.0863	474	67.4	Betaine
118.0873	117.079	-0.001	118.0863	276	81	Betaine
118.0873	117.079	-0.001	118.0863	409	61.5	Betaine
97.0774	114.104	0.0238	97.1012	34	22.5	Cyclohexanol, 1-Methyl-
186.0588	163.084	0.0149	186.0737	160	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	223.076	-0.0456	224.0837	47	100	Desmethyketamine
224.1293	223.084	-0.0376	224.0917	218	100	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	260	86.1	N-Acetyl-L-Tyrosine
400.3796	400.343	-0.0375	400.3421	191	27.7	Palmitoyl-L-Carnitine Cation
118.0873	117	0	118.09	319	25.8	Betaine
118.0873	117.079	-0.001	118.0863	417	43.4	Betaine
118.0873	117.079	-0.001	118.0863	346	84.3	Betaine
118.0873	117.079	-0.001	118.0863	269	72.2	Betaine
282.2797	281.272	-0.0006	282.2791	77	100	9-Octadecenamide, (Z)-
282.2797	281.272	-0.0006	282.2791	104	100	9-Octadecenamide, (Z)-
282.2797	281.272	-0.0006	282.2791	215	93.2	9-Octadecenamide, (Z)-
140.0692	139.027	-0.035	140.0342	100	100	3-Pyridinecarboxylic Acid, 1,6-Dihydro-6-Oxo-
186.0588	163.084	0.0149	186.0737	118	86.6	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	141	92	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	135	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	147	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	452	36.1	Betaine
118.0873	117	0	118.09	331	27.6	Betaine
118.0873	117.079	-0.001	118.0863	360	61.5	Betaine
186.0588	203.091	0.0285	186.0873	66	73.1	Ala-Asn
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
393.2988	392.293	0.0011	393.2999	89	100	Deoxycholic Acid
118.0873	117.079	-0.001	118.0863	264	33.9	Betaine
118.0873	117.079	-0.001	118.0863	427	65.1	Betaine
118.0873	117.079	-0.001	118.0863	295	49.6	Betaine
118.0873	117.079	-0.001	118.0863	413	59.4	Betaine
97.0774	114.104	0.0238	97.1012	26	45.3	Cyclohexanol, 2-Methyl-, Trans-
186.0588	370.196	0.0467	186.1055	60	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	180	100	N,N-Bis(2-Hydroxyethyl)Glycine
371.3164	370.308	-0.0009	371.3156	177	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	131	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	49	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester

371.3164	370.308	-0.0009	371.3156	170	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	329	60.7	Betaine
118.0873	117.079	-0.001	118.0863	419	47	Betaine
118.0873	117.079	-0.001	118.0863	339	98.2	Betaine
118.0873	117.079	-0.001	118.0863	341	59.5	Betaine
186.0588	163.084	0.0149	186.0737	192	92.6	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	146	93	N,N-Bis(2-Hydroxyethyl)Glycine
371.3164	370.308	-0.0009	371.3156	182	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	165	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	69	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	116	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	289	85.4	Betaine
118.0873	117.079	-0.001	118.0863	365	31.2	Betaine
118.0873	117.079	-0.001	118.0863	363	75.6	Betaine
118.0873	117.079	-0.001	118.0863	330	83	Betaine
118.0873	117.079	-0.001	118.0863	333	69.8	Betaine
118.0873	117.079	-0.001	118.0863	355	60.2	Betaine
118.0873	117.079	-0.001	118.0863	307	76.1	Betaine
118.0873	117.079	-0.001	118.0863	363	55.9	Betaine
97.0774	114.104	0.0238	97.1012	51	20	Cyclohexanol, 1-Methyl-
371.3164	370.308	-0.0009	371.3156	170	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	150	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	44	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	115	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
186.0588	163.084	0.0149	186.0737	98	57.3	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	203.091	0.0285	186.0873	49	68.7	Ala-Asn
186.0588	370.196	0.0467	186.1055	32	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	267	55.2	Betaine
118.0873	117.079	-0.001	118.0863	394	63.6	Betaine
118.0873	117.079	-0.001	118.0863	275	60.1	Betaine
118.0873	117.079	-0.001	118.0863	352	47	Betaine
186.0588	163.084	0.0149	186.0737	118	69.9	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	146	100	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105.079	-0.0009	106.0863	121	100	Diethanolamine
224.1293	223.106	-0.0164	224.1129	133	100	N-Acetyl-D-Galactosaminitol

224.1293	223.084	-0.0376	224.0917	189	70.6	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	284	89.6	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	263	86.8	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	406	71.7	Betaine
118.0873	117.079	-0.001	118.0863	289	56.5	Betaine
118.0873	117.079	-0.001	118.0863	377	61.8	Betaine
393.2988	392.293	0.0011	393.2999	78	100	Chenodeoxycholic Acid
371.3164	370.308	-0.0009	371.3156	207	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	174	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	66	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	117	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	444	60.1	Betaine
118.0873	117.079	-0.001	118.0863	308	69.2	Betaine
118.0873	117.079	-0.001	118.0863	364	41.6	Betaine
371.3164	370.308	-0.0009	371.3156	215	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	183	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	107	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	174	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
186.0588	163.084	0.0149	186.0737	145	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	256	39	Betaine
118.0873	117.079	-0.001	118.0863	387	31.2	Betaine
118.0873	117.079	-0.001	118.0863	251	65	Betaine
118.0873	117.079	-0.001	118.0863	242	66.5	Betaine
393.2988	392.293	0.0011	393.2999	45	100	Chenodeoxycholic Acid
393.2988	392.293	0.0011	393.2999	37	100	Chenodeoxycholic Acid
371.3164	370.308	-0.0009	371.3156	231	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	173	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	104	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	131	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
186.0588	163.084	0.0149	186.0737	145	100	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105	0	106.09	166	72.9	Diethanolamine
106.0872	105	0	106.09	161	81.4	Diethanolamine
118.0873	117.079	-0.001	118.0863	330	53.7	Betaine

118.0873	117.079	-0.001	118.0863	431	43.4	Betaine
118.0873	117.079	-0.001	118.0863	266	64.7	Betaine
118.0873	117.079	-0.001	118.0863	300	70.3	Betaine
371.3164	370.308	-0.0009	371.3156	219	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	136	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	138	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	123	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
140.0692	139.063	0.0014	140.0706	114	68.2	5-Amino-2-Methoxyphenol
118.0873	117.079	-0.001	118.0863	414	48.2	Betaine
118.0873	117.079	-0.001	118.0863	289	63.9	Betaine
118.0873	117.079	-0.001	118.0863	328	63	Betaine
371.3164	370.308	-0.0009	371.3156	243	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	177	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	85	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	105	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
140.0692	139.063	0.0014	140.0706	129	100	5-Amino-2-Methoxyphenol
118.0873	117.079	-0.001	118.0863	202	100	Betaine
118.0873	117.079	-0.001	118.0863	397	32.7	Betaine
118.0873	117.079	-0.001	118.0863	347	98.4	Betaine
118.0873	117	0	118.09	347	25.5	Betaine
371.3164	370.308	-0.0009	371.3156	243	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	144	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	109	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	97	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
97.0774	114.104	0.0238	97.1012	13	23.7	Cyclopentanemethanol, .Alpha.-Methyl-
118.0873	117.079	-0.001	118.0863	229	100	Betaine
118.0873	117.079	-0.001	118.0863	445	60.5	Betaine
118.0873	117.079	-0.001	118.0863	327	53.6	Betaine
118.0873	117.079	-0.001	118.0863	327	64	Betaine
186.0588	370.196	0.0467	186.1055	69	100	Ser-His-Lys
106.0872	105	0	106.09	189	80.2	Diethanolamine
118.0873	117.079	-0.001	118.0863	413	51.3	Betaine
118.0873	117.079	-0.001	118.0863	298	95.5	Betaine

118.0873	117.079	-0.001	118.0863	379	98.2	Betaine
371.3164	370.308	-0.0009	371.3156	226	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	188	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	106	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	152	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
106.0872	105	0	106.09	156	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	154	100	Diethanolamine
106.0872	105	0	106.09	225	53.4	Diethanolamine
118.0873	117.079	-0.001	118.0863	284	63.4	Betaine
118.0873	117.079	-0.001	118.0863	285	64.5	Betaine
118.0873	117	0	118.09	352	25.9	Betaine
371.3164	370.308	-0.0009	371.3156	196	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	155	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	141	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	145	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
106.0872	105	0	106.09	247	75.4	Diethanolamine
106.0872	105	0	106.09	196	79.6	Diethanolamine
393.2988	392.293	0.0011	393.2999	42	100	Chenodeoxycholic Acid
371.3164	370.308	-0.0009	371.3156	239	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	132	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	106	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	149	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
186.0588	370.196	0.0467	186.1055	58	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	154	100	N,N-Bis(2-Hydroxyethyl)Glycine
391.2862	390.277	-0.0019	391.2843	322	96.9	Diethyl Phthalate
391.2862	390.277	-0.0019	391.2843	230	55.9	Diethyl Phthalate
391.2862	390.277	-0.0019	391.2843	251	65.5	Diethyl Phthalate
391.2862	390.277	-0.0019	391.2843	229	53.6	Diethyl Phthalate
118.0873	117.079	-0.001	118.0863	398	56.6	Betaine
118.0873	117.079	-0.001	118.0863	340	83.5	Betaine
118.0873	117.079	-0.001	118.0863	339	42.9	Betaine
371.3164	370.308	-0.0009	371.3156	203	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	141	100	Hexanedioic Acid, Bis(2-

						Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	98	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	194	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
97.0774	114.104	0.0238	97.1012	44	23.5	Cyclohexanemethanol
106.0872	105	0	106.09	159	74.6	Diethanolamine
118.0873	117.079	-0.001	118.0863	374	47.5	Betaine
118.0873	117.079	-0.001	118.0863	241	86.4	Betaine
118.0873	117	0	118.09	347	22.7	Betaine
371.3164	370.308	-0.0009	371.3156	236	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	194	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	60	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	162	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
97.0774	114.104	0.0238	97.1012	12	53.1	Cyclohexanol, 2-Methyl-, Trans-
106.0872	105	0	106.09	159	75.6	Diethanolamine
106.0872	105	0	106.09	173	81.7	Diethanolamine
391.2862	390.277	-0.0019	391.2843	325	97.9	Diethyl Phthalate
391.2862	390.277	-0.0019	391.2843	245	95.4	Diethyl Phthalate
391.2862	390.277	-0.0019	391.2843	236	52.6	Diethyl Phthalate
391.2862	390.277	-0.0019	391.2843	190	55.2	Diethyl Phthalate
371.3164	370.308	-0.0009	371.3156	220	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	163	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	82	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	108	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	294	38.1	Betaine
118.0873	117	0	118.09	402	30.4	Betaine
118.0873	117.079	-0.001	118.0863	299	67.2	Betaine
118.0873	117.079	-0.001	118.0863	306	65.5	Betaine
106.0872	105	0	106.09	157	74.4	Diethanolamine
391.2862	390.277	-0.0019	391.2843	371	98.8	Diethyl Phthalate
391.2862	390.277	-0.0019	391.2843	244	52.5	Diethyl Phthalate
391.2862	390.277	-0.0019	391.2843	234	52	Diethyl Phthalate
391.2862	390.277	-0.0019	391.2843	202	54.8	Diethyl Phthalate
371.3164	370.308	-0.0009	371.3156	203	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	151	100	Hexanedioic Acid, Bis(2-

						Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	102	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	140	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	358	62.7	Betaine
118.0873	117.079	-0.001	118.0863	326	59.7	Betaine
118.0873	117.079	-0.001	118.0863	312	64.4	Betaine
391.2862	390.277	-0.0019	391.2843	347	98.5	Diocetyl Phthalate
391.2862	390.277	-0.0019	391.2843	221	95	Diocetyl Phthalate
391.2862	390.277	-0.0019	391.2843	196	55.1	Diocetyl Phthalate
391.2862	390.277	-0.0019	391.2843	238	53.9	Diocetyl Phthalate
371.3164	370.308	-0.0009	371.3156	213	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	163	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	152	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	151	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	358	61	Betaine
118.0873	117.079	-0.001	118.0863	304	67.6	Betaine
118.0873	117.079	-0.001	118.0863	287	63.7	Betaine
371.3164	370.308	-0.0009	371.3156	175	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	154	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	87	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	157	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	315	30.2	Betaine
118.0873	117.079	-0.001	118.0863	333	81.9	Betaine
118.0873	117.079	-0.001	118.0863	297	66.5	Betaine
97.0774	114.104	0.0238	97.1012	44	24	Cyclohexanol, 1-Methyl-
338.3423	337.334	-0.0005	338.3417	165	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	291	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	83	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	194	100	13-Docosenamide, (Z)-
371.3164	370.308	-0.0009	371.3156	195	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	161	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	105	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	183	100	Hexanedioic Acid, Bis(2-

						Ethylhexyl) Ester
419.3188	418.308	-0.0032	419.3156	158	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	202	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	208	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	209	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	160	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	204	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	209	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
371.3164	370.308	-0.0009	371.3156	218	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	153	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	93	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	84	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	286	42	Betaine
118.0873	117.079	-0.001	118.0863	319	63.4	Betaine
371.3164	370.308	-0.0009	371.3156	201	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	173	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	86	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	123	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	267	83.5	Betaine
118.0873	117.079	-0.001	118.0863	271	63.1	Betaine
118.0873	117.079	-0.001	118.0863	309	53.2	Betaine
97.0774	114.104	0.0238	97.1012	41	26.9	Cyclohexanol, 4-Methyl-, Trans-
419.3188	418.308	-0.0032	419.3156	181	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	204	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	206	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	206	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
118.0873	117.079	-0.001	118.0863	263	100	Betaine
118.0873	117.079	-0.001	118.0863	284	61.9	Betaine
97.0774	114.104	0.0238	97.1012	34	22.3	Cyclohexanol, 1-Methyl-

419.3188	418.308	-0.0032	419.3156	204	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	207	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	210	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	204	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
371.3239	370.308	-0.0083	371.3156	242	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3239	370.308	-0.0083	371.3156	148	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3239	370.308	-0.0083	371.3156	49	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3239	370.308	-0.0083	371.3156	169	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0941	117.079	-0.0078	118.0863	284	75.8	Betaine
118.0941	117.079	-0.0078	118.0863	383	53.6	Betaine
118.0941	117.079	-0.0078	118.0863	276	32.7	Betaine
118.0941	117.079	-0.0078	118.0863	309	44.9	Betaine
419.3188	418.308	-0.0032	419.3156	212	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	203	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	207	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	198	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
371.3164	370.308	-0.0009	371.3156	175	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	143	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	71	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	180	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	313	56.3	Betaine
118.0873	117.079	-0.001	118.0863	256	100	Betaine
118.0873	117.079	-0.001	118.0863	329	40.6	Betaine
118.0873	117.079	-0.001	118.0863	308	58.8	Betaine
118.0873	117.079	-0.001	118.0863	282	64.4	Betaine
118.0873	117.079	-0.001	118.0863	291	28.2	Betaine
371.3164	370.308	-0.0009	371.3156	174	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	128	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	103	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester

371.3164	370.308	-0.0009	371.3156	177	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
393.2988	392.293	0.0011	393.2999	45	100	Chenodeoxycholic Acid
419.3188	418.308	-0.0032	419.3156	210	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	203	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	211	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	196	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
118.0873	117.079	-0.001	118.0863	146	100	N-Methyl-.Alpha.-Aminoisobutyric Acid
118.0873	117.079	-0.001	118.0863	369	66.2	Betaine
118.0873	117.079	-0.001	118.0863	277	60.2	Betaine
118.0873	117.079	-0.001	118.0863	339	36.6	Betaine
106.0872	105	0	106.09	152	77.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	115	100	Diethanolamine
393.2988	392.293	0.0011	393.2999	36	100	Chenodeoxycholic Acid
419.3188	418.308	-0.0032	419.3156	204	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	208	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	202	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
419.3188	418.308	-0.0032	419.3156	206	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
371.3164	370.308	-0.0009	371.3156	195	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	138	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.3164	370.308	-0.0009	371.3156	115	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
393.2988	392.293	0.0011	393.2999	33	100	Chenodeoxycholic Acid
84.0822	102.092	-0.0014	84.0808	226	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	177	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	138	51	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	311	49.1	Betaine
118.0873	117.079	-0.001	118.0863	331	70.8	Betaine
118.0873	117.079	-0.001	118.0863	310	40.7	Betaine
106.0872	105	0	106.09	168	73.3	Diethanolamine
106.0872	105	0	106.09	150	78.2	Diethanolamine
106.0872	105	0	106.09	227	66	Diethanolamine
419.3188	418.308	-0.0032	419.3156	205	100	1,2-Benzenedicarboxylic Acid, Dinonyl Ester
118.0873	117.079	-0.001	118.0863	347	39.5	Betaine

118.0873	117.079	-0.001	118.0863	299	72.7	Betaine
118.0873	117.079	-0.001	118.0863	344	53.2	Betaine
106.0872	105	0	106.09	114	53.1	Diethanolamine
106.0872	105	0	106.09	210	68.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	253	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	211	50	Betaine Aldehyde Cation
186.0588	203.091	0.0285	186.0873	71	75.3	Ala-Asn
186.0588	163.084	0.0149	186.0737	146	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	395	37.1	Betaine
118.0873	117.079	-0.001	118.0863	301	67.1	Betaine
118.0873	117.079	-0.001	118.0863	354	48.8	Betaine
106.0872	105	0	106.09	159	78.9	Diethanolamine
106.0872	105	0	106.09	231	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	152	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	261	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	206	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	181	52	Betaine Aldehyde Cation
106.0872	105.079	-0.0009	106.0863	126	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	178	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	202	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	138	51	Betaine Aldehyde Cation
553.3927	530.4	-0.003	553.3897	1	17.2	Didodecyl 3,3'-Thiodipropionate Oxide
553.3927	530.4	-0.003	553.3897	4	7.7	Didodecyl 3,3'-Thiodipropionate Oxide
553.3927	530.4	-0.003	553.3897	10	8.5	Didodecyl 3,3'-Thiodipropionate Oxide
118.0873	117.079	-0.001	118.0863	336	55.2	Betaine
118.0873	117.079	-0.001	118.0863	269	62.3	Betaine
118.0873	117	0	118.09	343	24.5	Betaine
553.3927	530.4	-0.003	553.3897	88	14.4	Didodecyl 3,3'-Thiodipropionate Oxide
531.4089	530.4	-0.0011	531.4078	242	19.9	Didodecyl 3,3'-Thiodipropionate Oxide
531.4089	530.4	-0.0011	531.4078	318	17.5	Didodecyl 3,3'-Thiodipropionate Oxide
531.4089	530.4	-0.0011	531.4078	197	14	Didodecyl 3,3'-Thiodipropionate Oxide
531.4089	530.4	-0.0011	531.4078	297	35.6	Didodecyl 3,3'-Thiodipropionate Oxide
118.0873	117.079	-0.001	118.0863	366	24	Betaine
118.0873	117.079	-0.001	118.0863	278	62.9	Betaine
118.0873	117.079	-0.001	118.0863	337	42.2	Betaine
553.3927	530.4	-0.003	553.3897	3	21.3	Didodecyl 3,3'-Thiodipropionate

						Oxide
553.3927	530.4	-0.003	553.3897	38	10.8	Didodecyl 3,3'-Thiodipropionate Oxide
553.3927	530.4	-0.003	553.3897	78	14.4	Didodecyl 3,3'-Thiodipropionate Oxide
97.0774	114.104	0.0238	97.1012	28	35.8	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	29	21.7	Cyclohexanemethanol
531.4089	530.4	-0.0011	531.4078	358	19.2	Didodecyl 3,3'-Thiodipropionate Oxide
531.4089	530.4	-0.0011	531.4078	367	23.2	Didodecyl 3,3'-Thiodipropionate Oxide
531.4089	530.4	-0.0011	531.4078	241	28.3	Didodecyl 3,3'-Thiodipropionate Oxide
531.4089	530.4	-0.0011	531.4078	259	28.1	Didodecyl 3,3'-Thiodipropionate Oxide
106.0872	105	0	106.09	149	77.9	Diethanolamine
553.3927	530.4	-0.003	553.3897	14	15.3	Didodecyl 3,3'-Thiodipropionate Oxide
553.3927	530.4	-0.003	553.3897	6	8.3	Didodecyl 3,3'-Thiodipropionate Oxide
553.3927	530.4	-0.003	553.3897	1	20.6	Didodecyl 3,3'-Thiodipropionate Oxide
118.0873	117.079	-0.001	118.0863	177	100	Betaine
118.0873	117.079	-0.001	118.0863	381	62.8	Betaine
118.0873	117.079	-0.001	118.0863	321	98.8	Betaine
118.0873	117.079	-0.001	118.0863	343	37.3	Betaine
531.4089	530.4	-0.0011	531.4078	317	30.4	Didodecyl 3,3'-Thiodipropionate Oxide
531.4089	530.4	-0.0011	531.4078	269	13.2	Didodecyl 3,3'-Thiodipropionate Oxide
531.4089	530.4	-0.0011	531.4078	227	23.9	Didodecyl 3,3'-Thiodipropionate Oxide
531.4089	530.4	-0.0011	531.4078	218	15.9	Didodecyl 3,3'-Thiodipropionate Oxide
97.0774	114.104	0.0238	97.1012	71	25.7	Cyclohexanol, 1-Methyl-
84.0822	102.092	-0.0014	84.0808	244	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	210	51	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	137	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	154	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	340	32.5	Betaine
118.0873	117.079	-0.001	118.0863	330	39.3	Betaine
118.0873	117.079	-0.001	118.0863	323	56.6	Betaine
97.0774	114.104	0.0238	97.1012	43	26.6	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	152	74.8	Diethanolamine
553.3927	530.4	-0.003	553.3897	12	9	Didodecyl 3,3'-Thiodipropionate Oxide

118.0873	117.079	-0.001	118.0863	378	49.4	Betaine
118.0873	117.079	-0.001	118.0863	321	61.3	Betaine
118.0873	117.079	-0.001	118.0863	304	70.8	Betaine
97.0774	114.104	0.0238	97.1012	51	23.9	Cyclohexanemethanol
106.0872	105	0	106.09	144	74.9	Diethanolamine
106.0872	105	0	106.09	197	74.9	Diethanolamine
553.3927	530.4	-0.003	553.3897	70	13.7	Didodecyl 3,3'-Thiodipropionate Oxide
553.3927	530.4	-0.003	553.3897	57	15.6	Didodecyl 3,3'-Thiodipropionate Oxide
118.0873	117.079	-0.001	118.0863	365	35.7	Betaine
118.0873	117.079	-0.001	118.0863	374	49.7	Betaine
118.0873	117.079	-0.001	118.0863	351	55.1	Betaine
106.0872	105	0	106.09	157	77.6	Diethanolamine
118.0873	117.079	-0.001	118.0863	263	79.3	Betaine
118.0873	117.079	-0.001	118.0863	357	92.1	Betaine
118.0873	117.079	-0.001	118.0863	285	63	Betaine
118.0873	117.079	-0.001	118.0863	342	35.6	Betaine
97.0774	114.104	0.0238	97.1012	87	21.1	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	165	74.5	Diethanolamine
106.0872	105	0	106.09	151	78.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	207	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	183	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	147	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	186	95.3	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	341	34.4	Betaine
118.0873	117.079	-0.001	118.0863	282	61.1	Betaine
118.0873	117.079	-0.001	118.0863	281	66	Betaine
106.0872	105	0	106.09	155	75.8	Diethanolamine
106.0872	105	0	106.09	153	80.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	294	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	218	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	129	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	149	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	70	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	166	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	389	37.7	Betaine
118.0873	117.079	-0.001	118.0863	248	49.5	Betaine
118.0873	117.079	-0.001	118.0863	312	40.1	Betaine
97.0774	114.104	0.0238	97.1012	6	100	Cyclopentanemethanol, .Alpha.-Methyl-
106.0872	105	0	106.09	154	74.9	Diethanolamine

106.0872	105	0	106.09	155	78.6	Diethanolamine
610.5771	610	-0.04	610.54	125	50	DG 34:2; [M+NH4]+; DG(14:1/20:1/0:0)
610.5771	610	-0.04	610.54	120	50	DG 34:2; [M+NH4]+; DG(14:1/20:1/0:0)
610.5771	610	-0.04	610.54	81	50	DG 34:2; [M+NH4]+; DG(14:1/20:1/0:0)
640.5867	640	0	640.59	139	50	DG 36:1; [M+NH4]+; DG(14:1/22:0/0:0)
640.5867	640	0	640.59	128	50	DG 36:1; [M+NH4]+; DG(14:1/22:0/0:0)
640.5867	640	0	640.59	126	50	DG 36:1; [M+NH4]+; DG(14:1/22:0/0:0)
84.0822	102.092	-0.0014	84.0808	233	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	193	50	Betaine Aldehyde Cation
186.0588	203.091	0.0285	186.0873	82	82.7	Ala-Asn
186.0588	163.084	0.0149	186.0737	158	92.5	N,N-Bis(2-Hydroxyethyl)Glycine
640.5867	640	0	640.59	153	50	DG 36:1; [M+NH4]+; DG(14:1/22:0/0:0)
640.5867	640	0	640.59	154	50	DG 36:1; [M+NH4]+; DG(14:1/22:0/0:0)
118.0873	117.079	-0.001	118.0863	380	65.3	Betaine
118.0873	117.079	-0.001	118.0863	308	76.2	Betaine
118.0873	117.079	-0.001	118.0863	311	63.4	Betaine
610.5771	610	-0.04	610.54	156	50	DG 34:2; [M+NH4]+; DG(14:1/20:1/0:0)
636.5935	636	-0.03	636.56	155	50	DG 36:3; [M+NH4]+; DG(14:1/22:2/0:0)
636.5935	636	-0.03	636.56	155	50	DG 36:3; [M+NH4]+; DG(14:1/22:2/0:0)
636.5935	636	-0.03	636.56	153	50	DG 36:3; [M+NH4]+; DG(14:1/22:2/0:0)
97.0774	114.104	0.0238	97.1012	45	25.8	Cyclohexanol, 1-Methyl-
118.0873	117.079	-0.001	118.0863	330	89.7	Betaine
118.0873	117.079	-0.001	118.0863	415	47	Betaine
118.0873	117.079	-0.001	118.0863	325	78.9	Betaine
118.0873	117.079	-0.001	118.0863	449	57.4	Betaine
97.0774	114.104	0.0238	97.1012	33	26.6	Cyclohexanemethanol
106.0872	105	0	106.09	158	75.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	258	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	206	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	182	56	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	298	40.2	Betaine
118.0873	117.079	-0.001	118.0863	281	58	Betaine
118.0873	117.079	-0.001	118.0863	355	40.5	Betaine

106.0872	105	0	106.09	157	74.9	Diethanolamine
106.0872	105	0	106.09	159	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	150	100	Diethanolamine
666.6035	666	0	666.6	158	50	DG 38:2; [M+NH4] ⁺ ; DG(14:1/24:1/0:0)
666.6035	666	0	666.6	151	50	DG 38:2; [M+NH4] ⁺ ; DG(14:1/24:1/0:0)
186.0588	163.084	0.0149	186.0737	132	87.8	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	167	100	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105	0	106.09	156	79.6	Diethanolamine
106.0872	105	0	106.09	183	73.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	258	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	256	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	141	53.1	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	234	100	Betaine
118.0873	117.079	-0.001	118.0863	381	47.3	Betaine
118.0873	117.079	-0.001	118.0863	321	98.8	Betaine
118.0873	117.079	-0.001	118.0863	339	58.7	Betaine
97.0774	114.104	0.0238	97.1012	39	24.1	Cyclohexanol, 4-Methyl-, Trans-
186.0588	370.196	0.0467	186.1055	62	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	44	100	Ser-His-Lys
624.5931	624	-0.03	624.56	160	50	DG 35:2; [M+NH4] ⁺ ; DG(15:1/20:1/0:0)
118.0873	117.079	-0.001	118.0863	378	45.4	Betaine
118.0873	117.079	-0.001	118.0863	296	65.5	Betaine
118.0873	117.079	-0.001	118.0863	332	41.1	Betaine
106.0872	105	0	106.09	174	75	Diethanolamine
106.0872	105	0	106.09	159	75.2	Diethanolamine
118.0873	117.079	-0.001	118.0863	333	64.5	Betaine
118.0873	117.079	-0.001	118.0863	381	26.9	Betaine
118.0873	117.079	-0.001	118.0863	283	62.8	Betaine
118.0873	117.079	-0.001	118.0863	330	45.2	Betaine
106.0872	105	0	106.09	167	77.3	Diethanolamine
106.0872	105	0	106.09	158	80.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	274	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	216	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	162	52	Betaine Aldehyde Cation
106.0872	105.079	-0.0009	106.0863	113	100	Diethanolamine
186.0588	370.196	0.0467	186.1055	46	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	60	61.5	Ser-His-Lys
84.0822	102.092	-0.0014	84.0808	257	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	204	52	Betaine Aldehyde Cation

118.0873	117.079	-0.001	118.0863	295	48.9	Betaine
118.0873	117.079	-0.001	118.0863	417	63.4	Betaine
118.0873	117.079	-0.001	118.0863	254	100	Betaine
118.0873	117.079	-0.001	118.0863	325	37.9	Betaine
84.0822	102.092	-0.0014	84.0808	223	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	201	51	Betaine Aldehyde Cation
186.0588	203.091	0.0285	186.0873	62	100	Ala-Asn
186.0588	163.084	0.0149	186.0737	139	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	137	88.8	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	383	35.5	Betaine
118.0873	117.079	-0.001	118.0863	251	56.8	Betaine
118.0873	117.079	-0.001	118.0863	279	61.9	Betaine
97.0774	114.104	0.0238	97.1012	36	24.5	Cyclohexanol, 1-Methyl-
638.6087	638	-0.04	638.57	141	29.6	DG 36:2; [M+NH4]+; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	129	31.7	DG 36:2; [M+NH4]+; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	140	28	DG 36:2; [M+NH4]+; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	128	28	DG 36:2; [M+NH4]+; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	160	50	DG 36:2; [M+NH4]+; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	151	25.5	DG 36:2; [M+NH4]+; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	147	29.3	DG 36:2; [M+NH4]+; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	139	26	DG 36:2; [M+NH4]+; DG(16:1/20:1/0:0)
668.6187	668	0	668.62	152	31.7	DG 38:1; [M+NH4]+; DG(14:1/24:0/0:0)
668.6187	668	0	668.62	141	32.3	DG 38:1; [M+NH4]+; DG(16:1/22:0/0:0)
118.0873	117.079	-0.001	118.0863	308	70.7	Betaine
118.0873	117.079	-0.001	118.0863	316	61.7	Betaine
118.0873	117.079	-0.001	118.0863	329	78	Betaine
118.0873	117.079	-0.001	118.0863	327	63.5	Betaine
97.0774	114.104	0.0238	97.1012	27	23.1	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	156	80.7	Diethanolamine
106.0872	105	0	106.09	168	75.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	100	Diethanolamine
638.6087	638	-0.04	638.57	157	38.5	DG 36:2; [M+NH4]+; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	157	26	DG 36:2; [M+NH4]+; DG(16:1/20:1/0:0)

668.6187	668	0	668.62	151	31.7	DG 38:1; [M+NH4] ⁺ ; DG(14:1/24:0/0:0)
668.6187	668	0	668.62	149	35.1	DG 38:1; [M+NH4] ⁺ ; DG(16:1/22:0/0:0)
668.6187	668	0	668.62	137	39	DG 38:1; [M+NH4] ⁺ ; DG(14:1/24:0/0:0)
664.6234	664	-0.03	664.59	142	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	157	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	150	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
106.0872	105	0	106.09	169	80.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	236	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	223	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	117	54.2	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	181	88.4	N,N-Bis(2-Hydroxyethyl)Glycine
664.6234	664	-0.03	664.59	157	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	158	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
118.0873	117.079	-0.001	118.0863	298	82.7	Betaine
118.0873	117.079	-0.001	118.0863	449	99	Betaine
118.0873	117.079	-0.001	118.0863	313	71.5	Betaine
118.0873	117.079	-0.001	118.0863	378	47.3	Betaine
668.6187	668	0	668.62	215	50	DG 38:1; [M+NH4] ⁺ ; DG(16:1/22:0/0:0)
106.0872	105	0	106.09	190	77.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	175	100	Diethanolamine
118.0873	117.079	-0.001	118.0863	384	47.4	Betaine
118.0873	117.079	-0.001	118.0863	293	70.9	Betaine
118.0873	117.079	-0.001	118.0863	346	60.1	Betaine
97.0774	114.104	0.0238	97.1012	26	25.6	Cyclohexanemethanol
664.6234	664	-0.03	664.59	151	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	160	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	153	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
84.0822	102.092	-0.0014	84.0808	242	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	163	50	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	53	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-Hydroxyethyl)Glycine

118.0873	117.079	-0.001	118.0863	287	42.6	Betaine
118.0873	117.079	-0.001	118.0863	318	96.9	Betaine
118.0873	117.079	-0.001	118.0863	323	75.6	Betaine
97.0774	114.104	0.0238	97.1012	37	22.4	Cyclohexanemethanol
694.6329	694	0	694.63	160	50	DG 40:2; [M+NH4] ⁺ ; DG(16:1/24:1/0:0)
694.6329	694	0	694.63	160	50	DG 40:2; [M+NH4] ⁺ ; DG(16:1/24:1/0:0)
694.6329	694	0	694.63	159	50	DG 40:2; [M+NH4] ⁺ ; DG(16:1/24:1/0:0)
118.0873	117.079	-0.001	118.0863	319	42.8	Betaine
118.0873	117.079	-0.001	118.0863	331	93.5	Betaine
118.0873	117.079	-0.001	118.0863	300	68	Betaine
84.0822	102.092	-0.0014	84.0808	259	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	185	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	146	51	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	330	40.2	Betaine
118.0873	117.079	-0.001	118.0863	291	64.3	Betaine
118.0873	117.079	-0.001	118.0863	342	33.8	Betaine
186.0588	163.084	0.0149	186.0737	154	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	287	100	Betaine
118.0873	117.079	-0.001	118.0863	349	56.4	Betaine
118.0873	117.079	-0.001	118.0863	295	32.7	Betaine
118.0873	117.079	-0.001	118.0863	347	55	Betaine
106.0872	105	0	106.09	175	70.4	Diethanolamine
106.0872	105	0	106.09	154	73.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	239	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	178	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	171	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	144	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	116	50	Betaine Aldehyde Cation
148.0974	147	-0.04	148.06	57	52	O-Acetyl-L-Serine Hydrochloride
118.0873	117.079	-0.001	118.0863	318	30.8	Betaine
118.0873	117.079	-0.001	118.0863	321	32.8	Betaine
118.0873	117.079	-0.001	118.0863	308	60.2	Betaine
106.0872	105	0	106.09	172	69.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	138	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	279	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	210	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	127	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	79	73.2	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	129	92.4	N,N-Bis(2-Hydroxyethyl)Glycine

666.6406	666	-0.04	666.6	160	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	108	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	60	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	54	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
118.0873	117.079	-0.001	118.0863	256	75.4	Betaine
118.0873	117.079	-0.001	118.0863	433	43	Betaine
118.0873	117.079	-0.001	118.0863	290	63.6	Betaine
118.0873	117.079	-0.001	118.0863	399	54.5	Betaine
97.0774	114.104	0.0238	97.1012	34	27.9	Cyclohexanol, 4-Methyl-, Trans-
696.651	696	0	696.65	197	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	122	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	56	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	68	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
106.0872	105	0	106.09	154	83.5	Diethanolamine
666.6406	666	-0.04	666.6	156	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	112	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	111	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
696.651	696	0	696.65	159	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	127	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	89	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	71	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
118.0873	117.079	-0.001	118.0863	286	69.9	Betaine
118.0873	117.079	-0.001	118.0863	389	35.9	Betaine
118.0873	117.079	-0.001	118.0863	307	71.1	Betaine
118.0873	117	0	118.09	358	26.9	Betaine
97.0774	114.104	0.0238	97.1012	48	25.2	Cyclohexanemethanol
106.0872	105	0	106.09	228	77.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	100	Diethanolamine
696.651	696	0	696.65	159	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	159	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)

666.6406	666	-0.04	666.6	160	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
84.0822	102.092	-0.0014	84.0808	263	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	228	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	138	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	157	93.2	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	135	83.6	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	324	100	Betaine
118.0873	117	0	118.09	367	25.1	Betaine
118.0873	117.079	-0.001	118.0863	268	95.4	Betaine
118.0873	117.079	-0.001	118.0863	326	42.2	Betaine
97.0774	114.104	0.0238	97.1012	51	24.3	Cyclohexanol, 1-Methyl-
97.0774	114.104	0.0238	97.1012	37	24	Cyclohexanemethanol
106.0872	105	0	106.09	216	78.2	Diethanolamine
106.0872	105	0	106.09	159	79.3	Diethanolamine
118.0873	117.079	-0.001	118.0863	313	100	Betaine
118.0873	117.079	-0.001	118.0863	309	68.5	Betaine
118.0873	117.079	-0.001	118.0863	319	27.9	Betaine
97.0774	114.104	0.0238	97.1012	16	100	Cyclopentanemethanol, .Alpha.- Methyl-
97.0774	114.104	0.0238	97.1012	26	32.8	Cyclohexanemethanol
106.0872	105	0	106.09	152	80.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	303	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	241	50	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	307	59.5	Betaine
118.0873	117.079	-0.001	118.0863	306	68.6	Betaine
118.0873	117.079	-0.001	118.0863	353	43.5	Betaine
97.0774	114.104	0.0238	97.1012	44	23.5	Cyclohexanemethanol
106.0872	105	0	106.09	147	77.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	251	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	231	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	137	53.1	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	47	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	162	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	410	36.6	Betaine
118.0873	117.079	-0.001	118.0863	297	67	Betaine
118.0873	117.079	-0.001	118.0863	322	53.6	Betaine
97.0774	114.104	0.0238	97.1012	24	24.4	Cyclohexanemethanol
106.0872	105	0	106.09	159	75.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	191	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	260	51	Betaine Aldehyde Cation

84.0822	102.092	-0.0014	84.0808	198	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	151	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	151	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	360	25	Betaine
118.0873	117.079	-0.001	118.0863	302	67.7	Betaine
118.0873	117.079	-0.001	118.0863	289	64.6	Betaine
97.0774	114.104	0.0238	97.1012	29	20.9	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	148	80.2	Diethanolamine
186.0588	163.084	0.0149	186.0737	135	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	333	55	Betaine
118.0873	117.079	-0.001	118.0863	278	63	Betaine
118.0873	117.079	-0.001	118.0863	334	48.2	Betaine
97.0774	114.104	0.0238	97.1012	37	23.9	Cyclohexanemethanol
106.0872	105	0	106.09	196	69.9	Diethanolamine
106.0872	105	0	106.09	159	75.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	271	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	233	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	117	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	220	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	180	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	140	54.2	Betaine Aldehyde Cation
148.0974	147	-0.04	148.06	57	62.3	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	115	100	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	162	71.2	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	344	49.3	Betaine
118.0873	117.079	-0.001	118.0863	338	96.4	Betaine
118.0873	117.079	-0.001	118.0863	349	35.7	Betaine
97.0774	114.104	0.0238	97.1012	25	33.9	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	154	80.7	Diethanolamine
106.0872	105	0	106.09	155	78	Diethanolamine
186.0588	163.084	0.0149	186.0737	143	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	58	100	Ser-His-Lys
84.0822	102.092	-0.0014	84.0808	291	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	260	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	185	53.1	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	344	48.3	Betaine
118.0873	117.079	-0.001	118.0863	307	72	Betaine
118.0873	117.079	-0.001	118.0863	338	69.2	Betaine
106.0872	105	0	106.09	151	75.5	Diethanolamine

106.0872	105	0	106.09	145	70.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	275	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	212	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	156	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	139	51	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	196	94.9	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	116	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	323	34	Betaine
118.0873	117.079	-0.001	118.0863	280	62.3	Betaine
118.0873	117.079	-0.001	118.0863	367	35.9	Betaine
97.0774	114.104	0.0238	97.1012	30	24.4	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	153	75.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	286	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	238	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	164	54.2	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	293	32.4	Betaine
118.0873	117.079	-0.001	118.0863	327	39.4	Betaine
118.0873	117.079	-0.001	118.0863	362	44.4	Betaine
186.0588	203.091	0.0285	186.0873	65	71.9	Ala-Asn
186.0588	163.084	0.0149	186.0737	144	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	65	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	343	53.4	Betaine
118.0873	117.079	-0.001	118.0863	309	70.6	Betaine
118.0873	117.079	-0.001	118.0863	299	66.6	Betaine
97.0774	114.104	0.0238	97.1012	30	24.2	Cyclohexanol, 1-Methyl-
97.0774	114.104	0.0238	97.1012	46	23.4	Cyclohexanol, 4-Methyl-, Trans-
106.0872	105	0	106.09	165	71.4	Diethanolamine
106.0872	105	0	106.09	190	57.5	Diethanolamine
84.0822	102.092	-0.0014	84.0808	250	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	231	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	104	51	Betaine Aldehyde Cation
186.0588	203.091	0.0285	186.0873	36	100	Ala-Asn
118.0873	117.079	-0.001	118.0863	372	44.3	Betaine
118.0873	117.079	-0.001	118.0863	267	58.4	Betaine
118.0873	117.079	-0.001	118.0863	260	92.5	Betaine
106.0872	105	0	106.09	157	73.2	Diethanolamine
106.0872	105	0	106.09	155	79.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	262	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	233	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	188	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	139	77.2	N,N-Bis(2-Hydroxyethyl)Glycine

186.0588	163.084	0.0149	186.0737	137	86.6	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	151	92.7	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	345	31.4	Betaine
118.0873	117.079	-0.001	118.0863	309	98.8	Betaine
118.0873	117.079	-0.001	118.0863	351	98.7	Betaine
97.0774	114.104	0.0238	97.1012	16	39.8	Cyclohexanol, 4-Methyl-, Trans-
106.0872	105	0	106.09	154	77.7	Diethanolamine
106.0872	105	0	106.09	220	72.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	249	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	262	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	174	51	Betaine Aldehyde Cation
97.0774	114.104	0.0238	97.1012	29	22.4	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	157	75	Diethanolamine
84.0822	102.092	-0.0014	84.0808	267	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	233	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	137	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	155	54.2	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	170	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	155	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	59	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	331	96.2	Betaine
118.0873	117.079	-0.001	118.0863	290	65.8	Betaine
118.0873	117.079	-0.001	118.0863	352	54	Betaine
97.0774	114.104	0.0238	97.1012	82	19.4	Cyclohexanol, 2-Methyl-, Trans-
106.0872	105	0	106.09	159	77.1	Diethanolamine
106.0872	105	0	106.09	154	80.2	Diethanolamine
106.0872	105	0	106.09	159	76.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	298	56.6	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	245	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	236	52	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	383	45.4	Betaine
118.0873	117.079	-0.001	118.0863	335	58.5	Betaine
118.0873	117.079	-0.001	118.0863	354	35.4	Betaine
97.0774	114.104	0.0238	97.1012	30	23.8	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	156	79.6	Diethanolamine
106.0872	105	0	106.09	159	75	Diethanolamine
106.0872	105	0	106.09	155	79.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	275	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	253	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	143	51	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	117	100	N,N-Bis(2-Hydroxyethyl)Glycine

186.0588	163.084	0.0149	186.0737	148	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	151	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	317	32.4	Betaine
118.0873	117.079	-0.001	118.0863	282	61.1	Betaine
118.0873	117.079	-0.001	118.0863	344	59.6	Betaine
106.0872	105	0	106.09	158	78.6	Diethanolamine
106.0872	105	0	106.09	157	75.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	115	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	281	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	211	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	145	51	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	43	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
106.0872	105	0	106.09	159	79.6	Diethanolamine
106.0872	105	0	106.09	135	76.6	Diethanolamine
148.0974	147.053	-0.037	148.0604	93	56.5	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	141	100	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	384	97.4	Betaine
118.0873	117.079	-0.001	118.0863	281	61.2	Betaine
118.0873	117.079	-0.001	118.0863	294	41	Betaine
97.0774	114.104	0.0238	97.1012	36	20.9	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	159	75.5	Diethanolamine
106.0872	105	0	106.09	149	77.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	281	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	247	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	182	55.4	Betaine Aldehyde Cation
186.0588	203.091	0.0285	186.0873	99	74	Ala-Asn
186.0588	163.084	0.0149	186.0737	114	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	272	84	Betaine
118.0873	117.079	-0.001	118.0863	379	47.2	Betaine
118.0873	117.079	-0.001	118.0863	343	96	Betaine
118.0873	117.079	-0.001	118.0863	363	53.1	Betaine
97.0774	114.104	0.0238	97.1012	43	25.5	Cyclohexanemethanol
106.0872	105	0	106.09	152	77.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	288	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	232	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	125	54.2	Betaine Aldehyde Cation
106.0872	105	0	106.09	145	78.6	Diethanolamine
106.0872	105	0	106.09	161	79.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	259	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	207	53.1	Betaine Aldehyde Cation

84.0822	102.092	-0.0014	84.0808	161	54.2	Betaine Aldehyde Cation
186.0588	203.091	0.0285	186.0873	50	68.7	Ala-Asn
186.0588	163.084	0.0149	186.0737	123	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	360	59.5	Betaine
118.0873	117.079	-0.001	118.0863	297	64.4	Betaine
118.0873	117.079	-0.001	118.0863	380	48.9	Betaine
148.0974	147	-0.04	148.06	35	35.1	N-Acetyl-DL-Serine
148.0974	147	-0.04	148.06	36	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	171	100	O-Acetyl-L-Serine
393.2988	392.293	0.0011	393.2999	41	100	Chenodeoxycholic Acid
371.2972	370.308	0.0184	371.3156	227	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2972	370.308	0.0184	371.3156	123	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2972	370.308	0.0184	371.3156	67	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2972	370.308	0.0184	371.3156	104	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	372	54.7	Betaine
118.0873	117.079	-0.001	118.0863	339	39.5	Betaine
118.0873	117.079	-0.001	118.0863	354	57	Betaine
97.0774	114.104	0.0238	97.1012	37	24.1	Cyclohexanol, 1-Methyl-
106.0872	105.079	-0.0009	106.0863	120	100	Diethanolamine
106.0872	105	0	106.09	159	78.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	275	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	218	50	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	138	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	369	33.3	Betaine
118.0873	117.079	-0.001	118.0863	278	59.7	Betaine
118.0873	117.079	-0.001	118.0863	280	60.4	Betaine
97.0774	114.104	0.0238	97.1012	39	24.7	Cyclohexanol, 4-Methyl-, Trans-
106.0872	105.079	-0.0009	106.0863	124	100	Diethanolamine
106.0872	105	0	106.09	159	75.5	Diethanolamine
106.0872	105	0	106.09	153	80.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	257	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	228	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	145	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	156	53.1	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	61	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	164	92.8	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105	0	106.09	155	78.9	Diethanolamine
106.0872	105	0	106.09	157	67.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	267	53.1	Betaine Aldehyde Cation

84.0822	102.092	-0.0014	84.0808	186	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	172	51	Betaine Aldehyde Cation
148.0974	147.053	-0.037	148.0604	22	31.5	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	412	36.3	Betaine
118.0873	117.079	-0.001	118.0863	295	22.8	Betaine
118.0873	117.079	-0.001	118.0863	334	64.1	Betaine
148.0974	147.053	-0.037	148.0604	172	47	O-Acetyl-L-Serine
393.2988	392.293	0.0011	393.2999	16	100	Chenodeoxycholic Acid
371.2972	370.308	0.0184	371.3156	205	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2972	370.308	0.0184	371.3156	103	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2972	370.308	0.0184	371.3156	81	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2972	370.308	0.0184	371.3156	114	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	369	67.7	Betaine
118.0873	117.079	-0.001	118.0863	283	62.4	Betaine
118.0873	117.079	-0.001	118.0863	347	61.1	Betaine
106.0872	105	0	106.09	158	75.7	Diethanolamine
106.0872	105	0	106.09	152	74.2	Diethanolamine
106.0872	105	0	106.09	268	77.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	292	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	260	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	203	56	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	158	93.4	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	145	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	333	36.4	Betaine
118.0873	117.079	-0.001	118.0863	333	37.8	Betaine
118.0873	117.079	-0.001	118.0863	380	52.3	Betaine
97.0774	114.104	0.0238	97.1012	27	23.1	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	219	78.6	Diethanolamine
106.0872	105	0	106.09	181	64.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	255	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	228	56	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	160	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	113	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105	0	106.09	158	77.9	Diethanolamine
106.0872	105	0	106.09	159	72.3	Diethanolamine
106.0872	105	0	106.09	144	78.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	262	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	198	53.1	Betaine Aldehyde Cation

84.0822	102.092	-0.0014	84.0808	161	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	180	52	Betaine Aldehyde Cation
186.0588	203.091	0.0285	186.0873	83	100	Ala-Asn
186.0588	370.196	0.0467	186.1055	97	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	81	100	Ser-His-Lys
148.0974	147	-0.04	148.06	13	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	56	55.5	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	173	76.6	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	129	58	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	356	62.8	Betaine
118.0873	117.079	-0.001	118.0863	334	56.8	Betaine
118.0873	117.079	-0.001	118.0863	341	56	Betaine
106.0872	105	0	106.09	159	71.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	109	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	284	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	221	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	203	52	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	376	50.4	Betaine
118.0873	117.079	-0.001	118.0863	348	97.6	Betaine
118.0873	117	0	118.09	348	26.1	Betaine
84.0822	102.092	-0.0014	84.0808	231	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	212	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	142	54.2	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	41	100	O-Acetyl-L-Serine Hydrochloride
118.0873	117.079	-0.001	118.0863	367	36.4	Betaine
118.0873	117.079	-0.001	118.0863	316	75	Betaine
118.0873	117.079	-0.001	118.0863	355	51.9	Betaine
97.0774	114.104	0.0238	97.1012	41	100	Cyclohexanol, 4-Methyl-, Trans-
97.0774	114.104	0.0238	97.1012	48	25	Cyclohexanol, 4-Methyl-, Trans-
106.0872	105	0	106.09	158	76.9	Diethanolamine
106.0872	105	0	106.09	159	74.9	Diethanolamine
106.0872	105	0	106.09	158	79.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	280	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	259	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	160	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	205	51	Betaine Aldehyde Cation
106.0872	105	0	106.09	171	75.3	Diethanolamine
106.0872	105	0	106.09	159	78.9	Diethanolamine
106.0872	105	0	106.09	159	74.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	241	52	Betaine Aldehyde Cation

84.0822	102.092	-0.0014	84.0808	236	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	189	56	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	112	83.6	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	94	100	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	147	100	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	163	100	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	340	36	Betaine
118.0873	117.079	-0.001	118.0863	287	67.5	Betaine
118.0873	117.079	-0.001	118.0863	359	52.1	Betaine
148.0974	147	-0.04	148.06	31	67.3	O-Acetyl-L-Serine Hydrochloride
371.2927	370.308	0.0229	371.3156	184	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2927	370.308	0.0229	371.3156	178	76.9	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2927	370.308	0.0229	371.3156	81	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	322	29.1	Betaine
118.0873	117.079	-0.001	118.0863	323	99	Betaine
118.0873	117.079	-0.001	118.0863	343	31.4	Betaine
106.0872	105	0	106.09	166	71.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	266	56	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	279	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	167	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	163	51	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	356	53.9	Betaine
118.0873	117.079	-0.001	118.0863	329	82.7	Betaine
118.0873	117.079	-0.001	118.0863	323	29.3	Betaine
97.0774	114.104	0.0238	97.1012	49	32.3	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	208	76.5	Diethanolamine
106.0872	105	0	106.09	211	77	Diethanolamine
84.0822	102.092	-0.0014	84.0808	319	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	248	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	120	54.2	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	205	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	152	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	33	23.1	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	196	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	108	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	251	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	279	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	138	51	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	116	79.3	N,N-Bis(2-Hydroxyethyl)Glycine

186.0588	163.084	0.0149	186.0737	104	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	44	26.5	N-Acetyl-DL-Serine
148.0974	147	-0.04	148.06	36	28.1	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	103	52.8	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	362	33.5	Betaine
118.0873	117.079	-0.001	118.0863	321	49.9	Betaine
118.0873	117.079	-0.001	118.0863	337	62	Betaine
148.0974	147	-0.04	148.06	88	36.4	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	114	100	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	151	52.1	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	384	47.1	Betaine
118.0873	117.079	-0.001	118.0863	253	76.1	Betaine
118.0873	117.079	-0.001	118.0863	306	34.8	Betaine
106.0872	105	0	106.09	180	73.5	Diethanolamine
106.0872	105	0	106.09	159	74.3	Diethanolamine
106.0872	105	0	106.09	196	80.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	282	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	241	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	209	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	168	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	163	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	361	37.1	Betaine
118.0873	117.079	-0.001	118.0863	314	80.4	Betaine
118.0873	117.079	-0.001	118.0863	314	56.2	Betaine
97.0774	114.104	0.0238	97.1012	36	26.5	Cyclohexanemethanol
106.0872	105	0	106.09	228	76.3	Diethanolamine
106.0872	105	0	106.09	158	76.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	141	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	281	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	270	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	171	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	154	84	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105.079	-0.0009	106.0863	134	100	Diethanolamine
106.0872	105	0	106.09	170	79.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	204	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	267	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	230	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	200	53.1	Betaine Aldehyde Cation

186.0588	370.196	0.0467	186.1055	50	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	318	43.4	Betaine
118.0873	117.079	-0.001	118.0863	281	60.6	Betaine
118.0873	117.079	-0.001	118.0863	322	57	Betaine
148.0974	147.053	-0.037	148.0604	136	100	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	337	31.3	Betaine
118.0873	117.079	-0.001	118.0863	235	67.6	Betaine
118.0873	117.079	-0.001	118.0863	331	39	Betaine
106.0872	105	0	106.09	159	75.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	107	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	298	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	240	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	155	56	Betaine Aldehyde Cation
186.0588	168.042	0.0173	186.0761	26	100	3-Hydroxy-4-Methoxybenzoic Acid
186.0588	370.196	0.0467	186.1055	55	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	415	58.5	Betaine
118.0873	117.079	-0.001	118.0863	319	33.5	Betaine
118.0873	117.079	-0.001	118.0863	380	34.7	Betaine
97.0774	114.104	0.0238	97.1012	40	20.8	Cyclohexanemethanol
106.0872	105	0	106.09	171	77.9	Diethanolamine
106.0872	105	0	106.09	212	63.5	Diethanolamine
84.0822	102.092	-0.0014	84.0808	292	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	225	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	149	53.1	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	37	64.7	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	120	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	70	60	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	72	100	Ser-His-Lys
106.0872	105	0	106.09	153	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	131	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	279	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	233	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	173	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	126	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147.053	-0.037	148.0604	123	100	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	340	53.1	Betaine
118.0873	117.079	-0.001	118.0863	291	97.1	Betaine
118.0873	117.079	-0.001	118.0863	377	51.1	Betaine
393.2988	392.293	0.0011	393.2999	37	100	Chenodeoxycholic Acid
371.2927	370.308	0.0229	371.3156	186	100	Hexanedioic Acid, Bis(2-

						Ethylhexyl) Ester
371.2927	370.308	0.0229	371.3156	153	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2927	370.308	0.0229	371.3156	21	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2927	370.308	0.0229	371.3156	125	74.8	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	391	34.4	Betaine
118.0873	117.079	-0.001	118.0863	291	66.1	Betaine
118.0873	117.079	-0.001	118.0863	290	64.3	Betaine
97.0774	114.104	0.0238	97.1012	35	23	Cyclohexanemethanol
106.0872	105	0	106.09	159	79.3	Diethanolamine
106.0872	105	0	106.09	218	77.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	290	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	233	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	150	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	182	54.2	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	121	83.5	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	145	88.3	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	152	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147.053	-0.037	148.0604	98	45.8	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	272	75.6	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	212	79.6	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	35	19.5	Cyclohexanol, 1-Methyl-
97.0774	114.104	0.0238	97.1012	22	100	Cyclohexanol, 4-Methyl-, Trans-
118.0873	117.079	-0.001	118.0863	310	49.9	Betaine
118.0873	117.079	-0.001	118.0863	395	38	Betaine
118.0873	117.079	-0.001	118.0863	305	68.3	Betaine
118.0873	117.079	-0.001	118.0863	286	66	Betaine
106.0872	105	0	106.09	159	74.1	Diethanolamine
106.0872	105	0	106.09	152	74.8	Diethanolamine
106.0872	105	0	106.09	176	77.5	Diethanolamine
84.0822	102.092	-0.0014	84.0808	292	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	259	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	197	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	200	55.4	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	60	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	307	61.8	Betaine
118.0873	117.079	-0.001	118.0863	378	39.3	Betaine
118.0873	117.079	-0.001	118.0863	299	66.7	Betaine
118.0873	117.079	-0.001	118.0863	323	61.8	Betaine

106.0872	105	0	106.09	156	80.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	304	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	287	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	208	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	183	94	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	104	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	339	62.8	Betaine
118.0873	117.079	-0.001	118.0863	283	35.8	Betaine
118.0873	117.079	-0.001	118.0863	310	33.9	Betaine
97.0774	114.104	0.0238	97.1012	48	25	Cyclohexanemethanol
106.0872	105	0	106.09	160	73.8	Diethanolamine
106.0872	105	0	106.09	157	74.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	304	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	237	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	196	54.2	Betaine Aldehyde Cation
148.0974	147.053	-0.037	148.0604	134	100	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	320	60.8	Betaine
118.0873	117.079	-0.001	118.0863	267	60	Betaine
118.0873	117.079	-0.001	118.0863	313	35	Betaine
186.0588	370.196	0.0467	186.1055	48	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	46	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	166	94	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	63	60	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	168	74.9	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	37	26.2	Cyclohexanol, 1-Methyl-
97.0774	114.104	0.0238	97.1012	24	22.9	Cyclohexanol, 1-Methyl-
118.0873	117.079	-0.001	118.0863	278	83	Betaine
118.0873	117.079	-0.001	118.0863	433	34.6	Betaine
118.0873	117.079	-0.001	118.0863	294	75.4	Betaine
118.0873	117.079	-0.001	118.0863	273	56.9	Betaine
106.0872	105	0	106.09	170	79.9	Diethanolamine
106.0872	105	0	106.09	158	73.9	Diethanolamine
106.0872	105	0	106.09	136	78.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	315	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	195	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	119	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	213	54.2	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	58	32.2	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	140	85.2	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	344	100	Betaine
118.0873	117.079	-0.001	118.0863	437	56	Betaine

118.0873	117.079	-0.001	118.0863	287	62.8	Betaine
118.0873	117.079	-0.001	118.0863	327	46.7	Betaine
106.0872	105	0	106.09	210	74.1	Diethanolamine
106.0872	105	0	106.09	226	76.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	295	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	242	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	182	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	153	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	177	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	141	88.3	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	138	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	367	46	Betaine
118.0873	117.079	-0.001	118.0863	388	35.6	Betaine
118.0873	117.079	-0.001	118.0863	290	64.8	Betaine
118.0873	117.079	-0.001	118.0863	364	42.1	Betaine
106.0872	105	0	106.09	159	76.8	Diethanolamine
106.0872	105	0	106.09	225	80.4	Diethanolamine
106.0872	105	0	106.09	159	78.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	303	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	235	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	142	55.4	Betaine Aldehyde Cation
148.0974	147	-0.04	148.06	3	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	89	83.2	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	130	69.7	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	349	98.5	Betaine
118.0873	117.079	-0.001	118.0863	320	32.2	Betaine
118.0873	117.079	-0.001	118.0863	389	51.3	Betaine
106.0872	105	0	106.09	189	72.4	Diethanolamine
106.0872	105	0	106.09	148	78.6	Diethanolamine
106.0872	105	0	106.09	155	71.7	Diethanolamine
186.0588	370.196	0.0467	186.1055	88	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	66	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	135	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	36	21.9	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	280	100	Betaine
118.0873	117.079	-0.001	118.0863	300	64.9	Betaine
118.0873	117.079	-0.001	118.0863	360	56.5	Betaine
106.0872	105	0	106.09	130	72.8	Diethanolamine
106.0872	105	0	106.09	236	74.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	300	54.2	Betaine Aldehyde Cation

84.0822	102.092	-0.0014	84.0808	268	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	112	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	134	50	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	165	76.3	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	333	100	Betaine
118.0873	117.079	-0.001	118.0863	415	38.8	Betaine
118.0873	117.079	-0.001	118.0863	265	45.7	Betaine
118.0873	117.079	-0.001	118.0863	411	28.8	Betaine
106.0872	105	0	106.09	208	80.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	293	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	296	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	202	51	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	43	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	147	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	135	100	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105.079	-0.0009	106.0863	119	100	Diethanolamine
106.0872	105	0	106.09	158	75.2	Diethanolamine
106.0872	105	0	106.09	221	78.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	259	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	186	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	145	50	Betaine Aldehyde Cation
148.0974	147	-0.04	148.06	12	28.7	N-Acetyl-DL-Serine
148.0974	147.053	-0.037	148.0604	125	59	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	90	67.3	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	332	28.9	Betaine
118.0873	117.079	-0.001	118.0863	219	100	Betaine
118.0873	117.079	-0.001	118.0863	309	43.3	Betaine
186.0588	370.196	0.0467	186.1055	50	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	50	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	159	92.7	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	251	100	Betaine
118.0873	117.079	-0.001	118.0863	386	56.7	Betaine
118.0873	117.079	-0.001	118.0863	341	31.6	Betaine
118.0873	117.079	-0.001	118.0863	384	49.7	Betaine
106.0872	105	0	106.09	155	78.9	Diethanolamine
106.0872	105	0	106.09	169	79.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	318	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	223	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	198	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	114	83.5	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine

118.0873	117.079	-0.001	118.0863	402	37.4	Betaine
118.0873	117.079	-0.001	118.0863	305	58.7	Betaine
118.0873	117.079	-0.001	118.0863	329	66.4	Betaine
106.0872	105	0	106.09	159	74.9	Diethanolamine
106.0872	105	0	106.09	159	74.8	Diethanolamine
106.0872	105	0	106.09	148	79.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	297	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	223	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	115	53.1	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	74	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	145	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	118	89.8	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	31	19.4	Cyclohexanol, 1-Methyl-
97.0774	114.104	0.0238	97.1012	31	30.8	Cyclohexanemethanol
106.0872	105.079	-0.0009	106.0863	138	100	Diethanolamine
106.0872	105	0	106.09	202	77.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	296	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	244	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	225	51	Betaine Aldehyde Cation
148.0974	147	-0.04	148.06	47	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	222	64	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	348	49.7	Betaine
118.0873	117.079	-0.001	118.0863	300	40.4	Betaine
118.0873	117.079	-0.001	118.0863	325	62.3	Betaine
186.0588	163.084	0.0149	186.0737	155	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	394	27.4	Betaine
118.0873	117.079	-0.001	118.0863	333	81.4	Betaine
118.0873	117.079	-0.001	118.0863	362	69.9	Betaine
106.0872	105	0	106.09	156	74.4	Diethanolamine
106.0872	105	0	106.09	157	78.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	287	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	224	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	210	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	127	83.1	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	76	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	47	24.6	Cyclohexanol, 4-Methyl-, Trans-
118.0873	117.079	-0.001	118.0863	229	100	Betaine
118.0873	117.079	-0.001	118.0863	417	64.7	Betaine
118.0873	117.079	-0.001	118.0863	329	36	Betaine
118.0873	117.079	-0.001	118.0863	341	59.3	Betaine
106.0872	105	0	106.09	159	78.4	Diethanolamine

106.0872	105	0	106.09	157	75.7	Diethanolamine
106.0872	105	0	106.09	142	77.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	300	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	232	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	121	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	228	55.4	Betaine Aldehyde Cation
186.0588	203.095	0.0325	186.0913	112	60.2	Indole-3-Butyric Acid
186.0588	370.196	0.0467	186.1055	63	60.8	Ser-His-Lys
106.0872	105	0	106.09	203	66	Diethanolamine
106.0872	105	0	106.09	182	75.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	293	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	245	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	210	55.4	Betaine Aldehyde Cation
148.0974	147	-0.04	148.06	26	57.9	N-Acetyl-DL-Serine
118.0873	117.079	-0.001	118.0863	431	55.1	Betaine
118.0873	117.079	-0.001	118.0863	289	74.3	Betaine
118.0873	117.079	-0.001	118.0863	325	57.9	Betaine
106.0872	105	0	106.09	188	75.8	Diethanolamine
106.0872	105	0	106.09	252	77.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	307	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	186	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	236	54.2	Betaine Aldehyde Cation
186.0588	203.091	0.0285	186.0873	54	100	Ala-Asn
186.0588	163.084	0.0149	186.0737	166	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	33	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	117	74.9	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	393	54.7	Betaine
118.0873	117.079	-0.001	118.0863	274	63.3	Betaine
118.0873	117.079	-0.001	118.0863	314	44.2	Betaine
186.0588	370.196	0.0467	186.1055	27	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	76	100	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	123	62.3	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	280	95.5	Betaine
118.0873	117.079	-0.001	118.0863	414	54.1	Betaine
118.0873	117.079	-0.001	118.0863	312	73	Betaine
118.0873	117.079	-0.001	118.0863	271	60.3	Betaine
106.0872	105	0	106.09	157	72.6	Diethanolamine
106.0872	105	0	106.09	154	74.1	Diethanolamine
106.0872	105	0	106.09	158	79.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	309	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	279	53.1	Betaine Aldehyde Cation

84.0822	102.092	-0.0014	84.0808	244	51	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	89	74.8	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	42	23.6	Cyclohexanol, 4-Methyl-, Trans-
106.0872	105	0	106.09	159	74.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	278	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	261	55.4	Betaine Aldehyde Cation
148.0974	147.053	-0.037	148.0604	120	68.7	O-Acetyl-L-Serine
148.0974	147	-0.04	148.06	59	100	O-Acetyl-L-Serine Hydrochloride
118.0873	117.079	-0.001	118.0863	361	45.1	Betaine
118.0873	117.079	-0.001	118.0863	281	61.1	Betaine
118.0873	117.079	-0.001	118.0863	319	54.9	Betaine
186.0588	203.091	0.0285	186.0873	83	82.7	Ala-Asn
118.0873	117.079	-0.001	118.0863	260	71.2	Betaine
118.0873	117.079	-0.001	118.0863	293	64.4	Betaine
118.0873	117.079	-0.001	118.0863	318	75.5	Betaine
118.0873	117.079	-0.001	118.0863	323	49.9	Betaine
106.0872	105	0	106.09	159	74.9	Diethanolamine
106.0872	105	0	106.09	208	74.4	Diethanolamine
106.0872	105	0	106.09	303	76.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	328	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	231	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	124	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	199	51	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	83	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	35	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	259	85.3	Betaine
118.0873	117.079	-0.001	118.0863	403	97.4	Betaine
118.0873	117.079	-0.001	118.0863	292	68.4	Betaine
118.0873	117.079	-0.001	118.0863	407	40.4	Betaine
106.0872	105	0	106.09	195	76.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	307	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	251	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	229	53.1	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	39	59.3	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	133	83.3	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105	0	106.09	159	73.9	Diethanolamine
106.0872	105	0	106.09	158	74.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	292	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	239	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	146	56	Betaine Aldehyde Cation

148.0974	147	-0.04	148.06	28	100	O-Acetyl-L-Serine Hydrochloride
118.0873	117.079	-0.001	118.0863	378	100	Betaine
118.0873	117.079	-0.001	118.0863	301	67.3	Betaine
118.0873	117.079	-0.001	118.0863	356	38.2	Betaine
106.0872	105	0	106.09	158	80.9	Diethanolamine
106.0872	105	0	106.09	212	77.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	267	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	266	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	161	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	157	54.2	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	173	95.7	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	148	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	154	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	342	56.5	Betaine
118.0873	117.079	-0.001	118.0863	292	64.5	Betaine
118.0873	117.079	-0.001	118.0863	390	37.8	Betaine
84.0822	102.092	-0.0014	84.0808	297	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	252	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	217	52	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	30	100	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	94	59.4	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	27	26.4	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	352	99	Betaine
118.0873	117.079	-0.001	118.0863	312	98.6	Betaine
118.0873	117.079	-0.001	118.0863	347	44.6	Betaine
106.0872	105	0	106.09	191	71.7	Diethanolamine
106.0872	105	0	106.09	173	78.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	217	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	300	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	253	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	167	56	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	149	41.4	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	180	100	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105	0	106.09	230	61.9	Diethanolamine
106.0872	105	0	106.09	262	64.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	302	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	238	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	120	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	171	54.2	Betaine Aldehyde Cation
148.0974	147	-0.04	148.06	28	30.3	N-Acetyl-DL-Serine
148.0974	147.053	-0.037	148.0604	108	76.6	O-Acetyl-L-Serine

118.0873	117.079	-0.001	118.0863	224	100	Betaine
118.0873	117.079	-0.001	118.0863	417	40.4	Betaine
118.0873	117.079	-0.001	118.0863	326	59.1	Betaine
118.0873	117.079	-0.001	118.0863	323	38	Betaine
106.0872	105	0	106.09	133	73.3	Diethanolamine
106.0872	105	0	106.09	156	74.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	297	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	216	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	192	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	173	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	163	89.5	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	410	40	Betaine
118.0873	117.079	-0.001	118.0863	258	82.8	Betaine
118.0873	117.079	-0.001	118.0863	398	52.8	Betaine
106.0872	105	0	106.09	151	74.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	195	100	Diethanolamine
186.0588	370.196	0.0467	186.1055	36	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	52	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	70	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	8	100	Cyclopentanemethanol, .Alpha.-Methyl-
118.0873	117.079	-0.001	118.0863	354	66.2	Betaine
118.0873	117.079	-0.001	118.0863	331	96.8	Betaine
118.0873	117.079	-0.001	118.0863	376	33.3	Betaine
106.0872	105	0	106.09	176	74.7	Diethanolamine
106.0872	105	0	106.09	159	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	166	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	299	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	279	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	206	56.6	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	55	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	144	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	34	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147	-0.04	148.06	63	59.3	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	136	100	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	36	24.5	Cyclohexanemethanol
106.0872	105	0	106.09	155	77.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	276	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	238	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	184	53.1	Betaine Aldehyde Cation
148.0974	147	-0.04	148.06	37	100	O-Acetyl-L-Serine Hydrochloride

822.7532	822	0	822.75	332	82.7	TG 48:1; [M+NH4]+; TG(16:0/16:0/16:1)
822.7532	822	0	822.75	342	80.6	TG 48:1; [M+NH4]+; TG(16:0/16:0/16:1)
822.7532	822	0	822.75	280	56	TG 48:1; [M+NH4]+; TG(16:0/16:0/16:1)
822.7532	822	0	822.75	277	100	TG 48:1; [M+NH4]+; TG(16:0/16:0/16:1)
97.0774	114.104	0.0238	97.1012	30	32.3	Cyclohexanol, 1-Methyl-
118.0873	117.079	-0.001	118.0863	238	100	Betaine
118.0873	117.079	-0.001	118.0863	411	33.9	Betaine
118.0873	117.079	-0.001	118.0863	270	60.3	Betaine
118.0873	117.079	-0.001	118.0863	335	48.5	Betaine
106.0872	105	0	106.09	156	73.7	Diethanolamine
106.0872	105	0	106.09	158	80.2	Diethanolamine
106.0872	105	0	106.09	245	73.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	288	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	261	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	140	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	118	87.8	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	51	24	Cyclohexanol, 1-Methyl-
118.0873	117.079	-0.001	118.0863	260	79.5	Betaine
118.0873	117.079	-0.001	118.0863	351	32.3	Betaine
118.0873	117.079	-0.001	118.0863	266	80.8	Betaine
118.0873	117	0	118.09	358	24.3	Betaine
106.0872	105	0	106.09	133	78.2	Diethanolamine
106.0872	105	0	106.09	177	72.7	Diethanolamine
186.0588	163.084	0.0149	186.0737	172	83.3	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	107	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	117	88.3	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147.053	-0.037	148.0604	147	71	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	122	100	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	416	32.2	Betaine
118.0873	117.079	-0.001	118.0863	270	27.8	Betaine
118.0873	117.079	-0.001	118.0863	336	39.3	Betaine
106.0872	105	0	106.09	159	74	Diethanolamine
106.0872	105	0	106.09	155	79.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	303	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	267	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	150	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	140	90.4	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105	0	106.09	161	77.9	Diethanolamine

84.0822	102.092	-0.0014	84.0808	274	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	216	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	148	54.2	Betaine Aldehyde Cation
148.0974	147.053	-0.037	148.0604	20	37.1	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	123	70.2	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	41	100	Cyclohexanol, 4-Methyl-, Trans-
118.0873	117.079	-0.001	118.0863	335	68.9	Betaine
118.0873	117.079	-0.001	118.0863	431	57.5	Betaine
118.0873	117.079	-0.001	118.0863	300	43.9	Betaine
118.0873	117	0	118.09	323	28.9	Betaine
106.0872	105	0	106.09	158	76.3	Diethanolamine
106.0872	105	0	106.09	159	79.6	Diethanolamine
106.0872	105	0	106.09	218	52.8	Diethanolamine
106.0872	105	0	106.09	159	76.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	306	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	244	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	182	51	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	117	83	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	136	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	229	80.1	Betaine
118.0873	117.079	-0.001	118.0863	308	24.9	Betaine
118.0873	117.079	-0.001	118.0863	262	48.9	Betaine
118.0873	117.079	-0.001	118.0863	346	24.6	Betaine
148.0974	147.053	-0.037	148.0604	155	63.5	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	124	100	O-Acetyl-L-Serine
371.2885	370.308	0.0271	371.3156	198	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2885	370.308	0.0271	371.3156	165	88.8	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2885	370.308	0.0271	371.3156	144	81.9	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
118.0873	117.079	-0.001	118.0863	252	49.9	Betaine
118.0873	117.079	-0.001	118.0863	313	30.9	Betaine
106.0872	105	0	106.09	154	75.9	Diethanolamine
106.0872	105	0	106.09	224	80.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	298	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	223	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	159	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	183	54.2	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	137	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	56	100	Ser-His-Lys
170.0793	187.121	0.0383	170.1176	89	54.2	7-Keto-8-Aminopelargonic Acid

148.0974	147	-0.04	148.06	26	33.9	O-Acetyl-L-Serine Hydrochloride
148.0974	147	-0.04	148.06	3	100	O-Acetyl-L-Serine Hydrochloride
106.0872	105	0	106.09	171	75.1	Diethanolamine
106.0872	105	0	106.09	245	61.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	109	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	272	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	214	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	124	54.2	Betaine Aldehyde Cation
824.7703	824	0	824.77	250	73.2	TG 48:0; [M+NH4]+; TG(14:0/16:0/18:0)
824.7703	824	0	824.77	260	50	TG 48:0; [M+NH4]+; TG(14:0/16:0/18:0)
824.7703	824	0	824.77	235	74.9	TG 48:0; [M+NH4]+; TG(16:0/16:0/16:0)
824.7703	824	0	824.77	262	52	TG 48:0; [M+NH4]+; TG(16:0/16:0/16:0)
118.0873	117.079	-0.001	118.0863	332	41.8	Betaine
118.0873	117.079	-0.001	118.0863	387	28.1	Betaine
118.0873	117.079	-0.001	118.0863	250	56	Betaine
118.0873	117.079	-0.001	118.0863	305	34.3	Betaine
106.0872	105	0	106.09	159	80.2	Diethanolamine
106.0872	105	0	106.09	147	72.9	Diethanolamine
106.0872	105	0	106.09	151	77.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	282	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	277	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	220	51	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	139	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	142	91.7	N,N-Bis(2-Hydroxyethyl)Glycine
824.7703	824	0	824.77	311	85.4	TG 48:0; [M+NH4]+; TG(14:0/16:0/18:0)
824.7703	824	0	824.77	98	100	TG 48:0; [M+NH4]+; TG(14:0/16:0/18:0)
97.0774	114.104	0.0238	97.1012	65	25.2	Cyclohexanol, 4-Methyl-, Trans-
118.0873	117.079	-0.001	118.0863	277	100	Betaine
118.0873	117.079	-0.001	118.0863	398	62.9	Betaine
118.0873	117.079	-0.001	118.0863	302	72.8	Betaine
118.0873	117.079	-0.001	118.0863	371	53.1	Betaine
106.0872	105	0	106.09	160	75.2	Diethanolamine
106.0872	105	0	106.09	156	74.4	Diethanolamine
106.0872	105	0	106.09	170	80.7	Diethanolamine
186.0588	163.084	0.0149	186.0737	145	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	128	100	N,N-Bis(2-Hydroxyethyl)Glycine

876.8011	876	0	876.8	294	100	TG 52:2; [M+NH4]+; TG(16:0/18:1/18:1)
876.8011	876	0	876.8	310	86.6	TG 52:2; [M+NH4]+; TG(16:0/18:1/18:1)
876.8011	876	0	876.8	233	57.9	TG 52:2; [M+NH4]+; TG(16:0/18:1/18:1)
876.8011	876	0	876.8	306	90.4	TG 52:2; [M+NH4]+; TG(16:0/18:1/18:1)
118.0873	117.079	-0.001	118.0863	333	29.8	Betaine
118.0873	117.079	-0.001	118.0863	275	58.7	Betaine
118.0873	117.079	-0.001	118.0863	324	38.4	Betaine
84.0822	102.092	-0.0014	84.0808	259	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	229	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	130	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	133	56	Betaine Aldehyde Cation
186.0588	203.091	0.0285	186.0873	49	100	Ala-Asn
186.0588	370.196	0.0467	186.1055	58	100	Ser-His-Lys
148.0974	147	-0.04	148.06	10	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	122	100	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	26	28.9	Cyclohexanemethanol
106.0872	105	0	106.09	190	67.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	298	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	242	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	202	52	Betaine Aldehyde Cation
148.0974	147.053	-0.037	148.0604	120	73.2	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	39	30.9	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	302	38.3	Betaine
118.0873	117.079	-0.001	118.0863	358	60.1	Betaine
118.0873	117.079	-0.001	118.0863	323	78	Betaine
118.0873	117.079	-0.001	118.0863	293	65.5	Betaine
106.0872	105	0	106.09	158	80.2	Diethanolamine
106.0872	105	0	106.09	159	74.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	310	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	287	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	193	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	143	51	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	31	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	176	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	155	88.9	N,N-Bis(2-Hydroxyethyl)Glycine
170.0793	187.121	0.0383	170.1176	26	100	7-Keto-8-Aminopelargonic Acid
97.0774	114.104	0.0238	97.1012	28	24	Cyclohexanol, 1-Methyl-
118.0873	117.079	-0.001	118.0863	249	100	Betaine
118.0873	117.079	-0.001	118.0863	402	66.2	Betaine

118.0873	117.079	-0.001	118.0863	289	65.4	Betaine
118.0873	117.079	-0.001	118.0863	300	67.6	Betaine
106.0872	105	0	106.09	158	79.3	Diethanolamine
106.0872	105	0	106.09	156	75.1	Diethanolamine
106.0872	105	0	106.09	156	60.8	Diethanolamine
186.0588	203.091	0.0285	186.0873	78	100	Ala-Asn
186.0588	163.084	0.0149	186.0737	131	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	61	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	155	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	6	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	148	100	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	339	30.3	Betaine
118.0873	117.079	-0.001	118.0863	272	50.4	Betaine
118.0873	117.079	-0.001	118.0863	325	32.8	Betaine
84.0822	102.092	-0.0014	84.0808	251	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	207	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	176	52	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	46	35.9	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	83	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	24	55.4	Cyclohexanemethanol
106.0872	105	0	106.09	156	78.2	Diethanolamine
106.0872	105	0	106.09	159	75.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	276	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	265	51	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	415	93.2	Betaine
118.0873	117.079	-0.001	118.0863	327	33.7	Betaine
118.0873	117.079	-0.001	118.0863	308	58.5	Betaine
106.0872	105	0	106.09	149	74.5	Diethanolamine
106.0872	105	0	106.09	235	77.3	Diethanolamine
106.0872	105	0	106.09	159	76.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	299	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	267	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	221	56.6	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	184	90.9	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	172	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	33	20.3	Cyclohexanol, 1-Methyl-
118.0873	117.079	-0.001	118.0863	365	35.5	Betaine
118.0873	117.079	-0.001	118.0863	321	39.6	Betaine
118.0873	117.079	-0.001	118.0863	318	47.3	Betaine
106.0872	105	0	106.09	228	79.6	Diethanolamine

106.0872	105	0	106.09	158	80.9	Diethanolamine
106.0872	105	0	106.09	159	75.5	Diethanolamine
186.0588	203.091	0.0285	186.0873	106	70.2	Ala-Asn
186.0588	370.196	0.0467	186.1055	33	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	48	100	Ser-His-Lys
148.0974	147	-0.04	148.06	19	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	171	100	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	107	100	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	321	34.7	Betaine
84.0822	102.092	-0.0014	84.0808	269	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	213	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	222	55.4	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	113	84.9	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	107	100	Ser-His-Lys
148.0974	147	-0.04	148.06	35	30.6	O-Acetyl-L-Serine Hydrochloride
148.0974	147	-0.04	148.06	5	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	102	73.2	O-Acetyl-L-Serine
106.0872	105	0	106.09	158	79.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	280	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	242	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	225	54.2	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	376	99	Betaine
118.0873	117.079	-0.001	118.0863	276	57.9	Betaine
118.0873	117.079	-0.001	118.0863	301	69.2	Betaine
106.0872	105	0	106.09	159	78.6	Diethanolamine
106.0872	105	0	106.09	158	76	Diethanolamine
106.0872	105	0	106.09	277	60.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	302	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	265	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	162	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	216	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	142	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	164	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	23	55.4	O-Acetyl-L-Serine Hydrochloride
148.0974	147	-0.04	148.06	6	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	173	61.4	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	175	66.1	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	43	26.6	Cyclohexanol, 1-Methyl-
118.0873	117.079	-0.001	118.0863	383	100	Betaine
118.0873	117.079	-0.001	118.0863	269	56.3	Betaine

118.0873	117.079	-0.001	118.0863	380	50.1	Betaine
106.0872	105	0	106.09	114	71.4	Diethanolamine
106.0872	105	0	106.09	156	75.6	Diethanolamine
106.0872	105	0	106.09	163	100	Diethanolamine
106.0872	105	0	106.09	225	76.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	316	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	272	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	211	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	155	51	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	124	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	266	58.7	Betaine
118.0873	117.079	-0.001	118.0863	305	100	Betaine
84.0822	102.092	-0.0014	84.0808	274	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	217	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	148	50	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	60	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	118	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	59	100	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	147	100	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	122	100	O-Acetyl-L-Serine
106.0872	105	0	106.09	159	73.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	244	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	230	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	176	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	205	54.2	Betaine Aldehyde Cation
148.0974	147.053	-0.037	148.0604	168	76.6	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	29	28.4	Cyclohexanol, 1-Methyl-
97.0774	114.104	0.0238	97.1012	35	25.1	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	353	56.8	Betaine
118.0873	117.079	-0.001	118.0863	278	89.4	Betaine
118.0873	117.079	-0.001	118.0863	382	43.5	Betaine
106.0872	105	0	106.09	140	74.2	Diethanolamine
106.0872	105	0	106.09	221	80.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	299	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	290	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	223	55.4	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	165	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	410	49.1	Betaine
118.0873	117.079	-0.001	118.0863	266	53.6	Betaine
118.0873	117.079	-0.001	118.0863	352	98	Betaine
106.0872	105	0	106.09	166	73	Diethanolamine

106.0872	105	0	106.09	156	79.3	Diethanolamine
106.0872	105	0	106.09	267	56.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	113	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	328	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	273	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	197	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	140	90.1	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	162	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	275	84	Betaine
118.0873	117.079	-0.001	118.0863	273	62.7	Betaine
118.0873	117.079	-0.001	118.0863	264	58.7	Betaine
84.0822	102.092	-0.0014	84.0808	238	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	196	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	188	52	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	81	100	Ser-His-Lys
148.0974	147	-0.04	148.06	27	39.3	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	140	100	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	35	22.5	Cyclohexanol, 4-Methyl-, Trans-
106.0872	105	0	106.09	164	76.1	Diethanolamine
106.0872	105	0	106.09	158	75.4	Diethanolamine
148.0974	147.053	-0.037	148.0604	127	68.7	O-Acetyl-L-Serine
106.0872	105	0	106.09	185	78.1	Diethanolamine
106.0872	105	0	106.09	210	62.1	Diethanolamine
118.0873	117.079	-0.001	118.0863	231	93.3	Betaine
118.0873	117.079	-0.001	118.0863	434	33.8	Betaine
118.0873	117.079	-0.001	118.0863	321	80.7	Betaine
118.0873	117.079	-0.001	118.0863	338	36.6	Betaine
84.0822	102.092	-0.0014	84.0808	317	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	215	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	200	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	247	55.4	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	121	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	19	100	O-Acetyl-L-Serine Hydrochloride
118.0873	117.079	-0.001	118.0863	378	58.5	Betaine
118.0873	117.079	-0.001	118.0863	244	41.3	Betaine
118.0873	117.079	-0.001	118.0863	317	58.9	Betaine
106.0872	105	0	106.09	174	79.9	Diethanolamine
106.0872	105	0	106.09	202	78.9	Diethanolamine
106.0872	105	0	106.09	264	68.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	272	52	Betaine Aldehyde Cation

84.0822	102.092	-0.0014	84.0808	273	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	184	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	219	53.1	Betaine Aldehyde Cation
186.0588	203.091	0.0285	186.0873	60	100	Ala-Asn
186.0588	163.084	0.0149	186.0737	144	100	N,N-Bis(2-Hydroxyethyl)Glycine
118.0873	117.079	-0.001	118.0863	299	37.9	Betaine
118.0873	117.079	-0.001	118.0863	237	84.2	Betaine
118.0873	117.079	-0.001	118.0863	266	58	Betaine
84.0822	102.092	-0.0014	84.0808	245	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	246	51	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	154	91.4	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147.053	-0.037	148.0604	136	64.6	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	190	73.2	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	165	72.9	O-Acetyl-L-Serine
106.0872	105	0	106.09	203	75.2	Diethanolamine
106.0872	105	0	106.09	152	73.2	Diethanolamine
148.0974	147	-0.04	148.06	39	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147	-0.04	148.06	59	62.3	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	102	100	O-Acetyl-L-Serine
106.0872	105	0	106.09	155	75.9	Diethanolamine
106.0872	105	0	106.09	235	66	Diethanolamine
118.0873	117.079	-0.001	118.0863	195	100	Betaine
118.0873	117.079	-0.001	118.0863	377	30.8	Betaine
118.0873	117.079	-0.001	118.0863	301	67.5	Betaine
118.0873	117.079	-0.001	118.0863	365	37.1	Betaine
84.0822	102.092	-0.0014	84.0808	318	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	222	56	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	164	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	257	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	113	85.2	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	67	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147.053	-0.037	148.0604	2	100	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	119	73.2	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	130	68.7	O-Acetyl-L-Serine
106.0872	105.079	-0.0009	106.0863	123	100	Diethanolamine
106.0872	105	0	106.09	160	78.9	Diethanolamine
118.0873	117.079	-0.001	118.0863	258	82.9	Betaine
118.0873	117.079	-0.001	118.0863	400	67.5	Betaine
118.0873	117	0	118.09	334	23	Betaine
118.0873	117.079	-0.001	118.0863	361	31.6	Betaine

84.0822	102.092	-0.0014	84.0808	268	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	206	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	135	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	219	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	93	84.2	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105	0	106.09	211	69.8	Diethanolamine
118.0873	117.079	-0.001	118.0863	385	45.1	Betaine
118.0873	117.079	-0.001	118.0863	332	98.8	Betaine
118.0873	117.079	-0.001	118.0863	348	38.2	Betaine
84.0822	102.092	-0.0014	84.0808	308	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	285	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	218	56	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	132	84.2	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	137	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147.053	-0.037	148.0604	122	59.4	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	96	59.9	O-Acetyl-L-Serine
106.0872	105	0	106.09	158	76.6	Diethanolamine
106.0872	105	0	106.09	148	70.2	Diethanolamine
170.0793	187.121	0.0383	170.1176	70	39.2	7-Keto-8-Aminopelargonic Acid
106.0872	105	0	106.09	189	76.4	Diethanolamine
118.0873	117.079	-0.001	118.0863	349	57.7	Betaine
118.0873	117.079	-0.001	118.0863	277	61.8	Betaine
118.0873	117.079	-0.001	118.0863	364	58	Betaine
84.0822	102.092	-0.0014	84.0808	319	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	267	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	191	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	87	82.2	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	83	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	44	22.9	Cyclohexanemethanol
106.0872	105	0	106.09	166	75.3	Diethanolamine
106.0872	105	0	106.09	159	73.5	Diethanolamine
118.0873	117.079	-0.001	118.0863	397	99	Betaine
118.0873	117.079	-0.001	118.0863	323	98.3	Betaine
118.0873	117.079	-0.001	118.0863	370	32.5	Betaine
84.0822	102.092	-0.0014	84.0808	325	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	309	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	158	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	186	51	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	38	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	150	100	N,N-Bis(2-Hydroxyethyl)Glycine

148.0974	147	-0.04	148.06	18	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147	-0.04	148.06	13	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	215	78.6	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	55	22	Cyclohexanol, 4-Methyl-, Trans-
97.0774	114.104	0.0238	97.1012	34	26.6	Cyclohexanemethanol
106.0872	105	0	106.09	157	78.6	Diethanolamine
106.0872	105	0	106.09	202	76.1	Diethanolamine
118.0873	117.079	-0.001	118.0863	217	100	Betaine
118.0873	117.079	-0.001	118.0863	413	50.4	Betaine
118.0873	117	0	118.09	317	24.9	Betaine
118.0873	117	0	118.09	354	25.4	Betaine
84.0822	102.092	-0.0014	84.0808	307	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	269	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	173	52	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	125	100	N,N-Bis(2-Hydroxyethyl)Glycine
106.0872	105	0	106.09	186	74.1	Diethanolamine
106.0872	105	0	106.09	270	73.2	Diethanolamine
106.0872	105	0	106.09	157	80.9	Diethanolamine
118.0873	117.079	-0.001	118.0863	365	46.3	Betaine
118.0873	117.079	-0.001	118.0863	248	71.1	Betaine
118.0873	117	0	118.09	320	26.5	Betaine
84.0822	102.092	-0.0014	84.0808	315	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	299	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	155	50	Betaine Aldehyde Cation
148.0974	147	-0.04	148.06	31	56	N-Acetyl-DL-Serine
148.0974	147.053	-0.037	148.0604	116	73.5	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	143	65.7	O-Acetyl-L-Serine
118.0873	117.079	-0.001	118.0863	265	57.3	Betaine
84.0822	102.092	-0.0014	84.0808	276	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	256	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	103	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	149	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	177	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	152	92.7	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	82	68.7	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	169	59.3	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	60	29.1	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	159	75.9	Diethanolamine
106.0872	105	0	106.09	186	71.8	Diethanolamine
106.0872	105	0	106.09	157	78.6	Diethanolamine
118.0873	117.079	-0.001	118.0863	278	100	Betaine

118.0873	117.079	-0.001	118.0863	390	53.2	Betaine
118.0873	117.079	-0.001	118.0863	237	80.8	Betaine
118.0873	117.079	-0.001	118.0863	416	57.6	Betaine
84.0822	102.092	-0.0014	84.0808	317	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	292	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	190	53.1	Betaine Aldehyde Cation
186.0588	163.084	0.0149	186.0737	102	65.5	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	148	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	32	37.6	N-Acetyl-DL-Serine
148.0974	147.053	-0.037	148.0604	177	69.7	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	41	23.3	Cyclohexanol, 4-Methyl-, Trans-
106.0872	105	0	106.09	164	74	Diethanolamine
106.0872	105	0	106.09	154	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	167	100	Diethanolamine
186.0588	163.084	0.0149	186.0737	170	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
106.0872	105	0	106.09	170	75.8	Diethanolamine
106.0872	105	0	106.09	156	80.2	Diethanolamine
106.0872	105	0	106.09	187	68.4	Diethanolamine
106.0872	105	0	106.09	153	78.6	Diethanolamine
118.0873	117.079	-0.001	118.0863	374	66.3	Betaine
118.0873	117.079	-0.001	118.0863	333	30.3	Betaine
84.0822	102.092	-0.0014	84.0808	321	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	254	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	228	53.1	Betaine Aldehyde Cation
170.0793	187.121	0.0383	170.1176	40	100	7-Keto-8-Aminopelargonic Acid
148.0974	147	-0.04	148.06	15	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	133	100	O-Acetyl-L-Serine
84.0822	102.092	-0.0014	84.0808	187	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	182	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	136	51	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	402	71	Betaine
118.0873	117.079	-0.001	118.0863	295	66	Betaine
118.0873	117.079	-0.001	118.0863	332	98.8	Betaine
186.0588	370.196	0.0467	186.1055	61	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	131	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147.053	-0.037	148.0604	35	37.8	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	130	74.9	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	125	53.4	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	47	24.4	Cyclohexanol, 4-Methyl-, Trans-

106.0872	105	0	106.09	152	78.9	Diethanolamine
106.0872	105	0	106.09	157	78.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	285	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	267	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	252	51	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	390	38.2	Betaine
118.0873	117.079	-0.001	118.0863	291	65.3	Betaine
118.0873	117.079	-0.001	118.0863	365	55.7	Betaine
186.0588	370.196	0.0467	186.1055	56	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	129	76.9	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147.053	-0.037	148.0604	133	63.4	O-Acetyl-L-Serine
106.0872	105	0	106.09	158	75.1	Diethanolamine
106.0872	105	0	106.09	158	75.4	Diethanolamine
106.0872	105	0	106.09	154	78.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	311	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	244	52	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	177	100	5-Aminovaleric Acid
118.0873	117.079	-0.001	118.0863	416	98.5	Betaine
118.0873	117.079	-0.001	118.0863	278	59.1	Betaine
118.0873	117.079	-0.001	118.0863	340	48.1	Betaine
186.0588	370.196	0.0467	186.1055	46	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	153	91.8	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	65	51.2	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	170	100	O-Acetyl-L-Serine
106.0872	105	0	106.09	159	75.5	Diethanolamine
106.0872	105	0	106.09	261	79.6	Diethanolamine
371.2746	370.308	0.041	371.3156	228	89.2	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2746	370.308	0.041	371.3156	169	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2746	370.308	0.041	371.3156	85	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2746	370.214	-0.0529	371.2217	56	100	17-Phenyltrinor-13,14-Dihydroprostaglandin A2
97.0774	114.104	0.0238	97.1012	25	26.2	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	159	79.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	295	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	267	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	201	56	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	371	62.5	Betaine
118.0873	117.079	-0.001	118.0863	298	66.5	Betaine
118.0873	117.079	-0.001	118.0863	315	58.5	Betaine

186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	20	31.3	N-Acetyl-DL-Serine
148.0974	147.053	-0.037	148.0604	143	100	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	39	25.2	Cyclohexanemethanol
106.0872	105	0	106.09	156	71.7	Diethanolamine
106.0872	105	0	106.09	158	79.6	Diethanolamine
106.0872	105	0	106.09	230	76.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	290	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	248	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	178	54.2	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	359	39.7	Betaine
118.0873	117.079	-0.001	118.0863	305	68.2	Betaine
118.0873	117.079	-0.001	118.0863	315	47.1	Betaine
148.0974	147.053	-0.037	148.0604	112	50.2	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	131	54.7	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	184	70.3	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	33	25.4	Cyclohexanol, 2-Methyl-, Trans-
106.0872	105	0	106.09	151	78.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	173	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	105	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	317	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	271	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	207	54.2	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	207	100	Betaine
118.0873	117.079	-0.001	118.0863	397	50.6	Betaine
118.0873	117.079	-0.001	118.0863	277	58.4	Betaine
118.0873	117.079	-0.001	118.0863	351	53.1	Betaine
186.0588	163.084	0.0149	186.0737	134	91.1	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147	-0.04	148.06	26	24.2	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	41	32.1	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	81	100	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	71	49	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	24	52	Cyclohexanol, 4-Methyl-, Trans-
106.0872	105	0	106.09	158	78.3	Diethanolamine
106.0872	105	0	106.09	148	77.9	Diethanolamine
106.0872	105	0	106.09	214	75	Diethanolamine
84.0822	102.092	-0.0014	84.0808	309	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	247	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	154	100	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	169	56.6	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	364	61.1	Betaine

118.0873	117.079	-0.001	118.0863	386	98.5	Betaine
118.0873	117.079	-0.001	118.0863	281	66.6	Betaine
118.0873	117.079	-0.001	118.0863	327	27.1	Betaine
148.0974	147	-0.04	148.06	9	50	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	210	76.6	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	117	43.7	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	20	100	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	110	60	Cyclohexanemethanol
106.0872	105	0	106.09	245	75.7	Diethanolamine
186.0588	370.196	0.0467	186.1055	32	54.2	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	26	21	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	49	100	O-Acetyl-L-Serine
84.0822	102.092	-0.0014	84.0808	141	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	185	51	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	326	37.3	Betaine
118.0873	117.079	-0.001	118.0863	272	61.3	Betaine
118.0873	117.079	-0.001	118.0863	257	54.7	Betaine
186.0588	163.084	0.0149	186.0737	119	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	55	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	147	100	N,N-Bis(2-Hydroxyethyl)Glycine
148.0974	147.053	-0.037	148.0604	114	50.2	O-Acetyl-L-Serine
371.2746	370.308	0.041	371.3156	194	70.6	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2746	370.308	0.041	371.3156	170	78.3	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2746	370.308	0.041	371.3156	80	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
371.2746	370.308	0.041	371.3156	140	100	Hexanedioic Acid, Bis(2-Ethylhexyl) Ester
97.0774	114.104	0.0238	97.1012	75	21.6	Cyclohexanol, 1-Methyl-
106.0872	105	0	106.09	155	71.7	Diethanolamine
106.0872	105	0	106.09	232	78.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	289	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	252	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	113	53.1	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	319	32.2	Betaine
118.0873	117.079	-0.001	118.0863	276	61.7	Betaine
118.0873	117.079	-0.001	118.0863	372	45.1	Betaine
186.0588	370.196	0.0467	186.1055	52	100	Ser-His-Lys
186.0588	203.091	0.0285	186.0873	75	100	Ala-Asn
148.0974	147	-0.04	148.06	33	56	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	178	100	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	98	24.3	Cyclohexanol, 4-Methyl-, Trans-

106.0872	105	0	106.09	154	74.8	Diethanolamine
106.0872	105	0	106.09	253	76.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	300	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	253	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	228	55.4	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	321	50.1	Betaine
118.0873	117.079	-0.001	118.0863	365	55.6	Betaine
148.0974	147	-0.04	148.06	12	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	119	100	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	70	52	Cyclohexanemethanol
106.0872	105	0	106.09	157	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	111	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	289	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	253	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	157	55.4	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	171	54.2	Betaine Aldehyde Cation
118.0873	117.079	-0.001	118.0863	330	43.4	Betaine
118.0873	117.079	-0.001	118.0863	272	72.7	Betaine
118.0873	117.079	-0.001	118.0863	326	99	Betaine
97.0774	114.104	0.0238	97.1012	51	25.3	Cyclohexanol, 1-Methyl-
84.0822	102.092	-0.0014	84.0808	255	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	185	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	166	53.1	Betaine Aldehyde Cation
106.0872	105	0	106.09	159	78.9	Diethanolamine
106.0872	105	0	106.09	180	67.3	Diethanolamine
186.0588	370.196	0.0467	186.1055	38	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
148.0974	147	-0.04	148.06	21	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	140	100	O-Acetyl-L-Serine
84.0822	102.092	-0.0014	84.0808	168	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	149	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	147	52	Betaine Aldehyde Cation
186.0588	370.196	0.0467	186.1055	73	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	213	100	Betaine
121.1229	60.032	-0.051	121.072	21	64.7	Urea
121.1229	60.032	-0.051	121.072	37	78.9	Urea
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.032	-0.051	121.072	44	81.7	Urea
84.0822	102.092	-0.0014	84.0808	247	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	184	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	200	53.1	Betaine Aldehyde Cation

106.0872	105	0	106.09	151	75.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	100	Diethanolamine
106.0872	105	0	106.09	218	77.3	Diethanolamine
148.0974	147.053	-0.037	148.0604	89	69.5	O-Acetyl-L-Serine
121.1229	60.032	-0.051	121.072	29	77.9	Urea
121.1229	60.032	-0.051	121.072	31	78.2	Urea
121.1229	60.058	-0.0006	121.1223	10	100	1-Propanol
121.1229	60.032	-0.051	121.072	73	83.2	Urea
228.1067	227.12	0.021	228.1277	146	100	Ametryn
84.0822	102.092	-0.0014	84.0808	237	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	185	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	190	51	Betaine Aldehyde Cation
106.0872	105	0	106.09	160	75.3	Diethanolamine
106.0872	105	0	106.09	159	75.5	Diethanolamine
106.0872	105	0	106.09	159	74.3	Diethanolamine
121.1229	60.032	-0.051	121.072	26	76.9	Urea
121.1229	60.032	-0.051	121.072	38	68.7	Urea
121.1229	60.032	-0.051	121.072	64	85.6	Urea
228.1067	227.12	0.021	228.1277	67	100	Ametryn
84.0822	102.092	-0.0014	84.0808	262	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	219	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	132	51	Betaine Aldehyde Cation
106.0872	105	0	106.09	169	76	Diethanolamine
106.0872	105	0	106.09	151	76.6	Diethanolamine
106.0872	105	0	106.09	200	64.3	Diethanolamine
148.0974	147	-0.04	148.06	59	51	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	149	100	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	120	100	O-Acetyl-L-Serine
103.1124	102.068	-0.037	103.0754	114	82.4	Pentanoic Acid
103.1124	102.068	-0.037	103.0754	64	100	Pentanoic Acid
121.1229	60.032	-0.051	121.072	58	80.9	Urea
121.1229	60.032	-0.051	121.072	67	83.1	Urea
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
148.0974	147	-0.04	148.06	64	54.2	O-Acetyl-L-Serine Hydrochloride
103.1124	102.068	-0.037	103.0754	204	77.3	Pentanoic Acid
103.1124	102.116	0.011	103.123	166	52	1,5-Pentanediamine
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-Hydroxyethyl)Glycine
84.0822	102.092	-0.0014	84.0808	257	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	187	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	197	55.4	Betaine Aldehyde Cation
106.0872	105	0	106.09	159	73.7	Diethanolamine

106.0872	105	0	106.09	171	72.3	Diethanolamine
106.0872	105	0	106.09	201	62.3	Diethanolamine
121.1229	60.032	-0.051	121.072	20	68.7	Urea
121.1229	60.032	-0.051	121.072	28	77.6	Urea
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
228.1067	227.12	0.021	228.1277	116	100	Ametryn
103.1124	102.068	-0.037	103.0754	195	78.2	Pentanoic Acid
103.1124	102.116	0.011	103.123	218	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	216	100	1,5-Pentanediamine
106.0872	105	0	106.09	158	79.3	Diethanolamine
106.0872	105	0	106.09	151	78.9	Diethanolamine
121.1229	60.032	-0.051	121.072	20	63.5	Urea
121.1229	60.032	-0.051	121.072	45	82.2	Urea
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.032	-0.051	121.072	59	84	Urea
148.0974	147.053	-0.037	148.0604	117	53.2	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	156	77.3	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	177	71.9	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	7	100	Cyclopentanemethanol, .Alpha.-Methyl-
84.0822	102.092	-0.0014	84.0808	277	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	205	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	164	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	148	51	Betaine Aldehyde Cation
106.0872	105	0	106.09	193	73.4	Diethanolamine
106.0872	105	0	106.09	157	73.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	100	Diethanolamine
103.1124	102.116	0.011	103.123	106	73.2	1,5-Pentanediamine
84.0822	102.092	-0.0014	84.0808	194	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	192	51	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	134	51	Betaine Aldehyde Cation
121.1229	60.032	-0.051	121.072	26	71.7	Urea
121.1229	60.032	-0.051	121.072	38	77.3	Urea
121.1229	60.058	-0.0006	121.1223	3	100	1-Propanol
121.1229	60.032	-0.051	121.072	38	80.2	Urea
148.0974	147.053	-0.037	148.0604	116	61.8	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	159	67.3	O-Acetyl-L-Serine
103.1124	102.116	0.011	103.123	101	81.9	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	222	85.2	1,5-Pentanediamine
97.0774	114.104	0.0238	97.1012	17	100	Cyclohexanemethanol
106.0872	105	0	106.09	222	73.8	Diethanolamine

106.0872	105	0	106.09	159	73.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	284	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	257	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	231	55.4	Betaine Aldehyde Cation
228.1067	227.12	0.021	228.1277	118	100	Ametryn
121.1229	60.032	-0.051	121.072	14	61.5	Urea
121.1229	60.032	-0.051	121.072	25	76.6	Urea
121.1229	60.058	-0.0006	121.1223	4	100	1-Propanol
121.1229	60.032	-0.051	121.072	45	78.6	Urea
148.0974	147.053	-0.037	148.0604	106	59.9	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	136	100	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	187	75	O-Acetyl-L-Serine
106.0872	105	0	106.09	158	76.1	Diethanolamine
106.0872	105	0	106.09	235	75.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	303	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	239	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	139	54.2	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	186	56	Betaine Aldehyde Cation
228.1067	227.12	0.021	228.1277	104	100	Ametryn
121.1229	60.032	-0.051	121.072	63	85.6	Urea
121.1229	60.032	-0.051	121.072	45	80.4	Urea
121.1229	60.032	-0.051	121.072	46	82.2	Urea
121.1229	60.032	-0.051	121.072	37	79.9	Urea
148.0974	147	-0.04	148.06	25	100	O-Acetyl-L-Serine Hydrochloride
148.0974	147.053	-0.037	148.0604	165	100	O-Acetyl-L-Serine
148.0974	147.053	-0.037	148.0604	142	76.6	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	25	19.9	Cyclohexanol, 2-Methyl-, Trans-
106.0872	105	0	106.09	155	74.4	Diethanolamine
106.0872	105	0	106.09	183	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	151	100	Diethanolamine
121.1229	60.032	-0.051	121.072	41	81.4	Urea
121.1229	60.032	-0.051	121.072	40	80.9	Urea
121.1229	60.032	-0.051	121.072	44	81.9	Urea
103.1124	102.068	-0.037	103.0754	107	100	Pentanoic Acid
103.1124	102.116	0.011	103.123	164	91.8	1,5-Pentanediamine
84.0822	102.092	-0.0014	84.0808	191	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	167	52	Betaine Aldehyde Cation
228.1067	227.12	0.021	228.1277	54	100	Ametryn
103.1124	102.116	0.011	103.123	104	63.5	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	217	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	227	100	1,5-Pentanediamine

371.2569	370.214	-0.0352	371.2217	74	32.4	17-Phenyltrnor-13,14-Dihydroprostaglandin A2
371.2569	370.222	-0.028	371.2289	46	55.4	Pyroglu-Ile-Lys
371.2569	370.214	-0.0352	371.2217	57	100	17-Phenyltrnor-13,14-Dihydroprostaglandin A2
186.0588	370.196	0.0467	186.1055	60	100	Ser-His-Lys
106.0872	105	0	106.09	159	78.6	Diethanolamine
106.0872	105	0	106.09	157	78.9	Diethanolamine
106.0872	105	0	106.09	174	79.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	317	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	256	50	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	200	54.2	Betaine Aldehyde Cation
228.1067	227.12	0.021	228.1277	114	100	Ametryn
121.1229	60.032	-0.051	121.072	26	73.2	Urea
121.1229	60.032	-0.051	121.072	53	83.3	Urea
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.032	-0.051	121.072	41	80.9	Urea
148.0974	147.053	-0.037	148.0604	158	100	O-Acetyl-L-Serine
97.0774	114.104	0.0238	97.1012	50	33.9	Cyclohexanol, 1-Methyl-
106.0872	105.079	-0.0009	106.0863	119	100	Diethanolamine
228.1067	227.12	0.021	228.1277	70	100	Ametryn
121.1229	60.032	-0.051	121.072	47	82.7	Urea
121.1229	60.032	-0.051	121.072	40	80.9	Urea
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.032	-0.051	121.072	45	82.2	Urea
106.0872	105	0	106.09	169	75	Diethanolamine
106.0872	105	0	106.09	157	75	Diethanolamine
106.0872	105.079	-0.0009	106.0863	156	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	293	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	234	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	231	52	Betaine Aldehyde Cation
103.1124	102.116	0.011	103.123	127	87.3	1,5-Pentanediamine
103.1124	102.068	-0.037	103.0754	93	100	Pentanoic Acid
118.0873	117	0	118.09	263	30.2	Betaine
118.0873	117.079	-0.001	118.0863	257	59.8	Betaine
118.0873	117.079	-0.001	118.0863	345	48.4	Betaine
186.0588	163.084	0.0149	186.0737	156	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	86	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	150	100	N,N-Bis(2-Hydroxyethyl)Glycine
84.0822	102.092	-0.0014	84.0808	196	52	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	179	53.1	Betaine Aldehyde Cation
84.0822	102.092	-0.0014	84.0808	183	50	Betaine Aldehyde Cation

118.0873	117.079	-0.001	118.0863	454	73.9	Betaine
118.0873	117.079	-0.001	118.0863	324	79.5	Betaine
118.0873	117.079	-0.001	118.0863	366	62.6	Betaine
97.0774	114.104	0.0238	97.1012	45	26.4	Cyclohexanol, 1-Methyl-
97.0774	114.104	0.0238	97.1012	28	22.2	Cycloheptanol
106.0872	105	0	106.09	159	74.6	Diethanolamine
186.0588	370.196	0.0467	186.1055	39	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	165	93.8	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	446.228	-0.0081	224.1212	87	64.7	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	218	93.1	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	300	88.4	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	392	72.2	Betaine
118.0873	117.079	-0.001	118.0863	257	65.1	Betaine
118.0873	117.079	-0.001	118.0863	268	40.1	Betaine
97.0774	114.104	0.0238	97.1012	71	25.7	Cyclohexanol, 1-Methyl-
186.0588	370.196	0.0467	186.1055	55	35.3	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	50	100	Ser-His-Lys
224.1293	223.1	-0.022	224.107	159	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	146	51	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	254	93.8	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	279	91.5	N-Acetyl-L-Tyrosine
125.9874	125	0.04	126.03	169	91.8	2-Aminoethylphosphonic Acid
125.9874	125	0.04	126.03	151	100	2-Aminoethylphosphonic Acid
125.9874	125	0.04	126.03	145	100	2-Aminoethylphosphonic Acid
186.0588	163.084	0.0149	186.0737	183	89	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	45	55.1	Cyclohexanol, 4-Methyl-, Trans-
167.0138	166.049	0.0426	167.0564	272	91.3	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	280	96.3	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	264	90.9	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	329	96.2	7-Methylxanthine
118.0873	117.079	-0.001	118.0863	206	100	Betaine
118.0873	117.079	-0.001	118.0863	479	68.2	Betaine
118.0873	117.079	-0.001	118.0863	298	60.8	Betaine
118.0873	117.079	-0.001	118.0863	345	42.1	Betaine
186.0588	163.084	0.0149	186.0737	138	85.9	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	33	100	Cyclopentanemethanol, .Alpha.-Methyl-
97.0774	114.104	0.0238	97.1012	29	23.8	Cyclohexanol, 1-Methyl-
118.0873	117.079	-0.001	118.0863	367	29.5	Betaine
118.0873	117.079	-0.001	118.0863	508	74.5	Betaine
118.0873	117.079	-0.001	118.0863	302	66.9	Betaine
118.0873	117.079	-0.001	118.0863	293	71.8	Betaine

186.0588	203.091	0.0285	186.0873	61	84.7	Ala-Asn
186.0588	163.084	0.0149	186.0737	148	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	446.228	-0.0081	224.1212	115	88	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	296	94.1	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	275	81.5	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	335	48.9	Betaine
118.0873	117.079	-0.001	118.0863	387	56.3	Betaine
118.0873	117.079	-0.001	118.0863	316	83.4	Betaine
118.0873	117.079	-0.001	118.0863	319	62.9	Betaine
186.0588	163.084	0.0149	186.0737	134	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	55	52	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	59	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	265	100	Betaine
118.0873	117.079	-0.001	118.0863	444	62.9	Betaine
118.0873	117.079	-0.001	118.0863	207	67.7	Betaine
118.0873	117.079	-0.001	118.0863	291	59.3	Betaine
186.0588	163.084	0.0149	186.0737	147	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	147	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	22	33.6	Cyclohexanol, 2-Methyl-, Trans-
140.0692	139.1	0.038	140.107	96	100	Tropinone
118.0873	117.079	-0.001	118.0863	329	42.2	Betaine
118.0873	117.079	-0.001	118.0863	378	76.4	Betaine
118.0873	117.079	-0.001	118.0863	279	69.3	Betaine
118.0873	117.079	-0.001	118.0863	355	61.4	Betaine
186.0588	163.084	0.0149	186.0737	172	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	157	84.9	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	139	100	N,N-Bis(2-Hydroxyethyl)Glycine
195.1236	194.115	-0.0009	195.1227	280	98.4	Tetraethylene Glycol
195.1236	194.115	-0.0009	195.1227	241	100	Tetraethylene Glycol
118.0873	117	0	118.09	339	24.1	Betaine
118.0873	117.079	-0.001	118.0863	506	68.9	Betaine
118.0873	117.079	-0.001	118.0863	169	61.4	Betaine
118.0873	117.079	-0.001	118.0863	283	65.8	Betaine
186.0588	163.084	0.0149	186.0737	203	92.3	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	161	94	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139.063	0.0014	140.0706	55	100	5-Amino-2-Methoxyphenol
224.1293	223.1	-0.022	224.107	138	76.6	N-Fluorenylacetamide
224.1293	446.228	-0.0081	224.1212	134	49.4	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	204	87.1	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	274	91.7	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	215	80.1	Betaine

118.0873	117.079	-0.001	118.0863	423	77.2	Betaine
118.0873	117.079	-0.001	118.0863	350	87	Betaine
118.0873	117.079	-0.001	118.0863	293	81.6	Betaine
186.0588	163.084	0.0149	186.0737	168	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	223.084	-0.0376	224.0917	203	76	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	214	100	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	314	86.1	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	245	87.3	Betaine
118.0873	117	0	118.09	359	33.3	Betaine
118.0873	117.079	-0.001	118.0863	316	71.8	Betaine
186.0588	163.084	0.0149	186.0737	137	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	223.1	-0.022	224.107	166	96.6	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	123	39.4	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	258	79.9	N-Acetyl-L-Tyrosine
224.1293	446.228	-0.0081	224.1212	186	49.5	Tyr-His-Lys
118.0873	117.079	-0.001	118.0863	303	78.1	Betaine
118.0873	117.079	-0.001	118.0863	482	65	Betaine
118.0873	117.079	-0.001	118.0863	234	66.3	Betaine
118.0873	117.079	-0.001	118.0863	215	68.6	Betaine
186.0588	370.196	0.0467	186.1055	92	43.2	Ser-His-Lys
140.0692	139.1	0.038	140.107	45	41.8	Tropinone
97.0774	114.104	0.0238	97.1012	21	21	Cyclohexanol, 1-Methyl-
224.1293	223.1	-0.022	224.107	165	79.2	N-Fluorenylacetamide
224.1293	446.228	-0.0081	224.1212	145	50.1	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	169	92.3	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	303	76.5	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	279	63.6	Betaine
118.0873	117.079	-0.001	118.0863	519	69.9	Betaine
118.0873	117.079	-0.001	118.0863	340	84	Betaine
118.0873	117.079	-0.001	118.0863	264	98.3	Betaine
186.0588	163.084	0.0149	186.0737	165	87.2	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	138	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	223.106	-0.0164	224.1129	88	100	N-Acetyl-D-Galactosaminitol
224.1293	223.084	-0.0376	224.0917	103	100	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	295	93.4	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	336	84.5	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	338	54.8	Betaine
118.0873	117.079	-0.001	118.0863	499	46	Betaine
118.0873	117.079	-0.001	118.0863	372	62.9	Betaine

118.0873	117.079	-0.001	118.0863	182	64.6	Betaine
186.0588	163.084	0.0149	186.0737	150	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	223.084	-0.0376	224.0917	193	79.9	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	279	95.8	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	320	88.7	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	358	31.6	Betaine
118.0873	117.079	-0.001	118.0863	472	58.2	Betaine
118.0873	117.079	-0.001	118.0863	289	70.2	Betaine
118.0873	117.079	-0.001	118.0863	358	70.1	Betaine
186.0588	163.084	0.0149	186.0737	141	90.4	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	48	100	Ser-His-Lys
224.1293	223.1	-0.022	224.107	154	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	168	51.6	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	141	78.6	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	156	58.6	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	296	37.6	Betaine
118.0873	117.079	-0.001	118.0863	482	63.3	Betaine
118.0873	117.079	-0.001	118.0863	321	85.2	Betaine
118.0873	117.079	-0.001	118.0863	253	44.6	Betaine
186.0588	163.084	0.0149	186.0737	158	92.3	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139.027	-0.035	140.0342	120	55.4	3-Pyridinecarboxylic Acid, 1,6-Dihydro-6-Oxo-
97.0774	114.104	0.0238	97.1012	31	20.2	Cyclohexanemethanol
224.1293	223.1	-0.022	224.107	143	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	221	52.8	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	291	95.6	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	278	72	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	421	71.1	Betaine
118.0873	117.079	-0.001	118.0863	517	67	Betaine
118.0873	117.079	-0.001	118.0863	288	67.9	Betaine
118.0873	117.079	-0.001	118.0863	373	72.5	Betaine
186.0588	163.084	0.0149	186.0737	141	85.9	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139.063	0.0014	140.0706	89	100	5-Amino-2-Methoxyphenol
224.1293	223.106	-0.0164	224.1129	97	100	N-Acetyl-D-Galactosaminitol
224.1293	446.228	-0.0081	224.1212	94	36.8	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	215	87.8	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	273	82.7	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	435	97.3	Betaine
118.0873	117.079	-0.001	118.0863	385	97	Betaine
118.0873	117.079	-0.001	118.0863	305	73.6	Betaine
186.0588	163.084	0.0149	186.0737	122	81.3	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	155	100	N,N-Bis(2-Hydroxyethyl)Glycine

224.1293	446.228	-0.0081	224.1212	154	45.8	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	320	94.9	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	137	58.6	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	188	100	Betaine
118.0873	117.079	-0.001	118.0863	426	73.8	Betaine
118.0873	117.079	-0.001	118.0863	307	74.9	Betaine
118.0873	117.079	-0.001	118.0863	450	98.7	Betaine
186.0588	163.084	0.0149	186.0737	110	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	50	25.9	Cyclohexanol, 1-Methyl-
97.0774	114.104	0.0238	97.1012	30	23.8	Cyclohexanol, 1-Methyl-
224.1293	223.1	-0.022	224.107	171	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	179	48.5	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	354	91.2	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	236	78.9	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	220	69.2	Betaine
118.0873	117.079	-0.001	118.0863	498	67.3	Betaine
118.0873	117.079	-0.001	118.0863	292	73.6	Betaine
118.0873	117.079	-0.001	118.0863	296	49.5	Betaine
186.0588	370.196	0.0467	186.1055	54	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	37	26.6	Cyclohexanol, 1-Methyl-
224.1293	223.1	-0.022	224.107	151	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	205	80.4	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	262	93.7	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	294	89.1	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	573	78	Betaine
118.0873	117.079	-0.001	118.0863	252	80.8	Betaine
118.0873	117.079	-0.001	118.0863	360	75.3	Betaine
186.0588	203.091	0.0285	186.0873	70	72.7	Ala-Asn
186.0588	370.196	0.0467	186.1055	58	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	39	21.9	Cyclohexanol, 1-Methyl-
224.1293	223.1	-0.022	224.107	124	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	174	47.6	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	311	95.9	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	273	86.4	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	60	83	5-Aminovaleric Acid
118.0873	117.079	-0.001	118.0863	499	69	Betaine
118.0873	117.079	-0.001	118.0863	354	83.8	Betaine
118.0873	117.079	-0.001	118.0863	331	68.7	Betaine
186.0588	203.091	0.0285	186.0873	70	100	Ala-Asn
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	48	26.3	Cyclohexanol, 1-Methyl-

97.0774	114.104	0.0238	97.1012	38	25.3	Cyclohexanol, 1-Methyl-
224.1293	223.1	-0.022	224.107	157	84	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	126	56.6	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	257	100	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	265	88.3	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	342	72.3	Betaine
118.0873	117.079	-0.001	118.0863	430	43.8	Betaine
118.0873	117.079	-0.001	118.0863	295	78.8	Betaine
118.0873	117.079	-0.001	118.0863	265	72.3	Betaine
186.0588	163.084	0.0149	186.0737	179	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	150	87.5	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	154	100	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139	0.04	140.11	51	100	Tropinone
97.0774	114.104	0.0238	97.1012	69	20.1	Cyclohexanemethanol
224.1293	446.228	-0.0081	224.1212	167	46.8	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	181	87.5	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	288	86.9	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	313	66.2	Betaine
118.0873	117.079	-0.001	118.0863	439	44.1	Betaine
118.0873	117.079	-0.001	118.0863	372	59.1	Betaine
118.0873	117.079	-0.001	118.0863	291	44	Betaine
186.0588	370.196	0.0467	186.1055	105	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	149	100	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139.063	0.0014	140.0706	30	100	5-Amino-2-Methoxyphenol
97.0774	114.104	0.0238	97.1012	69	23.8	Cyclohexanol, 1-Methyl-
195.1236	194.115	-0.0009	195.1227	276	100	Tetraethylene Glycol
195.1236	194.115	-0.0009	195.1227	278	100	Tetraethylene Glycol
195.1236	194.115	-0.0009	195.1227	261	100	Tetraethylene Glycol
118.0873	117.079	-0.001	118.0863	246	100	Betaine
118.0873	117.079	-0.001	118.0863	443	34.9	Betaine
118.0873	117.079	-0.001	118.0863	372	100	Betaine
118.0873	117.079	-0.001	118.0863	264	75.6	Betaine
186.0588	163.084	0.0149	186.0737	132	80.4	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	150	91.4	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	370.196	0.0467	186.1055	54	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	176	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	223.1	-0.022	224.107	143	83.1	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	160	45.6	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	165	100	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	312	94.2	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	558	97.9	Betaine

118.0873	117.079	-0.001	118.0863	235	76.5	Betaine
118.0873	117.079	-0.001	118.0863	270	70.2	Betaine
186.0588	163.084	0.0149	186.0737	167	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	223.084	-0.0376	224.0917	233	71	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	302	96	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	267	81	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	485	44.5	Betaine
118.0873	117.079	-0.001	118.0863	259	81	Betaine
118.0873	117.079	-0.001	118.0863	397	67.4	Betaine
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	159	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	70	26.2	Cyclohexanol, 1-Methyl-
224.1293	446.228	-0.0081	224.1212	131	57.9	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	321	94.7	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	221	77.8	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	329	55.9	Betaine
118.0873	117.079	-0.001	118.0863	501	70.4	Betaine
118.0873	117.079	-0.001	118.0863	275	75.2	Betaine
118.0873	117.079	-0.001	118.0863	280	73.1	Betaine
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	155	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	46	23.7	Cyclohexanol, 1-Methyl-
224.1293	223.1	-0.022	224.107	133	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	146	54.5	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	213	91.4	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	192	76.3	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	306	77	Betaine
118.0873	117.079	-0.001	118.0863	445	63.7	Betaine
118.0873	117.079	-0.001	118.0863	232	62.8	Betaine
118.0873	117.079	-0.001	118.0863	237	69.5	Betaine
186.0588	203.091	0.0285	186.0873	68	100	Ala-Asn
186.0588	370.196	0.0467	186.1055	66	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	133	100	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139.063	0.0014	140.0706	59	52	5-Amino-2-Methoxyphenol
224.1293	446.228	-0.0081	224.1212	102	68.9	Tyr-His-Lys
224.1293	223.1	-0.022	224.107	133	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	173	100	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	346	94.3	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	485	43	Betaine
118.0873	117.079	-0.001	118.0863	236	72.2	Betaine
118.0873	117.079	-0.001	118.0863	267	42.2	Betaine

186.0588	163.084	0.0149	186.0737	153	92.1	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139.027	-0.035	140.0342	19	100	3-Pyridinecarboxylic Acid, 1,6-Dihydro-6-Oxo-
140.0692	139.027	-0.035	140.0342	80	100	3-Pyridinecarboxylic Acid, 1,6-Dihydro-6-Oxo-
97.0774	114.104	0.0238	97.1012	134	45.3	Cyclohexanol, 1-Methyl-
195.1236	194.115	-0.0009	195.1227	279	100	Tetraethylene Glycol
195.1236	194.115	-0.0009	195.1227	281	100	Tetraethylene Glycol
118.0873	117.079	-0.001	118.0863	262	83.6	Betaine
118.0873	117.079	-0.001	118.0863	491	65.7	Betaine
118.0873	117.079	-0.001	118.0863	227	69.4	Betaine
118.0873	117.079	-0.001	118.0863	310	63.7	Betaine
186.0588	370.196	0.0467	186.1055	55	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139.063	0.0014	140.0706	27	100	5-Amino-2-Methoxyphenol
97.0774	114.104	0.0238	97.1012	44	25.9	Cyclohexanemethanol
224.1293	223.1	-0.022	224.107	139	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	199	50.3	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	287	97.4	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	298	89.9	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	414	90	Betaine
118.0873	117.079	-0.001	118.0863	459	41.6	Betaine
118.0873	117.079	-0.001	118.0863	331	98.8	Betaine
118.0873	117.079	-0.001	118.0863	221	73.2	Betaine
186.0588	370.196	0.0467	186.1055	74	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	131	100	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139.1	0.038	140.107	38	100	Tropinone
224.1293	223.084	-0.0376	224.0917	178	100	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	161	45	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	362	96.5	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	308	90.6	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	361	28.4	Betaine
118.0873	117.079	-0.001	118.0863	441	72.7	Betaine
118.0873	117.079	-0.001	118.0863	354	85.7	Betaine
118.0873	117.079	-0.001	118.0863	433	64.6	Betaine
186.0588	163.084	0.0149	186.0737	137	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	90	44.5	Cyclohexanol, 1-Methyl-
97.0774	114.104	0.0238	97.1012	39	22.1	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	21	32.3	Cyclohexanol, 1-Methyl-
224.1293	223.084	-0.0376	224.0917	230	46.1	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	274	89.5	N-Acetyl-L-Tyrosine

224.1293	223.084	-0.0376	224.0917	209	89.6	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	331	59.8	Betaine
118.0873	117.079	-0.001	118.0863	532	67.2	Betaine
118.0873	117.079	-0.001	118.0863	286	76.1	Betaine
118.0873	117.079	-0.001	118.0863	234	65	Betaine
186.0588	203.091	0.0285	186.0873	75	76.9	Ala-Asn
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	152	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	223.106	-0.0164	224.1129	82	100	N-Acetyl-D-Galactosaminitol
224.1293	223.084	-0.0376	224.0917	174	54.2	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	267	91.7	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	173	68.1	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	220	100	Betaine
118.0873	117.079	-0.001	118.0863	416	55.2	Betaine
118.0873	117.079	-0.001	118.0863	256	69.3	Betaine
118.0873	117.079	-0.001	118.0863	296	73.5	Betaine
140.0692	139.063	0.0014	140.0706	40	100	5-Amino-2-Methoxyphenol
186.0588	163.084	0.0149	186.0737	89	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	24	33.6	Cyclohexanol, 1-Methyl-
195.1236	194.115	-0.0009	195.1227	345	100	Tetraethylene Glycol
195.1236	194.115	-0.0009	195.1227	297	100	Tetraethylene Glycol
195.1236	194.115	-0.0009	195.1227	266	100	Tetraethylene Glycol
195.1236	194.115	-0.0009	195.1227	263	100	Tetraethylene Glycol
118.0873	117.079	-0.001	118.0863	237	97.7	Betaine
118.0873	117.079	-0.001	118.0863	569	74.2	Betaine
118.0873	117.079	-0.001	118.0863	306	76.3	Betaine
118.0873	117.079	-0.001	118.0863	449	85.8	Betaine
186.0588	163.084	0.0149	186.0737	137	76.6	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	30	24.5	Cyclohexanol, 1-Methyl-
118.0873	117.079	-0.001	118.0863	278	60.5	Betaine
118.0873	117.079	-0.001	118.0863	490	47	Betaine
118.0873	117.079	-0.001	118.0863	424	98.2	Betaine
118.0873	117.079	-0.001	118.0863	316	74.8	Betaine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	26	58.6	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	25	33.6	Cyclohexanol, 1-Methyl-
224.1293	223.084	-0.0376	224.0917	184	55.3	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	300	92.1	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	259	83.3	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	306	70.4	Betaine

118.0873	117.079	-0.001	118.0863	542	75.2	Betaine
118.0873	117.079	-0.001	118.0863	361	94.6	Betaine
118.0873	117.079	-0.001	118.0863	399	63.6	Betaine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	223.1	-0.022	224.107	134	93.1	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	152	45.7	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	269	92.8	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	275	87	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	369	63	Betaine
118.0873	117.079	-0.001	118.0863	492	67.8	Betaine
118.0873	117.079	-0.001	118.0863	405	95.2	Betaine
118.0873	117.079	-0.001	118.0863	299	67.6	Betaine
186.0588	163.084	0.0149	186.0737	174	100	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139.063	0.0014	140.0706	78	59.3	3-Amino-2,3-Dihydrobenzoic Acid
97.0774	114.104	0.0238	97.1012	18	100	Cyclohexanemethanol
195.1236	194.115	-0.0009	195.1227	139	92.3	Tetraethylene Glycol
195.1236	194.115	-0.0009	195.1227	332	100	Tetraethylene Glycol
195.1236	194.115	-0.0009	195.1227	263	100	Tetraethylene Glycol
118.0873	117.079	-0.001	118.0863	325	69.7	Betaine
118.0873	117.079	-0.001	118.0863	459	57.5	Betaine
118.0873	117.079	-0.001	118.0863	322	61.6	Betaine
118.0873	117.079	-0.001	118.0863	313	64.9	Betaine
140.0692	139.1	0.038	140.107	131	100	Tropinone
186.0588	370.196	0.0467	186.1055	87	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	47	20.6	Cyclohexanol, 4-Methyl-, Trans-
97.0774	114.104	0.0238	97.1012	22	32	Cyclohexanol, 1-Methyl-
224.1293	446.228	-0.0081	224.1212	162	50.8	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	259	88.8	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	268	80.1	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	254	89.1	Betaine
118.0873	117.079	-0.001	118.0863	465	98.4	Betaine
118.0873	117.079	-0.001	118.0863	215	72.5	Betaine
118.0873	117.079	-0.001	118.0863	374	66.6	Betaine
186.0588	163.084	0.0149	186.0737	159	100	N,N-Bis(2-Hydroxyethyl)Glycine
140.0692	139.063	0.0014	140.0706	94	55.3	3-Amino-2,3-Dihydrobenzoic Acid
224.1293	241.117	-0.0151	224.1142	25	100	(6R)-5,6,7,8-Tetrahydrobiopterin
224.1293	223.1	-0.022	224.107	101	41.3	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	336	97.5	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	301	91.2	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	469	97.8	Betaine
118.0873	117.079	-0.001	118.0863	355	98.6	Betaine

118.0873	117.079	-0.001	118.0863	333	75.7	Betaine
186.0588	163.084	0.0149	186.0737	110	100	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	102	100	N,N-Bis(2-Hydroxyethyl)Glycine
97.0774	114.104	0.0238	97.1012	38	23.9	Cyclohexanol, 1-Methyl-
97.0774	114.104	0.0238	97.1012	44	19.2	Cyclohexanol, 4-Methyl-, Trans-
224.1293	223.106	-0.0164	224.1129	121	100	N-Acetyl-D-Galactosaminitol
224.1293	223.084	-0.0376	224.0917	151	49.2	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	261	93	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	230	90.7	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	278	100	Betaine
118.0873	117.079	-0.001	118.0863	479	67.2	Betaine
118.0873	117.079	-0.001	118.0863	364	77	Betaine
118.0873	117.079	-0.001	118.0863	178	61.7	Betaine
186.0588	163.084	0.0149	186.0737	86	54.5	N,N-Bis(2-Hydroxyethyl)Glycine
186.0588	163.084	0.0149	186.0737	158	100	N,N-Bis(2-Hydroxyethyl)Glycine
224.1293	446.228	-0.0081	224.1212	123	67.9	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	307	97.2	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	214	61.1	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	227	81.1	Betaine
118.0873	117.079	-0.001	118.0863	475	66.8	Betaine
118.0873	117.079	-0.001	118.0863	320	83.8	Betaine
118.0873	117.079	-0.001	118.0863	231	39	Betaine
186.0588	370.196	0.0467	186.1055	41	100	Ser-His-Lys
140.0692	139.063	0.0014	140.0706	41	100	5-Amino-2-Methoxyphenol
140.0692	139.063	0.0014	140.0706	89	56.6	3-Amino-2,3-Dihydrobenzoic Acid
97.0774	114.104	0.0238	97.1012	40	23.5	Cyclohexanol, 1-Methyl-
224.1293	223.084	-0.0376	224.0917	185	70.9	N-Acetyl-L-Tyrosine
224.1293	446.228	-0.0081	224.1212	95	76.9	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	276	97.1	N-Acetyl-L-Tyrosine
224.1293	223.084	-0.0376	224.0917	304	90.8	N-Acetyl-L-Tyrosine
118.0873	117.079	-0.001	118.0863	390	70.2	Betaine
118.0873	117.079	-0.001	118.0863	527	70.7	Betaine
118.0873	117.079	-0.001	118.0863	305	85.4	Betaine
118.0873	117.079	-0.001	118.0863	265	54	Betaine

Table A7. List of non-volatile metabolites (LC/MS) for managed population animals. Samples collected in Dec 2011 from multiple animals were pooled. Experiment was conducted using specialized lipids fraction protocol on RP column (refer to Materials and Methods section) in positive ion mode. Top three matches are given for each compound.

Parent m/z	Mass	Delta (m/z)	Library Precursor m/z	Match Score	Probability (%)	Chem ID
118.0873	117.079	-0.001	118.0863	220	67.5	Betaine
118.0873	117.079	-0.001	118.0863	213	67.5	Betaine
118.0873	117.079	-0.001	118.0863	212	67.5	Betaine
118.0873	117.079	-0.001	118.0863	452	58.8	Betaine
118.0873	117.079	-0.001	118.0863	450	58.8	Betaine
118.0873	117.079	-0.001	118.0863	446	58.8	Betaine
118.0873	117.079	-0.001	118.0863	340	82.5	Betaine
118.0873	117.079	-0.001	118.0863	334	82.5	Betaine
118.0873	117.079	-0.001	118.0863	321	82.5	Betaine
118.0873	117.079	-0.001	118.0863	352	65.8	Betaine
118.0873	117.079	-0.001	118.0863	351	65.8	Betaine
118.0873	117.079	-0.001	118.0863	350	65.8	Betaine
224.1293	223.106	-0.0164	224.1129	65	56.6	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	64	56.6	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	62	56.6	N-Acetyl-D-galactosaminitol
224.1293	223.084	-0.0376	224.0917	159	47	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	152	36	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	142	47	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	202	89.1	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	125	10.9	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	218	79.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	197	79.4	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	172	16.8	Tyr-His-Lys
118.0873	117.079	-0.001	118.0863	382	100	Betaine
118.0873	117.079	-0.001	118.0863	376	100	Betaine
118.0873	117.079	-0.001	118.0863	371	100	Betaine
118.0873	117.079	-0.001	118.0863	460	45.1	Betaine
118.0873	117.079	-0.001	118.0863	455	45.1	Betaine
118.0873	117.079	-0.001	118.0863	451	45.1	Betaine
118.0873	117.079	-0.001	118.0863	322	81.8	Betaine
118.0873	117.079	-0.001	118.0863	321	81.8	Betaine
118.0873	117.079	-0.001	118.0863	311	81.8	Betaine
118.0873	117.079	-0.001	118.0863	207	66.5	Betaine
118.0873	117.079	-0.001	118.0863	206	66.5	Betaine
118.0873	117.079	-0.001	118.0863	202	66.5	Betaine
186.0588	370.196	0.0467	186.1055	52	100	Ser-His-Lys
224.1293	223.084	-0.0376	224.0917	307	90.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	290	90.4	N-Acetyl-L-tyrosine

224.1293	223.084	-0.0376	224.0917	255	90.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	205	76.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	190	76.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	173	76.2	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	318	32.2	Betaine
118.0873	117.079	-0.001	118.0863	318	32.2	Betaine
118.0873	117.079	-0.001	118.0863	316	32.2	Betaine
118.0873	117.079	-0.001	118.0863	472	64.4	Betaine
118.0873	117.079	-0.001	118.0863	468	64.4	Betaine
118.0873	117.079	-0.001	118.0863	467	64.4	Betaine
118.0873	117.079	-0.001	118.0863	275	67.5	Betaine
118.0873	117.079	-0.001	118.0863	275	67.5	Betaine
118.0873	117.079	-0.001	118.0863	271	67.5	Betaine
118.0873	117.079	-0.001	118.0863	368	68.7	Betaine
118.0873	117.079	-0.001	118.0863	364	68.7	Betaine
118.0873	117.079	-0.001	118.0863	361	68.7	Betaine
186.0588	163.084	0.0149	186.0737	117	80.1	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	91	80.1	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	64	15.8	Ala-Asn
224.1293	223.106	-0.0164	224.1129	42	58.6	N-Acetyl-D-galactosaminitol
224.1293	241.117	-0.0151	224.1142	32	41.4	((6R)-5,6,7,8-Tetrahydrobiopterin
224.1293	446.228	-0.0081	224.1212	120	49.7	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	116	42	N-Acetyl-L-tyrosine
224.1293	223.106	-0.0164	224.1129	62	8.2	N-Acetyl-D-galactosaminitol
224.1293	223.084	-0.0376	224.0917	249	55.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	246	55.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	239	55.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	205	77.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	190	77.6	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	177	22.4	Tyr-His-Lys
224.1293	223.106	-0.0164	224.1129	93	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	92	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	89	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	86	100	N-Acetyl-D-galactosaminitol
243.1858	220.183	-0.0139	243.1719	64	100	Butylated hydroxytoluene
243.1858	220.183	-0.0139	243.1719	48	100	Butylated hydroxytoluene
118.0959	117.079	-0.0096	118.0863	295	100	Betaine
118.0959	117.079	-0.0096	118.0863	293	100	Betaine
118.0959	117.079	-0.0096	118.0863	288	100	Betaine
118.0959	117.079	-0.0096	118.0863	268	96.4	Betaine
118.0959	117.079	-0.0096	118.0863	263	96.4	Betaine
118.0959	117.079	-0.0096	118.0863	221	96.4	Betaine
118.0959	117.079	-0.0096	118.0863	332	31.6	Betaine
118.0959	117.079	-0.0096	118.0863	330	31.6	Betaine
118.0959	117.079	-0.0096	118.0863	328	31.6	Betaine
139.0603	138.032	-0.021	139.039	120	37.2	Salicylic acid
139.0603	138.068	0.0151	139.0754	116	31.4	Benzeneethanol, 2-hydroxy-

139.0603	138.068	0.0151	139.0754	115	31.4	Benzeneethanol, 2-hydroxy-
139.0603	138.043	-0.0101	139.0502	163	28.4	4-Imidazoleacrylic acid
139.0603	138.043	-0.0101	139.0502	161	28.4	4-Imidazoleacrylic acid
139.0603	138	-0.01	139.05	161	26.2	urocanic acid
139.0603	138.043	-0.0101	139.0502	163	72.5	4-Imidazoleacrylic acid
139.0603	138.043	-0.0101	139.0502	162	72.5	4-Imidazoleacrylic acid
139.0603	138.043	-0.0101	139.0502	159	72.5	4-Imidazoleacrylic acid
273.1777	290.225	0.0436	273.2213	67	73.2	5-Androsten-3.beta.,17.beta.-diol
273.1777	290.225	0.0436	273.2213	65	73.2	5-Androsten-3.beta.,17.beta.-diol
273.1777	290.225	0.0436	273.2213	65	73.2	5-Androsten-3.beta.,17.beta.-diol
273.1777	290.225	0.0436	273.2213	102	42	5-Androsten-3.beta.,17.beta.-diol
273.1777	290.225	0.0436	273.2213	101	42	5-Androsten-3.beta.,17.beta.-diol
273.1777	290.225	0.0436	273.2213	89	42	5-Androsten-3.beta.,17.beta.-diol
195.1333	194.115	-0.0106	195.1227	209	100	Tetraethylene glycol
195.1333	194.115	-0.0106	195.1227	205	100	Tetraethylene glycol
195.1333	194.115	-0.0106	195.1227	176	100	Tetraethylene glycol
432.2891	449.314	0.0217	432.3108	66	100	Glycodeoxycholic acid
387.1819	386	-0.05	387.13	258	28.5	1-O-b-D-glucopyranosyl sinapate
387.1819	386	-0.05	387.13	250	21.3	1-O-b-D-glucopyranosyl sinapate
387.1819	386	-0.05	387.13	244	16.7	1-O-b-D-glucopyranosyl sinapate
387.1819	193.074	-0.0268	387.1551	252	31.3	Hippuric acid, methyl ester
387.1819	193.074	-0.0268	387.1551	251	31.3	Hippuric acid, methyl ester
387.1819	193.074	-0.0268	387.1551	243	31.3	Hippuric acid, methyl ester
387.1819	193.074	-0.0268	387.1551	301	54.5	Hippuric acid, methyl ester
387.1819	193.074	-0.0268	387.1551	301	54.5	Hippuric acid, methyl ester
387.1819	193.074	-0.0268	387.1551	293	54.5	Hippuric acid, methyl ester
387.1819	193.074	-0.0268	387.1551	237	28.3	Hippuric acid, methyl ester
387.1819	193.074	-0.0268	387.1551	236	28.3	Hippuric acid, methyl ester
387.1819	193.074	-0.0268	387.1551	232	28.3	Hippuric acid, methyl ester
404.2081	403.207	0.006	404.214	79	12.7	Gln-Glu-Lys
404.2081	403.207	0.006	404.214	77	11.7	Gln-Glu-Lys
404.2081	403.207	0.006	404.214	75	10.8	Gln-Glu-Lys
404.2081	403.222	0.0211	404.2292	16	11.4	Trp-Ala-Lys
404.2081	403.222	0.0211	404.2292	15	11	Trp-Ala-Lys
404.2081	403.254	0.0535	404.2616	13	10.2	Arg-Thr-Lys
404.2081	403.207	0.006	404.214	49	42.5	Gln-Glu-Lys
404.2081	403.218	0.0171	404.2252	32	23.2	Thr-Gln-Arg
404.2081	403.207	0.006	404.214	10	9.2	Gln-Glu-Lys
404.2081	403.207	0.006	404.214	64	17.2	Gln-Glu-Lys
404.2081	403.207	0.006	404.214	55	12.5	Glu-Gln-Lys
404.2081	403.218	0.0171	404.2252	52	11.1	Thr-Gln-Arg
409.1633	386.17	-0.0038	409.1595	113	81.2	Aminophenyl)ethyladenosine
409.1633	408.186	0.0305	409.1938	73	18.8	Met-Met-Lys
409.1633	386.17	-0.0038	409.1595	42	81.2	Aminophenyl)ethyladenosine
343.291	408.288	-0.0267	343.2643	88	100	Cholic acid
343.291	408.288	-0.0267	343.2643	63	100	Cholic acid
343.291	408.288	-0.0267	343.2643	47	100	Cholic acid

387.176	193.074	-0.0209	387.1551	237	100	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	237	100	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	236	100	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	264	69	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	260	69	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	260	69	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	266	100	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	264	100	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	264	100	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	308	49.2	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	306	49.2	Hippuric acid, methyl ester
387.176	193.074	-0.0209	387.1551	304	49.2	Hippuric acid, methyl ester
118.0821	117.079	0.0042	118.0863	392	68.2	Betaine
118.0821	117.079	0.0042	118.0863	389	68.2	Betaine
118.0821	117.079	0.0042	118.0863	389	68.2	Betaine
118.0821	117.079	0.0042	118.0863	547	97.5	Betaine
118.0821	117.079	0.0042	118.0863	542	97.5	Betaine
118.0821	117.079	0.0042	118.0863	531	97.5	Betaine
118.0821	117.079	0.0042	118.0863	345	76.5	Betaine
118.0821	117.079	0.0042	118.0863	335	76.5	Betaine
118.0821	117.079	0.0042	118.0863	319	76.5	Betaine
118.0821	117.079	0.0042	118.0863	376	35.4	Betaine
118.0821	117.079	0.0042	118.0863	373	35.4	Betaine
118.0821	117	0.01	118.09	368	26.4	Betaine
118.0873	117.079	-0.001	118.0863	344	100	Betaine
118.0873	117.079	-0.001	118.0863	337	100	Betaine
118.0873	117.079	-0.001	118.0863	333	100	Betaine
118.0873	117.079	-0.001	118.0863	365	31.3	Betaine
118.0873	117.079	-0.001	118.0863	364	31.3	Betaine
118.0873	117.079	-0.001	118.0863	361	31.3	Betaine
118.0873	117.079	-0.001	118.0863	294	66.7	Betaine
118.0873	117.079	-0.001	118.0863	291	66.7	Betaine
118.0873	117.079	-0.001	118.0863	288	66.7	Betaine
118.0873	117	0	118.09	317	27.8	Betaine
118.0873	117.079	-0.001	118.0863	315	25.7	Betaine
118.0873	117.079	-0.001	118.0863	312	25.7	Betaine
118.0873	117.079	-0.001	118.0863	424	62.4	Betaine
118.0873	117.079	-0.001	118.0863	420	62.4	Betaine
118.0873	117.079	-0.001	118.0863	415	62.4	Betaine
118.0873	117.079	-0.001	118.0863	295	68.2	Betaine
118.0873	117.079	-0.001	118.0863	295	68.2	Betaine
118.0873	117.079	-0.001	118.0863	291	68.2	Betaine
118.0873	117.079	-0.001	118.0863	321	70.2	Betaine
118.0873	117.079	-0.001	118.0863	320	70.2	Betaine
118.0873	117.079	-0.001	118.0863	316	70.2	Betaine
288.2597	270.219	-0.0064	288.2533	61	100	Surfynol PSA-336
288.2547	287.196	-0.052	288.203	89	20.4	Leu-Arg

288.2547	287.196	-0.052	288.203	89	20.4	Arg-Leu
288.2547	287.196	-0.052	288.203	83	16	Leu-Arg
288.2547	287.196	-0.052	288.203	271	67.2	Leu-Arg
288.2547	287.196	-0.052	288.203	232	15.9	Arg-Leu
288.2547	287.196	-0.052	288.203	225	12.1	Arg-Ile
288.2547	287.196	-0.052	288.203	116	32.9	Leu-Arg
288.2547	287.196	-0.052	288.203	110	25.8	Arg-Leu
288.2547	287.196	-0.052	288.203	99	17.7	Arg-Ile
118.0873	117.079	-0.001	118.0863	449	66.5	Betaine
118.0873	117.079	-0.001	118.0863	444	66.5	Betaine
118.0873	117.079	-0.001	118.0863	438	66.5	Betaine
118.0873	117.079	-0.001	118.0863	309	68.9	Betaine
118.0873	117.079	-0.001	118.0863	308	68.9	Betaine
118.0873	117.079	-0.001	118.0863	304	68.9	Betaine
118.0873	117.079	-0.001	118.0863	299	73.6	Betaine
118.0873	117.079	-0.001	118.0863	297	73.6	Betaine
118.0873	117.079	-0.001	118.0863	291	73.6	Betaine
244.2278	226.193	-0.0007	244.2271	146	100	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
244.2278	226.193	-0.0007	244.2271	135	100	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
304.3018	304.3	-0.0019	304.2999	183	12.9	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	183	12.9	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	177	10.2	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	301	46	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	227	6.1	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	225	5.6	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	170	15.6	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	168	14.3	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	165	12.7	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	182	10.4	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	180	9.6	Benzyl dodecyl dimethylammonium cation
304.3018	304.3	-0.0019	304.2999	176	8.1	Benzyl dodecyl dimethylammonium cation
118.0873	117.079	-0.001	118.0863	378	34.6	Betaine
118.0873	117.079	-0.001	118.0863	376	34.6	Betaine

118.0873	117.079	-0.001	118.0863	372	34.6	Betaine
118.0873	117.079	-0.001	118.0863	333	81.7	Betaine
118.0873	117.079	-0.001	118.0863	332	81.7	Betaine
118.0873	117.079	-0.001	118.0863	323	81.7	Betaine
118.0873	117.079	-0.001	118.0863	376	62.6	Betaine
118.0873	117.079	-0.001	118.0863	373	62.6	Betaine
118.0873	117.079	-0.001	118.0863	372	62.6	Betaine
186.0588	370.196	0.0467	186.1055	65	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	62	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	302	68.4	Betaine
118.0873	117.079	-0.001	118.0863	301	68.4	Betaine
118.0873	117.079	-0.001	118.0863	293	68.4	Betaine
118.0873	117.079	-0.001	118.0863	391	39.1	Betaine
118.0873	117.079	-0.001	118.0863	389	39.1	Betaine
118.0873	117.079	-0.001	118.0863	383	39.1	Betaine
118.0873	117.079	-0.001	118.0863	320	100	Betaine
118.0873	117.079	-0.001	118.0863	318	100	Betaine
118.0873	117.079	-0.001	118.0863	308	100	Betaine
118.0873	117.079	-0.001	118.0863	346	60.5	Betaine
118.0873	117.079	-0.001	118.0863	343	60.5	Betaine
118.0873	117.079	-0.001	118.0863	341	60.5	Betaine
267.1739	266.165	-0.002	267.172	266	100	Tributyl phosphate
267.1739	266.165	-0.002	267.172	266	100	Tributyl phosphate
267.1739	266.165	-0.002	267.172	266	100	Tributyl phosphate
118.0873	117.079	-0.001	118.0863	331	98.4	Betaine
118.0873	117.079	-0.001	118.0863	326	98.4	Betaine
118.0873	117.079	-0.001	118.0863	323	98.4	Betaine
118.0873	117.079	-0.001	118.0863	437	72	Betaine
118.0873	117.079	-0.001	118.0863	426	72	Betaine
118.0873	117.079	-0.001	118.0863	421	72	Betaine
118.0873	117.079	-0.001	118.0863	317	74.1	Betaine
118.0873	117.079	-0.001	118.0863	317	74.1	Betaine
118.0873	117.079	-0.001	118.0863	308	74.1	Betaine
118.0873	117.079	-0.001	118.0863	312	55.2	Betaine
118.0873	117.079	-0.001	118.0863	310	55.2	Betaine
118.0873	117.079	-0.001	118.0863	308	55.2	Betaine
118.0873	117.079	-0.001	118.0863	409	52.8	Betaine
118.0873	117.079	-0.001	118.0863	409	52.8	Betaine
118.0873	117.079	-0.001	118.0863	401	52.8	Betaine
118.0873	117.079	-0.001	118.0863	350	59.1	Betaine
118.0873	117.079	-0.001	118.0863	346	59.1	Betaine
118.0873	117.079	-0.001	118.0863	344	59.1	Betaine
118.0873	117.079	-0.001	118.0863	347	58.6	Betaine
118.0873	117.079	-0.001	118.0863	342	58.6	Betaine
118.0873	117.079	-0.001	118.0863	342	58.6	Betaine
279.1625	278.152	-0.0035	279.1591	251	81.2	Dibutyl phthalate
279.1625	278.152	-0.0035	279.1591	251	81.2	Dibutyl phthalate

279.1625	278.152	-0.0035	279.1591	249	81.2	Dibutyl phthalate
279.1625	278.152	-0.0035	279.1591	250	96.5	Dibutyl phthalate
279.1625	278.152	-0.0035	279.1591	250	96.5	Dibutyl phthalate
279.1625	278.152	-0.0035	279.1591	248	96.5	Dibutyl phthalate
279.1625	278.152	-0.0035	279.1591	308	96	Dibutyl phthalate
279.1625	278.152	-0.0035	279.1591	300	96	Dibutyl phthalate
279.1625	278.152	-0.0035	279.1591	299	96	Dibutyl phthalate
279.1625	278.152	-0.0035	279.1591	284	97	Dibutyl phthalate
279.1625	278.152	-0.0035	279.1591	282	97	Dibutyl phthalate
279.1625	278.152	-0.0035	279.1591	281	97	Dibutyl phthalate
399.2537	398.243	-0.0031	399.2506	165	100	Tris(butoxyethyl) phosphate
399.2537	398.243	-0.0031	399.2506	164	100	Tris(butoxyethyl) phosphate
399.2537	398.243	-0.0031	399.2506	159	100	Tris(butoxyethyl) phosphate
399.2537	398.243	-0.0031	399.2506	113	100	Tris(butoxyethyl) phosphate
399.2537	398.243	-0.0031	399.2506	113	100	Tris(butoxyethyl) phosphate
399.2537	398.243	-0.0031	399.2506	110	100	Tris(butoxyethyl) phosphate
444.3346	443.297	-0.0305	444.3041	62	27.4	Arg-Ile-Arg
444.3346	443.297	-0.0305	444.3041	58	23.1	Arg-Ile-Arg
444.3346	443.297	-0.0305	444.3041	48	16.3	Arg-Ile-Arg
532.3865	514.318	-0.0351	532.3514	207	100	3,6,9,12,15-Pentaoxonacosan-1-ol, hydrogen sulfate
532.3865	514.318	-0.0351	532.3514	129	100	3,6,9,12,15-Pentaoxonacosan-1-ol, hydrogen sulfate
400.3098	399.259	-0.0431	400.2667	17	18.5	Arg-Pro-Lys
400.3098	399.259	-0.0431	400.2667	14	16.3	Arg-Pro-Lys
400.3098	399.259	-0.0431	400.2667	13	15.7	Arg-Pro-Lys
186.0588	163.084	0.0149	186.0737	128	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	448	48.6	Betaine
118.0873	117.079	-0.001	118.0863	447	48.6	Betaine
118.0873	117.079	-0.001	118.0863	442	48.6	Betaine
118.0873	117.079	-0.001	118.0863	319	74	Betaine
118.0873	117.079	-0.001	118.0863	311	74	Betaine
118.0873	117.079	-0.001	118.0863	295	74	Betaine
118.0873	117.079	-0.001	118.0863	343	65.7	Betaine
118.0873	117.079	-0.001	118.0863	342	65.7	Betaine
118.0873	117.079	-0.001	118.0863	341	65.7	Betaine
97.0774	114.104	0.0238	97.1012	23	62.3	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	15	62.3	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	15	62.3	Cyclohexanemethanol
332.332	332.332	-0.0009	332.3312	225	11.3	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	223	10.5	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	221	9.6	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	237	26.7	Benzyl tetradecyl dimethylammonium cation

332.332	332.332	-0.0009	332.3312	219	13.8	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	211	10.3	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	170	12.8	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	169	12.4	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	165	10.4	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	213	18.3	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	207	14.4	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	204	12.7	Benzyl tetradecyl dimethylammonium cation
118.0873	117.079	-0.001	118.0863	385	71.1	Betaine
118.0873	117.079	-0.001	118.0863	383	71.1	Betaine
118.0873	117.079	-0.001	118.0863	375	71.1	Betaine
118.0873	117.079	-0.001	118.0863	295	64.3	Betaine
118.0873	117.079	-0.001	118.0863	294	64.3	Betaine
118.0873	117.079	-0.001	118.0863	290	64.3	Betaine
118.0873	117.079	-0.001	118.0863	324	30.8	Betaine
118.0873	117.079	-0.001	118.0863	321	30.8	Betaine
118.0873	117.079	-0.001	118.0863	319	30.8	Betaine
118.0873	117.079	-0.001	118.0863	383	52.7	Betaine
118.0873	117.079	-0.001	118.0863	379	52.7	Betaine
118.0873	117.079	-0.001	118.0863	379	52.7	Betaine
118.0873	117.079	-0.001	118.0863	370	89.7	Betaine
118.0873	117.079	-0.001	118.0863	358	89.7	Betaine
118.0873	117.079	-0.001	118.0863	339	89.7	Betaine
118.0873	117.079	-0.001	118.0863	316	76.1	Betaine
118.0873	117.079	-0.001	118.0863	311	76.1	Betaine
118.0873	117.079	-0.001	118.0863	299	76.1	Betaine
332.332	332.332	-0.0009	332.3312	97	42	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	89	31.3	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	75	19.6	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	150	21.2	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	146	17.9	Benzyl tetradecyl dimethylammonium cation
332.332	332.332	-0.0009	332.3312	144	16.5	Benzyl tetradecyl dimethylammonium cation
186.0588	370.196	0.0467	186.1055	65	100	Ser-His-Lys

284.3311	284.332	0	284.3312	25	100	Hexadecyltrimethylammonium cation
284.3311	284.332	0	284.3312	202	84.5	Hexadecyltrimethylammonium cation
284.3311	284.332	0	284.3312	65	3.1	Hexadecyltrimethylammonium cation
284.3311	284.332	0	284.3312	47	1.6	Hexadecyltrimethylammonium cation
284.3311	284.332	0	284.3312	160	73.4	Hexadecyltrimethylammonium cation
284.3311	283.288	-0.0363	284.2948	70	6.3	Octadecanamide
284.3311	283.288	-0.0363	284.2948	70	6.3	Octadecanamide
284.3311	284.332	0	284.3312	163	78.8	Hexadecyltrimethylammonium cation
284.3311	283.288	-0.0363	284.2948	66	6.2	Octadecanamide
284.3311	283.288	-0.0363	284.2948	44	6.2	Octadecanamide
118.0873	117.079	-0.001	118.0863	234	100	Betaine
118.0873	117.079	-0.001	118.0863	233	100	Betaine
118.0873	117.079	-0.001	118.0863	221	100	Betaine
118.0873	117.079	-0.001	118.0863	430	60.3	Betaine
118.0873	117.079	-0.001	118.0863	425	60.3	Betaine
118.0873	117.079	-0.001	118.0863	420	60.3	Betaine
118.0873	117.079	-0.001	118.0863	337	80.8	Betaine
118.0873	117.079	-0.001	118.0863	336	80.8	Betaine
118.0873	117.079	-0.001	118.0863	326	80.8	Betaine
118.0873	117.079	-0.001	118.0863	392	63.6	Betaine
118.0873	117.079	-0.001	118.0863	391	63.6	Betaine
118.0873	117.079	-0.001	118.0863	388	63.6	Betaine
546.3998	523.364	-0.047	546.353	115	100	PAF C-16
546.3998	523.364	-0.047	546.353	104	100	PAF C-16
546.3998	523.364	-0.047	546.353	89	100	PAF C-16
546.3998	523.364	-0.047	546.353	95	100	PAF C-16
118.0873	117.079	-0.001	118.0863	358	48	Betaine
118.0873	117.079	-0.001	118.0863	357	48	Betaine
118.0873	117.079	-0.001	118.0863	357	48	Betaine
118.0873	117.079	-0.001	118.0863	419	100	Betaine
118.0873	117.079	-0.001	118.0863	416	100	Betaine
118.0873	117.079	-0.001	118.0863	412	100	Betaine
118.0873	117.079	-0.001	118.0863	386	98.4	Betaine
118.0873	117.079	-0.001	118.0863	374	98.4	Betaine
118.0873	117.079	-0.001	118.0863	350	98.4	Betaine
118.0873	117.079	-0.001	118.0863	310	66.3	Betaine
118.0873	117.079	-0.001	118.0863	310	66.3	Betaine
118.0873	117.079	-0.001	118.0863	305	66.3	Betaine
284.3311	284.332	0	284.3312	160	77.5	Hexadecyltrimethylammonium cation

284.3311	284.332	0	284.3312	19	2.6	Hexadecyltrimethylammonium cation
284.3311	284.332	0	284.3312	18	2.5	Hexadecyltrimethylammonium cation
186.0588	370.196	0.0467	186.1055	76	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	413	63.5	Betaine
118.0873	117.079	-0.001	118.0863	409	63.5	Betaine
118.0873	117.079	-0.001	118.0863	404	63.5	Betaine
118.0873	117.079	-0.001	118.0863	360	91.2	Betaine
118.0873	117.079	-0.001	118.0863	343	91.2	Betaine
118.0873	117.079	-0.001	118.0863	316	91.2	Betaine
118.0873	117.079	-0.001	118.0863	336	74.1	Betaine
118.0873	117.079	-0.001	118.0863	335	74.1	Betaine
118.0873	117.079	-0.001	118.0863	331	74.1	Betaine
140.0692	139.1	0.038	140.107	98	100	Tropinone
140.0692	139.1	0.038	140.107	97	100	Tropinone
140.0692	139.1	0.038	140.107	96	100	Tropinone
118.0873	117.079	-0.001	118.0863	421	62.4	Betaine
118.0873	117.079	-0.001	118.0863	417	62.4	Betaine
118.0873	117.079	-0.001	118.0863	409	62.4	Betaine
118.0873	117.079	-0.001	118.0863	320	63.9	Betaine
118.0873	117.079	-0.001	118.0863	320	63.9	Betaine
118.0873	117.079	-0.001	118.0863	317	63.9	Betaine
118.0873	117.079	-0.001	118.0863	282	64.4	Betaine
118.0873	117.079	-0.001	118.0863	281	64.4	Betaine
118.0873	117.079	-0.001	118.0863	275	64.4	Betaine
118.0873	117.079	-0.001	118.0863	286	41.8	Betaine
118.0873	117.079	-0.001	118.0863	285	41.8	Betaine
118.0873	117.079	-0.001	118.0863	281	41.8	Betaine
118.0873	117	0	118.09	431	31.7	Betaine
118.0873	117.079	-0.001	118.0863	425	24.9	Betaine
118.0873	117.079	-0.001	118.0863	422	24.9	Betaine
118.0873	117.079	-0.001	118.0863	287	70.3	Betaine
118.0873	117.079	-0.001	118.0863	285	70.3	Betaine
118.0873	117.079	-0.001	118.0863	281	70.3	Betaine
118.0873	117.079	-0.001	118.0863	383	75.4	Betaine
118.0873	117.079	-0.001	118.0863	382	75.4	Betaine
118.0873	117.079	-0.001	118.0863	379	75.4	Betaine
428.3751	427	0.03	428.41	233	51.5	N-Octanoylsphinganine,D-erythro
428.3751	427	0.03	428.41	224	37.4	N-Octanoylsphinganine,D-erythro
428.3751	427	0.03	428.41	198	11.2	N-Octanoylsphinganine,D-erythro
186.0588	163.084	0.0149	186.0737	151	89.1	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	97	89.1	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	47	6.2	Ala-Asn

118.0873	117.079	-0.001	118.0863	333	100	Betaine
118.0873	117.079	-0.001	118.0863	331	100	Betaine
118.0873	117.079	-0.001	118.0863	330	100	Betaine
118.0873	117.079	-0.001	118.0863	370	66.4	Betaine
118.0873	117.079	-0.001	118.0863	367	66.4	Betaine
118.0873	117.079	-0.001	118.0863	356	66.4	Betaine
118.0873	117.079	-0.001	118.0863	314	74.1	Betaine
118.0873	117.079	-0.001	118.0863	313	74.1	Betaine
118.0873	117.079	-0.001	118.0863	309	74.1	Betaine
118.0873	117.079	-0.001	118.0863	256	65.4	Betaine
118.0873	117.079	-0.001	118.0863	256	65.4	Betaine
118.0873	117.079	-0.001	118.0863	252	65.4	Betaine
186.0588	370.196	0.0467	186.1055	70	100	Ser-His-Lys
224.1293	446.228	-0.0081	224.1212	124	55.4	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	112	36.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	65	7.7	Bendiocarb
224.1293	223.084	-0.0376	224.0917	328	93.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	318	93.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	284	93.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	303	92.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	280	92.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	240	92.7	N-Acetyl-L-tyrosine
195.1236	194.115	-0.0009	195.1227	248	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	247	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	246	100	Tetraethylene glycol
118.0873	117.079	-0.001	118.0863	325	100	Betaine
118.0873	117.079	-0.001	118.0863	323	100	Betaine
118.0873	117.079	-0.001	118.0863	320	100	Betaine
118.0873	117.079	-0.001	118.0863	488	66.2	Betaine
118.0873	117.079	-0.001	118.0863	482	66.2	Betaine
118.0873	117.079	-0.001	118.0863	476	66.2	Betaine
118.0873	117.079	-0.001	118.0863	382	97.3	Betaine
118.0873	117.079	-0.001	118.0863	374	97.3	Betaine
118.0873	117.079	-0.001	118.0863	369	97.3	Betaine
118.0873	117.079	-0.001	118.0863	389	62.7	Betaine
118.0873	117.079	-0.001	118.0863	385	62.7	Betaine
118.0873	117.079	-0.001	118.0863	382	62.7	Betaine
360.3626	360.363	-0.0002	360.3625	283	40.4	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	261	16	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	260	15.4	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	299	41.1	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	281	21.2	Benzyl hexadecyl dimethylammonium cation

360.3626	360.363	-0.0002	360.3625	280	20.4	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	350	87.6	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	203	2.5	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	193	1.8	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	309	72.3	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	250	13.1	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	231	6.3	Benzyl hexadecyl dimethylammonium cation
97.0774	114.104	0.0238	97.1012	24	23.1	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	16	17.2	Cycloheptanol
97.0774	114.104	0.0238	97.1012	14	15.9	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	256	55.8	Betaine
118.0873	117.079	-0.001	118.0863	249	55.8	Betaine
118.0873	117.079	-0.001	118.0863	248	55.8	Betaine
118.0873	117.079	-0.001	118.0863	381	45	Betaine
118.0873	117.079	-0.001	118.0863	379	45	Betaine
118.0873	117.079	-0.001	118.0863	375	45	Betaine
118.0873	117.079	-0.001	118.0863	304	76.5	Betaine
118.0873	117.079	-0.001	118.0863	302	76.5	Betaine
118.0873	117.079	-0.001	118.0863	296	76.5	Betaine
118.0873	117.079	-0.001	118.0863	276	61.5	Betaine
118.0873	117.079	-0.001	118.0863	275	61.5	Betaine
118.0873	117.079	-0.001	118.0863	270	61.5	Betaine
360.3626	360.363	-0.0002	360.3625	285	56.7	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	206	6.5	Benzyl hexadecyl dimethylammonium cation
360.3626	360.363	-0.0002	360.3625	204	6	Benzyl hexadecyl dimethylammonium cation
118.0873	117.079	-0.001	118.0863	424	59.2	Betaine
118.0873	117.079	-0.001	118.0863	421	59.2	Betaine
118.0873	117.079	-0.001	118.0863	410	59.2	Betaine
118.0873	117.079	-0.001	118.0863	261	65.9	Betaine
118.0873	117.079	-0.001	118.0863	260	65.9	Betaine
118.0873	117.079	-0.001	118.0863	256	65.9	Betaine
118.0873	117.079	-0.001	118.0863	398	41.3	Betaine
118.0873	117.079	-0.001	118.0863	396	41.3	Betaine
118.0873	117.079	-0.001	118.0863	396	41.3	Betaine
369.3861	386.355	-0.0345	369.3516	260	55.4	Cholesterol
369.3861	386.355	-0.0345	369.3516	255	44.6	Cholestan-3-one, (5.alpha.)-
369.3861	386.355	-0.0345	369.3516	245	44.6	Cholestan-3-one, (5.alpha.)-

97.0774	114.104	0.0238	97.1012	71	100	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	62	100	Cyclopentanemethanol, .alpha.-methyl-
186.0588	370.196	0.0467	186.1055	50	100	Ser-His-Lys
385.3803	384.339	-0.0338	385.3465	21	53.1	Cholesta-5,7-dien-3-ol, (3.beta.)-
385.3803	402.35	-0.0338	385.3465	18	46.9	25-Hydroxycholesterol
385.3803	384.339	-0.0338	385.3465	18	53.1	Cholesta-5,7-dien-3-ol, (3.beta.)-
385.3803	384.339	-0.0338	385.3465	102	100	Cholecalciferol
385.3803	384.339	-0.0338	385.3465	96	100	Cholecalciferol
385.3803	384.339	-0.0338	385.3465	95	100	Cholecalciferol
385.3803	402.35	-0.0338	385.3465	3	100	25-Hydroxycholesterol
195.1236	194.115	-0.0009	195.1227	272	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	271	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	268	100	Tetraethylene glycol
118.0873	117.079	-0.001	118.0863	225	100	Betaine
118.0873	117.079	-0.001	118.0863	219	100	Betaine
118.0873	117.079	-0.001	118.0863	213	100	Betaine
118.0873	117.079	-0.001	118.0863	424	44.4	Betaine
118.0873	117	0	118.09	416	33.1	Betaine
118.0873	117.079	-0.001	118.0863	413	44.4	Betaine
118.0873	117.079	-0.001	118.0863	299	68.2	Betaine
118.0873	117.079	-0.001	118.0863	298	68.2	Betaine
118.0873	117.079	-0.001	118.0863	291	68.2	Betaine
118.0873	117.079	-0.001	118.0863	340	60.9	Betaine
118.0873	117.079	-0.001	118.0863	336	60.9	Betaine
118.0873	117.079	-0.001	118.0863	334	60.9	Betaine
224.1293	223.084	-0.0376	224.0917	222	76.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	215	76.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	201	76.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	265	83.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	255	83.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	247	83.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	251	89.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	236	89.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	210	89.1	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	353	32.5	Betaine
118.0873	117.079	-0.001	118.0863	351	32.5	Betaine
118.0873	117	0	118.09	349	27.4	Betaine
118.0873	117.079	-0.001	118.0863	474	67.4	Betaine
118.0873	117.079	-0.001	118.0863	468	67.4	Betaine
118.0873	117.079	-0.001	118.0863	466	67.4	Betaine
118.0873	117.079	-0.001	118.0863	276	81	Betaine
118.0873	117.079	-0.001	118.0863	266	81	Betaine
118.0873	117.079	-0.001	118.0863	266	81	Betaine
118.0873	117.079	-0.001	118.0863	409	61.5	Betaine
118.0873	117.079	-0.001	118.0863	406	61.5	Betaine

118.0873	117.079	-0.001	118.0863	399	61.5	Betaine
97.0774	114.104	0.0238	97.1012	34	22.5	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	28	17.7	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	27	17	Cyclohexanol, 4-methyl-, trans-
186.0588	163.084	0.0149	186.0737	160	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	223.076	-0.0456	224.0837	47	100	Desmethylketamine
224.1293	223.084	-0.0376	224.0917	218	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	192	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	161	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	260	86.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	245	86.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	215	86.1	N-Acetyl-L-tyrosine
400.3796	400.343	-0.0375	400.3421	191	27.7	Palmitoyl-L-carnitine cation
400.3796	400.343	-0.0375	400.3421	182	20.1	Palmitoyl-L-carnitine cation
400.3796	400.343	-0.0375	400.3421	175	15.4	Palmitoyl-L-carnitine cation
118.0873	117	0	118.09	319	25.8	Betaine
118.0873	117.079	-0.001	118.0863	315	21.8	Betaine
118.0873	117.079	-0.001	118.0863	315	21.8	Betaine
118.0873	117.079	-0.001	118.0863	417	43.4	Betaine
118.0873	117.079	-0.001	118.0863	412	43.4	Betaine
118.0873	117.079	-0.001	118.0863	408	43.4	Betaine
118.0873	117.079	-0.001	118.0863	346	84.3	Betaine
118.0873	117.079	-0.001	118.0863	345	84.3	Betaine
118.0873	117.079	-0.001	118.0863	337	84.3	Betaine
118.0873	117.079	-0.001	118.0863	269	72.2	Betaine
118.0873	117.079	-0.001	118.0863	268	72.2	Betaine
118.0873	117.079	-0.001	118.0863	259	72.2	Betaine
282.2797	281.272	-0.0006	282.2791	77	100	9-Octadecenamide, (Z)-
282.2797	281.272	-0.0006	282.2791	60	100	9-Octadecenamide, (Z)-
282.2797	281.272	-0.0006	282.2791	58	100	9-Octadecenamide, (Z)-
282.2797	281.272	-0.0006	282.2791	104	100	9-Octadecenamide, (Z)-
282.2797	281.272	-0.0006	282.2791	103	100	9-Octadecenamide, (Z)-
282.2797	281.272	-0.0006	282.2791	102	100	9-Octadecenamide, (Z)-
282.2797	281.272	-0.0006	282.2791	215	93.2	9-Octadecenamide, (Z)-
282.2797	281.272	-0.0006	282.2791	211	93.2	9-Octadecenamide, (Z)-
282.2797	281.272	-0.0006	282.2791	209	93.2	9-Octadecenamide, (Z)-
140.0692	139.027	-0.035	140.0342	100	100	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
140.0692	139.027	-0.035	140.0342	99	100	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
140.0692	139.027	-0.035	140.0342	89	100	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
186.0588	163.084	0.0149	186.0737	118	86.6	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	51	13.4	Ala-Asn
186.0588	163.084	0.0149	186.0737	141	92	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	52	8	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	135	100	N,N-Bis(2-hydroxyethyl)glycine

186.0588	163.084	0.0149	186.0737	106	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	147	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	452	36.1	Betaine
118.0873	117.079	-0.001	118.0863	448	36.1	Betaine
118.0873	117.079	-0.001	118.0863	448	36.1	Betaine
118.0873	117	0	118.09	331	27.6	Betaine
118.0873	117.079	-0.001	118.0863	326	22.3	Betaine
118.0873	117.079	-0.001	118.0863	326	22.3	Betaine
118.0873	117.079	-0.001	118.0863	360	61.5	Betaine
118.0873	117.079	-0.001	118.0863	356	61.5	Betaine
118.0873	117.079	-0.001	118.0863	353	61.5	Betaine
186.0588	203.091	0.0285	186.0873	66	73.1	Ala-Asn
186.0588	163.084	0.0149	186.0737	37	20.7	N,N-Bis(2-hydroxyethyl)glycine
186.0588	168.042	0.0173	186.0761	11	6.2	3-Hydroxy-4-methoxybenzoic acid
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
393.2988	392.293	0.0011	393.2999	89	100	Deoxycholic acid
118.0873	117.079	-0.001	118.0863	264	33.9	Betaine
118.0873	117.079	-0.001	118.0863	264	33.9	Betaine
118.0873	117	0	118.09	262	31.3	Betaine
118.0873	117.079	-0.001	118.0863	427	65.1	Betaine
118.0873	117.079	-0.001	118.0863	425	65.1	Betaine
118.0873	117.079	-0.001	118.0863	414	65.1	Betaine
118.0873	117.079	-0.001	118.0863	295	49.6	Betaine
118.0873	117.079	-0.001	118.0863	292	49.6	Betaine
118.0873	117.079	-0.001	118.0863	291	49.6	Betaine
118.0873	117.079	-0.001	118.0863	413	59.4	Betaine
118.0873	117.079	-0.001	118.0863	412	59.4	Betaine
118.0873	117.079	-0.001	118.0863	411	59.4	Betaine
97.0774	114.104	0.0238	97.1012	26	45.3	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	17	32.9	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	16	45.3	Cyclohexanol, 2-methyl-, trans-
186.0588	370.196	0.0467	186.1055	60	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	180	100	N,N-Bis(2-hydroxyethyl)glycine
371.3164	370.308	-0.0009	371.3156	177	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	118	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	111	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	131	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	128	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	126	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	49	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	40	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	22	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	170	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	150	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	106	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	329	60.7	Betaine
118.0873	117.079	-0.001	118.0863	329	60.7	Betaine
118.0873	117.079	-0.001	118.0863	319	60.7	Betaine
118.0873	117.079	-0.001	118.0863	419	47	Betaine
118.0873	117.079	-0.001	118.0863	417	47	Betaine
118.0873	117.079	-0.001	118.0863	415	47	Betaine
118.0873	117.079	-0.001	118.0863	339	98.2	Betaine
118.0873	117.079	-0.001	118.0863	334	98.2	Betaine
118.0873	117.079	-0.001	118.0863	317	98.2	Betaine
118.0873	117.079	-0.001	118.0863	341	59.5	Betaine
118.0873	117.079	-0.001	118.0863	341	59.5	Betaine
118.0873	117.079	-0.001	118.0863	331	59.5	Betaine
186.0588	163.084	0.0149	186.0737	192	92.6	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	159	92.6	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	96	7.4	Ala-Asn
186.0588	163.084	0.0149	186.0737	146	93	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	47	7	Ser-His-Lys
371.3164	370.308	-0.0009	371.3156	182	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	80	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	77	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	165	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	147	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	126	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	69	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	54	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	45	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	116	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	95	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	78	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	289	85.4	Betaine
118.0873	117.079	-0.001	118.0863	288	85.4	Betaine
118.0873	117.079	-0.001	118.0863	285	85.4	Betaine
118.0873	117.079	-0.001	118.0863	365	31.2	Betaine
118.0873	117.079	-0.001	118.0863	364	31.2	Betaine
118.0873	117.079	-0.001	118.0863	360	31.2	Betaine
118.0873	117.079	-0.001	118.0863	363	75.6	Betaine
118.0873	117.079	-0.001	118.0863	346	75.6	Betaine
118.0873	117.079	-0.001	118.0863	326	75.6	Betaine
118.0873	117.079	-0.001	118.0863	330	83	Betaine
118.0873	117.079	-0.001	118.0863	327	83	Betaine
118.0873	117.079	-0.001	118.0863	321	83	Betaine
118.0873	117.079	-0.001	118.0863	333	69.8	Betaine
118.0873	117.079	-0.001	118.0863	330	69.8	Betaine
118.0873	117.079	-0.001	118.0863	321	69.8	Betaine
118.0873	117.079	-0.001	118.0863	355	60.2	Betaine
118.0873	117.079	-0.001	118.0863	350	60.2	Betaine
118.0873	117.079	-0.001	118.0863	349	60.2	Betaine
118.0873	117.079	-0.001	118.0863	307	76.1	Betaine
118.0873	117.079	-0.001	118.0863	302	76.1	Betaine
118.0873	117.079	-0.001	118.0863	301	76.1	Betaine
118.0873	117.079	-0.001	118.0863	363	55.9	Betaine
118.0873	117.079	-0.001	118.0863	362	55.9	Betaine
118.0873	117.079	-0.001	118.0863	358	55.9	Betaine
97.0774	114.104	0.0238	97.1012	51	20	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	48	17.6	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	48	17.6	Cyclohexanol, 4-methyl-, trans-
371.3164	370.308	-0.0009	371.3156	170	100	Hexanedioic acid, bis(2-ethylhexyl)
371.3164	370.308	-0.0009	371.3156	105	100	Hexanedioic acid, bis(2-ethylhexyl)
371.3164	370.308	-0.0009	371.3156	99	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	150	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	134	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	110	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	44	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	19	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	115	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	93	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	66	100	Hexanedioic acid, bis(2-ethylhexyl) ester
186.0588	163.084	0.0149	186.0737	98	57.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	90	42.7	Ala-Asn
186.0588	163.084	0.0149	186.0737	49	57.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	49	68.7	Ala-Asn
186.0588	163.084	0.0149	186.0737	29	31.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	32	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	267	55.2	Betaine
118.0873	117.079	-0.001	118.0863	267	55.2	Betaine
118.0873	117.079	-0.001	118.0863	265	55.2	Betaine
118.0873	117.079	-0.001	118.0863	394	63.6	Betaine
118.0873	117.079	-0.001	118.0863	392	63.6	Betaine
118.0873	117.079	-0.001	118.0863	380	63.6	Betaine
118.0873	117.079	-0.001	118.0863	275	60.1	Betaine
118.0873	117.079	-0.001	118.0863	271	60.1	Betaine
118.0873	117.079	-0.001	118.0863	269	60.1	Betaine
118.0873	117.079	-0.001	118.0863	352	47	Betaine
118.0873	117.079	-0.001	118.0863	352	47	Betaine
118.0873	117.079	-0.001	118.0863	348	47	Betaine
186.0588	163.084	0.0149	186.0737	118	69.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	96	27.6	Ala-Asn
186.0588	163.084	0.0149	186.0737	29	69.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	146	100	N,N-Bis(2-hydroxyethyl)glycine
106.0872	105.079	-0.0009	106.0863	121	100	Diethanolamine
224.1293	223.106	-0.0164	224.1129	133	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	132	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	126	100	N-Acetyl-D-galactosaminitol
224.1293	223.084	-0.0376	224.0917	189	70.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	175	70.6	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	166	25.8	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	284	89.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	266	89.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	241	89.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	263	86.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	250	86.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	221	86.8	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	406	71.7	Betaine
118.0873	117.079	-0.001	118.0863	405	71.7	Betaine
118.0873	117.079	-0.001	118.0863	390	71.7	Betaine
118.0873	117.079	-0.001	118.0863	289	56.5	Betaine
118.0873	117.079	-0.001	118.0863	288	56.5	Betaine
118.0873	117.079	-0.001	118.0863	286	56.5	Betaine

118.0873	117.079	-0.001	118.0863	377	61.8	Betaine
118.0873	117.079	-0.001	118.0863	374	61.8	Betaine
118.0873	117.079	-0.001	118.0863	370	61.8	Betaine
393.2988	392.293	0.0011	393.2999	78	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	64	100	Chenodeoxycholic acid
371.3164	370.308	-0.0009	371.3156	207	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	130	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	117	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	174	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	126	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	112	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	66	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	62	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	56	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	117	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	95	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	68	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	444	60.1	Betaine
118.0873	117.079	-0.001	118.0863	443	60.1	Betaine
118.0873	117.079	-0.001	118.0863	436	60.1	Betaine
118.0873	117.079	-0.001	118.0863	308	69.2	Betaine
118.0873	117.079	-0.001	118.0863	307	69.2	Betaine
118.0873	117.079	-0.001	118.0863	301	69.2	Betaine
118.0873	117.079	-0.001	118.0863	364	41.6	Betaine
118.0873	117.079	-0.001	118.0863	362	41.6	Betaine
118.0873	117.079	-0.001	118.0863	358	41.6	Betaine
371.3164	370.308	-0.0009	371.3156	215	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	108	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	97	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	183	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	179	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	160	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	107	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	88	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	50	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	174	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	157	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	109	100	Hexanedioic acid, bis(2-ethylhexyl) ester
186.0588	163.084	0.0149	186.0737	145	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	256	39	Betaine
118.0873	117.079	-0.001	118.0863	254	39	Betaine
118.0873	117.079	-0.001	118.0863	253	39	Betaine
118.0873	117.079	-0.001	118.0863	387	31.2	Betaine
118.0873	117.079	-0.001	118.0863	386	31.2	Betaine
118.0873	117.079	-0.001	118.0863	385	31.2	Betaine
118.0873	117.079	-0.001	118.0863	251	65	Betaine
118.0873	117.079	-0.001	118.0863	250	65	Betaine
118.0873	117.079	-0.001	118.0863	245	65	Betaine
118.0873	117.079	-0.001	118.0863	242	66.5	Betaine
118.0873	117.079	-0.001	118.0863	240	66.5	Betaine
118.0873	117.079	-0.001	118.0863	235	66.5	Betaine
393.2988	392.293	0.0011	393.2999	45	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	44	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	40	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	37	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	31	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	30	100	Chenodeoxycholic acid
371.3164	370.308	-0.0009	371.3156	231	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	127	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	123	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	173	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	170	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	151	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	104	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	85	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	51	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	131	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	109	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	74	100	Hexanedioic acid, bis(2-ethylhexyl) ester
186.0588	163.084	0.0149	186.0737	145	100	N,N-Bis(2-hydroxyethyl)glycine
106.0872	105	0	106.09	166	72.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	16.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	16.6	Diethanolamine
106.0872	105	0	106.09	161	81.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	18.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	18.6	Diethanolamine
118.0873	117.079	-0.001	118.0863	330	53.7	Betaine
118.0873	117.079	-0.001	118.0863	330	53.7	Betaine
118.0873	117.079	-0.001	118.0863	329	53.7	Betaine
118.0873	117.079	-0.001	118.0863	431	43.4	Betaine
118.0873	117.079	-0.001	118.0863	422	43.4	Betaine
118.0873	117	0	118.09	421	30.7	Betaine
118.0873	117.079	-0.001	118.0863	266	64.7	Betaine
118.0873	117.079	-0.001	118.0863	264	64.7	Betaine
118.0873	117.079	-0.001	118.0863	260	64.7	Betaine
118.0873	117.079	-0.001	118.0863	300	70.3	Betaine
118.0873	117.079	-0.001	118.0863	297	70.3	Betaine
118.0873	117.079	-0.001	118.0863	297	70.3	Betaine
371.3164	370.308	-0.0009	371.3156	219	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	146	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	142	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	136	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	126	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	112	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	138	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	115	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	79	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	123	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	100	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	74	100	Hexanedioic acid, bis(2-ethylhexyl) ester
140.0692	139.063	0.0014	140.0706	114	68.2	5-Amino-2-methoxyphenol
140.0692	139.063	0.0014	140.0706	95	68.2	5-Amino-2-methoxyphenol
140.0692	139.063	0.0014	140.0706	85	68.2	5-Amino-2-methoxyphenol
118.0873	117.079	-0.001	118.0863	414	48.2	Betaine
118.0873	117.079	-0.001	118.0863	409	48.2	Betaine
118.0873	117.079	-0.001	118.0863	404	48.2	Betaine
118.0873	117.079	-0.001	118.0863	289	63.9	Betaine
118.0873	117.079	-0.001	118.0863	288	63.9	Betaine
118.0873	117.079	-0.001	118.0863	284	63.9	Betaine
118.0873	117.079	-0.001	118.0863	328	63	Betaine
118.0873	117.079	-0.001	118.0863	326	63	Betaine
118.0873	117.079	-0.001	118.0863	326	63	Betaine
371.3164	370.308	-0.0009	371.3156	243	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	144	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	140	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	177	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	154	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	148	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	85	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	70	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	59	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	105	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	85	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	82	100	Hexanedioic acid, bis(2-ethylhexyl) ester
140.0692	139.063	0.0014	140.0706	129	100	5-Amino-2-methoxyphenol
118.0873	117.079	-0.001	118.0863	202	100	Betaine
118.0873	117.079	-0.001	118.0863	199	100	Betaine

118.0873	117.079	-0.001	118.0863	191	100	Betaine
118.0873	117.079	-0.001	118.0863	397	32.7	Betaine
118.0873	117.079	-0.001	118.0863	396	32.7	Betaine
118.0873	117.079	-0.001	118.0863	394	32.7	Betaine
118.0873	117.079	-0.001	118.0863	347	98.4	Betaine
118.0873	117.079	-0.001	118.0863	345	98.4	Betaine
118.0873	117.079	-0.001	118.0863	339	98.4	Betaine
118.0873	117	0	118.09	347	25.5	Betaine
118.0873	117.079	-0.001	118.0863	346	24.5	Betaine
118.0873	117.079	-0.001	118.0863	345	24.5	Betaine
371.3164	370.308	-0.0009	371.3156	243	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	140	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	133	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	144	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	133	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	124	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	109	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	41	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	33	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	97	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	80	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	51	100	Hexanedioic acid, bis(2-ethylhexyl) ester
97.0774	114.104	0.0238	97.1012	13	23.7	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	10	23.7	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	10	20.9	Cyclohexanol, 2-methyl-, trans-
118.0873	117.079	-0.001	118.0863	229	100	Betaine
118.0873	117.079	-0.001	118.0863	4	100	Betaine
118.0873	117.079	-0.001	118.0863	2	100	Betaine
118.0873	117.079	-0.001	118.0863	445	60.5	Betaine
118.0873	117.079	-0.001	118.0863	443	60.5	Betaine
118.0873	117.079	-0.001	118.0863	441	60.5	Betaine
118.0873	117.079	-0.001	118.0863	327	53.6	Betaine
118.0873	117.079	-0.001	118.0863	325	53.6	Betaine

118.0873	117.079	-0.001	118.0863	325	53.6	Betaine
118.0873	117.079	-0.001	118.0863	327	64	Betaine
118.0873	117.079	-0.001	118.0863	326	64	Betaine
118.0873	117.079	-0.001	118.0863	324	64	Betaine
186.0588	370.196	0.0467	186.1055	69	100	Ser-His-Lys
106.0872	105	0	106.09	189	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	153	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	153	19.8	Diethanolamine
118.0873	117.079	-0.001	118.0863	413	51.3	Betaine
118.0873	117.079	-0.001	118.0863	411	51.3	Betaine
118.0873	117.079	-0.001	118.0863	408	51.3	Betaine
118.0873	117.079	-0.001	118.0863	298	95.5	Betaine
118.0873	117.079	-0.001	118.0863	296	95.5	Betaine
118.0873	117.079	-0.001	118.0863	286	95.5	Betaine
118.0873	117.079	-0.001	118.0863	379	98.2	Betaine
118.0873	117.079	-0.001	118.0863	379	98.2	Betaine
118.0873	117.079	-0.001	118.0863	373	98.2	Betaine
371.3164	370.308	-0.0009	371.3156	226	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	136	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	129	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	188	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	172	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	167	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	106	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	51	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	45	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	152	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	132	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	99	100	Hexanedioic acid, bis(2-ethylhexyl) ester
106.0872	105	0	106.09	156	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	154	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	153	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	152	100	Diethanolamine

106.0872	105	0	106.09	225	53.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	218	40.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	216	40.9	Diethanolamine
118.0873	117.079	-0.001	118.0863	284	63.4	Betaine
118.0873	117.079	-0.001	118.0863	283	63.4	Betaine
118.0873	117.079	-0.001	118.0863	278	63.4	Betaine
118.0873	117.079	-0.001	118.0863	285	64.5	Betaine
118.0873	117.079	-0.001	118.0863	284	64.5	Betaine
118.0873	117.079	-0.001	118.0863	282	64.5	Betaine
118.0873	117	0	118.09	352	25.9	Betaine
118.0873	117	0	118.09	350	23.9	Betaine
118.0873	117.079	-0.001	118.0863	341	17.3	Betaine
371.3164	370.308	-0.0009	371.3156	196	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	115	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	106	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	155	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	121	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	107	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	141	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	115	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	88	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	145	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	119	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	72	100	Hexanedioic acid, bis(2-ethylhexyl) ester
106.0872	105	0	106.09	247	75.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	221	22.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	220	22.6	Diethanolamine
106.0872	105	0	106.09	196	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	162	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	161	20.4	Diethanolamine
393.2988	392.293	0.0011	393.2999	42	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	39	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	37	100	Chenodeoxycholic acid
371.3164	370.308	-0.0009	371.3156	239	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	119	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	118	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	132	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	108	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	96	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	106	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	61	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	40	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	149	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	128	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	82	100	Hexanedioic acid, bis(2-ethylhexyl) ester
186.0588	370.196	0.0467	186.1055	58	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	154	100	N,N-Bis(2-hydroxyethyl)glycine
391.2862	390.277	-0.0019	391.2843	322	96.9	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	312	96.9	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	306	96.9	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	230	55.9	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	223	55.9	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	223	42.8	Bis(2-ethylhexyl) phthalate
391.2862	390.277	-0.0019	391.2843	251	65.5	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	241	65.5	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	238	65.5	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	229	53.6	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	225	45.3	Bis(2-ethylhexyl) phthalate
391.2862	390.277	-0.0019	391.2843	221	53.6	Diethyl phthalate
118.0873	117.079	-0.001	118.0863	398	56.6	Betaine
118.0873	117.079	-0.001	118.0863	397	56.6	Betaine
118.0873	117.079	-0.001	118.0863	393	56.6	Betaine
118.0873	117.079	-0.001	118.0863	340	83.5	Betaine
118.0873	117.079	-0.001	118.0863	334	83.5	Betaine
118.0873	117.079	-0.001	118.0863	318	83.5	Betaine
118.0873	117.079	-0.001	118.0863	339	42.9	Betaine
118.0873	117.079	-0.001	118.0863	333	42.9	Betaine
118.0873	117.079	-0.001	118.0863	332	42.9	Betaine
371.3164	370.308	-0.0009	371.3156	203	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	77	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	75	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	141	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	138	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	122	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	98	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	96	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	76	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	194	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	170	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	127	100	Hexanedioic acid, bis(2-ethylhexyl) ester
97.0774	114.104	0.0238	97.1012	44	23.5	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	42	21.6	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	35	16.6	Cyclohexanol, 1-methyl-
106.0872	105	0	106.09	159	74.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	19.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	19.5	Diethanolamine
118.0873	117.079	-0.001	118.0863	374	47.5	Betaine
118.0873	117.079	-0.001	118.0863	374	47.5	Betaine
118.0873	117.079	-0.001	118.0863	372	47.5	Betaine
118.0873	117.079	-0.001	118.0863	241	86.4	Betaine
118.0873	117.079	-0.001	118.0863	226	86.4	Betaine
118.0873	117.079	-0.001	118.0863	223	86.4	Betaine
118.0873	117	0	118.09	347	22.7	Betaine
118.0873	117	0	118.09	347	22.7	Betaine
118.0873	117.079	-0.001	118.0863	346	21.8	Betaine
371.3164	370.308	-0.0009	371.3156	236	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	123	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	117	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	194	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	167	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	144	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	60	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	50	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	49	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	162	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	140	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	112	100	Hexanedioic acid, bis(2-ethylhexyl) ester
97.0774	114.104	0.0238	97.1012	12	53.1	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	10	53.1	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	9	46.9	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	159	75.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	18.4	Diethanolamine
106.0872	105	0	106.09	173	81.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	131	18.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	131	18.3	Diethanolamine
391.2862	390.277	-0.0019	391.2843	325	97.9	Diocetyl phthalate
391.2862	390.277	-0.0019	391.2843	324	97.9	Diocetyl phthalate
391.2862	390.277	-0.0019	391.2843	316	97.9	Diocetyl phthalate
391.2862	390.277	-0.0019	391.2843	245	95.4	Diocetyl phthalate
391.2862	390.277	-0.0019	391.2843	193	95.4	Diocetyl phthalate
391.2862	390.277	-0.0019	391.2843	182	95.4	Diocetyl phthalate
391.2862	390.277	-0.0019	391.2843	236	52.6	Diocetyl phthalate
391.2862	390.277	-0.0019	391.2843	233	46.5	Bis(2-ethylhexyl) phthalate
391.2862	390.277	-0.0019	391.2843	230	52.6	Diocetyl phthalate
391.2862	390.277	-0.0019	391.2843	190	55.2	Diocetyl phthalate
391.2862	390.277	-0.0019	391.2843	183	42.3	Bis(2-ethylhexyl) phthalate
391.2862	390.277	-0.0019	391.2843	182	55.2	Diocetyl phthalate
371.3164	370.308	-0.0009	371.3156	220	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	122	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	122	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	163	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	142	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	104	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	82	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	108	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	88	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	70	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	294	38.1	Betaine
118.0873	117.079	-0.001	118.0863	291	38.1	Betaine
118.0873	117.079	-0.001	118.0863	289	38.1	Betaine
118.0873	117	0	118.09	402	30.4	Betaine
118.0873	117.079	-0.001	118.0863	395	23.3	Betaine
118.0873	117.079	-0.001	118.0863	392	23.3	Betaine
118.0873	117.079	-0.001	118.0863	299	67.2	Betaine
118.0873	117.079	-0.001	118.0863	298	67.2	Betaine
118.0873	117.079	-0.001	118.0863	289	67.2	Betaine
118.0873	117.079	-0.001	118.0863	306	65.5	Betaine
118.0873	117.079	-0.001	118.0863	304	65.5	Betaine
118.0873	117.079	-0.001	118.0863	302	65.5	Betaine
106.0872	105	0	106.09	157	74.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20.3	Diethanolamine
391.2862	390.277	-0.0019	391.2843	371	98.8	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	346	98.8	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	338	98.8	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	244	52.5	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	241	46.4	Bis(2-ethylhexyl) phthalate
391.2862	390.277	-0.0019	391.2843	233	52.5	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	234	52	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	231	45.9	Bis(2-ethylhexyl) phthalate
391.2862	390.277	-0.0019	391.2843	226	52	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	202	54.8	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	197	44.2	Bis(2-ethylhexyl) phthalate
391.2862	390.277	-0.0019	391.2843	194	54.8	Diethyl phthalate
371.3164	370.308	-0.0009	371.3156	203	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	130	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	125	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	151	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	111	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	97	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	102	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	83	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	70	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	140	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	115	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	67	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	358	62.7	Betaine
118.0873	117.079	-0.001	118.0863	354	62.7	Betaine
118.0873	117.079	-0.001	118.0863	349	62.7	Betaine
118.0873	117.079	-0.001	118.0863	326	59.7	Betaine
118.0873	117.079	-0.001	118.0863	323	59.7	Betaine
118.0873	117.079	-0.001	118.0863	319	59.7	Betaine
118.0873	117.079	-0.001	118.0863	312	64.4	Betaine
118.0873	117.079	-0.001	118.0863	312	64.4	Betaine
118.0873	117.079	-0.001	118.0863	306	64.4	Betaine
391.2862	390.277	-0.0019	391.2843	347	98.5	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	338	98.5	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	323	98.5	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	221	95	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	169	95	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	160	95	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	196	55.1	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	190	43.3	Bis(2-ethylhexyl) phthalate
391.2862	390.277	-0.0019	391.2843	189	55.1	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	238	53.9	Diethyl phthalate
391.2862	390.277	-0.0019	391.2843	234	45.5	Bis(2-ethylhexyl) phthalate
391.2862	390.277	-0.0019	391.2843	231	53.9	Diethyl phthalate
371.3164	370.308	-0.0009	371.3156	213	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	108	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	105	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	163	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	144	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	106	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	152	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	137	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	104	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	151	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	137	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	117	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	358	61	Betaine
118.0873	117.079	-0.001	118.0863	355	61	Betaine
118.0873	117.079	-0.001	118.0863	351	61	Betaine
118.0873	117.079	-0.001	118.0863	304	67.6	Betaine
118.0873	117.079	-0.001	118.0863	301	67.6	Betaine
118.0873	117.079	-0.001	118.0863	299	67.6	Betaine
118.0873	117.079	-0.001	118.0863	287	63.7	Betaine
118.0873	117.079	-0.001	118.0863	287	63.7	Betaine
118.0873	117.079	-0.001	118.0863	284	63.7	Betaine
371.3164	370.308	-0.0009	371.3156	175	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	115	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	110	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	154	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	143	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	142	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	87	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	77	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	65	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	157	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	140	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	125	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	315	30.2	Betaine
118.0873	117.079	-0.001	118.0863	313	30.2	Betaine
118.0873	117.079	-0.001	118.0863	311	30.2	Betaine
118.0873	117.079	-0.001	118.0863	333	81.9	Betaine

118.0873	117.079	-0.001	118.0863	325	81.9	Betaine
118.0873	117.079	-0.001	118.0863	312	81.9	Betaine
118.0873	117.079	-0.001	118.0863	297	66.5	Betaine
118.0873	117.079	-0.001	118.0863	294	66.5	Betaine
118.0873	117.079	-0.001	118.0863	290	66.5	Betaine
97.0774	114.104	0.0238	97.1012	44	24	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	36	17.9	Cycloheptanol
97.0774	114.104	0.0238	97.1012	32	15.1	Cyclohexanemethanol
338.3423	337.334	-0.0005	338.3417	165	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	161	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	159	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	291	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	278	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	274	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	83	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	74	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	74	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	194	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	191	100	13-Docosenamide, (Z)-
338.3423	337.334	-0.0005	338.3417	187	100	13-Docosenamide, (Z)-
371.3164	370.308	-0.0009	371.3156	195	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	150	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	149	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	161	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	148	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	142	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	105	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	91	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	59	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	183	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	158	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	107	100	Hexanedioic acid, bis(2-ethylhexyl) ester
419.3188	418.308	-0.0032	419.3156	158	100	1,2-Benzenedicarboxylic acid, dinonyl ester

419.3188	418.308	-0.0032	419.3156	202	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	208	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	209	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	160	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	204	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	209	100	1,2-Benzenedicarboxylic acid, dinonyl ester
371.3164	370.308	-0.0009	371.3156	218	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	81	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	76	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	153	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	142	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	140	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	93	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	56	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	84	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	70	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	60	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	286	42	Betaine
118.0873	117.079	-0.001	118.0863	285	42	Betaine
118.0873	117.079	-0.001	118.0863	285	42	Betaine
118.0873	117.079	-0.001	118.0863	319	63.4	Betaine
118.0873	117.079	-0.001	118.0863	316	63.4	Betaine
118.0873	117.079	-0.001	118.0863	315	63.4	Betaine
371.3164	370.308	-0.0009	371.3156	201	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	130	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	129	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	173	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	168	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	158	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	86	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	69	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	57	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	123	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	103	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	71	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	267	83.5	Betaine
118.0873	117.079	-0.001	118.0863	266	83.5	Betaine
118.0873	117.079	-0.001	118.0863	265	83.5	Betaine
118.0873	117.079	-0.001	118.0863	271	63.1	Betaine
118.0873	117.079	-0.001	118.0863	269	63.1	Betaine
118.0873	117.079	-0.001	118.0863	268	63.1	Betaine
118.0873	117.079	-0.001	118.0863	309	53.2	Betaine
118.0873	117.079	-0.001	118.0863	307	53.2	Betaine
118.0873	117.079	-0.001	118.0863	304	53.2	Betaine
97.0774	114.104	0.0238	97.1012	41	26.9	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	31	19	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	30	18.3	Cyclohexanol, 2-methyl-, trans-
419.3188	418.308	-0.0032	419.3156	181	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	204	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	206	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	206	100	1,2-Benzenedicarboxylic acid, dinonyl ester
118.0873	117.079	-0.001	118.0863	263	100	Betaine
118.0873	117.079	-0.001	118.0863	220	100	Betaine
118.0873	117.079	-0.001	118.0863	220	100	Betaine
118.0873	117.079	-0.001	118.0863	284	61.9	Betaine
118.0873	117.079	-0.001	118.0863	284	61.9	Betaine
118.0873	117.079	-0.001	118.0863	281	61.9	Betaine
97.0774	114.104	0.0238	97.1012	34	22.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	27	17.1	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	26	16.4	Cycloheptanol

419.3188	418.308	-0.0032	419.3156	204	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	207	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	210	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	204	100	1,2-Benzenedicarboxylic acid, dinonyl ester
371.3239	370.308	-0.0083	371.3156	242	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3239	370.308	-0.0083	371.3156	94	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3239	370.308	-0.0083	371.3156	90	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3239	370.308	-0.0083	371.3156	148	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3239	370.308	-0.0083	371.3156	130	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3239	370.308	-0.0083	371.3156	114	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3239	370.308	-0.0083	371.3156	49	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3239	370.308	-0.0083	371.3156	169	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3239	370.308	-0.0083	371.3156	154	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3239	370.308	-0.0083	371.3156	137	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0941	117.079	-0.0078	118.0863	284	75.8	Betaine
118.0941	117.079	-0.0078	118.0863	281	75.8	Betaine
118.0941	117.079	-0.0078	118.0863	277	75.8	Betaine
118.0941	117.079	-0.0078	118.0863	383	53.6	Betaine
118.0941	117.079	-0.0078	118.0863	381	53.6	Betaine
118.0941	117.079	-0.0078	118.0863	376	53.6	Betaine
118.0941	117.079	-0.0078	118.0863	276	32.7	Betaine
118.0941	117.079	-0.0078	118.0863	275	32.7	Betaine
118.0941	117.079	-0.0078	118.0863	275	32.7	Betaine
118.0941	117.079	-0.0078	118.0863	309	44.9	Betaine
118.0941	117.079	-0.0078	118.0863	308	44.9	Betaine
118.0941	117.079	-0.0078	118.0863	307	44.9	Betaine
419.3188	418.308	-0.0032	419.3156	212	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	203	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	207	100	1,2-Benzenedicarboxylic acid, dinonyl ester

419.3188	418.308	-0.0032	419.3156	198	100	1,2-Benzenedicarboxylic acid, dinonyl ester
371.3164	370.308	-0.0009	371.3156	175	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	69	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	64	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	143	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	108	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	96	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	71	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	58	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	44	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	180	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	158	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	108	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	313	56.3	Betaine
118.0873	117.079	-0.001	118.0863	313	56.3	Betaine
118.0873	117.079	-0.001	118.0863	303	56.3	Betaine
118.0873	117.079	-0.001	118.0863	256	100	Betaine
118.0873	117.079	-0.001	118.0863	254	100	Betaine
118.0873	117.079	-0.001	118.0863	253	100	Betaine
118.0873	117.079	-0.001	118.0863	329	40.6	Betaine
118.0873	117.079	-0.001	118.0863	326	40.6	Betaine
118.0873	117.079	-0.001	118.0863	323	40.6	Betaine
118.0873	117.079	-0.001	118.0863	308	58.8	Betaine
118.0873	117.079	-0.001	118.0863	307	58.8	Betaine
118.0873	117.079	-0.001	118.0863	299	58.8	Betaine
118.0873	117.079	-0.001	118.0863	282	64.4	Betaine
118.0873	117.079	-0.001	118.0863	281	64.4	Betaine
118.0873	117.079	-0.001	118.0863	279	64.4	Betaine
118.0873	117.079	-0.001	118.0863	291	28.2	Betaine
118.0873	117.079	-0.001	118.0863	289	28.2	Betaine
118.0873	117.079	-0.001	118.0863	289	28.2	Betaine
371.3164	370.308	-0.0009	371.3156	174	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.3164	370.308	-0.0009	371.3156	109	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	95	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	128	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	111	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	98	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	103	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	75	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	70	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	177	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	157	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	118	100	Hexanedioic acid, bis(2-ethylhexyl) ester
393.2988	392.293	0.0011	393.2999	45	100	Chenodeoxycholic acid
419.3188	418.308	-0.0032	419.3156	210	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	203	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	211	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	196	100	1,2-Benzenedicarboxylic acid, dinonyl ester
118.0873	117.079	-0.001	118.0863	146	100	N-Methyl-.alpha.-aminoisobutyric acid
118.0873	117.079	-0.001	118.0863	144	100	N-Methyl-.alpha.-aminoisobutyric acid
118.0873	117.079	-0.001	118.0863	143	100	N-Methyl-.alpha.-aminoisobutyric acid
118.0873	117.079	-0.001	118.0863	369	66.2	Betaine
118.0873	117.079	-0.001	118.0863	366	66.2	Betaine
118.0873	117.079	-0.001	118.0863	360	66.2	Betaine
118.0873	117.079	-0.001	118.0863	277	60.2	Betaine
118.0873	117.079	-0.001	118.0863	275	60.2	Betaine
118.0873	117.079	-0.001	118.0863	275	60.2	Betaine
118.0873	117.079	-0.001	118.0863	339	36.6	Betaine
118.0873	117.079	-0.001	118.0863	338	36.6	Betaine
118.0873	117.079	-0.001	118.0863	331	36.6	Betaine
106.0872	105	0	106.09	152	77.2	Diethanolamine

106.0872	105.079	-0.0009	106.0863	121	21	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	21	Diethanolamine
106.0872	105.079	-0.0009	106.0863	115	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	100	Diethanolamine
393.2988	392.293	0.0011	393.2999	36	100	Chenodeoxycholic acid
419.3188	418.308	-0.0032	419.3156	204	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	208	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	202	100	1,2-Benzenedicarboxylic acid, dinonyl ester
419.3188	418.308	-0.0032	419.3156	206	100	1,2-Benzenedicarboxylic acid, dinonyl ester
371.3164	370.308	-0.0009	371.3156	195	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	117	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	111	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	138	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	120	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	88	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	115	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	77	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.3164	370.308	-0.0009	371.3156	65	100	Hexanedioic acid, bis(2-ethylhexyl) ester
393.2988	392.293	0.0011	393.2999	33	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	29	100	Chenodeoxycholic acid
84.0822	102.092	-0.0014	84.0808	226	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	225	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	177	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	176	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	138	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	137	49	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	311	49.1	Betaine
118.0873	117.079	-0.001	118.0863	307	49.1	Betaine
118.0873	117.079	-0.001	118.0863	305	49.1	Betaine
118.0873	117.079	-0.001	118.0863	331	70.8	Betaine
118.0873	117.079	-0.001	118.0863	327	70.8	Betaine
118.0873	117.079	-0.001	118.0863	321	70.8	Betaine
118.0873	117.079	-0.001	118.0863	310	40.7	Betaine

118.0873	117.079	-0.001	118.0863	310	40.7	Betaine
118.0873	117.079	-0.001	118.0863	310	40.7	Betaine
106.0872	105	0	106.09	168	73.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	139	20.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	138	20.8	Diethanolamine
106.0872	105	0	106.09	150	78.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	21.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	21.8	Diethanolamine
106.0872	105	0	106.09	227	66	Diethanolamine
106.0872	105.079	-0.0009	106.0863	209	34	Diethanolamine
106.0872	105.079	-0.0009	106.0863	207	34	Diethanolamine
419.3188	418.308	-0.0032	419.3156	205	100	1,2-Benzenedicarboxylic acid, dinonyl ester
118.0873	117.079	-0.001	118.0863	347	39.5	Betaine
118.0873	117.079	-0.001	118.0863	346	39.5	Betaine
118.0873	117.079	-0.001	118.0863	343	39.5	Betaine
118.0873	117.079	-0.001	118.0863	299	72.7	Betaine
118.0873	117.079	-0.001	118.0863	291	72.7	Betaine
118.0873	117.079	-0.001	118.0863	279	72.7	Betaine
118.0873	117.079	-0.001	118.0863	344	53.2	Betaine
118.0873	117.079	-0.001	118.0863	339	53.2	Betaine
118.0873	117.079	-0.001	118.0863	338	53.2	Betaine
106.0872	105	0	106.09	114	53.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	111	46.9	Diethanolamine
106.0872	105	0	106.09	210	68.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	190	31.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	190	31.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	253	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	250	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	211	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	211	50	Betaine aldehyde cation
186.0588	203.091	0.0285	186.0873	71	75.3	Ala-Asn
186.0588	163.084	0.0149	186.0737	33	18.1	N,N-Bis(2-hydroxyethyl)glycine
186.0588	168.042	0.0173	186.0761	10	6.6	3-Hydroxy-4-methoxybenzoic acid
186.0588	163.084	0.0149	186.0737	146	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	395	37.1	Betaine
118.0873	117.079	-0.001	118.0863	394	37.1	Betaine
118.0873	117.079	-0.001	118.0863	389	37.1	Betaine
118.0873	117.079	-0.001	118.0863	301	67.1	Betaine
118.0873	117.079	-0.001	118.0863	298	67.1	Betaine
118.0873	117.079	-0.001	118.0863	293	67.1	Betaine
118.0873	117.079	-0.001	118.0863	354	48.8	Betaine
118.0873	117.079	-0.001	118.0863	353	48.8	Betaine
118.0873	117.079	-0.001	118.0863	349	48.8	Betaine
106.0872	105	0	106.09	159	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	21.1	Diethanolamine

106.0872	105.079	-0.0009	106.0863	127	21.1	Diethanolamine
106.0872	105	0	106.09	231	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	198	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	197	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	152	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	152	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	147	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	261	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	260	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	206	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	205	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	181	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	179	48	Betaine aldehyde cation
106.0872	105.079	-0.0009	106.0863	126	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	178	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	178	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	202	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	201	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	138	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	137	49	Betaine aldehyde cation
553.3927	530.4	-0.003	553.3897	1	17.2	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	4	7.7	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	3	7.4	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	3	7.4	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	10	8.5	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	10	8.5	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	10	8.5	Didodecyl 3,3'-thiodipropionate oxide
118.0873	117.079	-0.001	118.0863	336	55.2	Betaine
118.0873	117.079	-0.001	118.0863	334	55.2	Betaine
118.0873	117.079	-0.001	118.0863	329	55.2	Betaine
118.0873	117.079	-0.001	118.0863	269	62.3	Betaine
118.0873	117.079	-0.001	118.0863	267	62.3	Betaine
118.0873	117.079	-0.001	118.0863	265	62.3	Betaine
118.0873	117	0	118.09	343	24.5	Betaine
118.0873	117	0	118.09	341	22.6	Betaine
118.0873	117.079	-0.001	118.0863	336	18.2	Betaine
553.3927	530.4	-0.003	553.3897	88	14.4	Didodecyl 3,3'-thiodipropionate oxide

553.3927	530.4	-0.003	553.3897	88	14.4	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	87	13.8	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	242	19.9	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	239	17.6	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	236	15.6	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	318	17.5	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	315	15.5	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	311	13.1	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	197	14	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	197	14	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	196	13.5	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	297	35.6	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	293	30.1	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	264	8.5	Didodecyl 3,3'-thiodipropionate oxide
118.0873	117.079	-0.001	118.0863	366	24	Betaine
118.0873	117	0	118.09	366	24	Betaine
118.0873	117.079	-0.001	118.0863	365	24	Betaine
118.0873	117.079	-0.001	118.0863	278	62.9	Betaine
118.0873	117.079	-0.001	118.0863	278	62.9	Betaine
118.0873	117.079	-0.001	118.0863	276	62.9	Betaine
118.0873	117.079	-0.001	118.0863	337	42.2	Betaine
118.0873	117.079	-0.001	118.0863	335	42.2	Betaine
118.0873	117.079	-0.001	118.0863	334	42.2	Betaine
553.3927	530.4	-0.003	553.3897	3	21.3	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	2	20.5	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	1	19.7	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	38	10.8	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	38	10.8	Didodecyl 3,3'-thiodipropionate oxide

553.3927	530.4	-0.003	553.3897	38	10.8	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	78	14.4	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	77	13.8	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	76	13.3	Didodecyl 3,3'-thiodipropionate oxide
97.0774	114.104	0.0238	97.1012	28	35.8	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	23	35.8	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	21	27.4	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	29	21.7	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	26	21.7	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	26	19.2	Cyclohexanol, 4-methyl-, trans-
531.4089	530.4	-0.0011	531.4078	358	19.2	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	356	17.7	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	355	17	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	367	23.2	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	360	17.8	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	352	13.2	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	241	28.3	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	238	25	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	220	12.9	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	259	28.1	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	258	27	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	236	10.7	Didodecyl 3,3'-thiodipropionate oxide
106.0872	105	0	106.09	149	77.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	22.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	22.1	Diethanolamine
553.3927	530.4	-0.003	553.3897	14	15.3	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	14	15.3	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	13	14.7	Didodecyl 3,3'-thiodipropionate oxide

553.3927	530.4	-0.003	553.3897	6	8.3	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	6	8.3	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	5	8	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	1	20.6	Didodecyl 3,3'-thiodipropionate oxide
118.0873	117.079	-0.001	118.0863	177	100	Betaine
118.0873	117.079	-0.001	118.0863	13	100	Betaine
118.0873	117.079	-0.001	118.0863	381	62.8	Betaine
118.0873	117.079	-0.001	118.0863	380	62.8	Betaine
118.0873	117.079	-0.001	118.0863	372	62.8	Betaine
118.0873	117.079	-0.001	118.0863	321	98.8	Betaine
118.0873	117.079	-0.001	118.0863	318	98.8	Betaine
118.0873	117.079	-0.001	118.0863	308	98.8	Betaine
118.0873	117.079	-0.001	118.0863	343	37.3	Betaine
118.0873	117.079	-0.001	118.0863	343	37.3	Betaine
118.0873	117.079	-0.001	118.0863	338	37.3	Betaine
531.4089	530.4	-0.0011	531.4078	317	30.4	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	296	12.9	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	288	9.6	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	269	13.2	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	268	12.7	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	268	12.7	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	227	23.9	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	221	18.8	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	212	13.6	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	218	15.9	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	218	15.9	Didodecyl 3,3'-thiodipropionate oxide
531.4089	530.4	-0.0011	531.4078	214	13.5	Didodecyl 3,3'-thiodipropionate oxide
97.0774	114.104	0.0238	97.1012	71	25.7	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	59	17.1	Cycloheptanol
97.0774	114.104	0.0238	97.1012	57	15.8	Cyclohexanemethanol
84.0822	102.092	-0.0014	84.0808	244	50	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	244	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	210	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	209	49	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	137	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	154	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	340	32.5	Betaine
118.0873	117.079	-0.001	118.0863	336	32.5	Betaine
118.0873	117.079	-0.001	118.0863	335	32.5	Betaine
118.0873	117.079	-0.001	118.0863	330	39.3	Betaine
118.0873	117.079	-0.001	118.0863	327	39.3	Betaine
118.0873	117.079	-0.001	118.0863	326	39.3	Betaine
118.0873	117.079	-0.001	118.0863	323	56.6	Betaine
118.0873	117.079	-0.001	118.0863	323	56.6	Betaine
118.0873	117.079	-0.001	118.0863	322	56.6	Betaine
97.0774	114.104	0.0238	97.1012	43	26.6	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	33	18.7	Cycloheptanol
97.0774	114.104	0.0238	97.1012	26	14.4	Cyclopentanemethanol, .alpha.-methyl-
106.0872	105	0	106.09	152	74.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	18.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	18.5	Diethanolamine
553.3927	530.4	-0.003	553.3897	12	9	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	11	8.6	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	11	8.6	Didodecyl 3,3'-thiodipropionate oxide
118.0873	117.079	-0.001	118.0863	378	49.4	Betaine
118.0873	117.079	-0.001	118.0863	374	49.4	Betaine
118.0873	117.079	-0.001	118.0863	371	49.4	Betaine
118.0873	117.079	-0.001	118.0863	321	61.3	Betaine
118.0873	117.079	-0.001	118.0863	318	61.3	Betaine
118.0873	117.079	-0.001	118.0863	316	61.3	Betaine
118.0873	117.079	-0.001	118.0863	304	70.8	Betaine
118.0873	117.079	-0.001	118.0863	302	70.8	Betaine
118.0873	117.079	-0.001	118.0863	300	70.8	Betaine
97.0774	114.104	0.0238	97.1012	51	23.9	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	51	23.9	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	40	16.4	Cyclohexanol, 1-methyl-
106.0872	105	0	106.09	144	74.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	25.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	25.1	Diethanolamine
106.0872	105	0	106.09	197	74.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	173	25.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	173	25.1	Diethanolamine
553.3927	530.4	-0.003	553.3897	70	13.7	Didodecyl 3,3'-thiodipropionate oxide

553.3927	530.4	-0.003	553.3897	70	13.7	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	69	13.2	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	57	15.6	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	56	14.9	Didodecyl 3,3'-thiodipropionate oxide
553.3927	530.4	-0.003	553.3897	56	14.9	Didodecyl 3,3'-thiodipropionate oxide
118.0873	117.079	-0.001	118.0863	365	35.7	Betaine
118.0873	117.079	-0.001	118.0863	365	35.7	Betaine
118.0873	117.079	-0.001	118.0863	363	35.7	Betaine
118.0873	117.079	-0.001	118.0863	374	49.7	Betaine
118.0873	117.079	-0.001	118.0863	373	49.7	Betaine
118.0873	117.079	-0.001	118.0863	369	49.7	Betaine
118.0873	117.079	-0.001	118.0863	351	55.1	Betaine
118.0873	117.079	-0.001	118.0863	347	55.1	Betaine
118.0873	117.079	-0.001	118.0863	344	55.1	Betaine
106.0872	105	0	106.09	157	77.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	22.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	22.4	Diethanolamine
118.0873	117.079	-0.001	118.0863	263	79.3	Betaine
118.0873	117.079	-0.001	118.0863	259	79.3	Betaine
118.0873	117.079	-0.001	118.0863	252	79.3	Betaine
118.0873	117.079	-0.001	118.0863	357	92.1	Betaine
118.0873	117.079	-0.001	118.0863	353	92.1	Betaine
118.0873	117.079	-0.001	118.0863	351	92.1	Betaine
118.0873	117.079	-0.001	118.0863	285	63	Betaine
118.0873	117.079	-0.001	118.0863	283	63	Betaine
118.0873	117.079	-0.001	118.0863	278	63	Betaine
118.0873	117.079	-0.001	118.0863	342	35.6	Betaine
118.0873	117.079	-0.001	118.0863	339	35.6	Betaine
118.0873	117.079	-0.001	118.0863	336	35.6	Betaine
97.0774	114.104	0.0238	97.1012	87	21.1	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	87	21.1	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	86	20.3	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	165	74.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	133	19.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	132	19.9	Diethanolamine
106.0872	105	0	106.09	151	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	21.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	207	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	204	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	183	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	181	48	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	147	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	145	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	186	95.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	64	4.7	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	341	34.4	Betaine
118.0873	117.079	-0.001	118.0863	338	34.4	Betaine
118.0873	117.079	-0.001	118.0863	337	34.4	Betaine
118.0873	117.079	-0.001	118.0863	282	61.1	Betaine
118.0873	117.079	-0.001	118.0863	279	61.1	Betaine
118.0873	117.079	-0.001	118.0863	275	61.1	Betaine
118.0873	117.079	-0.001	118.0863	281	66	Betaine
118.0873	117.079	-0.001	118.0863	279	66	Betaine
118.0873	117.079	-0.001	118.0863	277	66	Betaine
106.0872	105	0	106.09	155	75.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	18.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	18.2	Diethanolamine
106.0872	105	0	106.09	153	80.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	19.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	294	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	291	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	218	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	213	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	129	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	127	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	149	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	70	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	166	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	389	37.7	Betaine
118.0873	117.079	-0.001	118.0863	386	37.7	Betaine
118.0873	117.079	-0.001	118.0863	381	37.7	Betaine
118.0873	117.079	-0.001	118.0863	248	49.5	Betaine
118.0873	117.079	-0.001	118.0863	246	49.5	Betaine
118.0873	117.079	-0.001	118.0863	245	49.5	Betaine
118.0873	117.079	-0.001	118.0863	312	40.1	Betaine
118.0873	117.079	-0.001	118.0863	310	40.1	Betaine
118.0873	117.079	-0.001	118.0863	305	40.1	Betaine
97.0774	114.104	0.0238	97.1012	6	100	Cyclopentanemethanol, .alpha.-methyl-
106.0872	105	0	106.09	154	74.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	19.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	19.2	Diethanolamine
106.0872	105	0	106.09	155	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	21.4	Diethanolamine
610.5771	610	-0.04	610.54	125	50	DG 34:2; [M+NH4]+; DG(14:1/20:1/0:0)

610.5771	610	-0.04	610.54	125	50	DG 34:2; [M+NH4] ⁺ ; DG(20:1/14:1/0:0)
610.5771	610	-0.04	610.54	120	50	DG 34:2; [M+NH4] ⁺ ; DG(14:1/20:1/0:0)
610.5771	610	-0.04	610.54	120	50	DG 34:2; [M+NH4] ⁺ ; DG(20:1/14:1/0:0)
610.5771	610	-0.04	610.54	81	50	DG 34:2; [M+NH4] ⁺ ; DG(14:1/20:1/0:0)
610.5771	610	-0.04	610.54	81	50	DG 34:2; [M+NH4] ⁺ ; DG(20:1/14:1/0:0)
640.5867	640	0	640.59	139	50	DG 36:1; [M+NH4] ⁺ ; DG(14:1/22:0/0:0)
640.5867	640	0	640.59	139	50	DG 36:1; [M+NH4] ⁺ ; DG(22:0/14:1/0:0)
640.5867	640	0	640.59	128	50	DG 36:1; [M+NH4] ⁺ ; DG(14:1/22:0/0:0)
640.5867	640	0	640.59	128	50	DG 36:1; [M+NH4] ⁺ ; DG(22:0/14:1/0:0)
640.5867	640	0	640.59	126	50	DG 36:1; [M+NH4] ⁺ ; DG(14:1/22:0/0:0)
640.5867	640	0	640.59	126	50	DG 36:1; [M+NH4] ⁺ ; DG(22:0/14:1/0:0)
84.0822	102.092	-0.0014	84.0808	233	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	229	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	193	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	193	50	Betaine aldehyde cation
186.0588	203.091	0.0285	186.0873	82	82.7	Ala-Asn
186.0588	163.084	0.0149	186.0737	35	17.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	158	92.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	63	7.5	Ser-His-Lys
640.5867	640	0	640.59	153	50	DG 36:1; [M+NH4] ⁺ ; DG(14:1/22:0/0:0)
640.5867	640	0	640.59	153	50	DG 36:1; [M+NH4] ⁺ ; DG(22:0/14:1/0:0)
640.5867	640	0	640.59	154	50	DG 36:1; [M+NH4] ⁺ ; DG(14:1/22:0/0:0)
640.5867	640	0	640.59	154	50	DG 36:1; [M+NH4] ⁺ ; DG(22:0/14:1/0:0)
118.0873	117.079	-0.001	118.0863	380	65.3	Betaine
118.0873	117.079	-0.001	118.0863	374	65.3	Betaine
118.0873	117.079	-0.001	118.0863	368	65.3	Betaine
118.0873	117.079	-0.001	118.0863	308	76.2	Betaine
118.0873	117.079	-0.001	118.0863	305	76.2	Betaine
118.0873	117.079	-0.001	118.0863	299	76.2	Betaine
118.0873	117.079	-0.001	118.0863	311	63.4	Betaine
118.0873	117.079	-0.001	118.0863	310	63.4	Betaine
118.0873	117.079	-0.001	118.0863	309	63.4	Betaine

610.5771	610	-0.04	610.54	156	50	DG 34:2; [M+NH4] ⁺ ; DG(14:1/20:1/0:0)
610.5771	610	-0.04	610.54	156	50	DG 34:2; [M+NH4] ⁺ ; DG(20:1/14:1/0:0)
636.5935	636	-0.03	636.56	155	50	DG 36:3; [M+NH4] ⁺ ; DG(14:1/22:2/0:0)
636.5935	636	-0.03	636.56	155	50	DG 36:3; [M+NH4] ⁺ ; DG(22:2/14:1/0:0)
636.5935	636	-0.03	636.56	155	50	DG 36:3; [M+NH4] ⁺ ; DG(14:1/22:2/0:0)
636.5935	636	-0.03	636.56	155	50	DG 36:3; [M+NH4] ⁺ ; DG(22:2/14:1/0:0)
636.5935	636	-0.03	636.56	153	50	DG 36:3; [M+NH4] ⁺ ; DG(14:1/22:2/0:0)
636.5935	636	-0.03	636.56	153	50	DG 36:3; [M+NH4] ⁺ ; DG(22:2/14:1/0:0)
97.0774	114.104	0.0238	97.1012	45	25.8	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	34	17.7	Cycloheptanol
97.0774	114.104	0.0238	97.1012	30	15	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	330	89.7	Betaine
118.0873	117.079	-0.001	118.0863	322	89.7	Betaine
118.0873	117.079	-0.001	118.0863	308	89.7	Betaine
118.0873	117.079	-0.001	118.0863	415	47	Betaine
118.0873	117.079	-0.001	118.0863	410	47	Betaine
118.0873	117.079	-0.001	118.0863	409	47	Betaine
118.0873	117.079	-0.001	118.0863	325	78.9	Betaine
118.0873	117.079	-0.001	118.0863	325	78.9	Betaine
118.0873	117.079	-0.001	118.0863	318	78.9	Betaine
118.0873	117.079	-0.001	118.0863	449	57.4	Betaine
118.0873	117.079	-0.001	118.0863	448	57.4	Betaine
118.0873	117.079	-0.001	118.0863	442	57.4	Betaine
97.0774	114.104	0.0238	97.1012	33	26.6	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	32	26.6	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	29	22.4	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	158	75.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	18	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	18	Diethanolamine
84.0822	102.092	-0.0014	84.0808	258	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	257	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	206	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	203	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	182	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	176	44	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	298	40.2	Betaine
118.0873	117.079	-0.001	118.0863	298	40.2	Betaine
118.0873	117.079	-0.001	118.0863	295	40.2	Betaine
118.0873	117.079	-0.001	118.0863	281	58	Betaine

118.0873	117.079	-0.001	118.0863	278	58	Betaine
118.0873	117.079	-0.001	118.0863	278	58	Betaine
118.0873	117.079	-0.001	118.0863	355	40.5	Betaine
118.0873	117.079	-0.001	118.0863	352	40.5	Betaine
118.0873	117.079	-0.001	118.0863	351	40.5	Betaine
106.0872	105	0	106.09	157	74.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	133	25.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	132	25.1	Diethanolamine
106.0872	105	0	106.09	159	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	150	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	149	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	148	100	Diethanolamine
666.6035	666	0	666.6	158	50	DG 38:2; [M+NH4]+; DG(14:1/24:1/0:0)
666.6035	666	0	666.6	158	50	DG 38:2; [M+NH4]+; DG(24:1/14:1/0:0)
666.6035	666	0	666.6	151	50	DG 38:2; [M+NH4]+; DG(14:1/24:1/0:0)
666.6035	666	0	666.6	151	50	DG 38:2; [M+NH4]+; DG(24:1/14:1/0:0)
186.0588	163.084	0.0149	186.0737	132	87.8	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	60	12.2	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	167	100	N,N-Bis(2-hydroxyethyl)glycine
106.0872	105	0	106.09	156	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	20.4	Diethanolamine
106.0872	105	0	106.09	183	73.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	160	26.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	159	26.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	258	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	257	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	256	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	254	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	141	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	138	46.9	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	234	100	Betaine
118.0873	117.079	-0.001	118.0863	227	100	Betaine
118.0873	117.079	-0.001	118.0863	170	100	Betaine
118.0873	117.079	-0.001	118.0863	381	47.3	Betaine
118.0873	117.079	-0.001	118.0863	380	47.3	Betaine
118.0873	117.079	-0.001	118.0863	376	47.3	Betaine
118.0873	117.079	-0.001	118.0863	321	98.8	Betaine
118.0873	117.079	-0.001	118.0863	317	98.8	Betaine
118.0873	117.079	-0.001	118.0863	306	98.8	Betaine
118.0873	117.079	-0.001	118.0863	339	58.7	Betaine

118.0873	117.079	-0.001	118.0863	338	58.7	Betaine
118.0873	117.079	-0.001	118.0863	337	58.7	Betaine
97.0774	114.104	0.0238	97.1012	39	24.1	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	34	19.5	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	31	17.2	Cyclohexanemethanol
186.0588	370.196	0.0467	186.1055	62	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	44	100	Ser-His-Lys
624.5931	624	-0.03	624.56	160	50	DG 35:2; [M+NH4]+; DG(15:1/20:1/0:0)
624.5931	624	-0.03	624.56	160	50	DG 35:2; [M+NH4]+; DG(20:1/15:1/0:0)
118.0873	117.079	-0.001	118.0863	378	45.4	Betaine
118.0873	117.079	-0.001	118.0863	376	45.4	Betaine
118.0873	117.079	-0.001	118.0863	370	45.4	Betaine
118.0873	117.079	-0.001	118.0863	296	65.5	Betaine
118.0873	117.079	-0.001	118.0863	293	65.5	Betaine
118.0873	117.079	-0.001	118.0863	291	65.5	Betaine
118.0873	117.079	-0.001	118.0863	332	41.1	Betaine
118.0873	117.079	-0.001	118.0863	331	41.1	Betaine
118.0873	117.079	-0.001	118.0863	329	41.1	Betaine
106.0872	105	0	106.09	174	75	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	15.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	15.8	Diethanolamine
106.0872	105	0	106.09	159	75.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	19.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	19.7	Diethanolamine
118.0873	117.079	-0.001	118.0863	333	64.5	Betaine
118.0873	117.079	-0.001	118.0863	329	64.5	Betaine
118.0873	117.079	-0.001	118.0863	321	64.5	Betaine
118.0873	117.079	-0.001	118.0863	381	26.9	Betaine
118.0873	117	0	118.09	380	25.9	Betaine
118.0873	117.079	-0.001	118.0863	379	26.9	Betaine
118.0873	117.079	-0.001	118.0863	283	62.8	Betaine
118.0873	117.079	-0.001	118.0863	282	62.8	Betaine
118.0873	117.079	-0.001	118.0863	278	62.8	Betaine
118.0873	117.079	-0.001	118.0863	330	45.2	Betaine
118.0873	117.079	-0.001	118.0863	327	45.2	Betaine
118.0873	117.079	-0.001	118.0863	324	45.2	Betaine
106.0872	105	0	106.09	167	77.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	140	22.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	138	22.7	Diethanolamine
106.0872	105	0	106.09	158	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	274	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	274	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	216	52	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	214	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	162	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	160	48	Betaine aldehyde cation
106.0872	105.079	-0.0009	106.0863	113	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	111	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	107	100	Diethanolamine
186.0588	370.196	0.0467	186.1055	46	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	60	61.5	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	46	38.5	Ser-His-Lys
84.0822	102.092	-0.0014	84.0808	257	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	255	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	204	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	202	48	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	295	48.9	Betaine
118.0873	117.079	-0.001	118.0863	292	48.9	Betaine
118.0873	117.079	-0.001	118.0863	291	48.9	Betaine
118.0873	117.079	-0.001	118.0863	417	63.4	Betaine
118.0873	117.079	-0.001	118.0863	412	63.4	Betaine
118.0873	117.079	-0.001	118.0863	405	63.4	Betaine
118.0873	117.079	-0.001	118.0863	254	100	Betaine
118.0873	117.079	-0.001	118.0863	253	100	Betaine
118.0873	117.079	-0.001	118.0863	250	100	Betaine
118.0873	117.079	-0.001	118.0863	325	37.9	Betaine
118.0873	117.079	-0.001	118.0863	323	37.9	Betaine
118.0873	117.079	-0.001	118.0863	320	37.9	Betaine
84.0822	102.092	-0.0014	84.0808	223	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	223	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	201	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	200	49	Betaine aldehyde cation
186.0588	203.091	0.0285	186.0873	62	100	Ala-Asn
186.0588	163.084	0.0149	186.0737	139	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	137	88.8	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	61	11.2	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	383	35.5	Betaine
118.0873	117.079	-0.001	118.0863	382	35.5	Betaine
118.0873	117.079	-0.001	118.0863	381	35.5	Betaine
118.0873	117.079	-0.001	118.0863	251	56.8	Betaine
118.0873	117.079	-0.001	118.0863	249	56.8	Betaine
118.0873	117.079	-0.001	118.0863	248	56.8	Betaine
118.0873	117.079	-0.001	118.0863	279	61.9	Betaine
118.0873	117.079	-0.001	118.0863	279	61.9	Betaine
118.0873	117.079	-0.001	118.0863	276	61.9	Betaine
97.0774	114.104	0.0238	97.1012	36	24.5	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	27	17.8	Cycloheptanol
97.0774	114.104	0.0238	97.1012	23	15	Cyclohexanemethanol
638.6087	638	-0.04	638.57	141	29.6	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)

638.6087	638	-0.04	638.57	141	29.6	DG 36:2; [M+NH4] ⁺ ; DG(22:1/14:1/0:0)
638.6087	638	-0.04	638.57	130	20.3	DG 36:2; [M+NH4] ⁺ ; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	129	31.7	DG 36:2; [M+NH4] ⁺ ; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	129	31.7	DG 36:2; [M+NH4] ⁺ ; DG(20:1/16:1/0:0)
638.6087	638	-0.04	638.57	113	18.3	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	140	28	DG 36:2; [M+NH4] ⁺ ; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	140	28	DG 36:2; [M+NH4] ⁺ ; DG(20:1/16:1/0:0)
638.6087	638	-0.04	638.57	134	22	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	128	28	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	128	28	DG 36:2; [M+NH4] ⁺ ; DG(22:1/14:1/0:0)
638.6087	638	-0.04	638.57	122	22	DG 36:2; [M+NH4] ⁺ ; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	160	50	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	160	50	DG 36:2; [M+NH4] ⁺ ; DG(22:1/14:1/0:0)
638.6087	638	-0.04	638.57	151	25.5	DG 36:2; [M+NH4] ⁺ ; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	151	25.5	DG 36:2; [M+NH4] ⁺ ; DG(20:1/16:1/0:0)
638.6087	638	-0.04	638.57	150	24.5	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	147	29.3	DG 36:2; [M+NH4] ⁺ ; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	147	29.3	DG 36:2; [M+NH4] ⁺ ; DG(20:1/16:1/0:0)
638.6087	638	-0.04	638.57	137	20.7	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	139	26	DG 36:2; [M+NH4] ⁺ ; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	139	26	DG 36:2; [M+NH4] ⁺ ; DG(20:1/16:1/0:0)
638.6087	638	-0.04	638.57	137	24	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)
668.6187	668	0	668.62	152	31.7	DG 38:1; [M+NH4] ⁺ ; DG(14:1/24:0/0:0)

668.6187	668	0	668.62	152	31.7	DG 38:1; [M+NH4] ⁺ ; DG(24:0/14:1/0:0)
668.6187	668	0	668.62	136	18.3	DG 38:1; [M+NH4] ⁺ ; DG(16:1/22:0/0:0)
668.6187	668	0	668.62	141	32.3	DG 38:1; [M+NH4] ⁺ ; DG(16:1/22:0/0:0)
668.6187	668	0	668.62	141	32.3	DG 38:1; [M+NH4] ⁺ ; DG(22:0/16:1/0:0)
668.6187	668	0	668.62	124	17.6	DG 38:1; [M+NH4] ⁺ ; DG(14:1/24:0/0:0)
118.0873	117.079	-0.001	118.0863	308	70.7	Betaine
118.0873	117.079	-0.001	118.0863	303	70.7	Betaine
118.0873	117.079	-0.001	118.0863	300	70.7	Betaine
118.0873	117.079	-0.001	118.0863	316	61.7	Betaine
118.0873	117.079	-0.001	118.0863	312	61.7	Betaine
118.0873	117.079	-0.001	118.0863	312	61.7	Betaine
118.0873	117.079	-0.001	118.0863	329	78	Betaine
118.0873	117.079	-0.001	118.0863	328	78	Betaine
118.0873	117.079	-0.001	118.0863	317	78	Betaine
118.0873	117.079	-0.001	118.0863	327	63.5	Betaine
118.0873	117.079	-0.001	118.0863	327	63.5	Betaine
118.0873	117.079	-0.001	118.0863	322	63.5	Betaine
97.0774	114.104	0.0238	97.1012	27	23.1	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	19	17.2	Cycloheptanol
97.0774	114.104	0.0238	97.1012	16	15.2	Cyclopentanemethanol, .alpha.-methyl-
106.0872	105	0	106.09	156	80.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	19.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	19.3	Diethanolamine
106.0872	105	0	106.09	168	75.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	142	22.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	141	22.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	115	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	105	100	Diethanolamine
638.6087	638	-0.04	638.57	157	38.5	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)
638.6087	638	-0.04	638.57	157	38.5	DG 36:2; [M+NH4] ⁺ ; DG(22:1/14:1/0:0)
638.6087	638	-0.04	638.57	131	11.5	DG 36:2; [M+NH4] ⁺ ; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	157	26	DG 36:2; [M+NH4] ⁺ ; DG(16:1/20:1/0:0)
638.6087	638	-0.04	638.57	157	26	DG 36:2; [M+NH4] ⁺ ; DG(20:1/16:1/0:0)
638.6087	638	-0.04	638.57	155	24	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)

668.6187	668	0	668.62	151	31.7	DG 38:1; [M+NH4]+; DG(14:1/24:0/0:0)
668.6187	668	0	668.62	151	31.7	DG 38:1; [M+NH4]+; DG(24:0/14:1/0:0)
668.6187	668	0	668.62	135	18.3	DG 38:1; [M+NH4]+; DG(16:1/22:0/0:0)
668.6187	668	0	668.62	149	35.1	DG 38:1; [M+NH4]+; DG(16:1/22:0/0:0)
668.6187	668	0	668.62	149	35.1	DG 38:1; [M+NH4]+; DG(22:0/16:1/0:0)
668.6187	668	0	668.62	128	14.9	DG 38:1; [M+NH4]+; DG(14:1/24:0/0:0)
668.6187	668	0	668.62	137	39	DG 38:1; [M+NH4]+; DG(14:1/24:0/0:0)
668.6187	668	0	668.62	137	39	DG 38:1; [M+NH4]+; DG(24:0/14:1/0:0)
668.6187	668	0	668.62	108	11	DG 38:1; [M+NH4]+; DG(16:1/22:0/0:0)
664.6234	664	-0.03	664.59	142	50	DG 38:3; [M+NH4]+; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	142	50	DG 38:3; [M+NH4]+; DG(22:2/16:1/0:0)
664.6234	664	-0.03	664.59	157	50	DG 38:3; [M+NH4]+; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	157	50	DG 38:3; [M+NH4]+; DG(22:2/16:1/0:0)
664.6234	664	-0.03	664.59	150	50	DG 38:3; [M+NH4]+; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	150	50	DG 38:3; [M+NH4]+; DG(22:2/16:1/0:0)
106.0872	105	0	106.09	169	80.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	130	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	236	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	233	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	223	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	222	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	117	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	113	45.8	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	181	88.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	141	88.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	76	6	Ser-His-Lys
664.6234	664	-0.03	664.59	157	50	DG 38:3; [M+NH4]+; DG(16:1/22:2/0:0)

664.6234	664	-0.03	664.59	157	50	DG 38:3; [M+NH4] ⁺ ; DG(22:2/16:1/0:0)
664.6234	664	-0.03	664.59	158	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	158	50	DG 38:3; [M+NH4] ⁺ ; DG(22:2/16:1/0:0)
118.0873	117.079	-0.001	118.0863	298	82.7	Betaine
118.0873	117.079	-0.001	118.0863	293	82.7	Betaine
118.0873	117.079	-0.001	118.0863	288	82.7	Betaine
118.0873	117.079	-0.001	118.0863	449	99	Betaine
118.0873	117.079	-0.001	118.0863	446	99	Betaine
118.0873	117.079	-0.001	118.0863	443	99	Betaine
118.0873	117.079	-0.001	118.0863	313	71.5	Betaine
118.0873	117.079	-0.001	118.0863	309	71.5	Betaine
118.0873	117.079	-0.001	118.0863	306	71.5	Betaine
118.0873	117.079	-0.001	118.0863	378	47.3	Betaine
118.0873	117.079	-0.001	118.0863	377	47.3	Betaine
118.0873	117.079	-0.001	118.0863	374	47.3	Betaine
668.6187	668	0	668.62	215	50	DG 38:1; [M+NH4] ⁺ ; DG(16:1/22:0/0:0)
668.6187	668	0	668.62	215	50	DG 38:1; [M+NH4] ⁺ ; DG(22:0/16:1/0:0)
106.0872	105	0	106.09	190	77.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	150	17.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	149	17.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	175	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	163	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	154	100	Diethanolamine
118.0873	117.079	-0.001	118.0863	384	47.4	Betaine
118.0873	117.079	-0.001	118.0863	382	47.4	Betaine
118.0873	117.079	-0.001	118.0863	380	47.4	Betaine
118.0873	117.079	-0.001	118.0863	293	70.9	Betaine
118.0873	117.079	-0.001	118.0863	292	70.9	Betaine
118.0873	117.079	-0.001	118.0863	282	70.9	Betaine
118.0873	117.079	-0.001	118.0863	346	60.1	Betaine
118.0873	117.079	-0.001	118.0863	346	60.1	Betaine
118.0873	117.079	-0.001	118.0863	344	60.1	Betaine
97.0774	114.104	0.0238	97.1012	26	25.6	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	24	23.6	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	22	25.6	Cyclohexanemethanol
664.6234	664	-0.03	664.59	151	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	151	50	DG 38:3; [M+NH4] ⁺ ; DG(22:2/16:1/0:0)

664.6234	664	-0.03	664.59	160	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	160	50	DG 38:3; [M+NH4] ⁺ ; DG(22:2/16:1/0:0)
664.6234	664	-0.03	664.59	153	50	DG 38:3; [M+NH4] ⁺ ; DG(16:1/22:2/0:0)
664.6234	664	-0.03	664.59	153	50	DG 38:3; [M+NH4] ⁺ ; DG(22:2/16:1/0:0)
84.0822	102.092	-0.0014	84.0808	242	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	241	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	163	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	163	50	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	53	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	287	42.6	Betaine
118.0873	117.079	-0.001	118.0863	286	42.6	Betaine
118.0873	117.079	-0.001	118.0863	282	42.6	Betaine
118.0873	117.079	-0.001	118.0863	318	96.9	Betaine
118.0873	117.079	-0.001	118.0863	317	96.9	Betaine
118.0873	117.079	-0.001	118.0863	311	96.9	Betaine
118.0873	117.079	-0.001	118.0863	323	75.6	Betaine
118.0873	117.079	-0.001	118.0863	320	75.6	Betaine
118.0873	117.079	-0.001	118.0863	318	75.6	Betaine
97.0774	114.104	0.0238	97.1012	37	22.4	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	34	19.8	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	32	18.3	Cyclohexanol, 1-methyl-
694.6329	694	0	694.63	160	50	DG 40:2; [M+NH4] ⁺ ; DG(16:1/24:1/0:0)
694.6329	694	0	694.63	160	50	DG 40:2; [M+NH4] ⁺ ; DG(24:1/16:1/0:0)
694.6329	694	0	694.63	160	50	DG 40:2; [M+NH4] ⁺ ; DG(16:1/24:1/0:0)
694.6329	694	0	694.63	160	50	DG 40:2; [M+NH4] ⁺ ; DG(24:1/16:1/0:0)
694.6329	694	0	694.63	159	50	DG 40:2; [M+NH4] ⁺ ; DG(16:1/24:1/0:0)
694.6329	694	0	694.63	159	50	DG 40:2; [M+NH4] ⁺ ; DG(24:1/16:1/0:0)
118.0873	117.079	-0.001	118.0863	319	42.8	Betaine
118.0873	117.079	-0.001	118.0863	317	42.8	Betaine
118.0873	117.079	-0.001	118.0863	317	42.8	Betaine
118.0873	117.079	-0.001	118.0863	331	93.5	Betaine
118.0873	117.079	-0.001	118.0863	328	93.5	Betaine
118.0873	117.079	-0.001	118.0863	328	93.5	Betaine
118.0873	117.079	-0.001	118.0863	300	68	Betaine
118.0873	117.079	-0.001	118.0863	299	68	Betaine
118.0873	117.079	-0.001	118.0863	292	68	Betaine

84.0822	102.092	-0.0014	84.0808	259	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	258	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	185	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	184	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	146	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	145	49	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	330	40.2	Betaine
118.0873	117.079	-0.001	118.0863	330	40.2	Betaine
118.0873	117.079	-0.001	118.0863	327	40.2	Betaine
118.0873	117.079	-0.001	118.0863	291	64.3	Betaine
118.0873	117.079	-0.001	118.0863	290	64.3	Betaine
118.0873	117.079	-0.001	118.0863	284	64.3	Betaine
118.0873	117.079	-0.001	118.0863	342	33.8	Betaine
118.0873	117.079	-0.001	118.0863	340	33.8	Betaine
118.0873	117.079	-0.001	118.0863	338	33.8	Betaine
186.0588	163.084	0.0149	186.0737	154	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	287	100	Betaine
118.0873	117.079	-0.001	118.0863	286	100	Betaine
118.0873	117.079	-0.001	118.0863	275	100	Betaine
118.0873	117.079	-0.001	118.0863	349	56.4	Betaine
118.0873	117.079	-0.001	118.0863	349	56.4	Betaine
118.0873	117.079	-0.001	118.0863	337	56.4	Betaine
118.0873	117.079	-0.001	118.0863	295	32.7	Betaine
118.0873	117.079	-0.001	118.0863	295	32.7	Betaine
118.0873	117.079	-0.001	118.0863	294	32.7	Betaine
118.0873	117.079	-0.001	118.0863	347	55	Betaine
118.0873	117.079	-0.001	118.0863	344	55	Betaine
118.0873	117.079	-0.001	118.0863	340	55	Betaine
106.0872	105	0	106.09	175	70.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	151	23.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	150	23.6	Diethanolamine
106.0872	105	0	106.09	154	73.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	20.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	239	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	236	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	178	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	178	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	171	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	170	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	144	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	143	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	116	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	116	50	Betaine aldehyde cation
148.0974	147	-0.04	148.06	57	52	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	55	48	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	318	30.8	Betaine

118.0873	117.079	-0.001	118.0863	316	30.8	Betaine
118.0873	117.079	-0.001	118.0863	312	30.8	Betaine
118.0873	117.079	-0.001	118.0863	321	32.8	Betaine
118.0873	117.079	-0.001	118.0863	320	32.8	Betaine
118.0873	117.079	-0.001	118.0863	317	32.8	Betaine
118.0873	117.079	-0.001	118.0863	308	60.2	Betaine
118.0873	117.079	-0.001	118.0863	306	60.2	Betaine
118.0873	117.079	-0.001	118.0863	305	60.2	Betaine
106.0872	105	0	106.09	172	69.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	148	23.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	147	23.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	138	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	137	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	131	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	279	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	278	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	210	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	207	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	127	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	124	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	79	73.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	56	26.8	Ala-Asn
186.0588	163.084	0.0149	186.0737	12	73.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	129	92.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	35	7.6	Ser-His-Lys
666.6406	666	-0.04	666.6	160	50	DG 38:2; [M+NH4]+; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	160	50	DG 38:2; [M+NH4]+; DG(22:1/16:1/0:0)
666.6406	666	-0.04	666.6	108	50	DG 38:2; [M+NH4]+; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	108	50	DG 38:2; [M+NH4]+; DG(22:1/16:1/0:0)
666.6406	666	-0.04	666.6	60	50	DG 38:2; [M+NH4]+; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	60	50	DG 38:2; [M+NH4]+; DG(22:1/16:1/0:0)
666.6406	666	-0.04	666.6	54	50	DG 38:2; [M+NH4]+; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	54	50	DG 38:2; [M+NH4]+; DG(22:1/16:1/0:0)
118.0873	117.079	-0.001	118.0863	256	75.4	Betaine
118.0873	117.079	-0.001	118.0863	255	75.4	Betaine
118.0873	117.079	-0.001	118.0863	252	75.4	Betaine
118.0873	117.079	-0.001	118.0863	433	43	Betaine
118.0873	117.079	-0.001	118.0863	433	43	Betaine
118.0873	117.079	-0.001	118.0863	428	43	Betaine

118.0873	117.079	-0.001	118.0863	290	63.6	Betaine
118.0873	117.079	-0.001	118.0863	289	63.6	Betaine
118.0873	117.079	-0.001	118.0863	286	63.6	Betaine
118.0873	117.079	-0.001	118.0863	399	54.5	Betaine
118.0873	117.079	-0.001	118.0863	397	54.5	Betaine
118.0873	117.079	-0.001	118.0863	394	54.5	Betaine
97.0774	114.104	0.0238	97.1012	34	27.9	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	31	24.6	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	28	24.6	Cyclohexanemethanol
696.651	696	0	696.65	197	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	197	50	DG 40:1; [M+NH4] ⁺ ; DG(24:0/16:1/0:0)
696.651	696	0	696.65	122	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	122	50	DG 40:1; [M+NH4] ⁺ ; DG(24:0/16:1/0:0)
696.651	696	0	696.65	56	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	56	50	DG 40:1; [M+NH4] ⁺ ; DG(24:0/16:1/0:0)
696.651	696	0	696.65	68	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	68	50	DG 40:1; [M+NH4] ⁺ ; DG(24:0/16:1/0:0)
106.0872	105	0	106.09	154	83.5	Diethanolamine
106.0872	105	0	106.09	101	16.5	Diethanolamine
666.6406	666	-0.04	666.6	156	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	156	50	DG 38:2; [M+NH4] ⁺ ; DG(22:1/16:1/0:0)
666.6406	666	-0.04	666.6	112	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	112	50	DG 38:2; [M+NH4] ⁺ ; DG(22:1/16:1/0:0)
666.6406	666	-0.04	666.6	111	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	111	50	DG 38:2; [M+NH4] ⁺ ; DG(22:1/16:1/0:0)
696.651	696	0	696.65	159	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	159	50	DG 40:1; [M+NH4] ⁺ ; DG(24:0/16:1/0:0)
696.651	696	0	696.65	127	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	127	50	DG 40:1; [M+NH4] ⁺ ; DG(24:0/16:1/0:0)

696.651	696	0	696.65	89	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	89	50	DG 40:1; [M+NH4] ⁺ ; DG(24:0/16:1/0:0)
696.651	696	0	696.65	71	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	71	50	DG 40:1; [M+NH4] ⁺ ; DG(24:0/16:1/0:0)
118.0873	117.079	-0.001	118.0863	286	69.9	Betaine
118.0873	117.079	-0.001	118.0863	277	69.9	Betaine
118.0873	117.079	-0.001	118.0863	269	69.9	Betaine
118.0873	117.079	-0.001	118.0863	389	35.9	Betaine
118.0873	117.079	-0.001	118.0863	386	35.9	Betaine
118.0873	117.079	-0.001	118.0863	384	35.9	Betaine
118.0873	117.079	-0.001	118.0863	307	71.1	Betaine
118.0873	117.079	-0.001	118.0863	305	71.1	Betaine
118.0873	117.079	-0.001	118.0863	301	71.1	Betaine
118.0873	117	0	118.09	358	26.9	Betaine
118.0873	117.079	-0.001	118.0863	357	25.9	Betaine
118.0873	117.079	-0.001	118.0863	354	25.9	Betaine
97.0774	114.104	0.0238	97.1012	48	25.2	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	45	22.3	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	37	25.2	Cyclohexanemethanol
106.0872	105	0	106.09	228	77.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	199	22.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	199	22.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	112	100	Diethanolamine
696.651	696	0	696.65	159	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	159	50	DG 40:1; [M+NH4] ⁺ ; DG(24:0/16:1/0:0)
696.651	696	0	696.65	159	50	DG 40:1; [M+NH4] ⁺ ; DG(16:1/24:0/0:0)
696.651	696	0	696.65	159	50	DG 40:1; [M+NH4] ⁺ ; DG(24:0/16:1/0:0)
666.6406	666	-0.04	666.6	160	50	DG 38:2; [M+NH4] ⁺ ; DG(16:1/22:1/0:0)
666.6406	666	-0.04	666.6	160	50	DG 38:2; [M+NH4] ⁺ ; DG(22:1/16:1/0:0)
84.0822	102.092	-0.0014	84.0808	263	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	263	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	228	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	227	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	138	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	135	46.9	Betaine aldehyde cation

186.0588	163.084	0.0149	186.0737	157	93.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	97	93.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	56	6.8	Ala-Asn
186.0588	163.084	0.0149	186.0737	135	83.6	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	81	16.4	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	324	100	Betaine
118.0873	117.079	-0.001	118.0863	323	100	Betaine
118.0873	117.079	-0.001	118.0863	322	100	Betaine
118.0873	117	0	118.09	367	25.1	Betaine
118.0873	117.079	-0.001	118.0863	367	25.1	Betaine
118.0873	117.079	-0.001	118.0863	365	25.1	Betaine
118.0873	117.079	-0.001	118.0863	268	95.4	Betaine
118.0873	117.079	-0.001	118.0863	259	95.4	Betaine
118.0873	117.079	-0.001	118.0863	225	95.4	Betaine
118.0873	117.079	-0.001	118.0863	326	42.2	Betaine
118.0873	117.079	-0.001	118.0863	325	42.2	Betaine
118.0873	117.079	-0.001	118.0863	320	42.2	Betaine
97.0774	114.104	0.0238	97.1012	51	24.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	47	20.5	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	41	16.1	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	37	24	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	34	21.2	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	31	24	Cyclohexanemethanol
106.0872	105	0	106.09	216	78.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	186	21.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	185	21.8	Diethanolamine
106.0872	105	0	106.09	159	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.7	Diethanolamine
118.0873	117.079	-0.001	118.0863	313	100	Betaine
118.0873	117.079	-0.001	118.0863	308	100	Betaine
118.0873	117.079	-0.001	118.0863	307	100	Betaine
118.0873	117.079	-0.001	118.0863	309	68.5	Betaine
118.0873	117.079	-0.001	118.0863	309	68.5	Betaine
118.0873	117.079	-0.001	118.0863	301	68.5	Betaine
118.0873	117.079	-0.001	118.0863	319	27.9	Betaine
118.0873	117.079	-0.001	118.0863	316	27.9	Betaine
118.0873	117.079	-0.001	118.0863	315	27.9	Betaine
97.0774	114.104	0.0238	97.1012	16	100	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	9	100	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	7	100	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	26	32.8	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	22	32.8	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	21	26.4	Cyclohexanol, 2-methyl-, trans-

106.0872	105	0	106.09	152	80.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	115	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	112	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	303	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	301	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	241	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	241	50	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	307	59.5	Betaine
118.0873	117.079	-0.001	118.0863	306	59.5	Betaine
118.0873	117.079	-0.001	118.0863	299	59.5	Betaine
118.0873	117.079	-0.001	118.0863	306	68.6	Betaine
118.0873	117.079	-0.001	118.0863	305	68.6	Betaine
118.0873	117.079	-0.001	118.0863	301	68.6	Betaine
118.0873	117.079	-0.001	118.0863	353	43.5	Betaine
118.0873	117.079	-0.001	118.0863	351	43.5	Betaine
118.0873	117.079	-0.001	118.0863	350	43.5	Betaine
97.0774	114.104	0.0238	97.1012	44	23.5	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	43	22.6	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	34	16.4	Cyclohexanol, 1-methyl-
106.0872	105	0	106.09	147	77.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	22.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	22.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	251	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	249	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	231	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	231	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	137	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	134	46.9	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	47	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	162	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	410	36.6	Betaine
118.0873	117.079	-0.001	118.0863	408	36.6	Betaine
118.0873	117.079	-0.001	118.0863	405	36.6	Betaine
118.0873	117.079	-0.001	118.0863	297	67	Betaine
118.0873	117.079	-0.001	118.0863	295	67	Betaine
118.0873	117.079	-0.001	118.0863	288	67	Betaine
118.0873	117.079	-0.001	118.0863	322	53.6	Betaine
118.0873	117.079	-0.001	118.0863	321	53.6	Betaine
118.0873	117.079	-0.001	118.0863	316	53.6	Betaine
97.0774	114.104	0.0238	97.1012	24	24.4	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	24	24.4	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	21	21.5	Cyclohexanol, 1-methyl-
106.0872	105	0	106.09	159	75.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.1	Diethanolamine

106.0872	105.079	-0.0009	106.0863	123	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	191	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	190	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	189	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	260	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	259	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	198	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	198	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	151	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	148	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	151	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	360	25	Betaine
118.0873	117.079	-0.001	118.0863	357	25	Betaine
118.0873	117	0	118.09	356	21.1	Betaine
118.0873	117.079	-0.001	118.0863	302	67.7	Betaine
118.0873	117.079	-0.001	118.0863	300	67.7	Betaine
118.0873	117.079	-0.001	118.0863	297	67.7	Betaine
118.0873	117.079	-0.001	118.0863	289	64.6	Betaine
118.0873	117.079	-0.001	118.0863	285	64.6	Betaine
118.0873	117.079	-0.001	118.0863	284	64.6	Betaine
97.0774	114.104	0.0238	97.1012	29	20.9	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	29	20.9	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	26	18.5	Cyclohexanemethanol
106.0872	105	0	106.09	148	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	112	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	112	19.8	Diethanolamine
186.0588	163.084	0.0149	186.0737	135	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	333	55	Betaine
118.0873	117.079	-0.001	118.0863	333	55	Betaine
118.0873	117.079	-0.001	118.0863	326	55	Betaine
118.0873	117.079	-0.001	118.0863	278	63	Betaine
118.0873	117.079	-0.001	118.0863	277	63	Betaine
118.0873	117.079	-0.001	118.0863	275	63	Betaine
118.0873	117.079	-0.001	118.0863	334	48.2	Betaine
118.0873	117.079	-0.001	118.0863	333	48.2	Betaine
118.0873	117.079	-0.001	118.0863	327	48.2	Betaine
97.0774	114.104	0.0238	97.1012	37	23.9	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	33	23.9	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	33	20.2	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	196	69.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	173	25.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	172	25.5	Diethanolamine
106.0872	105	0	106.09	159	75.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19	Diethanolamine

106.0872	105.079	-0.0009	106.0863	123	19	Diethanolamine
84.0822	102.092	-0.0014	84.0808	271	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	271	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	233	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	232	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	117	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	113	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	220	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	218	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	180	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	179	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	140	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	136	45.8	Betaine aldehyde cation
148.0974	147	-0.04	148.06	57	62.3	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	42	37.7	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	115	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	162	71.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	152	71.2	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	137	21.7	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	344	49.3	Betaine
118.0873	117.079	-0.001	118.0863	342	49.3	Betaine
118.0873	117.079	-0.001	118.0863	338	49.3	Betaine
118.0873	117.079	-0.001	118.0863	338	96.4	Betaine
118.0873	117.079	-0.001	118.0863	338	96.4	Betaine
118.0873	117.079	-0.001	118.0863	337	96.4	Betaine
118.0873	117.079	-0.001	118.0863	349	35.7	Betaine
118.0873	117.079	-0.001	118.0863	347	35.7	Betaine
118.0873	117.079	-0.001	118.0863	345	35.7	Betaine
97.0774	114.104	0.0238	97.1012	25	33.9	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	18	25.9	Cycloheptanol
97.0774	114.104	0.0238	97.1012	13	20.9	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	154	80.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	19.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	19.3	Diethanolamine
106.0872	105	0	106.09	155	78	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	20.4	Diethanolamine
186.0588	163.084	0.0149	186.0737	143	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	58	100	Ser-His-Lys
84.0822	102.092	-0.0014	84.0808	291	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	288	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	260	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	257	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	185	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	182	46.9	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	344	48.3	Betaine
118.0873	117.079	-0.001	118.0863	343	48.3	Betaine

118.0873	117.079	-0.001	118.0863	341	48.3	Betaine
118.0873	117.079	-0.001	118.0863	307	72	Betaine
118.0873	117.079	-0.001	118.0863	306	72	Betaine
118.0873	117.079	-0.001	118.0863	297	72	Betaine
118.0873	117.079	-0.001	118.0863	338	69.2	Betaine
118.0873	117.079	-0.001	118.0863	337	69.2	Betaine
118.0873	117.079	-0.001	118.0863	336	69.2	Betaine
106.0872	105	0	106.09	151	75.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	18.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	18.4	Diethanolamine
106.0872	105	0	106.09	145	70.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	29.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	29.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	275	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	275	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	212	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	211	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	156	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	152	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	139	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	138	49	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	196	94.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	144	94.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	77	5.1	Ala-Asn
186.0588	163.084	0.0149	186.0737	116	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	323	34	Betaine
118.0873	117.079	-0.001	118.0863	319	34	Betaine
118.0873	117.079	-0.001	118.0863	318	34	Betaine
118.0873	117.079	-0.001	118.0863	280	62.3	Betaine
118.0873	117.079	-0.001	118.0863	276	62.3	Betaine
118.0873	117.079	-0.001	118.0863	276	62.3	Betaine
118.0873	117.079	-0.001	118.0863	367	35.9	Betaine
118.0873	117.079	-0.001	118.0863	366	35.9	Betaine
118.0873	117.079	-0.001	118.0863	365	35.9	Betaine
97.0774	114.104	0.0238	97.1012	30	24.4	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	22	18.2	Cycloheptanol
97.0774	114.104	0.0238	97.1012	17	14.6	Cyclohexanemethanol
106.0872	105	0	106.09	153	75.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	18.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	18.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	286	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	286	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	238	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	238	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	164	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	160	45.8	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	293	32.4	Betaine

118.0873	117.079	-0.001	118.0863	293	32.4	Betaine
118.0873	117.079	-0.001	118.0863	292	32.4	Betaine
118.0873	117.079	-0.001	118.0863	327	39.4	Betaine
118.0873	117.079	-0.001	118.0863	324	39.4	Betaine
118.0873	117.079	-0.001	118.0863	324	39.4	Betaine
118.0873	117.079	-0.001	118.0863	362	44.4	Betaine
118.0873	117.079	-0.001	118.0863	361	44.4	Betaine
118.0873	117.079	-0.001	118.0863	360	44.4	Betaine
186.0588	203.091	0.0285	186.0873	65	71.9	Ala-Asn
186.0588	163.084	0.0149	186.0737	25	16.7	N,N-Bis(2-hydroxyethyl)glycine
186.0588	168.042	0.0173	186.0761	14	11.4	3-Hydroxy-4-methoxybenzoic acid
186.0588	163.084	0.0149	186.0737	144	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	65	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	343	53.4	Betaine
118.0873	117.079	-0.001	118.0863	342	53.4	Betaine
118.0873	117.079	-0.001	118.0863	339	53.4	Betaine
118.0873	117.079	-0.001	118.0863	309	70.6	Betaine
118.0873	117.079	-0.001	118.0863	309	70.6	Betaine
118.0873	117.079	-0.001	118.0863	300	70.6	Betaine
118.0873	117.079	-0.001	118.0863	299	66.6	Betaine
118.0873	117.079	-0.001	118.0863	298	66.6	Betaine
118.0873	117.079	-0.001	118.0863	291	66.6	Betaine
97.0774	114.104	0.0238	97.1012	30	24.2	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	24	19	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	21	16.8	Cycloheptanol
97.0774	114.104	0.0238	97.1012	46	23.4	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	44	21.6	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	39	17.4	Cyclohexanemethanol
106.0872	105	0	106.09	165	71.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	17.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	17.4	Diethanolamine
106.0872	105	0	106.09	190	57.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	174	33.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	173	33.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	250	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	246	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	231	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	228	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	104	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	103	49	Betaine aldehyde cation
186.0588	203.091	0.0285	186.0873	36	100	Ala-Asn
118.0873	117.079	-0.001	118.0863	372	44.3	Betaine
118.0873	117.079	-0.001	118.0863	372	44.3	Betaine
118.0873	117.079	-0.001	118.0863	364	44.3	Betaine
118.0873	117.079	-0.001	118.0863	267	58.4	Betaine
118.0873	117.079	-0.001	118.0863	266	58.4	Betaine

118.0873	117.079	-0.001	118.0863	264	58.4	Betaine
118.0873	117.079	-0.001	118.0863	260	92.5	Betaine
118.0873	117.079	-0.001	118.0863	260	92.5	Betaine
118.0873	117.079	-0.001	118.0863	259	92.5	Betaine
106.0872	105	0	106.09	157	73.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20.4	Diethanolamine
106.0872	105	0	106.09	155	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	20.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	262	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	260	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	233	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	231	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	188	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	186	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	139	77.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	66	10.5	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	51	6.4	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	137	86.6	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	70	13.4	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	151	92.7	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	54	7.3	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	345	31.4	Betaine
118.0873	117.079	-0.001	118.0863	345	31.4	Betaine
118.0873	117.079	-0.001	118.0863	342	31.4	Betaine
118.0873	117.079	-0.001	118.0863	309	98.8	Betaine
118.0873	117.079	-0.001	118.0863	307	98.8	Betaine
118.0873	117.079	-0.001	118.0863	300	98.8	Betaine
118.0873	117.079	-0.001	118.0863	351	98.7	Betaine
118.0873	117.079	-0.001	118.0863	350	98.7	Betaine
118.0873	117.079	-0.001	118.0863	347	98.7	Betaine
97.0774	114.104	0.0238	97.1012	16	39.8	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	14	39.8	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	10	31.3	Cyclopentanemethanol, .alpha.-methyl-
106.0872	105	0	106.09	154	77.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	20.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	20.3	Diethanolamine
106.0872	105	0	106.09	220	72.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	196	24.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	196	24.2	Diethanolamine
84.0822	102.092	-0.0014	84.0808	249	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	249	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	262	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	262	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	174	51	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	173	49	Betaine aldehyde cation
97.0774	114.104	0.0238	97.1012	29	22.4	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	25	18.9	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	20	15.3	Cycloheptanol
106.0872	105	0	106.09	157	75	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	267	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	266	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	233	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	230	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	137	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	137	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	155	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	151	45.8	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	170	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	155	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	59	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	331	96.2	Betaine
118.0873	117.079	-0.001	118.0863	330	96.2	Betaine
118.0873	117.079	-0.001	118.0863	322	96.2	Betaine
118.0873	117.079	-0.001	118.0863	290	65.8	Betaine
118.0873	117.079	-0.001	118.0863	283	65.8	Betaine
118.0873	117.079	-0.001	118.0863	276	65.8	Betaine
118.0873	117.079	-0.001	118.0863	352	54	Betaine
118.0873	117.079	-0.001	118.0863	352	54	Betaine
118.0873	117.079	-0.001	118.0863	351	54	Betaine
97.0774	114.104	0.0238	97.1012	82	19.4	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	82	19.4	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	82	19.4	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	159	77.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	17.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	17.6	Diethanolamine
106.0872	105	0	106.09	154	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	19.8	Diethanolamine
106.0872	105	0	106.09	159	76.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	21.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	298	56.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	291	43.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	245	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	243	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	236	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	234	48	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	383	45.4	Betaine
118.0873	117.079	-0.001	118.0863	382	45.4	Betaine

118.0873	117.079	-0.001	118.0863	378	45.4	Betaine
118.0873	117.079	-0.001	118.0863	335	58.5	Betaine
118.0873	117.079	-0.001	118.0863	333	58.5	Betaine
118.0873	117.079	-0.001	118.0863	331	58.5	Betaine
118.0873	117.079	-0.001	118.0863	354	35.4	Betaine
118.0873	117.079	-0.001	118.0863	351	35.4	Betaine
118.0873	117.079	-0.001	118.0863	351	35.4	Betaine
97.0774	114.104	0.0238	97.1012	30	23.8	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	24	18.7	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	22	17.3	Cycloheptanol
106.0872	105	0	106.09	156	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	20.4	Diethanolamine
106.0872	105	0	106.09	159	75	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	18.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	18.5	Diethanolamine
106.0872	105	0	106.09	155	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	20.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	275	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	272	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	253	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	253	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	143	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	142	49	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	117	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	148	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	151	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	317	32.4	Betaine
118.0873	117.079	-0.001	118.0863	317	32.4	Betaine
118.0873	117.079	-0.001	118.0863	314	32.4	Betaine
118.0873	117.079	-0.001	118.0863	282	61.1	Betaine
118.0873	117.079	-0.001	118.0863	282	61.1	Betaine
118.0873	117.079	-0.001	118.0863	278	61.1	Betaine
118.0873	117.079	-0.001	118.0863	344	59.6	Betaine
118.0873	117.079	-0.001	118.0863	341	59.6	Betaine
118.0873	117.079	-0.001	118.0863	338	59.6	Betaine
106.0872	105	0	106.09	158	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	21.4	Diethanolamine
106.0872	105	0	106.09	157	75.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	115	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	113	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	281	54.2	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	277	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	211	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	211	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	145	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	144	49	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	43	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
106.0872	105	0	106.09	159	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.4	Diethanolamine
106.0872	105	0	106.09	135	76.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	110	23.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	108	23.4	Diethanolamine
148.0974	147.053	-0.037	148.0604	93	56.5	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	68	17.2	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	65	15.2	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	141	100	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	384	97.4	Betaine
118.0873	117.079	-0.001	118.0863	382	97.4	Betaine
118.0873	117.079	-0.001	118.0863	377	97.4	Betaine
118.0873	117.079	-0.001	118.0863	281	61.2	Betaine
118.0873	117.079	-0.001	118.0863	278	61.2	Betaine
118.0873	117.079	-0.001	118.0863	275	61.2	Betaine
118.0873	117.079	-0.001	118.0863	294	41	Betaine
118.0873	117.079	-0.001	118.0863	292	41	Betaine
118.0873	117.079	-0.001	118.0863	291	41	Betaine
97.0774	114.104	0.0238	97.1012	36	20.9	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	34	19.3	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	34	19.3	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	159	75.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	18.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	18.7	Diethanolamine
106.0872	105	0	106.09	149	77.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	22.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	22.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	281	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	280	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	247	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	246	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	182	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	177	44.6	Betaine aldehyde cation
186.0588	203.091	0.0285	186.0873	99	74	Ala-Asn
186.0588	163.084	0.0149	186.0737	50	15.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	40	10.7	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	114	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	83	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	272	84	Betaine

118.0873	117.079	-0.001	118.0863	270	84	Betaine
118.0873	117.079	-0.001	118.0863	269	84	Betaine
118.0873	117.079	-0.001	118.0863	379	47.2	Betaine
118.0873	117.079	-0.001	118.0863	377	47.2	Betaine
118.0873	117.079	-0.001	118.0863	377	47.2	Betaine
118.0873	117.079	-0.001	118.0863	343	96	Betaine
118.0873	117.079	-0.001	118.0863	334	96	Betaine
118.0873	117.079	-0.001	118.0863	318	96	Betaine
118.0873	117.079	-0.001	118.0863	363	53.1	Betaine
118.0873	117.079	-0.001	118.0863	361	53.1	Betaine
118.0873	117.079	-0.001	118.0863	358	53.1	Betaine
97.0774	114.104	0.0238	97.1012	43	25.5	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	42	24.5	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	33	25.5	Cyclohexanemethanol
106.0872	105	0	106.09	152	77.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	21	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	21	Diethanolamine
84.0822	102.092	-0.0014	84.0808	288	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	287	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	232	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	232	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	125	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	121	45.8	Betaine aldehyde cation
106.0872	105	0	106.09	145	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	21.4	Diethanolamine
106.0872	105	0	106.09	161	79.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	259	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	259	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	207	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	204	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	161	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	157	45.8	Betaine aldehyde cation
186.0588	203.091	0.0285	186.0873	50	68.7	Ala-Asn
186.0588	370.196	0.0467	186.1055	30	31.3	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	123	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	360	59.5	Betaine
118.0873	117.079	-0.001	118.0863	360	59.5	Betaine
118.0873	117.079	-0.001	118.0863	351	59.5	Betaine
118.0873	117.079	-0.001	118.0863	297	64.4	Betaine
118.0873	117.079	-0.001	118.0863	295	64.4	Betaine
118.0873	117.079	-0.001	118.0863	292	64.4	Betaine
118.0873	117.079	-0.001	118.0863	380	48.9	Betaine
118.0873	117.079	-0.001	118.0863	379	48.9	Betaine
118.0873	117.079	-0.001	118.0863	377	48.9	Betaine

148.0974	147	-0.04	148.06	35	35.1	N-acetyl-DL-serine
148.0974	147	-0.04	148.06	33	32.4	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	33	32.4	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	36	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	171	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	159	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	143	100	O-Acetyl-L-serine
393.2988	392.293	0.0011	393.2999	41	100	Chenodeoxycholic acid
371.2972	370.308	0.0184	371.3156	227	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	157	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	155	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	123	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	111	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	97	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	67	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	54	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	46	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	104	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	77	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	62	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	372	54.7	Betaine
118.0873	117.079	-0.001	118.0863	370	54.7	Betaine
118.0873	117.079	-0.001	118.0863	366	54.7	Betaine
118.0873	117.079	-0.001	118.0863	339	39.5	Betaine
118.0873	117.079	-0.001	118.0863	337	39.5	Betaine
118.0873	117.079	-0.001	118.0863	336	39.5	Betaine
118.0873	117.079	-0.001	118.0863	354	57	Betaine
118.0873	117.079	-0.001	118.0863	350	57	Betaine
118.0873	117.079	-0.001	118.0863	347	57	Betaine
97.0774	114.104	0.0238	97.1012	37	24.1	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	28	17.5	Cycloheptanol
97.0774	114.104	0.0238	97.1012	24	14.8	Cyclohexanemethanol
106.0872	105.079	-0.0009	106.0863	120	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	100	Diethanolamine

106.0872	105	0	106.09	159	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	21.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	275	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	274	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	218	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	218	50	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	138	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	369	33.3	Betaine
118.0873	117.079	-0.001	118.0863	368	33.3	Betaine
118.0873	117.079	-0.001	118.0863	364	33.3	Betaine
118.0873	117.079	-0.001	118.0863	278	59.7	Betaine
118.0873	117.079	-0.001	118.0863	274	59.7	Betaine
118.0873	117.079	-0.001	118.0863	273	59.7	Betaine
118.0873	117.079	-0.001	118.0863	280	60.4	Betaine
118.0873	117.079	-0.001	118.0863	278	60.4	Betaine
118.0873	117.079	-0.001	118.0863	276	60.4	Betaine
97.0774	114.104	0.0238	97.1012	39	24.7	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	35	20.9	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	32	24.7	Cyclohexanol, 4-methyl-, trans-
106.0872	105.079	-0.0009	106.0863	124	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	100	Diethanolamine
106.0872	105	0	106.09	159	75.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.4	Diethanolamine
106.0872	105	0	106.09	153	80.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	115	19.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	115	19.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	257	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	256	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	228	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	226	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	145	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	141	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	156	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	153	46.9	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	61	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	164	92.8	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	66	7.2	Ser-His-Lys
106.0872	105	0	106.09	155	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	21.1	Diethanolamine
106.0872	105	0	106.09	157	67.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	138	32.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	137	32.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	267	53.1	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	264	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	186	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	186	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	172	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	171	49	Betaine aldehyde cation
148.0974	147.053	-0.037	148.0604	22	31.5	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	21	31.5	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	20	31.5	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	412	36.3	Betaine
118.0873	117.079	-0.001	118.0863	410	36.3	Betaine
118.0873	117.079	-0.001	118.0863	407	36.3	Betaine
118.0873	117.079	-0.001	118.0863	295	22.8	Betaine
118.0873	117	0	118.09	295	22.8	Betaine
118.0873	117.079	-0.001	118.0863	294	22.8	Betaine
118.0873	117.079	-0.001	118.0863	334	64.1	Betaine
118.0873	117.079	-0.001	118.0863	333	64.1	Betaine
118.0873	117.079	-0.001	118.0863	328	64.1	Betaine
148.0974	147.053	-0.037	148.0604	172	47	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	170	43.3	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	166	47	O-Acetyl-L-serine
393.2988	392.293	0.0011	393.2999	16	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	15	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	15	100	Chenodeoxycholic acid
371.2972	370.308	0.0184	371.3156	205	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	181	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	176	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	103	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	102	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	98	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	81	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	45	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	14	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	114	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	93	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2972	370.308	0.0184	371.3156	80	100	Hexanedioic acid, bis(2-ethylhexyl) ester

118.0873	117.079	-0.001	118.0863	369	67.7	Betaine
118.0873	117.079	-0.001	118.0863	368	67.7	Betaine
118.0873	117.079	-0.001	118.0863	357	67.7	Betaine
118.0873	117.079	-0.001	118.0863	283	62.4	Betaine
118.0873	117.079	-0.001	118.0863	283	62.4	Betaine
118.0873	117.079	-0.001	118.0863	280	62.4	Betaine
118.0873	117.079	-0.001	118.0863	347	61.1	Betaine
118.0873	117.079	-0.001	118.0863	345	61.1	Betaine
118.0873	117.079	-0.001	118.0863	343	61.1	Betaine
106.0872	105	0	106.09	158	75.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19	Diethanolamine
106.0872	105	0	106.09	152	74.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	19	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	19	Diethanolamine
106.0872	105	0	106.09	268	77.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	234	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	232	19.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	292	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	288	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	260	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	257	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	203	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	197	44	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	158	93.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	98	93.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	55	6.6	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	145	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	333	36.4	Betaine
118.0873	117.079	-0.001	118.0863	331	36.4	Betaine
118.0873	117.079	-0.001	118.0863	326	36.4	Betaine
118.0873	117.079	-0.001	118.0863	333	37.8	Betaine
118.0873	117.079	-0.001	118.0863	331	37.8	Betaine
118.0873	117.079	-0.001	118.0863	329	37.8	Betaine
118.0873	117.079	-0.001	118.0863	380	52.3	Betaine
118.0873	117.079	-0.001	118.0863	379	52.3	Betaine
118.0873	117.079	-0.001	118.0863	377	52.3	Betaine
97.0774	114.104	0.0238	97.1012	27	23.1	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	18	16.8	Cycloheptanol
97.0774	114.104	0.0238	97.1012	16	15.5	Cyclohexanemethanol
106.0872	105	0	106.09	219	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	188	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	187	21.4	Diethanolamine
106.0872	105	0	106.09	181	64.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	160	27.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	159	27.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	255	51	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	254	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	228	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	222	44	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	160	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	157	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	113	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-hydroxyethyl)glycine
106.0872	105	0	106.09	158	77.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	22.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	22.1	Diethanolamine
106.0872	105	0	106.09	159	72.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	133	21.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	133	21.7	Diethanolamine
106.0872	105	0	106.09	144	78.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	21.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	21.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	262	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	259	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	198	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	195	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	161	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	160	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	180	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	178	48	Betaine aldehyde cation
186.0588	203.091	0.0285	186.0873	83	100	Ala-Asn
186.0588	370.196	0.0467	186.1055	97	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	81	100	Ser-His-Lys
148.0974	147	-0.04	148.06	13	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	56	55.5	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	30	55.5	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	28	16	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	173	76.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	162	76.6	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	148	23.4	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	129	58	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	122	58	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	113	33.4	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	356	62.8	Betaine
118.0873	117.079	-0.001	118.0863	353	62.8	Betaine
118.0873	117.079	-0.001	118.0863	347	62.8	Betaine
118.0873	117.079	-0.001	118.0863	334	56.8	Betaine
118.0873	117.079	-0.001	118.0863	332	56.8	Betaine
118.0873	117.079	-0.001	118.0863	331	56.8	Betaine
118.0873	117.079	-0.001	118.0863	341	56	Betaine
118.0873	117.079	-0.001	118.0863	339	56	Betaine
118.0873	117.079	-0.001	118.0863	339	56	Betaine
106.0872	105	0	106.09	159	71.7	Diethanolamine

106.0872	105.079	-0.0009	106.0863	137	28.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	136	28.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	109	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	109	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	103	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	284	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	283	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	221	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	220	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	203	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	201	48	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	376	50.4	Betaine
118.0873	117.079	-0.001	118.0863	372	50.4	Betaine
118.0873	117.079	-0.001	118.0863	368	50.4	Betaine
118.0873	117.079	-0.001	118.0863	348	97.6	Betaine
118.0873	117.079	-0.001	118.0863	337	97.6	Betaine
118.0873	117.079	-0.001	118.0863	322	97.6	Betaine
118.0873	117	0	118.09	348	26.1	Betaine
118.0873	117.079	-0.001	118.0863	344	22	Betaine
118.0873	117	0	118.09	342	20.3	Betaine
84.0822	102.092	-0.0014	84.0808	231	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	230	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	212	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	212	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	142	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	138	45.8	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	41	100	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	367	36.4	Betaine
118.0873	117.079	-0.001	118.0863	366	36.4	Betaine
118.0873	117.079	-0.001	118.0863	361	36.4	Betaine
118.0873	117.079	-0.001	118.0863	316	75	Betaine
118.0873	117.079	-0.001	118.0863	312	75	Betaine
118.0873	117.079	-0.001	118.0863	301	75	Betaine
118.0873	117.079	-0.001	118.0863	355	51.9	Betaine
118.0873	117.079	-0.001	118.0863	354	51.9	Betaine
118.0873	117.079	-0.001	118.0863	350	51.9	Betaine
97.0774	114.104	0.0238	97.1012	41	100	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	48	25	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	40	18.6	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	40	18.6	Cyclohexanol, 1-methyl-
106.0872	105	0	106.09	158	76.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	132	23.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	131	23.1	Diethanolamine
106.0872	105	0	106.09	159	74.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	20	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20	Diethanolamine

106.0872	105	0	106.09	158	79.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	20.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	280	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	280	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	259	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	257	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	160	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	159	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	205	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	204	49	Betaine aldehyde cation
106.0872	105	0	106.09	171	75.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	136	18.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	18.9	Diethanolamine
106.0872	105	0	106.09	159	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	21.1	Diethanolamine
106.0872	105	0	106.09	159	74.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	20.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	20.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	241	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	239	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	236	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	233	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	189	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	183	44	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	112	83.6	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	83	83.6	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	58	16.4	Ala-Asn
186.0588	370.196	0.0467	186.1055	94	100	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	147	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	138	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	163	100	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	340	36	Betaine
118.0873	117.079	-0.001	118.0863	336	36	Betaine
118.0873	117.079	-0.001	118.0863	335	36	Betaine
118.0873	117.079	-0.001	118.0863	287	67.5	Betaine
118.0873	117.079	-0.001	118.0863	284	67.5	Betaine
118.0873	117.079	-0.001	118.0863	282	67.5	Betaine
118.0873	117.079	-0.001	118.0863	359	52.1	Betaine
118.0873	117.079	-0.001	118.0863	356	52.1	Betaine
118.0873	117.079	-0.001	118.0863	355	52.1	Betaine
148.0974	147	-0.04	148.06	31	67.3	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	12	32.7	N-acetyl-DL-serine
371.2927	370.308	0.0229	371.3156	184	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.2927	370.308	0.0229	371.3156	107	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	98	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	178	76.9	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	166	76.9	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	130	76.9	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	81	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	78	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	65	100	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	322	29.1	Betaine
118.0873	117.079	-0.001	118.0863	321	29.1	Betaine
118.0873	117.079	-0.001	118.0863	318	29.1	Betaine
118.0873	117.079	-0.001	118.0863	323	99	Betaine
118.0873	117.079	-0.001	118.0863	321	99	Betaine
118.0873	117.079	-0.001	118.0863	313	99	Betaine
118.0873	117.079	-0.001	118.0863	343	31.4	Betaine
118.0873	117.079	-0.001	118.0863	342	31.4	Betaine
118.0873	117.079	-0.001	118.0863	339	31.4	Betaine
106.0872	105	0	106.09	166	71.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	19.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	19.5	Diethanolamine
84.0822	102.092	-0.0014	84.0808	266	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	260	44	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	279	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	278	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	167	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	166	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	163	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	162	49	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	356	53.9	Betaine
118.0873	117.079	-0.001	118.0863	352	53.9	Betaine
118.0873	117.079	-0.001	118.0863	349	53.9	Betaine
118.0873	117.079	-0.001	118.0863	329	82.7	Betaine
118.0873	117.079	-0.001	118.0863	321	82.7	Betaine
118.0873	117.079	-0.001	118.0863	306	82.7	Betaine
118.0873	117.079	-0.001	118.0863	323	29.3	Betaine
118.0873	117	0	118.09	320	25.9	Betaine
118.0873	117.079	-0.001	118.0863	319	29.3	Betaine
97.0774	114.104	0.0238	97.1012	49	32.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	35	20.2	Cycloheptanol

97.0774	114.104	0.0238	97.1012	32	17.9	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	208	76.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	174	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	174	19.6	Diethanolamine
106.0872	105	0	106.09	211	77	Diethanolamine
106.0872	105.079	-0.0009	106.0863	174	18.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	172	18.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	319	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	316	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	248	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	245	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	120	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	116	45.8	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	205	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	132	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	152	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	33	23.1	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	26	17.7	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	25	17.7	Cyclohexanemethanol
106.0872	105	0	106.09	196	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	164	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	164	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	108	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	108	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	108	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	251	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	247	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	279	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	277	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	138	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	137	49	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	116	79.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	96	79.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	83	20.7	Ala-Asn
186.0588	163.084	0.0149	186.0737	104	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	44	26.5	N-acetyl-DL-serine
148.0974	147.053	-0.037	148.0604	35	19.2	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	35	19.2	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	36	28.1	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	34	25.9	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	32	23.9	N-acetyl-DL-serine
148.0974	147.053	-0.037	148.0604	103	52.8	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	97	52.8	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	92	36.2	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	362	33.5	Betaine
118.0873	117.079	-0.001	118.0863	362	33.5	Betaine
118.0873	117.079	-0.001	118.0863	358	33.5	Betaine

118.0873	117.079	-0.001	118.0863	321	49.9	Betaine
118.0873	117.079	-0.001	118.0863	319	49.9	Betaine
118.0873	117.079	-0.001	118.0863	318	49.9	Betaine
118.0873	117.079	-0.001	118.0863	337	62	Betaine
118.0873	117.079	-0.001	118.0863	334	62	Betaine
118.0873	117.079	-0.001	118.0863	330	62	Betaine
148.0974	147	-0.04	148.06	88	36.4	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	80	27.2	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	73	20.8	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	114	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	107	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	151	52.1	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	148	52.1	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	142	52.1	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	384	47.1	Betaine
118.0873	117.079	-0.001	118.0863	380	47.1	Betaine
118.0873	117.079	-0.001	118.0863	379	47.1	Betaine
118.0873	117.079	-0.001	118.0863	253	76.1	Betaine
118.0873	117.079	-0.001	118.0863	246	76.1	Betaine
118.0873	117.079	-0.001	118.0863	240	76.1	Betaine
118.0873	117.079	-0.001	118.0863	306	34.8	Betaine
118.0873	117.079	-0.001	118.0863	305	34.8	Betaine
118.0873	117.079	-0.001	118.0863	303	34.8	Betaine
106.0872	105	0	106.09	180	73.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	136	15.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	15.9	Diethanolamine
106.0872	105	0	106.09	159	74.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	19.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	19.9	Diethanolamine
106.0872	105	0	106.09	196	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	160	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	159	19.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	282	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	282	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	241	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	236	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	209	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	205	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	168	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	165	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	163	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	361	37.1	Betaine
118.0873	117.079	-0.001	118.0863	361	37.1	Betaine
118.0873	117.079	-0.001	118.0863	357	37.1	Betaine
118.0873	117.079	-0.001	118.0863	314	80.4	Betaine

118.0873	117.079	-0.001	118.0863	301	80.4	Betaine
118.0873	117.079	-0.001	118.0863	282	80.4	Betaine
118.0873	117.079	-0.001	118.0863	314	56.2	Betaine
118.0873	117.079	-0.001	118.0863	314	56.2	Betaine
118.0873	117.079	-0.001	118.0863	312	56.2	Betaine
97.0774	114.104	0.0238	97.1012	36	26.5	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	33	26.5	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	30	20.8	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	228	76.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	194	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	192	19.6	Diethanolamine
106.0872	105	0	106.09	158	76.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	141	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	141	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	139	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	281	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	277	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	270	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	267	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	171	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	169	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	154	84	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	98	16	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-hydroxyethyl)glycine
106.0872	105.079	-0.0009	106.0863	134	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	100	Diethanolamine
106.0872	105	0	106.09	170	79.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	134	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	204	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	204	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	194	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	267	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	266	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	230	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	230	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	200	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	197	46.9	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	50	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	318	43.4	Betaine
118.0873	117.079	-0.001	118.0863	317	43.4	Betaine
118.0873	117.079	-0.001	118.0863	312	43.4	Betaine
118.0873	117.079	-0.001	118.0863	281	60.6	Betaine
118.0873	117.079	-0.001	118.0863	280	60.6	Betaine

118.0873	117.079	-0.001	118.0863	274	60.6	Betaine
118.0873	117.079	-0.001	118.0863	322	57	Betaine
118.0873	117.079	-0.001	118.0863	320	57	Betaine
118.0873	117.079	-0.001	118.0863	314	57	Betaine
148.0974	147.053	-0.037	148.0604	136	100	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	337	31.3	Betaine
118.0873	117.079	-0.001	118.0863	336	31.3	Betaine
118.0873	117.079	-0.001	118.0863	333	31.3	Betaine
118.0873	117.079	-0.001	118.0863	235	67.6	Betaine
118.0873	117.079	-0.001	118.0863	232	67.6	Betaine
118.0873	117.079	-0.001	118.0863	230	67.6	Betaine
118.0873	117.079	-0.001	118.0863	331	39	Betaine
118.0873	117.079	-0.001	118.0863	329	39	Betaine
118.0873	117.079	-0.001	118.0863	324	39	Betaine
106.0872	105	0	106.09	159	75.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19	Diethanolamine
106.0872	105.079	-0.0009	106.0863	107	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	107	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	106	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	298	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	298	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	240	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	240	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	155	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	149	44	Betaine aldehyde cation
186.0588	168.042	0.0173	186.0761	26	100	3-Hydroxy-4-methoxybenzoic acid
186.0588	370.196	0.0467	186.1055	55	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	415	58.5	Betaine
118.0873	117.079	-0.001	118.0863	413	58.5	Betaine
118.0873	117.079	-0.001	118.0863	408	58.5	Betaine
118.0873	117.079	-0.001	118.0863	319	33.5	Betaine
118.0873	117.079	-0.001	118.0863	318	33.5	Betaine
118.0873	117.079	-0.001	118.0863	315	33.5	Betaine
118.0873	117.079	-0.001	118.0863	380	34.7	Betaine
118.0873	117.079	-0.001	118.0863	379	34.7	Betaine
118.0873	117.079	-0.001	118.0863	375	34.7	Betaine
97.0774	114.104	0.0238	97.1012	40	20.8	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	39	19.9	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	39	19.9	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	171	77.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	142	22.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	141	22.1	Diethanolamine
106.0872	105	0	106.09	212	63.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	191	27	Diethanolamine

106.0872	105.079	-0.0009	106.0863	187	27	Diethanolamine
84.0822	102.092	-0.0014	84.0808	292	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	287	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	225	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	223	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	149	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	146	46.9	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	37	64.7	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	20	35.3	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	120	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	70	60	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	58	40	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	72	100	Ser-His-Lys
106.0872	105	0	106.09	153	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	131	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	279	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	277	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	233	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	229	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	173	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	171	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	126	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147.053	-0.037	148.0604	123	100	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	340	53.1	Betaine
118.0873	117.079	-0.001	118.0863	340	53.1	Betaine
118.0873	117.079	-0.001	118.0863	337	53.1	Betaine
118.0873	117.079	-0.001	118.0863	291	97.1	Betaine
118.0873	117.079	-0.001	118.0863	277	97.1	Betaine
118.0873	117.079	-0.001	118.0863	259	97.1	Betaine
118.0873	117.079	-0.001	118.0863	377	51.1	Betaine
118.0873	117.079	-0.001	118.0863	377	51.1	Betaine
118.0873	117.079	-0.001	118.0863	374	51.1	Betaine
393.2988	392.293	0.0011	393.2999	37	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	36	100	Chenodeoxycholic acid
393.2988	392.293	0.0011	393.2999	35	100	Chenodeoxycholic acid
371.2927	370.308	0.0229	371.3156	186	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	160	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	152	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	153	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.2927	370.308	0.0229	371.3156	152	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	148	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	21	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	1	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	125	74.8	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	110	74.8	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2927	370.308	0.0229	371.3156	94	74.8	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	391	34.4	Betaine
118.0873	117.079	-0.001	118.0863	389	34.4	Betaine
118.0873	117.079	-0.001	118.0863	387	34.4	Betaine
118.0873	117.079	-0.001	118.0863	291	66.1	Betaine
118.0873	117.079	-0.001	118.0863	289	66.1	Betaine
118.0873	117.079	-0.001	118.0863	283	66.1	Betaine
118.0873	117.079	-0.001	118.0863	290	64.3	Betaine
118.0873	117.079	-0.001	118.0863	290	64.3	Betaine
118.0873	117.079	-0.001	118.0863	286	64.3	Betaine
97.0774	114.104	0.0238	97.1012	35	23	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	35	23	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	34	23	Cyclohexanemethanol
106.0872	105	0	106.09	159	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.7	Diethanolamine
106.0872	105	0	106.09	218	77.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	189	22.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	189	22.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	290	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	289	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	233	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	232	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	150	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	145	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	182	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	178	45.8	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	121	83.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	93	83.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	68	16.5	Ala-Asn
186.0588	163.084	0.0149	186.0737	145	88.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	71	11.7	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	152	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147.053	-0.037	148.0604	98	45.8	O-Acetyl-L-serine

148.0974	147.053	-0.037	148.0604	94	45.8	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	90	34.1	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	272	75.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	255	75.6	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	241	20.6	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	212	79.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	201	79.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	183	79.6	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	35	19.5	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	35	19.5	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	35	19.5	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	22	100	Cyclohexanol, 4-methyl-, trans-
118.0873	117.079	-0.001	118.0863	310	49.9	Betaine
118.0873	117.079	-0.001	118.0863	307	49.9	Betaine
118.0873	117.079	-0.001	118.0863	304	49.9	Betaine
118.0873	117.079	-0.001	118.0863	395	38	Betaine
118.0873	117.079	-0.001	118.0863	393	38	Betaine
118.0873	117.079	-0.001	118.0863	388	38	Betaine
118.0873	117.079	-0.001	118.0863	305	68.3	Betaine
118.0873	117.079	-0.001	118.0863	303	68.3	Betaine
118.0873	117.079	-0.001	118.0863	298	68.3	Betaine
118.0873	117.079	-0.001	118.0863	286	66	Betaine
118.0873	117.079	-0.001	118.0863	283	66	Betaine
118.0873	117.079	-0.001	118.0863	282	66	Betaine
106.0872	105	0	106.09	159	74.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	19.4	Diethanolamine
106.0872	105	0	106.09	152	74.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	19.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	19.2	Diethanolamine
106.0872	105	0	106.09	176	77.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	145	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	144	21.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	292	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	288	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	259	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	259	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	197	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	193	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	200	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	195	44.6	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	60	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	307	61.8	Betaine
118.0873	117.079	-0.001	118.0863	301	61.8	Betaine
118.0873	117.079	-0.001	118.0863	291	61.8	Betaine
118.0873	117.079	-0.001	118.0863	378	39.3	Betaine

118.0873	117.079	-0.001	118.0863	373	39.3	Betaine
118.0873	117.079	-0.001	118.0863	373	39.3	Betaine
118.0873	117.079	-0.001	118.0863	299	66.7	Betaine
118.0873	117.079	-0.001	118.0863	299	66.7	Betaine
118.0873	117.079	-0.001	118.0863	295	66.7	Betaine
118.0873	117.079	-0.001	118.0863	323	61.8	Betaine
118.0873	117.079	-0.001	118.0863	322	61.8	Betaine
118.0873	117.079	-0.001	118.0863	320	61.8	Betaine
106.0872	105	0	106.09	156	80.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	19.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	19.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	304	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	300	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	287	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	282	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	208	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	205	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	183	94	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	125	94	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	72	5.9	Ala-Asn
186.0588	370.196	0.0467	186.1055	104	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	339	62.8	Betaine
118.0873	117.079	-0.001	118.0863	339	62.8	Betaine
118.0873	117.079	-0.001	118.0863	331	62.8	Betaine
118.0873	117.079	-0.001	118.0863	283	35.8	Betaine
118.0873	117.079	-0.001	118.0863	282	35.8	Betaine
118.0873	117.079	-0.001	118.0863	280	35.8	Betaine
118.0873	117.079	-0.001	118.0863	310	33.9	Betaine
118.0873	117.079	-0.001	118.0863	310	33.9	Betaine
118.0873	117.079	-0.001	118.0863	308	33.9	Betaine
97.0774	114.104	0.0238	97.1012	48	25	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	43	20.2	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	36	15.4	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	160	73.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	18.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	18.5	Diethanolamine
106.0872	105	0	106.09	157	74.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	304	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	302	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	237	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	237	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	196	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	192	45.8	Betaine aldehyde cation
148.0974	147.053	-0.037	148.0604	134	100	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	320	60.8	Betaine

118.0873	117.079	-0.001	118.0863	317	60.8	Betaine
118.0873	117.079	-0.001	118.0863	316	60.8	Betaine
118.0873	117.079	-0.001	118.0863	267	60	Betaine
118.0873	117.079	-0.001	118.0863	267	60	Betaine
118.0873	117.079	-0.001	118.0863	264	60	Betaine
118.0873	117.079	-0.001	118.0863	313	35	Betaine
118.0873	117.079	-0.001	118.0863	312	35	Betaine
118.0873	117.079	-0.001	118.0863	312	35	Betaine
186.0588	370.196	0.0467	186.1055	48	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	46	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	166	94	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	56	6	Ser-His-Lys
148.0974	147	-0.04	148.06	63	60	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	51	40	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	168	74.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	157	74.9	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	144	25.1	O-acetyl-L-serine hydrochloride
97.0774	114.104	0.0238	97.1012	37	26.2	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	27	18.5	Cycloheptanol
97.0774	114.104	0.0238	97.1012	22	14.9	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	24	22.9	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	16	17.1	Cycloheptanol
97.0774	114.104	0.0238	97.1012	14	15.8	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	278	83	Betaine
118.0873	117.079	-0.001	118.0863	278	83	Betaine
118.0873	117.079	-0.001	118.0863	268	83	Betaine
118.0873	117.079	-0.001	118.0863	433	34.6	Betaine
118.0873	117.079	-0.001	118.0863	432	34.6	Betaine
118.0873	117.079	-0.001	118.0863	428	34.6	Betaine
118.0873	117.079	-0.001	118.0863	294	75.4	Betaine
118.0873	117.079	-0.001	118.0863	287	75.4	Betaine
118.0873	117.079	-0.001	118.0863	286	75.4	Betaine
118.0873	117.079	-0.001	118.0863	273	56.9	Betaine
118.0873	117.079	-0.001	118.0863	273	56.9	Betaine
118.0873	117.079	-0.001	118.0863	270	56.9	Betaine
106.0872	105	0	106.09	170	79.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	20.1	Diethanolamine
106.0872	105	0	106.09	158	73.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	19.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	19.7	Diethanolamine
106.0872	105	0	106.09	136	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	104	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	103	21.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	315	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	313	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	195	51	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	194	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	119	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	115	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	213	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	209	45.8	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	58	32.2	Ser-His-Lys
186.0588	203.091	0.0285	186.0873	53	26	Ala-Asn
186.0588	370.196	0.0467	186.1055	42	17.8	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	140	85.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	79	14.8	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	344	100	Betaine
118.0873	117.079	-0.001	118.0863	343	100	Betaine
118.0873	117.079	-0.001	118.0863	341	100	Betaine
118.0873	117.079	-0.001	118.0863	437	56	Betaine
118.0873	117.079	-0.001	118.0863	432	56	Betaine
118.0873	117.079	-0.001	118.0863	429	56	Betaine
118.0873	117.079	-0.001	118.0863	287	62.8	Betaine
118.0873	117.079	-0.001	118.0863	287	62.8	Betaine
118.0873	117.079	-0.001	118.0863	284	62.8	Betaine
118.0873	117.079	-0.001	118.0863	327	46.7	Betaine
118.0873	117.079	-0.001	118.0863	326	46.7	Betaine
118.0873	117.079	-0.001	118.0863	326	46.7	Betaine
106.0872	105	0	106.09	210	74.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	180	20.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	180	20.6	Diethanolamine
106.0872	105	0	106.09	226	76.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	201	23.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	201	23.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	295	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	295	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	242	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	242	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	182	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	182	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	153	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	150	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	177	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	116	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	141	88.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	67	11.7	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	138	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	367	46	Betaine
118.0873	117.079	-0.001	118.0863	366	46	Betaine
118.0873	117.079	-0.001	118.0863	362	46	Betaine
118.0873	117.079	-0.001	118.0863	388	35.6	Betaine
118.0873	117.079	-0.001	118.0863	387	35.6	Betaine
118.0873	117.079	-0.001	118.0863	384	35.6	Betaine

118.0873	117.079	-0.001	118.0863	290	64.8	Betaine
118.0873	117.079	-0.001	118.0863	289	64.8	Betaine
118.0873	117.079	-0.001	118.0863	284	64.8	Betaine
118.0873	117.079	-0.001	118.0863	364	42.1	Betaine
118.0873	117.079	-0.001	118.0863	364	42.1	Betaine
118.0873	117.079	-0.001	118.0863	358	42.1	Betaine
106.0872	105	0	106.09	159	76.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	17.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	17.8	Diethanolamine
106.0872	105	0	106.09	225	80.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	188	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	187	19.6	Diethanolamine
106.0872	105	0	106.09	159	78.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	303	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	299	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	235	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	233	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	142	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	137	44.6	Betaine aldehyde cation
148.0974	147	-0.04	148.06	3	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	89	83.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	87	83.2	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	38	16.8	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	130	69.7	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	75	13.5	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	64	9.3	N-acetyl-DL-serine
118.0873	117.079	-0.001	118.0863	349	98.5	Betaine
118.0873	117.079	-0.001	118.0863	348	98.5	Betaine
118.0873	117.079	-0.001	118.0863	347	98.5	Betaine
118.0873	117.079	-0.001	118.0863	320	32.2	Betaine
118.0873	117.079	-0.001	118.0863	320	32.2	Betaine
118.0873	117.079	-0.001	118.0863	319	32.2	Betaine
118.0873	117.079	-0.001	118.0863	389	51.3	Betaine
118.0873	117.079	-0.001	118.0863	388	51.3	Betaine
118.0873	117.079	-0.001	118.0863	387	51.3	Betaine
106.0872	105	0	106.09	189	72.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	161	20.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	159	20.9	Diethanolamine
106.0872	105	0	106.09	148	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	21.4	Diethanolamine
106.0872	105	0	106.09	155	71.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	133	28.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	132	28.3	Diethanolamine
186.0588	370.196	0.0467	186.1055	88	100	Ser-His-Lys

186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	66	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	135	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	36	21.9	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	35	21	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	31	17.8	Cyclohexanol, 1-methyl-
118.0873	117.079	-0.001	118.0863	280	100	Betaine
118.0873	117.079	-0.001	118.0863	279	100	Betaine
118.0873	117.079	-0.001	118.0863	277	100	Betaine
118.0873	117.079	-0.001	118.0863	300	64.9	Betaine
118.0873	117.079	-0.001	118.0863	298	64.9	Betaine
118.0873	117.079	-0.001	118.0863	296	64.9	Betaine
118.0873	117.079	-0.001	118.0863	360	56.5	Betaine
118.0873	117.079	-0.001	118.0863	356	56.5	Betaine
118.0873	117.079	-0.001	118.0863	355	56.5	Betaine
106.0872	105	0	106.09	130	72.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	98	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	97	19.4	Diethanolamine
106.0872	105	0	106.09	236	74.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	212	25.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	211	25.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	300	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	296	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	268	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	268	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	112	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	110	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	134	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	134	50	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	165	76.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	154	76.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	127	18.3	Ala-Asn
118.0873	117.079	-0.001	118.0863	333	100	Betaine
118.0873	117.079	-0.001	118.0863	330	100	Betaine
118.0873	117.079	-0.001	118.0863	330	100	Betaine
118.0873	117.079	-0.001	118.0863	415	38.8	Betaine
118.0873	117.079	-0.001	118.0863	413	38.8	Betaine
118.0873	117.079	-0.001	118.0863	408	38.8	Betaine
118.0873	117.079	-0.001	118.0863	265	45.7	Betaine
118.0873	117.079	-0.001	118.0863	264	45.7	Betaine
118.0873	117.079	-0.001	118.0863	263	45.7	Betaine
118.0873	117.079	-0.001	118.0863	411	28.8	Betaine
118.0873	117.079	-0.001	118.0863	410	28.8	Betaine
118.0873	117	0	118.09	409	26.6	Betaine
106.0872	105	0	106.09	208	80.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	171	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	169	19.6	Diethanolamine

84.0822	102.092	-0.0014	84.0808	293	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	292	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	296	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	291	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	202	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	201	49	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	43	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	147	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	135	100	N,N-Bis(2-hydroxyethyl)glycine
106.0872	105.079	-0.0009	106.0863	119	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
106.0872	105	0	106.09	158	75.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	19.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	19.7	Diethanolamine
106.0872	105	0	106.09	221	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	190	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	190	21.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	259	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	257	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	186	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	186	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	145	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	145	50	Betaine aldehyde cation
148.0974	147	-0.04	148.06	12	28.7	N-acetyl-DL-serine
148.0974	147.053	-0.037	148.0604	9	25.4	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	7	23.4	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	125	59	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	122	59	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	116	59	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	90	67.3	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	85	67.3	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	77	67.3	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	332	28.9	Betaine
118.0873	117.079	-0.001	118.0863	332	28.9	Betaine
118.0873	117.079	-0.001	118.0863	328	28.9	Betaine
118.0873	117.079	-0.001	118.0863	219	100	Betaine
118.0873	117.079	-0.001	118.0863	217	100	Betaine
118.0873	117.079	-0.001	118.0863	217	100	Betaine
118.0873	117.079	-0.001	118.0863	309	43.3	Betaine
118.0873	117.079	-0.001	118.0863	308	43.3	Betaine
118.0873	117.079	-0.001	118.0863	306	43.3	Betaine
186.0588	370.196	0.0467	186.1055	50	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	50	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	159	92.7	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	62	7.3	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	251	100	Betaine

118.0873	117.079	-0.001	118.0863	249	100	Betaine
118.0873	117.079	-0.001	118.0863	244	100	Betaine
118.0873	117.079	-0.001	118.0863	386	56.7	Betaine
118.0873	117.079	-0.001	118.0863	381	56.7	Betaine
118.0873	117.079	-0.001	118.0863	377	56.7	Betaine
118.0873	117.079	-0.001	118.0863	341	31.6	Betaine
118.0873	117.079	-0.001	118.0863	341	31.6	Betaine
118.0873	117.079	-0.001	118.0863	336	31.6	Betaine
118.0873	117.079	-0.001	118.0863	384	49.7	Betaine
118.0873	117.079	-0.001	118.0863	380	49.7	Betaine
118.0873	117.079	-0.001	118.0863	380	49.7	Betaine
106.0872	105	0	106.09	155	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	21.1	Diethanolamine
106.0872	105	0	106.09	169	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	136	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	20.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	318	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	316	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	223	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	222	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	198	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	195	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	114	83.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	95	83.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	61	16.5	Ala-Asn
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	402	37.4	Betaine
118.0873	117.079	-0.001	118.0863	402	37.4	Betaine
118.0873	117.079	-0.001	118.0863	398	37.4	Betaine
118.0873	117.079	-0.001	118.0863	305	58.7	Betaine
118.0873	117.079	-0.001	118.0863	303	58.7	Betaine
118.0873	117.079	-0.001	118.0863	302	58.7	Betaine
118.0873	117.079	-0.001	118.0863	329	66.4	Betaine
118.0873	117.079	-0.001	118.0863	328	66.4	Betaine
118.0873	117.079	-0.001	118.0863	324	66.4	Betaine
106.0872	105	0	106.09	159	74.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	25.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	25.1	Diethanolamine
106.0872	105	0	106.09	159	74.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	19.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.2	Diethanolamine
106.0872	105	0	106.09	148	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	20.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	297	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	293	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	223	52	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	221	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	115	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	112	46.9	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	74	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	145	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	93	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	118	89.8	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	39	10.2	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	31	19.4	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	31	19.4	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	31	19.4	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	31	30.8	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	26	30.8	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	23	23	Cyclohexanol, 4-methyl-, trans-
106.0872	105.079	-0.0009	106.0863	138	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	137	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	136	100	Diethanolamine
106.0872	105	0	106.09	202	77.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	174	22.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	173	22.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	296	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	295	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	244	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	241	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	225	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	224	49	Betaine aldehyde cation
148.0974	147	-0.04	148.06	47	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	222	64	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	209	64	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	202	29.1	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	348	49.7	Betaine
118.0873	117.079	-0.001	118.0863	347	49.7	Betaine
118.0873	117.079	-0.001	118.0863	345	49.7	Betaine
118.0873	117.079	-0.001	118.0863	300	40.4	Betaine
118.0873	117.079	-0.001	118.0863	299	40.4	Betaine
118.0873	117.079	-0.001	118.0863	297	40.4	Betaine
118.0873	117.079	-0.001	118.0863	325	62.3	Betaine
118.0873	117.079	-0.001	118.0863	324	62.3	Betaine
118.0873	117.079	-0.001	118.0863	323	62.3	Betaine
186.0588	163.084	0.0149	186.0737	155	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	394	27.4	Betaine
118.0873	117.079	-0.001	118.0863	393	27.4	Betaine
118.0873	117	0	118.09	393	26.4	Betaine
118.0873	117.079	-0.001	118.0863	333	81.4	Betaine
118.0873	117.079	-0.001	118.0863	325	81.4	Betaine
118.0873	117.079	-0.001	118.0863	313	81.4	Betaine
118.0873	117.079	-0.001	118.0863	362	69.9	Betaine

118.0873	117.079	-0.001	118.0863	362	69.9	Betaine
118.0873	117.079	-0.001	118.0863	359	69.9	Betaine
106.0872	105	0	106.09	156	74.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	19.1	Diethanolamine
106.0872	105	0	106.09	157	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	21.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	287	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	286	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	224	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	222	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	210	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	208	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	127	83.1	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	111	83.1	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	77	16.9	Ala-Asn
186.0588	370.196	0.0467	186.1055	76	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	47	24.6	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	41	19.4	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	38	24.6	Cyclohexanol, 4-methyl-, trans-
118.0873	117.079	-0.001	118.0863	229	100	Betaine
118.0873	117.079	-0.001	118.0863	225	100	Betaine
118.0873	117.079	-0.001	118.0863	222	100	Betaine
118.0873	117.079	-0.001	118.0863	417	64.7	Betaine
118.0873	117.079	-0.001	118.0863	411	64.7	Betaine
118.0873	117.079	-0.001	118.0863	410	64.7	Betaine
118.0873	117.079	-0.001	118.0863	329	36	Betaine
118.0873	117.079	-0.001	118.0863	328	36	Betaine
118.0873	117.079	-0.001	118.0863	326	36	Betaine
118.0873	117.079	-0.001	118.0863	341	59.3	Betaine
118.0873	117.079	-0.001	118.0863	340	59.3	Betaine
118.0873	117.079	-0.001	118.0863	339	59.3	Betaine
106.0872	105	0	106.09	159	78.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.1	Diethanolamine
106.0872	105	0	106.09	157	75.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	18.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	18.4	Diethanolamine
106.0872	105	0	106.09	142	77.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	22.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	112	22.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	300	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	298	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	232	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	228	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	121	55.4	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	116	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	228	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	223	44.6	Betaine aldehyde cation
186.0588	203.095	0.0325	186.0913	112	60.2	Indole-3-butyric acid
186.0588	203.095	0.0325	186.0913	105	60.2	Indole-3-butyric acid
186.0588	203.095	0.0325	186.0913	98	60.2	Indole-3-butyric acid
186.0588	370.196	0.0467	186.1055	63	60.8	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	50	39.2	Ser-His-Lys
106.0872	105	0	106.09	203	66	Diethanolamine
106.0872	105.079	-0.0009	106.0863	185	34	Diethanolamine
106.0872	105.079	-0.0009	106.0863	185	34	Diethanolamine
106.0872	105	0	106.09	182	75.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	151	20.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	150	20.5	Diethanolamine
84.0822	102.092	-0.0014	84.0808	293	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	288	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	245	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	242	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	210	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	205	44.6	Betaine aldehyde cation
148.0974	147	-0.04	148.06	26	57.9	N-acetyl-DL-serine
148.0974	147	-0.04	148.06	17	42.1	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	431	55.1	Betaine
118.0873	117.079	-0.001	118.0863	431	55.1	Betaine
118.0873	117.079	-0.001	118.0863	426	55.1	Betaine
118.0873	117.079	-0.001	118.0863	289	74.3	Betaine
118.0873	117.079	-0.001	118.0863	286	74.3	Betaine
118.0873	117.079	-0.001	118.0863	286	74.3	Betaine
118.0873	117.079	-0.001	118.0863	325	57.9	Betaine
118.0873	117.079	-0.001	118.0863	324	57.9	Betaine
118.0873	117.079	-0.001	118.0863	321	57.9	Betaine
106.0872	105	0	106.09	188	75.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	151	18.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	149	18.4	Diethanolamine
106.0872	105	0	106.09	252	77.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	224	22.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	223	22.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	307	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	305	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	186	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	182	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	236	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	232	45.8	Betaine aldehyde cation
186.0588	203.091	0.0285	186.0873	54	100	Ala-Asn
186.0588	163.084	0.0149	186.0737	166	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	33	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	117	74.9	O-Acetyl-L-serine

148.0974	147.053	-0.037	148.0604	113	74.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	103	74.9	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	393	54.7	Betaine
118.0873	117.079	-0.001	118.0863	391	54.7	Betaine
118.0873	117.079	-0.001	118.0863	388	54.7	Betaine
118.0873	117.079	-0.001	118.0863	274	63.3	Betaine
118.0873	117.079	-0.001	118.0863	272	63.3	Betaine
118.0873	117.079	-0.001	118.0863	270	63.3	Betaine
118.0873	117.079	-0.001	118.0863	314	44.2	Betaine
118.0873	117.079	-0.001	118.0863	312	44.2	Betaine
118.0873	117.079	-0.001	118.0863	309	44.2	Betaine
186.0588	370.196	0.0467	186.1055	27	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	76	100	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	123	62.3	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	115	62.3	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	108	37.7	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	280	95.5	Betaine
118.0873	117.079	-0.001	118.0863	278	95.5	Betaine
118.0873	117.079	-0.001	118.0863	270	95.5	Betaine
118.0873	117.079	-0.001	118.0863	414	54.1	Betaine
118.0873	117.079	-0.001	118.0863	413	54.1	Betaine
118.0873	117.079	-0.001	118.0863	411	54.1	Betaine
118.0873	117.079	-0.001	118.0863	312	73	Betaine
118.0873	117.079	-0.001	118.0863	309	73	Betaine
118.0873	117.079	-0.001	118.0863	306	73	Betaine
118.0873	117.079	-0.001	118.0863	271	60.3	Betaine
118.0873	117.079	-0.001	118.0863	269	60.3	Betaine
118.0873	117.079	-0.001	118.0863	266	60.3	Betaine
106.0872	105	0	106.09	157	72.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	21	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	21	Diethanolamine
106.0872	105	0	106.09	154	74.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	19.4	Diethanolamine
106.0872	105	0	106.09	158	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	20.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	309	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	306	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	279	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	276	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	244	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	243	49	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	89	74.8	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	59	20.8	Ala-Asn
186.0588	163.084	0.0149	186.0737	18	74.8	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	42	23.6	Cyclohexanol, 4-methyl-, trans-

97.0774	114.104	0.0238	97.1012	40	21.8	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	34	17.1	Cyclohexanol, 1-methyl-
106.0872	105	0	106.09	159	74.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	20	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20	Diethanolamine
84.0822	102.092	-0.0014	84.0808	278	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	276	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	261	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	256	44.6	Betaine aldehyde cation
148.0974	147.053	-0.037	148.0604	120	68.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	113	68.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	102	68.7	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	59	100	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	361	45.1	Betaine
118.0873	117.079	-0.001	118.0863	358	45.1	Betaine
118.0873	117.079	-0.001	118.0863	355	45.1	Betaine
118.0873	117.079	-0.001	118.0863	281	61.1	Betaine
118.0873	117.079	-0.001	118.0863	281	61.1	Betaine
118.0873	117.079	-0.001	118.0863	278	61.1	Betaine
118.0873	117.079	-0.001	118.0863	319	54.9	Betaine
118.0873	117.079	-0.001	118.0863	319	54.9	Betaine
118.0873	117.079	-0.001	118.0863	317	54.9	Betaine
186.0588	203.091	0.0285	186.0873	83	82.7	Ala-Asn
186.0588	168.042	0.0173	186.0761	36	17.3	3-Hydroxy-4-methoxybenzoic acid
118.0873	117.079	-0.001	118.0863	260	71.2	Betaine
118.0873	117.079	-0.001	118.0863	258	71.2	Betaine
118.0873	117.079	-0.001	118.0863	256	71.2	Betaine
118.0873	117.079	-0.001	118.0863	293	64.4	Betaine
118.0873	117.079	-0.001	118.0863	291	64.4	Betaine
118.0873	117.079	-0.001	118.0863	281	64.4	Betaine
118.0873	117.079	-0.001	118.0863	318	75.5	Betaine
118.0873	117.079	-0.001	118.0863	314	75.5	Betaine
118.0873	117.079	-0.001	118.0863	302	75.5	Betaine
118.0873	117.079	-0.001	118.0863	323	49.9	Betaine
118.0873	117.079	-0.001	118.0863	322	49.9	Betaine
118.0873	117.079	-0.001	118.0863	320	49.9	Betaine
106.0872	105	0	106.09	159	74.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	20	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20	Diethanolamine
106.0872	105	0	106.09	208	74.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	180	21.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	180	21.5	Diethanolamine
106.0872	105	0	106.09	303	76.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	277	23.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	276	23.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	328	54.2	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	324	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	231	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	228	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	124	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	121	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	199	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	198	49	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	83	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	35	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	259	85.3	Betaine
118.0873	117.079	-0.001	118.0863	259	85.3	Betaine
118.0873	117.079	-0.001	118.0863	256	85.3	Betaine
118.0873	117.079	-0.001	118.0863	403	97.4	Betaine
118.0873	117.079	-0.001	118.0863	403	97.4	Betaine
118.0873	117.079	-0.001	118.0863	401	97.4	Betaine
118.0873	117.079	-0.001	118.0863	292	68.4	Betaine
118.0873	117.079	-0.001	118.0863	290	68.4	Betaine
118.0873	117.079	-0.001	118.0863	287	68.4	Betaine
118.0873	117.079	-0.001	118.0863	407	40.4	Betaine
118.0873	117.079	-0.001	118.0863	406	40.4	Betaine
118.0873	117.079	-0.001	118.0863	402	40.4	Betaine
106.0872	105	0	106.09	195	76.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	161	19.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	161	19.5	Diethanolamine
84.0822	102.092	-0.0014	84.0808	307	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	305	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	251	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	247	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	229	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	226	46.9	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	39	59.3	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	28	40.7	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	133	83.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	81	16.6	Ser-His-Lys
106.0872	105	0	106.09	159	73.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	130	20.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	130	20.9	Diethanolamine
106.0872	105	0	106.09	158	74.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	292	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	291	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	239	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	238	49	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	146	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	140	44	Betaine aldehyde cation
148.0974	147	-0.04	148.06	28	100	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	378	100	Betaine
118.0873	117.079	-0.001	118.0863	376	100	Betaine
118.0873	117.079	-0.001	118.0863	370	100	Betaine
118.0873	117.079	-0.001	118.0863	301	67.3	Betaine
118.0873	117.079	-0.001	118.0863	301	67.3	Betaine
118.0873	117.079	-0.001	118.0863	297	67.3	Betaine
118.0873	117.079	-0.001	118.0863	356	38.2	Betaine
118.0873	117.079	-0.001	118.0863	355	38.2	Betaine
118.0873	117.079	-0.001	118.0863	349	38.2	Betaine
106.0872	105	0	106.09	158	80.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	19.1	Diethanolamine
106.0872	105	0	106.09	212	77.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	174	18.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	174	18.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	267	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	266	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	266	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	264	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	161	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	159	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	157	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	153	45.8	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	173	95.7	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	100	95.7	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	48	4.3	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	148	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	154	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	342	56.5	Betaine
118.0873	117.079	-0.001	118.0863	335	56.5	Betaine
118.0873	117.079	-0.001	118.0863	334	56.5	Betaine
118.0873	117.079	-0.001	118.0863	292	64.5	Betaine
118.0873	117.079	-0.001	118.0863	292	64.5	Betaine
118.0873	117.079	-0.001	118.0863	289	64.5	Betaine
118.0873	117.079	-0.001	118.0863	390	37.8	Betaine
118.0873	117.079	-0.001	118.0863	389	37.8	Betaine
118.0873	117.079	-0.001	118.0863	384	37.8	Betaine
84.0822	102.092	-0.0014	84.0808	297	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	294	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	252	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	249	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	217	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	215	48	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	30	100	Ser-His-Lys

148.0974	147.053	-0.037	148.0604	94	59.4	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	73	25.3	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	58	15.3	O-acetyl-L-serine hydrochloride
97.0774	114.104	0.0238	97.1012	27	26.4	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	24	26.4	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	22	21.3	Cyclohexanol, 4-methyl-, trans-
118.0873	117.079	-0.001	118.0863	352	99	Betaine
118.0873	117.079	-0.001	118.0863	349	99	Betaine
118.0873	117.079	-0.001	118.0863	349	99	Betaine
118.0873	117.079	-0.001	118.0863	312	98.6	Betaine
118.0873	117.079	-0.001	118.0863	308	98.6	Betaine
118.0873	117.079	-0.001	118.0863	305	98.6	Betaine
118.0873	117.079	-0.001	118.0863	347	44.6	Betaine
118.0873	117.079	-0.001	118.0863	345	44.6	Betaine
118.0873	117.079	-0.001	118.0863	343	44.6	Betaine
106.0872	105	0	106.09	191	71.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	166	21.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	161	21.9	Diethanolamine
106.0872	105	0	106.09	173	78.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	134	18.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	133	18.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	217	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	216	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	213	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	300	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	297	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	253	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	250	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	167	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	161	44	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	149	41.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	139	29.2	Ala-Asn
186.0588	203.095	0.0325	186.0913	138	28.1	Indole-3-butyric acid
186.0588	163.084	0.0149	186.0737	180	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	106	100	N,N-Bis(2-hydroxyethyl)glycine
106.0872	105	0	106.09	230	61.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	213	33.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	211	33.8	Diethanolamine
106.0872	105	0	106.09	262	64.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	245	35.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	244	35.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	302	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	302	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	238	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	237	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	120	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	118	48	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	171	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	167	45.8	Betaine aldehyde cation
148.0974	147	-0.04	148.06	28	30.3	N-acetyl-DL-serine
148.0974	147	-0.04	148.06	25	26.8	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	24	25.7	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	108	76.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	103	76.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	94	76.6	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	224	100	Betaine
118.0873	117.079	-0.001	118.0863	220	100	Betaine
118.0873	117.079	-0.001	118.0863	212	100	Betaine
118.0873	117.079	-0.001	118.0863	417	40.4	Betaine
118.0873	117.079	-0.001	118.0863	415	40.4	Betaine
118.0873	117.079	-0.001	118.0863	410	40.4	Betaine
118.0873	117.079	-0.001	118.0863	326	59.1	Betaine
118.0873	117.079	-0.001	118.0863	324	59.1	Betaine
118.0873	117.079	-0.001	118.0863	321	59.1	Betaine
118.0873	117.079	-0.001	118.0863	323	38	Betaine
118.0873	117.079	-0.001	118.0863	322	38	Betaine
118.0873	117.079	-0.001	118.0863	321	38	Betaine
106.0872	105	0	106.09	133	73.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	98	18.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	98	18.4	Diethanolamine
106.0872	105	0	106.09	156	74.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	19.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	297	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	297	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	216	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	215	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	192	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	189	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	173	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	163	89.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	59	6.2	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	48	4.3	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	410	40	Betaine
118.0873	117.079	-0.001	118.0863	409	40	Betaine
118.0873	117.079	-0.001	118.0863	406	40	Betaine
118.0873	117.079	-0.001	118.0863	258	82.8	Betaine
118.0873	117.079	-0.001	118.0863	257	82.8	Betaine
118.0873	117.079	-0.001	118.0863	256	82.8	Betaine
118.0873	117.079	-0.001	118.0863	398	52.8	Betaine
118.0873	117.079	-0.001	118.0863	397	52.8	Betaine
118.0873	117.079	-0.001	118.0863	395	52.8	Betaine
106.0872	105	0	106.09	151	74.3	Diethanolamine

106.0872	105.079	-0.0009	106.0863	118	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	195	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	195	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	193	100	Diethanolamine
186.0588	370.196	0.0467	186.1055	36	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	52	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	70	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	8	100	Cyclopentanemethanol, .alpha.-methyl-
118.0873	117.079	-0.001	118.0863	354	66.2	Betaine
118.0873	117.079	-0.001	118.0863	350	66.2	Betaine
118.0873	117.079	-0.001	118.0863	349	66.2	Betaine
118.0873	117.079	-0.001	118.0863	331	96.8	Betaine
118.0873	117.079	-0.001	118.0863	330	96.8	Betaine
118.0873	117.079	-0.001	118.0863	319	96.8	Betaine
118.0873	117.079	-0.001	118.0863	376	33.3	Betaine
118.0873	117.079	-0.001	118.0863	374	33.3	Betaine
118.0873	117.079	-0.001	118.0863	370	33.3	Betaine
106.0872	105	0	106.09	176	74.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	144	19.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	143	19.9	Diethanolamine
106.0872	105	0	106.09	159	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	166	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	165	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	164	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	299	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	299	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	279	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	279	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	206	56.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	199	43.4	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	55	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	144	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	34	100	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	63	59.3	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	52	40.7	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	136	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	128	100	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	36	24.5	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	34	24.5	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	33	21.6	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	155	77.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	22.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	22.4	Diethanolamine

84.0822	102.092	-0.0014	84.0808	276	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	276	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	238	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	236	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	184	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	181	46.9	Betaine aldehyde cation
148.0974	147	-0.04	148.06	37	100	O-acetyl-L-serine hydrochloride
822.7532	822	0	822.75	332	82.7	TG 48:1; [M+NH4]+; TG(16:0/16:0/16:1)
822.7532	822	0	822.75	285	17.3	TG 48:1; [M+NH4]+; TG(14:0/16:0/18:1)
822.7532	822	0	822.75	342	80.6	TG 48:1; [M+NH4]+; TG(16:0/16:0/16:1)
822.7532	822	0	822.75	297	17.2	TG 48:1; [M+NH4]+; TG(14:0/16:0/18:1)
822.7532	822	0	822.75	222	2.2	TG 48:1; [M+NH4]+; TG(14:0/16:1/18:0)
822.7532	822	0	822.75	280	56	TG 48:1; [M+NH4]+; TG(16:0/16:0/16:1)
822.7532	822	0	822.75	274	44	TG 48:1; [M+NH4]+; TG(14:0/16:0/18:1)
822.7532	822	0	822.75	277	100	TG 48:1; [M+NH4]+; TG(16:0/16:0/16:1)
97.0774	114.104	0.0238	97.1012	30	32.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	22	24.1	Cycloheptanol
97.0774	114.104	0.0238	97.1012	20	22.2	Cyclohexanol, 2-methyl-, trans-
118.0873	117.079	-0.001	118.0863	238	100	Betaine
118.0873	117.079	-0.001	118.0863	233	100	Betaine
118.0873	117.079	-0.001	118.0863	411	33.9	Betaine
118.0873	117.079	-0.001	118.0863	411	33.9	Betaine
118.0873	117.079	-0.001	118.0863	408	33.9	Betaine
118.0873	117.079	-0.001	118.0863	270	60.3	Betaine
118.0873	117.079	-0.001	118.0863	268	60.3	Betaine
118.0873	117.079	-0.001	118.0863	263	60.3	Betaine
118.0873	117.079	-0.001	118.0863	335	48.5	Betaine
118.0873	117.079	-0.001	118.0863	333	48.5	Betaine
118.0873	117.079	-0.001	118.0863	331	48.5	Betaine
106.0872	105	0	106.09	156	73.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19.7	Diethanolamine
106.0872	105	0	106.09	158	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19.8	Diethanolamine
106.0872	105	0	106.09	245	73.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	222	26.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	220	26.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	288	54.2	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	284	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	261	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	257	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	140	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	137	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	118	87.8	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	82	87.8	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	46	12.2	Ala-Asn
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	51	24	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	41	16.9	Cycloheptanol
97.0774	114.104	0.0238	97.1012	40	16.3	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	260	79.5	Betaine
118.0873	117.079	-0.001	118.0863	253	79.5	Betaine
118.0873	117.079	-0.001	118.0863	253	79.5	Betaine
118.0873	117.079	-0.001	118.0863	351	32.3	Betaine
118.0873	117.079	-0.001	118.0863	350	32.3	Betaine
118.0873	117.079	-0.001	118.0863	349	32.3	Betaine
118.0873	117.079	-0.001	118.0863	266	80.8	Betaine
118.0873	117.079	-0.001	118.0863	263	80.8	Betaine
118.0873	117.079	-0.001	118.0863	262	80.8	Betaine
118.0873	117	0	118.09	358	24.3	Betaine
118.0873	117	0	118.09	356	22.4	Betaine
118.0873	117.079	-0.001	118.0863	355	21.5	Betaine
106.0872	105	0	106.09	133	78.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	103	21.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	103	21.8	Diethanolamine
106.0872	105	0	106.09	177	72.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	149	21	Diethanolamine
106.0872	105.079	-0.0009	106.0863	148	21	Diethanolamine
186.0588	163.084	0.0149	186.0737	172	83.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	111	14.5	Ala-Asn
186.0588	163.084	0.0149	186.0737	45	83.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	107	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	117	88.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	43	11.7	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	147	71	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	140	71	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	128	71	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	122	100	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	416	32.2	Betaine
118.0873	117.079	-0.001	118.0863	414	32.2	Betaine
118.0873	117.079	-0.001	118.0863	412	32.2	Betaine
118.0873	117.079	-0.001	118.0863	270	27.8	Betaine
118.0873	117.079	-0.001	118.0863	270	27.8	Betaine
118.0873	117.079	-0.001	118.0863	268	27.8	Betaine
118.0873	117.079	-0.001	118.0863	336	39.3	Betaine

118.0873	117.079	-0.001	118.0863	332	39.3	Betaine
118.0873	117.079	-0.001	118.0863	331	39.3	Betaine
106.0872	105	0	106.09	159	74	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	20.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	20.2	Diethanolamine
106.0872	105	0	106.09	155	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	20.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	303	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	300	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	267	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	262	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	150	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	148	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	140	90.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	59	9.6	Ser-His-Lys
106.0872	105	0	106.09	161	77.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	132	22.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	132	22.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	274	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	273	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	216	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	214	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	148	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	144	45.8	Betaine aldehyde cation
148.0974	147.053	-0.037	148.0604	20	37.1	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	20	37.1	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	19	35.6	N-acetyl-DL-serine
148.0974	147.053	-0.037	148.0604	123	70.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	116	70.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	104	70.2	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	41	100	Cyclohexanol, 4-methyl-, trans-
118.0873	117.079	-0.001	118.0863	335	68.9	Betaine
118.0873	117.079	-0.001	118.0863	333	68.9	Betaine
118.0873	117.079	-0.001	118.0863	326	68.9	Betaine
118.0873	117.079	-0.001	118.0863	431	57.5	Betaine
118.0873	117.079	-0.001	118.0863	424	57.5	Betaine
118.0873	117.079	-0.001	118.0863	421	57.5	Betaine
118.0873	117.079	-0.001	118.0863	300	43.9	Betaine
118.0873	117.079	-0.001	118.0863	299	43.9	Betaine
118.0873	117.079	-0.001	118.0863	296	43.9	Betaine
118.0873	117	0	118.09	323	28.9	Betaine
118.0873	117.079	-0.001	118.0863	313	20.4	Betaine
118.0873	117.079	-0.001	118.0863	313	20.4	Betaine
106.0872	105	0	106.09	158	76.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	18.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	18.6	Diethanolamine

106.0872	105	0	106.09	159	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.4	Diethanolamine
106.0872	105	0	106.09	218	52.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	198	24	Diethanolamine
106.0872	105.079	-0.0009	106.0863	197	24	Diethanolamine
106.0872	105	0	106.09	159	76.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	17.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	17.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	306	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	304	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	244	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	239	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	182	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	181	49	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	117	83	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	94	83	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	68	17	Ala-Asn
186.0588	163.084	0.0149	186.0737	136	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	229	80.1	Betaine
118.0873	117.079	-0.001	118.0863	222	80.1	Betaine
118.0873	117.079	-0.001	118.0863	216	80.1	Betaine
118.0873	117.079	-0.001	118.0863	308	24.9	Betaine
118.0873	117	0	118.09	308	24.9	Betaine
118.0873	117.079	-0.001	118.0863	306	24.9	Betaine
118.0873	117.079	-0.001	118.0863	262	48.9	Betaine
118.0873	117.079	-0.001	118.0863	261	48.9	Betaine
118.0873	117.079	-0.001	118.0863	258	48.9	Betaine
118.0873	117.079	-0.001	118.0863	346	24.6	Betaine
118.0873	117.079	-0.001	118.0863	346	24.6	Betaine
118.0873	117.079	-0.001	118.0863	345	24.6	Betaine
148.0974	147.053	-0.037	148.0604	155	63.5	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	146	63.5	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	139	36.5	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	124	100	O-Acetyl-L-serine
371.2885	370.308	0.0271	371.3156	198	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2885	370.308	0.0271	371.3156	126	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2885	370.308	0.0271	371.3156	118	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2885	370.308	0.0271	371.3156	165	88.8	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2885	370.308	0.0271	371.3156	154	88.8	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2885	370.308	0.0271	371.3156	120	88.8	Hexanedioic acid, bis(2-ethylhexyl) ester

371.2885	370.308	0.0271	371.3156	144	81.9	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2885	370.308	0.0271	371.3156	120	81.9	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2885	370.308	0.0271	371.3156	70	81.9	Hexanedioic acid, bis(2-ethylhexyl) ester
118.0873	117.079	-0.001	118.0863	252	49.9	Betaine
118.0873	117.079	-0.001	118.0863	252	49.9	Betaine
118.0873	117.079	-0.001	118.0863	249	49.9	Betaine
118.0873	117.079	-0.001	118.0863	313	30.9	Betaine
118.0873	117.079	-0.001	118.0863	310	30.9	Betaine
118.0873	117.079	-0.001	118.0863	310	30.9	Betaine
106.0872	105	0	106.09	154	75.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	18.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	18.5	Diethanolamine
106.0872	105	0	106.09	224	80.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	187	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	186	19.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	298	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	295	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	223	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	223	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	159	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	154	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	183	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	179	45.8	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	137	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	56	100	Ser-His-Lys
170.0793	187.121	0.0383	170.1176	89	54.2	7-Keto-8-aminopelargonic acid
170.0793	187.121	0.0383	170.1176	85	45.8	7-Keto-8-aminopelargonic acid
148.0974	147	-0.04	148.06	26	33.9	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	24	31.2	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	9	18.9	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	3	100	O-acetyl-L-serine hydrochloride
106.0872	105	0	106.09	171	75.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	136	18.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	136	18.8	Diethanolamine
106.0872	105	0	106.09	245	61.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	230	37.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	229	37.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	109	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	103	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	272	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	270	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	214	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	212	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	124	54.2	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	120	45.8	Betaine aldehyde cation
824.7703	824	0	824.77	250	73.2	TG 48:0; [M+NH4] ⁺ ; TG(14:0/16:0/18:0)
824.7703	824	0	824.77	227	26.8	TG 48:0; [M+NH4] ⁺ ; TG(16:0/16:0/16:0)
824.7703	824	0	824.77	260	50	TG 48:0; [M+NH4] ⁺ ; TG(14:0/16:0/18:0)
824.7703	824	0	824.77	260	50	TG 48:0; [M+NH4] ⁺ ; TG(16:0/16:0/16:0)
824.7703	824	0	824.77	235	74.9	TG 48:0; [M+NH4] ⁺ ; TG(16:0/16:0/16:0)
824.7703	824	0	824.77	211	25.1	TG 48:0; [M+NH4] ⁺ ; TG(14:0/16:0/18:0)
824.7703	824	0	824.77	262	52	TG 48:0; [M+NH4] ⁺ ; TG(16:0/16:0/16:0)
824.7703	824	0	824.77	260	48	TG 48:0; [M+NH4] ⁺ ; TG(14:0/16:0/18:0)
118.0873	117.079	-0.001	118.0863	332	41.8	Betaine
118.0873	117.079	-0.001	118.0863	332	41.8	Betaine
118.0873	117.079	-0.001	118.0863	327	41.8	Betaine
118.0873	117.079	-0.001	118.0863	387	28.1	Betaine
118.0873	117.079	-0.001	118.0863	384	28.1	Betaine
118.0873	117.079	-0.001	118.0863	384	28.1	Betaine
118.0873	117.079	-0.001	118.0863	250	56	Betaine
118.0873	117.079	-0.001	118.0863	250	56	Betaine
118.0873	117.079	-0.001	118.0863	247	56	Betaine
118.0873	117.079	-0.001	118.0863	305	34.3	Betaine
118.0873	117.079	-0.001	118.0863	305	34.3	Betaine
118.0873	117.079	-0.001	118.0863	302	34.3	Betaine
106.0872	105	0	106.09	159	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19.8	Diethanolamine
106.0872	105	0	106.09	147	72.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	20.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	20.3	Diethanolamine
106.0872	105	0	106.09	151	77.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	22.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	22.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	282	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	280	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	277	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	277	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	220	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	219	49	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	139	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	97	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys

186.0588	163.084	0.0149	186.0737	142	91.7	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	57	8.3	Ser-His-Lys
824.7703	824	0	824.77	311	85.4	TG 48:0; [M+NH4] ⁺ ; TG(14:0/16:0/18:0)
824.7703	824	0	824.77	249	14.6	TG 48:0; [M+NH4] ⁺ ; TG(16:0/16:0/16:0)
824.7703	824	0	824.77	98	100	TG 48:0; [M+NH4] ⁺ ; TG(14:0/16:0/18:0)
97.0774	114.104	0.0238	97.1012	65	25.2	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	58	19.3	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	56	19.3	Cyclohexanol, 2-methyl-, trans-
118.0873	117.079	-0.001	118.0863	277	100	Betaine
118.0873	117.079	-0.001	118.0863	275	100	Betaine
118.0873	117.079	-0.001	118.0863	274	100	Betaine
118.0873	117.079	-0.001	118.0863	398	62.9	Betaine
118.0873	117.079	-0.001	118.0863	393	62.9	Betaine
118.0873	117.079	-0.001	118.0863	390	62.9	Betaine
118.0873	117.079	-0.001	118.0863	302	72.8	Betaine
118.0873	117.079	-0.001	118.0863	296	72.8	Betaine
118.0873	117.079	-0.001	118.0863	283	72.8	Betaine
118.0873	117.079	-0.001	118.0863	371	53.1	Betaine
118.0873	117.079	-0.001	118.0863	370	53.1	Betaine
118.0873	117.079	-0.001	118.0863	366	53.1	Betaine
106.0872	105	0	106.09	160	75.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	18	Diethanolamine
106.0872	105	0	106.09	156	74.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	19.1	Diethanolamine
106.0872	105	0	106.09	170	80.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	132	19.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	130	19.3	Diethanolamine
186.0588	163.084	0.0149	186.0737	145	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	128	100	N,N-Bis(2-hydroxyethyl)glycine
876.8011	876	0	876.8	294	100	TG 52:2; [M+NH4] ⁺ ; TG(16:0/18:1/18:1)
876.8011	876	0	876.8	310	86.6	TG 52:2; [M+NH4] ⁺ ; TG(16:0/18:1/18:1)
876.8011	876	0	876.8	212	6.7	TG 52:2; [M+NH4] ⁺ ; TG(17:0/17:1/18:1)
876.8011	876	0	876.8	207	5.4	TG 52:2; [M+NH4] ⁺ ; TG(16:1/18:0/18:1)
876.8011	876	0	876.8	233	57.9	TG 52:2; [M+NH4] ⁺ ; TG(16:0/18:1/18:1)
876.8011	876	0	876.8	224	42.1	TG 52:2; [M+NH4] ⁺ ; TG(16:1/18:0/18:1)

876.8011	876	0	876.8	306	90.4	TG 52:2; [M+NH4] ⁺ ; TG(16:0/18:1/18:1)
876.8011	876	0	876.8	216	7.7	TG 52:2; [M+NH4] ⁺ ; TG(16:1/18:0/18:1)
876.8011	876	0	876.8	178	1.9	TG 52:2; [M+NH4] ⁺ ; TG(16:0/18:0/18:2)
118.0873	117.079	-0.001	118.0863	333	29.8	Betaine
118.0873	117.079	-0.001	118.0863	333	29.8	Betaine
118.0873	117.079	-0.001	118.0863	330	29.8	Betaine
118.0873	117.079	-0.001	118.0863	275	58.7	Betaine
118.0873	117.079	-0.001	118.0863	275	58.7	Betaine
118.0873	117.079	-0.001	118.0863	272	58.7	Betaine
118.0873	117.079	-0.001	118.0863	324	38.4	Betaine
118.0873	117.079	-0.001	118.0863	324	38.4	Betaine
118.0873	117.079	-0.001	118.0863	320	38.4	Betaine
84.0822	102.092	-0.0014	84.0808	259	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	258	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	229	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	229	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	130	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	129	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	133	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	127	44	Betaine aldehyde cation
186.0588	203.091	0.0285	186.0873	49	100	Ala-Asn
186.0588	370.196	0.0467	186.1055	58	100	Ser-His-Lys
148.0974	147	-0.04	148.06	10	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	122	100	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	26	28.9	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	22	24.4	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	22	24.4	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	190	67.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	168	26.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	166	26.6	Diethanolamine
84.0822	102.092	-0.0014	84.0808	298	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	297	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	242	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	238	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	202	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	200	48	Betaine aldehyde cation
148.0974	147.053	-0.037	148.0604	120	73.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	113	73.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	102	73.2	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	39	30.9	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	38	29.7	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	37	30.9	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	302	38.3	Betaine
118.0873	117.079	-0.001	118.0863	299	38.3	Betaine

118.0873	117.079	-0.001	118.0863	299	38.3	Betaine
118.0873	117.079	-0.001	118.0863	358	60.1	Betaine
118.0873	117.079	-0.001	118.0863	355	60.1	Betaine
118.0873	117.079	-0.001	118.0863	351	60.1	Betaine
118.0873	117.079	-0.001	118.0863	323	78	Betaine
118.0873	117.079	-0.001	118.0863	310	78	Betaine
118.0873	117.079	-0.001	118.0863	298	78	Betaine
118.0873	117.079	-0.001	118.0863	293	65.5	Betaine
118.0873	117.079	-0.001	118.0863	293	65.5	Betaine
118.0873	117.079	-0.001	118.0863	289	65.5	Betaine
106.0872	105	0	106.09	158	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19.8	Diethanolamine
106.0872	105	0	106.09	159	74.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	19.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	19.9	Diethanolamine
84.0822	102.092	-0.0014	84.0808	310	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	308	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	287	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	287	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	193	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	192	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	143	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	142	49	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	31	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	176	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	155	88.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	56	6.7	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	43	4.3	Ser-His-Lys
170.0793	187.121	0.0383	170.1176	26	100	7-Keto-8-aminopelargonic acid
97.0774	114.104	0.0238	97.1012	28	24	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	20	17.9	Cycloheptanol
97.0774	114.104	0.0238	97.1012	17	15.9	Cyclohexanol, 2-methyl-, trans-
118.0873	117.079	-0.001	118.0863	249	100	Betaine
118.0873	117.079	-0.001	118.0863	233	100	Betaine
118.0873	117.079	-0.001	118.0863	211	100	Betaine
118.0873	117.079	-0.001	118.0863	402	66.2	Betaine
118.0873	117.079	-0.001	118.0863	398	66.2	Betaine
118.0873	117.079	-0.001	118.0863	388	66.2	Betaine
118.0873	117.079	-0.001	118.0863	289	65.4	Betaine
118.0873	117.079	-0.001	118.0863	287	65.4	Betaine
118.0873	117.079	-0.001	118.0863	284	65.4	Betaine
118.0873	117.079	-0.001	118.0863	300	67.6	Betaine
118.0873	117.079	-0.001	118.0863	300	67.6	Betaine
118.0873	117.079	-0.001	118.0863	296	67.6	Betaine
106.0872	105	0	106.09	158	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.7	Diethanolamine

106.0872	105.079	-0.0009	106.0863	125	20.7	Diethanolamine
106.0872	105	0	106.09	156	75.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	18.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	18.3	Diethanolamine
106.0872	105	0	106.09	156	60.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	141	36.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	140	36.9	Diethanolamine
186.0588	203.091	0.0285	186.0873	78	100	Ala-Asn
186.0588	163.084	0.0149	186.0737	131	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	61	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	155	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	6	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	148	100	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	339	30.3	Betaine
118.0873	117.079	-0.001	118.0863	339	30.3	Betaine
118.0873	117.079	-0.001	118.0863	335	30.3	Betaine
118.0873	117.079	-0.001	118.0863	272	50.4	Betaine
118.0873	117.079	-0.001	118.0863	272	50.4	Betaine
118.0873	117.079	-0.001	118.0863	270	50.4	Betaine
118.0873	117.079	-0.001	118.0863	325	32.8	Betaine
118.0873	117.079	-0.001	118.0863	322	32.8	Betaine
118.0873	117.079	-0.001	118.0863	322	32.8	Betaine
84.0822	102.092	-0.0014	84.0808	251	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	250	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	207	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	203	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	176	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	174	48	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	46	35.9	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	38	26.8	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	29	19.4	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	83	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	24	55.4	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	20	55.4	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	19	44.6	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	156	78.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	21.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	21.8	Diethanolamine
106.0872	105	0	106.09	159	75.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19	Diethanolamine
84.0822	102.092	-0.0014	84.0808	276	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	276	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	265	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	264	49	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	415	93.2	Betaine
118.0873	117.079	-0.001	118.0863	412	93.2	Betaine

118.0873	117.079	-0.001	118.0863	406	93.2	Betaine
118.0873	117.079	-0.001	118.0863	327	33.7	Betaine
118.0873	117.079	-0.001	118.0863	324	33.7	Betaine
118.0873	117.079	-0.001	118.0863	323	33.7	Betaine
118.0873	117.079	-0.001	118.0863	308	58.5	Betaine
118.0873	117.079	-0.001	118.0863	307	58.5	Betaine
118.0873	117.079	-0.001	118.0863	302	58.5	Betaine
106.0872	105	0	106.09	149	74.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	18.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	113	18.7	Diethanolamine
106.0872	105	0	106.09	235	77.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	200	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	198	19.4	Diethanolamine
106.0872	105	0	106.09	159	76.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	17.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	17.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	299	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	299	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	267	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	265	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	221	56.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	214	43.4	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	184	90.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	142	90.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	89	7.4	Ala-Asn
186.0588	163.084	0.0149	186.0737	172	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	99	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	33	20.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	33	20.3	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	29	17.2	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	365	35.5	Betaine
118.0873	117.079	-0.001	118.0863	364	35.5	Betaine
118.0873	117.079	-0.001	118.0863	359	35.5	Betaine
118.0873	117.079	-0.001	118.0863	321	39.6	Betaine
118.0873	117.079	-0.001	118.0863	317	39.6	Betaine
118.0873	117.079	-0.001	118.0863	316	39.6	Betaine
118.0873	117.079	-0.001	118.0863	318	47.3	Betaine
118.0873	117.079	-0.001	118.0863	316	47.3	Betaine
118.0873	117.079	-0.001	118.0863	315	47.3	Betaine
106.0872	105	0	106.09	228	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	194	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	193	20.4	Diethanolamine
106.0872	105	0	106.09	158	80.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	19.1	Diethanolamine
106.0872	105	0	106.09	159	75.5	Diethanolamine

106.0872	105.079	-0.0009	106.0863	125	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.4	Diethanolamine
186.0588	203.091	0.0285	186.0873	106	70.2	Ala-Asn
186.0588	203.095	0.0325	186.0913	85	29.8	Indole-3-butyric acid
186.0588	370.196	0.0467	186.1055	33	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	48	100	Ser-His-Lys
148.0974	147	-0.04	148.06	19	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	171	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	160	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	107	100	O-Acetyl-L-serine
118.0873	117.079	-0.001	118.0863	321	34.7	Betaine
118.0873	117.079	-0.001	118.0863	319	34.7	Betaine
118.0873	117.079	-0.001	118.0863	318	34.7	Betaine
84.0822	102.092	-0.0014	84.0808	269	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	266	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	213	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	212	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	222	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	217	44.6	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	113	84.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	78	84.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	53	15.1	Ala-Asn
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	107	100	Ser-His-Lys
148.0974	147	-0.04	148.06	35	30.6	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	35	30.6	N-acetyl-DL-serine
148.0974	147.053	-0.037	148.0604	29	24.1	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	5	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	102	73.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	96	73.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	87	73.2	O-Acetyl-L-serine
106.0872	105	0	106.09	158	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	20.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	280	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	279	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	242	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	241	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	225	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	221	45.8	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	376	99	Betaine
118.0873	117.079	-0.001	118.0863	375	99	Betaine
118.0873	117.079	-0.001	118.0863	373	99	Betaine
118.0873	117.079	-0.001	118.0863	276	57.9	Betaine
118.0873	117.079	-0.001	118.0863	274	57.9	Betaine
118.0873	117.079	-0.001	118.0863	271	57.9	Betaine
118.0873	117.079	-0.001	118.0863	301	69.2	Betaine

118.0873	117.079	-0.001	118.0863	296	69.2	Betaine
118.0873	117.079	-0.001	118.0863	293	69.2	Betaine
106.0872	105	0	106.09	159	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	21.4	Diethanolamine
106.0872	105	0	106.09	158	76	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	18.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	18.5	Diethanolamine
106.0872	105	0	106.09	277	60.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	262	36.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	261	36.7	Diethanolamine
84.0822	102.092	-0.0014	84.0808	302	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	299	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	265	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	262	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	162	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	161	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	216	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	214	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	142	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	164	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	23	55.4	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	18	44.6	N-acetyl-DL-serine
148.0974	147	-0.04	148.06	6	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	173	61.4	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	162	61.4	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	154	29.8	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	175	66.1	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	162	66.1	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	153	26.1	O-acetyl-L-serine hydrochloride
97.0774	114.104	0.0238	97.1012	43	26.6	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	31	17.7	Cycloheptanol
97.0774	114.104	0.0238	97.1012	29	16.3	Cyclohexanol, 4-methyl-, trans-
118.0873	117.079	-0.001	118.0863	383	100	Betaine
118.0873	117.079	-0.001	118.0863	379	100	Betaine
118.0873	117.079	-0.001	118.0863	377	100	Betaine
118.0873	117.079	-0.001	118.0863	269	56.3	Betaine
118.0873	117.079	-0.001	118.0863	269	56.3	Betaine
118.0873	117.079	-0.001	118.0863	266	56.3	Betaine
118.0873	117.079	-0.001	118.0863	380	50.1	Betaine
118.0873	117.079	-0.001	118.0863	379	50.1	Betaine
118.0873	117.079	-0.001	118.0863	376	50.1	Betaine
106.0872	105	0	106.09	114	71.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	83	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	83	19.4	Diethanolamine
106.0872	105	0	106.09	156	75.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	18.4	Diethanolamine

106.0872	105.079	-0.0009	106.0863	118	18.4	Diethanolamine
106.0872	105	0	106.09	163	100	Diethanolamine
106.0872	105	0	106.09	225	76.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	199	23.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	198	23.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	316	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	312	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	272	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	271	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	211	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	209	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	155	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	154	49	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	124	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	266	58.7	Betaine
118.0873	117.079	-0.001	118.0863	265	58.7	Betaine
118.0873	117.079	-0.001	118.0863	262	58.7	Betaine
118.0873	117.079	-0.001	118.0863	305	100	Betaine
118.0873	117.079	-0.001	118.0863	305	100	Betaine
118.0873	117.079	-0.001	118.0863	297	100	Betaine
84.0822	102.092	-0.0014	84.0808	274	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	271	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	217	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	215	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	148	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	148	50	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	60	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	118	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	59	100	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	147	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	122	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	116	100	O-Acetyl-L-serine
106.0872	105	0	106.09	159	73.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	131	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	130	21.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	244	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	242	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	230	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	229	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	176	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	173	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	205	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	201	45.8	Betaine aldehyde cation
148.0974	147.053	-0.037	148.0604	168	76.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	157	76.6	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	143	23.4	O-acetyl-L-serine hydrochloride
97.0774	114.104	0.0238	97.1012	29	28.4	Cyclohexanol, 1-methyl-

97.0774	114.104	0.0238	97.1012	22	21.7	Cycloheptanol
97.0774	114.104	0.0238	97.1012	16	17.1	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	35	25.1	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	33	23.2	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	30	25.1	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	353	56.8	Betaine
118.0873	117.079	-0.001	118.0863	350	56.8	Betaine
118.0873	117.079	-0.001	118.0863	346	56.8	Betaine
118.0873	117.079	-0.001	118.0863	278	89.4	Betaine
118.0873	117.079	-0.001	118.0863	271	89.4	Betaine
118.0873	117.079	-0.001	118.0863	267	89.4	Betaine
118.0873	117.079	-0.001	118.0863	382	43.5	Betaine
118.0873	117.079	-0.001	118.0863	381	43.5	Betaine
118.0873	117.079	-0.001	118.0863	377	43.5	Betaine
106.0872	105	0	106.09	140	74.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	107	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	106	19.4	Diethanolamine
106.0872	105	0	106.09	221	80.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	183	19.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	183	19.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	299	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	297	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	290	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	289	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	223	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	218	44.6	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	165	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	410	49.1	Betaine
118.0873	117.079	-0.001	118.0863	410	49.1	Betaine
118.0873	117.079	-0.001	118.0863	406	49.1	Betaine
118.0873	117.079	-0.001	118.0863	266	53.6	Betaine
118.0873	117.079	-0.001	118.0863	265	53.6	Betaine
118.0873	117.079	-0.001	118.0863	263	53.6	Betaine
118.0873	117.079	-0.001	118.0863	352	98	Betaine
118.0873	117.079	-0.001	118.0863	348	98	Betaine
118.0873	117.079	-0.001	118.0863	346	98	Betaine
106.0872	105	0	106.09	166	73	Diethanolamine
106.0872	105.079	-0.0009	106.0863	136	20.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	136	20.3	Diethanolamine
106.0872	105	0	106.09	156	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	20.7	Diethanolamine
106.0872	105	0	106.09	267	56.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	257	40	Diethanolamine
106.0872	105.079	-0.0009	106.0863	256	40	Diethanolamine
106.0872	105.079	-0.0009	106.0863	113	100	Diethanolamine

106.0872	105.079	-0.0009	106.0863	113	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	110	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	328	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	328	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	273	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	273	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	197	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	194	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	140	90.1	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	60	9.9	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	162	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	275	84	Betaine
118.0873	117.079	-0.001	118.0863	274	84	Betaine
118.0873	117.079	-0.001	118.0863	274	84	Betaine
118.0873	117.079	-0.001	118.0863	273	62.7	Betaine
118.0873	117.079	-0.001	118.0863	273	62.7	Betaine
118.0873	117.079	-0.001	118.0863	267	62.7	Betaine
118.0873	117.079	-0.001	118.0863	264	58.7	Betaine
118.0873	117.079	-0.001	118.0863	261	58.7	Betaine
118.0873	117.079	-0.001	118.0863	259	58.7	Betaine
84.0822	102.092	-0.0014	84.0808	238	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	238	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	196	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	196	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	188	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	186	48	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	81	100	Ser-His-Lys
148.0974	147	-0.04	148.06	27	39.3	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	21	30.9	N-acetyl-DL-serine
148.0974	147.053	-0.037	148.0604	20	29.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	140	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	129	100	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	35	22.5	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	35	22.5	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	32	19.9	Cyclohexanemethanol
106.0872	105	0	106.09	164	76.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	17.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	17.7	Diethanolamine
106.0872	105	0	106.09	158	75.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.3	Diethanolamine
148.0974	147.053	-0.037	148.0604	127	68.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	120	68.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	108	68.7	O-Acetyl-L-serine
106.0872	105	0	106.09	185	78.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	153	20.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	152	20.9	Diethanolamine

106.0872	105	0	106.09	210	62.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	189	26.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	188	26.4	Diethanolamine
118.0873	117.079	-0.001	118.0863	231	93.3	Betaine
118.0873	117.079	-0.001	118.0863	223	93.3	Betaine
118.0873	117.079	-0.001	118.0863	220	93.3	Betaine
118.0873	117.079	-0.001	118.0863	434	33.8	Betaine
118.0873	117.079	-0.001	118.0863	431	33.8	Betaine
118.0873	117.079	-0.001	118.0863	423	33.8	Betaine
118.0873	117.079	-0.001	118.0863	321	80.7	Betaine
118.0873	117.079	-0.001	118.0863	312	80.7	Betaine
118.0873	117.079	-0.001	118.0863	296	80.7	Betaine
118.0873	117.079	-0.001	118.0863	338	36.6	Betaine
118.0873	117.079	-0.001	118.0863	337	36.6	Betaine
118.0873	117.079	-0.001	118.0863	335	36.6	Betaine
84.0822	102.092	-0.0014	84.0808	317	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	315	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	215	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	212	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	200	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	199	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	247	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	242	44.6	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	121	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	19	100	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	378	58.5	Betaine
118.0873	117.079	-0.001	118.0863	370	58.5	Betaine
118.0873	117.079	-0.001	118.0863	370	58.5	Betaine
118.0873	117.079	-0.001	118.0863	244	41.3	Betaine
118.0873	117.079	-0.001	118.0863	243	41.3	Betaine
118.0873	117.079	-0.001	118.0863	243	41.3	Betaine
118.0873	117.079	-0.001	118.0863	317	58.9	Betaine
118.0873	117.079	-0.001	118.0863	315	58.9	Betaine
118.0873	117.079	-0.001	118.0863	314	58.9	Betaine
106.0872	105	0	106.09	174	79.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	139	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	138	20.1	Diethanolamine
106.0872	105	0	106.09	202	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	170	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	170	21.1	Diethanolamine
106.0872	105	0	106.09	264	68.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	244	31.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	243	31.3	Diethanolamine
84.0822	102.092	-0.0014	84.0808	272	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	270	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	273	51	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	272	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	184	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	179	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	219	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	216	46.9	Betaine aldehyde cation
186.0588	203.091	0.0285	186.0873	60	100	Ala-Asn
186.0588	163.084	0.0149	186.0737	144	100	N,N-Bis(2-hydroxyethyl)glycine
118.0873	117.079	-0.001	118.0863	299	37.9	Betaine
118.0873	117.079	-0.001	118.0863	297	37.9	Betaine
118.0873	117	0	118.09	294	30.5	Betaine
118.0873	117.079	-0.001	118.0863	237	84.2	Betaine
118.0873	117.079	-0.001	118.0863	236	84.2	Betaine
118.0873	117.079	-0.001	118.0863	236	84.2	Betaine
118.0873	117.079	-0.001	118.0863	266	58	Betaine
118.0873	117.079	-0.001	118.0863	264	58	Betaine
118.0873	117.079	-0.001	118.0863	261	58	Betaine
84.0822	102.092	-0.0014	84.0808	245	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	244	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	246	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	245	49	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	154	91.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	70	8.6	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	136	64.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	129	64.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	117	64.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	190	73.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	179	73.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	164	73.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	165	72.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	155	72.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	141	72.9	O-Acetyl-L-serine
106.0872	105	0	106.09	203	75.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	171	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	171	20.1	Diethanolamine
106.0872	105	0	106.09	152	73.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	26.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	26.8	Diethanolamine
148.0974	147	-0.04	148.06	39	100	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	59	62.3	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	44	37.7	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	102	100	O-Acetyl-L-serine
106.0872	105	0	106.09	155	75.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	19	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	19	Diethanolamine
106.0872	105	0	106.09	235	66	Diethanolamine
106.0872	105.079	-0.0009	106.0863	217	34	Diethanolamine
106.0872	105.079	-0.0009	106.0863	216	34	Diethanolamine

118.0873	117.079	-0.001	118.0863	195	100	Betaine
118.0873	117.079	-0.001	118.0863	3	100	Betaine
118.0873	117.079	-0.001	118.0863	377	30.8	Betaine
118.0873	117.079	-0.001	118.0863	376	30.8	Betaine
118.0873	117.079	-0.001	118.0863	373	30.8	Betaine
118.0873	117.079	-0.001	118.0863	301	67.5	Betaine
118.0873	117.079	-0.001	118.0863	300	67.5	Betaine
118.0873	117.079	-0.001	118.0863	296	67.5	Betaine
118.0873	117.079	-0.001	118.0863	365	37.1	Betaine
118.0873	117.079	-0.001	118.0863	364	37.1	Betaine
118.0873	117.079	-0.001	118.0863	363	37.1	Betaine
84.0822	102.092	-0.0014	84.0808	318	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	318	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	222	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	216	44	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	164	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	162	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	257	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	255	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	113	85.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	87	85.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	52	14.8	Ala-Asn
186.0588	370.196	0.0467	186.1055	67	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147.053	-0.037	148.0604	2	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	2	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	119	73.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	112	73.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	100	73.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	130	68.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	122	68.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	110	68.7	O-Acetyl-L-serine
106.0872	105.079	-0.0009	106.0863	123	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	116	100	Diethanolamine
106.0872	105	0	106.09	160	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	21.1	Diethanolamine
118.0873	117.079	-0.001	118.0863	258	82.9	Betaine
118.0873	117.079	-0.001	118.0863	257	82.9	Betaine
118.0873	117.079	-0.001	118.0863	254	82.9	Betaine
118.0873	117.079	-0.001	118.0863	400	67.5	Betaine
118.0873	117.079	-0.001	118.0863	393	67.5	Betaine
118.0873	117.079	-0.001	118.0863	390	67.5	Betaine
118.0873	117	0	118.09	334	23	Betaine
118.0873	117.079	-0.001	118.0863	334	23	Betaine
118.0873	117.079	-0.001	118.0863	332	23	Betaine

118.0873	117.079	-0.001	118.0863	361	31.6	Betaine
118.0873	117.079	-0.001	118.0863	357	31.6	Betaine
118.0873	117.079	-0.001	118.0863	356	31.6	Betaine
84.0822	102.092	-0.0014	84.0808	268	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	267	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	206	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	203	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	135	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	133	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	219	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	216	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	93	84.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	36	15.8	Ala-Asn
106.0872	105	0	106.09	211	69.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	188	25.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	186	25.5	Diethanolamine
118.0873	117.079	-0.001	118.0863	385	45.1	Betaine
118.0873	117.079	-0.001	118.0863	380	45.1	Betaine
118.0873	117.079	-0.001	118.0863	379	45.1	Betaine
118.0873	117.079	-0.001	118.0863	332	98.8	Betaine
118.0873	117.079	-0.001	118.0863	330	98.8	Betaine
118.0873	117.079	-0.001	118.0863	319	98.8	Betaine
118.0873	117.079	-0.001	118.0863	348	38.2	Betaine
118.0873	117.079	-0.001	118.0863	348	38.2	Betaine
118.0873	117.079	-0.001	118.0863	344	38.2	Betaine
84.0822	102.092	-0.0014	84.0808	308	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	306	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	285	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	285	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	218	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	212	44	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	132	84.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	101	84.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	75	15.8	Ala-Asn
186.0588	163.084	0.0149	186.0737	137	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147.053	-0.037	148.0604	122	59.4	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	115	59.4	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	103	59.4	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	96	59.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	92	59.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	83	59.9	O-Acetyl-L-serine
106.0872	105	0	106.09	158	76.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	133	23.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	132	23.4	Diethanolamine
106.0872	105	0	106.09	148	70.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	29.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	29.8	Diethanolamine

170.0793	187.121	0.0383	170.1176	70	39.2	7-Keto-8-aminopelargonic acid
170.0793	187.121	0.0383	170.1176	65	31.6	7-Keto-8-aminopelargonic acid
170.0793	187.121	0.0383	170.1176	63	29.2	7-Keto-8-aminopelargonic acid
106.0872	105	0	106.09	189	76.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	151	18.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	150	18.3	Diethanolamine
118.0873	117.079	-0.001	118.0863	349	57.7	Betaine
118.0873	117.079	-0.001	118.0863	347	57.7	Betaine
118.0873	117.079	-0.001	118.0863	342	57.7	Betaine
118.0873	117.079	-0.001	118.0863	277	61.8	Betaine
118.0873	117.079	-0.001	118.0863	274	61.8	Betaine
118.0873	117.079	-0.001	118.0863	274	61.8	Betaine
118.0873	117.079	-0.001	118.0863	364	58	Betaine
118.0873	117.079	-0.001	118.0863	361	58	Betaine
118.0873	117.079	-0.001	118.0863	360	58	Betaine
84.0822	102.092	-0.0014	84.0808	319	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	316	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	267	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	265	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	191	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	189	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	87	82.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	64	82.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	43	17.8	Ala-Asn
186.0588	163.084	0.0149	186.0737	83	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	44	22.9	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	42	21.1	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	38	17.8	Cyclohexanol, 2-methyl-, trans-
106.0872	105	0	106.09	166	75.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	130	18.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	18.6	Diethanolamine
106.0872	105	0	106.09	159	73.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	20	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	20	Diethanolamine
118.0873	117.079	-0.001	118.0863	397	99	Betaine
118.0873	117.079	-0.001	118.0863	396	99	Betaine
118.0873	117.079	-0.001	118.0863	394	99	Betaine
118.0873	117.079	-0.001	118.0863	323	98.3	Betaine
118.0873	117.079	-0.001	118.0863	322	98.3	Betaine
118.0873	117.079	-0.001	118.0863	316	98.3	Betaine
118.0873	117.079	-0.001	118.0863	370	32.5	Betaine
118.0873	117.079	-0.001	118.0863	368	32.5	Betaine
118.0873	117.079	-0.001	118.0863	364	32.5	Betaine
84.0822	102.092	-0.0014	84.0808	325	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	323	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	309	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	306	46.9	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	158	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	154	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	186	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	185	49	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	38	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	150	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	18	100	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	13	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	215	78.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	201	78.6	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	184	21.4	O-acetyl-L-serine hydrochloride
97.0774	114.104	0.0238	97.1012	55	22	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	53	20.3	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	51	22	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	34	26.6	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	31	23.5	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	27	19.9	Cyclohexanol, 4-methyl-, trans-
106.0872	105	0	106.09	157	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	19.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	19.7	Diethanolamine
106.0872	105	0	106.09	202	76.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	167	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	166	19.1	Diethanolamine
118.0873	117.079	-0.001	118.0863	217	100	Betaine
118.0873	117.079	-0.001	118.0863	206	100	Betaine
118.0873	117.079	-0.001	118.0863	201	100	Betaine
118.0873	117.079	-0.001	118.0863	413	50.4	Betaine
118.0873	117.079	-0.001	118.0863	409	50.4	Betaine
118.0873	117.079	-0.001	118.0863	409	50.4	Betaine
118.0873	117	0	118.09	317	24.9	Betaine
118.0873	117.079	-0.001	118.0863	316	23.9	Betaine
118.0873	117.079	-0.001	118.0863	316	23.9	Betaine
118.0873	117	0	118.09	354	25.4	Betaine
118.0873	117	0	118.09	351	22.5	Betaine
118.0873	117.079	-0.001	118.0863	348	19.9	Betaine
84.0822	102.092	-0.0014	84.0808	307	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	305	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	269	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	269	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	173	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	171	48	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	125	100	N,N-Bis(2-hydroxyethyl)glycine
106.0872	105	0	106.09	186	74.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	162	24.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	161	24.8	Diethanolamine
106.0872	105	0	106.09	270	73.2	Diethanolamine

106.0872	105.079	-0.0009	106.0863	246	24.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	245	24.5	Diethanolamine
106.0872	105	0	106.09	157	80.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	19.1	Diethanolamine
118.0873	117.079	-0.001	118.0863	365	46.3	Betaine
118.0873	117.079	-0.001	118.0863	363	46.3	Betaine
118.0873	117.079	-0.001	118.0863	361	46.3	Betaine
118.0873	117.079	-0.001	118.0863	248	71.1	Betaine
118.0873	117.079	-0.001	118.0863	245	71.1	Betaine
118.0873	117.079	-0.001	118.0863	238	71.1	Betaine
118.0873	117	0	118.09	320	26.5	Betaine
118.0873	117.079	-0.001	118.0863	319	25.5	Betaine
118.0873	117.079	-0.001	118.0863	318	25.5	Betaine
84.0822	102.092	-0.0014	84.0808	315	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	313	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	299	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	299	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	155	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	155	50	Betaine aldehyde cation
148.0974	147	-0.04	148.06	31	56	N-acetyl-DL-serine
148.0974	147	-0.04	148.06	25	44	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	116	73.5	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	69	15.4	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	60	11.2	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	143	65.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	134	65.7	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	122	27.9	O-acetyl-L-serine hydrochloride
118.0873	117.079	-0.001	118.0863	265	57.3	Betaine
118.0873	117.079	-0.001	118.0863	265	57.3	Betaine
118.0873	117.079	-0.001	118.0863	262	57.3	Betaine
84.0822	102.092	-0.0014	84.0808	276	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	273	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	256	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	253	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	103	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	99	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	149	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	146	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	177	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	152	92.7	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	55	7.3	Ser-His-Lys
148.0974	147	-0.04	148.06	82	68.7	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	62	31.3	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	169	59.3	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	158	40.7	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	155	59.3	O-Acetyl-L-serine

97.0774	114.104	0.0238	97.1012	60	29.1	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	52	21.7	Cycloheptanol
97.0774	114.104	0.0238	97.1012	47	17.5	Cyclohexanol, 2-methyl-, trans-
106.0872	105	0	106.09	159	75.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19	Diethanolamine
106.0872	105	0	106.09	186	71.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	161	21.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	160	21.9	Diethanolamine
106.0872	105	0	106.09	157	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	21.4	Diethanolamine
118.0873	117.079	-0.001	118.0863	278	100	Betaine
118.0873	117.079	-0.001	118.0863	278	100	Betaine
118.0873	117.079	-0.001	118.0863	276	100	Betaine
118.0873	117.079	-0.001	118.0863	390	53.2	Betaine
118.0873	117.079	-0.001	118.0863	387	53.2	Betaine
118.0873	117.079	-0.001	118.0863	387	53.2	Betaine
118.0873	117.079	-0.001	118.0863	237	80.8	Betaine
118.0873	117.079	-0.001	118.0863	234	80.8	Betaine
118.0873	117.079	-0.001	118.0863	233	80.8	Betaine
118.0873	117.079	-0.001	118.0863	416	57.6	Betaine
118.0873	117.079	-0.001	118.0863	415	57.6	Betaine
118.0873	117.079	-0.001	118.0863	414	57.6	Betaine
84.0822	102.092	-0.0014	84.0808	317	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	313	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	292	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	291	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	190	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	187	46.9	Betaine aldehyde cation
186.0588	163.084	0.0149	186.0737	102	65.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	95	65.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	76	19.6	Ala-Asn
186.0588	163.084	0.0149	186.0737	148	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	32	37.6	N-acetyl-DL-serine
148.0974	147	-0.04	148.06	28	31.8	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	27	30.6	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	177	69.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	168	69.7	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	153	23.3	O-acetyl-L-serine hydrochloride
97.0774	114.104	0.0238	97.1012	41	23.3	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	39	21.5	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	34	17.3	Cyclohexanol, 1-methyl-
106.0872	105	0	106.09	164	74	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	17.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	17.2	Diethanolamine

106.0872	105	0	106.09	154	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	167	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	166	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	166	100	Diethanolamine
186.0588	163.084	0.0149	186.0737	170	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
106.0872	105	0	106.09	170	75.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	17.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	17.3	Diethanolamine
106.0872	105	0	106.09	156	80.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	19.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	19.8	Diethanolamine
106.0872	105	0	106.09	187	68.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	166	29.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	164	29.1	Diethanolamine
106.0872	105	0	106.09	153	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	21.4	Diethanolamine
118.0873	117.079	-0.001	118.0863	374	66.3	Betaine
118.0873	117.079	-0.001	118.0863	371	66.3	Betaine
118.0873	117.079	-0.001	118.0863	362	66.3	Betaine
118.0873	117.079	-0.001	118.0863	333	30.3	Betaine
118.0873	117.079	-0.001	118.0863	333	30.3	Betaine
118.0873	117	0	118.09	330	26.8	Betaine
84.0822	102.092	-0.0014	84.0808	321	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	321	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	254	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	249	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	228	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	225	46.9	Betaine aldehyde cation
170.0793	187.121	0.0383	170.1176	40	100	7-Keto-8-aminopelargonic acid
148.0974	147	-0.04	148.06	15	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	133	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	127	100	O-Acetyl-L-serine
84.0822	102.092	-0.0014	84.0808	187	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	187	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	182	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	180	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	136	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	135	49	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	402	71	Betaine
118.0873	117.079	-0.001	118.0863	400	71	Betaine
118.0873	117.079	-0.001	118.0863	391	71	Betaine
118.0873	117.079	-0.001	118.0863	295	66	Betaine
118.0873	117.079	-0.001	118.0863	293	66	Betaine

118.0873	117.079	-0.001	118.0863	284	66	Betaine
118.0873	117.079	-0.001	118.0863	332	98.8	Betaine
118.0873	117.079	-0.001	118.0863	328	98.8	Betaine
118.0873	117.079	-0.001	118.0863	328	98.8	Betaine
186.0588	370.196	0.0467	186.1055	61	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	131	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147.053	-0.037	148.0604	35	37.8	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	35	37.8	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	34	37.8	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	130	74.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	122	74.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	111	74.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	125	53.4	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	120	53.4	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	112	53.4	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	47	24.4	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	44	21.6	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	39	17.4	Cyclohexanol, 2-methyl-, trans-
106.0872	105	0	106.09	152	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	21.1	Diethanolamine
106.0872	105	0	106.09	157	78.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	21.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	21.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	285	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	285	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	267	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	265	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	252	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	251	49	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	390	38.2	Betaine
118.0873	117.079	-0.001	118.0863	389	38.2	Betaine
118.0873	117.079	-0.001	118.0863	385	38.2	Betaine
118.0873	117.079	-0.001	118.0863	291	65.3	Betaine
118.0873	117.079	-0.001	118.0863	288	65.3	Betaine
118.0873	117.079	-0.001	118.0863	287	65.3	Betaine
118.0873	117.079	-0.001	118.0863	365	55.7	Betaine
118.0873	117.079	-0.001	118.0863	364	55.7	Betaine
118.0873	117.079	-0.001	118.0863	359	55.7	Betaine
186.0588	370.196	0.0467	186.1055	56	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	129	76.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	116	76.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	92	18.7	Ala-Asn
148.0974	147.053	-0.037	148.0604	133	63.4	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	125	63.4	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	113	63.4	O-Acetyl-L-serine
106.0872	105	0	106.09	158	75.1	Diethanolamine

106.0872	105.079	-0.0009	106.0863	125	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.6	Diethanolamine
106.0872	105	0	106.09	158	75.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19.3	Diethanolamine
106.0872	105	0	106.09	154	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	21.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	311	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	310	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	244	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	242	48	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	177	100	5-Aminovaleric acid
118.0873	117.079	-0.001	118.0863	168	100	5-Aminovaleric acid
118.0873	117.079	-0.001	118.0863	416	98.5	Betaine
118.0873	117.079	-0.001	118.0863	413	98.5	Betaine
118.0873	117.079	-0.001	118.0863	410	98.5	Betaine
118.0873	117.079	-0.001	118.0863	278	59.1	Betaine
118.0873	117.079	-0.001	118.0863	274	59.1	Betaine
118.0873	117.079	-0.001	118.0863	274	59.1	Betaine
118.0873	117.079	-0.001	118.0863	340	48.1	Betaine
118.0873	117.079	-0.001	118.0863	336	48.1	Betaine
118.0873	117.079	-0.001	118.0863	335	48.1	Betaine
186.0588	370.196	0.0467	186.1055	46	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	153	91.8	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	107	91.8	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	67	8.2	Ala-Asn
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	65	51.2	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	48	27.9	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	40	20.8	N-acetyl-DL-serine
148.0974	147.053	-0.037	148.0604	170	100	O-Acetyl-L-serine
106.0872	105	0	106.09	159	75.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	18.4	Diethanolamine
106.0872	105	0	106.09	261	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	227	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	226	20.4	Diethanolamine
371.2746	370.308	0.041	371.3156	228	89.2	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	105	89.2	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	103	89.2	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	169	100	Hexanedioic acid, bis(2-ethylhexyl) ester

371.2746	370.308	0.041	371.3156	153	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	119	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	85	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	72	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	40	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.214	-0.0529	371.2217	56	100	17-Phenyltrilor-13,14-dihydroprostaglandin A2
371.2746	370.214	-0.0529	371.2217	48	100	17-Phenyltrilor-13,14-dihydroprostaglandin A2
97.0774	114.104	0.0238	97.1012	25	26.2	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	15	18.5	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	12	18.5	Cyclopentanemethanol, .alpha.-methyl-
106.0872	105	0	106.09	159	79.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	295	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	293	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	267	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	266	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	201	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	195	44	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	371	62.5	Betaine
118.0873	117.079	-0.001	118.0863	371	62.5	Betaine
118.0873	117.079	-0.001	118.0863	360	62.5	Betaine
118.0873	117.079	-0.001	118.0863	298	66.5	Betaine
118.0873	117.079	-0.001	118.0863	297	66.5	Betaine
118.0873	117.079	-0.001	118.0863	289	66.5	Betaine
118.0873	117.079	-0.001	118.0863	315	58.5	Betaine
118.0873	117.079	-0.001	118.0863	314	58.5	Betaine
118.0873	117.079	-0.001	118.0863	313	58.5	Betaine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147	-0.04	148.06	20	31.3	N-acetyl-DL-serine
148.0974	147	-0.04	148.06	15	25.2	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	15	25.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	143	100	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	39	25.2	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	32	19.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	32	25.2	Cyclohexanemethanol
106.0872	105	0	106.09	156	71.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	134	28.3	Diethanolamine

106.0872	105.079	-0.0009	106.0863	133	28.3	Diethanolamine
106.0872	105	0	106.09	158	79.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	20.4	Diethanolamine
106.0872	105	0	106.09	230	76.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	205	23.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	205	23.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	290	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	290	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	248	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	247	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	178	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	174	45.8	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	359	39.7	Betaine
118.0873	117.079	-0.001	118.0863	358	39.7	Betaine
118.0873	117.079	-0.001	118.0863	357	39.7	Betaine
118.0873	117.079	-0.001	118.0863	305	68.2	Betaine
118.0873	117.079	-0.001	118.0863	304	68.2	Betaine
118.0873	117.079	-0.001	118.0863	296	68.2	Betaine
118.0873	117.079	-0.001	118.0863	315	47.1	Betaine
118.0873	117.079	-0.001	118.0863	314	47.1	Betaine
118.0873	117.079	-0.001	118.0863	314	47.1	Betaine
148.0974	147.053	-0.037	148.0604	112	50.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	106	50.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	96	50.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	131	54.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	125	54.7	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	118	35.3	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	184	70.3	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	169	70.3	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	158	21.1	O-acetyl-L-serine hydrochloride
97.0774	114.104	0.0238	97.1012	33	25.4	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	32	24.5	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	28	24.5	Cyclohexanemethanol
106.0872	105	0	106.09	151	78.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	21.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	21.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	173	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	165	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	105	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	105	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	104	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	317	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	315	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	271	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	269	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	207	54.2	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	203	45.8	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	207	100	Betaine
118.0873	117.079	-0.001	118.0863	397	50.6	Betaine
118.0873	117.079	-0.001	118.0863	395	50.6	Betaine
118.0873	117.079	-0.001	118.0863	389	50.6	Betaine
118.0873	117.079	-0.001	118.0863	277	58.4	Betaine
118.0873	117.079	-0.001	118.0863	274	58.4	Betaine
118.0873	117.079	-0.001	118.0863	273	58.4	Betaine
118.0873	117.079	-0.001	118.0863	351	53.1	Betaine
118.0873	117.079	-0.001	118.0863	345	53.1	Betaine
118.0873	117.079	-0.001	118.0863	345	53.1	Betaine
186.0588	163.084	0.0149	186.0737	134	91.1	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	51	8.9	Ser-His-Lys
148.0974	147	-0.04	148.06	26	24.2	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	25	23.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	25	23.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	41	32.1	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	36	25.9	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	35	32.1	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	81	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	71	49	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	68	49	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	61	49	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	24	52	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	22	48	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	16	48	Cyclohexanemethanol
106.0872	105	0	106.09	158	78.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.1	Diethanolamine
106.0872	105	0	106.09	148	77.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	22.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	22.1	Diethanolamine
106.0872	105	0	106.09	214	75	Diethanolamine
106.0872	105.079	-0.0009	106.0863	183	20.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	182	20.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	309	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	306	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	247	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	245	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	154	100	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	169	56.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	162	43.4	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	364	61.1	Betaine
118.0873	117.079	-0.001	118.0863	361	61.1	Betaine
118.0873	117.079	-0.001	118.0863	359	61.1	Betaine
118.0873	117.079	-0.001	118.0863	386	98.5	Betaine
118.0873	117.079	-0.001	118.0863	382	98.5	Betaine

118.0873	117.079	-0.001	118.0863	377	98.5	Betaine
118.0873	117.079	-0.001	118.0863	281	66.6	Betaine
118.0873	117.079	-0.001	118.0863	278	66.6	Betaine
118.0873	117.079	-0.001	118.0863	275	66.6	Betaine
118.0873	117.079	-0.001	118.0863	327	27.1	Betaine
118.0873	117.079	-0.001	118.0863	326	27.1	Betaine
118.0873	117	0	118.09	325	25	Betaine
148.0974	147	-0.04	148.06	9	50	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	9	50	N-acetyl-DL-serine
148.0974	147.053	-0.037	148.0604	210	76.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	197	76.6	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	185	23.4	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	117	43.7	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	115	43.7	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	114	38.6	O-acetyl-L-serine hydrochloride
97.0774	114.104	0.0238	97.1012	20	100	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	110	60	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	107	60	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	106	60	Cyclohexanemethanol
106.0872	105	0	106.09	245	75.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	214	20.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	212	20.6	Diethanolamine
186.0588	370.196	0.0467	186.1055	32	54.2	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	28	45.8	Ser-His-Lys
148.0974	147.053	-0.037	148.0604	26	21	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	26	21	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	26	21	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	49	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	49	100	O-Acetyl-L-serine
84.0822	102.092	-0.0014	84.0808	141	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	139	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	185	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	184	49	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	326	37.3	Betaine
118.0873	117.079	-0.001	118.0863	324	37.3	Betaine
118.0873	117.079	-0.001	118.0863	323	37.3	Betaine
118.0873	117.079	-0.001	118.0863	272	61.3	Betaine
118.0873	117.079	-0.001	118.0863	272	61.3	Betaine
118.0873	117.079	-0.001	118.0863	269	61.3	Betaine
118.0873	117.079	-0.001	118.0863	257	54.7	Betaine
118.0873	117.079	-0.001	118.0863	257	54.7	Betaine
118.0873	117.079	-0.001	118.0863	255	54.7	Betaine
186.0588	163.084	0.0149	186.0737	119	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	55	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	147	100	N,N-Bis(2-hydroxyethyl)glycine
148.0974	147.053	-0.037	148.0604	114	50.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	108	50.2	O-Acetyl-L-serine

148.0974	147.053	-0.037	148.0604	97	50.2	O-Acetyl-L-serine
371.2746	370.308	0.041	371.3156	194	70.6	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	138	70.6	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	136	70.6	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	170	78.3	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	149	78.3	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	109	78.3	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	80	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	68	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	54	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	140	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	122	100	Hexanedioic acid, bis(2-ethylhexyl) ester
371.2746	370.308	0.041	371.3156	102	100	Hexanedioic acid, bis(2-ethylhexyl) ester
97.0774	114.104	0.0238	97.1012	75	21.6	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	74	20.7	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	74	20.7	Cyclohexanemethanol
106.0872	105	0	106.09	155	71.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	133	28.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	133	28.3	Diethanolamine
106.0872	105	0	106.09	232	78.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	202	21.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	201	21.8	Diethanolamine
84.0822	102.092	-0.0014	84.0808	289	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	288	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	252	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	249	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	113	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	110	46.9	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	319	32.2	Betaine
118.0873	117.079	-0.001	118.0863	318	32.2	Betaine
118.0873	117.079	-0.001	118.0863	318	32.2	Betaine
118.0873	117.079	-0.001	118.0863	276	61.7	Betaine
118.0873	117.079	-0.001	118.0863	273	61.7	Betaine
118.0873	117.079	-0.001	118.0863	272	61.7	Betaine

118.0873	117.079	-0.001	118.0863	372	45.1	Betaine
118.0873	117.079	-0.001	118.0863	370	45.1	Betaine
118.0873	117.079	-0.001	118.0863	367	45.1	Betaine
186.0588	370.196	0.0467	186.1055	52	100	Ser-His-Lys
186.0588	203.091	0.0285	186.0873	75	100	Ala-Asn
148.0974	147	-0.04	148.06	33	56	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	27	44	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	178	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	167	100	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	98	24.3	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	87	16.6	Cycloheptanol
97.0774	114.104	0.0238	97.1012	87	16.6	Cyclopentanemethanol, .alpha.-methyl-
106.0872	105	0	106.09	154	74.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	18.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	18.5	Diethanolamine
106.0872	105	0	106.09	253	76.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	228	23.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	228	23.4	Diethanolamine
84.0822	102.092	-0.0014	84.0808	300	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	295	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	253	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	250	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	228	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	223	44.6	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	321	50.1	Betaine
118.0873	117.079	-0.001	118.0863	320	50.1	Betaine
118.0873	117.079	-0.001	118.0863	319	50.1	Betaine
118.0873	117.079	-0.001	118.0863	365	55.6	Betaine
118.0873	117.079	-0.001	118.0863	364	55.6	Betaine
118.0873	117.079	-0.001	118.0863	361	55.6	Betaine
148.0974	147	-0.04	148.06	12	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	119	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	112	100	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	70	52	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	68	48	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	66	48	Cyclopentanemethanol, .alpha.-methyl-
106.0872	105	0	106.09	157	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	111	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	110	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	109	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	289	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	288	49	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	253	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	252	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	157	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	152	44.6	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	171	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	167	45.8	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	330	43.4	Betaine
118.0873	117.079	-0.001	118.0863	326	43.4	Betaine
118.0873	117.079	-0.001	118.0863	324	43.4	Betaine
118.0873	117.079	-0.001	118.0863	272	72.7	Betaine
118.0873	117.079	-0.001	118.0863	272	72.7	Betaine
118.0873	117.079	-0.001	118.0863	271	72.7	Betaine
118.0873	117.079	-0.001	118.0863	326	99	Betaine
118.0873	117.079	-0.001	118.0863	325	99	Betaine
118.0873	117.079	-0.001	118.0863	322	99	Betaine
97.0774	114.104	0.0238	97.1012	51	25.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	44	19.4	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	40	16.4	Cyclopentanemethanol, .alpha.-methyl-
84.0822	102.092	-0.0014	84.0808	255	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	255	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	185	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	184	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	166	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	163	46.9	Betaine aldehyde cation
106.0872	105	0	106.09	159	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	21.1	Diethanolamine
106.0872	105	0	106.09	180	67.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	161	32.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	160	32.7	Diethanolamine
186.0588	370.196	0.0467	186.1055	38	100	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
148.0974	147	-0.04	148.06	21	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	140	100	O-Acetyl-L-serine
84.0822	102.092	-0.0014	84.0808	168	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	167	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	149	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	149	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	147	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	145	48	Betaine aldehyde cation
186.0588	370.196	0.0467	186.1055	73	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	213	100	Betaine
118.0873	117.079	-0.001	118.0863	212	100	Betaine
118.0873	117.079	-0.001	118.0863	211	100	Betaine
121.1229	60.032	-0.051	121.072	21	64.7	Urea
121.1229	60.032	-0.051	121.072	20	64.7	Urea

121.1229	60.032	-0.051	121.072	20	64.7	Urea
121.1229	60.032	-0.051	121.072	37	78.9	Urea
121.1229	60.032	-0.051	121.072	30	78.9	Urea
121.1229	60.032	-0.051	121.072	24	78.9	Urea
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.032	-0.051	121.072	44	81.7	Urea
121.1229	60.032	-0.051	121.072	37	81.7	Urea
121.1229	60.032	-0.051	121.072	27	81.7	Urea
84.0822	102.092	-0.0014	84.0808	247	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	246	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	184	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	182	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	200	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	197	46.9	Betaine aldehyde cation
106.0872	105	0	106.09	151	75.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	114	18.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	113	18.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	100	Diethanolamine
106.0872	105	0	106.09	218	77.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	191	22.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	190	22.7	Diethanolamine
148.0974	147.053	-0.037	148.0604	89	69.5	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	85	69.5	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	78	69.5	O-Acetyl-L-serine
121.1229	60.032	-0.051	121.072	29	77.9	Urea
121.1229	60.032	-0.051	121.072	28	77.9	Urea
121.1229	60.032	-0.051	121.072	27	77.9	Urea
121.1229	60.032	-0.051	121.072	31	78.2	Urea
121.1229	60.032	-0.051	121.072	25	78.2	Urea
121.1229	60.032	-0.051	121.072	20	78.2	Urea
121.1229	60.058	-0.0006	121.1223	10	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	8	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	8	100	1-Propanol
121.1229	60.032	-0.051	121.072	73	83.2	Urea
121.1229	60.032	-0.051	121.072	64	83.2	Urea
121.1229	60.032	-0.051	121.072	53	83.2	Urea
228.1067	227.12	0.021	228.1277	146	100	Ametryn
228.1067	227.12	0.021	228.1277	111	100	Ametryn
228.1067	227.12	0.021	228.1277	99	100	Ametryn
84.0822	102.092	-0.0014	84.0808	237	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	234	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	185	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	184	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	190	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	189	49	Betaine aldehyde cation

106.0872	105	0	106.09	160	75.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18	Diethanolamine
106.0872	105	0	106.09	159	75.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	19.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.4	Diethanolamine
106.0872	105	0	106.09	159	74.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	129	20.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	20.6	Diethanolamine
121.1229	60.032	-0.051	121.072	26	76.9	Urea
121.1229	60.032	-0.051	121.072	24	76.9	Urea
121.1229	60.032	-0.051	121.072	23	76.9	Urea
121.1229	60.032	-0.051	121.072	38	68.7	Urea
121.1229	60.032	-0.051	121.072	32	68.7	Urea
121.1229	60.032	-0.051	121.072	25	68.7	Urea
121.1229	60.032	-0.051	121.072	64	85.6	Urea
121.1229	60.032	-0.051	121.072	59	85.6	Urea
121.1229	60.032	-0.051	121.072	58	85.6	Urea
228.1067	227.12	0.021	228.1277	67	100	Ametryn
84.0822	102.092	-0.0014	84.0808	262	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	260	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	219	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	218	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	132	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	131	49	Betaine aldehyde cation
106.0872	105	0	106.09	169	76	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	17.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	17.3	Diethanolamine
106.0872	105	0	106.09	151	76.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	23.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	23.4	Diethanolamine
106.0872	105	0	106.09	200	64.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	178	25.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	177	25.4	Diethanolamine
148.0974	147	-0.04	148.06	59	51	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	58	49	N-acetyl-DL-serine
148.0974	147.053	-0.037	148.0604	149	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	139	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	120	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	113	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	102	100	O-Acetyl-L-serine
103.1124	102.068	-0.037	103.0754	114	82.4	Pentanoic acid
103.1124	102.068	-0.037	103.0754	107	82.4	Pentanoic acid
103.1124	102.068	-0.037	103.0754	79	82.4	Pentanoic acid
103.1124	102.068	-0.037	103.0754	64	100	Pentanoic acid
103.1124	102.068	-0.037	103.0754	56	100	Pentanoic acid
103.1124	102.068	-0.037	103.0754	40	100	Pentanoic acid

121.1229	60.032	-0.051	121.072	58	80.9	Urea
121.1229	60.032	-0.051	121.072	55	80.9	Urea
121.1229	60.032	-0.051	121.072	54	80.9	Urea
121.1229	60.032	-0.051	121.072	67	83.1	Urea
121.1229	60.032	-0.051	121.072	59	83.1	Urea
121.1229	60.032	-0.051	121.072	48	83.1	Urea
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
148.0974	147	-0.04	148.06	64	54.2	O-acetyl-L-serine hydrochloride
148.0974	147	-0.04	148.06	60	45.8	O-acetyl-L-serine hydrochloride
103.1124	102.068	-0.037	103.0754	204	77.3	Pentanoic acid
103.1124	102.068	-0.037	103.0754	202	77.3	Pentanoic acid
103.1124	102.116	0.011	103.123	177	22.7	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	166	52	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	165	52	1,5-Pentanediamine
103.1124	102.068	-0.037	103.0754	164	48	Pentanoic acid
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	108	100	N,N-Bis(2-hydroxyethyl)glycine
84.0822	102.092	-0.0014	84.0808	257	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	253	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	187	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	185	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	197	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	192	44.6	Betaine aldehyde cation
106.0872	105	0	106.09	159	73.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	19.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	19.7	Diethanolamine
106.0872	105	0	106.09	171	72.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	146	22	Diethanolamine
106.0872	105.079	-0.0009	106.0863	145	22	Diethanolamine
106.0872	105	0	106.09	201	62.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	186	37.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	184	37.7	Diethanolamine
121.1229	60.032	-0.051	121.072	20	68.7	Urea
121.1229	60.032	-0.051	121.072	19	68.7	Urea
121.1229	60.032	-0.051	121.072	18	68.7	Urea
121.1229	60.032	-0.051	121.072	28	77.6	Urea
121.1229	60.032	-0.051	121.072	25	77.6	Urea
121.1229	60.032	-0.051	121.072	23	77.6	Urea
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
228.1067	227.12	0.021	228.1277	116	100	Ametryn

228.1067	227.12	0.021	228.1277	87	100	Ametryn
228.1067	227.12	0.021	228.1277	82	100	Ametryn
103.1124	102.068	-0.037	103.0754	195	78.2	Pentanoic acid
103.1124	102.068	-0.037	103.0754	180	78.2	Pentanoic acid
103.1124	102.116	0.011	103.123	165	21.8	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	218	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	215	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	213	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	216	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	214	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	211	100	1,5-Pentanediamine
106.0872	105	0	106.09	158	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	20.7	Diethanolamine
106.0872	105	0	106.09	151	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	118	21.1	Diethanolamine
121.1229	60.032	-0.051	121.072	20	63.5	Urea
121.1229	60.032	-0.051	121.072	18	63.5	Urea
121.1229	60.032	-0.051	121.072	16	63.5	Urea
121.1229	60.032	-0.051	121.072	45	82.2	Urea
121.1229	60.032	-0.051	121.072	38	82.2	Urea
121.1229	60.032	-0.051	121.072	31	82.2	Urea
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.032	-0.051	121.072	59	84	Urea
121.1229	60.032	-0.051	121.072	51	84	Urea
121.1229	60.058	-0.0006	121.1223	3	16	1-Propanol
148.0974	147.053	-0.037	148.0604	117	53.2	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	109	53.2	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	107	37.5	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	156	77.3	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	143	77.3	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	133	77.3	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	177	71.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	165	71.9	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	151	21.5	O-acetyl-L-serine hydrochloride
97.0774	114.104	0.0238	97.1012	7	100	Cyclopentanemethanol, .alpha.-methyl-
84.0822	102.092	-0.0014	84.0808	277	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	277	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	205	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	204	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	164	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	160	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	148	51	Betaine aldehyde cation

84.0822	102.092	-0.0014	84.0808	147	49	Betaine aldehyde cation
106.0872	105	0	106.09	193	73.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	165	21.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	164	21.2	Diethanolamine
106.0872	105	0	106.09	157	73.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	100	Diethanolamine
103.1124	102.116	0.011	103.123	106	73.2	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	103	73.2	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	103	73.2	1,5-Pentanediamine
84.0822	102.092	-0.0014	84.0808	194	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	191	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	192	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	191	49	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	134	51	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	133	49	Betaine aldehyde cation
121.1229	60.032	-0.051	121.072	26	71.7	Urea
121.1229	60.032	-0.051	121.072	24	71.7	Urea
121.1229	60.032	-0.051	121.072	21	71.7	Urea
121.1229	60.032	-0.051	121.072	38	77.3	Urea
121.1229	60.032	-0.051	121.072	34	77.3	Urea
121.1229	60.032	-0.051	121.072	32	77.3	Urea
121.1229	60.058	-0.0006	121.1223	3	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.032	-0.051	121.072	38	80.2	Urea
121.1229	60.032	-0.051	121.072	31	80.2	Urea
121.1229	60.032	-0.051	121.072	23	80.2	Urea
148.0974	147.053	-0.037	148.0604	116	61.8	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	109	61.8	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	99	61.8	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	159	67.3	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	148	67.3	O-Acetyl-L-serine
148.0974	147	-0.04	148.06	140	32.7	O-acetyl-L-serine hydrochloride
103.1124	102.116	0.011	103.123	101	81.9	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	98	81.9	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	97	81.9	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	222	85.2	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	221	85.2	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	215	85.2	1,5-Pentanediamine
97.0774	114.104	0.0238	97.1012	17	100	Cyclohexanemethanol
106.0872	105	0	106.09	222	73.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	197	22.5	Diethanolamine
106.0872	105.079	-0.0009	106.0863	196	22.5	Diethanolamine

106.0872	105	0	106.09	159	73.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	20	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	20	Diethanolamine
84.0822	102.092	-0.0014	84.0808	284	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	282	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	257	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	257	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	231	55.4	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	226	44.6	Betaine aldehyde cation
228.1067	227.12	0.021	228.1277	118	100	Ametryn
228.1067	227.12	0.021	228.1277	94	100	Ametryn
228.1067	227.12	0.021	228.1277	89	100	Ametryn
121.1229	60.032	-0.051	121.072	14	61.5	Urea
121.1229	60.032	-0.051	121.072	12	61.5	Urea
121.1229	60.032	-0.051	121.072	10	61.5	Urea
121.1229	60.032	-0.051	121.072	25	76.6	Urea
121.1229	60.032	-0.051	121.072	20	76.6	Urea
121.1229	60.032	-0.051	121.072	17	76.6	Urea
121.1229	60.058	-0.0006	121.1223	4	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.032	-0.051	121.072	45	78.6	Urea
121.1229	60.032	-0.051	121.072	36	78.6	Urea
121.1229	60.032	-0.051	121.072	28	78.6	Urea
148.0974	147.053	-0.037	148.0604	106	59.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	101	59.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	91	59.9	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	136	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	128	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	187	75	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	175	75	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	158	75	O-Acetyl-L-serine
106.0872	105	0	106.09	158	76.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	122	18.8	Diethanolamine
106.0872	105	0	106.09	235	75.8	Diethanolamine
106.0872	105.079	-0.0009	106.0863	205	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	204	21.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	303	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	301	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	239	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	236	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	139	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	135	45.8	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	186	56	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	180	44	Betaine aldehyde cation
228.1067	227.12	0.021	228.1277	104	100	Ametryn

228.1067	227.12	0.021	228.1277	98	100	Ametryn
228.1067	227.12	0.021	228.1277	94	100	Ametryn
121.1229	60.032	-0.051	121.072	63	85.6	Urea
121.1229	60.032	-0.051	121.072	62	85.6	Urea
121.1229	60.032	-0.051	121.072	61	85.6	Urea
121.1229	60.032	-0.051	121.072	45	80.4	Urea
121.1229	60.032	-0.051	121.072	38	80.4	Urea
121.1229	60.032	-0.051	121.072	31	80.4	Urea
121.1229	60.032	-0.051	121.072	46	82.2	Urea
121.1229	60.058	-0.0006	121.1223	2	17.8	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	17.8	1-Propanol
121.1229	60.032	-0.051	121.072	37	79.9	Urea
121.1229	60.032	-0.051	121.072	30	79.9	Urea
121.1229	60.032	-0.051	121.072	23	79.9	Urea
148.0974	147	-0.04	148.06	25	100	O-acetyl-L-serine hydrochloride
148.0974	147.053	-0.037	148.0604	165	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	154	100	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	142	76.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	133	76.6	O-Acetyl-L-serine
148.0974	147.053	-0.037	148.0604	120	76.6	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	25	19.9	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	23	18.4	Cycloheptanol
97.0774	114.104	0.0238	97.1012	22	17.7	Cyclopentanemethanol, .alpha.-methyl-
106.0872	105	0	106.09	155	74.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	121	19.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	120	19.1	Diethanolamine
106.0872	105	0	106.09	183	79.3	Diethanolamine
106.0872	105.079	-0.0009	106.0863	150	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	150	20.7	Diethanolamine
106.0872	105.079	-0.0009	106.0863	151	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	150	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	144	100	Diethanolamine
121.1229	60.032	-0.051	121.072	41	81.4	Urea
121.1229	60.032	-0.051	121.072	38	81.4	Urea
121.1229	60.032	-0.051	121.072	35	81.4	Urea
121.1229	60.032	-0.051	121.072	40	80.9	Urea
121.1229	60.032	-0.051	121.072	32	80.9	Urea
121.1229	60.032	-0.051	121.072	25	80.9	Urea
121.1229	60.032	-0.051	121.072	44	81.9	Urea
121.1229	60.032	-0.051	121.072	36	81.9	Urea
121.1229	60.058	-0.0006	121.1223	1	18.1	1-Propanol
103.1124	102.068	-0.037	103.0754	107	100	Pentanoic acid
103.1124	102.068	-0.037	103.0754	68	100	Pentanoic acid
103.1124	102.068	-0.037	103.0754	67	100	Pentanoic acid
103.1124	102.116	0.011	103.123	164	91.8	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	161	91.8	1,5-Pentanediamine

103.1124	102.068	-0.037	103.0754	78	8.2	Pentanoic acid
84.0822	102.092	-0.0014	84.0808	191	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	191	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	167	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	165	48	Betaine aldehyde cation
228.1067	227.12	0.021	228.1277	54	100	Ametryn
103.1124	102.116	0.011	103.123	104	63.5	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	103	63.5	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	102	63.5	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	217	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	215	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	213	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	227	100	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	225	100	1,5-Pentanediamine
371.2569	370.214	-0.0352	371.2217	74	32.4	17-Phenyltrinor-13,14-dihydroprostaglandin A2
371.2569	370.214	-0.0352	371.2217	74	32.4	Spiromesifen
371.2569	370.214	-0.0352	371.2217	72	32.4	17-Phenyltrinor-13,14-dihydroprostaglandin A2
371.2569	370.222	-0.028	371.2289	46	55.4	PyroGlu-Ile-Lys
371.2569	370.222	-0.028	371.2289	41	44.6	PyroGlu-Ile-Lys
371.2569	370.214	-0.0352	371.2217	57	100	17-Phenyltrinor-13,14-dihydroprostaglandin A2
371.2569	370.214	-0.0352	371.2217	51	100	17-Phenyltrinor-13,14-dihydroprostaglandin A2
186.0588	370.196	0.0467	186.1055	60	100	Ser-His-Lys
106.0872	105	0	106.09	159	78.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	128	21.4	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	21.4	Diethanolamine
106.0872	105	0	106.09	157	78.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	125	21.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	21.1	Diethanolamine
106.0872	105	0	106.09	174	79.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	139	20.1	Diethanolamine
106.0872	105.079	-0.0009	106.0863	139	20.1	Diethanolamine
84.0822	102.092	-0.0014	84.0808	317	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	315	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	256	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	256	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	200	54.2	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	196	45.8	Betaine aldehyde cation
228.1067	227.12	0.021	228.1277	114	100	Ametryn
228.1067	227.12	0.021	228.1277	74	100	Ametryn
228.1067	227.12	0.021	228.1277	63	100	Ametryn
121.1229	60.032	-0.051	121.072	26	73.2	Urea
121.1229	60.032	-0.051	121.072	24	73.2	Urea
121.1229	60.032	-0.051	121.072	24	73.2	Urea

121.1229	60.032	-0.051	121.072	53	83.3	Urea
121.1229	60.032	-0.051	121.072	45	83.3	Urea
121.1229	60.032	-0.051	121.072	37	83.3	Urea
121.1229	60.058	-0.0006	121.1223	2	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.032	-0.051	121.072	41	80.9	Urea
121.1229	60.032	-0.051	121.072	34	80.9	Urea
121.1229	60.032	-0.051	121.072	26	80.9	Urea
148.0974	147.053	-0.037	148.0604	158	100	O-Acetyl-L-serine
97.0774	114.104	0.0238	97.1012	50	33.9	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	43	25.9	Cycloheptanol
97.0774	114.104	0.0238	97.1012	38	20.9	Cyclohexanol, 4-methyl-, trans-
106.0872	105.079	-0.0009	106.0863	119	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	119	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	117	100	Diethanolamine
228.1067	227.12	0.021	228.1277	70	100	Ametryn
121.1229	60.032	-0.051	121.072	47	82.7	Urea
121.1229	60.032	-0.051	121.072	47	82.7	Urea
121.1229	60.032	-0.051	121.072	47	82.7	Urea
121.1229	60.032	-0.051	121.072	40	80.9	Urea
121.1229	60.032	-0.051	121.072	33	80.9	Urea
121.1229	60.032	-0.051	121.072	27	80.9	Urea
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.058	-0.0006	121.1223	1	100	1-Propanol
121.1229	60.032	-0.051	121.072	45	82.2	Urea
121.1229	60.032	-0.051	121.072	37	82.2	Urea
121.1229	60.058	-0.0006	121.1223	1	17.8	1-Propanol
106.0872	105	0	106.09	169	75	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	19.2	Diethanolamine
106.0872	105.079	-0.0009	106.0863	135	19.2	Diethanolamine
106.0872	105	0	106.09	157	75	Diethanolamine
106.0872	105.079	-0.0009	106.0863	124	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	123	19.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	156	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	155	100	Diethanolamine
106.0872	105.079	-0.0009	106.0863	154	100	Diethanolamine
84.0822	102.092	-0.0014	84.0808	293	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	291	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	234	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	232	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	231	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	229	48	Betaine aldehyde cation
103.1124	102.116	0.011	103.123	127	87.3	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	127	87.3	1,5-Pentanediamine
103.1124	102.116	0.011	103.123	119	87.3	1,5-Pentanediamine
103.1124	102.068	-0.037	103.0754	93	100	Pentanoic acid

103.1124	102.068	-0.037	103.0754	66	100	Pentanoic acid
103.1124	102.068	-0.037	103.0754	64	100	Pentanoic acid
118.0873	117	0	118.09	263	30.2	Betaine
118.0873	117	0	118.09	263	30.2	Betaine
118.0873	117.079	-0.001	118.0863	260	26.7	Betaine
118.0873	117.079	-0.001	118.0863	257	59.8	Betaine
118.0873	117.079	-0.001	118.0863	254	59.8	Betaine
118.0873	117.079	-0.001	118.0863	252	59.8	Betaine
118.0873	117.079	-0.001	118.0863	345	48.4	Betaine
118.0873	117.079	-0.001	118.0863	342	48.4	Betaine
118.0873	117.079	-0.001	118.0863	341	48.4	Betaine
186.0588	163.084	0.0149	186.0737	156	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	86	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	150	100	N,N-Bis(2-hydroxyethyl)glycine
84.0822	102.092	-0.0014	84.0808	196	52	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	194	48	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	179	53.1	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	176	46.9	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	183	50	Betaine aldehyde cation
84.0822	102.092	-0.0014	84.0808	183	50	Betaine aldehyde cation
118.0873	117.079	-0.001	118.0863	454	73.9	Betaine
118.0873	117.079	-0.001	118.0863	442	73.9	Betaine
118.0873	117.079	-0.001	118.0863	442	73.9	Betaine
118.0873	117.079	-0.001	118.0863	324	79.5	Betaine
118.0873	117.079	-0.001	118.0863	316	79.5	Betaine
118.0873	117.079	-0.001	118.0863	316	79.5	Betaine
118.0873	117.079	-0.001	118.0863	366	62.6	Betaine
118.0873	117.079	-0.001	118.0863	363	62.6	Betaine
118.0873	117.079	-0.001	118.0863	358	62.6	Betaine
97.0774	114.104	0.0238	97.1012	45	26.4	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	34	18.1	Cycloheptanol
97.0774	114.104	0.0238	97.1012	30	15.3	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	28	22.2	Cycloheptanol
97.0774	114.104	0.0238	97.1012	24	18.7	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	20	15.8	Cyclopentanemethanol, .alpha.-methyl-
106.0872	105	0	106.09	159	74.6	Diethanolamine
106.0872	105.079	-0.0009	106.0863	127	19.9	Diethanolamine
106.0872	105.079	-0.0009	106.0863	126	19.9	Diethanolamine
186.0588	370.196	0.0467	186.1055	39	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	165	93.8	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	58	6.2	Ser-His-Lys
224.1293	446.228	-0.0081	224.1212	87	64.7	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	70	35.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	55	35.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	218	93.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	196	93.1	N-Acetyl-L-tyrosine

224.1293	223.084	-0.0376	224.0917	171	93.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	300	88.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	288	88.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	267	88.4	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	392	72.2	Betaine
118.0873	117.079	-0.001	118.0863	389	72.2	Betaine
118.0873	117.079	-0.001	118.0863	378	72.2	Betaine
118.0873	117.079	-0.001	118.0863	257	65.1	Betaine
118.0873	117.079	-0.001	118.0863	255	65.1	Betaine
118.0873	117.079	-0.001	118.0863	251	65.1	Betaine
118.0873	117.079	-0.001	118.0863	268	40.1	Betaine
118.0873	117.079	-0.001	118.0863	266	40.1	Betaine
118.0873	117.079	-0.001	118.0863	266	40.1	Betaine
97.0774	114.104	0.0238	97.1012	71	25.7	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	66	20.7	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	60	16.3	Cycloheptanol
186.0588	370.196	0.0467	186.1055	55	35.3	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	49	27.7	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	37	18.5	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	50	100	Ser-His-Lys
224.1293	223.1	-0.022	224.107	159	100	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	155	100	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	147	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	146	51	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	145	49	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	144	51	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	254	93.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	246	93.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	216	93.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	279	91.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	245	91.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	213	91.5	N-Acetyl-L-tyrosine
125.9874	125	0.04	126.03	169	91.8	2-Aminoethylphosphonic acid
125.9874	125.015	0.0345	126.0219	83	8.2	Taurine
125.9874	125	0.04	126.03	151	100	2-Aminoethylphosphonic acid
125.9874	125	0.04	126.03	145	100	2-Aminoethylphosphonic acid
186.0588	163.084	0.0149	186.0737	183	89	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	116	89	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	57	3.9	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	45	55.1	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	25	25.1	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	19	19.7	Cycloheptanol
167.0138	166.049	0.0426	167.0564	272	91.3	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	267	91.3	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	264	91.3	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	280	96.3	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	275	96.3	7-Methylxanthine

167.0138	166.049	0.0426	167.0564	251	96.3	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	264	90.9	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	263	90.9	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	249	90.9	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	329	96.2	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	313	96.2	7-Methylxanthine
167.0138	166.049	0.0426	167.0564	311	96.2	7-Methylxanthine
118.0873	117.079	-0.001	118.0863	206	100	Betaine
118.0873	117.079	-0.001	118.0863	30	100	Betaine
118.0873	117.079	-0.001	118.0863	30	100	Betaine
118.0873	117.079	-0.001	118.0863	479	68.2	Betaine
118.0873	117.079	-0.001	118.0863	475	68.2	Betaine
118.0873	117.079	-0.001	118.0863	467	68.2	Betaine
118.0873	117.079	-0.001	118.0863	298	60.8	Betaine
118.0873	117.079	-0.001	118.0863	298	60.8	Betaine
118.0873	117.079	-0.001	118.0863	295	60.8	Betaine
118.0873	117.079	-0.001	118.0863	345	42.1	Betaine
118.0873	117.079	-0.001	118.0863	340	42.1	Betaine
118.0873	117.079	-0.001	118.0863	337	42.1	Betaine
186.0588	163.084	0.0149	186.0737	138	85.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	74	14.1	Ala-Asn
97.0774	114.104	0.0238	97.1012	33	100	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	29	23.8	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	20	17.3	Cycloheptanol
97.0774	114.104	0.0238	97.1012	17	15.3	Cyclohexanemethanol
118.0873	117.079	-0.001	118.0863	367	29.5	Betaine
118.0873	117.079	-0.001	118.0863	362	29.5	Betaine
118.0873	117.079	-0.001	118.0863	361	29.5	Betaine
118.0873	117.079	-0.001	118.0863	508	74.5	Betaine
118.0873	117.079	-0.001	118.0863	500	74.5	Betaine
118.0873	117.079	-0.001	118.0863	490	74.5	Betaine
118.0873	117.079	-0.001	118.0863	302	66.9	Betaine
118.0873	117.079	-0.001	118.0863	297	66.9	Betaine
118.0873	117.079	-0.001	118.0863	292	66.9	Betaine
118.0873	117.079	-0.001	118.0863	293	71.8	Betaine
118.0873	117.079	-0.001	118.0863	291	71.8	Betaine
118.0873	117.079	-0.001	118.0863	288	71.8	Betaine
186.0588	203.091	0.0285	186.0873	61	84.7	Ala-Asn
186.0588	163.084	0.0149	186.0737	2	15.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	148	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	446.228	-0.0081	224.1212	115	88	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	42	12	Bendiocarb
224.1293	223.084	-0.0376	224.0917	296	94.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	273	94.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	249	94.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	275	81.5	N-Acetyl-L-tyrosine

224.1293	223.084	-0.0376	224.0917	256	81.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	226	81.5	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	335	48.9	Betaine
118.0873	117.079	-0.001	118.0863	328	48.9	Betaine
118.0873	117.079	-0.001	118.0863	323	48.9	Betaine
118.0873	117.079	-0.001	118.0863	387	56.3	Betaine
118.0873	117.079	-0.001	118.0863	385	56.3	Betaine
118.0873	117.079	-0.001	118.0863	380	56.3	Betaine
118.0873	117.079	-0.001	118.0863	316	83.4	Betaine
118.0873	117.079	-0.001	118.0863	314	83.4	Betaine
118.0873	117.079	-0.001	118.0863	304	83.4	Betaine
118.0873	117.079	-0.001	118.0863	319	62.9	Betaine
118.0873	117.079	-0.001	118.0863	315	62.9	Betaine
118.0873	117.079	-0.001	118.0863	313	62.9	Betaine
186.0588	163.084	0.0149	186.0737	134	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	55	52	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	53	48	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	59	100	Ser-His-Lys
118.0873	117.079	-0.001	118.0863	265	100	Betaine
118.0873	117.079	-0.001	118.0863	257	100	Betaine
118.0873	117.079	-0.001	118.0863	243	100	Betaine
118.0873	117.079	-0.001	118.0863	444	62.9	Betaine
118.0873	117.079	-0.001	118.0863	441	62.9	Betaine
118.0873	117.079	-0.001	118.0863	432	62.9	Betaine
118.0873	117.079	-0.001	118.0863	207	67.7	Betaine
118.0873	117.079	-0.001	118.0863	206	67.7	Betaine
118.0873	117.079	-0.001	118.0863	201	67.7	Betaine
118.0873	117.079	-0.001	118.0863	291	59.3	Betaine
118.0873	117.079	-0.001	118.0863	288	59.3	Betaine
118.0873	117.079	-0.001	118.0863	283	59.3	Betaine
186.0588	163.084	0.0149	186.0737	147	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	147	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	22	33.6	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	16	26.4	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	14	26.4	Cyclohexanol, 4-methyl-, trans-
140.0692	139.1	0.038	140.107	96	100	Tropinone
140.0692	139.1	0.038	140.107	95	100	Tropinone
140.0692	139.1	0.038	140.107	91	100	Tropinone
118.0873	117.079	-0.001	118.0863	329	42.2	Betaine
118.0873	117.079	-0.001	118.0863	329	42.2	Betaine
118.0873	117.079	-0.001	118.0863	326	42.2	Betaine
118.0873	117.079	-0.001	118.0863	378	76.4	Betaine
118.0873	117.079	-0.001	118.0863	371	76.4	Betaine
118.0873	117.079	-0.001	118.0863	362	76.4	Betaine
118.0873	117.079	-0.001	118.0863	279	69.3	Betaine
118.0873	117.079	-0.001	118.0863	279	69.3	Betaine
118.0873	117.079	-0.001	118.0863	275	69.3	Betaine

118.0873	117.079	-0.001	118.0863	355	61.4	Betaine
118.0873	117.079	-0.001	118.0863	350	61.4	Betaine
118.0873	117.079	-0.001	118.0863	349	61.4	Betaine
186.0588	163.084	0.0149	186.0737	172	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	157	84.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.095	0.0325	186.0913	97	15.1	Indole-3-butyric acid
186.0588	203.095	0.0325	186.0913	83	15.1	Indole-3-butyric acid
186.0588	163.084	0.0149	186.0737	139	100	N,N-Bis(2-hydroxyethyl)glycine
195.1236	194.115	-0.0009	195.1227	280	98.4	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	279	98.4	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	277	98.4	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	241	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	241	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	239	100	Tetraethylene glycol
118.0873	117	0	118.09	339	24.1	Betaine
118.0873	117.079	-0.001	118.0863	336	21.3	Betaine
118.0873	117	0	118.09	336	21.3	Betaine
118.0873	117.079	-0.001	118.0863	506	68.9	Betaine
118.0873	117.079	-0.001	118.0863	501	68.9	Betaine
118.0873	117.079	-0.001	118.0863	501	68.9	Betaine
118.0873	117.079	-0.001	118.0863	169	61.4	Betaine
118.0873	117.079	-0.001	118.0863	169	61.4	Betaine
118.0873	117.079	-0.001	118.0863	163	61.4	Betaine
118.0873	117.079	-0.001	118.0863	283	65.8	Betaine
118.0873	117.079	-0.001	118.0863	282	65.8	Betaine
118.0873	117.079	-0.001	118.0863	278	65.8	Betaine
186.0588	163.084	0.0149	186.0737	203	92.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	146	92.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	99	6.4	Ala-Asn
186.0588	163.084	0.0149	186.0737	161	94	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	51	6	Ser-His-Lys
140.0692	139.063	0.0014	140.0706	55	100	5-Amino-2-methoxyphenol
224.1293	223.1	-0.022	224.107	138	76.6	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	131	76.6	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	130	76.6	N-Fluorenylacetamide
224.1293	446.228	-0.0081	224.1212	134	49.4	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	124	34.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	113	34.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	204	87.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	194	87.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	168	87.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	274	91.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	258	91.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	221	91.7	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	215	80.1	Betaine
118.0873	117.079	-0.001	118.0863	211	80.1	Betaine
118.0873	117.079	-0.001	118.0863	205	80.1	Betaine

118.0873	117.079	-0.001	118.0863	423	77.2	Betaine
118.0873	117.079	-0.001	118.0863	414	77.2	Betaine
118.0873	117.079	-0.001	118.0863	401	77.2	Betaine
118.0873	117.079	-0.001	118.0863	350	87	Betaine
118.0873	117.079	-0.001	118.0863	344	87	Betaine
118.0873	117.079	-0.001	118.0863	340	87	Betaine
118.0873	117.079	-0.001	118.0863	293	81.6	Betaine
118.0873	117.079	-0.001	118.0863	293	81.6	Betaine
118.0873	117.079	-0.001	118.0863	289	81.6	Betaine
186.0588	163.084	0.0149	186.0737	168	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	223.084	-0.0376	224.0917	203	76	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	200	76	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	194	76	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	214	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	198	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	162	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	314	86.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	296	86.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	275	86.1	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	245	87.3	Betaine
118.0873	117.079	-0.001	118.0863	236	87.3	Betaine
118.0873	117.079	-0.001	118.0863	230	87.3	Betaine
118.0873	117	0	118.09	359	33.3	Betaine
118.0873	117	0	118.09	349	23.5	Betaine
118.0873	117.079	-0.001	118.0863	339	16.6	Betaine
118.0873	117.079	-0.001	118.0863	316	71.8	Betaine
118.0873	117.079	-0.001	118.0863	313	71.8	Betaine
118.0873	117.079	-0.001	118.0863	313	71.8	Betaine
186.0588	163.084	0.0149	186.0737	137	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	223.1	-0.022	224.107	166	96.6	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	165	96.6	N-Fluorenylacetamide
224.1293	241.117	-0.0151	224.1142	27	3.4	(6R)-5,6,7,8-Tetrahydrobiopterin
224.1293	223.084	-0.0376	224.0917	123	39.4	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	115	29.4	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	110	39.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	258	79.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	257	79.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	243	79.9	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	186	49.5	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	183	43.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	171	43.7	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	303	78.1	Betaine
118.0873	117.079	-0.001	118.0863	293	78.1	Betaine
118.0873	117.079	-0.001	118.0863	271	78.1	Betaine
118.0873	117.079	-0.001	118.0863	482	65	Betaine

118.0873	117.079	-0.001	118.0863	481	65	Betaine
118.0873	117.079	-0.001	118.0863	476	65	Betaine
118.0873	117.079	-0.001	118.0863	234	66.3	Betaine
118.0873	117.079	-0.001	118.0863	234	66.3	Betaine
118.0873	117.079	-0.001	118.0863	229	66.3	Betaine
118.0873	117.079	-0.001	118.0863	215	68.6	Betaine
118.0873	117.079	-0.001	118.0863	215	68.6	Betaine
118.0873	117.079	-0.001	118.0863	214	68.6	Betaine
186.0588	370.196	0.0467	186.1055	92	43.2	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	91	41.6	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	68	15.2	Ser-His-Lys
140.0692	139.1	0.038	140.107	45	41.8	Tropinone
140.0692	139.1	0.038	140.107	44	41.8	Tropinone
140.0692	139.1	0.038	140.107	44	41.8	Tropinone
97.0774	114.104	0.0238	97.1012	21	21	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	16	16.9	Cycloheptanol
97.0774	114.104	0.0238	97.1012	15	16.3	Cyclohexanemethanol
224.1293	223.1	-0.022	224.107	165	79.2	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	164	79.2	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	154	79.2	N-Fluorenylacetamide
224.1293	446.228	-0.0081	224.1212	145	50.1	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	133	33.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	125	33.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	169	92.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	153	92.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	123	92.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	303	76.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	302	76.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	297	76.5	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	279	63.6	Betaine
118.0873	117.079	-0.001	118.0863	271	63.6	Betaine
118.0873	117.079	-0.001	118.0863	267	63.6	Betaine
118.0873	117.079	-0.001	118.0863	519	69.9	Betaine
118.0873	117.079	-0.001	118.0863	510	69.9	Betaine
118.0873	117.079	-0.001	118.0863	510	69.9	Betaine
118.0873	117.079	-0.001	118.0863	340	84	Betaine
118.0873	117.079	-0.001	118.0863	335	84	Betaine
118.0873	117.079	-0.001	118.0863	322	84	Betaine
118.0873	117.079	-0.001	118.0863	264	98.3	Betaine
118.0873	117.079	-0.001	118.0863	264	98.3	Betaine
118.0873	117.079	-0.001	118.0863	247	98.3	Betaine
186.0588	163.084	0.0149	186.0737	165	87.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	117	87.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	87	10.3	Ala-Asn
186.0588	163.084	0.0149	186.0737	138	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	223.106	-0.0164	224.1129	88	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	86	100	N-Acetyl-D-galactosaminitol

224.1293	223.106	-0.0164	224.1129	84	100	N-Acetyl-D-galactosaminitol
224.1293	223.084	-0.0376	224.0917	103	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	95	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	295	93.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	270	93.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	234	93.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	336	84.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	332	84.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	328	84.5	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	338	54.8	Betaine
118.0873	117.079	-0.001	118.0863	338	54.8	Betaine
118.0873	117.079	-0.001	118.0863	331	54.8	Betaine
118.0873	117.079	-0.001	118.0863	499	46	Betaine
118.0873	117.079	-0.001	118.0863	495	46	Betaine
118.0873	117.079	-0.001	118.0863	493	46	Betaine
118.0873	117.079	-0.001	118.0863	372	62.9	Betaine
118.0873	117.079	-0.001	118.0863	372	62.9	Betaine
118.0873	117.079	-0.001	118.0863	364	62.9	Betaine
118.0873	117.079	-0.001	118.0863	182	64.6	Betaine
118.0873	117.079	-0.001	118.0863	179	64.6	Betaine
118.0873	117.079	-0.001	118.0863	174	64.6	Betaine
186.0588	163.084	0.0149	186.0737	150	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	223.084	-0.0376	224.0917	193	79.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	183	79.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	171	79.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	279	95.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	251	95.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	228	95.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	320	88.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	302	88.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	267	88.7	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	358	31.6	Betaine
118.0873	117	0	118.09	355	27.9	Betaine
118.0873	117.079	-0.001	118.0863	352	31.6	Betaine
118.0873	117.079	-0.001	118.0863	472	58.2	Betaine
118.0873	117.079	-0.001	118.0863	467	58.2	Betaine
118.0873	117.079	-0.001	118.0863	462	58.2	Betaine
118.0873	117.079	-0.001	118.0863	289	70.2	Betaine
118.0873	117.079	-0.001	118.0863	287	70.2	Betaine
118.0873	117.079	-0.001	118.0863	282	70.2	Betaine
118.0873	117.079	-0.001	118.0863	358	70.1	Betaine
118.0873	117.079	-0.001	118.0863	355	70.1	Betaine
118.0873	117.079	-0.001	118.0863	352	70.1	Betaine
186.0588	163.084	0.0149	186.0737	141	90.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	60	9.6	Ser-His-Lys
186.0588	370.196	0.0467	186.1055	48	100	Ser-His-Lys
224.1293	223.1	-0.022	224.107	154	100	N-Fluorenylacetamide

224.1293	223.1	-0.022	224.107	141	100	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	137	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	168	51.6	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	158	36.4	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	138	51.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	141	78.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	128	78.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	103	78.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	156	58.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	150	58.6	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	146	41.4	Tyr-His-Lys
118.0873	117.079	-0.001	118.0863	296	37.6	Betaine
118.0873	117.079	-0.001	118.0863	295	37.6	Betaine
118.0873	117.079	-0.001	118.0863	294	37.6	Betaine
118.0873	117.079	-0.001	118.0863	482	63.3	Betaine
118.0873	117.079	-0.001	118.0863	480	63.3	Betaine
118.0873	117.079	-0.001	118.0863	472	63.3	Betaine
118.0873	117.079	-0.001	118.0863	321	85.2	Betaine
118.0873	117.079	-0.001	118.0863	320	85.2	Betaine
118.0873	117.079	-0.001	118.0863	307	85.2	Betaine
118.0873	117.079	-0.001	118.0863	253	44.6	Betaine
118.0873	117.079	-0.001	118.0863	252	44.6	Betaine
118.0873	117.079	-0.001	118.0863	250	44.6	Betaine
186.0588	163.084	0.0149	186.0737	158	92.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	65	7.6	Ser-His-Lys
140.0692	139.027	-0.035	140.0342	120	55.4	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
140.0692	139.027	-0.035	140.0342	116	55.4	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
140.0692	139.063	0.0014	140.0706	115	44.6	3-Amino-2,3-dihydrobenzoic acid
97.0774	114.104	0.0238	97.1012	31	20.2	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	31	20.2	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	30	19.4	Cyclohexanol, 4-methyl-, trans-
224.1293	223.1	-0.022	224.107	143	100	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	134	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	221	52.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	220	52.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	210	52.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	291	95.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	277	95.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	242	95.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	278	72	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	260	72	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	252	21.6	Tyr-His-Lys
118.0873	117.079	-0.001	118.0863	421	71.1	Betaine
118.0873	117.079	-0.001	118.0863	421	71.1	Betaine

118.0873	117.079	-0.001	118.0863	416	71.1	Betaine
118.0873	117.079	-0.001	118.0863	517	67	Betaine
118.0873	117.079	-0.001	118.0863	513	67	Betaine
118.0873	117.079	-0.001	118.0863	509	67	Betaine
118.0873	117.079	-0.001	118.0863	288	67.9	Betaine
118.0873	117.079	-0.001	118.0863	287	67.9	Betaine
118.0873	117.079	-0.001	118.0863	283	67.9	Betaine
118.0873	117.079	-0.001	118.0863	373	72.5	Betaine
118.0873	117.079	-0.001	118.0863	373	72.5	Betaine
118.0873	117.079	-0.001	118.0863	363	72.5	Betaine
186.0588	163.084	0.0149	186.0737	141	85.9	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	77	14.1	Ser-His-Lys
140.0692	139.063	0.0014	140.0706	89	100	5-Amino-2-methoxyphenol
140.0692	139.063	0.0014	140.0706	85	100	5-Amino-2-methoxyphenol
140.0692	139.063	0.0014	140.0706	84	100	5-Amino-2-methoxyphenol
224.1293	223.106	-0.0164	224.1129	97	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	93	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	91	100	N-Acetyl-D-galactosaminitol
224.1293	446.228	-0.0081	224.1212	94	36.8	Tyr-His-Lys
224.1293	223.106	-0.0164	224.1129	87	28.2	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	87	28.2	N-Acetyl-D-galactosaminitol
224.1293	223.084	-0.0376	224.0917	215	87.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	205	87.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	174	87.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	273	82.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	265	82.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	249	82.7	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	435	97.3	Betaine
118.0873	117.079	-0.001	118.0863	432	97.3	Betaine
118.0873	117.079	-0.001	118.0863	421	97.3	Betaine
118.0873	117.079	-0.001	118.0863	385	97	Betaine
118.0873	117.079	-0.001	118.0863	368	97	Betaine
118.0873	117.079	-0.001	118.0863	342	97	Betaine
118.0873	117.079	-0.001	118.0863	305	73.6	Betaine
118.0873	117.079	-0.001	118.0863	296	73.6	Betaine
118.0873	117.079	-0.001	118.0863	295	73.6	Betaine
186.0588	163.084	0.0149	186.0737	122	81.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	106	81.3	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	66	15.5	Ala-Asn
186.0588	163.084	0.0149	186.0737	155	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	446.228	-0.0081	224.1212	154	45.8	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	150	38.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	148	38.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	320	94.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	306	94.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	274	94.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	137	58.6	N-Acetyl-L-tyrosine

224.1293	223.084	-0.0376	224.0917	130	58.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	130	58.6	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	188	100	Betaine
118.0873	117.079	-0.001	118.0863	4	100	Betaine
118.0873	117.079	-0.001	118.0863	3	100	Betaine
118.0873	117.079	-0.001	118.0863	426	73.8	Betaine
118.0873	117.079	-0.001	118.0863	424	73.8	Betaine
118.0873	117.079	-0.001	118.0863	405	73.8	Betaine
118.0873	117.079	-0.001	118.0863	307	74.9	Betaine
118.0873	117.079	-0.001	118.0863	301	74.9	Betaine
118.0873	117.079	-0.001	118.0863	300	74.9	Betaine
118.0873	117.079	-0.001	118.0863	450	98.7	Betaine
118.0873	117.079	-0.001	118.0863	450	98.7	Betaine
118.0873	117.079	-0.001	118.0863	448	98.7	Betaine
186.0588	163.084	0.0149	186.0737	110	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	50	25.9	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	40	18.3	Cycloheptanol
97.0774	114.104	0.0238	97.1012	38	16.9	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	30	23.8	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	21	17.3	Cycloheptanol
97.0774	114.104	0.0238	97.1012	19	15.9	Cyclohexanol, 2-methyl-, trans-
224.1293	223.1	-0.022	224.107	171	100	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	161	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	179	48.5	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	174	39.1	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	169	48.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	354	91.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	319	91.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	263	91.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	236	78.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	210	78.9	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	193	17.4	Tyr-His-Lys
118.0873	117.079	-0.001	118.0863	220	69.2	Betaine
118.0873	117.079	-0.001	118.0863	216	69.2	Betaine
118.0873	117.079	-0.001	118.0863	211	69.2	Betaine
118.0873	117.079	-0.001	118.0863	498	67.3	Betaine
118.0873	117.079	-0.001	118.0863	481	67.3	Betaine
118.0873	117.079	-0.001	118.0863	477	67.3	Betaine
118.0873	117.079	-0.001	118.0863	292	73.6	Betaine
118.0873	117.079	-0.001	118.0863	290	73.6	Betaine
118.0873	117.079	-0.001	118.0863	289	73.6	Betaine
118.0873	117.079	-0.001	118.0863	296	49.5	Betaine
118.0873	117.079	-0.001	118.0863	291	49.5	Betaine
118.0873	117.079	-0.001	118.0863	285	49.5	Betaine
186.0588	370.196	0.0467	186.1055	54	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	37	26.6	Cyclohexanol, 1-methyl-

97.0774	114.104	0.0238	97.1012	26	18.3	Cycloheptanol
97.0774	114.104	0.0238	97.1012	23	16.1	Cyclopentanemethanol, .alpha.-methyl-
224.1293	223.1	-0.022	224.107	151	100	N-Fluorenylacетamide
224.1293	223.1	-0.022	224.107	149	100	N-Fluorenylacетamide
224.1293	223.1	-0.022	224.107	147	100	N-Fluorenylacетamide
224.1293	223.084	-0.0376	224.0917	205	80.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	191	80.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	172	80.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	262	93.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	239	93.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	215	93.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	294	89.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	287	89.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	267	89.1	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	573	78	Betaine
118.0873	117.079	-0.001	118.0863	566	78	Betaine
118.0873	117.079	-0.001	118.0863	555	78	Betaine
118.0873	117.079	-0.001	118.0863	252	80.8	Betaine
118.0873	117.079	-0.001	118.0863	249	80.8	Betaine
118.0873	117.079	-0.001	118.0863	241	80.8	Betaine
118.0873	117.079	-0.001	118.0863	360	75.3	Betaine
118.0873	117.079	-0.001	118.0863	358	75.3	Betaine
118.0873	117.079	-0.001	118.0863	349	75.3	Betaine
186.0588	203.091	0.0285	186.0873	70	72.7	Ala-Asn
186.0588	163.084	0.0149	186.0737	18	14.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.095	0.0325	186.0913	15	12.8	Indole-3-butyric acid
186.0588	370.196	0.0467	186.1055	58	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	39	21.9	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	35	18.5	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	33	17.1	Cyclohexanemethanol
224.1293	223.1	-0.022	224.107	124	100	N-Fluorenylacетamide
224.1293	223.084	-0.0376	224.0917	174	47.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	168	47.6	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	168	37.5	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	311	95.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	299	95.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	262	95.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	273	86.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	252	86.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	225	86.4	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	60	83	5-Aminovaleric acid
118.0873	117.079	-0.001	118.0863	57	83	5-Aminovaleric acid
118.0873	117.079	-0.001	118.0863	51	83	5-Aminovaleric acid
118.0873	117.079	-0.001	118.0863	499	69	Betaine
118.0873	117.079	-0.001	118.0863	497	69	Betaine
118.0873	117.079	-0.001	118.0863	492	69	Betaine

118.0873	117.079	-0.001	118.0863	354	83.8	Betaine
118.0873	117.079	-0.001	118.0863	343	83.8	Betaine
118.0873	117.079	-0.001	118.0863	322	83.8	Betaine
118.0873	117.079	-0.001	118.0863	331	68.7	Betaine
118.0873	117.079	-0.001	118.0863	328	68.7	Betaine
118.0873	117.079	-0.001	118.0863	323	68.7	Betaine
186.0588	203.091	0.0285	186.0873	70	100	Ala-Asn
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	48	26.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	36	17.5	Cyclohexanol, 2-methyl-, trans-
97.0774	114.104	0.0238	97.1012	36	17.5	Cycloheptanol
97.0774	114.104	0.0238	97.1012	38	25.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	27	17.4	Cycloheptanol
97.0774	114.104	0.0238	97.1012	25	16	Cyclohexanemethanol
224.1293	223.1	-0.022	224.107	157	84	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	151	84	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	147	84	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	126	56.6	N-Acetyl-L-tyrosine
224.1293	223.106	-0.0164	224.1129	119	43.4	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	118	43.4	N-Acetyl-D-galactosaminitol
224.1293	223.084	-0.0376	224.0917	257	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	233	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	201	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	265	88.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	242	88.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	211	88.3	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	342	72.3	Betaine
118.0873	117.079	-0.001	118.0863	335	72.3	Betaine
118.0873	117.079	-0.001	118.0863	329	72.3	Betaine
118.0873	117.079	-0.001	118.0863	430	43.8	Betaine
118.0873	117.079	-0.001	118.0863	425	43.8	Betaine
118.0873	117.079	-0.001	118.0863	424	43.8	Betaine
118.0873	117.079	-0.001	118.0863	295	78.8	Betaine
118.0873	117.079	-0.001	118.0863	295	78.8	Betaine
118.0873	117.079	-0.001	118.0863	291	78.8	Betaine
118.0873	117.079	-0.001	118.0863	265	72.3	Betaine
118.0873	117.079	-0.001	118.0863	258	72.3	Betaine
118.0873	117.079	-0.001	118.0863	253	72.3	Betaine
186.0588	163.084	0.0149	186.0737	179	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	136	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	150	87.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	79	12.5	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	154	100	N,N-Bis(2-hydroxyethyl)glycine
140.0692	139	0.04	140.11	51	100	Tropinone
97.0774	114.104	0.0238	97.1012	69	20.1	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	69	20.1	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	68	19.3	Cyclohexanol, 1-methyl-

224.1293	446.228	-0.0081	224.1212	167	46.8	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	159	34.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	150	34.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	181	87.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	155	87.5	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	110	12.5	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	288	86.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	275	86.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	248	86.9	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	313	66.2	Betaine
118.0873	117.079	-0.001	118.0863	308	66.2	Betaine
118.0873	117.079	-0.001	118.0863	296	66.2	Betaine
118.0873	117.079	-0.001	118.0863	439	44.1	Betaine
118.0873	117.079	-0.001	118.0863	435	44.1	Betaine
118.0873	117.079	-0.001	118.0863	431	44.1	Betaine
118.0873	117.079	-0.001	118.0863	372	59.1	Betaine
118.0873	117.079	-0.001	118.0863	368	59.1	Betaine
118.0873	117.079	-0.001	118.0863	366	59.1	Betaine
118.0873	117.079	-0.001	118.0863	291	44	Betaine
118.0873	117.079	-0.001	118.0863	285	44	Betaine
118.0873	117.079	-0.001	118.0863	284	44	Betaine
186.0588	370.196	0.0467	186.1055	105	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	149	100	N,N-Bis(2-hydroxyethyl)glycine
140.0692	139.063	0.0014	140.0706	30	100	5-Amino-2-methoxyphenol
97.0774	114.104	0.0238	97.1012	69	23.8	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	61	17.8	Cycloheptanol
97.0774	114.104	0.0238	97.1012	60	17.1	Cyclohexanemethanol
195.1236	194.115	-0.0009	195.1227	276	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	270	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	263	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	278	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	276	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	271	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	261	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	258	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	258	100	Tetraethylene glycol
118.0873	117.079	-0.001	118.0863	246	100	Betaine
118.0873	117.079	-0.001	118.0863	243	100	Betaine
118.0873	117.079	-0.001	118.0863	235	100	Betaine
118.0873	117.079	-0.001	118.0863	443	34.9	Betaine
118.0873	117.079	-0.001	118.0863	439	34.9	Betaine
118.0873	117.079	-0.001	118.0863	439	34.9	Betaine
118.0873	117.079	-0.001	118.0863	372	100	Betaine
118.0873	117.079	-0.001	118.0863	369	100	Betaine
118.0873	117.079	-0.001	118.0863	365	100	Betaine
118.0873	117.079	-0.001	118.0863	264	75.6	Betaine
118.0873	117.079	-0.001	118.0863	262	75.6	Betaine

118.0873	117.079	-0.001	118.0863	256	75.6	Betaine
186.0588	163.084	0.0149	186.0737	132	80.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	95	19.6	Ala-Asn
186.0588	163.084	0.0149	186.0737	56	80.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	150	91.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	96	91.4	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	66	8.6	Ala-Asn
186.0588	370.196	0.0467	186.1055	54	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	176	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	223.1	-0.022	224.107	143	83.1	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	138	83.1	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	134	83.1	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	160	45.6	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	157	40.3	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	150	45.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	165	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	158	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	137	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	312	94.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	293	94.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	257	94.2	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	558	97.9	Betaine
118.0873	117.079	-0.001	118.0863	548	97.9	Betaine
118.0873	117.079	-0.001	118.0863	541	97.9	Betaine
118.0873	117.079	-0.001	118.0863	235	76.5	Betaine
118.0873	117.079	-0.001	118.0863	233	76.5	Betaine
118.0873	117.079	-0.001	118.0863	223	76.5	Betaine
118.0873	117.079	-0.001	118.0863	270	70.2	Betaine
118.0873	117.079	-0.001	118.0863	268	70.2	Betaine
118.0873	117.079	-0.001	118.0863	266	70.2	Betaine
186.0588	163.084	0.0149	186.0737	167	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	96	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	223.084	-0.0376	224.0917	233	71	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	225	71	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	203	19.7	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	302	96	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	266	96	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	219	96	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	267	81	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	253	81	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	227	81	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	485	44.5	Betaine
118.0873	117.079	-0.001	118.0863	484	44.5	Betaine
118.0873	117.079	-0.001	118.0863	480	44.5	Betaine
118.0873	117.079	-0.001	118.0863	259	81	Betaine
118.0873	117.079	-0.001	118.0863	255	81	Betaine
118.0873	117.079	-0.001	118.0863	245	81	Betaine

118.0873	117.079	-0.001	118.0863	397	67.4	Betaine
118.0873	117.079	-0.001	118.0863	394	67.4	Betaine
118.0873	117.079	-0.001	118.0863	392	67.4	Betaine
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	159	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	70	26.2	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	61	19.1	Cycloheptanol
97.0774	114.104	0.0238	97.1012	53	14.2	Cyclohexanol, 2-methyl-, trans-
224.1293	446.228	-0.0081	224.1212	131	57.9	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	122	42.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	121	42.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	321	94.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	311	94.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	299	94.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	221	77.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	210	77.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	198	77.8	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	329	55.9	Betaine
118.0873	117.079	-0.001	118.0863	324	55.9	Betaine
118.0873	117.079	-0.001	118.0863	317	55.9	Betaine
118.0873	117.079	-0.001	118.0863	501	70.4	Betaine
118.0873	117.079	-0.001	118.0863	496	70.4	Betaine
118.0873	117.079	-0.001	118.0863	485	70.4	Betaine
118.0873	117.079	-0.001	118.0863	275	75.2	Betaine
118.0873	117.079	-0.001	118.0863	269	75.2	Betaine
118.0873	117.079	-0.001	118.0863	267	75.2	Betaine
118.0873	117.079	-0.001	118.0863	280	73.1	Betaine
118.0873	117.079	-0.001	118.0863	278	73.1	Betaine
118.0873	117.079	-0.001	118.0863	274	73.1	Betaine
186.0588	370.196	0.0467	186.1055	68	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	155	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	46	23.7	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	37	17.2	Cycloheptanol
97.0774	114.104	0.0238	97.1012	35	15.9	Cyclohexanol, 4-methyl-, trans-
224.1293	223.1	-0.022	224.107	133	100	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	128	100	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	126	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	146	54.5	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	139	41.8	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	133	54.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	213	91.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	207	91.4	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	129	8.6	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	192	76.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	178	76.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	162	76.3	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	306	77	Betaine

118.0873	117.079	-0.001	118.0863	299	77	Betaine
118.0873	117.079	-0.001	118.0863	292	77	Betaine
118.0873	117.079	-0.001	118.0863	445	63.7	Betaine
118.0873	117.079	-0.001	118.0863	443	63.7	Betaine
118.0873	117.079	-0.001	118.0863	433	63.7	Betaine
118.0873	117.079	-0.001	118.0863	232	62.8	Betaine
118.0873	117.079	-0.001	118.0863	232	62.8	Betaine
118.0873	117.079	-0.001	118.0863	227	62.8	Betaine
118.0873	117.079	-0.001	118.0863	237	69.5	Betaine
118.0873	117.079	-0.001	118.0863	236	69.5	Betaine
118.0873	117.079	-0.001	118.0863	231	69.5	Betaine
186.0588	203.091	0.0285	186.0873	68	100	Ala-Asn
186.0588	370.196	0.0467	186.1055	66	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	133	100	N,N-Bis(2-hydroxyethyl)glycine
140.0692	139.063	0.0014	140.0706	59	52	5-Amino-2-methoxyphenol
140.0692	139.1	0.038	140.107	57	48	Tropinone
140.0692	139.1	0.038	140.107	55	48	Tropinone
224.1293	446.228	-0.0081	224.1212	102	68.9	Tyr-His-Lys
224.1293	446.228	-0.0081	224.1212	72	19.1	Tyr-His-Lys
224.1293	446.228	-0.0081	224.1212	58	12	Tyr-His-Lys
224.1293	223.1	-0.022	224.107	133	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	173	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	155	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	126	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	346	94.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	331	94.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	307	94.3	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	485	43	Betaine
118.0873	117.079	-0.001	118.0863	478	43	Betaine
118.0873	117.079	-0.001	118.0863	473	43	Betaine
118.0873	117.079	-0.001	118.0863	236	72.2	Betaine
118.0873	117.079	-0.001	118.0863	236	72.2	Betaine
118.0873	117.079	-0.001	118.0863	231	72.2	Betaine
118.0873	117.079	-0.001	118.0863	267	42.2	Betaine
118.0873	117	0	118.09	261	33.2	Betaine
118.0873	117.079	-0.001	118.0863	260	42.2	Betaine
186.0588	163.084	0.0149	186.0737	153	92.1	N,N-Bis(2-hydroxyethyl)glycine
186.0588	370.196	0.0467	186.1055	63	7.9	Ser-His-Lys
140.0692	139.027	-0.035	140.0342	19	100	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
140.0692	139.027	-0.035	140.0342	10	100	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
140.0692	139.027	-0.035	140.0342	7	100	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
140.0692	139.027	-0.035	140.0342	80	100	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-

140.0692	139.027	-0.035	140.0342	79	100	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
140.0692	139.027	-0.035	140.0342	78	100	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
97.0774	114.104	0.0238	97.1012	134	45.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	131	40	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	108	14.6	Cyclopentanemethanol, .alpha.-methyl-
195.1236	194.115	-0.0009	195.1227	279	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	278	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	276	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	281	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	279	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	278	100	Tetraethylene glycol
118.0873	117.079	-0.001	118.0863	262	83.6	Betaine
118.0873	117.079	-0.001	118.0863	261	83.6	Betaine
118.0873	117.079	-0.001	118.0863	253	83.6	Betaine
118.0873	117.079	-0.001	118.0863	491	65.7	Betaine
118.0873	117.079	-0.001	118.0863	487	65.7	Betaine
118.0873	117.079	-0.001	118.0863	479	65.7	Betaine
118.0873	117.079	-0.001	118.0863	227	69.4	Betaine
118.0873	117.079	-0.001	118.0863	227	69.4	Betaine
118.0873	117.079	-0.001	118.0863	222	69.4	Betaine
118.0873	117.079	-0.001	118.0863	310	63.7	Betaine
118.0873	117.079	-0.001	118.0863	305	63.7	Betaine
118.0873	117.079	-0.001	118.0863	299	63.7	Betaine
186.0588	370.196	0.0467	186.1055	55	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	157	100	N,N-Bis(2-hydroxyethyl)glycine
140.0692	139.063	0.0014	140.0706	27	100	5-Amino-2-methoxyphenol
97.0774	114.104	0.0238	97.1012	44	25.9	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	42	23.9	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	35	25.9	Cyclohexanemethanol
224.1293	223.1	-0.022	224.107	139	100	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	133	100	N-Fluorenylacetamide
224.1293	223.1	-0.022	224.107	126	100	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	199	50.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	188	50.3	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	186	32.5	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	287	97.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	263	97.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	220	97.4	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	298	89.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	279	89.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	256	89.9	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	414	90	Betaine
118.0873	117.079	-0.001	118.0863	411	90	Betaine

118.0873	117.079	-0.001	118.0863	398	90	Betaine
118.0873	117.079	-0.001	118.0863	459	41.6	Betaine
118.0873	117.079	-0.001	118.0863	458	41.6	Betaine
118.0873	117.079	-0.001	118.0863	450	41.6	Betaine
118.0873	117.079	-0.001	118.0863	331	98.8	Betaine
118.0873	117.079	-0.001	118.0863	318	98.8	Betaine
118.0873	117.079	-0.001	118.0863	297	98.8	Betaine
118.0873	117.079	-0.001	118.0863	221	73.2	Betaine
118.0873	117.079	-0.001	118.0863	218	73.2	Betaine
118.0873	117.079	-0.001	118.0863	213	73.2	Betaine
186.0588	370.196	0.0467	186.1055	74	100	Ser-His-Lys
186.0588	163.084	0.0149	186.0737	131	100	N,N-Bis(2-hydroxyethyl)glycine
140.0692	139.1	0.038	140.107	38	100	Tropinone
140.0692	139.1	0.038	140.107	37	100	Tropinone
140.0692	139.1	0.038	140.107	36	100	Tropinone
224.1293	223.084	-0.0376	224.0917	178	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	170	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	167	100	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	161	45	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	160	45	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	157	45	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	362	96.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	347	96.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	305	96.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	308	90.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	293	90.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	254	90.6	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	361	28.4	Betaine
118.0873	117.079	-0.001	118.0863	358	28.4	Betaine
118.0873	117	0	118.09	357	24	Betaine
118.0873	117.079	-0.001	118.0863	441	72.7	Betaine
118.0873	117.079	-0.001	118.0863	433	72.7	Betaine
118.0873	117.079	-0.001	118.0863	423	72.7	Betaine
118.0873	117.079	-0.001	118.0863	354	85.7	Betaine
118.0873	117.079	-0.001	118.0863	354	85.7	Betaine
118.0873	117.079	-0.001	118.0863	342	85.7	Betaine
118.0873	117.079	-0.001	118.0863	433	64.6	Betaine
118.0873	117.079	-0.001	118.0863	431	64.6	Betaine
118.0873	117.079	-0.001	118.0863	421	64.6	Betaine
186.0588	163.084	0.0149	186.0737	137	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	90	44.5	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	80	31.4	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	73	24.1	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	39	22.1	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	37	20.4	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	34	18	Cyclohexanol, 1-methyl-

97.0774	114.104	0.0238	97.1012	21	32.3	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	14	24.7	Cycloheptanol
97.0774	114.104	0.0238	97.1012	12	22.8	Cyclohexanol, 4-methyl-, trans-
224.1293	223.084	-0.0376	224.0917	230	46.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	230	46.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	226	46.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	274	89.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	269	89.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	253	89.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	209	89.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	192	89.6	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	163	89.6	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	331	59.8	Betaine
118.0873	117.079	-0.001	118.0863	321	59.8	Betaine
118.0873	117.079	-0.001	118.0863	314	59.8	Betaine
118.0873	117.079	-0.001	118.0863	532	67.2	Betaine
118.0873	117.079	-0.001	118.0863	524	67.2	Betaine
118.0873	117.079	-0.001	118.0863	511	67.2	Betaine
118.0873	117.079	-0.001	118.0863	286	76.1	Betaine
118.0873	117.079	-0.001	118.0863	282	76.1	Betaine
118.0873	117.079	-0.001	118.0863	276	76.1	Betaine
118.0873	117.079	-0.001	118.0863	234	65	Betaine
118.0873	117.079	-0.001	118.0863	232	65	Betaine
118.0873	117.079	-0.001	118.0863	231	65	Betaine
186.0588	203.091	0.0285	186.0873	75	76.9	Ala-Asn
186.0588	163.084	0.0149	186.0737	29	16.2	N,N-Bis(2-hydroxyethyl)glycine
186.0588	168.042	0.0173	186.0761	8	6.9	3-Hydroxy-4-methoxybenzoic acid
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	152	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	223.106	-0.0164	224.1129	82	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	81	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	81	100	N-Acetyl-D-galactosaminitol
224.1293	223.084	-0.0376	224.0917	174	54.2	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	170	45.8	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	167	54.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	267	91.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	236	91.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	196	91.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	173	68.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	165	68.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	160	68.1	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	220	100	Betaine
118.0873	117.079	-0.001	118.0863	215	100	Betaine
118.0873	117.079	-0.001	118.0863	214	100	Betaine
118.0873	117.079	-0.001	118.0863	416	55.2	Betaine
118.0873	117.079	-0.001	118.0863	415	55.2	Betaine

118.0873	117.079	-0.001	118.0863	413	55.2	Betaine
118.0873	117.079	-0.001	118.0863	256	69.3	Betaine
118.0873	117.079	-0.001	118.0863	255	69.3	Betaine
118.0873	117.079	-0.001	118.0863	251	69.3	Betaine
118.0873	117.079	-0.001	118.0863	296	73.5	Betaine
118.0873	117.079	-0.001	118.0863	293	73.5	Betaine
118.0873	117.079	-0.001	118.0863	291	73.5	Betaine
140.0692	139.063	0.0014	140.0706	40	100	5-Amino-2-methoxyphenol
140.0692	139.063	0.0014	140.0706	33	100	5-Amino-2-methoxyphenol
140.0692	139.063	0.0014	140.0706	28	100	5-Amino-2-methoxyphenol
186.0588	163.084	0.0149	186.0737	89	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	140	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	24	33.6	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	18	26.4	Cycloheptanol
97.0774	114.104	0.0238	97.1012	13	21.3	Cyclohexanol, 4-methyl-, trans-
195.1236	194.115	-0.0009	195.1227	345	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	340	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	334	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	297	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	295	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	294	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	266	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	266	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	266	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	266	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	263	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	262	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	259	100	Tetraethylene glycol
118.0873	117.079	-0.001	118.0863	237	97.7	Betaine
118.0873	117.079	-0.001	118.0863	234	97.7	Betaine
118.0873	117.079	-0.001	118.0863	224	97.7	Betaine
118.0873	117.079	-0.001	118.0863	569	74.2	Betaine
118.0873	117.079	-0.001	118.0863	561	74.2	Betaine
118.0873	117.079	-0.001	118.0863	555	74.2	Betaine
118.0873	117.079	-0.001	118.0863	306	76.3	Betaine
118.0873	117.079	-0.001	118.0863	304	76.3	Betaine
118.0873	117.079	-0.001	118.0863	293	76.3	Betaine
118.0873	117.079	-0.001	118.0863	449	85.8	Betaine
118.0873	117.079	-0.001	118.0863	448	85.8	Betaine
118.0873	117.079	-0.001	118.0863	445	85.8	Betaine
186.0588	163.084	0.0149	186.0737	137	76.6	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	122	76.6	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	103	19.6	Ala-Asn
97.0774	114.104	0.0238	97.1012	30	24.5	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	22	18.3	Cycloheptanol
97.0774	114.104	0.0238	97.1012	18	15.4	Cyclohexanol, 2-methyl-, trans-
118.0873	117.079	-0.001	118.0863	278	60.5	Betaine
118.0873	117.079	-0.001	118.0863	271	60.5	Betaine

118.0873	117.079	-0.001	118.0863	270	60.5	Betaine
118.0873	117.079	-0.001	118.0863	490	47	Betaine
118.0873	117.079	-0.001	118.0863	483	47	Betaine
118.0873	117.079	-0.001	118.0863	480	47	Betaine
118.0873	117.079	-0.001	118.0863	424	98.2	Betaine
118.0873	117.079	-0.001	118.0863	420	98.2	Betaine
118.0873	117.079	-0.001	118.0863	415	98.2	Betaine
118.0873	117.079	-0.001	118.0863	316	74.8	Betaine
118.0873	117.079	-0.001	118.0863	316	74.8	Betaine
118.0873	117.079	-0.001	118.0863	313	74.8	Betaine
186.0588	163.084	0.0149	186.0737	141	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	26	58.6	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	20	58.6	Cyclohexanemethanol
97.0774	114.104	0.0238	97.1012	16	41.4	Cyclopentanemethanol, .alpha.-methyl-
97.0774	114.104	0.0238	97.1012	25	33.6	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	19	26.4	Cycloheptanol
97.0774	114.104	0.0238	97.1012	14	21.3	Cyclohexanol, 4-methyl-, trans-
224.1293	223.084	-0.0376	224.0917	184	55.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	165	55.3	N-Acetyl-L-tyrosine
224.1293	223.1	-0.022	224.107	162	21.8	N-Fluorenylacetamide
224.1293	223.084	-0.0376	224.0917	300	92.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	268	92.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	234	92.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	259	83.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	243	83.3	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	216	83.3	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	306	70.4	Betaine
118.0873	117.079	-0.001	118.0863	301	70.4	Betaine
118.0873	117.079	-0.001	118.0863	285	70.4	Betaine
118.0873	117.079	-0.001	118.0863	542	75.2	Betaine
118.0873	117.079	-0.001	118.0863	536	75.2	Betaine
118.0873	117.079	-0.001	118.0863	525	75.2	Betaine
118.0873	117.079	-0.001	118.0863	361	94.6	Betaine
118.0873	117.079	-0.001	118.0863	342	94.6	Betaine
118.0873	117.079	-0.001	118.0863	310	94.6	Betaine
118.0873	117.079	-0.001	118.0863	399	63.6	Betaine
118.0873	117.079	-0.001	118.0863	398	63.6	Betaine
118.0873	117.079	-0.001	118.0863	396	63.6	Betaine
186.0588	163.084	0.0149	186.0737	153	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	223.1	-0.022	224.107	134	93.1	N-Fluorenylacetamide
224.1293	241.117	-0.0151	224.1142	34	6.9	(6R)-5,6,7,8-Tetrahydrobiopterin
224.1293	223.084	-0.0376	224.0917	152	45.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	150	45.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	149	45.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	269	92.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	262	92.8	N-Acetyl-L-tyrosine

224.1293	223.084	-0.0376	224.0917	229	92.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	275	87	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	251	87	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	224	87	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	369	63	Betaine
118.0873	117.079	-0.001	118.0863	362	63	Betaine
118.0873	117.079	-0.001	118.0863	350	63	Betaine
118.0873	117.079	-0.001	118.0863	492	67.8	Betaine
118.0873	117.079	-0.001	118.0863	491	67.8	Betaine
118.0873	117.079	-0.001	118.0863	480	67.8	Betaine
118.0873	117.079	-0.001	118.0863	405	95.2	Betaine
118.0873	117.079	-0.001	118.0863	375	95.2	Betaine
118.0873	117.079	-0.001	118.0863	347	95.2	Betaine
118.0873	117.079	-0.001	118.0863	299	67.6	Betaine
118.0873	117.079	-0.001	118.0863	298	67.6	Betaine
118.0873	117.079	-0.001	118.0863	296	67.6	Betaine
186.0588	163.084	0.0149	186.0737	174	100	N,N-Bis(2-hydroxyethyl)glycine
140.0692	139.063	0.0014	140.0706	78	59.3	3-Amino-2,3-dihydrobenzoic acid
140.0692	139.027	-0.035	140.0342	67	40.7	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
140.0692	139.027	-0.035	140.0342	58	40.7	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
97.0774	114.104	0.0238	97.1012	18	100	Cyclohexanemethanol
195.1236	194.115	-0.0009	195.1227	139	92.3	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	133	92.3	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	128	92.3	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	332	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	332	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	328	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	263	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	262	100	Tetraethylene glycol
195.1236	194.115	-0.0009	195.1227	261	100	Tetraethylene glycol
118.0873	117.079	-0.001	118.0863	325	69.7	Betaine
118.0873	117.079	-0.001	118.0863	320	69.7	Betaine
118.0873	117.079	-0.001	118.0863	311	69.7	Betaine
118.0873	117.079	-0.001	118.0863	459	57.5	Betaine
118.0873	117.079	-0.001	118.0863	457	57.5	Betaine
118.0873	117.079	-0.001	118.0863	455	57.5	Betaine
118.0873	117.079	-0.001	118.0863	322	61.6	Betaine
118.0873	117.079	-0.001	118.0863	317	61.6	Betaine
118.0873	117.079	-0.001	118.0863	317	61.6	Betaine
118.0873	117.079	-0.001	118.0863	313	64.9	Betaine
118.0873	117.079	-0.001	118.0863	306	64.9	Betaine
118.0873	117.079	-0.001	118.0863	303	64.9	Betaine
140.0692	139.1	0.038	140.107	131	100	Tropinone
140.0692	139.1	0.038	140.107	129	100	Tropinone

140.0692	139.1	0.038	140.107	126	100	Tropinone
186.0588	370.196	0.0467	186.1055	87	100	Ser-His-Lys
97.0774	114.104	0.0238	97.1012	47	20.6	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	45	20.6	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	43	17.4	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	22	32	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	16	25.2	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	16	25.2	Cyclohexanol, 4-methyl-, trans-
224.1293	446.228	-0.0081	224.1212	162	50.8	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	157	41	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	140	41	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	259	88.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	243	88.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	220	88.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	268	80.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	244	80.1	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	222	16.9	Tyr-His-Lys
118.0873	117.079	-0.001	118.0863	254	89.1	Betaine
118.0873	117.079	-0.001	118.0863	244	89.1	Betaine
118.0873	117.079	-0.001	118.0863	242	89.1	Betaine
118.0873	117.079	-0.001	118.0863	465	98.4	Betaine
118.0873	117.079	-0.001	118.0863	458	98.4	Betaine
118.0873	117.079	-0.001	118.0863	449	98.4	Betaine
118.0873	117.079	-0.001	118.0863	215	72.5	Betaine
118.0873	117.079	-0.001	118.0863	210	72.5	Betaine
118.0873	117.079	-0.001	118.0863	204	72.5	Betaine
118.0873	117.079	-0.001	118.0863	374	66.6	Betaine
118.0873	117.079	-0.001	118.0863	371	66.6	Betaine
118.0873	117.079	-0.001	118.0863	366	66.6	Betaine
186.0588	163.084	0.0149	186.0737	159	100	N,N-Bis(2-hydroxyethyl)glycine
140.0692	139.063	0.0014	140.0706	94	55.3	3-Amino-2,3-dihydrobenzoic acid
140.0692	139.063	0.0014	140.0706	75	26.8	5-Amino-2-methoxyphenol
140.0692	139.027	-0.035	140.0342	63	17.9	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
224.1293	241.117	-0.0151	224.1142	25	100	(6R)-5,6,7,8-Tetrahydrobiopterin
224.1293	223.1	-0.022	224.107	101	41.3	N-Fluorenylacetamide
224.1293	446.228	-0.0081	224.1212	98	36.5	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	83	22.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	336	97.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	329	97.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	292	97.5	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	301	91.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	288	91.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	252	91.2	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	469	97.8	Betaine
118.0873	117.079	-0.001	118.0863	467	97.8	Betaine

118.0873	117.079	-0.001	118.0863	463	97.8	Betaine
118.0873	117.079	-0.001	118.0863	355	98.6	Betaine
118.0873	117.079	-0.001	118.0863	350	98.6	Betaine
118.0873	117.079	-0.001	118.0863	336	98.6	Betaine
118.0873	117.079	-0.001	118.0863	333	75.7	Betaine
118.0873	117.079	-0.001	118.0863	330	75.7	Betaine
118.0873	117.079	-0.001	118.0863	328	75.7	Betaine
186.0588	163.084	0.0149	186.0737	110	100	N,N-Bis(2-hydroxyethyl)glycine
186.0588	163.084	0.0149	186.0737	102	100	N,N-Bis(2-hydroxyethyl)glycine
97.0774	114.104	0.0238	97.1012	38	23.9	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	28	16.9	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	28	16.9	Cycloheptanol
97.0774	114.104	0.0238	97.1012	44	19.2	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	44	19.2	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	41	17	Cyclopentanemethanol, .alpha.-methyl-
224.1293	223.106	-0.0164	224.1129	121	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	114	100	N-Acetyl-D-galactosaminitol
224.1293	223.106	-0.0164	224.1129	108	100	N-Acetyl-D-galactosaminitol
224.1293	223.084	-0.0376	224.0917	151	49.2	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	150	47.3	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	141	49.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	261	93	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	248	93	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	219	93	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	230	90.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	206	90.7	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	169	90.7	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	278	100	Betaine
118.0873	117.079	-0.001	118.0863	272	100	Betaine
118.0873	117.079	-0.001	118.0863	259	100	Betaine
118.0873	117.079	-0.001	118.0863	479	67.2	Betaine
118.0873	117.079	-0.001	118.0863	473	67.2	Betaine
118.0873	117.079	-0.001	118.0863	468	67.2	Betaine
118.0873	117.079	-0.001	118.0863	364	77	Betaine
118.0873	117.079	-0.001	118.0863	362	77	Betaine
118.0873	117.079	-0.001	118.0863	359	77	Betaine
118.0873	117.079	-0.001	118.0863	178	61.7	Betaine
118.0873	117.079	-0.001	118.0863	177	61.7	Betaine
118.0873	117.079	-0.001	118.0863	172	61.7	Betaine
186.0588	163.084	0.0149	186.0737	86	54.5	N,N-Bis(2-hydroxyethyl)glycine
186.0588	203.091	0.0285	186.0873	70	31.4	Ala-Asn
186.0588	168.042	0.0173	186.0761	16	6.1	3-Hydroxy-4-methoxybenzoic acid
186.0588	163.084	0.0149	186.0737	158	100	N,N-Bis(2-hydroxyethyl)glycine
224.1293	446.228	-0.0081	224.1212	123	67.9	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	79	14.7	N-Acetyl-L-tyrosine

224.1293	223.106	-0.0164	224.1129	77	13.6	N-Acetyl-D-galactosaminitol
224.1293	223.084	-0.0376	224.0917	307	97.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	286	97.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	242	97.2	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	214	61.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	198	61.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	196	61.1	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	227	81.1	Betaine
118.0873	117.079	-0.001	118.0863	226	81.1	Betaine
118.0873	117.079	-0.001	118.0863	224	81.1	Betaine
118.0873	117.079	-0.001	118.0863	475	66.8	Betaine
118.0873	117.079	-0.001	118.0863	472	66.8	Betaine
118.0873	117.079	-0.001	118.0863	467	66.8	Betaine
118.0873	117.079	-0.001	118.0863	320	83.8	Betaine
118.0873	117.079	-0.001	118.0863	317	83.8	Betaine
118.0873	117.079	-0.001	118.0863	312	83.8	Betaine
118.0873	117.079	-0.001	118.0863	231	39	Betaine
118.0873	117	0	118.09	228	34.5	Betaine
118.0873	117.079	-0.001	118.0863	225	39	Betaine
186.0588	370.196	0.0467	186.1055	41	100	Ser-His-Lys
140.0692	139.063	0.0014	140.0706	41	100	5-Amino-2-methoxyphenol
140.0692	139.063	0.0014	140.0706	89	56.6	3-Amino-2,3-dihydrobenzoic acid
140.0692	139.027	-0.035	140.0342	82	43.4	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
140.0692	139.027	-0.035	140.0342	75	43.4	3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-
97.0774	114.104	0.0238	97.1012	40	23.5	Cyclohexanol, 1-methyl-
97.0774	114.104	0.0238	97.1012	34	18.5	Cyclohexanol, 4-methyl-, trans-
97.0774	114.104	0.0238	97.1012	31	16.3	Cycloheptanol
224.1293	223.084	-0.0376	224.0917	185	70.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	168	70.9	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	166	70.9	N-Acetyl-L-tyrosine
224.1293	446.228	-0.0081	224.1212	95	76.9	Tyr-His-Lys
224.1293	223.084	-0.0376	224.0917	69	23.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	276	97.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	263	97.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	227	97.1	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	304	90.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	282	90.8	N-Acetyl-L-tyrosine
224.1293	223.084	-0.0376	224.0917	248	90.8	N-Acetyl-L-tyrosine
118.0873	117.079	-0.001	118.0863	390	70.2	Betaine
118.0873	117.079	-0.001	118.0863	389	70.2	Betaine
118.0873	117.079	-0.001	118.0863	382	70.2	Betaine
118.0873	117.079	-0.001	118.0863	527	70.7	Betaine
118.0873	117.079	-0.001	118.0863	522	70.7	Betaine
118.0873	117.079	-0.001	118.0863	516	70.7	Betaine

118.0873	117.079	-0.001	118.0863	305	85.4	Betaine
118.0873	117.079	-0.001	118.0863	305	85.4	Betaine
118.0873	117.079	-0.001	118.0863	292	85.4	Betaine
118.0873	117.079	-0.001	118.0863	265	54	Betaine
118.0873	117.079	-0.001	118.0863	263	54	Betaine
118.0873	117.079	-0.001	118.0863	260	54	Betaine

Table A8. List of non-volatile metabolites (LC/MS) for managed population animals. Samples collected in Dec 2011 from multiple animals were pooled. Experiment was conducted using specialized lipids fraction protocol on RP column (refer to Materials and Methods section) in negative ion mode. Only top match is given for each compound.

Parent m/z	Mass	Delta (m/z)	Library Precursor m/z	Match Score	Probability (%)	Chem ID
187.0432	186.046	0.0104	187.0536	195	86.	Carbimazole
187.0432	186.046	0.0104	187.0536	190	87.	Carbimazole
311.1692	310.193	0.0314	311.2006	40	10	Cannabinol
311.1692	310.193	0.0314	311.2006	45	10	Mestranol
311.1692	310.193	0.0314	311.2006	45	10	Mestranol
311.1692	310.193	0.0314	311.2006	34	10	Mestranol
297.153	296.178	0.0319	297.1849	17	10	5,8,11,14-Eicosatetraynoic acid
309.1749	310.181	-8E-04	309.1741	214	21.	(Oxyethylene)lauryl sulfate
309.1749	310.181	-8E-04	309.1741	209	58.	(Oxyethylene)lauryl sulfate
325.1848	324.184	0.0063	325.1911	46	10	Quinine
325.1848	324.184	0.0063	325.1911	53	10	Quinine
325.1848	324.184	0.0063	325.1911	52	10	Quinine
325.1848	326.192	-5E-04	325.1843	129	90.	Dodecylbenzenesulfonic acid
325.1848	324.184	0.0063	325.1911	40	10	Quinine
325.1848	324.184	0.0063	325.1911	27	10	Quinine
325.1848	324.184	0.0063	325.1911	41	10	Quinine
325.1848	324.184	0.0063	325.1911	36	10	Quinine
325.1848	324.184	0.0063	325.1911	50	10	Quinine
325.1848	324.184	0.0063	325.1911	31	10	Quinine
311.1692	310.193	0.0314	311.2006	60	10	Mestranol
311.1692	310.193	0.0314	311.2006	60	10	Mestranol
311.1692	310.193	0.0314	311.2006	31	10	Mestranol
325.1848	324.184	0.0063	325.1911	37	10	Quinine
325.1848	324.184	0.0063	325.1911	32	10	Quinine
325.1848	324.184	0.0063	325.1911	82	10	Quinine
311.1692	310.116	-0.045	311.1238	50	10	.alpha.-L-Glu-L-Tyr
325.1848	324.184	0.0063	325.1911	45	10	Quinine
325.1848	324.184	0.0063	325.1911	18	10	Quinine
325.1848	324.184	0.0063	325.1911	39	10	Quinine
325.1848	324.184	0.0063	325.1911	51	73.	Quinine
325.1848	324.184	0.0063	325.1911	59	10	Quinine
325.1848	324.184	0.0063	325.1911	38	10	Quinine
325.1848	324.184	0.0063	325.1911	37	10	Quinine
325.1848	324.184	0.0063	325.1911	66	59.	Quinine
325.1848	324.184	0.0063	325.1911	45	10	Quinine
325.1848	324.184	0.0063	325.1911	40	10	Quinine
325.1848	324.184	0.0063	325.1911	50	10	Quinine
325.1848	324.184	0.0063	325.1911	63	10	Quinine

325.1848	324.184	0.0063	325.1911	35	100	Quinine
311.1692	310.116	-0.045	311.1238	48	100	.alpha.-L-Glu-L-Tyr
283.2642	282.256	-0.001	283.2632	25	54.2	6-Octadecenoic acid, (Z)-
283.2642	282.256	-0.001	283.2632	26	100	6-Octadecenoic acid, (Z)-
325.1848	324.184	0.0063	325.1911	67	100	Quinine
325.1848	324.184	0.0063	325.1911	57	100	Quinine
325.1848	324.184	0.0063	325.1911	54	100	Quinine
325.1848	324.184	0.0063	325.1911	48	100	Quinine
311.1692	310.193	0.0314	311.2006	56	100	Mestranol
311.1692	312.176	-6E-04	311.1686	38	100	Benzenesulfonic acid, 4-undecyl-
311.1692	310.193	0.0314	311.2006	20	100	Mestranol
325.1848	324.184	0.0063	325.1911	57	100	Quinine
325.1848	324.184	0.0063	325.1911	46	100	Quinine
325.1848	324.184	0.0063	325.1911	44	100	Quinine
325.1848	324.184	0.0063	325.1911	47	100	Quinine
325.1848	324.184	0.0063	325.1911	49	100	Quinine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	43	100	Quinine
325.1848	324.184	0.0063	325.1911	54	100	Quinine
325.1848	324.184	0.0063	325.1911	32	100	Quinine
325.1848	324.184	0.0063	325.1911	34	100	Quinine
325.1848	324.184	0.0063	325.1911	30	100	Quinine
325.1848	324.184	0.0063	325.1911	65	100	Quinine
325.1848	324.184	0.0063	325.1911	39	100	Quinine
325.1848	324.184	0.0063	325.1911	79	100	Quinine
311.1692	310.116	-0.045	311.1238	39	59.3	.alpha.-L-Glu-L-Tyr
112.9862	112.027	0.0484	113.0346	97	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	186	100	4,6-Dihydroxypyrimidine
311.1692	310.148	-0.014	311.1554	37	100	Desmethylocitalopram
311.1692	310.193	0.0314	311.2006	50	100	Mestranol
325.1848	324.184	0.0063	325.1911	52	100	Quinine
325.1848	324.184	0.0063	325.1911	55	100	Quinine
325.1848	324.184	0.0063	325.1911	40	100	Quinine
325.1848	324.184	0.0063	325.1911	72	100	Quinine
311.1692	310.193	0.0314	311.2006	17	100	Mestranol
112.9862	112.027	0.0484	113.0346	74	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	124	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	89	100	4,6-Dihydroxypyrimidine
112.9862	130.027	0.0371	113.0233	191	95.7	Butanedioic acid, methylene-
325.1848	324.184	0.0063	325.1911	27	100	Quinine
325.1848	324.184	0.0063	325.1911	62	100	Quinine
325.1848	324.184	0.0063	325.1911	51	100	Quinine
112.9862	112.027	0.0484	113.0346	70	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	60	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	84	100	4,6-Dihydroxypyrimidine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	55	100	Quinine

325.1848	324.184	0.0063	325.1911	36	100	Quinine
325.1848	324.184	0.0063	325.1911	58	100	Quinine
112.9862	112.027	0.0484	113.0346	93	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	60	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	85	100	4,6-Dihydroxypyrimidine
311.1692	310.193	0.0314	311.2006	40	100	Mestranol
112.9862	112.027	0.0484	113.0346	96	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	100	100	4,6-Dihydroxypyrimidine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	59	100	Quinine
325.1848	324.184	0.0063	325.1911	59	100	Quinine
325.1848	324.184	0.0063	325.1911	42	100	Quinine
112.9862	112.027	0.0484	113.0346	106	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	94	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	78	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	97	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	108	100	4,6-Dihydroxypyrimidine
112.9862	130.027	0.0371	113.0233	146	100	Butanedioic acid, methylene-
112.9862	112.027	0.0484	113.0346	95	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	103	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	81	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	89	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	218	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	120	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	80	100	4,6-Dihydroxypyrimidine

Table A9. List of non-volatile metabolites (LC/MS) for managed population animals. Samples collected in Dec 2011 from multiple animals were pooled. Experiment was conducted using specialized lipids fraction protocol on RP column (refer to Materials and Methods section) in negative ion mode. Top three matches are given for each compound.

Parent m/z	Mass	Delta (m/z)	Library Precurs or m/z	Match Score	Probability (%)	Chem ID
187.0432	186.046	0.0104	187.0536	195	86.1	Carbimazole
187.0432	186.046	0.0104	187.0536	130	13.9	Ethyl 2-amino-4-methylthiazole-5-carboxylate
187.0432	186.046	0.0104	187.0536	127	13.9	Ethyl 2-amino-4-methylthiazole-5-carboxylate
187.0432	186.046	0.0104	187.0536	190	87.3	Carbimazole
187.0432	186.046	0.0104	187.0536	178	87.3	Carbimazole
187.0432	186.046	0.0104	187.0536	120	12.7	Ethyl 2-amino-4-methylthiazole-5-carboxylate
311.1692	310.193	0.0314	311.2006	40	100	Cannabinol
311.1692	310.193	0.0314	311.2006	45	100	Mestranol
311.1692	310.193	0.0314	311.2006	33	100	Mestranol
311.1692	310.193	0.0314	311.2006	45	100	Mestranol
311.1692	310.193	0.0314	311.2006	34	100	Mestranol
311.1692	310.193	0.0314	311.2006	29	100	Mestranol
311.1692	310.193	0.0314	311.2006	23	100	Mestranol
297.153	296.178	0.0319	297.1849	17	100	5,8,11,14-Eicosatetraynoic acid
309.1749	310.181	-0.0008	309.1741	214	21.9	(Oxyethylene)lauryl sulfate
309.1749	310.181	-0.0008	309.1741	199	13.3	(Oxyethylene)lauryl sulfate
309.1749	310.181	-0.0008	309.1741	198	12.8	(Oxyethylene)lauryl sulfate
309.1749	310.181	-0.0008	309.1741	209	58.1	(Oxyethylene)lauryl sulfate
309.1749	310.181	-0.0008	309.1741	175	14.9	(Oxyethylene)lauryl sulfate
309.1749	310.181	-0.0008	309.1741	174	14.3	(Oxyethylene)lauryl sulfate
325.1848	324.184	0.0063	325.1911	46	100	Quinine
325.1848	324.184	0.0063	325.1911	44	100	Quinine
325.1848	324.184	0.0063	325.1911	42	100	Quinine
325.1848	324.184	0.0063	325.1911	53	100	Quinine
325.1848	324.184	0.0063	325.1911	52	100	Quinine
325.1848	324.184	0.0063	325.1911	51	100	Quinine
325.1848	324.184	0.0063	325.1911	52	100	Quinine
325.1848	324.184	0.0063	325.1911	25	100	Quinine
325.1848	326.192	-0.0005	325.1843	129	90.4	Dodecylbenzenesulfonic acid
325.1848	324.184	0.0063	325.1911	48	9.6	Quinine
325.1848	324.184	0.0063	325.1911	47	9.6	Quinine
325.1848	324.184	0.0063	325.1911	40	100	Quinine
325.1848	324.184	0.0063	325.1911	40	100	Quinine
325.1848	324.184	0.0063	325.1911	39	100	Quinine
325.1848	324.184	0.0063	325.1911	27	100	Quinine

325.1848	324.184	0.0063	325.1911	41	100	Quinine
325.1848	324.184	0.0063	325.1911	36	100	Quinine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	32	100	Quinine
325.1848	324.184	0.0063	325.1911	50	100	Quinine
325.1848	324.184	0.0063	325.1911	49	100	Quinine
325.1848	324.184	0.0063	325.1911	48	100	Quinine
325.1848	324.184	0.0063	325.1911	31	100	Quinine
311.1692	310.193	0.0314	311.2006	60	100	Mestranol
311.1692	310.193	0.0314	311.2006	52	100	Mestranol
311.1692	310.193	0.0314	311.2006	60	100	Mestranol
311.1692	310.193	0.0314	311.2006	31	100	Mestranol
311.1692	310.193	0.0314	311.2006	29	100	Mestranol
311.1692	310.193	0.0314	311.2006	26	100	Mestranol
325.1848	324.184	0.0063	325.1911	37	100	Quinine
325.1848	324.184	0.0063	325.1911	34	100	Quinine
325.1848	324.184	0.0063	325.1911	32	100	Quinine
325.1848	324.184	0.0063	325.1911	32	100	Quinine
325.1848	324.184	0.0063	325.1911	31	100	Quinine
325.1848	324.184	0.0063	325.1911	30	100	Quinine
325.1848	324.184	0.0063	325.1911	82	100	Quinine
325.1848	324.184	0.0063	325.1911	80	100	Quinine
325.1848	324.184	0.0063	325.1911	78	100	Quinine
311.1692	310.116	-0.0454	311.1238	50	100	.alpha.-L-Glu-L-Tyr
325.1848	324.184	0.0063	325.1911	45	100	Quinine
325.1848	324.184	0.0063	325.1911	45	100	Quinine
325.1848	324.184	0.0063	325.1911	43	100	Quinine
325.1848	324.184	0.0063	325.1911	18	100	Quinine
325.1848	324.184	0.0063	325.1911	17	100	Quinine
325.1848	324.184	0.0063	325.1911	16	100	Quinine
325.1848	324.184	0.0063	325.1911	39	100	Quinine
325.1848	324.184	0.0063	325.1911	37	100	Quinine
325.1848	324.184	0.0063	325.1911	34	100	Quinine
325.1848	324.184	0.0063	325.1911	51	73.2	Quinine
325.1848	324.184	0.0063	325.1911	50	73.2	Quinine
325.1848	324.184	0.0063	325.1911	47	73.2	Quinine
325.1848	324.184	0.0063	325.1911	59	100	Quinine
325.1848	324.184	0.0063	325.1911	53	100	Quinine
325.1848	324.184	0.0063	325.1911	51	100	Quinine
325.1848	324.184	0.0063	325.1911	38	100	Quinine
325.1848	324.184	0.0063	325.1911	37	100	Quinine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	37	100	Quinine
325.1848	324.184	0.0063	325.1911	36	100	Quinine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	66	59.3	Quinine
325.1848	324.184	0.0063	325.1911	64	59.3	Quinine

325.1848	324.184	0.0063	325.1911	64	59.3	Quinine
325.1848	324.184	0.0063	325.1911	45	100	Quinine
325.1848	324.184	0.0063	325.1911	43	100	Quinine
325.1848	324.184	0.0063	325.1911	38	100	Quinine
325.1848	324.184	0.0063	325.1911	40	100	Quinine
325.1848	324.184	0.0063	325.1911	37	100	Quinine
325.1848	324.184	0.0063	325.1911	32	100	Quinine
325.1848	324.184	0.0063	325.1911	50	100	Quinine
325.1848	324.184	0.0063	325.1911	48	100	Quinine
325.1848	324.184	0.0063	325.1911	47	100	Quinine
325.1848	324.184	0.0063	325.1911	63	100	Quinine
325.1848	324.184	0.0063	325.1911	62	100	Quinine
325.1848	324.184	0.0063	325.1911	62	100	Quinine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
311.1692	310.116	-0.0454	311.1238	48	100	.alpha.-L-Glu-L-Tyr
283.2642	282.256	-0.001	283.2632	25	54.2	6-Octadecenoic acid, (Z)-
283.2642	282.256	-0.001	283.2632	21	45.8	Elaidic acid
283.2642	282.256	-0.001	283.2632	26	100	6-Octadecenoic acid, (Z)-
325.1848	324.184	0.0063	325.1911	67	100	Quinine
325.1848	324.184	0.0063	325.1911	66	100	Quinine
325.1848	324.184	0.0063	325.1911	65	100	Quinine
325.1848	324.184	0.0063	325.1911	57	100	Quinine
325.1848	324.184	0.0063	325.1911	53	100	Quinine
325.1848	324.184	0.0063	325.1911	47	100	Quinine
325.1848	324.184	0.0063	325.1911	54	100	Quinine
325.1848	324.184	0.0063	325.1911	52	100	Quinine
325.1848	324.184	0.0063	325.1911	51	100	Quinine
325.1848	324.184	0.0063	325.1911	48	100	Quinine
325.1848	324.184	0.0063	325.1911	46	100	Quinine
325.1848	324.184	0.0063	325.1911	44	100	Quinine
311.1692	310.193	0.0314	311.2006	56	100	Mestranol
311.1692	310.193	0.0314	311.2006	51	100	Mestranol
311.1692	310.193	0.0314	311.2006	48	100	Mestranol
311.1692	312.176	-0.0006	311.1686	38	100	Benzenesulfonic acid, 4-undecyl-
311.1692	310.193	0.0314	311.2006	20	100	Mestranol
325.1848	324.184	0.0063	325.1911	57	100	Quinine
325.1848	324.184	0.0063	325.1911	55	100	Quinine
325.1848	324.184	0.0063	325.1911	53	100	Quinine
325.1848	324.184	0.0063	325.1911	46	100	Quinine
325.1848	324.184	0.0063	325.1911	45	100	Quinine
325.1848	324.184	0.0063	325.1911	41	100	Quinine
325.1848	324.184	0.0063	325.1911	44	100	Quinine
325.1848	324.184	0.0063	325.1911	47	100	Quinine
325.1848	324.184	0.0063	325.1911	43	100	Quinine
325.1848	324.184	0.0063	325.1911	42	100	Quinine
325.1848	324.184	0.0063	325.1911	49	100	Quinine

325.1848	324.184	0.0063	325.1911	47	100	Quinine
325.1848	324.184	0.0063	325.1911	44	100	Quinine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	43	100	Quinine
325.1848	324.184	0.0063	325.1911	40	100	Quinine
325.1848	324.184	0.0063	325.1911	39	100	Quinine
325.1848	324.184	0.0063	325.1911	54	100	Quinine
325.1848	324.184	0.0063	325.1911	53	100	Quinine
325.1848	324.184	0.0063	325.1911	51	100	Quinine
325.1848	324.184	0.0063	325.1911	32	100	Quinine
325.1848	324.184	0.0063	325.1911	32	100	Quinine
325.1848	324.184	0.0063	325.1911	28	100	Quinine
325.1848	324.184	0.0063	325.1911	34	100	Quinine
325.1848	324.184	0.0063	325.1911	30	100	Quinine
325.1848	324.184	0.0063	325.1911	28	100	Quinine
325.1848	324.184	0.0063	325.1911	26	100	Quinine
325.1848	324.184	0.0063	325.1911	65	100	Quinine
325.1848	324.184	0.0063	325.1911	63	100	Quinine
325.1848	324.184	0.0063	325.1911	58	100	Quinine
325.1848	324.184	0.0063	325.1911	39	100	Quinine
325.1848	324.184	0.0063	325.1911	39	100	Quinine
325.1848	324.184	0.0063	325.1911	38	100	Quinine
325.1848	324.184	0.0063	325.1911	79	100	Quinine
325.1848	324.184	0.0063	325.1911	76	100	Quinine
325.1848	324.184	0.0063	325.1911	76	100	Quinine
311.1692	310.116	-0.0454	311.1238	39	59.3	.alpha.-L-Glu-L-Tyr
311.1692	310.193	0.0314	311.2006	28	40.7	Mestranol
112.9862	112.027	0.0484	113.0346	97	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	96	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	93	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	186	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	166	100	4,6-Dihydroxypyrimidine
311.1692	310.148	-0.0138	311.1554	37	100	Desmethylcitalopram
311.1692	310.193	0.0314	311.2006	50	100	Mestranol
325.1848	324.184	0.0063	325.1911	52	100	Quinine
325.1848	324.184	0.0063	325.1911	52	100	Quinine
325.1848	324.184	0.0063	325.1911	51	100	Quinine
325.1848	324.184	0.0063	325.1911	55	100	Quinine
325.1848	324.184	0.0063	325.1911	54	100	Quinine
325.1848	324.184	0.0063	325.1911	49	100	Quinine
325.1848	324.184	0.0063	325.1911	40	100	Quinine
325.1848	324.184	0.0063	325.1911	72	100	Quinine
311.1692	310.193	0.0314	311.2006	17	100	Mestranol
112.9862	112.027	0.0484	113.0346	74	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	73	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	72	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	124	100	4,6-Dihydroxypyrimidine

112.9862	112.027	0.0484	113.0346	120	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	115	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	89	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	87	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	86	100	4,6-Dihydroxypyrimidine
112.9862	130.027	0.0371	113.0233	191	95.7	Butanedioic acid, methylene-
112.9862	130.027	0.0371	113.0233	173	95.7	Butanedioic acid, methylene-
112.9862	130.027	0.0371	113.0233	172	95.7	Butanedioic acid, methylene-
325.1848	324.184	0.0063	325.1911	27	100	Quinine
325.1848	324.184	0.0063	325.1911	24	100	Quinine
325.1848	324.184	0.0063	325.1911	23	100	Quinine
325.1848	324.184	0.0063	325.1911	62	100	Quinine
325.1848	324.184	0.0063	325.1911	61	100	Quinine
325.1848	324.184	0.0063	325.1911	61	100	Quinine
325.1848	324.184	0.0063	325.1911	51	100	Quinine
112.9862	112.027	0.0484	113.0346	70	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	69	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	68	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	60	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	59	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	58	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	84	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	82	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	82	100	4,6-Dihydroxypyrimidine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	55	100	Quinine
325.1848	324.184	0.0063	325.1911	36	100	Quinine
325.1848	324.184	0.0063	325.1911	58	100	Quinine
325.1848	324.184	0.0063	325.1911	56	100	Quinine
325.1848	324.184	0.0063	325.1911	55	100	Quinine
112.9862	112.027	0.0484	113.0346	93	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	89	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	60	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	59	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	57	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	85	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	82	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	79	100	4,6-Dihydroxypyrimidine
311.1692	310.193	0.0314	311.2006	40	100	Mestranol
112.9862	112.027	0.0484	113.0346	96	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	95	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	92	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	100	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	100	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	96	100	4,6-Dihydroxypyrimidine

325.1848	324.184	0.0063	325.1911	35	100	Quinine
325.1848	324.184	0.0063	325.1911	30	100	Quinine
325.1848	324.184	0.0063	325.1911	27	100	Quinine
325.1848	324.184	0.0063	325.1911	59	100	Quinine
325.1848	324.184	0.0063	325.1911	57	100	Quinine
325.1848	324.184	0.0063	325.1911	55	100	Quinine
325.1848	324.184	0.0063	325.1911	59	100	Quinine
325.1848	324.184	0.0063	325.1911	58	100	Quinine
325.1848	324.184	0.0063	325.1911	57	100	Quinine
325.1848	324.184	0.0063	325.1911	42	100	Quinine
112.9862	112.027	0.0484	113.0346	106	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	94	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	93	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	88	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	78	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	76	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	71	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	97	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	95	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	95	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	108	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	108	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	103	100	4,6-Dihydroxypyrimidine
112.9862	130.027	0.0371	113.0233	146	100	Butanedioic acid, methylene-
112.9862	130.027	0.0371	113.0233	129	100	Butanedioic acid, methylene-
112.9862	112.027	0.0484	113.0346	95	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	90	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	90	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	103	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	102	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	94	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	81	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	79	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	78	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	89	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	87	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	83	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	218	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	215	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	203	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	120	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	119	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	109	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	80	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	79	100	4,6-Dihydroxypyrimidine
112.9862	112.027	0.0484	113.0346	75	100	4,6-Dihydroxypyrimidine

Table A10. List of non-volatile metabolites (LC/MS) for wild population animals. Sample was pooled from multiple animals (FB246, FB127, F268, F242, F142 collected in May 2011, 2012). Experiment was conducted using specialized lipids fraction protocol on RP column (refer to Materials and Methods section) in positive ion mode. Only top match is given for each compound.

Parent m/z	Mass	Delta (m/z)	Library Precursor m/z	Match Score	Probability (%)	Chem ID
170.1251	187.121	-0.0075	170.1176	397	76	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	51	100	Leu-Trp-Arg
400.3206	400.343	0.0215	400.3421	163	21	Palmitoyl-L-carnitine cation
170.1251	187.121	-0.0075	170.1176	386	61	7-Keto-8-aminopelargonic acid
461.3108	460.28	-0.0237	461.2871	52	100	Trp-Lys-Lys
472.291	471.314	0.03	472.321	74	100	Terfenadine
170.1251	187.121	-0.0075	170.1176	378	72	7-Keto-8-aminopelargonic acid
400.3206	400.343	0.0215	400.3421	110	10	Palmitoyl-L-carnitine cation
472.291	471.314	0.03	472.321	108	100	Terfenadine
400.3206	400.343	0.0215	400.3421	76	57	Palmitoyl-L-carnitine cation
170.1251	187.121	-0.0075	170.1176	394	78	7-Keto-8-aminopelargonic acid
370.2484	369.288	0.0468	370.2952	279	20	N-Oleoyl-L-serine
414.2746	413.239	-0.0287	414.2459	84	100	PyroGlu-Arg-Lys
472.291	471.314	0.03	472.321	102	100	Terfenadine
170.1251	187.121	-0.0075	170.1176	367	45	7-Keto-8-aminopelargonic acid
655.4667	654.492	0.0324	655.4991	112	38	Deca(propylene glycol) monobutyl ether
516.3205	515.292	-0.0216	516.2989	69	100	Taurocholic acid
170.1251	169.085	-0.0327	170.0924	452	49	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	36	55	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	420	75	7-Keto-8-aminopelargonic acid
400.3206	400.343	0.0215	400.3421	112	42	Palmitoyl-L-carnitine cation
516.3205	515.292	-0.0216	516.2989	74	100	Taurocholic acid
170.1251	187.121	-0.0075	170.1176	351	57	7-Keto-8-aminopelargonic acid
472.291	471.314	0.03	472.321	162	100	Terfenadine
461.2688	461	-0.04	461.23	6	27	PA 17:0; [M+Na] ⁺ ; GPA(4:0/13:0)
516.3205	515.292	-0.0216	516.2989	59	100	Taurocholic acid
472.291	471.314	0.03	472.321	111	100	Terfenadine
414.2891	449.314	0.0112	414.3003	98	100	Glycodeoxycholic acid
472.291	471.314	0.03	472.321	150	100	Terfenadine

516.3205	515.292	-0.0216	516.2989	269	100	Taurocholic acid
472.3318	471.314	-0.011	472.321	181	100	Terfenadine
170.14	169.085	-0.0476	170.0924	221	53.7	L-Histidine, 3-methyl-
391.2847	390.277	-0.0005	391.2843	89	51.2	Bis(2-ethylhexyl) phthalate
419.3154	418.308	0.0002	419.3156	196	100	1,2-Benzenedicarboxylic acid, dinonyl ester
149.0233	166.027	0	149.0233	451	99	1,2-Benzenedicarboxylic acid
311.1646	310.193	0.036	311.2006	99	67.9	Mestranol
279.159	278.152	0.0001	279.1591	235	96.3	Dibutyl phthalate
516.3205	515.292	-0.0216	516.2989	261	100	Taurocholic acid
170.135	187.121	-0.0174	170.1176	346	66.5	7-Keto-8-aminopelargonic acid
399.2511	398.243	-0.0005	399.2506	236	100	Tris(butoxyethyl) phosphate
163.0749	179.095	0.0005	163.0754	250	75.1	3,4-Methylenedioxyamphetamine
516.3205	515.292	-0.0216	516.2989	261	100	Taurocholic acid
472.291	471.314	0.03	472.321	281	100	Terfenadine
387.1826	386	-0.05	387.13	229	23.8	1-O-b-D-glucopyranosyl sinapate
267.172	266.165	0	267.172	221	99	Tributyl phosphate
458.3056	435.281	-0.0357	458.2699	90	100	N-Acetyl-S-geranylgeranyl-L-cysteine
391.2847	390.277	-0.0005	391.2843	142	49.7	Diocetyl phthalate
404.2083	403.207	0.006	404.214	55	8.7	Glu-Gln-Lys
474.2907	473.275	-0.0084	474.2823	107	68.4	Leu-Trp-Arg
170.1251	169.085	-0.0327	170.0924	332	34.4	L-Histidine, 1-methyl-
518.3165	495.332	0.0052	518.3217	89	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
516.3205	515.292	-0.0216	516.2989	172	100	Taurocholic acid
170.1251	187.121	-0.0075	170.1176	373	68.1	7-Keto-8-aminopelargonic acid
472.291	471.314	0.03	472.321	197	100	Terfenadine
279.0943	278.086	-0.0009	279.0933	30	100	Triphenylphosphine oxide
387.1826	386	-0.05	387.13	241	22.8	1-O-b-D-glucopyranosyl sinapate
288.2521	287.196	-0.049	288.203	122	26.1	Leu-Arg
516.3205	515.292	-0.0216	516.2989	199	100	Taurocholic acid
474.2907	473.275	-0.0084	474.2823	180	62.2	Leu-Trp-Arg
655.4667	654.492	0.0324	655.4991	198	19.8	Deca(propylene glycol) monobutyl ether
170.1251	187.121	-0.0075	170.1176	383	71.5	7-Keto-8-aminopelargonic acid
370.2484	369.288	0.0468	370.2952	295	18.9	N-Oleoyl-L-serine
249.1125	249.139	0.0261	249.1386	217	69.6	1H-Pyrazolium, 1,2-dimethyl-3,5-diphenyl-

207.157	206.152	0.0021	207.1591	350	78.9	Tri(propylene glycol) methyl ether
496.417	495.369	-0.0408	496.3762	145	100	2-O-Methyl PAF C-16
414.2891	449.314	0.0112	414.3003	269	95	Glycodeoxycholic acid
472.291	471.314	0.03	472.321	55	100	Terfenadine
170.1122	187.121	0.0054	170.1176	415	71	7-Keto-8-aminopelargonic acid
655.4943	654.492	0.0048	655.4991	249	20.2	Deca(propylene glycol) monobutyl ether
170.1251	187.121	-0.0075	170.1176	419	70.6	7-Keto-8-aminopelargonic acid
472.3318	471.314	-0.011	472.321	102	100	Terfenadine
655.4667	654.492	0.0324	655.4991	141	52	Deca(propylene glycol) monobutyl ether
472.3318	471.314	-0.011	472.321	63	100	Terfenadine
516.3205	515.292	-0.0216	516.2989	79	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	140	100	Taurocholic acid
170.1122	169.085	-0.0198	170.0924	346	45.1	L-Histidine, 1-methyl-
472.3318	471.314	-0.011	472.321	192	100	Terfenadine
516.3205	515.292	-0.0216	516.2989	130	100	Taurocholic acid
170.1122	169.085	-0.0198	170.0924	354	58.9	L-Histidine, 3-methyl-
170.1251	169.085	-0.0327	170.0924	342	68.3	L-Histidine, 3-methyl-
206.1384	223.106	-0.0361	206.1023	157	76.7	N-Acetyl-D-galactosaminitol
114.091	113.059	-0.0248	114.0662	308	28.3	Creatinine
414.2891	413	0.05	414.34	191	100	Solasodine
474.2907	473.275	-0.0084	474.2823	84	62.3	Trp-Ile-Arg
328.1988	327.147	-0.0445	328.1543	81	39.3	Naloxone
516.3205	515.292	-0.0216	516.2989	274	100	Taurocholic acid
370.2484	369.288	0.0468	370.2952	192	16.9	N-Oleoyl-L-serine
472.3318	471.314	-0.011	472.321	109	100	Terfenadine
461.2688	460.28	0.0183	461.2871	61	100	Trp-Lys-Lys
206.1384	223.106	-0.0361	206.1023	227	96.4	N-Acetyl-D-galactosaminitol
474.2907	473.275	-0.0084	474.2823	133	34	Leu-Trp-Arg
422.2707	421.233	-0.0309	422.2398	101	39.7	Gln-Phe-Lys
370.2484	369.288	0.0468	370.2952	147	15.1	N-Oleoyl-L-serine
414.259	449.314	0.0413	414.3003	258	96.6	Glycodeoxycholic acid
518.3165	495.332	0.0052	518.3217	49	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
461.2688	460.243	-0.0181	461.2507	127	22.6	Trp-Gln-Lys
422.2573	421.233	-0.0175	422.2398	129	25.6	Phe-Gln-Lys
458.3056	435.281	-0.0357	458.2699	64	100	N-Acetyl-S-geranylgeranyl-L-cysteine
239.141	239	0.04	239.18	7	37.6	MG 9:0; [M+Li]+; MG(9:0/0:0/0:0)

169.0621	169	0.05	169.11	55	71	MG 4:0; [M+Li]+; MG(4:0/0:0/0:0)
458.3056	435.281	-0.0357	458.2699	100	100	N-Acetyl-S-geranylgeranyl-L-cysteine
422.2345	421.269	0.0417	422.2762	32	100	Phe-Lys-Lys
461.2688	460.243	-0.0181	461.2507	151	20.4	Trp-Gln-Lys
472.291	471.314	0.03	472.321	82	100	Terfenadine
370.2484	369.288	0.0468	370.2952	114	20.4	N-Oleoyl-L-serine
195.1223	194.115	0.0004	195.1227	305	100	Tetraethylene glycol
516.3205	515.292	-0.0216	516.2989	97	100	Taurocholic acid
170.1251	169.085	-0.0327	170.0924	386	51.7	L-Histidine, 1-methyl-
244.1904	226.193	0.0367	244.2271	494	98.2	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
226.1797	225.136	-0.0359	226.1438	157	73.3	3,4,5-TrimethoxyAmphetamine
474.2907	473.275	-0.0084	474.2823	44	33.5	Ile-Trp-Arg
472.291	471.314	0.03	472.321	77	100	Terfenadine
370.2484	369.288	0.0468	370.2952	107	16.6	N-Oleoyl-L-serine
414.259	413.202	-0.0494	414.2096	38	100	PyroGlu-Gln-Arg
422.2417	421.233	-0.0019	422.2398	98	26.6	Gln-Phe-Lys
474.2907	473.275	-0.0084	474.2823	58	48.6	Ile-Trp-Arg
518.3165	495.332	0.0052	518.3217	69	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
195.1223	194.115	0.0004	195.1227	356	99	Tetraethylene glycol
244.1904	226.193	0.0367	244.2271	393	97.4	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
474.2907	473.275	-0.0084	474.2823	84	35.2	Ile-Trp-Arg
518.3165	495.332	0.0052	518.3217	74	55.4	1-Hexadecanoyl-sn-glycero-3-phosphocholine
370.2484	370	-0.04	370.21	111	40.2	MGDG 7:0; [M+NH4-CO]+; MGDG(3:0/4:0)
239.1487	238.099	-0.043	239.106	26	100	4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid
137.0453	136.039	0.0005	137.0458	386	91.9	Hypoxanthine
474.2907	473.275	-0.0084	474.2823	100	68.7	Ile-Trp-Arg
370.2484	370	-0.04	370.21	133	14.6	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
655.4667	654.492	0.0324	655.4991	130	43.4	Deca(propylene glycol)monobutyl ether
474.2907	473.275	-0.0084	474.2823	59	100	Leu-Trp-Arg
472.291	471.314	0.03	472.321	105	100	Terfenadine
414.2746	449.314	0.0257	414.3003	70	100	Glycodeoxycholic acid
787.6688	786.661	0	787.6688	54	100	N-Docosanoyl-4-sphingenyl-1-O-phosphorylcholine
139.0503	138.043	-0.0001	139.0502	596	80.3	4-Imidazoleacrylic acid
414.259	449.314	0.0413	414.3003	121	100	Glycodeoxycholic acid

170.1444	169.085	-0.052	170.0924	358	47.4	L-Histidine, 3-methyl-
638.6067	638	-0.04	638.57	122	36.6	DG 36:2; [M+NH ₄] ⁺ ; DG(14:1/22:1/0:0)
402.2682	401.278	0.017	402.285	24	100	Myriocin
474.2907	473.275	-0.0084	474.2823	60	37.8	Leu-Trp-Arg
170.14	187.121	-0.0224	170.1176	205	60	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	260	59.6	L-Histidine, 1-methyl-
458.3056	435.281	-0.0357	458.2699	44	100	N-Acetyl-S-geranylgeranyl-L- cysteine
474.2907	473.275	-0.0084	474.2823	52	43.1	Trp-Ile-Arg
170.1251	169.085	-0.0327	170.0924	237	75.8	L-Histidine, 3-methyl-
474.2907	473.275	-0.0084	474.2823	67	56.2	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	48	56.7	Leu-Trp-Arg
458.3056	435.281	-0.0357	458.2699	11	100	N-Acetyl-S-geranylgeranyl-L- cysteine
400.355	400.343	-0.0129	400.3421	36	18.8	Palmitoyl-L-carnitine cation
437.2353	436.207	-0.021	437.2143	94	100	Phe-Asp-Arg
170.1251	187.121	-0.0075	170.1176	11	50	7-Keto-8-aminopelargonic acid
655.4667	654.492	0.0324	655.4991	247	27.6	Deca(propylene glycol) monobutyl ether
170.1251	187.121	-0.0075	170.1176	105	27.5	7-Keto-8-aminopelargonic acid
400.3206	400.343	0.0215	400.3421	15	100	Palmitoyl-L-carnitine cation
170.1251	169.085	-0.0327	170.0924	262	41.6	L-Histidine, 1-methyl-
343.2943	408.288	-0.03	343.2643	17	100	Cholic acid
170.135	187.121	-0.0174	170.1176	190	36.4	7-Keto-8-aminopelargonic acid
461.2453	460.243	0.0054	461.2507	62	37.5	Trp-Gln-Lys
170.1251	169.085	-0.0327	170.0924	218	38.8	L-Histidine, 3-methyl-
787.6248	786.661	0.044	787.6688	211	18.6	N-Docosanoyl-4-sphingeny-1- O-phosphorylcholine
461.2688	230.152	0.0421	461.3109	30	100	Dodecanedioic acid
170.135	187.121	-0.0174	170.1176	236	37	7-Keto-8-aminopelargonic acid
655.4667	654.492	0.0324	655.4991	129	41.9	Deca(propylene glycol) monobutyl ether
461.2904	230.163	0.043	461.3334	189	93.4	Leu-Val
655.4667	654.492	0.0324	655.4991	124	37.2	Deca(propylene glycol) monobutyl ether
400.3206	400.343	0.0215	400.3421	149	8.9	Palmitoyl-L-carnitine cation
170.14	187.121	-0.0224	170.1176	341	56.5	7-Keto-8-aminopelargonic acid
400.3206	400.343	0.0215	400.3421	343	16.5	Palmitoyl-L-carnitine cation
655.4667	654.492	0.0324	655.4991	113	38.1	Deca(propylene glycol) monobutyl ether

695.4097	672.473	0.0525	695.4622	14	100	1-Hexadecanoyl-2-(9Z,12Z-octadecadienyl)-sn-glycero-3-phosphoric acid
170.1444	187.121	-0.0268	170.1176	120	46.6	7-Keto-8-aminopelargonic acid
695.4097	672.473	0.0525	695.4622	31	100	1-Hexadecanoyl-2-(9Z,12Z-octadecadienyl)-sn-glycero-3-phosphoric acid
400.3206	400.343	0.0215	400.3421	197	10	Palmitoyl-L-carnitine cation
343.2827	342.256	-0.0195	343.2632	93	100	Retinyl propionate
400.3206	400.343	0.0215	400.3421	302	12.5	Palmitoyl-L-carnitine cation
170.1251	187.121	-0.0075	170.1176	68	25.6	7-Keto-8-aminopelargonic acid
472.291	471.314	0.03	472.321	47	100	Terfenadine
458.3056	435.281	-0.0357	458.2699	65	100	N-Acetyl-S-geranylgeranyl-L-cysteine
414.2891	413	0.05	414.34	28	100	Solasodine
474.2907	473.275	-0.0084	474.2823	24	100	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	81	23.3	7-Keto-8-aminopelargonic acid
414.259	413.239	-0.0131	414.2459	40	29.8	PyroGlu-Lys-Arg
458.3056	435.281	-0.0357	458.2699	30	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.3056	435.281	-0.0357	458.2699	51	100	N-Acetyl-S-geranylgeranyl-L-cysteine
414.2746	449.314	0.0257	414.3003	50	100	Glycodeoxycholic acid
474.2907	473.275	-0.0084	474.2823	58	50.9	Leu-Trp-Arg
518.3165	495.332	0.0052	518.3217	92	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
474.2907	473.275	-0.0084	474.2823	46	100	Leu-Trp-Arg
458.3056	435.281	-0.0357	458.2699	64	100	N-Acetyl-S-geranylgeranyl-L-cysteine
474.2907	473.275	-0.0084	474.2823	87	27.5	Ile-Trp-Arg
170.1251	169	-0.04	170.09	278	32.5	3-Methyl-L-histidine
474.2907	473.275	-0.0084	474.2823	27	30.1	Leu-Trp-Arg
655.4667	654.492	0.0324	655.4991	145	45.5	Deca(propylene glycol) monobutyl ether
170.1251	187.121	-0.0075	170.1176	31	23.4	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	53	64.7	Leu-Trp-Arg
170.1251	187.121	-0.0075	170.1176	50	25.9	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	23	100	Leu-Trp-Arg
170.1251	187.121	-0.0075	170.1176	71	36.4	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	59	19.8	Ile-Trp-Arg

170.1251	187.121	-0.0075	170.1176	133	46.7	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	75	24.5	7-Keto-8-aminopelargonic acid
422.2573	421.269	0.0189	422.2762	25	100	Phe-Lys-Lys
170.1251	187.121	-0.0075	170.1176	113	32.2	7-Keto-8-aminopelargonic acid
472.261	471.223	-0.0307	472.2303	66	100	PyroGlu-Trp-Arg
458.3056	435.281	-0.0357	458.2699	80	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	90	39	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	61	100	Ile-Trp-Arg
458.2695	435.281	0.0004	458.2699	35	100	N-Acetyl-S-geranylgeranyl-L-cysteine
518.277	495.332	0.0447	518.3217	60	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
458.3056	435.281	-0.0357	458.2699	33	100	N-Acetyl-S-geranylgeranyl-L-cysteine
474.2449	473.275	0.0374	474.2823	68	38.8	Trp-Ile-Arg
515.3745	246.211	0.0373	515.4117	29	100	Dodecyldimethylphosphine oxide
170.1251	187.121	-0.0075	170.1176	124	37.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	129	38.4	7-Keto-8-aminopelargonic acid
515.3601	246.211	0.0516	515.4117	44	100	Dodecyldimethylphosphine oxide
474.2449	473.275	0.0374	474.2823	101	67.3	Trp-Ile-Arg
458.2695	435.281	0.0004	458.2699	67	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	169	39.6	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	90	48.2	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	187	49.9	7-Keto-8-aminopelargonic acid
458.2578	435.281	0.0121	458.2699	132	100	N-Acetyl-S-geranylgeranyl-L-cysteine
474.2907	473.275	-0.0084	474.2823	77	56	Trp-Ile-Arg
518.3165	495.332	0.0052	518.3217	72	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
170.1251	187.121	-0.0075	170.1176	196	53	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	146	33.3	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	48	100	Ile-Trp-Arg
400.3206	400.343	0.0215	400.3421	36	56	Palmitoyl-L-carnitine cation

458.3056	435.281	-0.0357	458.2699	66	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	194	46.8	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	143	40.3	7-Keto-8-aminopelargonic acid
458.2403	435.281	0.0296	458.2699	85	79.3	N-Acetyl-S-geranylgeranyl-L-cysteine
400.3206	401.278	-0.0501	400.2705	60	73.2	Myriocin
170.1251	187.121	-0.0075	170.1176	204	65.7	7-Keto-8-aminopelargonic acid
458.3056	435.281	-0.0357	458.2699	58	100	N-Acetyl-S-geranylgeranyl-L-cysteine
655.4667	654.492	0.0324	655.4991	107	45.9	Deca(propylene glycol) monobutyl ether
170.1251	187.121	-0.0075	170.1176	122	38.5	7-Keto-8-aminopelargonic acid
414.259	413.202	-0.0494	414.2096	115	49.9	PyroGlu-Gln-Arg
370.2484	370	-0.04	370.21	205	41.3	MGDG 7:0; [M+NH ₄ -CO] ⁺ ; MGDG(2:0/5:0)
343.2757	342.256	-0.0125	343.2632	109	56.3	Retinyl propionate
170.1251	187.121	-0.0075	170.1176	201	48.4	7-Keto-8-aminopelargonic acid
518.3165	495.332	0.0052	518.3217	83	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
458.3056	435.281	-0.0357	458.2699	46	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	142	59.5	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	59	36.5	Leu-Trp-Arg
458.3056	435.281	-0.0357	458.2699	48	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	156	48.5	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	50	40.2	Ile-Trp-Arg
458.3056	435.281	-0.0357	458.2699	39	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	221	52	7-Keto-8-aminopelargonic acid
414.259	413.202	-0.0494	414.2096	75	100	PyroGlu-Gln-Arg
458.3056	435.281	-0.0357	458.2699	56	100	N-Acetyl-S-geranylgeranyl-L-cysteine
474.2907	473.275	-0.0084	474.2823	39	100	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	215	62.3	7-Keto-8-aminopelargonic acid
400.3206	401.278	-0.0501	400.2705	48	44.7	Myriocin

170.1251	187.121	-0.0075	170.1176	192	59.3	7-Keto-8-aminopelargonic acid
518.3165	495.332	0.0052	518.3217	133	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
170.1251	187.121	-0.0075	170.1176	227	50.4	7-Keto-8-aminopelargonic acid
458.3056	435.281	-0.0357	458.2699	65	100	N-Acetyl-S-geranylgeranyl-L-cysteine
400.3206	400.343	0.0215	400.3421	38	100	Palmitoyl-L-carnitine cation
170.1251	187.121	-0.0075	170.1176	248	45.4	7-Keto-8-aminopelargonic acid
518.3165	495.332	0.0052	518.3217	64	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
170.135	187.121	-0.0174	170.1176	175	41.8	7-Keto-8-aminopelargonic acid
400.3206	400.343	0.0215	400.3421	82	37	Palmitoyl-L-carnitine cation
414.2746	413.239	-0.0287	414.2459	75	35.7	PyroGlu-Lys-Arg
414.2746	413.239	-0.0287	414.2459	49	39	PyroGlu-Lys-Arg
170.1251	187.121	-0.0075	170.1176	235	62.2	7-Keto-8-aminopelargonic acid
343.2873	408.288	-0.0231	343.2643	45	100	Cholic acid
414.2746	413.239	-0.0287	414.2459	101	68.7	PyroGlu-Lys-Arg
170.135	187.121	-0.0174	170.1176	219	47.1	7-Keto-8-aminopelargonic acid
458.3056	435.281	-0.0357	458.2699	58	100	N-Acetyl-S-geranylgeranyl-L-cysteine
518.3165	495.332	0.0052	518.3217	63	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
400.3206	400.343	0.0215	400.3421	87	25.1	Palmitoyl-L-carnitine cation
474.2907	473.275	-0.0084	474.2823	32	100	Ile-Trp-Arg
170.1251	169.085	-0.0327	170.0924	166	36.4	L-Histidine, 1-methyl-
343.2757	342.256	-0.0125	343.2632	95	100	Retinyl propionate
458.3056	435.281	-0.0357	458.2699	76	100	N-Acetyl-S-geranylgeranyl-L-cysteine
414.2746	413.239	-0.0287	414.2459	95	100	PyroGlu-Lys-Arg
170.1251	187.121	-0.0075	170.1176	262	50.8	7-Keto-8-aminopelargonic acid
458.3056	435.281	-0.0357	458.2699	65	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	229	44.8	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	235	37	L-Histidine, 1-methyl-
458.3056	435.281	-0.0357	458.2699	58	100	N-Acetyl-S-geranylgeranyl-L-cysteine
474.2642	473.275	0.0181	474.2823	53	41.8	Leu-Trp-Arg
170.1251	169.085	-0.0327	170.0924	206	37.1	L-Histidine, 1-methyl-

458.3056	435.281	-0.0357	458.2699	39	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	225	40.9	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	41	73.2	Ile-Trp-Arg
343.2757	342.256	-0.0125	343.2632	117	86.1	Retinyl propionate
370.2484	370	-0.04	370.21	167	31.2	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
170.1251	169.085	-0.0327	170.0924	253	46.6	L-Histidine, 1-methyl-
370.2217	370	-0.01	370.21	148	50	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
170.1251	169.085	-0.0327	170.0924	382	79.6	L-Histidine, 1-methyl-
343.2757	408.288	-0.0114	343.2643	55	100	Cholic acid
370.2484	369.288	0.0468	370.2952	208	12.1	N-Oleoyl-L-serine
170.1251	169.085	-0.0327	170.0924	336	71.4	L-Histidine, 1-methyl-
370.2484	370	-0.04	370.21	181	34	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
518.3165	495.332	0.0052	518.3217	79	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
474.2907	473.275	-0.0084	474.2823	57	100	Leu-Trp-Arg
170.1251	169.085	-0.0327	170.0924	266	44.5	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	269	60.2	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	25	42.4	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	299	40.6	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	29	100	Ile-Trp-Arg
170.1251	169.085	-0.0327	170.0924	222	51.4	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	322	47	7-Keto-8-aminopelargonic acid
370.2484	370	-0.04	370.21	141	13.7	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
170.1251	169.085	-0.0327	170.0924	361	78.9	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	35	48	Leu-Trp-Arg
170.1251	169.085	-0.0327	170.0924	309	65.2	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	237	30.7	7-Keto-8-aminopelargonic acid
370.1994	370	0.01	370.21	195	49.5	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
170.1251	169.085	-0.0327	170.0924	313	76.5	L-Histidine, 1-methyl-
370.1994	370	0.01	370.21	138	48.5	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
170.1251	169.085	-0.0327	170.0924	217	61.2	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	17	100	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	208	36.6	7-Keto-8-aminopelargonic acid
458.3056	435.281	-0.0357	458.2699	35	100	N-Acetyl-S-geranylgeranyl-L-cysteine

370.2084	370	0	370.21	131	48	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
170.1251	187.121	-0.0075	170.1176	205	36.7	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	45	100	Leu-Trp-Arg
370.2484	370	-0.04	370.21	127	29.6	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
170.1251	187.121	-0.0075	170.1176	251	40.8	7-Keto-8-aminopelargonic acid
370.2484	370	-0.04	370.21	127	33.2	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2484	370	-0.04	370.21	145	16.9	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
170.1251	187.121	-0.0075	170.1176	223	38.3	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	299	60.9	L-Histidine, 1-methyl-
458.2578	435.281	0.0121	458.2699	47	43.4	N-Acetyl-S-geranylgeranyl-L- cysteine
170.1251	187.121	-0.0075	170.1176	264	55.1	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	23	100	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	222	55.9	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	211	46.9	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	197	57.1	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	265	58.1	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	25	40.2	Ile-Trp-Arg
370.2484	370	-0.04	370.21	148	37.6	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
414.2746	449.314	0.0257	414.3003	67	100	Glycodeoxycholic acid
472.291	471.314	0.03	472.321	51	100	Terfenadine
170.1251	187.121	-0.0075	170.1176	385	73.1	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	424	69.7	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	398	73.5	7-Keto-8-aminopelargonic acid
414.2746	413.239	-0.0287	414.2459	115	43.7	PyroGlu-Arg-Lys
170.1444	187.121	-0.0268	170.1176	390	78.1	7-Keto-8-aminopelargonic acid
787.6248	786.661	0.044	787.6688	111	100	N-Docosanoyl-4-sphingenyl-1- O-phosphorylcholine
195.1223	388.243	0.007	195.129	52	100	Leu-Thr-Arg
474.2907	473.275	-0.0084	474.2823	55	100	Leu-Trp-Arg

170.14	187.121	-0.0224	170.1176	279	70.4	7-Keto-8-aminopelargonic acid
472.291	471.314	0.03	472.321	102	100	Terfenadine
518.3165	495.332	0.0052	518.3217	50	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
655.5166	654.492	-0.0175	655.4991	241	100	Deca(propylene glycol) monobutyl ether
170.1251	169.085	-0.0327	170.0924	362	66.9	L-Histidine, 1-methyl-
461.3108	460.28	-0.0237	461.2871	31	57.3	Trp-Lys-Lys

Table A11. List of non-volatile metabolites (LC/MS) for managed population animals. Samples collected in Dec 2011 from multiple animals were pooled. Experiment was conducted using specialized lipids fraction protocol on RP column (refer to Materials and Methods section) in positive ion mode. Top three matches are given for each compound.

Parent m/z	Mass	Delta (m/z)	Library Precurs or m/z	Match Score	Probability (%)	Chem ID
170.1251	187.121	-0.0075	170.1176	397	76.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	358	18.1	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	309	3.7	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	51	100	Leu-Trp-Arg
400.3206	400.343	0.0215	400.3421	163	21.4	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	158	17.2	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	156	15.9	Palmitoyl-L-carnitine cation
170.1251	187.121	-0.0075	170.1176	386	61.8	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	362	20.7	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	360	20.7	L-Histidine, 1-methyl-
461.3108	460.28	-0.0237	461.2871	52	100	Trp-Lys-Lys
472.291	471.314	0.03	472.321	74	100	Terfenadine
170.1251	187.121	-0.0075	170.1176	378	72.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	350	20.9	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	295	4.1	L-Histidine, 1-methyl-
400.3206	400.343	0.0215	400.3421	110	10.2	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	110	10.2	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	109	9.8	Palmitoyl-L-carnitine cation
472.291	471.314	0.03	472.321	108	100	Terfenadine
400.3206	400.343	0.0215	400.3421	76	57.9	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	67	42.1	Palmitoyl-L-carnitine cation
170.1251	187.121	-0.0075	170.1176	394	78.3	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	351	17.3	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	303	3.6	L-Histidine, 1-methyl-
370.2484	369.288	0.0468	370.2952	279	20.2	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	277	18.6	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	267	13.1	N-Oleoyl-L-serine
414.2746	413.239	-0.0287	414.2459	84	100	PyroGlu-Arg-Lys
472.291	471.314	0.03	472.321	102	100	Terfenadine
170.1251	187.121	-0.0075	170.1176	367	45	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	347	20.5	L-Histidine, 3-methyl-
170.1251	169.085	-0.0327	170.0924	343	17.3	L-Histidine, 1-methyl-
655.4667	654.492	0.0324	655.4991	112	38.6	Deca(propylene glycol) monobutyl
655.4667	654.492	0.0324	655.4991	108	32.6	Deca(propylene glycol) monobutyl
655.4667	654.492	0.0324	655.4991	105	28.8	Deca(propylene glycol) monobutyl

516.3205	515.292	-0.0216	516.2989	69	100	Taurocholic acid
170.1251	169.085	-0.0327	170.0924	452	49.4	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	452	49.4	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	451	49.4	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	36	55.4	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	31	44.6	Leu-Trp-Arg
170.1251	187.121	-0.0075	170.1176	420	75.7	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	360	13.4	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	344	7.7	L-Histidine, 1-methyl-
400.3206	400.343	0.0215	400.3421	112	42.6	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	101	29.2	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	100	28.1	Palmitoyl-L-carnitine cation
516.3205	515.292	-0.0216	516.2989	74	100	Taurocholic acid
170.1251	187.121	-0.0075	170.1176	351	57.5	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	329	22.7	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	328	22.7	L-Histidine, 1-methyl-
472.291	471.314	0.03	472.321	162	100	Terfenadine
472.291	471.314	0.03	472.321	149	100	Terfenadine
461.2688	461	-0.04	461.23	6	27.1	PA 17:0; [M+Na] ⁺ ; GPA(4:0/13:0)
461.2688	461	-0.04	461.23	6	27.1	PA 17:0; [M+Na] ⁺ ; GPA(13:0/4:0)
461.2688	461	-0.04	461.23	2	22.9	PA 17:0; [M+Na] ⁺ ; GPA(2:0/15:0)
516.3205	515.292	-0.0216	516.2989	59	100	Taurocholic acid
472.291	471.314	0.03	472.321	111	100	Terfenadine
414.2891	449.314	0.0112	414.3003	98	100	Glycodeoxycholic acid
414.2891	449.314	0.0112	414.3003	88	100	Glycodeoxycholic acid
472.291	471.314	0.03	472.321	150	100	Terfenadine
472.291	471.314	0.03	472.321	131	100	Terfenadine
516.3205	515.292	-0.0216	516.2989	269	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	252	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	250	100	Taurocholic acid
472.3318	471.314	-0.011	472.321	181	100	Terfenadine
472.3318	471.314	-0.011	472.321	153	100	Terfenadine
170.14	169.085	-0.0476	170.0924	221	53.7	L-Histidine, 3-methyl-
170.14	169.085	-0.0476	170.0924	220	53.7	L-Histidine, 3-methyl-
170.14	169.085	-0.0476	170.0924	211	53.7	L-Histidine, 3-methyl-
391.2847	390.277	-0.0005	391.2843	89	51.2	Bis(2-ethylhexyl) phthalate
391.2847	390.277	-0.0005	391.2843	85	43.2	Diethyl phthalate
391.2847	390.277	-0.0005	391.2843	77	43.2	Diethyl phthalate
419.3154	418.308	0.0002	419.3156	196	100	1,2-Benzenedicarboxylic acid, dinonyl ester
149.0233	166.027	0	149.0233	451	99	1,2-Benzenedicarboxylic acid
149.0233	166.027	0	149.0233	447	99	1,2-Benzenedicarboxylic acid
149.0233	166.027	0	149.0233	441	99	1,2-Benzenedicarboxylic acid
311.1646	310.193	0.036	311.2006	99	67.9	Mestranol
311.1646	310.193	0.036	311.2006	95	67.9	Mestranol
311.1646	310.193	0.036	311.2006	92	67.9	Mestranol
279.159	278.152	0.0001	279.1591	235	96.3	Dibutyl phthalate

279.159	278.152	0.0001	279.1591	235	96.3	Dibutyl phthalate
279.159	278.152	0.0001	279.1591	233	96.3	Dibutyl phthalate
516.3205	515.292	-0.0216	516.2989	261	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	255	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	222	100	Taurocholic acid
170.135	187.121	-0.0174	170.1176	346	66.5	7-Keto-8-aminopelargonic acid
170.135	187.121	-0.0174	170.1176	296	13.5	7-Keto-8-aminopelargonic acid
170.135	169.085	-0.0426	170.0924	284	9	L-Histidine, 1-methyl-
399.2511	398.243	-0.0005	399.2506	236	100	Tris(butoxyethyl) phosphate
399.2511	398.243	-0.0004	399.2506	90	100	Tris(butoxyethyl) phosphate
399.2511	398.243	-0.0004	399.2506	89	100	Tris(butoxyethyl) phosphate
163.0749	179.095	0.0005	163.0754	250	75.1	3,4-Methylenedioxyamphetamine
163.0749	179.095	0.0005	163.0754	247	75.1	3,4-Methylenedioxyamphetamine
163.0749	179.095	0.0005	163.0754	244	75.1	3,4-Methylenedioxyamphetamine
516.3205	515.292	-0.0216	516.2989	261	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	261	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	248	100	Taurocholic acid
472.291	471.314	0.03	472.321	281	100	Terfenadine
472.291	471.314	0.03	472.321	242	100	Terfenadine
472.291	471.314	0.03	472.321	173	100	Terfenadine
387.1826	386	-0.05	387.13	229	23.8	1-O-b-D-glucopyranosyl sinapate
387.1826	386	-0.05	387.13	224	19.2	1-O-b-D-glucopyranosyl sinapate
387.1826	386	-0.05	387.13	220	16.2	1-O-b-D-glucopyranosyl sinapate
267.172	266.165	0	267.172	221	99	Tributyl phosphate
267.172	266.165	0	267.172	221	99	Tributyl phosphate
267.172	266.165	0	267.172	220	99	Tributyl phosphate
458.3056	435.281	-0.0357	458.2699	90	100	N-Acetyl-S-geranylgeranyl-L-cysteine
391.2847	390.277	-0.0005	391.2843	142	49.7	Diocetyl phthalate
391.2847	390.277	-0.0005	391.2843	141	47.8	Bis(2-ethylhexyl) phthalate
391.2847	390.277	-0.0005	391.2843	128	49.7	Diocetyl phthalate
404.2083	403.207	0.006	404.214	55	8.7	Glu-Gln-Lys
404.2083	403.207	0.006	404.214	49	6.8	Glu-Gln-Lys
404.2083	403.207	0.006	404.214	49	6.8	Gln-Glu-Lys
474.2907	473.275	-0.0084	474.2823	107	68.4	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	64	15.1	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	61	13.3	Leu-Trp-Arg
170.1251	169.085	-0.0327	170.0924	332	34.4	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	330	34.4	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	327	34.4	L-Histidine, 1-methyl-
518.3165	495.332	0.0052	518.3217	89	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
516.3205	515.292	-0.0216	516.2989	172	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	166	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	166	100	Taurocholic acid
170.1251	187.121	-0.0075	170.1176	373	68.1	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	329	14.8	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	313	8.5	L-Histidine, 1-methyl-

472.291	471.314	0.03	472.321	197	100	Terfenadine
472.291	471.314	0.03	472.321	164	100	Terfenadine
279.0943	278.086	-0.0009	279.0933	30	100	Triphenylphosphine oxide
279.0943	278.086	-0.0009	279.0933	22	100	Triphenylphosphine oxide
279.0943	278.086	-0.0009	279.0933	20	100	Triphenylphosphine oxide
387.1826	386	-0.05	387.13	241	22.8	1-O-b-D-glucofuranosyl sinapate
387.1826	386	-0.05	387.13	241	22.8	1-O-b-D-glucofuranosyl sinapate
387.1826	386	-0.05	387.13	233	17	1-O-b-D-glucofuranosyl sinapate
288.2521	287.196	-0.049	288.203	122	26.1	Leu-Arg
288.2521	287.196	-0.049	288.203	119	23.1	Arg-Leu
288.2521	287.196	-0.049	288.203	106	14.9	Arg-Ile
516.3205	515.292	-0.0216	516.2989	199	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	193	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	192	100	Taurocholic acid
474.2907	473.275	-0.0084	474.2823	180	62.2	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	136	13.5	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	117	6.5	Ile-Trp-Arg
655.4667	654.492	0.0324	655.4991	198	19.8	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	194	16.7	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	188	13.1	Deca(propylene glycol) monobutyl ether
170.1251	187.121	-0.0075	170.1176	383	71.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	329	14	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	319	9.9	L-Histidine, 1-methyl-
370.2484	369.288	0.0468	370.2952	295	18.9	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	288	14.4	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	285	12.8	N-Oleoyl-L-serine
249.1125	249.139	0.0261	249.1386	217	69.6	1H-Pyrazolium, 1,2-dimethyl-3,5-diphenyl
249.1125	249.139	0.0261	249.1386	211	69.6	1H-Pyrazolium, 1,2-dimethyl-3,5-diphenyl
249.1125	249.139	0.0261	249.1386	210	69.6	1H-Pyrazolium, 1,2-dimethyl-3,5-diphenyl
207.157	206.152	0.0021	207.1591	350	78.9	Tri(propylene glycol) methyl ether
207.157	206.152	0.0021	207.1591	343	78.9	Tri(propylene glycol) methyl ether
207.157	206.152	0.0021	207.1591	342	78.9	Tri(propylene glycol) methyl ether
496.417	495.369	-0.0408	496.3762	145	100	2-O-Methyl PAF C-16
496.417	495.369	-0.0408	496.3762	142	100	2-O-Methyl PAF C-16
496.417	495.369	-0.0408	496.3762	139	100	2-O-Methyl PAF C-16
414.2891	449.314	0.0112	414.3003	269	95	Glycodeoxycholic acid
414.2891	449.314	0.0112	414.3003	262	95	Glycodeoxycholic acid
414.2891	413	0.05	414.34	141	4.1	Solasodine
472.291	471.314	0.03	472.321	55	100	Terfenadine
170.1122	187.121	0.0054	170.1176	415	71	7-Keto-8-aminopelargonic acid
170.1122	187.121	0.0054	170.1176	365	14.4	7-Keto-8-aminopelargonic acid

170.1122	169.085	-0.0198	170.0924	359	11.4	L-Histidine, 1-methyl-
655.4943	654.492	0.0048	655.4991	249	20.2	Deca(propylene glycol) monobutyl ether
655.4943	654.492	0.0048	655.4991	248	19.4	Deca(propylene glycol) monobutyl ether
655.4943	654.492	0.0048	655.4991	239	14.1	Deca(propylene glycol) monobutyl ether
170.1251	187.121	-0.0075	170.1176	419	70.6	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	370	14.5	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	362	10.8	L-Histidine, 1-methyl-
472.3318	471.314	-0.011	472.321	102	100	Terfenadine
472.3318	471.314	-0.011	472.321	85	100	Terfenadine
655.4667	654.492	0.0324	655.4991	141	52	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	139	48	Deca(propylene glycol) monobutyl ether
472.3318	471.314	-0.011	472.321	63	100	Terfenadine
472.3318	471.314	-0.011	472.321	58	100	Terfenadine
516.3205	515.292	-0.0216	516.2989	79	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	77	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	77	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	140	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	140	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	136	100	Taurocholic acid
170.1122	169.085	-0.0198	170.0924	346	45.1	L-Histidine, 1-methyl-
170.1122	169.085	-0.0198	170.0924	346	45.1	L-Histidine, 1-methyl-
170.1122	169.085	-0.0198	170.0924	344	41.6	L-Histidine, 3-methyl-
472.3318	471.314	-0.011	472.321	192	100	Terfenadine
472.3318	471.314	-0.011	472.321	171	100	Terfenadine
472.3318	471.314	-0.011	472.321	131	100	Terfenadine
516.3205	515.292	-0.0216	516.2989	130	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	123	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	123	100	Taurocholic acid
170.1122	169.085	-0.0198	170.0924	354	58.9	L-Histidine, 3-methyl-
170.1122	169.085	-0.0198	170.0924	351	58.9	L-Histidine, 3-methyl-
170.1122	169.085	-0.0198	170.0924	350	58.9	L-Histidine, 3-methyl-
170.1251	169.085	-0.0327	170.0924	342	68.3	L-Histidine, 3-methyl-
170.1251	169.085	-0.0327	170.0924	334	68.3	L-Histidine, 3-methyl-
170.1251	169.085	-0.0327	170.0924	323	68.3	L-Histidine, 3-methyl-
206.1384	223.106	-0.0361	206.1023	157	76.7	N-Acetyl-D-galactosaminitol
206.1384	410.217	-0.0229	206.1155	114	16.9	Tyr-Thr-Lys
206.1384	223.106	-0.0361	206.1023	111	76.7	N-Acetyl-D-galactosaminitol
114.091	113.059	-0.0248	114.0662	308	28.3	Creatinine
114.091	113.059	-0.0248	114.0662	308	28.3	Creatinine
114.091	113.059	-0.0248	114.0662	306	28.3	Creatinine
414.2891	413	0.05	414.34	191	100	Solasodine
474.2907	473.275	-0.0084	474.2823	84	62.3	Trp-Ile-Arg

474.2907	473.275	-0.0084	474.2823	69	37.7	Trp-Ile-Arg
328.1988	327.147	-0.0445	328.1543	81	39.3	Naloxone
328.1988	327.147	-0.0445	328.1543	80	37.8	6-Monoacetylmorphine
328.1988	327.147	-0.0445	328.1543	69	37.8	6-Monoacetylmorphine
516.3205	515.292	-0.0216	516.2989	274	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	267	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	266	100	Taurocholic acid
370.2484	369.288	0.0468	370.2952	192	16.9	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	189	14.9	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	179	10.5	N-Oleoyl-L-serine
472.3318	471.314	-0.011	472.321	109	100	Terfenadine
472.3318	471.314	-0.011	472.321	88	100	Terfenadine
461.2688	460.28	0.0183	461.2871	61	100	Trp-Lys-Lys
206.1384	223.106	-0.0361	206.1023	227	96.4	N-Acetyl-D-galactosaminitol
206.1384	223.106	-0.0361	206.1023	157	96.4	N-Acetyl-D-galactosaminitol
206.1384	223.106	-0.0361	206.1023	152	96.4	N-Acetyl-D-galactosaminitol
474.2907	473.275	-0.0084	474.2823	133	34	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	117	19.6	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	116	18.8	Trp-Ile-Arg
422.2707	421.233	-0.0309	422.2398	101	39.7	Gln-Phe-Lys
422.2707	421.233	-0.0309	422.2398	96	32	Gln-Phe-Lys
422.2707	421.233	-0.0309	422.2398	93	28.3	Gln-Phe-Lys
370.2484	369.288	0.0468	370.2952	147	15.1	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	139	11.3	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	138	10.8	N-Oleoyl-L-serine
414.259	449.314	0.0413	414.3003	258	96.6	Glycodeoxycholic acid
414.259	449.314	0.0413	414.3003	210	96.6	Glycodeoxycholic acid
414.259	413.202	-0.0494	414.2096	106	2.6	PyroGlu-Gln-Arg
518.3165	495.332	0.0052	518.3217	49	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
461.2688	460.243	-0.0181	461.2507	127	22.6	Trp-Gln-Lys
461.2688	460.243	-0.0181	461.2507	117	15.9	Trp-Gln-Lys
461.2688	460.243	-0.0181	461.2507	115	14.7	Trp-Gln-Lys
422.2573	421.233	-0.0175	422.2398	129	25.6	Phe-Gln-Lys
422.2573	421.233	-0.0175	422.2398	123	20.1	Phe-Gln-Lys
422.2573	421.233	-0.0175	422.2398	121	18.6	Phe-Gln-Lys
458.3056	435.281	-0.0357	458.2699	64	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.3056	435.281	-0.0357	458.2699	56	100	N-Acetyl-S-geranylgeranyl-L-cysteine
239.141	239	0.04	239.18	7	37.6	MG 9:0; [M+Li] ⁺ ; MG(9:0/0:0/0:0)
239.141	238.099	-0.035	239.106	3	31.8	4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid
239.141	238.099	-0.035	239.106	3	31.8	4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid
169.0621	169	0.05	169.11	55	71	MG 4:0; [M+Li] ⁺ ; MG(4:0/0:0/0:0)
169.0621	210.1	-0.0013	169.0608	14	16.2	Aprobarbital
169.0621	146.069	-0.0037	169.0584	8	12.7	Ala-Gly
458.3056	435.281	-0.0357	458.2699	100	100	N-Acetyl-S-geranylgeranyl-L-cysteine

458.3056	435.281	-0.0357	458.2699	93	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.3056	435.281	-0.0357	458.2699	65	100	N-Acetyl-S-geranylgeranyl-L-cysteine
422.2345	421.269	0.0417	422.2762	32	100	Phe-Lys-Lys
461.2688	460.243	-0.0181	461.2507	151	20.4	Trp-Gln-Lys
461.2688	460.28	0.0183	461.2871	136	12.4	Lys-Trp-Lys
461.2688	460.243	-0.0181	461.2507	135	11.9	Trp-Gln-Lys
472.291	471.314	0.03	472.321	82	100	Terfenadine
370.2484	369.288	0.0468	370.2952	114	20.4	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	113	19.6	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	113	19.6	N-Oleoyl-L-serine
195.1223	194.115	0.0004	195.1227	305	100	Tetraethylene glycol
195.1223	194.115	0.0004	195.1227	303	100	Tetraethylene glycol
195.1223	194.115	0.0004	195.1227	298	100	Tetraethylene glycol
516.3205	515.292	-0.0216	516.2989	97	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	92	100	Taurocholic acid
516.3205	515.292	-0.0216	516.2989	86	100	Taurocholic acid
170.1251	169.085	-0.0327	170.0924	386	51.7	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	385	51.7	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	379	51.7	L-Histidine, 1-methyl-
244.1904	226.193	0.0367	244.2271	494	98.2	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
244.1904	226.193	0.0367	244.2271	234	98.2	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
244.1904	243.158	-0.0248	244.1656	156	1	Pro-Lys
226.1797	225.136	-0.0359	226.1438	157	73.3	3,4,5-TrimethoxyAmphetamine
226.1797	450.259	-0.0429	226.1368	117	17	Ile-Tyr-Arg
226.1797	450.259	-0.0429	226.1368	86	4.6	Ile-Tyr-Arg
474.2907	473.275	-0.0084	474.2823	44	33.5	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	36	25	Trp-Ile-Arg
474.2907	473.275	-0.0084	474.2823	29	19.2	Leu-Trp-Arg
472.291	471.314	0.03	472.321	77	100	Terfenadine
370.2484	369.288	0.0468	370.2952	107	16.6	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	102	13.4	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	99	11.9	N-Oleoyl-L-serine
414.259	413.202	-0.0494	414.2096	38	100	PyroGlu-Gln-Arg
422.2417	421.233	-0.0019	422.2398	98	26.6	Gln-Phe-Lys
422.2417	421.233	-0.0019	422.2398	93	21.5	Gln-Phe-Lys
422.2417	421.233	-0.0019	422.2398	90	19	Phe-Gln-Lys
474.2907	473.275	-0.0084	474.2823	58	48.6	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	50	36.3	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	11	8.6	Leu-Trp-Arg
518.3165	495.332	0.0052	518.3217	69	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
195.1223	194.115	0.0004	195.1227	356	99	Tetraethylene glycol
195.1223	194.115	0.0004	195.1227	354	99	Tetraethylene glycol
195.1223	194.115	0.0004	195.1227	353	99	Tetraethylene glycol
244.1904	226.193	0.0367	244.2271	393	97.4	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
244.1904	226.193	0.0367	244.2271	189	97.4	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
244.1904	243.158	-0.0248	244.1656	133	1	Pro-Lys

474.2907	473.275	-0.0084	474.2823	84	35.2	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	81	31.1	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	65	17.9	Trp-Ile-Arg
518.3165	495.332	0.0052	518.3217	74	55.4	1-Hexadecanoyl-sn-glycero-3-phosphocholine
518.3165	495.332	0.0052	518.3217	69	44.6	1-Hexadecanoyl-sn-glycero-3-phosphocholine
370.2484	370	-0.04	370.21	111	40.2	MGDG 7:0; [M+NH4-CO]+; MGDG(3:0/4:0)
370.2484	370	-0.04	370.21	111	40.2	MGDG 7:0; [M+NH4-CO]+; MGDG(4:0/3:0)
370.2484	370	-0.04	370.21	74	9.8	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
239.1487	238.099	-0.043	239.106	26	100	4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid
239.1487	238.099	-0.043	239.106	21	100	4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid
137.0453	136.039	0.0005	137.0458	386	91.9	Hypoxanthine
137.0453	136.039	0.0005	137.0458	374	91.9	Hypoxanthine
137.0453	136.039	0.0005	137.0458	368	91.9	Hypoxanthine
474.2907	473.275	-0.0084	474.2823	100	68.7	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	80	31.3	Leu-Trp-Arg
370.2484	370	-0.04	370.21	133	14.6	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2484	370	-0.04	370.21	133	14.6	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.2484	369.288	0.0468	370.2952	131	13.5	N-Oleoyl-L-serine
655.4667	654.492	0.0324	655.4991	130	43.4	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	122	32.4	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	114	24.2	Deca(propylene glycol) monobutyl ether
474.2907	473.275	-0.0084	474.2823	59	100	Leu-Trp-Arg
472.291	471.314	0.03	472.321	105	100	Terfenadine
414.2746	449.314	0.0257	414.3003	70	100	Glycodeoxycholic acid
414.2746	449.314	0.0257	414.3003	56	100	Glycodeoxycholic acid
414.2746	449.314	0.0257	414.3003	42	100	Glycodeoxycholic acid
787.6688	786.661	0	787.6688	54	100	N-Docosanoyl-4-sphingenyl-1-O-phosphorylcholine
139.0503	138.043	-0.0001	139.0502	596	80.3	4-Imidazoleacrylic acid
139.0503	138.043	-0.0001	139.0502	589	80.3	4-Imidazoleacrylic acid
139.0503	138.043	-0.0001	139.0502	586	80.3	4-Imidazoleacrylic acid
414.259	449.314	0.0413	414.3003	121	100	Glycodeoxycholic acid
414.259	449.314	0.0413	414.3003	96	100	Glycodeoxycholic acid
414.259	449.314	0.0413	414.3003	71	100	Glycodeoxycholic acid
170.1444	169.085	-0.052	170.0924	358	47.4	L-Histidine, 3-methyl-

170.1444	169.085	-0.052	170.0924	357	47.4	L-Histidine, 3-methyl-
170.1444	169.085	-0.052	170.0924	352	47.4	L-Histidine, 3-methyl-
638.6067	638	-0.04	638.57	122	36.6	DG 36:2; [M+NH4] ⁺ ; DG(14:1/22:1/0:0)
638.6067	638	-0.04	638.57	122	36.6	DG 36:2; [M+NH4] ⁺ ; DG(22:1/14:1/0:0)
638.6067	638	-0.04	638.57	99	13.4	DG 36:2; [M+NH4] ⁺ ; DG(16:1/20:1/0:0)
402.2682	401.278	0.017	402.285	24	100	Myriocin
474.2907	473.275	-0.0084	474.2823	60	37.8	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	44	21.8	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	43	20.9	Trp-Ile-Arg
170.14	187.121	-0.0224	170.1176	205	60	7-Keto-8-aminopelargonic acid
170.14	187.121	-0.0224	170.1176	189	34.6	7-Keto-8-aminopelargonic acid
170.14	169.089	-0.0436	170.0964	122	5.3	Pyridine, 4-benzyl-
170.1251	169.085	-0.0327	170.0924	260	59.6	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	260	59.6	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	249	59.6	L-Histidine, 1-methyl-
458.3056	435.281	-0.0357	458.2699	44	100	N-Acetyl-S-geranylgeranyl-L-cysteine
474.2907	473.275	-0.0084	474.2823	52	43.1	Trp-Ile-Arg
474.2907	473.275	-0.0084	474.2823	44	32.2	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	37	24.6	Ile-Trp-Arg
170.1251	169.085	-0.0327	170.0924	237	75.8	L-Histidine, 3-methyl-
170.1251	187.121	-0.0075	170.1176	199	18.1	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	175	6.1	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	67	56.2	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	34	14.7	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	19	8.9	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	48	56.7	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	24	19	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	14	13.4	Leu-Trp-Arg
458.3056	435.281	-0.0357	458.2699	11	100	N-Acetyl-S-geranylgeranyl-L-cysteine
400.355	400.343	-0.0129	400.3421	36	18.8	Palmitoyl-L-carnitine cation
400.355	400.343	-0.0129	400.3421	36	18.8	Palmitoyl-L-carnitine cation
400.355	400.343	-0.0129	400.3421	34	17.3	Palmitoyl-L-carnitine cation
437.2353	436.207	-0.021	437.2143	94	100	Phe-Asp-Arg
170.1251	187.121	-0.0075	170.1176	11	50	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	11	50	7-Keto-8-aminopelargonic acid
655.4667	654.492	0.0324	655.4991	247	27.6	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	240	21.1	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	234	16.6	Deca(propylene glycol) monobutyl ether
170.1251	187.121	-0.0075	170.1176	105	27.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	101	23.3	7-Keto-8-aminopelargonic acid
170.1251	169.074	-0.0439	170.0812	89	15.5	Pyridoxine

400.3206	400.343	0.0215	400.3421	15	100	Palmitoyl-L-carnitine cation
170.1251	169.085	-0.0327	170.0924	262	41.6	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	261	41.6	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	259	41.6	L-Histidine, 1-methyl-
343.2943	408.288	-0.03	343.2643	17	100	Cholic acid
170.135	187.121	-0.0174	170.1176	190	36.4	7-Keto-8-aminopelargonic acid
170.135	187.121	-0.0174	170.1176	186	30.7	7-Keto-8-aminopelargonic acid
170.135	169.089	-0.0386	170.0964	176	21.7	Pyridine, 4-benzyl-
461.2453	460.243	0.0054	461.2507	62	37.5	Trp-Gln-Lys
461.2453	460.243	0.0054	461.2507	60	34.6	Trp-Gln-Lys
461.2453	460.243	0.0054	461.2507	55	27.9	Trp-Gln-Lys
170.1251	169.085	-0.0327	170.0924	218	38.8	L-Histidine, 3-methyl-
170.1251	187.121	-0.0075	170.1176	218	38.8	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	217	38.8	L-Histidine, 3-methyl-
787.6248	786.661	0.044	787.6688	211	18.6	N-Docosanoyl-4-sphingenyl-1-O-phosphorylcholine
787.6248	786.661	0.044	787.6688	203	13.9	N-Docosanoyl-4-sphingenyl-1-O-phosphorylcholine
787.6248	786.661	0.044	787.6688	198	11.2	N-Docosanoyl-4-sphingenyl-1-O-phosphorylcholine
461.2688	230.152	0.0421	461.3109	30	100	Dodecanedioic acid
170.135	187.121	-0.0174	170.1176	236	37	7-Keto-8-aminopelargonic acid
170.135	169	-0.04	170.09	220	21.3	3-Methyl-L-histidine
170.135	169.085	-0.0426	170.0924	213	16.3	L-Histidine, 3-methyl-
655.4667	654.492	0.0324	655.4991	129	41.9	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	119	29.6	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	118	28.4	Deca(propylene glycol) monobutyl ether
461.2904	230.163	0.043	461.3334	189	93.4	Leu-Val
461.2904	230.152	0.0205	461.3109	86	6.6	Dodecanedioic acid
461.2904	230.163	0.043	461.3334	8	93.4	Leu-Val
655.4667	654.492	0.0324	655.4991	124	37.2	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	120	31.4	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	120	31.4	Deca(propylene glycol) monobutyl ether
400.3206	400.343	0.0215	400.3421	149	8.9	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	148	8.6	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	148	8.6	Palmitoyl-L-carnitine cation
170.14	187.121	-0.0224	170.1176	341	56.5	7-Keto-8-aminopelargonic acid
170.14	187.121	-0.0224	170.1176	322	27.4	7-Keto-8-aminopelargonic acid
170.14	169.085	-0.0476	170.0924	283	6.5	L-Histidine, 3-methyl-
400.3206	400.343	0.0215	400.3421	343	16.5	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	338	13.3	Palmitoyl-L-carnitine cation

400.3206	400.343	0.0215	400.3421	338	13.3	Palmitoyl-L-carnitine cation
655.4667	654.492	0.0324	655.4991	113	38.1	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	109	32.2	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	107	29.7	Deca(propylene glycol) monobutyl ether
695.4097	672.473	0.0525	695.4622	14	100	1-Hexadecanoyl-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoric acid
170.1444	187.121	-0.0268	170.1176	120	46.6	7-Keto-8-aminopelargonic acid
170.1444	187.121	-0.0268	170.1176	107	30.1	7-Keto-8-aminopelargonic acid
170.1444	169.085	-0.052	170.0924	69	7.2	L-Histidine, 3-methyl-
695.4097	672.473	0.0525	695.4622	31	100	1-Hexadecanoyl-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoric acid
400.3206	400.343	0.0215	400.3421	197	10	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	194	8.8	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	194	8.8	Palmitoyl-L-carnitine cation
343.2827	342.256	-0.0195	343.2632	93	100	Retinyl propionate
400.3206	400.343	0.0215	400.3421	302	12.5	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	302	12.5	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	302	12.5	Palmitoyl-L-carnitine cation
170.1251	187.121	-0.0075	170.1176	68	25.6	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	61	19.6	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	53	14.6	L-Histidine, 1-methyl-
472.291	471.314	0.03	472.321	47	100	Terfenadine
472.291	471.314	0.03	472.321	36	100	Terfenadine
458.3056	435.281	-0.0357	458.2699	65	100	N-Acetyl-S-geranylgeranyl-L-cysteine
414.2891	413	0.05	414.34	28	100	Solasodine
474.2907	473.275	-0.0084	474.2823	24	100	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	81	23.3	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	78	20.5	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	65	13.3	L-Histidine, 3-methyl-
414.259	413.239	-0.0131	414.2459	40	29.8	PyroGlu-Lys-Arg
414.259	413.239	-0.0131	414.2459	39	28.6	PyroGlu-Lys-Arg
414.259	413.239	-0.0131	414.2459	37	26.4	PyroGlu-Lys-Arg
458.3056	435.281	-0.0357	458.2699	30	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.3056	435.281	-0.0357	458.2699	51	100	N-Acetyl-S-geranylgeranyl-L-cysteine
414.2746	449.314	0.0257	414.3003	50	100	Glycodeoxycholic acid
474.2907	473.275	-0.0084	474.2823	58	50.9	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	41	27.8	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	34	21.3	Trp-Ile-Arg
518.3165	495.332	0.0052	518.3217	92	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
474.2907	473.275	-0.0084	474.2823	46	100	Leu-Trp-Arg
458.3056	435.281	-0.0357	458.2699	64	100	N-Acetyl-S-geranylgeranyl-L-cysteine

474.2907	473.275	-0.0084	474.2823	87	27.5	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	66	11.7	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	61	9.4	Trp-Ile-Arg
170.1251	169	-0.04	170.09	278	32.5	3-Methyl-L-histidine
170.1251	187.121	-0.0075	170.1176	276	30	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	272	25.4	L-Histidine, 3-methyl-
474.2907	473.275	-0.0084	474.2823	27	30.1	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	26	28.9	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	23	25.5	Ile-Trp-Arg
655.4667	654.492	0.0324	655.4991	145	45.5	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	140	36.7	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	121	17.8	Deca(propylene glycol) monobutyl ether
170.1251	187.121	-0.0075	170.1176	31	23.4	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	31	23.4	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	21	16.5	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	53	64.7	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	36	35.3	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	50	25.9	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	48	23.9	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	31	13	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	23	100	Leu-Trp-Arg
170.1251	187.121	-0.0075	170.1176	71	36.4	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	68	32.2	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	47	13.7	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	59	19.8	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	57	18.2	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	54	16.1	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	133	46.7	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	120	30.2	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	77	6.7	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	75	24.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	73	22.6	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	72	21.7	L-Histidine, 3-methyl-
422.2573	421.269	0.0189	422.2762	25	100	Phe-Lys-Lys
170.1251	187.121	-0.0075	170.1176	113	32.2	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	111	29.7	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	108	26.2	L-Histidine, 1-methyl-
472.261	471.223	-0.0307	472.2303	66	100	PyroGlu-Trp-Arg
458.3056	435.281	-0.0357	458.2699	80	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	90	39	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	88	36	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	62	10.8	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	61	100	Ile-Trp-Arg
458.2695	435.281	0.0004	458.2699	35	100	N-Acetyl-S-geranylgeranyl-L-cysteine

458.2695	435.281	0.0004	458.2699	23	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.2695	435.281	0.0004	458.2699	21	100	N-Acetyl-S-geranylgeranyl-L-cysteine
518.277	495.332	0.0447	518.3217	60	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
458.3056	435.281	-0.0357	458.2699	33	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.3056	435.281	-0.0357	458.2699	30	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.3056	435.281	-0.0357	458.2699	27	100	N-Acetyl-S-geranylgeranyl-L-cysteine
474.2449	473.275	0.0374	474.2823	68	38.8	Trp-Ile-Arg
474.2449	473.275	0.0374	474.2823	68	38.8	Trp-Leu-Arg
474.2449	473.275	0.0374	474.2823	52	22.4	Ile-Trp-Arg
515.3745	246.211	0.0373	515.4117	29	100	Dodecyldimethylphosphine oxide
515.3745	246.211	0.0373	515.4117	9	100	Dodecyldimethylphosphine oxide
515.3745	246.211	0.0373	515.4117	7	100	Dodecyldimethylphosphine oxide
170.1251	187.121	-0.0075	170.1176	124	37.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	122	34.6	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	117	27.9	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	129	38.4	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	128	36.9	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	116	24.6	L-Histidine, 1-methyl-
515.3601	246.211	0.0516	515.4117	44	100	Dodecyldimethylphosphine oxide
474.2449	473.275	0.0374	474.2823	101	67.3	Trp-Ile-Arg
474.2449	473.275	0.0374	474.2823	82	32.7	Ile-Trp-Arg
458.2695	435.281	0.0004	458.2699	67	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	169	39.6	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	158	27.2	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	143	16.5	L-Histidine, 3-methyl-
474.2907	473.275	-0.0084	474.2823	90	48.2	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	85	38.8	Trp-Ile-Arg
474.2907	473.275	-0.0084	474.2823	61	13	Leu-Trp-Arg
170.1251	187.121	-0.0075	170.1176	187	49.9	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	174	32.2	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	133	7.3	L-Histidine, 1-methyl-
458.2578	435.281	0.0121	458.2699	132	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.2578	435.281	0.0121	458.2699	99	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.2578	435.281	0.0121	458.2699	97	100	N-Acetyl-S-geranylgeranyl-L-cysteine
474.2907	473.275	-0.0084	474.2823	77	56	Trp-Ile-Arg
474.2907	473.275	-0.0084	474.2823	71	44	Ile-Trp-Arg
518.3165	495.332	0.0052	518.3217	72	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
170.1251	187.121	-0.0075	170.1176	196	53	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	183	34.3	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	138	7.3	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	146	33.3	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	143	29.5	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	138	23.8	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	48	100	Ile-Trp-Arg
400.3206	400.343	0.0215	400.3421	36	56	Palmitoyl-L-carnitine cation

400.3206	400.343	0.0215	400.3421	30	44	Palmitoyl-L-carnitine cation
458.3056	435.281	-0.0357	458.2699	66	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	194	46.8	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	185	34	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	143	7.6	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	143	40.3	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	132	27.7	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	116	15.9	L-Histidine, 1-methyl-
458.2403	435.281	0.0296	458.2699	85	79.3	N-Acetyl-S-geranylgeranyl-L-cysteine
458.2403	457.244	0.011	458.251	52	20.7	Pro-Trp-Arg
400.3206	401.278	-0.0501	400.2705	60	73.2	Myriocin
400.3206	400.343	0.0215	400.3421	37	26.8	Palmitoyl-L-carnitine cation
170.1251	187.121	-0.0075	170.1176	204	65.7	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	181	24	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	132	4.9	L-Histidine, 1-methyl-
458.3056	435.281	-0.0357	458.2699	58	100	N-Acetyl-S-geranylgeranyl-L-cysteine
655.4667	654.492	0.0324	655.4991	107	45.9	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	93	28.7	Deca(propylene glycol) monobutyl ether
655.4667	654.492	0.0324	655.4991	90	25.4	Deca(propylene glycol) monobutyl ether
170.1251	187.121	-0.0075	170.1176	122	38.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	120	35.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	85	8.9	7-Keto-8-aminopelargonic acid
414.259	413.202	-0.0494	414.2096	115	49.9	PyroGlu-Gln-Arg
414.259	413.202	-0.0494	414.2096	101	31.2	PyroGlu-Gln-Arg
414.259	413.202	-0.0494	414.2096	86	18.9	PyroGlu-Gln-Arg
370.2484	370	-0.04	370.21	205	41.3	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2484	370	-0.04	370.21	205	41.3	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.2484	369.288	0.0468	370.2952	113	3.5	N-Oleoyl-L-serine
343.2757	342.256	-0.0125	343.2632	109	56.3	Retinyl propionate
343.2757	408.288	-0.0114	343.2643	95	35.2	Cholic acid
343.2757	408.288	-0.0114	343.2643	92	35.2	Cholic acid
170.1251	187.121	-0.0075	170.1176	201	48.4	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	195	38	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	145	7.7	L-Histidine, 1-methyl-
518.3165	495.332	0.0052	518.3217	83	100	1-Hexadecanoyl-sn-glycero-3- phosphocholine
458.3056	435.281	-0.0357	458.2699	46	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	142	59.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	125	32.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	89	8	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	59	36.5	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	43	21	Ile-Trp-Arg

474.2907	473.275	-0.0084	474.2823	38	16.9	Trp-Ile-Arg
458.3056	435.281	-0.0357	458.2699	48	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.3056	435.281	-0.0357	458.2699	36	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.3056	435.281	-0.0357	458.2699	35	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	156	48.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	152	41	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	110	9.2	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	50	40.2	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	49	38.7	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	32	21.1	Ile-Trp-Arg
458.3056	435.281	-0.0357	458.2699	39	100	N-Acetyl-S-geranylgeranyl-L-cysteine
458.3056	435.281	-0.0357	458.2699	28	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	221	52	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	213	38.8	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	158	7.5	7-Keto-8-aminopelargonic acid
414.259	413.202	-0.0494	414.2096	75	100	PyroGlu-Gln-Arg
458.3056	435.281	-0.0357	458.2699	56	100	N-Acetyl-S-geranylgeranyl-L-cysteine
474.2907	473.275	-0.0084	474.2823	39	100	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	215	62.3	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	195	28.4	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	128	4.4	7-Keto-8-aminopelargonic acid
400.3206	401.278	-0.0501	400.2705	48	44.7	Myriocin
400.3206	401.278	-0.0501	400.2705	47	44.7	Myriocin
400.3206	400.343	0.0215	400.3421	28	20.4	Palmitoyl-L-carnitine cation
170.1251	187.121	-0.0075	170.1176	192	59.3	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	174	30.6	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	142	8.2	L-Histidine, 1-methyl-
518.3165	495.332	0.0052	518.3217	133	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
170.1251	187.121	-0.0075	170.1176	227	50.4	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	218	36.6	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	180	8.8	7-Keto-8-aminopelargonic acid
458.3056	435.281	-0.0357	458.2699	65	100	N-Acetyl-S-geranylgeranyl-L-cysteine
400.3206	400.343	0.0215	400.3421	38	100	Palmitoyl-L-carnitine cation
170.1251	187.121	-0.0075	170.1176	248	45.4	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	246	41.9	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	203	9.2	L-Histidine, 1-methyl-
518.3165	495.332	0.0052	518.3217	64	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
170.135	187.121	-0.0174	170.1176	175	41.8	7-Keto-8-aminopelargonic acid
170.135	187.121	-0.0174	170.1176	173	38.5	7-Keto-8-aminopelargonic acid
170.135	169.085	-0.0426	170.0924	118	7.5	L-Histidine, 1-methyl-
400.3206	400.343	0.0215	400.3421	82	37	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	80	34.1	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	76	28.8	Palmitoyl-L-carnitine cation
414.2746	413.239	-0.0287	414.2459	75	35.7	PyroGlu-Lys-Arg
414.2746	413.239	-0.0287	414.2459	67	26.6	PyroGlu-Lys-Arg

414.2746	413.239	-0.0287	414.2459	60	20.4	PyroGlu-Lys-Arg
414.2746	413.239	-0.0287	414.2459	49	39	PyroGlu-Lys-Arg
414.2746	413.239	-0.0287	414.2459	30	18.9	PyroGlu-Lys-Arg
414.2746	413.239	-0.0287	414.2459	28	17.5	PyroGlu-Lys-Arg
170.1251	187.121	-0.0075	170.1176	235	62.2	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	213	24.6	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	189	8.2	L-Histidine, 1-methyl-
343.2873	408.288	-0.0231	343.2643	45	100	Cholic acid
343.2873	408.288	-0.0231	343.2643	34	100	Cholic acid
343.2873	408.288	-0.0231	343.2643	24	100	Cholic acid
414.2746	413.239	-0.0287	414.2459	101	68.7	PyroGlu-Lys-Arg
414.2746	413.239	-0.0287	414.2459	81	31.3	PyroGlu-Lys-Arg
170.135	187.121	-0.0174	170.1176	219	47.1	7-Keto-8-aminopelargonic acid
170.135	187.121	-0.0174	170.1176	208	32.3	7-Keto-8-aminopelargonic acid
170.135	187.121	-0.0174	170.1176	152	6.2	7-Keto-8-aminopelargonic acid
458.3056	435.281	-0.0357	458.2699	58	100	N-Acetyl-S-geranylgeranyl-L-cysteine
518.3165	495.332	0.0052	518.3217	63	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
400.3206	400.343	0.0215	400.3421	87	25.1	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	85	23.2	Palmitoyl-L-carnitine cation
400.3206	400.343	0.0215	400.3421	82	20.5	Palmitoyl-L-carnitine cation
474.2907	473.275	-0.0084	474.2823	32	100	Ile-Trp-Arg
170.1251	169.085	-0.0327	170.0924	166	36.4	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	165	36.4	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	164	36.4	L-Histidine, 1-methyl-
343.2757	342.256	-0.0125	343.2632	95	100	Retinyl propionate
458.3056	435.281	-0.0357	458.2699	76	100	N-Acetyl-S-geranylgeranyl-L-cysteine
414.2746	413.239	-0.0287	414.2459	95	100	PyroGlu-Lys-Arg
170.1251	187.121	-0.0075	170.1176	262	50.8	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	253	36.9	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	208	7.9	L-Histidine, 3-methyl-
458.3056	435.281	-0.0357	458.2699	65	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	229	44.8	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	216	28.9	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	197	14.1	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	235	37	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	233	37	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	232	37	L-Histidine, 1-methyl-
458.3056	435.281	-0.0357	458.2699	58	100	N-Acetyl-S-geranylgeranyl-L-cysteine
474.2642	473.275	0.0181	474.2823	53	41.8	Leu-Trp-Arg
474.2642	473.275	0.0181	474.2823	48	33.7	Ile-Trp-Arg
474.2642	473.275	0.0181	474.2823	39	24.5	Ile-Trp-Arg
170.1251	169.085	-0.0327	170.0924	206	37.1	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	204	37.1	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	204	37.1	L-Histidine, 1-methyl-
458.3056	435.281	-0.0357	458.2699	39	100	N-Acetyl-S-geranylgeranyl-L-cysteine
170.1251	187.121	-0.0075	170.1176	225	40.9	7-Keto-8-aminopelargonic acid

170.1251	187.121	-0.0075	170.1176	223	37.7	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	168	7.3	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	41	73.2	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	18	26.8	Ile-Trp-Arg
343.2757	342.256	-0.0125	343.2632	117	86.1	Retinyl propionate
343.2757	408.288	-0.0114	343.2643	52	13.9	Cholic acid
343.2757	408.288	-0.0114	343.2643	42	13.9	Cholic acid
370.2484	370	-0.04	370.21	167	31.2	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2484	370	-0.04	370.21	167	31.2	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.2484	369.288	0.0468	370.2952	101	4.9	N-Oleoyl-L-serine
170.1251	169.085	-0.0327	170.0924	253	46.6	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	251	46.6	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	247	46.6	L-Histidine, 1-methyl-
370.2217	370	-0.01	370.21	148	50	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2217	370	-0.01	370.21	148	50	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
170.1251	169.085	-0.0327	170.0924	382	79.6	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	381	79.6	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	377	79.6	L-Histidine, 1-methyl-
343.2757	408.288	-0.0114	343.2643	55	100	Cholic acid
343.2757	408.288	-0.0114	343.2643	50	100	Cholic acid
343.2757	408.288	-0.0114	343.2643	40	100	Cholic acid
370.2484	369.288	0.0468	370.2952	208	12.1	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	207	11.7	N-Oleoyl-L-serine
370.2484	369.288	0.0468	370.2952	206	11.2	N-Oleoyl-L-serine
170.1251	169.085	-0.0327	170.0924	336	71.4	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	336	71.4	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	331	71.4	L-Histidine, 1-methyl-
370.2484	370	-0.04	370.21	181	34	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2484	370	-0.04	370.21	181	34	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.2484	369.288	0.0468	370.2952	125	6.5	N-Oleoyl-L-serine
518.3165	495.332	0.0052	518.3217	79	100	1-Hexadecanoyl-sn-glycero-3- phosphocholine
474.2907	473.275	-0.0084	474.2823	57	100	Leu-Trp-Arg
170.1251	169.085	-0.0327	170.0924	266	44.5	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	258	33.2	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	256	44.5	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	269	60.2	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	266	60.2	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	264	60.2	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	25	42.4	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	20	34.2	Ile-Trp-Arg

474.2907	473.275	-0.0084	474.2823	9	23.4	Leu-Trp-Arg
170.1251	187.121	-0.0075	170.1176	299	40.6	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	287	27	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	286	27	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	29	100	Ile-Trp-Arg
170.1251	169.085	-0.0327	170.0924	222	51.4	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	216	51.4	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	215	51.4	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	322	47	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	305	25.6	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	304	25.6	L-Histidine, 1-methyl-
370.2484	370	-0.04	370.21	141	13.7	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2484	370	-0.04	370.21	141	13.7	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.2484	369.288	0.0468	370.2952	135	10.8	N-Oleoyl-L-serine
170.1251	169.085	-0.0327	170.0924	361	78.9	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	355	78.9	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	353	78.9	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	35	48	Leu-Trp-Arg
474.2907	473.275	-0.0084	474.2823	19	27.6	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	16	24.4	Ile-Trp-Arg
170.1251	169.085	-0.0327	170.0924	309	65.2	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	308	65.2	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	307	65.2	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	237	30.7	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	235	28.3	L-Histidine, 3-methyl-
170.1251	169.085	-0.0327	170.0924	231	28.3	L-Histidine, 3-methyl-
370.1994	370	0.01	370.21	195	49.5	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.1994	370	0.01	370.21	195	49.5	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.1994	369.158	-0.0345	370.1649	23	1	Heroin
170.1251	169.085	-0.0327	170.0924	313	76.5	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	310	76.5	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	309	76.5	L-Histidine, 1-methyl-
370.1994	370	0.01	370.21	138	48.5	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.1994	370	0.01	370.21	138	48.5	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.1994	369.158	-0.0345	370.1649	24	3	Heroin
170.1251	169.085	-0.0327	170.0924	217	61.2	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	213	61.2	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	210	61.2	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	17	100	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	208	36.6	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	204	30.9	7-Keto-8-aminopelargonic acid

170.1251	169.085	-0.0327	170.0924	193	21.2	L-Histidine, 1-methyl-
458.3056	435.281	-0.0357	458.2699	35	100	N-Acetyl-S-geranylgeranyl-L-cysteine
370.2084	370	0	370.21	131	48	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2084	370	0	370.21	131	48	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.2084	369.158	-0.0435	370.1649	41	4.1	Heroin
170.1251	187.121	-0.0075	170.1176	205	36.7	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	196	26.6	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	195	25.6	L-Histidine, 1-methyl-
474.2907	473.275	-0.0084	474.2823	45	100	Leu-Trp-Arg
370.2484	370	-0.04	370.21	127	29.6	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2484	370	-0.04	370.21	127	29.6	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.2484	369.288	0.0468	370.2952	61	4.7	N-Oleoyl-L-serine
170.1251	187.121	-0.0075	170.1176	251	40.8	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	235	23.5	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	235	23.5	7-Keto-8-aminopelargonic acid
370.2484	370	-0.04	370.21	127	33.2	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2484	370	-0.04	370.21	127	33.2	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.2484	369.288	0.0468	370.2952	52	4.3	N-Oleoyl-L-serine
370.2484	370	-0.04	370.21	145	16.9	MGDG 7:0; [M+NH4-CO]+; MGDG(2:0/5:0)
370.2484	370	-0.04	370.21	145	16.9	MGDG 7:0; [M+NH4-CO]+; MGDG(5:0/2:0)
370.2484	369.288	0.0468	370.2952	122	6.2	N-Oleoyl-L-serine
170.1251	187.121	-0.0075	170.1176	223	38.3	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	217	30.1	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	212	30.1	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	299	60.9	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	293	60.9	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	293	60.9	L-Histidine, 1-methyl-
458.2578	435.281	0.0121	458.2699	47	43.4	N-Acetyl-S-geranylgeranyl-L-cysteine
458.2578	457.244	-0.007	458.251	29	22.4	Pro-Trp-Arg
458.2578	457.244	-0.007	458.251	25	18.9	Trp-Pro-Arg
170.1251	187.121	-0.0075	170.1176	264	55.1	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	250	34.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	195	6.7	7-Keto-8-aminopelargonic acid
474.2907	473.275	-0.0084	474.2823	23	100	Ile-Trp-Arg
170.1251	187.121	-0.0075	170.1176	222	55.9	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	206	32.2	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	170	8	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	211	46.9	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	203	35	7-Keto-8-aminopelargonic acid

170.1251	169.085	-0.0327	170.0924	150	6.9	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	197	57.1	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	178	27.7	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	125	5.5	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	265	58.1	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	245	26.5	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	208	6.4	L-Histidine, 3-methyl-
474.2907	473.275	-0.0084	474.2823	25	40.2	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	20	32.4	Ile-Trp-Arg
474.2907	473.275	-0.0084	474.2823	16	27.4	Leu-Trp-Arg
370.2484	370	-0.04	370.21	148	37.6	MGDG 7:0; [M+NH ₄ -CO] ⁺ ; MGDG(2:0/5:0)
370.2484	370	-0.04	370.21	148	37.6	MGDG 7:0; [M+NH ₄ -CO] ⁺ ; MGDG(5:0/2:0)
370.2484	369.288	0.0468	370.2952	67	4	N-Oleoyl-L-serine
414.2746	449.314	0.0257	414.3003	67	100	Glycodeoxycholic acid
414.2746	449.314	0.0257	414.3003	51	100	Glycodeoxycholic acid
472.291	471.314	0.03	472.321	51	100	Terfenadine
170.1251	187.121	-0.0075	170.1176	385	73.1	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	358	21.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	287	3.1	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	424	69.7	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	384	16.2	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	370	10.1	L-Histidine, 1-methyl-
170.1251	187.121	-0.0075	170.1176	398	73.5	7-Keto-8-aminopelargonic acid
170.1251	187.121	-0.0075	170.1176	361	17.9	7-Keto-8-aminopelargonic acid
170.1251	169.085	-0.0327	170.0924	337	6	L-Histidine, 1-methyl-
414.2746	413.239	-0.0287	414.2459	115	43.7	PyroGlu-Arg-Lys
414.2746	413.239	-0.0287	414.2459	103	29.1	PyroGlu-Arg-Lys
414.2746	413.239	-0.0287	414.2459	72	7.9	PyroGlu-Lys-Arg
170.1444	187.121	-0.0268	170.1176	390	78.1	7-Keto-8-aminopelargonic acid
170.1444	187.121	-0.0268	170.1176	338	15.6	7-Keto-8-aminopelargonic acid
170.1444	169.085	-0.052	170.0924	291	3.3	L-Histidine, 1-methyl-
787.6248	786.661	0.044	787.6688	111	100	N-Docosanoyl-4-sphinganyl-1-O-phosphorylcholine
195.1223	388.243	0.007	195.129	52	100	Leu-Thr-Arg
474.2907	473.275	-0.0084	474.2823	55	100	Leu-Trp-Arg
170.14	187.121	-0.0224	170.1176	279	70.4	7-Keto-8-aminopelargonic acid
170.14	187.121	-0.0224	170.1176	246	18.4	7-Keto-8-aminopelargonic acid
170.14	169.085	-0.0476	170.0924	212	4.7	L-Histidine, 1-methyl-
472.291	471.314	0.03	472.321	102	100	Terfenadine
518.3165	495.332	0.0052	518.3217	50	100	1-Hexadecanoyl-sn-glycero-3-phosphocholine
655.5166	654.492	-0.0175	655.4991	241	100	Deca(propylene glycol) monobutyl ether
170.1251	169.085	-0.0327	170.0924	362	66.9	L-Histidine, 1-methyl-
170.1251	169.085	-0.0327	170.0924	362	66.9	L-Histidine, 1-methyl-

170.1251	169.085	-0.0327	170.0924	359	66.9	L-Histidine, 1-methyl-
461.3108	460.28	-0.0237	461.2871	31	57.3	Trp-Lys-Lys
461.3108	460.28	-0.0237	461.2871	23	42.7	Trp-Lys-Lys

Table A12. List of non-volatile metabolites (LC/MS) in sea water. Experiment was conducted using HILIC column in positive ion mode (refer to Materials and Methods section).

Parent m/z	Mass	Delta (m/z)	Library Precursor	Match Score	Probability (%)	Chem ID
276.1945	275.159	-0.0279	276.1666	174	68.4	Arg-Thr
276.1945	319.133	-0.0438	276.1507	79	100	Norfloxacin
276.1945	275.152	-0.0351	276.1594	176	74.1	Methylenedioxypropylvalerone
276.1945	275.152	-0.0351	276.1594	218	89.8	Methylenedioxypropylvalerone
276.1945	275.159	-0.0279	276.1666	131	57.5	Arg-Thr
276.1945	275.159	-0.0279	276.1666	154	34.9	Thr-Arg
276.1945	275.159	-0.0279	276.1666	142	62.3	Arg-Thr
276.1945	275.152	-0.0351	276.1594	134	66.1	Methylenedioxypropylvalerone
276.1945	275.152	-0.0351	276.1594	142	54	Methylenedioxypropylvalerone
276.1945	275.159	-0.0279	276.1666	157	55.8	Arg-Thr
276.1945	319.133	-0.0438	276.1507	171	79.5	Norfloxacin
276.1945	275.152	-0.0351	276.1594	152	78.1	Methylenedioxypropylvalerone
150.1003	167.095	-0.009	150.0913	264	90.4	Synephrine
150.1003	167.095	-0.009	150.0913	325	87.6	Synephrine
150.1003	167.095	-0.009	150.0913	203	45.9	Synephrine
150.1003	167.095	-0.009	150.0913	225	60.8	Synephrine
150.0885	167.095	0.0028	150.0913	195	53.5	Synephrine
150.0885	149.07	-0.0111	150.0774	343	94	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	244	86.3	Adenine, N6-methyl
150.0885	167.095	0.0028	150.0913	262	42.8	Synephrine
205.1202	204.072	-0.0408	205.0794	136	75.1	Levamisole
205.1202	408.237	0.0057	205.1259	154	16.9	Tyr-Val-Lys
205.1202	204.072	-0.0408	205.0794	200	12.7	Levamisole
205.1202	204.072	-0.0408	205.0794	257	56.2	Levamisole
205.1202	204.075	-0.0383	205.0819	82	76.9	Gly-Glu
205.1202	188.116	-0.0008	205.1194	173	75.3	Glycyl-L-norleucine
205.1202	204.075	-0.0383	205.0819	164	27.6	Ala-Asp
205.1202	408.212	-0.0069	205.1133	227	23.1	Phe-Ser-Arg
150.0831	167.095	0.0082	150.0913	225	80.2	Synephrine
150.0831	167.095	0.0082	150.0913	261	38.8	Synephrine
150.0831	149.07	-0.0057	150.0774	316	80.7	Adenine, N6-methyl
150.0831	167.095	0.0082	150.0913	278	92	Synephrine
257.1363	256.117	-0.0119	257.1244	103	34.5	Thr-His
257.1363	256.117	-0.0119	257.1244	169	67	Thr-His
257.1363	256.117	-0.0119	257.1244	201	24.7	Thr-His
257.1363	256.117	-0.0119	257.1244	213	53.7	Thr-His
150.1003	303.147	-0.009	150.0913	253	75.7	Cocaine
150.1003	149	-0.02	150.08	277	39.7	3-Methyladenine
150.1003	149.07	-0.0229	150.0774	213	69.4	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	293	36.4	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	180	86.9	Synephrine

150.1003	149.105	0.0122	150.1125	218	67.1	Triethanolamine
150.1003	167.095	-0.009	150.0913	254	82.6	Synephrine
150.1003	167.058	-0.045	150.055	287	70.8	3-Methyl-2-nitrobenzyl alcohol
150.0831	149.12	0.0446	150.1277	280	79	Methamphetamine
150.0831	149.07	-0.0057	150.0774	359	94	Adenine, N6-methyl
150.0831	149.12	0.0446	150.1277	236	43	Methamphetamine
150.0831	167.095	0.0082	150.0913	236	80.7	Synephrine
150.0885	167.095	0.0028	150.0913	150	43.1	Synephrine
150.0885	149.07	-0.0111	150.0774	204	51.2	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	269	83.4	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	153	76.4	Adenine, N6-methyl
176.0975	175	-0.03	176.07	191	70.3	1-Methoxy-3-carbaldehyde
176.0975	175	-0.03	176.07	79	79.6	1-Methoxy-3-carbaldehyde
176.0975	175	-0.03	176.07	84	66	1-Methoxy-3-carbaldehyde
283.1685	282.122	-0.0396	283.1289	139	54.6	Thr-Tyr
283.1685	282.179	0.0179	283.1864	260	67.7	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	282.179	0.0179	283.1864	313	70.1	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	282.179	0.0179	283.1864	309	79.3	1,3-Bis(tris(hydroxymethyl)methylamino)propane
257.1363	256.117	-0.0119	257.1244	133	67.2	Thr-His
257.1363	256.11	-0.0191	257.1172	128	79.1	Pterostilbene
257.1363	256.11	-0.0191	257.1172	82	100	Pterostilbene
257.1363	256.11	-0.0191	257.1172	147	100	Pterostilbene
225.1677	224.127	-0.0331	225.1346	22	100	Pirimicarb-desmethyl
225.1677	448.229	-0.046	225.122	177	26.1	His-His-Arg
225.1677	0	-0.02	225.15	177	55.5	Methyl jasmonate
225.1677	224.116	-0.0443	225.1234	177	82.8	Butalbital
238.1427	237.103	-0.0319	238.1108	76	100	3-(Cyclohexylamino)-2-hydroxy-1-propanesulfonic acid
238.1427	0	-0.05	238.09	157	39.7	Biopterin
238.1427	237.092	-0.0434	238.0993	189	48.4	Ketamine
238.1427	237.103	-0.0319	238.1108	217	58.8	Methionine sulphone, butyl ester
150.1003	149	-0.02	150.08	146	35.3	3-Methyladenine
150.1003	149.07	-0.0229	150.0774	224	52.6	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	346	89.9	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	340	72.7	Synephrine
176.1195	175	-0.05	176.07	129	100	1-Methoxy-3-carbaldehyde
176.1195	175	-0.05	176.07	136	71.4	1-Methoxy-3-carbaldehyde
176.1195	175.096	-0.017	176.103	46	37.1	L-Citrulline

266.1194	283.128	0.0054	266.1248	101	84.8	His-Gln
284.1259	283.164	0.0458	284.1717	142	51.9	His-Lys
284.1259	283.164	0.0458	284.1717	238	69.7	His-Lys
284.1259	283.164	0.0458	284.1717	150	34.8	His-Lys
284.1259	0	0.01	284.14	230	74.6	His Gln
150.0831	149	0	150.08	129	33.1	3-Methyladenine
150.0831	149.07	-0.0057	150.0774	309	96.5	Adenine, N6-methyl
150.0831	167.095	0.0082	150.0913	436	89.9	Synephrine
150.0831	149.07	-0.0057	150.0774	146	47.8	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	291	64.7	Synephrine
150.1003	167.058	-0.045	150.055	277	68.6	3-Methyl-2-nitrobenzyl alcohol
150.1003	149.07	-0.0229	150.0774	232	35.8	Adenine, N6-methyl
150.1003	167.058	-0.045	150.055	264	78.8	3-Methyl-2-nitrobenzyl alcohol
257.1594	256.117	-0.035	257.1244	92	40.7	His-Thr
257.1594	256.11	-0.0422	257.1172	187	49.6	Pterostilbene
257.1594	256.117	-0.035	257.1244	228	39.1	His-Thr
257.1594	256.117	-0.035	257.1244	235	38.2	His-Thr
289.1998	288.209	0.0164	289.2162	4	100	5-Androsten-3.beta.-ol-17-one
289.1998	288.209	0.0164	289.2162	16	12.5	5-Androsten-3.beta.-ol-17-one
289.1998	288.209	0.0164	289.2162	21	11.5	5.alpha.-Androstane-3,17-dione
289.1998	288.209	0.0164	289.2162	42	13.9	5.alpha.-Androstane-3,17-dione
276.1945	275.159	-0.0279	276.1666	99	20.1	Thr-Arg
276.1945	275.159	-0.0279	276.1666	99	52.6	Arg-Thr
276.1945	319.133	-0.0438	276.1507	171	62.8	Norfloxacin
276.1945	0	-0.03	276.16	189	24.6	Homatropine
276.1945	275.159	-0.0279	276.1666	165	48.7	Arg-Thr
276.1945	275.152	-0.0351	276.1594	139	57.4	Methylenedioxypropyvalerone
276.1945	275.152	-0.0351	276.1594	135	60	Methylenedioxypropyvalerone
276.1945	275.152	-0.0351	276.1594	104	57.4	Methylenedioxypropyvalerone
276.1945	275.159	-0.0279	276.1666	123	34	Thr-Arg
276.1945	275.152	-0.0351	276.1594	159	47.9	Methylenedioxypropyvalerone
276.1945	275.159	-0.0279	276.1666	107	23.1	Thr-Arg
276.1945	275.152	-0.0351	276.1594	170	79.3	Methylenedioxypropyvalerone
205.1202	204.075	-0.0383	205.0819	154	76.3	Gly-Glu
205.1202	204.09	-0.023	205.0972	200	60.7	L-Tryptophan
205.1202	204.09	-0.023	205.0972	253	57.5	Fenozolone
205.1202	204.072	-0.0408	205.0794	352	57	Levamisole
205.1202	204.075	-0.0383	205.0819	71	73	Gly-Glu
205.1202	204.09	-0.023	205.0972	297	76.1	L-Tryptophan
205.1202	408.223	-0.001	205.119	207	35.9	Pro-His-Arg
205.1202	204.072	-0.0408	205.0794	331	70.2	Levamisole

150.0787	167.058	-0.024	150.055	210	47.7	3-Methyl-2-nitrobenzyl alcohol
150.0787	167.095	0.0126	150.0913	372	69.1	Synephrine
150.0787	167.058	-0.024	150.055	235	51	3-Methyl-2-nitrobenzyl alcohol
150.0787	167.095	0.0126	150.0913	198	45.9	Synephrine
205.1202	204.075	-0.0383	205.0819	160	40.2	Gly-Glu
205.1202	204.072	-0.0408	205.0794	235	47.4	Levamisole
205.1202	204.072	-0.0408	205.0794	198	20.4	Tetramisole
205.1202	204.072	-0.0408	205.0794	291	73.3	Levamisole
258.1748	275.148	-0.03	258.1448	82	72.8	Lys-Glu
258.1748	275.127	-0.0511	258.1237	124	75.2	Trp-Ala
258.1748	0	0.02	258.19	117	32.6	Dextroprphan
258.1748	257.142	-0.026	258.1488	268	93.2	Medifoxamine
205.1202	204.075	-0.0383	205.0819	82	53.1	Gly-Glu
205.1202	204.075	-0.0383	205.0819	184	94	Gly-Glu
205.1202	204.09	-0.023	205.0972	203	35.9	L-Tryptophan
205.1202	408.237	0.0057	205.1259	258	41.4	Tyr-Val-Lys
205.1202	204.072	-0.0408	205.0794	80	65.5	Levamisole
205.1202	204.09	-0.023	205.0972	278	70.4	L-Tryptophan
205.1202	204.1	-0.013	205.107	224	30.2	1,6-Anhydro-b-D-glucose, permethyl-
205.1202	204.072	-0.0408	205.0794	244	47.7	Tetramisole
150.0885	149.07	-0.0111	150.0774	281	60.4	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	392	93.2	Adenine, N6-methyl
150.0885	149	-0.01	150.08	280	51.8	3-Methyladenine
150.0885	149.07	-0.0111	150.0774	291	80.3	Adenine, N6-methyl
150.0885	167.095	0.0028	150.0913	200	63.7	Synephrine
150.0885	149.07	-0.0111	150.0774	212	77.3	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	301	74.4	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	294	47.4	Adenine, N6-methyl
176.1041	193.058	-0.0494	176.0547	13	58.6	S-(2-Boronoethyl)-L-cysteine
176.1041	175	-0.03	176.07	250	63.2	1-Methoxy-3-carbaldehyde
283.1685	282.179	0.0179	283.1864	128	43.5	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	282.179	0.0179	283.1864	221	49.6	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	282.179	0.0179	283.1864	294	61.8	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	0	-0.02	283.15	193	48.6	Artemisinin
205.1202	204.075	-0.0383	205.0819	96	51.3	Gly-Glu
205.1202	204.072	-0.0408	205.0794	247	71.7	Levamisole
205.1202	204.09	-0.023	205.0972	305	65.5	Fenozolone

205.1202	204.072	-0.0408	205.0794	217	31.4	Tetramisole
134.0966	151.1	-0.0002	134.0964	18	11.6	Norephedrine
134.0966	283.164	-0.0204	134.0762	223	27	Lys-His
134.0966	134.11	0.012	134.109	206	20.7	Benzene, n-butyl-
134.0966	135	-0.05	134.05	220	72.1	Adenine
150.0885	167.095	0.0028	150.0913	195	88.2	Synephrine
150.0885	149.07	-0.0111	150.0774	228	50.2	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	244	54.9	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	247	84.4	Adenine, N6-methyl
205.1202	204.075	-0.0383	205.0819	165	76.5	Gly-Glu
205.1202	408.201	-0.0125	205.1077	160	18.4	Phe-Asp-Lys
205.1202	204.1	-0.013	205.107	171	26.8	1,6-Anhydro-b-D-glucose, permethyl-
205.1202	408.223	-0.001	205.119	237	23.6	Pro-His-Arg
176.0975	175	-0.03	176.07	111	100	1-Methoxy-3-carbaldehyde
176.0975	175.048	-0.0421	176.0554	67	33.5	N-Acetyl-L-aspartic acid
176.0975	175.063	-0.0269	176.0706	31	100	3-Indoleacetic acid
257.1363	256.117	-0.0119	257.1244	144	47	Thr-His
257.1363	256.117	-0.0119	257.1244	128	78.9	Thr-His
257.1363	256.11	-0.0191	257.1172	128	80.4	Pterostilbene
257.1363	256.117	-0.0119	257.1244	112	40.6	Thr-His
238.1227	237.103	-0.0119	238.1108	152	78	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1227	237.086	-0.0292	238.0935	130	37.5	6-Biopterin
238.1227	237.092	-0.0234	238.0993	182	79	Ketamine
238.1227	237.092	-0.0234	238.0993	179	61.4	Ketamine
150.0831	167.095	0.0082	150.0913	129	33.9	Synephrine
150.0831	167.095	0.0082	150.0913	272	79.3	Synephrine
150.0831	149.07	-0.0057	150.0774	352	93.4	Adenine, N6-methyl
150.0831	149.07	-0.0057	150.0774	229	92.3	Adenine, N6-methyl
176.0975	175	-0.03	176.07	138	88.9	1-Methoxy-3-carbaldehyde
176.0975	175	-0.03	176.07	125	73.4	1-Methoxy-3-carbaldehyde
176.0975	175	-0.03	176.07	58	100	1-Methoxy-3-carbaldehyde
176.0975	175.063	-0.0269	176.0706	131	100	3-Indoleacetic acid
150.1003	167.095	-0.009	150.0913	239	79.8	Synephrine
150.1003	149.07	-0.0229	150.0774	292	64.1	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	346	90.7	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	189	77.8	Adenine, N6-methyl
150.1003	169.074	-0.0442	150.0561	226	47	DL-Norepinephrine
150.1003	167.095	-0.009	150.0913	319	41	Synephrine
150.1003	149.07	-0.0229	150.0774	227	80	Adenine, N6-methyl
150.1003	149.12	0.0274	150.1277	361	78.8	Methamphetamine
231.0825	230.09	0.0151	231.0976	30	100	Asp-Pro
231.0825	230.103	0.0279	231.1104	83	53.1	(m- Trifluoromethylphenyl)piperazi ne

231.0825	0	0.03	231.11	122	62.1	N- (3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP)
231.0825	0	0.03	231.11	93	100	N- (3-TRIFLUOROMETHYLPHENYL)PIPERAZINE (TFMPP)
276.1945	275.159	-0.0279	276.1666	205	77.4	Arg-Thr
276.1945	275.159	-0.0279	276.1666	121	62.3	Arg-Thr
276.1945	319.133	-0.0438	276.1507	182	68	Norfloxacin
276.1945	275.152	-0.0351	276.1594	264	77.6	Methylenedioxypropylvalerone
276.1945	275.159	-0.0279	276.1666	167	73.6	Arg-Thr
276.1945	275.152	-0.0351	276.1594	165	83.7	Methylenedioxypropylvalerone
276.1945	275.163	-0.0238	276.1707	117	69	Physostigmine
276.1945	275.152	-0.0351	276.1594	246	69.8	Methylenedioxypropylvalerone
276.1945	275.159	-0.0279	276.1666	203	83.2	Arg-Thr
276.1945	319.133	-0.0438	276.1507	170	74.8	Norfloxacin
276.1945	275.159	-0.0279	276.1666	114	38.2	Arg-Thr
276.1945	275.159	-0.0279	276.1666	155	25	Arg-Thr
150.1003	303.147	-0.009	150.0913	136	68.4	Cocaine
150.1003	149.07	-0.0229	150.0774	204	70	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	158	72	Adenine, N6-methyl
150.1003	167.058	-0.045	150.055	325	79.9	3-Methyl-2-nitrobenzyl alcohol
150.1003	167.095	-0.009	150.0913	159	78	Synephrine
150.1003	149.07	-0.0229	150.0774	289	73.6	Adenine, N6-methyl
150.1003	149.12	0.0274	150.1277	261	69.5	Methamphetamine
150.1003	149.07	-0.0229	150.0774	236	92.2	Adenine, N6-methyl
205.1202	204.075	-0.0383	205.0819	115	46.7	Gly-Glu
205.1202	408.223	-0.001	205.119	198	67.7	Pro-His-Arg
205.1202	204.072	-0.0408	205.0794	249	20.1	Levamisole
205.1202	204.1	-0.013	205.107	202	35.6	1,6-Anhydro-b-D-glucose, permethyl-
150.1003	167.095	-0.009	150.0913	264	76.1	Synephrine
150.1003	149.07	-0.0229	150.0774	344	98.5	Adenine, N6-methyl
150.1003	149.12	0.0274	150.1277	177	61.2	Methamphetamine
150.1003	149.07	-0.0229	150.0774	157	42.1	Adenine, N6-methyl
176.1041	175	-0.03	176.07	59	82.2	1-Methoxy-3-carbaldehyde
176.1041	175	-0.03	176.07	80	85.6	1-Methoxy-3-carbaldehyde
176.1041	175.063	-0.0335	176.0706	254	84	3-Indoleacetic acid
205.1202	204.072	-0.0408	205.0794	192	93.3	Tetramisole
205.1202	408.223	-0.001	205.119	146	26.1	Pro-His-Arg
205.1202	204.09	-0.023	205.0972	319	70.7	Fenozolone
205.1202	408.212	-0.0069	205.1133	266	18.5	Tyr-Ala-Arg
205.1202	204.075	-0.0383	205.0819	81	62.3	Ala-Asp
205.1202	204.09	-0.023	205.0972	254	74.9	Fenozolone

205.1202	204.1	-0.013	205.107	202	37.4	1,6-Anhydro-b-D-glucose, permethyl-
205.1202	204.09	-0.023	205.0972	284	39.1	Fenozolone
150.1003	303.147	-0.009	150.0913	118	70.5	Cocaine
150.1003	149.07	-0.0229	150.0774	195	71.2	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	288	76.2	Synephrine
150.1003	150.128	0.0274	150.1277	215	60.7	N-Butyl-4-methylpyridinium
205.1202	204.072	-0.0408	205.0794	66	56.6	Levamisole
205.1202	204.09	-0.023	205.0972	119	77	Fenozolone
205.1202	408.223	-0.001	205.119	119	36.3	Pro-His-Arg
205.1202	204.072	-0.0408	205.0794	145	35.1	Levamisole
276.1945	275.159	-0.0279	276.1666	100	40.5	Thr-Arg
276.1945	275.152	-0.0351	276.1594	186	79.8	Methylenedioxypropylvalerone
276.1945	275.152	-0.0351	276.1594	122	80.9	Methylenedioxypropylvalerone
276.1945	275.152	-0.0351	276.1594	229	92.7	Methylenedioxypropylvalerone
205.1202	204.075	-0.0383	205.0819	114	100	Gly-Glu
205.1202	204.09	-0.023	205.0972	151	38.2	Fenozolone
205.1202	204.09	-0.023	205.0972	191	35.6	Ethotoin
150.1003	149.07	-0.0229	150.0774	50	43.9	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	85	45.3	Adenine, N6-methyl
150.1003	150.128	0.0274	150.1277	236	73.8	N-Butyl-4-methylpyridinium
150.1003	149.07	-0.0229	150.0774	72	66	Adenine, N6-methyl
163.1358	162.116	-0.013	163.123	18	21	Anabasine
163.1358	162.116	-0.013	163.123	13	100	Nicotine
163.1358	162.126	-0.0029	163.1329	274	94.1	Ethanol, 2-(2-butoxyethoxy)-
163.1358	162.116	-0.013	163.123	247	68.8	Nicotine
515.4017	514.406	0.0112	515.4129	192	100	Propanoic acid, 3,3'-thiobis-, didodecyl ester
515.4017	514.406	0.0112	515.4129	279	100	Propanoic acid, 3,3'-thiobis-, didodecyl ester
515.4017	514.406	0.0112	515.4129	284	100	Propanoic acid, 3,3'-thiobis-, didodecyl ester
425.2912	426.295	-0.003	425.2882	77	38.7	Leupeptin
425.2912	424.255	-0.0293	425.2619	134	51	His-Ile-Arg
303.2336	320.235	-0.0017	303.2319	51	16.3	15(S)-Hydroxy-(5Z,8Z,11Z,13E)-eicosatetraenoic acid
303.2336	320.235	-0.0017	303.2319	121	43.9	15(S)-Hydroxy-(5Z,8Z,11Z,13E)-eicosatetraenoic acid
303.2336	302.225	-0.0017	303.2319	206	34.4	17.alpha.-Methyltestosterone
303.2336	320.235	-0.0017	303.2319	356	66.3	15(S)-Hydroxy-(5Z,8Z,11Z,13E)-eicosatetraenoic acid
211.1671	0	-0.04	211.13	238	45.2	Jasmonic acid
211.1671	210.126	-0.0342	211.1329	279	66.9	Jasmonic Acid
211.1671	210.126	-0.0342	211.1329	470	74.7	Jasmonic Acid

211.1671	210.126	-0.0342	211.1329	408	60.3	Jasmonic Acid
283.1685	260.148	-0.0308	283.1377	108	29.9	Lys-Asn
283.1685	282.179	0.0179	283.1864	61	33	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	0	-0.02	283.15	145	54.9	Artemisinin
283.1685	0	-0.02	283.15	149	58.9	Artemisinin
283.1685	0	-0.02	283.15	103	49.8	Artemisinin
283.1685	282.122	-0.0396	283.1289	14	54.2	Tyr-Thr
283.1685	282.179	0.0179	283.1864	74	61.1	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	0	-0.02	283.15	150	72.5	Artemisinin
115.0768	114.025	-0.0444	115.0324	3	100	Methimazole
211.1441	210.1	-0.0364	211.1077	234	77.9	Aprobarbital
211.1441	0	-0.01	211.13	232	36.5	Jasmonic acid
211.1441	210.126	-0.0112	211.1329	266	69.1	Jasmonic Acid
211.1441	420.249	-0.0126	211.1315	228	33.9	Phe-Val-Arg
211.1441	210.126	-0.0112	211.1329	195	42.8	Jasmonic Acid
211.1441	228.147	0	211.1441	308	78.2	Ile-Pro
211.1441	420.249	-0.0126	211.1315	267	38.5	Phe-Val-Arg
211.1441	420.249	-0.0126	211.1315	266	67.4	Phe-Val-Arg
211.1441	420.179	-0.0473	211.0968	244	59.8	Met-Asp-Arg
211.1441	228.147	0	211.1441	268	67.7	Ile-Pro
211.1441	210.1	-0.0364	211.1077	244	44	Aprobarbital
211.1441	420.179	-0.0473	211.0968	201	48.8	Met-Asp-Arg
532.3931	509.385	-0.0194	532.3737	43	100	Lyso-PAF C-18
532.3931	514.318	-0.0417	532.3514	297	100	3,6,9,12,15-Pentaoxonacosan-1-ol, hydrogen sulfate
532.3931	514.318	-0.0417	532.3514	289	100	3,6,9,12,15-Pentaoxonacosan-1-ol, hydrogen sulfate
532.3931	514.318	-0.0417	532.3514	190	100	3,6,9,12,15-Pentaoxonacosan-1-ol, hydrogen sulfate
532.3856	509.385	-0.0119	532.3737	50	100	Lyso-PAF C-18
532.3856	514.318	-0.0342	532.3514	275	100	3,6,9,12,15-Pentaoxonacosan-1-ol, hydrogen sulfate
532.3856	514.318	-0.0342	532.3514	343	100	3,6,9,12,15-Pentaoxonacosan-1-ol, hydrogen sulfate
532.3856	514.318	-0.0342	532.3514	128	100	3,6,9,12,15-Pentaoxonacosan-1-ol, hydrogen sulfate
283.1685	260.148	-0.0308	283.1377	174	63.6	Lys-Asn

283.1685	300.173	0.0008	283.1693	107	41.3	2-Methoxyestrone
283.1685	282.122	-0.0396	283.1289	147	64.5	Tyr-Thr
283.1685	0	-0.02	283.15	103	71	Artemisinin
211.1813	210.159	-0.0147	211.1666	18	100	Altretamine
211.1813	420.249	-0.0498	211.1315	268	56.1	Phe-Val-Arg
211.1813	0	-0.05	211.13	257	34.4	Jasmonic acid
211.1813	210.126	-0.0484	211.1329	89	43.9	Jasmonic Acid
276.2063	275.159	-0.0397	276.1666	105	47.1	Thr-Arg
276.2063	275.152	-0.0469	276.1594	173	38.4	Homatropine
276.2063	275.159	-0.0397	276.1666	106	44.3	Arg-Thr
276.2063	275.152	-0.0469	276.1594	185	75.5	Methylenedioxypropylvalerone
163.0993	164.068	-0.0381	163.0612	288	68.5	L-(+)-Rhamnose
163.0993	179.095	-0.0239	163.0754	295	79.4	3,4-Methylenedioxyamphetamine
163.0993	179.095	-0.0239	163.0754	338	37.3	3,4-Methylenedioxyamphetamine
163.0993	179.095	-0.0239	163.0754	343	82.7	3,4-Methylenedioxyamphetamine
211.1113	0	0.02	211.13	182	52	Jasmonic acid
211.1113	210.126	0.0216	211.1329	236	21.8	Jasmonic Acid
211.1113	210.126	0.0216	211.1329	268	54	Jasmonic Acid
211.1113	210.1	-0.0036	211.1077	145	45.6	Aprobarbital
211.1113	0	0.02	211.13	115	30.8	Jasmonic acid
211.1113	210.1	-0.0036	211.1077	206	35.7	Aprobarbital
211.1113	210.1	-0.0036	211.1077	245	23	Aprobarbital
211.1113	420.249	0.0202	211.1315	188	37.6	Phe-Val-Arg
283.1823	300.209	0.0233	283.2056	130	46	9-cis-Retinoic acid
283.1823	282.181	0.0061	283.1884	278	71.3	Doxepin-D3
283.1823	300.173	-0.013	283.1693	222	56	2-Methoxyestrone
283.1823	0	-0.03	283.15	235	72.3	Artemisinin
211.132	188.116	-0.0267	211.1053	21	40.2	Ile-Gly
211.132	0	0	211.13	227	43	Jasmonic acid
211.132	228.147	0.0121	211.1441	279	38.2	Ile-Pro
211.132	0	-0.03	211.1	243	38.6	Sinapyl alcohol
150.0885	167.095	0.0028	150.0913	153	71.3	Synephrine
150.0885	167.095	0.0028	150.0913	372	65.5	Synephrine
150.0885	149.07	-0.0111	150.0774	272	82.1	Adenine, N6-methyl
150.0885	149.12	0.0392	150.1277	345	53.8	Methamphetamine
205.1202	204.075	-0.0383	205.0819	192	36	Gly-Glu
205.1202	204.075	-0.0383	205.0819	181	42.6	alpha.-L-Glu-Gly
205.1202	204.072	-0.0408	205.0794	228	22.3	Tetramisole
205.1202	204.09	-0.023	205.0972	259	20	L-Tryptophan
205.1202	204.075	-0.0383	205.0819	142	33.6	alpha.-L-Glu-Gly
205.1202	204.072	-0.0408	205.0794	207	19.2	Levamisole
205.1202	0	-0.04	205.08	258	28.4	gamma-D-Glutamylglycine
205.1202	408.237	0.0057	205.1259	335	81.2	Tyr-Val-Lys
205.1202	408.161	-0.0323	205.0879	128	44	Cys-Met-Arg

205.1202	0	-0.04	205.08	260	49.7	gamma-D-Glutamylglycine
205.1202	204.09	-0.023	205.0972	221	29.3	L-Tryptophan
205.1202	408.237	0.0057	205.1259	232	21.4	Tyr-Val-Lys
115.0571	0	-0.03	115.03	189	62.9	Methimazole
211.1548	210.126	-0.0219	211.1329	243	69.8	Jasmonic Acid
211.1548	210.126	-0.0219	211.1329	266	44.8	Jasmonic Acid
211.1548	210.126	-0.0219	211.1329	236	33.5	Jasmonic Acid
211.1548	420.249	-0.0233	211.1315	256	25.6	Phe-Val-Arg
205.1202	0	-0.04	205.08	116	18.4	gamma-D-Glutamylglycine
205.1202	204.1	-0.013	205.107	262	45	1,6-Anhydro-b-D-glucose, permethyl-
205.1202	408.237	0.0057	205.1259	255	24	Tyr-Val-Lys
205.1202	204.1	-0.013	205.107	200	19.5	1,6-Anhydro-b-D-glucose, permethyl-
211.1548	210.126	-0.0219	211.1329	182	31.1	Jasmonic Acid
211.1548	0	-0.02	211.13	250	71.6	Jasmonic acid
211.1548	210.1	-0.0471	211.1077	256	38.7	Aprobarbital
211.1548	210.1	-0.0471	211.1077	268	48.6	Aprobarbital
115.0571	114.025	-0.0247	115.0324	50	32	Methimazole
115.0571	0	-0.01	115.05	196	50.1	Dihydrouracil
115.0571	0	-0.03	115.03	8	36.1	Methimazole
115.0571	114.043	-0.0069	115.0502	17	100	Dihydrouracil
115.0571	132.042	-0.018	115.039	86	55.1	Glutaric acid
176.0975	193.058	-0.0428	176.0547	99	73.7	S-(2-Boronoethyl)-L-cysteine
176.0975	175	-0.03	176.07	152	76.5	1-Methoxy-3-carbaldehyde
176.0975	175.063	-0.0269	176.0706	238	55.4	3-Indoleacetic acid
258.1677	0	-0.05	258.12	195	76.3	4'-(DIMETHYLAMINO)AZOXY BENZENE N-OXIDE
258.1677	0	-0.05	258.12	162	81.2	4'-(DIMETHYLAMINO)AZOXY BENZENE N-OXIDE
258.1677	0	0.02	258.19	81	100	Dextrorphan
258.1677	0	0.02	258.19	265	74.9	Dextrorphan
343.2033	342.215	0.0194	343.2227	29	100	Loxistatin
343.2033	344.235	0.0246	343.2279	168	67.7	(+/-)-10-hydroxy-4Z,7Z,11E,13Z,16Z,19Z-docosahexaenoic acid
343.2033	342.215	0.0194	343.2227	136	82.8	Loxistatin
343.2033	342.227	0.031	343.234	139	66.8	Val-Pro-Lys
266.1481	265.168	0.027	266.1751	41	100	Oxprenolol
266.1481	265.095	-0.0458	266.1023	181	83.7	3,4-Dihydroxycinnamic acid (L-alanine methyl ester) amide
266.1481	265.15	0.0092	266.1573	196	29.6	Esprocarb
266.1481	265.168	0.027	266.1751	44	100	Oxprenolol

283.1685	300.173	0.0008	283.1693	95	62.5	2-Methoxyestrone
283.1685	0	-0.02	283.15	223	43	Artemisinin
283.1685	0	-0.02	283.15	306	81.1	Artemisinin
283.1685	0	-0.02	283.15	313	90.3	Artemisinin
176.0975	175.084	-0.0058	176.0917	97	79	N-Carboxyethyl-.gamma.-aminobutyric acid
176.0975	175	-0.03	176.07	143	70.4	1-Methoxy-3-carbaldehyde
150.1003	149.07	-0.0229	150.0774	150	75.7	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	294	84.7	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	317	74.7	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	241	50.6	Synephrine
150.1003	149.084	-0.009	150.0913	54	48.9	S(-)-Cathinone
150.1003	149.105	0.0122	150.1125	220	67.5	Triethanolamine
150.1003	167.095	-0.009	150.0913	229	72.5	Synephrine
150.1003	149.07	-0.0229	150.0774	310	56.8	Adenine, N6-methyl
211.1441	188.116	-0.0388	211.1053	93	68.4	Ile-Gly
211.1441	210.126	-0.0112	211.1329	140	32.2	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	209	31.9	Jasmonic Acid
211.1441	210.1	-0.0364	211.1077	288	79.5	Aprobarbital
276.1945	275.159	-0.0279	276.1666	114	51.4	Thr-Arg
276.1945	319.133	-0.0438	276.1507	61	60.8	Norfloxacin
276.1945	319.133	-0.0438	276.1507	137	69.9	Norfloxacin
276.1945	275.152	-0.0351	276.1594	200	48	Homatropine
276.1945	275.148	-0.0391	276.1554	104	20.5	Glu-Lys
276.1945	275.152	-0.0351	276.1594	145	34.7	4-Hydroxypropranolol
276.1945	319.133	-0.0438	276.1507	105	53.5	Norfloxacin
276.1945	275.152	-0.0351	276.1594	136	66.1	Homatropine
276.1945	275.159	-0.0279	276.1666	174	39.5	Thr-Arg
276.1945	275.152	-0.0351	276.1594	129	47.1	Methylenedioxyprovalerone
276.1945	275.159	-0.0279	276.1666	179	21.1	Thr-Arg
276.1945	319.133	-0.0438	276.1507	202	45.1	Norfloxacin
150.0885	167.095	0.0028	150.0913	182	60	Synephrine
150.0885	149.07	-0.0111	150.0774	337	96.3	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	307	87.6	Adenine, N6-methyl
150.0885	167.095	0.0028	150.0913	316	82.8	Synephrine
115.0709	0	-0.02	115.05	126	43.7	3-Cyano-L-alanine
115.0709	132.053	-0.0207	115.0502	11	100	3-Ureidopropionic acid
211.1441	210.126	-0.0112	211.1329	87	29.6	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	71	15.5	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	232	40.6	Jasmonic Acid
211.1441	0	-0.01	211.13	264	42.3	Jasmonic acid
211.1113	188.116	-0.006	211.1053	77	26.8	Ile-Gly
211.1113	210.126	0.0216	211.1329	192	28.2	Jasmonic Acid
211.1113	210.1	-0.0036	211.1077	260	62.5	Aprobarbital
211.1113	210.1	-0.0036	211.1077	207	43.4	Aprobarbital
115.0692	0	-0.02	115.05	113	25.6	Dihydrouracil
115.0692	114.025	-0.0368	115.0324	48	56.6	Methimazole

276.1945	275.159	-0.0279	276.1666	130	28.9	Thr-Arg
276.1945	275.159	-0.0279	276.1666	144	22.2	Arg-Thr
276.1945	275.152	-0.0351	276.1594	170	52.7	Methylenedioxypropylvalerone
276.1945	275.159	-0.0279	276.1666	202	25.5	Thr-Arg
343.209	342.202	-0.0002	343.2088	170	12.4	Ala-Pro-Arg
343.209	342.215	0.0137	343.2227	190	55.9	Loxistatin
343.209	342.215	0.0137	343.2227	182	33.4	Loxistatin
343.209	342.215	0.0137	343.2227	231	49.8	Loxistatin
276.1945	275.159	-0.0279	276.1666	214	58.7	Thr-Arg
276.1945	275.159	-0.0279	276.1666	206	55.9	Thr-Arg
276.1945	319.133	-0.0438	276.1507	157	37.2	Norfloxacin
276.1945	275.152	-0.0351	276.1594	185	43.2	Homatropine
343.2127	344.235	0.0152	343.2279	189	78	(+/-)-4-hydroxy-5E,7Z,10Z,13Z,16Z,19Z-docosahexaenoic acid
343.2127	342.256	0.0505	343.2632	170	52.8	Retinyl propionate
343.2127	171.126	0.0464	343.2591	251	54.4	Gabapentin
343.2127	171.126	0.0464	343.2591	236	47.7	Gabapentin
257.1363	256.117	-0.0119	257.1244	176	25.3	His-Thr
257.1363	256.117	-0.0119	257.1244	200	45	Thr-His
257.1363	256.117	-0.0119	257.1244	301	28.7	Thr-His
257.1363	256.117	-0.0119	257.1244	164	38.3	Thr-His
150.0787	149.07	-0.0013	150.0774	145	41.4	Adenine, N6-methyl
150.0787	149.07	-0.0013	150.0774	351	97.5	Adenine, N6-methyl
150.0787	167.095	0.0126	150.0913	363	82.6	Synephrine
150.0787	149.07	-0.0013	150.0774	343	52.5	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	229	72.7	Synephrine
150.1003	167.095	-0.009	150.0913	303	55.9	Synephrine
150.1003	149.07	-0.0229	150.0774	372	93	Adenine, N6-methyl
150.1003	167.058	-0.045	150.055	286	52.9	3-Methyl-2-nitrobenzyl alcohol
150.0885	149.07	-0.0111	150.0774	353	89.7	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	266	43.9	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	409	96.3	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	263	56	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	242	46	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	261	71.1	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	342	75.2	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	231	47.4	Adenine, N6-methyl
225.1804	0	-0.03	225.15	261	79.9	Methyl jasmonate
225.1804	0	-0.03	225.15	357	84.5	Methyl jasmonate
225.1804	0	-0.03	225.15	286	86.2	Methyl jasmonate
225.1804	0	-0.03	225.15	403	97.7	Methyl jasmonate
211.1548	0	-0.02	211.13	139	35.6	Jasmonic acid
211.1548	210.126	-0.0219	211.1329	280	45.6	Jasmonic Acid
211.1548	210.126	-0.0219	211.1329	255	34.7	Jasmonic Acid
211.1548	0	-0.02	211.13	303	53.8	Jasmonic acid

150.1003	149.07	-0.0229	150.0774	292	87.2	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	292	92.3	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	266	55.6	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	254	67.7	Adenine, N6-methyl
205.1202	204.075	-0.0383	205.0819	169	97.4	Gly-Glu
205.1202	204.1	-0.013	205.107	189	44.3	1,6-Anhydro-b-D-glucose, permethyl-
205.1202	204.072	-0.0408	205.0794	299	54.4	Tetramisole
205.1202	204.072	-0.0408	205.0794	251	26.3	Levamisole
137.0462	136.039	-0.0004	137.0458	26	8.8	Allopurinol
137.0462	136.039	-0.0004	137.0458	314	81.8	Hypoxanthine
137.0462	136.039	-0.0004	137.0458	91	13.6	Hypoxanthine
137.0462	154.063	0.0135	137.0597	134	24.6	2-Hydroxy-3-methoxybenzyl alcohol
205.1202	204.072	-0.0408	205.0794	196	60.3	Tetramisole
205.1202	204.1	-0.013	205.107	251	54.9	1,6-Anhydro-b-D-glucose, permethyl-
205.1202	204.072	-0.0408	205.0794	185	36.5	Levamisole
205.1202	204.072	-0.0408	205.0794	357	53.9	Levamisole
150.0885	149	-0.01	150.08	135	41.8	3-Methyladenine
150.0885	149.07	-0.0111	150.0774	408	96.2	Adenine, N6-methyl
150.0885	149.07	-0.0111	150.0774	378	81.4	Adenine, N6-methyl
150.0885	167.095	0.0028	150.0913	295	81	Synephrine
137.0462	154.027	-0.0229	137.0233	2	100	.beta.-Resorcylic acid
137.0462	154.027	-0.0229	137.0233	114	18.3	Benzoic acid, 2,3-dihydroxy-
137.0462	136.039	-0.0004	137.0458	20	8.3	Hypoxanthine
137.0462	136.039	-0.0004	137.0458	58	20.6	Hypoxanthine
283.1685	282.179	0.0179	283.1864	101	66	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	0	-0.02	283.15	219	68	Artemisinin
283.1685	282.122	-0.0396	283.1289	241	28.1	Thr-Tyr
283.1685	282.179	0.0179	283.1864	276	64.3	1,3-Bis(tris(hydroxymethyl)methylamino)propane
205.1202	204.075	-0.0383	205.0819	178	51.4	Gly-Glu
205.1202	408.161	-0.0323	205.0879	173	22.4	Cys-Met-Arg
205.1202	204.072	-0.0408	205.0794	201	21.3	Levamisole
205.1202	204.072	-0.0408	205.0794	356	69.3	Tetramisole
150.1003	167.095	-0.009	150.0913	264	93.6	Synephrine
150.1003	149.07	-0.0229	150.0774	321	73.5	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	387	94.8	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	265	56	Synephrine
276.1945	275.159	-0.0279	276.1666	199	70.5	Arg-Thr
276.1945	275.159	-0.0279	276.1666	133	24.9	Thr-Arg
276.1945	275.152	-0.0351	276.1594	207	90.8	Methylenedioxyprovalerone
276.1945	275.152	-0.0351	276.1594	276	78.4	Methylenedioxyprovalerone

276.2063	275.159	-0.0397	276.1666	235	70.1	Arg-Thr
276.2063	275.159	-0.0397	276.1666	219	78.4	Arg-Thr
276.2063	275.152	-0.0469	276.1594	152	80.4	Methylenedioxypropylvalerone
276.2063	275.152	-0.0469	276.1594	255	74.9	Homatropine
211.1247	188.116	-0.0194	211.1053	18	16.6	Ile-Gly
211.1247	420.223	-0.006	211.119	36	11.8	His-His-Lys
211.1247	210.126	0.0082	211.1329	94	20.7	Jasmonic Acid
211.1247	210.126	0.0082	211.1329	152	28.6	Jasmonic Acid
211.1247	0	0.01	211.13	40	16.3	Jasmonic acid
211.1247	0	0.01	211.13	92	44	Jasmonic acid
211.1247	0	-0.04	211.08	96	17.4	D-Glucoheptose
211.1247	420.249	0.0068	211.1315	75	14.4	Phe-Val-Arg
211.128	210.126	0.0049	211.1329	37	11.4	Jasmonic Acid
211.128	0	0	211.13	138	17.1	Jasmonic acid
211.128	210.126	0.0049	211.1329	99	17.1	Jasmonic Acid
211.128	0	0	211.13	146	44.4	Jasmonic acid
163.1098	162	0	163.11	171	47.4	DL-5-Hydroxylysine hydrochloride
163.1098	162.1	-0.0021	163.1077	248	52.8	DL-Lysine, 5-hydroxy-
163.1098	162	0	163.11	275	33.5	DL-5-Hydroxylysine hydrochloride
163.1098	162.116	0.013	163.123	319	60.7	Anabasine
133.097	150.079	-0.021	133.076	10	50	3-Methylbenzamide oxime
133.097	150.068	-0.032	133.0648	236	68.1	(2S,3S)-(-)-3-Phenylglycidol
133.097	150.068	-0.032	133.0648	320	73.2	(2S,3S)-(-)-3-Phenylglycidol
133.097	150.068	-0.032	133.0648	253	41.2	(2S,3S)-(-)-3-Phenylglycidol
276.2157	0	-0.05	276.17	82	67.3	cyclobenzaprine
205.1375	188.116	-0.0181	205.1194	172	73.5	Glycyl-L-norleucine
205.1375	408.223	-0.018	205.119	185	44.2	Pro-His-Arg
205.1375	408.237	-0.0116	205.1259	158	62.8	Tyr-Val-Lys
205.1375	408.212	-0.0242	205.1133	344	58.2	Phe-Ser-Arg
276.2157	258.183	0.0012	276.2169	55	100	Tetradecanedioic acid
276.2157	258.183	0.0012	276.2169	77	83.8	Tetradecanedioic acid
276.2157	0	-0.05	276.17	85	100	cyclobenzaprine
276.2157	0	-0.05	276.17	128	87.1	cyclobenzaprine
176.1125	175.096	-0.009	176.103	43	100	L-Citrulline
176.1125	175	-0.04	176.07	167	73.6	1-Methoxy-3-carbaldehyde
163.1098	162.064	-0.0385	163.0713	103	48.3	Gly-Ser
163.1098	179.095	-0.0344	163.0754	148	32.1	3,4- Methylenedioxyamphetamine
163.1098	162	0	163.11	254	43.6	DL-5-Hydroxylysine hydrochloride
163.1098	162.116	0.013	163.123	231	60	Anabasine
149.0962	148.074	-0.0154	149.0808	279	76.8	Mevalonic acid
149.0962	165.115	-0.0001	149.0961	347	99	(+/-)-p-Methoxyamphetamine

149.0962	165.115	-0.0001	149.0961	343	91.5	(+/-)-p-Methoxyamphetamine
149.0962	165.115	-0.0001	149.0961	306	69.7	(+/-)-p-Methoxyamphetamine
205.1375	188.116	-0.0181	205.1194	132	60.6	Glycyl-L-norleucine
205.1375	188.116	-0.0181	205.1194	114	21.1	Glycyl-L-norleucine
205.1375	408.161	-0.0496	205.0879	127	30.5	Cys-Met-Arg
205.1375	204.09	-0.0403	205.0972	267	30.7	Fenozolone
205.1375	188.116	-0.0181	205.1194	163	94.1	Glycyl-L-norleucine
205.1375	188.116	-0.0181	205.1194	126	20.9	Glycyl-L-norleucine
205.1375	408.223	-0.018	205.119	303	65.8	Pro-His-Arg
205.1375	408.237	-0.0116	205.1259	325	44.9	Tyr-Val-Lys
163.1064	179.095	-0.031	163.0754	140	74.8	3,4-Methylenedioxyamphetamine
163.1064	162.126	0.0264	163.1329	211	67	Ethanol, 2-(2-butoxyethoxy)-
163.1064	164.068	-0.0452	163.0612	222	44.6	L-(+)-Rhamnose
163.1064	162.116	0.017	163.123	241	38	Anabasine
163.1098	179.095	-0.0344	163.0754	97	22.9	3,4-Methylenedioxyamphetamine
163.1098	162.1	-0.0021	163.1077	131	33.8	DL-Lysine, 5-hydroxy-
163.1098	162.116	0.013	163.123	302	63.5	Anabasine
163.1098	162.1	-0.0021	163.1077	282	69.2	DL-Lysine, 5-hydroxy-
327.2164	344.235	0.0155	327.2319	115	72	Medroxyprogesterone
327.2164	344.199	-0.0209	327.1955	144	46.9	Tetrahydrocannabinol(nor-delta-9-HOOC)
327.2164	344.199	-0.0209	327.1955	170	35.5	Tetrahydrocannabinol(nor-delta-9-HOOC)
283.1898	0	-0.04	283.15	134	37.5	Artemisinin
283.1898	300.173	-0.0205	283.1693	147	39.9	2-Methoxyestrone
283.1898	0	-0.04	283.15	275	76.3	Artemisinin
283.1898	0	-0.04	283.15	239	49.2	Artemisinin
283.1898	0	-0.04	283.15	127	47.4	Artemisinin
283.1898	282.179	-0.0034	283.1864	182	48.1	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1898	0	-0.04	283.15	222	68.3	Artemisinin
283.1898	0	-0.04	283.15	263	78.1	Artemisinin
283.1898	0	-0.04	283.15	111	42.7	Artemisinin
283.1898	282.179	-0.0034	283.1864	236	62.8	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1898	300.173	-0.0205	283.1693	187	41	2-Methoxyestrone
283.1898	300.173	-0.0205	283.1693	218	49.2	2-Methoxyestrone
257.1488	256.117	-0.0244	257.1244	187	43	Thr-His
257.1488	256.117	-0.0244	257.1244	180	53.3	Thr-His
257.1488	256.117	-0.0244	257.1244	157	26.3	Thr-His
257.1488	256.117	-0.0244	257.1244	188	38.9	His-Thr

205.1202	204.075	-0.0383	205.0819	131	63.4	Gly-Glu
205.1202	204.1	-0.013	205.107	146	27.3	1,6-Anhydro-b-D-glucose, permethyl-
205.1202	204.072	-0.0408	205.0794	340	74.8	Levamisole
205.1202	408.223	-0.001	205.119	206	20.7	His-Pro-Arg
283.1854	0	-0.04	283.15	102	43.1	Artemisinin
283.1854	282.179	0.001	283.1864	224	91.1	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1854	282.179	0.001	283.1864	244	77.7	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1854	0	-0.04	283.15	308	69.3	Artemisinin
283.1898	0	-0.04	283.15	122	44.3	Artemisinin
283.1898	282.179	-0.0034	283.1864	220	71.4	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1898	0	-0.04	283.15	198	44.7	Artemisinin
283.1898	0	-0.04	283.15	264	75.4	Artemisinin
343.3048	342.256	-0.0416	343.2632	34	77.3	Retinyl propionate
343.3048	342.256	-0.0416	343.2632	71	70	Retinyl propionate
327.2164	344.199	-0.0209	327.1955	96	58	Tetrahydrocannabinol(nor-delta-9-HOOC)
327.2164	326.199	-0.0097	327.2067	224	51.8	Ajmaline
327.2164	0	-0.01	327.21	139	70.8	Hydroquinidine
327.2164	326.192	-0.0176	327.1988	75	60	Dodecylbenzenesulfonic acid
327.2164	0	-0.01	327.21	172	59	Ajmaline
327.2164	326.192	-0.0176	327.1988	118	31.3	Dodecylbenzenesulfonic acid
176.1195	175	-0.05	176.07	128	48.8	1-Methoxy-3-carbaldehyde
176.1195	175	-0.05	176.07	122	45.8	1-Methoxy-3-carbaldehyde
176.1195	175	-0.05	176.07	121	70.2	1-Methoxy-3-carbaldehyde
169.1192	168.115	0.0031	169.1223	166	81.1	Jasmine lactone
169.1192	168.115	0.0031	169.1223	228	84.8	Jasmine lactone
169.1192	168.115	0.0031	169.1223	228	88.9	Jasmine lactone
169.1192	168.09	-0.022	169.0972	308	55.4	Pyridoxamine
169.1215	336.147	-0.0409	169.0806	159	45.2	Ser-Cys-Lys
169.1215	336.147	-0.0409	169.0806	250	65	Ser-Cys-Lys
169.1215	168.115	0.0008	169.1223	209	69.9	Jasmine lactone
169.1215	168.09	-0.0243	169.0972	170	42.4	Pyridoxamine
163.1028	162.064	-0.0315	163.0713	83	41.7	Gly-Ser
163.1028	162.126	0.0301	163.1329	215	46.6	Ethanol, 2-(2-butoxyethoxy)-
163.1028	162.116	0.02	163.123	345	80	Anabasine
163.1028	162.116	0.02	163.123	474	90.9	Anabasine
276.1945	275.159	-0.0279	276.1666	171	39.1	Arg-Thr
276.1945	0	-0.03	276.16	160	30.8	Homatropine
276.1945	0	-0.03	276.16	220	77.4	Homatropine
276.1945	275.152	-0.0351	276.1594	285	74.2	Homatropine

164.0069	163.046	0.0459	164.0528	74	44	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	118	67.7	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	151	80	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	147	60	4-Hydroxy-L-glutamic acid
327.2164	326.199	-0.0097	327.2067	70	60	Ajmaline
327.2164	344.199	-0.0209	327.1955	128	100	Tetrahydrocannabinol(nor-delta-9-HOOC)
327.2164	326.192	-0.0176	327.1988	156	47.8	Dodecylbenzenesulfonic acid
176.1195	175.121	0.0086	176.1281	301	65.6	Threonine, butyl ester
176.1195	175	-0.05	176.07	78	79.6	1-Methoxy-3-carbaldehyde
176.1195	175	-0.05	176.07	105	56.6	1-Methoxy-3-carbaldehyde
205.1375	188.116	-0.0181	205.1194	155	90.1	Glycyl-L-norleucine
205.1375	204.09	-0.0403	205.0972	201	92.9	Fenozolone
205.1375	204.09	-0.0403	205.0972	263	73.3	Fenozolone
205.1375	408.201	-0.0298	205.1077	341	52.1	Phe-Asp-Lys
149.0908	148	-0.05	149.04	89	64.1	(S)-(+)-Citramalic acid
149.0908	148.1	0.0165	149.1073	130	76.5	Normicotine
149.0908	165.115	0.0053	149.0961	146	78.2	(+/-)-p-Methoxyamphetamine
149.0908	148.1	0.0165	149.1073	197	64.7	N-Benzylacetamidine
149.1107	148.1	-0.0034	149.1073	11	39	N-Benzylacetamidine
149.1107	165.115	-0.0146	149.0961	142	86.8	(+/-)-p-Methoxyamphetamine
149.1107	148.1	-0.0034	149.1073	196	55.4	N-Benzylacetamidine
149.1107	166.063	-0.051	149.0597	261	71.6	Tropic acid
149.0962	165.115	-0.0001	149.0961	169	95.2	(+/-)-p-Methoxyamphetamine
149.0962	165.115	-0.0001	149.0961	177	76.2	(+/-)-p-Methoxyamphetamine
149.0962	165.115	-0.0001	149.0961	118	81.2	(+/-)-p-Methoxyamphetamine
149.0962	165.115	-0.0001	149.0961	239	80.7	(+/-)-p-Methoxyamphetamine
371.2391	370.196	-0.0354	371.2037	19	100	His-Ser-Lys
149.0962	165.115	-0.0001	149.0961	86	82.8	(+/-)-p-Methoxyamphetamine
149.0962	165.115	-0.0001	149.0961	201	80.4	(+/-)-p-Methoxyamphetamine
149.0962	165.115	-0.0001	149.0961	191	83.8	(+/-)-p-Methoxyamphetamine
149.0962	165.115	-0.0001	149.0961	219	77.3	(+/-)-p-Methoxyamphetamine
150.1003	167.095	-0.009	150.0913	139	49.6	Synephrine
150.1003	149.07	-0.0229	150.0774	288	70.8	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	286	87.5	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	285	66.6	Adenine, N6-methyl
205.1202	188.116	-0.0008	205.1194	188	78.3	Glycyl-L-norleucine

205.1202	204.075	-0.0383	205.0819	142	60.4	Gly-Glu
205.1202	408.223	-0.001	205.119	214	12	His-Pro-Arg
205.1202	204.09	-0.023	205.0972	221	19	Fenozolone
176.1125	350.195	-0.007	176.105	61	65.8	Phe-Gly-Lys
176.1125	175	-0.04	176.07	101	78.2	1-Methoxy-3-carbaldehyde
149.1041	148.1	0.0032	149.1073	69	59.3	N-Benzylacetamidine
149.1041	165.115	-0.008	149.0961	191	94	(.+/-)-p-Methoxyamphetamine
149.1041	165.115	-0.008	149.0961	243	81.9	(.+/-)-p-Methoxyamphetamine
149.1041	165.115	-0.008	149.0961	260	53.8	(.+/-)-p-Methoxyamphetamine
176.1125	175.121	0.0156	176.1281	58	68.7	Threonine, butyl ester
164.0069	163.046	0.0459	164.0528	119	54.1	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	129	74.1	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	15	100	Pterine
257.1488	256.117	-0.0244	257.1244	69	54.2	Thr-His
257.1488	256.117	-0.0244	257.1244	118	43.5	Thr-His
257.1488	256.11	-0.0316	257.1172	108	62.9	Pterostilbene
257.1488	256.11	-0.0316	257.1172	148	100	Pterostilbene
164.0069	163.046	0.0459	164.0528	151	80.2	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	109	67.3	Pterine
164.0069	163.046	0.0459	164.0528	79	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	128	62.8	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	164	86.3	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	109	72.4	Benzothiazole, 2,5-dimethyl-
164.0069	163	0.03	164.04	71	84.7	N-Acetyl-L-cysteine
164.0069	163.049	0.0498	164.0567	51	56	Pterine
238.168	474.234	-0.0438	238.1242	80	41.7	Trp-Asn-Arg
238.168	474.234	-0.0438	238.1242	44	35.5	Trp-Asn-Arg
238.168	237.136	-0.0242	238.1438	33	100	Viloxazine
176.1195	175.121	0.0086	176.1281	4	100	Threonine, butyl ester
176.1195	175	-0.05	176.07	31	100	1-Methoxy-3-carbaldehyde
205.1375	188.116	-0.0181	205.1194	100	60.9	Glycyl-L-norleucine
205.1375	188.116	-0.0181	205.1194	37	79.6	Glycyl-L-norleucine
205.1375	204.09	-0.0403	205.0972	56	100	Fenozolone
205.1375	204.09	-0.0403	205.0972	289	82.1	Ethotoin
205.1375	188.116	-0.0181	205.1194	176	59.4	Glycyl-L-norleucine
205.1375	408.201	-0.0298	205.1077	165	15.8	Phe-Asp-Lys
205.1375	204.09	-0.0403	205.0972	173	65.6	Fenozolone
205.1375	408.212	-0.0242	205.1133	305	56.1	Phe-Ser-Arg
169.1265	168.115	-0.0042	169.1223	37	33.6	Jasmine lactone
169.1265	336.147	-0.0459	169.0806	125	75.1	Ser-Cys-Lys
169.1265	168.115	-0.0042	169.1223	136	61.6	Jasmine lactone
150.1003	167.095	-0.009	150.0913	116	33.3	Synephrine
150.1003	149.07	-0.0229	150.0774	62	41.2	Adenine, N6-methyl
150.1003	149.105	0.0122	150.1125	172	55.1	Triethanolamine

150.1003	167.095	-0.009	150.0913	353	77.4	Synephrine
150.1003	303.147	-0.009	150.0913	79	56.6	Cocaine
150.1003	149.084	-0.009	150.0913	169	24.3	S(-)-Cathinone
150.1003	149.07	-0.0229	150.0774	95	52.4	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	87	100	Adenine, N6-methyl
169.1115	146.069	-0.0531	169.0584	53	18.6	Gly-Ala
169.1115	168.115	0.0108	169.1223	179	94.7	Jasmine lactone
169.1115	186.1	-0.0143	169.0972	183	89.3	Ala-Pro
285.284	302.246	-0.0416	285.2424	30	100	Glycerol 1-myristate
285.284	302.246	-0.0416	285.2424	63	100	Glycerol 1-myristate
285.284	302.246	-0.0416	285.2424	87	100	Glycerol 1-myristate
285.284	302.246	-0.0416	285.2424	183	100	Glycerol 1-myristate
164.0069	163.046	0.0459	164.0528	68	51.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	100	84.5	Benzothiazole, 2,5-dimethyl-
164.0069	163.038	0.0386	164.0455	37	100	7-Nitroindazole
164.0069	163.046	0.0459	164.0528	116	76.7	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	94	39.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	42	100	Pterine
164.0069	163.046	0.0459	164.0528	114	66.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	69	79.3	Pterine
164.0069	163.038	0.0386	164.0455	6	100	7-Nitroindazole
164.0069	163.046	0.0459	164.0528	123	82.5	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	67	79.6	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	86	81.2	Pterine
164.0069	163.048	0.0484	164.0553	51	100	4-Hydroxy-L-glutamic acid
225.154	0	0	225.15	44	80.9	Methyl jasmonate
225.154	224.116	-0.0306	225.1234	42	77.6	Butalbital
225.154	448.207	-0.0432	225.1108	49	19.6	PyroGlu-Tyr-Arg
164.0069	163.046	0.0459	164.0528	78	66.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	152	93.2	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	28	61.5	Pterine
164.0069	163.038	0.0386	164.0455	30	100	7-Nitroindazole
134.1002	151.1	-0.0038	134.0964	134	53.9	Norephedrine
134.1002	283.164	-0.024	134.0762	187	20.9	Lys-His
134.1002	0	-0.04	134.06	199	81.1	Oxindole
134.1002	151.1	-0.0038	134.0964	1	51	Norephedrine
343.2942	342.256	-0.031	343.2632	158	77	Retinyl propionate
343.2942	342.256	-0.031	343.2632	209	50.4	Retinyl propionate
569.3045	1138	-0.037	569.2675	9	100	CYFVNCPRG/2
150.1003	167.095	-0.009	150.0913	108	48	Synephrine
150.1003	149.12	0.0274	150.1277	138	71.1	N,N-Diethylaniline
150.1003	149.12	0.0274	150.1277	117	49.2	Methamphetamine
150.1003	0	-0.01	150.09	74	11.4	2-Aminopropiophenone
343.2942	171.126	-0.0351	343.2591	193	78.2	Gabapentin
343.2942	342.256	-0.031	343.2632	71	60.8	Retinyl propionate
150.1003	167.095	-0.009	150.0913	108	86.6	Synephrine

150.1003	167.058	-0.045	150.055	183	76.5	3-Methyl-2-nitrobenzyl alcohol
150.1003	150.128	0.0274	150.1277	174	77.9	N-Butyl-4-methylpyridinium
150.1003	149.07	-0.0229	150.0774	102	71.9	Adenine, N6-methyl
211.1743	210.159	-0.0077	211.1666	27	100	Altretamine
211.1743	437.264	-0.0484	211.1259	17	100	Lys-Tyr-Lys
211.1743	0	0	211.17	296	80.4	altretamine
211.1743	210.126	-0.0414	211.1329	145	63.3	Jasmonic Acid
180.0344	362.082	-0.0008	180.0336	78	100	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
180.0344	362.082	-0.0008	180.0336	176	81.3	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
180.0344	362.082	-0.0008	180.0336	17	57.3	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
149.0908	165.115	0.0053	149.0961	204	76.6	(.+/-)-p-Methoxyamphetamine
149.0908	148.1	0.0165	149.1073	149	86.8	N-Benzylacetamidine
149.0908	165.115	0.0053	149.0961	80	71.4	(.+/-)-p-Methoxyamphetamine
326.1619	325.135	-0.02	326.1419	118	50	Clemizole
343.2942	342.256	-0.031	343.2632	74	68.4	Retinyl propionate
343.2942	342.256	-0.031	343.2632	35	100	Retinyl propionate
150.1003	149.07	-0.0229	150.0774	184	57.2	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	160	79	Synephrine
150.1003	149.12	0.0274	150.1277	142	50.7	Methamphetamine
150.1003	167.095	-0.009	150.0913	121	75	Synephrine
343.2942	342.256	-0.031	343.2632	95	84.5	Retinyl propionate
164.0069	163.046	0.0459	164.0528	111	77.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	136	52	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	47	69.5	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	128	85.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.038	0.0386	164.0455	7	100	7-Nitroindazole
164.0069	163.046	0.0459	164.0528	77	59.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	106	92.5	Benzothiazole, 2,5-dimethyl-
164.0069	163	0.03	164.04	50	48.3	N-Acetyl-L-cysteine
180.0344	181.041	-0.0008	180.0336	7	100	Acamprosate
180.0344	179.058	0.0311	180.0655	1	100	Hippuric acid
180.0344	362.082	-0.0008	180.0336	197	83	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
180.0344	179.025	-0.0019	180.0325	16	100	S-Carboxymethyl-L-cysteine
343.2942	408.288	-0.0299	343.2643	23	100	Cholic acid
211.1113	210.126	0.0216	211.1329	13	100	Jasmonic Acid
211.1113	210.126	0.0216	211.1329	26	56	Jasmonic Acid
211.1113	420.179	-0.0145	211.0968	173	74.5	Met-Asp-Arg
211.1113	210.1	-0.0036	211.1077	25	66	Aprobarbital
257.1488	256.117	-0.0244	257.1244	40	100	Thr-His
257.1488	256.117	-0.0244	257.1244	37	100	Thr-His

257.1488	256.117	-0.0244	257.1244	9	39.5	Thr-His
257.1488	256.11	-0.0316	257.1172	67	100	Pterostilbene
176.1195	350.195	-0.015	176.105	16	100	Phe-Gly-Lys
150.1003	167.095	-0.009	150.0913	131	72	Synephrine
150.1003	167.095	-0.009	150.0913	100	54.7	Synephrine
150.1003	149.07	-0.0229	150.0774	86	67.1	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	135	62.5	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	24	66	Synephrine
150.1003	149.07	-0.0229	150.0774	168	49.6	Adenine, N6-methyl
150.1003	303.147	-0.009	150.0913	92	56.6	Cocaine
150.1003	149	-0.04	150.06	265	71.9	L-Methionine
150.1003	167.058	-0.045	150.055	144	72.1	3-Methyl-2-nitrobenzyl alcohol
150.1003	149.07	-0.0229	150.0774	33	29.7	Adenine, N6-methyl
150.1003	150.128	0.0274	150.1277	191	71.3	N-Butyl-4-methylpyridinium
150.1003	167.095	-0.009	150.0913	66	59.7	Synephrine
343.3048	342.256	-0.0416	343.2632	147	72.2	Retinyl propionate
343.3048	408.288	-0.0405	343.2643	5	100	Cholic acid
134.0966	151.1	-0.0002	134.0964	58	100	Norephedrine
134.0966	133.089	-0.0002	134.0964	128	28.4	Cyclopropanamine, 2-phenyl-, trans-
134.0966	0	-0.04	134.06	190	45	Oxindole
134.0966	151.1	-0.0002	134.0964	90	43.4	Norephedrine
285.284	302.246	-0.0416	285.2424	29	100	Glycerol 1-myristate
285.284	302.246	-0.0416	285.2424	210	100	Glycerol 1-myristate
205.1202	204.09	-0.023	205.0972	92	39.1	Fenozolone
205.1202	204.075	-0.0383	205.0819	163	70.3	Gly-Glu
205.1202	408.201	-0.0125	205.1077	187	20.4	Phe-Asp-Lys
205.1202	204.09	-0.023	205.0972	212	72.8	Fenozolone
287.2379	286.193	-0.0373	287.2006	84	45.9	4,6-Androstadien-17.beta.-ol-3-one
287.2379	286.193	-0.0373	287.2006	97	74.9	4,6-Androstadien-17.beta.-ol-3-one
287.2379	286.23	-0.001	287.2369	53	100	Retinol
257.1488	256.11	-0.0316	257.1172	105	100	Pterostilbene
343.2942	408.288	-0.0299	343.2643	15	100	Cholic acid
343.2942	408.288	-0.0299	343.2643	59	100	Cholic acid
343.2942	408.288	-0.0299	343.2643	61	100	Cholic acid
343.2942	342.256	-0.031	343.2632	13	100	Retinyl propionate
164.0069	163.046	0.0459	164.0528	99	62.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	108	84.5	Benzothiazole, 2,5-dimethyl-
164.0069	163.038	0.0386	164.0455	9	100	7-Nitroindazole
164.0069	163.046	0.0459	164.0528	86	75.5	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	94	80	Benzothiazole, 2,5-dimethyl-
285.284	302.246	-0.0416	285.2424	93	100	Glycerol 1-myristate
164.0069	163.046	0.0459	164.0528	86	69.8	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	127	89.3	Benzothiazole, 2,5-dimethyl-

164.0069	163.046	0.0459	164.0528	112	78.6	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	33	58.6	Pterine
169.1067	168.115	0.0156	169.1223	59	100	Jasmine lactone
169.1067	168.09	-0.0095	169.0972	28	59.9	Pyridoxamine
169.1067	168.069	-0.031	169.076	3	100	Norharmane
211.1441	210.159	0.0225	211.1666	20	100	Altretamine
211.1441	0	-0.01	211.13	47	44.7	Jasmonic acid
211.1441	210.126	-0.0112	211.1329	97	41.1	Jasmonic Acid
211.1441	420.249	-0.0126	211.1315	97	39.7	Phe-Val-Arg
211.1441	210.159	0.0225	211.1666	12	100	Altretamine
211.1441	210.126	-0.0112	211.1329	61	100	Jasmonic Acid
211.1441	420.179	-0.0473	211.0968	26	100	Met-Asp-Arg
211.1441	420.179	-0.0473	211.0968	152	34.3	Met-Asp-Arg
283.1685	282.179	0.0179	283.1864	23	100	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	260.148	-0.0308	283.1377	90	69.6	Lys-Asn
283.1685	282.122	-0.0396	283.1289	145	41.4	Thr-Tyr
283.1685	282.122	-0.0396	283.1289	151	58.2	Tyr-Thr
176.1195	175.121	0.0086	176.1281	24	44	Threonine, butyl ester
211.1441	210.126	-0.0112	211.1329	126	87	Jasmonic Acid
211.1441	0	-0.01	211.13	47	34.9	Jasmonic acid
211.1441	0	-0.01	211.13	34	55.4	Jasmonic acid
211.1441	210.1	-0.0364	211.1077	182	27.7	Aprobarbital
169.1299	168.115	-0.0076	169.1223	61	100	Jasmine lactone
169.1299	168.115	-0.0076	169.1223	95	100	Jasmine lactone
176.1195	175	-0.05	176.07	7	100	1-Methoxy-3-carbaldehyde
176.1195	175.121	0.0086	176.1281	14	53.1	Threonine, butyl ester
211.1441	228.136	-0.0112	211.1329	73	62.8	trans-Traumatic acid
211.1441	210.126	-0.0112	211.1329	100	40.7	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	52	38.7	Jasmonic Acid
211.1441	0	-0.04	211.1	158	35.4	Sinapyl alcohol
211.1441	210.116	-0.021	211.123	21	58.6	Naphtazoline
211.1441	210.126	-0.0112	211.1329	138	72.3	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	148	35.5	Jasmonic Acid
649.4343	2597	-0.0288	649.4055	7	100	YGRKKRRQRRRGPKRRLD L/4
164.0069	163.046	0.0459	164.0528	71	56.3	Benzothiazole, 2,5-dimethyl-
164.0069	0	0.03	164.04	156	74.6	Acetylcysteine
164.0069	163.038	0.0386	164.0455	3	100	7-Nitroindazole
164.0069	163.046	0.0459	164.0528	80	74.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	110	92.7	Benzothiazole, 2,5-dimethyl-
180.0344	181.041	-0.0008	180.0336	3	100	Acamprosate
180.0344	362.082	-0.0008	180.0336	58	100	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
180.0344	157.074	0.0287	180.0631	1	100	N-Tigloylglycine
225.154	0	0	225.15	45	100	Methyl jasmonate

225.154	448.207	-0.0432	225.1108	54	100	PyroGlu-Tyr-Arg
164.0069	163.046	0.0459	164.0528	86	69.1	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	70	64.9	Benzothiazole, 2,5-dimethyl-
225.1606	448.229	-0.039	225.122	137	33.3	His-His-Arg
225.1606	202.143	-0.0284	225.1322	28	100	N(G),N(G')-Dimethyl-L-arginine
225.1606	224.116	-0.0372	225.1234	38	29.4	Butalbital
205.1202	204.072	-0.0408	205.0794	71	38	Levamisole
205.1202	204.075	-0.0383	205.0819	146	43.6	Gly-Glu
205.1202	204.075	-0.0383	205.0819	88	20.3	Gly-Glu
205.1202	204.1	-0.013	205.107	130	36.8	1,6-Anhydro-b-D-glucose, permethyl-
225.1606	0	-0.01	225.15	7	100	Methyl jasmonate
225.1606	224.127	-0.026	225.1346	121	93.3	Pirimicarb-desmethyl
180.0344	181.041	-0.0008	180.0336	7	100	Acamprosate
180.0344	362.082	-0.0008	180.0336	180	84.2	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
180.0344	362.082	-0.0008	180.0336	110	100	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
180.0344	362.082	-0.0008	180.0336	76	76.9	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
163.1098	162.126	0.0231	163.1329	122	69.7	Ethanol, 2-(2-butoxyethoxy)-
163.1098	162.126	0.0231	163.1329	207	62	Ethanol, 2-(2-butoxyethoxy)-
163.1098	179.095	-0.0344	163.0754	40	25.9	3,4-Methylenedioxyamphetamine
163.1098	162.1	-0.0021	163.1077	86	25.8	DL-Lysine, 5-hydroxy-
134.0898	151.1	0.0066	134.0964	27	39.4	Norephedrine
134.0898	135	-0.04	134.05	87	30.7	Adenine
320.1349	362.139	0.0056	320.1405	7	100	Marbofloxacin
320.1349	320.092	-0.0432	320.0917	21	100	Coptisine cation
134.0898	134.11	0.019	134.109	48	77.3	Benzene, n-butyl-
134.0898	0	-0.03	134.06	136	82.3	Oxindole
134.0898	0	-0.03	134.06	288	88.4	Oxindole
149.0908	165.115	0.0053	149.0961	9	29	(.+/-)-p-Methoxyamphetamine
149.0908	150.053	-0.0453	149.0455	312	37.6	D-Lyxose
149.0908	148.1	0.0165	149.1073	48	61.5	N-Benzylacetamidine
211.1441	210.126	-0.0112	211.1329	81	44.9	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	201	75	Jasmonic Acid
211.1441	420.179	-0.0473	211.0968	225	66	Met-Asp-Arg
211.1441	420.223	-0.025	211.119	182	59.8	His-His-Lys
211.1441	210.159	0.0225	211.1666	12	51	Altretamine
211.1441	210.126	-0.0112	211.1329	134	64.2	Jasmonic Acid
211.1441	420.223	-0.025	211.119	216	52.9	His-His-Lys
211.1441	210.126	-0.0112	211.1329	29	55.4	Jasmonic Acid
211.1441	210	-0.01	211.13	152	78.7	(+)-Jasmonic acid
211.1441	210.126	-0.0112	211.1329	131	43.7	Jasmonic Acid

211.1441	210.126	-0.0112	211.1329	96	42.9	Jasmonic Acid
211.1441	0	-0.01	211.13	228	59.4	Jasmonic acid
310.1687	287.196	0.016	310.185	29	63.5	Ile-Arg
310.1687	309.194	0.0326	310.2013	136	39.3	Nadolol
211.1441	210.116	-0.021	211.123	58	76.9	Naphtazoline
211.1441	210.126	-0.0112	211.1329	150	70	Jasmonic Acid
211.1441	210.116	-0.021	211.123	1	100	Naphtazoline
211.1441	210.126	-0.0112	211.1329	160	32	Jasmonic Acid
169.1265	168	-0.03	169.1	122	100	Pyridoxamine dihydrochloride
169.1265	0	-0.05	169.08	29	100	Norharman
257.1488	256.117	-0.0244	257.1244	47	49	His-Thr
257.1488	256.117	-0.0244	257.1244	34	100	Thr-His
257.1488	256.117	-0.0244	257.1244	40	70.2	His-Thr
225.154	0	-0.05	225.1	131	100	7- HYDROXYETHYLTHEOPHY LLINE
225.154	224.127	-0.0194	225.1346	127	94.7	Pirimicarb-desmethyl
225.154	202.143	-0.0218	225.1322	71	64	NG,NG-Dimethyl-L-arginine
225.154	448.229	-0.032	225.122	152	38.1	His-His-Arg
164.0069	163.046	0.0459	164.0528	47	45.6	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	53	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	88	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	86	64.5	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	51	55.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.038	0.0386	164.0455	31	51	7-Nitroindazole
164.0069	163.038	0.0386	164.0455	2	100	7-Nitroindazole
164.0069	163.046	0.0459	164.0528	80	74.8	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	137	91.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	79	100	Benzothiazole, 2,5-dimethyl-
225.154	202.143	-0.0218	225.1322	115	75.2	NG,NG-Dimethyl-L-arginine
225.154	448.207	-0.0432	225.1108	192	76	PyroGlu-Tyr-Arg
225.154	0	0	225.15	165	49.8	Methyl jasmonate
176.1257	350.195	-0.021	176.105	44	100	Phe-Gly-Lys
225.1677	202.143	-0.0355	225.1322	71	83.3	N(G),N(G')-Dimethyl-L- arginine
225.1677	224.116	-0.0443	225.1234	37	28.4	Butalbital
225.1677	448.229	-0.046	225.122	86	44.9	His-His-Arg
225.1606	0	-0.01	225.15	32	36.9	Methyl jasmonate
225.1606	448.229	-0.039	225.122	194	49.3	His-His-Arg
225.1606	0	-0.01	225.15	136	51.6	Methyl jasmonate
169.1299	168.115	-0.0076	169.1223	39	100	Jasmine lactone
169.1299	168.115	-0.0076	169.1223	116	75.3	Jasmine lactone
169.1299	168.09	-0.0327	169.0972	65	82.7	Pyridoxamine
211.1441	210.126	-0.0112	211.1329	262	81.6	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	190	55.9	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	115	28.3	Jasmonic Acid

211.1441	420.223	-0.025	211.119	196	42.6	His-His-Lys
205.1202	204.072	-0.0408	205.0794	69	68.3	Levamisole
205.1202	204.1	-0.013	205.107	143	39.7	1,6-Anhydro-b-D-glucose, permethyl-
205.1202	204.09	-0.023	205.0972	213	62.5	Ethotoin
205.1202	204.075	-0.0383	205.0819	174	73.3	Gly-Glu
211.1441	228.136	-0.0112	211.1329	100	66.5	trans-Traumatic acid
211.1441	210.126	-0.0112	211.1329	72	60.9	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	143	48.5	Jasmonic Acid
211.1441	420.223	-0.025	211.119	176	70.1	His-His-Lys
211.1441	228.136	-0.0112	211.1329	19	27.3	trans-Traumatic acid
211.1441	210.126	-0.0112	211.1329	173	74	Jasmonic Acid
211.1441	210.1	-0.0364	211.1077	161	81.7	Aprobarbital
211.1441	210.126	-0.0112	211.1329	128	35.7	Jasmonic Acid
211.1441	210.159	0.0225	211.1666	11	100	Altretamine
211.1441	210.126	-0.0112	211.1329	104	42.2	Jasmonic Acid
211.1441	0	-0.01	211.13	129	27.7	Jasmonic acid
211.1441	420.179	-0.0473	211.0968	160	64.1	Met-Asp-Arg
225.1606	448.207	-0.0498	225.1108	52	28.9	PyroGlu-Tyr-Arg
225.1606	448.207	-0.0498	225.1108	75	83.8	PyroGlu-Tyr-Arg
163.1028	162.126	0.0301	163.1329	206	94.2	Ethanol, 2-(2-butoxyethoxy)-
163.1028	180.063	-0.0427	163.0601	85	33.5	D-(+)-Galactose
163.1028	179.095	-0.0274	163.0754	68	28.1	3-Amino-3-(4-methylphenyl)propionic acid
163.1028	162.1	0.0049	163.1077	3	50	DL-Lysine, 5-hydroxy-
164.0069	163.049	0.0498	164.0567	43	44.6	Pterine
164.0069	163.046	0.0459	164.0528	46	40.1	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	41	47.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	49	70.2	Benzothiazole, 2,5-dimethyl-
164.0069	163	0.03	164.04	31	100	N-Acetyl-L-cysteine
164.0069	163.049	0.0498	164.0567	13	58.6	Pterine
164.0069	163.046	0.0459	164.0528	75	52.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	38	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.038	0.0386	164.0455	4	100	7-Nitroindazole
164.0069	163.049	0.0498	164.0567	76	34.9	Pterine
164.0069	163.046	0.0459	164.0528	127	89.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.038	0.0386	164.0455	25	62.3	7-Nitroindazole
205.1202	204.075	-0.0383	205.0819	42	57.6	Gly-Glu
205.1202	204.09	-0.023	205.0972	13	100	Fenozolone
205.1202	204.072	-0.0408	205.0794	103	68.4	Tetramisole
205.1202	204.072	-0.0408	205.0794	56	19.9	Tetramisole
211.1441	228.136	-0.0112	211.1329	32	43.8	trans-Traumatic acid
211.1441	0	-0.01	211.13	69	66	Jasmonic acid
289.1777	266.165	-0.0238	289.1539	51	65.4	Tributyl phosphate
180.0344	362.082	-0.0008	180.0336	73	100	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
150.1003	149.084	-0.009	150.0913	130	14.6	S(-)-Cathinone

150.1003	167.095	-0.009	150.0913	32	49.8	Synephrine
289.1998	288.18	-0.013	289.187	10	100	Ala-Ala-Lys
164.0069	163.046	0.0459	164.0528	65	63.1	Benzothiazole, 2,5-dimethyl-
164.0069	165.065	0.0509	164.0578	4	100	1-Methylguanine
164.0069	163.046	0.0459	164.0528	15	60	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	76	77.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	36	57.9	Benzothiazole, 2,5-dimethyl-
268.9982	432.106	0.0473	269.0455	1	100	Genistin
164.0069	165.065	0.0509	164.0578	55	54.2	1-Methylguanine
164.0069	163.046	0.0459	164.0528	26	100	Benzothiazole, 2,5-dimethyl-
289.1729	266.165	-0.0189	289.1539	1	100	Tributyl phosphate
289.1729	288.209	0.0433	289.2162	34	60	9(11),(5.alpha.)-Androsten-3.beta.-ol-17-one
289.1729	288.18	0.014	289.187	9	100	Ala-Ala-Lys
205.1202	204.072	-0.0408	205.0794	27	40.4	Levamisole
205.1202	204.072	-0.0408	205.0794	35	51	Levamisole
205.1202	204.072	-0.0408	205.0794	34	100	Tetramisole
205.1202	204.1	-0.013	205.107	73	75.3	1,6-Anhydro-b-D-glucose, permethyl-
164.0069	163.046	0.0459	164.0528	62	69.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	120	92.5	Benzothiazole, 2,5-dimethyl-
289.1638	0	-0.02	289.14	97	51	4-Methylumbelliferyl heptanoate
164.0069	163.046	0.0459	164.0528	34	78.2	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	30	44	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	57	63.7	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	14	55.4	Pterine
211.1441	210.126	-0.0112	211.1329	84	67.4	Jasmonic Acid
211.1441	420.179	-0.0473	211.0968	135	69.4	Met-Asp-Arg
211.1441	0	-0.04	211.1	76	33.2	Sinapyl alcohol
692.4407	1384	0.0165	692.4572	8	56	GFLRRIRPKLK/2
205.1375	204.09	-0.0403	205.0972	1	100	Fenozolone
205.1375	204	-0.04	205.1	130	31.9	L-Tryptophane
205.1375	204.1	-0.03	205.107	168	40.8	1,6-Anhydro-b-D-glucose, permethyl-
205.1375	204.1	-0.03	205.107	80	81.2	1,6-Anhydro-b-D-glucose, permethyl-
164.0069	163.046	0.0459	164.0528	53	45.2	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	12	100	Pterine
164.0069	163.038	0.0386	164.0455	29	100	7-Nitroindazole
150.1003	149.07	-0.0229	150.0774	44	39.7	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	27	100	Adenine, N6-methyl
149.1041	165.115	-0.008	149.0961	18	100	(.+/-)-p-Methoxyamphetamine
149.1041	148.1	0.0032	149.1073	3	100	N-Benzylacetamidine
149.1041	148.1	0.0032	149.1073	9	57.9	N-Benzylacetamidine
164.0069	163.046	0.0459	164.0528	41	80.7	Benzothiazole, 2,5-dimethyl-

164.0069	165.065	0.0509	164.0578	101	84	1-Methylguanine
150.1003	149.07	-0.0229	150.0774	63	32.5	Adenine, N6-methyl
150.1003	167.058	-0.045	150.055	17	45.9	3-Methyl-2-nitrobenzyl alcohol
809.4807	1619	0.0292	809.5099	66	100	YAGFLRRIRPKLK/2
809.4807	1619	0.0292	809.5099	3	100	YAGFLRRIRPKLK/2
180.0344	181.041	-0.0008	180.0336	3	100	Acamprosate
180.0344	362.082	-0.0008	180.0336	47	100	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
180.0344	362.082	-0.0008	180.0336	99	80.9	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
180.0344	362.082	-0.0008	180.0336	15	100	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
303.1743	302.138	-0.0291	303.1452	25	55.4	His-Phe
303.1743	0	0.03	303.2	49	100	11beta-hydroxyandrost-4-ene-3,17-dione
164.0069	165.065	0.0509	164.0578	22	60	1-Methylguanine
164.0069	163.046	0.0459	164.0528	30	41.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	78	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	58	57	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	36	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	37	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	21	56	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	9	52	Benzothiazole, 2,5-dimethyl-
164.0069	163.038	0.0386	164.0455	2	100	7-Nitroindazole
225.154	202.143	-0.0218	225.1322	96	64.7	N(G),N(G')-Dimethyl-L-arginine
225.154	224.116	-0.0306	225.1234	57	70.5	Butalbital
211.1671	210.159	-0.0005	211.1666	10	100	Altretamine
211.1671	210.126	-0.0342	211.1329	67	100	Jasmonic Acid
134.0898	0	-0.03	134.06	18	56	Oxindole
211.1441	210.126	-0.0112	211.1329	37	55.6	Jasmonic Acid
211.1441	210.1	-0.0364	211.1077	178	85.9	Aprobarbital
180.0344	181.041	-0.0008	180.0336	3	100	Acamprosate
180.0344	157.074	0.0287	180.0631	2	100	N-Tigloylglycine
180.0344	362.082	-0.0008	180.0336	71	70.2	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
180.0344	362.082	-0.0008	180.0336	97	57.9	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
743.4303	2973	-0.0027	743.4276	1	100	MLTKFETKSARVKGLSFHP KRPWIL/4
150.1003	149.12	0.0274	150.1277	111	70.6	Methamphetamine
150.1003	167.095	-0.009	150.0913	153	66.3	Synephrine
180.0344	362.082	-0.0008	180.0336	57	100	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)
180.0344	362.082	-0.0008	180.0336	108	81.2	Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid)

205.1202	204.075	-0.0383	205.0819	30	25.6	Gly-Glu
205.1202	204.075	-0.0383	205.0819	40	79.3	Gly-Glu
205.1202	408.237	0.0057	205.1259	165	9.8	Tyr-Val-Lys
205.1202	204.075	-0.0383	205.0819	138	24.9	Gly-Glu
150.1003	149.105	0.0122	150.1125	200	94.5	Triethanolamine
150.1003	149.07	-0.0229	150.0774	17	100	Adenine, N6-methyl
787.6188	786.661	0.05	787.6688	43	100	N-Docosanoyl-4-sphingeny-1-O-phosphorylcholine
164.0069	163.046	0.0459	164.0528	86	80.8	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	67	66.7	Pterine
164.0069	163.046	0.0459	164.0528	111	77.6	Benzothiazole, 2,5-dimethyl-
164.0069	163	0.03	164.04	63	42.3	N-Acetyl-L-cysteine
164.0069	163.046	0.0459	164.0528	98	80.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	42	65	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	59	70.2	Benzothiazole, 2,5-dimethyl-
134.0931	151.1	0.0033	134.0964	3	100	Norephedrine
134.0931	0	-0.03	134.06	174	73.3	Oxindole
134.0966	135	-0.05	134.05	146	60.4	Adenine
134.0966	0	-0.04	134.06	230	73.2	Oxindole
283.1685	282.179	0.0179	283.1864	10	100	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	282.122	-0.0396	283.1289	87	66.2	Tyr-Thr
283.1685	282.179	0.0179	283.1864	14	58.6	1,3-Bis(tris(hydroxymethyl)methylamino)propane
211.1441	210.126	-0.0112	211.1329	40	100	Jasmonic Acid
211.1441	420.223	-0.025	211.119	21	36.8	His-His-Lys
205.1375	408.237	-0.0116	205.1259	258	41.2	Tyr-Val-Lys
205.1375	204.09	-0.0403	205.0972	215	81.9	Ethotoin
176.1125	175.063	-0.0419	176.0706	9	100	3-Indoleacetic acid
211.1441	210.159	0.0225	211.1666	2	100	Altretamine
211.1441	210.126	-0.0112	211.1329	151	70.8	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	35	100	Jasmonic Acid
205.1375	408.186	-0.037	205.1005	77	100	Met-Met-Lys
205.1375	204.09	-0.0403	205.0972	63	100	Fenozolone
150.1003	167.095	-0.009	150.0913	31	100	Synephrine
150.1003	149.12	0.0274	150.1277	259	74.4	Methamphetamine
205.1375	204	-0.04	205.1	74	28.7	L-Tryptophane
205.1375	222.1	-0.0403	205.0972	105	78.7	Gly-Phe
205.1375	188.116	-0.0181	205.1194	45	61.5	Glycyl-L-norleucine
205.1375	408.237	-0.0116	205.1259	110	12.5	Tyr-Val-Lys
180.0344	181.041	-0.0008	180.0336	18	100	Acamprosate
238.1427	237.092	-0.0434	238.0993	48	100	Ketamine
238.1427	237.103	-0.0319	238.1108	8	100	3-(Cyclohexylamino)-2-hydroxy-1-propanesulfonic acid

238.1427	474.234	-0.0185	238.1242	103	75.8	Trp-Asn-Arg
163.1064	162.126	0.0264	163.1329	187	80.9	Ethanol, 2-(2-butoxyethoxy)-
163.1064	162.064	-0.0351	163.0713	114	54	Gly-Ser
163.1064	162.064	-0.0351	163.0713	88	28.1	Gly-Ser
257.1052	256.117	0.0192	257.1244	34	78.6	Thr-His
164.0069	163.046	0.0459	164.0528	84	73.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	71	83.5	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	19	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	84	78.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	67	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	19	52	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	37	51.8	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	62	82.6	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	36	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.038	0.0386	164.0455	54	80.4	7-Nitroindazole
169.1048	168.115	0.0175	169.1223	22	33	Jasmine lactone
169.1048	210.1	-0.044	169.0608	45	25.1	Aprobarbital
169.1048	336.147	-0.0242	169.0806	24	57.3	Ser-Cys-Lys
134.1137	0	0.01	134.12	41	56.7	Bis (2-hydroxypropyl) amine
134.1137	0	-0.03	134.08	223	44.2	1,4-Dideoxy-1,4-Imino-D-Arabinitol
134.1137	0	-0.03	134.08	132	33.1	1,4-Dideoxy-1,4-Imino-D-Arabinitol
134.1137	0	-0.05	134.06	2	51	4-Hydroxyindole
169.1018	146.069	-0.0434	169.0584	15	20.9	Gly-Ala
169.1018	146.069	-0.0434	169.0584	74	45.5	Gly-Ala
169.1018	336.147	-0.0212	169.0806	28	100	Ser-Cys-Lys
169.1018	0	-0.05	169.05	15	100	p-Hydroxymandelic acid
134.1002	151.1	-0.0038	134.0964	25	21.7	Norephedrine
134.1002	134.11	0.009	134.109	20	39.6	Benzene, n-butyl-
150.1003	0	-0.01	150.09	114	31.2	2-Aminopropiophenone
150.1003	149.12	0.0274	150.1277	148	60.9	N,N-Diethylaniline
150.1003	149.105	0.0122	150.1125	213	71.8	Triethanolamine
150.1003	167.095	-0.009	150.0913	44	100	Synephrine
134.1137	283.164	-0.0375	134.0762	55	23	Lys-His
134.1137	0	-0.05	134.06	77	66	Oxindole
134.1137	283.164	-0.0375	134.0762	3	25.2	Lys-His
238.1427	237.103	-0.0319	238.1108	9	100	3-(Cyclohexylamino)-2-hydroxy-1-propanesulfonic acid
238.1427	237.136	0.0011	238.1438	9	100	Viloxazine
238.1427	237.092	-0.0434	238.0993	13	54.2	Ketamine
211.1548	210.126	-0.0219	211.1329	56	53.6	Jasmonic Acid
731.5822	730.599	0.024	731.6062	54	100	N-Stearoyl-4-sphingeny-1-O-phosphorylcholine
150.1003	149.07	-0.0229	150.0774	74	47.9	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	27	100	Adenine, N6-methyl

150.1003	149.07	-0.0229	150.0774	38	63.5	Adenine, N6-methyl
150.1003	303.147	-0.009	150.0913	32	68.7	Cocaine
164.0069	165.065	0.0509	164.0578	64	43.6	1-Methylguanine
164.0069	163.049	0.0498	164.0567	2	100	Pterine
164.0069	165.065	0.0509	164.0578	61	41	1-Methylguanine
164.0069	163.046	0.0459	164.0528	53	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	76	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	110	74.8	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	43	100	Benzothiazole, 2,5-dimethyl-
164.0069	163	0.03	164.04	19	52	N-Acetyl-L-cysteine
225.1606	448.229	-0.039	225.122	114	36.3	His-His-Arg
225.1606	0	-0.01	225.15	102	58.6	Methyl jasmonate
225.1606	0	-0.01	225.15	96	55.4	Methyl jasmonate
225.1606	0	-0.01	225.15	58	100	Methyl jasmonate
163.1064	162.064	-0.0351	163.0713	103	68.4	Gly-Ser
163.1064	162.126	0.0264	163.1329	259	87.9	Ethanol, 2-(2-butoxyethoxy)-
163.1064	162.116	0.017	163.123	87	24.3	Nicotine
163.1064	162.126	0.0264	163.1329	99	42.1	Ethanol, 2-(2-butoxyethoxy)-
163.1028	162.064	-0.0315	163.0713	70	71.5	Gly-Ser
163.1028	162.064	-0.0315	163.0713	80	50.6	Gly-Ser
163.1028	162.126	0.0301	163.1329	123	68.7	Ethanol, 2-(2-butoxyethoxy)-
163.1028	179.095	-0.0274	163.0754	27	25.5	3-Amino-3-(4-methylphenyl)propionic acid
163.1064	162.064	-0.0351	163.0713	129	64.4	Gly-Ser
163.1064	162.064	-0.0351	163.0713	135	60.2	Gly-Ser
163.1064	162.064	-0.0351	163.0713	56	34.8	Gly-Ser
163.1064	162.1	0.0013	163.1077	72	36.8	DL-Lysine, 5-hydroxy-
134.1137	283.164	-0.0375	134.0762	1	100	Lys-His
134.1137	0	-0.05	134.06	90	54.2	4-Hydroxyindole
205.1202	204.072	-0.0408	205.0794	10	56	Levamisole
205.1202	204.09	-0.023	205.0972	108	34.6	Fenozolone
205.1202	204.09	-0.023	205.0972	63	84.5	Ethotoin
205.1202	408.237	0.0057	205.1259	188	13.6	Tyr-Val-Lys
266.1327	265.095	-0.0304	266.1023	180	97.8	3,4-Dihydroxycinnamic acid (L-alanine methyl ester) amide
266.1327	265.131	0.006	266.1387	16	58.6	L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-
266.1327	265.088	-0.0369	266.0958	33	33.8	Albendazole
266.1327	265.131	0.006	266.1387	39	32.6	L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-
169.1018	336.147	-0.0212	169.0806	86	75.5	Ser-Cys-Lys
169.1018	186.1	-0.0046	169.0972	38	48.4	Ala-Pro
169.1018	186.1	-0.0046	169.0972	16	26	Ala-Pro
169.1018	336.147	-0.0212	169.0806	14	100	Ser-Cys-Lys
134.1137	151.1	-0.0173	134.0964	1	51	Norephedrine
134.1137	283.164	-0.0375	134.0762	15	100	Lys-His

134.1137	0	-0.05	134.06	152	35	4-Hydroxyindole
134.1137	151.1	-0.0173	134.0964	52	35.1	Norpseudoephedrine
257.1594	256.11	-0.0422	257.1172	12	100	Pterostilbene
163.1028	162.126	0.0301	163.1329	203	84.5	Ethanol, 2-(2-butoxyethoxy)-
163.1028	162.126	0.0301	163.1329	214	83.8	Ethanol, 2-(2-butoxyethoxy)-
163.1028	162.064	-0.0315	163.0713	14	21.1	Gly-Ser
163.1028	179.095	-0.0274	163.0754	31	23.9	3,4-Methylenedioxyamphetamine
238.1255	237.103	-0.0147	238.1108	55	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1255	237.092	-0.0262	238.0993	72	66	Ketamine
238.1255	237.1	-0.0181	238.1074	88	53.2	3-Hydroxy carbofuran
164.0069	163.046	0.0459	164.0528	82	72.6	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	120	75.3	Benzothiazole, 2,5-dimethyl-
164.0069	163	0.03	164.04	44	53.1	N-Acetyl-L-cysteine
164.0069	163.046	0.0459	164.0528	108	87.6	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	11	56.6	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	93	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	87	53	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	42	100	Benzothiazole, 2,5-dimethyl-
257.1488	128.059	-0.0244	257.1244	28	100	5-Methyl-5,6-Dihydrouracil
257.1488	256.117	-0.0244	257.1244	113	24.4	Thr-His
266.1655	265.131	-0.0268	266.1387	6	100	L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-
266.1655	265.131	-0.0268	266.1387	23	100	L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-
134.0898	0	-0.03	134.06	378	38.7	Oxindole
134.0898	133.064	-0.0185	134.0713	145	90.4	1H-Benzimidazol-2-amine
134.0898	0	-0.03	134.06	293	89.1	Oxindole
134.0898	0	-0.03	134.06	39	35.2	Oxindole
205.1202	204.075	-0.0383	205.0819	128	100	Gly-Glu
205.1202	204.075	-0.0383	205.0819	102	83.6	Gly-Glu
205.1202	204.09	-0.023	205.0972	133	54.1	Ethotoin
205.1202	204.075	-0.0383	205.0819	163	72.5	Gly-Glu
205.1375	204.09	-0.0403	205.0972	28	100	Fenozolone
205.1375	188.116	-0.0181	205.1194	117	91.4	Glycyl-L-norleucine
205.1375	204.09	-0.0403	205.0972	198	91	L-Tryptophan
205.1375	408.237	-0.0116	205.1259	185	44.7	Tyr-Val-Lys
176.1041	175	-0.03	176.07	15	100	1-Methoxy-3-carbaldehyde
176.1041	175.048	-0.0488	176.0553	98	61.5	Dimethyloxallylglycine
238.1427	237.103	-0.0319	238.1108	52	77.9	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.136	0.0011	238.1438	17	100	Viloxazine

283.1685	282.179	0.0179	283.1864	26	51	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	282.122	-0.0396	283.1289	47	47.3	Thr-Tyr
283.1685	282.179	0.0179	283.1864	157	100	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	0	-0.02	283.15	32	100	Artemisinin
238.1427	237.092	-0.0434	238.0993	59	81.7	Ketamine
238.1427	237.103	-0.0319	238.1108	9	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.103	-0.0319	238.1108	101	77.4	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.103	-0.0319	238.1108	144	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
205.1202	204.09	-0.023	205.0972	50	100	Fenozolone
205.1202	204.09	-0.023	205.0972	72	100	Fenozolone
205.1202	204.09	-0.023	205.0972	150	31.1	Ethotoin
238.1427	237.103	-0.0319	238.1108	9	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	0	-0.05	238.09	34	77.9	Biopterin
238.1427	0	-0.04	238.1	233	77.2	Mebendazole metabolite (2-Amino-5-benzoylbenzimidazole)
238.1427	237.136	0.0011	238.1438	8	100	Viloxazine
150.1003	169.074	-0.0442	150.0561	154	85.4	DL-Norepinephrine
150.1003	149.07	-0.0229	150.0774	117	42.5	Adenine, N6-methyl
150.1003	150.128	0.0274	150.1277	237	81.7	N-Butyl-4-methylpyridinium
150.1003	167.095	-0.009	150.0913	21	53.1	Synephrine
238.1311	237.103	-0.0203	238.1108	74	67.9	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1311	237.092	-0.0318	238.0993	63	100	Ketamine
238.1311	237.103	-0.0203	238.1108	18	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1311	237.103	-0.0203	238.1108	102	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
176.1041	193.058	-0.0494	176.0547	42	42.4	S-(2-Boronoethyl)-L-cysteine
211.1215	188.116	-0.0162	211.1053	229	89.3	L-Lysine, N2-acetyl-
211.1215	210.126	0.0114	211.1329	52	77.9	Jasmonic Acid

211.1215	210.126	0.0114	211.1329	131	53.5	Jasmonic Acid
164.0069	163.046	0.0459	164.0528	67	73.2	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	76	71.2	Pterine
164.0069	163.038	0.0386	164.0455	27	100	7-Nitroindazole
164.0069	163.046	0.0459	164.0528	52	71.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	100	100	Benzothiazole, 2,5-dimethyl-
164.0069	163	0.03	164.04	54	100	N-Acetyl-L-cysteine
164.0069	163.038	0.0386	164.0455	34	100	7-Nitroindazole
164.0069	163.046	0.0459	164.0528	75	73.7	Benzothiazole, 2,5-dimethyl-
164.0069	0	0.03	164.04	107	71	Acetylcysteine
164.0069	163.046	0.0459	164.0528	25	66	Benzothiazole, 2,5-dimethyl-
134.1096	0	-0.05	134.06	190	74.8	Oxindole
134.1096	0	-0.05	134.06	92	46.1	4-Hydroxyindole
134.1096	133.064	-0.0383	134.0713	45	20.6	1H-Benzimidazol-2-amine
326.182	325.131	-0.0433	326.1387	137	100	4-Hydroxycinnamic acid (L-phenylalanine methyl ester) amide
211.1441	210.159	0.0225	211.1666	4	100	Altretamine
211.1441	210.116	-0.021	211.123	6	100	Naphtazoline
211.1441	0	-0.01	211.13	200	47.2	Jasmonic acid
211.1441	0	-0.01	211.13	84	49.5	Jasmonic acid
176.1257	175.121	0.0024	176.1281	14	100	Threonine, butyl ester
176.1257	175.121	0.0024	176.1281	40	100	Threonine, butyl ester
257.1488	256.117	-0.0244	257.1244	82	71.9	His-Thr
257.1488	256.117	-0.0244	257.1244	76	100	Thr-His
257.1488	256.117	-0.0244	257.1244	90	50.9	Thr-His
211.1441	210.116	-0.021	211.123	40	79.6	Naphtazoline
211.1441	0	-0.01	211.13	145	41	Jasmonic acid
211.1441	210.126	-0.0112	211.1329	174	24.6	Jasmonic Acid
211.1441	0	-0.01	211.13	19	36.1	Jasmonic acid
176.1257	175.121	0.0024	176.1281	51	63.5	Threonine, butyl ester
176.1257	175.121	0.0024	176.1281	2	100	Threonine, butyl ester
149.0962	165.115	-0.0001	149.0961	31	100	(.+/-)-p-Methoxyamphetamine
149.0962	148.1	0.0111	149.1073	46	100	N-Benzylacetamide
149.0908	148	-0.05	149.04	90	100	(S)-(+)-Citramalic acid
149.0908	166.063	-0.0311	149.0597	173	23.8	Tropic acid
211.1441	210.116	-0.021	211.123	49	81.9	Naphtazoline
211.1441	210.126	-0.0112	211.1329	221	71.4	Jasmonic Acid
211.1441	420.223	-0.025	211.119	56	29	His-His-Lys
211.1441	188.116	-0.0388	211.1053	240	93.1	L-Lysine, N2-acetyl-
211.1671	228.147	-0.023	211.1441	59	33.8	Ile-Pro
211.1671	210.116	-0.044	211.123	7	100	Naphtazoline
211.1671	210.159	-0.0005	211.1666	140	85	Altretamine
211.1671	210.126	-0.0342	211.1329	66	45.5	Jasmonic Acid

238.1427	237.103	-0.0319	238.1108	16	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.103	-0.0319	238.1108	30	73.2	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	0	-0.04	238.1	106	78.4	Mebendazole metabolite (2- Amino-5- benzoylbenzimidazole)
238.1427	0	-0.04	238.1	216	95.8	Mebendazole metabolite (2- Amino-5- benzoylbenzimidazole)
238.1427	237.103	-0.0319	238.1108	45	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.136	0.0011	238.1438	25	68.7	Viloxazine
238.1427	0	-0.05	238.09	92	52.9	Biopterin
238.1427	0	-0.04	238.1	259	66.2	Mebendazole metabolite (2- Amino-5- benzoylbenzimidazole)
257.1594	256.117	-0.035	257.1244	101	78.2	Thr-His
257.1594	256.117	-0.035	257.1244	45	100	His-Thr
164.0069	163.046	0.0459	164.0528	54	63.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	45	64.7	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	87	65.4	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	118	71	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	83	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	25	100	4-Hydroxy-L-glutamic acid
164.0069	163.049	0.0498	164.0567	13	100	Pterine
164.0069	163.046	0.0459	164.0528	72	63.8	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	108	100	Pterine
164.0069	163.038	0.0386	164.0455	35	76.6	7-Nitroindazole
164.0069	163.046	0.0459	164.0528	78	76.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	37	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	39	79.9	Pterine
150.1003	150.053	-0.0242	150.0761	99	42	D-(-)-Ribose
150.1003	167.095	-0.009	150.0913	10	100	Synephrine
150.1003	149.07	-0.0229	150.0774	49	51.8	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	46	100	Adenine, N6-methyl
164.0069	163.046	0.0459	164.0528	61	41.8	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	27	73.2	Benzothiazole, 2,5-dimethyl-
163.1231	162.064	-0.0518	163.0713	23	42.7	Gly-Ser
163.1231	162.126	0.0098	163.1329	231	88.6	Ethanol, 2-(2-butoxyethoxy)-
163.1231	162.126	0.0098	163.1329	103	21.3	Ethanol, 2-(2-butoxyethoxy)-
163.1231	179.095	-0.0477	163.0754	80	35.5	3,4- Methylenedioxyamphetamine
205.1202	204.09	-0.023	205.0972	27	60	Fenozolone

205.1202	408.237	0.0057	205.1259	200	15	Tyr-Val-Lys
205.1202	408.201	-0.0125	205.1077	132	13.6	Phe-Asp-Lys
137.0611	136.039	-0.0153	137.0458	24	70.2	Allopurinol
137.0611	136.039	-0.0153	137.0458	72	11.1	Hypoxanthine
137.0611	154.027	-0.0378	137.0233	14	52	.beta.-Resorcylic acid
137.0611	0	0.01	137.07	115	29.6	PRALIDOXIME
164.0069	163.046	0.0459	164.0528	84	62.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	117	77.2	Pterine
149.1007	148.1	0.0066	149.1073	4	100	N-Benzylacetamide
149.1007	148.1	0.0066	149.1073	61	73.2	Normicotine
149.1007	150	-0.05	149.05	130	62.8	D-(-)-Arabinose
238.1427	237.092	-0.0434	238.0993	33	37.8	Ketamine
238.1427	237.092	-0.0434	238.0993	91	72.3	Ketamine
238.1427	474.234	-0.0185	238.1242	48	32.1	Trp-Asn-Arg
238.1427	0	-0.04	238.1	260	64.3	Mebendazole metabolite (2-Amino-5-benzoylbenzimidazole)
205.1375	408.186	-0.037	205.1005	143	95.1	Met-Met-Lys
205.1375	204.1	-0.03	205.107	4	100	1,6-Anhydro-b-D-glucose, permethyl-
205.1375	204.09	-0.0403	205.0972	109	29.3	Fenozolone
205.1202	204.075	-0.0383	205.0819	121	63.5	Gly-Glu
205.1202	204.09	-0.023	205.0972	123	100	Fenozolone
205.1202	408.201	-0.0125	205.1077	88	70.5	Phe-Asp-Lys
205.1202	408.186	-0.0197	205.1005	88	39.2	Met-Met-Lys
276.1945	275.159	-0.0279	276.1666	56	37.5	Thr-Arg
276.1945	319.133	-0.0438	276.1507	106	56	Norfloxacin
276.1945	275.159	-0.0279	276.1666	83	32.5	Arg-Thr
276.1945	319.133	-0.0438	276.1507	84	55.9	Norfloxacin
276.1945	319.133	-0.0438	276.1507	86	58	Norfloxacin
276.1945	275.152	-0.0351	276.1594	102	50.3	Homatropine
150.1003	150.128	0.0274	150.1277	187	77.6	N-Butyl-4-methylpyridinium
150.1003	167.095	-0.009	150.0913	30	100	Synephrine
150.1003	149.07	-0.0229	150.0774	174	44	Adenine, N6-methyl
238.1311	237.092	-0.0318	238.0993	17	36	Ketamine
238.1311	237.092	-0.0318	238.0993	76	57.7	Ketamine
238.1311	474.234	-0.0069	238.1242	99	29.1	His-Tyr-Arg
238.1311	474.234	-0.0069	238.1242	67	100	Trp-Asn-Arg
286.0528	285.067	0.0214	286.0742	80	100	7-Aminoclonazepam
647.333	0	-0.01	647.32	65	100	GARCINOLIC ACID
164.0069	163.046	0.0459	164.0528	50	81.2	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	1	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	6	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	14	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	67	84.7	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	4	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	6	100	4-Hydroxy-L-glutamic acid

164.0069	163.048	0.0484	164.0553	2	100	4-Hydroxy-L-glutamic acid
176.0975	175.084	-0.0058	176.0917	33	30.9	N-Carboxyethyl-.gamma.-aminobutyric acid
176.0975	175.048	-0.0422	176.0553	75	43.1	N-Acetyl-L-aspartic acid
176.0975	193.058	-0.0428	176.0547	34	100	S-(2-Boronoethyl)-L-cysteine
176.0975	175.084	-0.0058	176.0917	45	42.4	N-Carboxyethyl-.gamma.-aminobutyric acid
164.0069	163.046	0.0459	164.0528	47	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	3	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	1	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	14	100	4-Hydroxy-L-glutamic acid
176.1125	175	-0.04	176.07	61	54.2	1-Methoxy-3-carbaldehyde
176.1125	350.195	-0.007	176.105	16	100	Gly-Phe-Lys
176.1125	175.063	-0.0419	176.0706	117	100	3-Indoleacetic acid
211.1548	210.159	0.0118	211.1666	68	100	Altretamine
211.1548	188.116	-0.0495	211.1053	14	100	L-Lysine, N2-acetyl-
211.1548	420.223	-0.036	211.119	36	35.1	His-His-Lys
211.1548	0	0.02	211.17	103	28.8	altretamine
289.1861	288.209	0.0301	289.2162	100	63.1	Epitestosterone
289.1861	0	0.03	289.22	22	60	trans-Dehydroandrosterone
150.1003	149	-0.02	150.08	49	55.1	3-Methyladenine
150.1003	303.147	-0.009	150.0913	22	53.1	Cocaine
150.1003	149	-0.02	150.08	163	36.6	3-Methyladenine
276.1945	275.159	-0.0279	276.1666	41	31.8	Thr-Arg
276.1945	275.159	-0.0279	276.1666	45	35.6	Thr-Arg
276.1945	275.152	-0.0351	276.1594	134	88.5	Methylenedioxyprovalerone
276.1945	275.159	-0.0279	276.1666	95	43.9	Thr-Arg
276.1945	275.163	-0.0238	276.1707	165	90	Physostigmine
276.1945	319.133	-0.0438	276.1507	80	100	Norfloxacin
276.1945	275.152	-0.0351	276.1594	79	100	Methylenedioxyprovalerone
150.1003	150.053	-0.0242	150.0761	102	28.7	DL-Arabinose
150.1003	149.07	-0.0229	150.0774	38	100	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	61	100	Adenine, N6-methyl
150.1003	149.051	-0.042	150.0583	8	100	L-Methionine
276.1945	319.133	-0.0438	276.1507	87	51.7	Norfloxacin
276.1945	275.152	-0.0351	276.1594	31	56.6	4-Hydroxypropranolol
276.1945	275.159	-0.0279	276.1666	102	91.4	Arg-Thr
176.1195	175.121	0.0086	176.1281	33	100	Threonine, butyl ester
176.1195	175.084	-0.0278	176.0917	10	51	N-(tert-Butoxycarbonyl)glycine
176.1195	0	-0.05	176.07	22	61.5	Guanidinosuccinic Acid
286.0474	285.067	0.0268	286.0742	112	100	7-Aminoclonazepam
286.0474	285.067	0.0268	286.0742	63	100	7-Aminoclonazepam
286.0474	285.067	0.0268	286.0742	73	100	7-Aminoclonazepam
286.0474	285.067	0.0268	286.0742	49	100	7-Aminoclonazepam
164.0069	163.046	0.0459	164.0528	49	82.6	Benzothiazole, 2,5-dimethyl-

164.0069	163.048	0.0484	164.0553	1	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	1	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	2	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	46	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	4	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	3	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	22	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	45	81.7	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	2	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	2	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	7	100	4-Hydroxy-L-glutamic acid
169.1018	146.069	-0.0434	169.0584	32	13.5	Gly-Ala
169.1018	186.1	-0.0046	169.0972	11	31.4	Ala-Pro
169.1018	186.1	-0.0046	169.0972	60	54.2	Ala-Pro
169.1018	186.1	-0.0046	169.0972	60	100	Ala-Pro
176.0975	193.058	-0.0428	176.0547	39	26.7	S-(2-Boronoethyl)-L-cysteine
176.0975	175.063	-0.0269	176.0706	61	50	3-Indoleacetic acid
176.0975	193.058	-0.0428	176.0547	66	80.4	S-(2-Boronoethyl)-L-cysteine
287.247	286.193	-0.0464	287.2006	110	35.3	4-Androsten-3,17-dione
287.247	286.193	-0.0464	287.2006	144	58.6	4-Androsten-3,17-dione
591.2992	590.289	-0.0026	591.2966	40	100	Protoporphyrin IX dimethyl ester
205.1202	204.075	-0.0383	205.0819	40	19.8	Gly-Glu
205.1202	204.072	-0.0408	205.0794	20	7.7	Levamisole
205.1202	408.237	0.0057	205.1259	100	24.9	Tyr-Val-Lys
276.1945	275.159	-0.0279	276.1666	76	38.2	Thr-Arg
276.1945	275.159	-0.0279	276.1666	25	34.6	Thr-Arg
276.1945	0	-0.02	276.17	103	66.6	cyclobenzaprine
276.1945	275.159	-0.0279	276.1666	49	42.7	Thr-Arg
225.1677	224.116	-0.0443	225.1234	227	86.7	Butalbital
225.1677	224.116	-0.0443	225.1234	130	72.7	Butalbital
225.1677	0	-0.02	225.15	128	78.2	Methyl jasmonate
276.1945	258.183	0.0224	276.2169	102	37.2	Tetradecanedioic acid
276.1945	275.159	-0.0279	276.1666	24	27.6	Thr-Arg
276.1945	275.152	-0.0351	276.1594	25	100	4-Hydroxypropranolol
276.1945	275.148	-0.0391	276.1554	49	45.5	Glu-Lys
211.1113	210.116	0.012	211.123	14	100	Naphtazoline
211.1113	0	0.02	211.13	81	55.5	Jasmonic acid
211.1113	210	0.03	211.14	128	36.5	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-[(1S)-1-methylpropyl]-, (3S,8aS)-
211.1113	420.179	-0.0145	211.0968	84	39.9	Met-Asp-Arg
266.1134	243.078	-0.0465	266.0669	34	100	3-[N,N-Bis(2-hydroxyethyl)amino]-2-hydroxypropanesulfonic acid

266.1134	243.078	-0.0465	266.0669	35	100	3-[N,N-Bis(2-hydroxyethyl)amino]-2-hydroxypropanesulfonic acid
176.1195	175	-0.05	176.07	112	56	1-Methoxy-3-carbaldehyde
176.1195	175.121	0.0086	176.1281	6	100	Threonine, butyl ester
176.1195	175.063	-0.0489	176.0706	82	49.5	3-Indoleacetic acid
169.1084	73.053	-0.0136	169.0948	168	90.5	Formamide, N,N-dimethyl-
169.1084	186.1	-0.0112	169.0972	59	47.4	Ala-Pro
169.1084	186.1	-0.0112	169.0972	38	100	Ala-Pro
164.0069	163.046	0.0459	164.0528	50	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	2	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	2	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	10	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	42	81.2	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	5	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	1	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	59	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	48	82.2	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	3	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	2	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	8	100	4-Hydroxy-L-glutamic acid
176.1041	175	-0.03	176.07	36	47	3-Indoleacetic acid
176.1041	193.058	-0.0494	176.0547	12	52	S-(2-Boronoethyl)-L-cysteine
176.1041	193.058	-0.0494	176.0547	160	80.1	S-(2-Boronoethyl)-L-cysteine
149.0962	148.052	-0.0365	149.0597	177	76	trans-Cinnamic acid
149.0962	148.052	-0.0365	149.0597	190	57.4	trans-Cinnamic acid
149.0962	165.115	-0.0001	149.0961	39	100	(.+/-)-p-Methoxyamphetamine
150.1003	167.095	-0.009	150.0913	19	36.1	Synephrine
150.1003	167.095	-0.009	150.0913	130	47.1	Synephrine
150.1003	303.147	-0.009	150.0913	115	74.9	Cocaine
150.1003	149.07	-0.0229	150.0774	122	61.3	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	73	83.3	Synephrine
150.1003	149.07	-0.0229	150.0774	53	78.2	Adenine, N6-methyl
150.1003	167.058	-0.045	150.055	50	45.9	3-Methyl-2-nitrobenzyl alcohol
211.1441	210.116	-0.021	211.123	28	50	Naphtazoline
211.1441	210	-0.01	211.13	90	37.1	(+)-Jasmonic acid
211.1441	210.126	-0.0112	211.1329	56	33.8	Jasmonic Acid
211.1441	210.126	-0.0112	211.1329	10	100	Jasmonic Acid
276.1945	275.159	-0.0279	276.1666	74	21.8	Arg-Thr
276.1945	275.152	-0.0351	276.1594	51	52	4-Hydroxypropranolol
276.1945	319.133	-0.0438	276.1507	20	100	Norfloxacin
276.1945	275.159	-0.0279	276.1666	70	83	Thr-Arg
176.1257	175.096	-0.023	176.103	5	100	L-Citrulline

276.1945	275.159	-0.0279	276.1666	62	23	Thr-Arg
276.1945	275.159	-0.0279	276.1666	158	72.9	Arg-Thr
276.1945	275.152	-0.0351	276.1594	53	56.6	Homatropine
276.1945	258.183	0.0224	276.2169	71	35.5	Tetradecanedioic acid
276.1945	275.159	-0.0279	276.1666	20	59.3	Thr-Arg
276.1945	319.133	-0.0438	276.1507	44	100	Norfloxacin
276.1945	275.148	-0.0391	276.1554	38	50.7	.gamma.-L-Glu.-epsilon.-L-Lys
238.1427	237.103	-0.0319	238.1108	18	52	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.103	-0.0319	238.1108	20	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.103	-0.0319	238.1108	90	77.5	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.136	0.0011	238.1438	61	81.2	Viloxazine
176.1041	0	-0.03	176.07	114	21.2	3-Indoleacetic Acid
176.1041	175.063	-0.0335	176.0706	4	100	3-Indoleacetic acid
176.1041	193.058	-0.0494	176.0547	78	56.6	S-(2-Boronoethyl)-L-cysteine
176.1041	193.058	-0.0494	176.0547	278	99	S-(2-Boronoethyl)-L-cysteine
327.2164	326.199	-0.0097	327.2067	33	55.4	Hydroquinidine
327.2164	326.199	-0.0097	327.2067	48	60.8	Hydroquinidine
164.0069	163.046	0.0459	164.0528	45	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	3	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	3	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	5	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	57	83	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	9	56.6	Pterine
164.0069	163.048	0.0484	164.0553	3	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	53	83	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	5	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	2	100	4-Hydroxy-L-glutamic acid
164.0069	163.049	0.0498	164.0567	19	100	Pterine
289.1638	288.114	-0.0424	289.1214	137	82.5	Myclobutanil
289.1638	288.114	-0.0423	289.1215	72	100	Myclobutanil
150.1003	167.095	-0.009	150.0913	25	67.3	Synephrine
150.1003	149.07	-0.0229	150.0774	39	100	Adenine, N6-methyl
150.1003	149.105	0.0122	150.1125	204	69.2	Triethanolamine
150.1003	150.128	0.0274	150.1277	239	81.4	N-Butyl-4-methylpyridinium
150.1003	149.07	-0.0229	150.0774	95	74.5	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	248	54.3	Adenine, N6-methyl
150.1003	167.058	-0.045	150.055	84	73.2	3-Methyl-2-nitrobenzyl alcohol

150.1003	149.07	-0.0229	150.0774	197	83.2	Adenine, N6-methyl
150.1003	303.147	-0.009	150.0913	141	56	Cocaine
150.1003	149.07	-0.0229	150.0774	38	62.3	Adenine, N6-methyl
150.1003	149.12	0.0274	150.1277	137	56.1	Methamphetamine
569.3045	1138	0.0342	569.3387	10	100	YGGFLRRIR/2
150.1003	149.084	-0.009	150.0913	86	16.4	S(-)-Cathinone
150.1003	167.095	-0.009	150.0913	127	92	Synephrine
150.1003	149.105	0.0122	150.1125	122	47.5	Triethanolamine
150.1003	149.07	-0.0229	150.0774	2	100	Adenine, N6-methyl
276.1778	319.133	-0.0271	276.1507	86	78.9	Norfloxacin
276.1778	319.133	-0.0271	276.1507	30	100	Norfloxacin
276.1778	275.148	-0.0224	276.1554	75	38.4	Glu-Lys
176.1195	175.084	-0.0278	176.0917	22	100	N-Carboxyethyl-.gamma.-aminobutyric acid
176.1195	175.121	0.0086	176.1281	63	57.3	Threonine, butyl ester
176.1195	175.084	-0.0278	176.0917	61	47.6	N-Carboxyethyl-.gamma.-aminobutyric acid
276.1945	275.159	-0.0279	276.1666	45	36.2	Thr-Arg
276.1945	319.133	-0.0438	276.1507	56	62.3	Norfloxacin
276.1945	275.152	-0.0351	276.1594	42	100	4-Hydroxypropranolol
257.1488	274.128	-0.0244	257.1244	86	71.1	Gln-Gln
257.1488	256.117	-0.0244	257.1244	31	100	Thr-His
257.1488	256.117	-0.0244	257.1244	110	65	His-Thr
176.1298	175.096	-0.027	176.103	23	100	L-Citrulline
176.1298	175.084	-0.0381	176.0917	26	100	N-Carboxyethyl-.gamma.-aminobutyric acid
238.1427	237.092	-0.0434	238.0993	91	89.1	Ketamine
238.1427	474.234	-0.0185	238.1242	31	31.5	Trp-Asn-Arg
238.1427	237.103	-0.0319	238.1108	167	100	3-(Cyclohexylamino)-2-hydroxy-1-propanesulfonic acid
238.1427	474.234	-0.0185	238.1242	109	20.7	His-Tyr-Arg
164.0069	163.046	0.0459	164.0528	80	86.8	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	11	55.4	Pterine
164.0069	163.048	0.0484	164.0553	19	100	4-Hydroxy-L-glutamic acid
164.0069	163.038	0.0386	164.0455	34	100	7-Nitroindazole
164.0069	163.046	0.0459	164.0528	55	82.6	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	28	76.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	30	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	59	83.8	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	28	57.3	Pterine
164.0069	163.048	0.0484	164.0553	1	100	4-Hydroxy-L-glutamic acid
164.0069	163.038	0.0386	164.0455	28	100	7-Nitroindazole
205.1202	408.201	-0.0125	205.1077	20	16.5	Phe-Asp-Lys
205.1202	0	-0.04	205.08	102	33.9	Levamisole
205.1202	204.09	-0.023	205.0972	164	22.1	Fenozolone
205.1202	204.072	-0.0408	205.0794	156	21	Levamisole

205.1202	204.075	-0.0383	205.0819	25	12.4	Gly-Glu
205.1202	204.075	-0.0383	205.0819	67	22.4	Gly-Glu
205.1202	204.075	-0.0383	205.0819	81	14.5	Gly-Glu
205.1202	204.075	-0.0383	205.0819	113	12.4	Gly-Glu
164.0069	163.046	0.0459	164.0528	39	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	16	57.3	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	15	100	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	26	100	4-Hydroxy-L-glutamic acid
257.1279	128.059	-0.0035	257.1244	30	100	5-Methyl-5,6-Dihydrouracil
257.1279	256.117	-0.0035	257.1244	114	37.5	His-Thr
205.1375	204	-0.04	205.1	90	34	L-Tryptophane
205.1375	188.116	-0.0181	205.1194	120	69	Glycyl-L-norleucine
205.1375	204.1	-0.03	205.107	175	42.6	1,6-Anhydro-b-D-glucose, permethyl-
205.1375	408.237	-0.0116	205.1259	91	10.9	Tyr-Val-Lys
169.1265	168.115	-0.0042	169.1223	45	100	Jasmine lactone
169.1265	186.1	-0.0293	169.0972	63	44.7	Ala-Pro
169.1265	186.1	-0.0293	169.0972	83	77.8	Ala-Pro
169.1265	186.1	-0.0293	169.0972	78	71.8	Ala-Pro
134.0898	116.011	-0.045	134.0448	82	29.5	Maleic acid
134.0898	134.11	0.019	134.109	228	57.3	Benzene, n-butyl-
134.0898	283.164	-0.0136	134.0762	62	53.1	Lys-His
134.0898	0	-0.01	134.08	36	27.4	1,4-Dideoxy-1,4-Imino-D-Arabinitol
169.0986	146.069	-0.0402	169.0584	77	18.1	Gly-Ala
169.0986	336.147	-0.018	169.0806	185	75.7	Ser-Cys-Lys
169.0986	186.1	-0.0014	169.0972	89	73.2	Ala-Pro
169.1018	146.069	-0.0434	169.0584	81	40.5	Gly-Ala
169.1018	168.115	0.0205	169.1223	63	49.8	Jasmine lactone
169.1018	186.1	-0.0046	169.0972	108	82.2	Ala-Pro
169.1018	186.1	-0.0046	169.0972	80	62.9	Ala-Pro
276.1945	319.133	-0.0438	276.1507	97	59.6	Norfloxacin
276.1945	319.133	-0.0438	276.1507	23	100	Norfloxacin
276.1945	275.152	-0.0351	276.1594	92	85.9	Homatropine
169.1115	168.115	0.0108	169.1223	48	31.1	Jasmine lactone
169.1115	186.1	-0.0143	169.0972	86	67.9	Ala-Pro
169.1115	186.1	-0.0143	169.0972	95	100	Ala-Pro
169.1115	186.1	-0.0143	169.0972	35	79.6	Ala-Pro
276.1945	275.163	-0.0238	276.1707	147	88.8	Physostigmine
276.1945	319.133	-0.0438	276.1507	37	51	Norfloxacin
276.1945	319.133	-0.0438	276.1507	47	100	Norfloxacin
276.1945	319.133	-0.0438	276.1507	93	39.3	Norfloxacin
276.1945	319.133	-0.0438	276.1507	59	100	Norfloxacin
276.1945	275.152	-0.0351	276.1594	104	78.2	4-Hydroxypropranolol
276.1945	319.133	-0.0438	276.1507	7	100	Norfloxacin
276.1945	275.148	-0.0391	276.1554	108	56.9	Glu-Lys
276.1945	275.159	-0.0279	276.1666	26	73.2	Thr-Arg

276.1945	275.159	-0.0279	276.1666	123	57.6	Thr-Arg
276.1945	275.152	-0.0351	276.1594	90	57.8	4-Hydroxypropranolol
164.0069	163.046	0.0459	164.0528	51	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	52	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	31	56.6	Pterine
164.0069	163.049	0.0498	164.0567	40	100	Pterine
164.0069	163.046	0.0459	164.0528	51	70.6	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	6	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	59	100	Pterine
276.1945	275.159	-0.0279	276.1666	55	51.2	Arg-Thr
276.1945	275.159	-0.0279	276.1666	85	56	Arg-Thr
276.1945	319.133	-0.0438	276.1507	53	100	Norfloxacin
248.1168	498.175	-0.04	248.08	10	100	Benzenesulfonic acid, dodecyl(sulfophenoxy)-
238.1427	237.092	-0.0434	238.0993	42	80.4	Ketamine
238.1427	0	-0.05	238.09	54	41.1	Biopterin
238.1427	474.234	-0.0185	238.1242	128	37.1	Tyr-His-Arg
238.1427	474.234	-0.0185	238.1242	66	25.2	Tyr-His-Arg
163.1209	162.116	0.002	163.123	30	35.1	Anabasine
163.1209	162.126	0.0119	163.1329	74	22.3	Ethanol, 2-(2-butoxyethoxy)-
163.1209	162	-0.01	163.11	156	46.4	DL-5-Hydroxylysine hydrochloride
163.1209	162	-0.01	163.11	53	61.3	DL-5-Hydroxylysine hydrochloride
257.1488	256.117	-0.0244	257.1244	144	67.9	Thr-His
257.1488	256.117	-0.0244	257.1244	218	60.1	His-Thr
257.1488	256.117	-0.0244	257.1244	212	50.5	His-Thr
257.1488	256.11	-0.0316	257.1172	36	100	Pterostilbene
134.0966	134.11	0.012	134.109	92	56.4	Benzene, n-butyl-
134.0966	0	-0.04	134.06	62	29.8	Oxindole
134.0966	283.164	-0.0204	134.0762	43	100	Lys-His
134.0966	0	-0.04	134.06	202	73.5	Oxindole
257.1488	256.11	-0.0316	257.1172	40	100	Pterostilbene
257.1488	256.117	-0.0244	257.1244	92	79.6	Thr-His
257.1488	256.117	-0.0244	257.1244	94	55.4	Thr-His
238.1311	237.103	-0.0203	238.1108	19	38.4	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1311	237.136	0.0127	238.1438	18	57.9	Viloxazine
238.1311	474.234	-0.0069	238.1242	73	43.6	His-Tyr-Arg
211.1113	188.116	-0.006	211.1053	39	39.3	Ile-Gly
211.1113	188.116	-0.006	211.1053	279	95.7	L-Lysine, N2-acetyl-
211.1113	420.223	0.008	211.119	64	38	His-His-Lys
211.1113	210.1	-0.0036	211.1077	232	71.5	Aprobarbital
238.1427	215.116	-0.038	238.105	9	55.4	L-Proline, N-[(1,1- dimethylethoxy)carbonyl]-

238.1427	237.103	-0.0319	238.1108	125	60	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.136	0.0011	238.1438	102	64.3	Tyrosine, butyl ester
238.1427	474.234	-0.0185	238.1242	38	100	Trp-Asn-Arg
205.1375	204.09	-0.0403	205.0972	16	56.6	Fenozolone
205.1375	408.201	-0.0298	205.1077	100	55.4	Phe-Asp-Lys
205.1375	408.201	-0.0298	205.1077	230	27.7	Phe-Asp-Lys
205.1375	408.212	-0.0242	205.1133	183	18.4	Phe-Ser-Arg
238.1504	237.103	-0.0396	238.1108	20	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1504	237.136	-0.0066	238.1438	63	77.6	Viloxazine
238.1504	237.136	-0.0066	238.1438	19	37.1	Viloxazine
238.1504	237.103	-0.0396	238.1108	112	54.4	Methionine sulphone, butyl ester
326.1909	325.225	0.0417	326.2326	9	100	Bisoprolol
326.1909	325.225	0.0417	326.2326	56	76.6	Bisoprolol
205.1202	204.09	-0.023	205.0972	82	100	Fenozolone
205.1202	408.237	0.0057	205.1259	140	18.3	Tyr-Val-Lys
205.1202	408.223	-0.001	205.119	198	22.3	Pro-His-Arg
205.1202	204.072	-0.0408	205.0794	115	38.5	Tetramisole
205.1375	188.116	-0.0181	205.1194	222	100	Glycyl-L-norleucine
205.1375	204.09	-0.0403	205.0972	124	100	Fenozolone
205.1375	204.09	-0.0403	205.0972	257	82.2	Ethotoin
205.1375	204.09	-0.0403	205.0972	6	100	Fenozolone
211.132	188.116	-0.0267	211.1053	39	47.1	Ile-Gly
211.132	0	-0.03	211.1	132	77.2	Sinapyl alcohol
211.132	0	-0.03	211.1	112	77.5	Sinapyl alcohol
211.132	0	-0.05	211.08	154	27	D-Glucoheptose
150.1003	150.128	0.0274	150.1277	45	68.2	N-Butyl-4-methylpyridinium
150.1003	167.058	-0.045	150.055	57	52.3	3-Methyl-2-nitrobenzyl alcohol
150.1003	149.07	-0.0229	150.0774	112	92.1	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	47	33.3	Adenine, N6-methyl
164.0069	163.046	0.0459	164.0528	95	73.5	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	34	56	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	86	100	4-Hydroxy-L-glutamic acid
164.0069	163.038	0.0386	164.0455	47	100	7-Nitroindazole
205.1202	408.201	-0.0125	205.1077	77	22.5	Phe-Asp-Lys
205.1202	204.09	-0.023	205.0972	242	78	Ethotoin
205.1202	204.09	-0.023	205.0972	219	74.1	Fenozolone
205.1202	204.072	-0.0408	205.0794	163	26.1	Tetramisole
266.1596	265.168	0.0155	266.1751	13	100	Oxprenolol
266.1596	265.131	-0.0209	266.1387	218	97.6	L-Phenylalanine, N-[(1,1- dimethylethoxy)carbonyl]-
276.1945	275.159	-0.0279	276.1666	41	20.8	Thr-Arg

276.1945	275.159	-0.0279	276.1666	126	87.1	Arg-Thr
276.1945	319.133	-0.0438	276.1507	52	100	Norfloxacin
276.1945	275.148	-0.0391	276.1554	86	40.1	Glu-Lys
164.0069	163.046	0.0459	164.0528	71	38.7	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	67	81.2	Pterine
164.0069	163.048	0.0484	164.0553	79	57.3	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	81	73.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	63	100	Benzothiazole, 2,5-dimethyl-
150.1003	167.095	-0.009	150.0913	7	55.4	Synephrine
150.1003	167.058	-0.045	150.055	205	69	3-Methyl-2-nitrobenzyl alcohol
150.1003	167.095	-0.009	150.0913	71	100	Synephrine
149.0962	165.115	-0.0001	149.0961	224	84.8	(+/-)-p-Methoxyamphetamine
149.0962	148.1	0.0111	149.1073	253	97.1	N-Benzylacetamidine
149.0962	150	-0.05	149.05	293	82	D-(-)-Arabinose
149.0962	165.115	-0.0001	149.0961	7	100	(+/-)-p-Methoxyamphetamine
276.1945	275.159	-0.0279	276.1666	154	52.1	Thr-Arg
276.1945	275.152	-0.0351	276.1594	138	86.2	Methylenedioxypropylvalerone
276.1945	275.159	-0.0279	276.1666	51	39.1	Thr-Arg
276.1945	275.152	-0.0351	276.1594	128	100	Methylenedioxypropylvalerone
134.0898	0	-0.03	134.06	210	74.6	Oxindole
134.0898	135	-0.04	134.05	194	59.3	Adenine
134.0898	151.1	0.0066	134.0964	36	35.3	Norephedrine
176.0975	175	-0.03	176.07	59	67	1-Methoxy-3-carbaldehyde
176.0975	175.121	0.0306	176.1281	2	100	Threonine, butyl ester
176.0975	193.058	-0.0428	176.0547	47	69.3	S-(2-Boronoethyl)-L-cysteine
176.0975	193.058	-0.0428	176.0547	85	100	S-(2-Boronoethyl)-L-cysteine
134.0966	135	-0.05	134.05	71	59.2	Adenine
134.0966	283.164	-0.0204	134.0762	144	30.4	Lys-His
134.0966	0	-0.04	134.06	68	68.7	Oxindole
134.0966	151.1	-0.0002	134.0964	99	80.2	Norephedrine
238.1427	237.103	-0.0319	238.1108	11	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	474.234	-0.0185	238.1242	61	33.5	Trp-Asn-Arg
238.1427	474.234	-0.0185	238.1242	35	39	Tyr-His-Arg
276.2063	275.159	-0.0397	276.1666	25	100	Thr-Arg
276.2063	275.159	-0.0397	276.1666	44	32.8	Arg-Thr
276.2063	275.159	-0.0397	276.1666	59	64.7	Arg-Thr
276.2063	275.159	-0.0397	276.1666	61	74.9	Arg-Thr
205.1202	204.09	-0.023	205.0972	36	52.4	Fenozolone
205.1202	204.09	-0.023	205.0972	143	39.4	L-Tryptophan
205.1202	204.09	-0.023	205.0972	146	68	Ethotoin

205.1202	204.1	-0.013	205.107	132	53.4	1,6-Anhydro-b-D-glucose, permethyl-
276.1945	275.159	-0.0279	276.1666	86	60.8	Thr-Arg
276.1945	275.159	-0.0279	276.1666	58	100	Thr-Arg
276.1945	275.159	-0.0279	276.1666	68	52.5	Thr-Arg
276.1945	275.152	-0.0351	276.1594	51	39.5	4-Hydroxypropranolol
150.1003	167.095	-0.009	150.0913	97	76.4	Synephrine
150.1003	303.147	-0.009	150.0913	59	79.6	Cocaine
150.1003	149.12	0.0274	150.1277	145	48.5	Methamphetamine
150.1003	150.053	-0.0242	150.0761	7	52	D-(+)-Xylose
205.1202	204.09	-0.023	205.0972	99	77.6	L-Tryptophan
205.1202	204.072	-0.0408	205.0794	161	51.9	Tetramisole
205.1202	204.09	-0.023	205.0972	167	68.6	Fenozolone
205.1202	204.09	-0.023	205.0972	145	75.5	Ethotoin
205.1202	204.075	-0.0383	205.0819	73	73.1	Gly-Glu
205.1202	204.075	-0.0383	205.0819	144	76.7	Gly-Glu
205.1202	408.223	-0.001	205.119	58	24.4	Pro-His-Arg
205.1202	204.072	-0.0408	205.0794	18	32.9	Tetramisole
176.1041	175.059	-0.0375	176.0666	61	83.6	Guanidinosuccinic acid
176.1041	175.121	0.024	176.1281	47	70.2	Threonine, butyl ester
176.1041	175.063	-0.0335	176.0706	75	50	3-Indoleacetic acid
176.1041	175.048	-0.0488	176.0553	27	50	Dimethyloxallylglycine
276.1945	275.159	-0.0279	276.1666	44	41.9	Thr-Arg
276.1945	275.163	-0.0238	276.1707	91	66.1	Physostigmine
276.1945	319.133	-0.0438	276.1507	71	100	Norfloxacin
205.1375	408.212	-0.0242	205.1133	66	9.3	Phe-Ser-Arg
205.1375	204.09	-0.0403	205.0972	170	71.3	L-Tryptophan
205.1202	204.072	-0.0408	205.0794	21	19.9	Levamisole
205.1202	204.075	-0.0383	205.0819	109	52.6	Gly-Glu
205.1202	204.075	-0.0383	205.0819	208	89.9	Gly-Glu
205.1202	204.072	-0.0408	205.0794	122	39.2	Levamisole
238.1311	237.092	-0.0318	238.0993	102	80.1	Ketamine
238.1311	0	-0.02	238.11	57	30.5	COTARNINE
238.1311	237.103	-0.0203	238.1108	125	63	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1311	237.103	-0.0203	238.1108	79	51.1	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
150.1003	167.095	-0.009	150.0913	13	100	Synephrine
150.1003	167.095	-0.009	150.0913	11	37.6	Synephrine
150.1003	150.053	-0.0242	150.0761	72	46.2	D-(+)-Xylose
164.0069	163.046	0.0459	164.0528	127	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	69	61.5	4-Hydroxy-L-glutamic acid
164.0069	163.048	0.0484	164.0553	85	100	4-Hydroxy-L-glutamic acid
149.0962	148.11	0.021	149.1172	46	77.3	1-(2-Methoxyethoxy)-2-methyl-2-propanol

149.0962	148.11	0.021	149.1172	38	61.3	1-(2-Methoxyethoxy)-2-methyl-2-propanol
164.0069	163.049	0.0498	164.0567	69	45.4	Pterine
164.0069	163.046	0.0459	164.0528	56	47.6	Benzothiazole, 2,5-dimethyl-
276.1945	275.159	-0.0279	276.1666	127	74	Arg-Thr
276.1945	0	-0.02	276.17	153	87	cyclobenzaprine
276.1945	275.159	-0.0279	276.1666	89	53.1	Arg-Thr
164.0069	163.046	0.0459	164.0528	108	92.3	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	75	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	62	66.7	Benzothiazole, 2,5-dimethyl-
163.1064	162.116	0.017	163.123	32	12.2	Nicotine
163.1064	179.095	-0.031	163.0754	148	32.6	3,4-Methylenedioxyamphetamine
163.1064	162.116	0.017	163.123	38	27.8	Anabasine
257.1488	256.117	-0.0244	257.1244	76	35.7	His-Thr
257.1488	274.128	-0.0244	257.1244	98	77.1	Gln-Gln
205.1202	408.201	-0.0125	205.1077	65	37.1	Phe-Asp-Lys
205.1202	204.09	-0.023	205.0972	96	45.5	L-Tryptophan
205.1202	408.223	-0.001	205.119	80	16.5	Pro-His-Arg
205.1202	408.212	-0.0069	205.1133	122	20	Phe-Ser-Arg
205.1202	204.075	-0.0383	205.0819	161	79.1	Gly-Glu
205.1202	204.075	-0.0383	205.0819	84	64.1	Gly-Glu
205.1202	204.09	-0.023	205.0972	137	17.8	Fenozolone
205.1202	408.212	-0.0069	205.1133	190	9.8	Tyr-Ala-Arg
276.1945	275.159	-0.0279	276.1666	51	17.2	Thr-Arg
276.1945	319.133	-0.0438	276.1507	72	81.4	Norfloxacin
276.1945	275.152	-0.0351	276.1594	54	32.3	4-Hydroxypropranolol
276.1945	319.133	-0.0438	276.1507	66	85.2	Norfloxacin
150.1003	167.095	-0.009	150.0913	5	100	Synephrine
150.1003	150.053	-0.0242	150.0761	118	25.5	D-(-)-Ribose
150.1003	149	-0.02	150.08	249	85.8	3-Methyladenine
150.1003	167.095	-0.009	150.0913	154	79.2	Synephrine
238.1427	237.092	-0.0434	238.0993	77	83.8	Ketamine
238.1427	237.136	0.0011	238.1438	24	41.7	Viloxazine
238.1427	0	-0.05	238.09	80	31.9	Biopterin
238.1427	0	-0.05	238.09	73	84	Biopterin
327.1725	326.199	0.0342	327.2067	72	100	Ajmaline
327.1725	0	0.04	327.21	14	59.3	Ajmaline
327.1725	344.199	0.023	327.1955	107	77.2	Tetrahydrocannabinol(nor-delta-9-HOOC)
326.2095	652	-0.0459	326.1636	90	80.9	YAFPGP/2
238.1427	237.103	-0.0319	238.1108	4	100	3-(Cyclohexylamino)-2-hydroxy-1-propanesulfonic acid
238.1427	474.234	-0.0185	238.1242	66	33	Trp-Asn-Arg
238.1427	0	-0.03	238.11	187	94.4	COTARNINE
238.1427	237.092	-0.0434	238.0993	16	55.4	Ketamine

276.1945	275.148	-0.0391	276.1554	32	100	Glu-Lys
276.1945	275.163	-0.0238	276.1707	133	85.6	Physostigmine
150.1003	150.053	-0.0242	150.0761	71	36.3	D-(+)-Xylose
150.1003	149.07	-0.0229	150.0774	67	38.4	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	109	41.8	Adenine, N6-methyl
150.1003	303.147	-0.009	150.0913	79	83.6	Cocaine
150.1003	167.095	-0.009	150.0913	90	50.2	Synephrine
150.1003	149.07	-0.0229	150.0774	70	100	Adenine, N6-methyl
150.1003	149.12	0.0274	150.1277	169	73.7	Methamphetamine
149.0962	165.115	-0.0001	149.0961	64	84.9	(./-.)-p-Methoxyamphetamine
149.0962	165.115	-0.0001	149.0961	57	100	(./-.)-p-Methoxyamphetamine
149.0962	166.063	-0.0365	149.0597	43	57.8	Tropic acid
149.0962	166.063	-0.0365	149.0597	67	81.2	Tropic acid
205.1202	204.09	-0.023	205.0972	19	100	Fenozolone
205.1202	204	-0.02	205.1	88	30.2	L-Tryptophane
205.1202	103.063	-0.0008	205.1194	185	65.8	Butanoic acid, 2-amino-, (R)-
205.1202	204.1	-0.013	205.107	64	77.3	1,6-Anhydro-b-D-glucose, permethyl-
164.0069	163.046	0.0459	164.0528	76	86.6	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	48	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	80	100	Pterine
164.0069	163.048	0.0484	164.0553	66	100	4-Hydroxy-L-glutamic acid
176.1257	175.096	-0.023	176.103	45	32.2	L-Citrulline
176.1257	175.121	0.0024	176.1281	8	100	Threonine, butyl ester
164.0069	163.046	0.0459	164.0528	51	61.5	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	12	38.3	4-Hydroxy-L-glutamic acid
164.0069	163.038	0.0386	164.0455	95	100	7-Nitroindazole
176.1041	175.096	-0.001	176.103	35	27.3	L-Citrulline
176.1041	193.058	-0.0494	176.0547	69	62.9	S-(2-Boronoethyl)-L-cysteine
176.1041	193.058	-0.0494	176.0547	25	60.8	S-(2-Boronoethyl)-L-cysteine
176.1041	193.058	-0.0494	176.0547	55	68.7	S-(2-Boronoethyl)-L-cysteine
164.0069	163.046	0.0459	164.0528	83	61	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	128	86.8	Benzothiazole, 2,5-dimethyl-
164.0069	163.048	0.0484	164.0553	6	100	4-Hydroxy-L-glutamic acid
211.1775	210.126	-0.0446	211.1329	119	48.5	Jasmonic Acid
211.1775	210.126	-0.0446	211.1329	36	29.4	Jasmonic Acid
211.1775	420.249	-0.046	211.1315	39	34.8	Phe-Val-Arg
205.1202	204.075	-0.0383	205.0819	24	100	Gly-Glu
205.1202	204.075	-0.0383	205.0819	89	35.6	Gly-Glu
205.1202	204.072	-0.0408	205.0794	92	37.9	Tetramisole
205.1202	204.072	-0.0408	205.0794	96	28.3	Tetramisole
205.1375	204.09	-0.0403	205.0972	20	100	Fenozolone

205.1375	204.09	-0.0403	205.0972	54	35	L-Tryptophan
205.1375	103.063	-0.0181	205.1194	184	89.4	Butanoic acid, 2-amino-, (S)-
205.1375	204.09	-0.0403	205.0972	157	68	L-Tryptophan
276.1809	275.167	-0.0062	276.1747	123	62.3	Cyclobenzaprine
276.1809	319.133	-0.0302	276.1507	49	82.2	Norfloxacin
276.1809	275.152	-0.0215	276.1594	129	74.4	4-Hydroxypropranolol
276.1809	275.152	-0.0215	276.1594	126	57.3	Homatropine
163.1064	162.064	-0.0351	163.0713	69	50.3	Gly-Ser
163.1064	162.126	0.0264	163.1329	80	35.5	Ethanol, 2-(2-butoxyethoxy)-
163.1064	162.126	0.0264	163.1329	92	55.2	Ethanol, 2-(2-butoxyethoxy)-
163.1064	486.314	0.0055	163.1119	94	26.9	Arg-Arg-Arg
276.1945	275.159	-0.0279	276.1666	72	50.4	Thr-Arg
276.1945	275.159	-0.0279	276.1666	52	48.5	Thr-Arg
276.1945	275.148	-0.0391	276.1554	28	30.1	Glu-Lys
276.1945	275.152	-0.0351	276.1594	151	82.5	Methylenedioxypropylvalerone
176.1125	175.059	-0.0459	176.0666	9	24.6	Guanidinosuccinic acid
176.1125	175.063	-0.0419	176.0706	14	54.2	3-Indoleacetic acid
276.1945	275.159	-0.0279	276.1666	42	46.8	Thr-Arg
276.1945	275.159	-0.0279	276.1666	32	39.9	Arg-Thr
276.1945	275.159	-0.0279	276.1666	59	100	Thr-Arg
205.1202	204.075	-0.0383	205.0819	133	100	Gly-Glu
205.1202	204.075	-0.0383	205.0819	113	57.3	Gly-Glu
205.1202	204.072	-0.0408	205.0794	216	38.8	Tetramisole
205.1202	204.09	-0.023	205.0972	67	35.8	Ethotoin
238.1427	215.116	-0.038	238.105	39	51	L-Proline, N-[(1,1-dimethylethoxy)carbonyl]-
238.1427	237.092	-0.0434	238.0993	27	44	Ketamine
238.1427	0	-0.03	238.11	43	47.1	COTARNINE
238.1427	237.103	-0.0319	238.1108	111	56.7	3-(Cyclohexylamino)-2-hydroxy-1-propanesulfonic acid
276.1945	275.159	-0.0279	276.1666	120	54.4	Thr-Arg
276.1945	319.133	-0.0438	276.1507	59	100	Norfloxacin
276.1945	319.133	-0.0438	276.1507	56	82.2	Norfloxacin
276.1945	275.152	-0.0351	276.1594	139	63.3	4-Hydroxypropranolol
211.1345	188.116	-0.0292	211.1053	34	41.6	Ile-Gly
211.1345	210.1	-0.0268	211.1077	46	100	Aprobarbital
211.1345	420.179	-0.0377	211.0968	27	34.1	Met-Asp-Arg
211.1345	210.1	-0.0268	211.1077	156	78.4	Aprobarbital
134.1002	135	-0.05	134.05	238	78.8	Adenine
134.1002	0	-0.04	134.06	377	88.4	Oxindole
134.1002	283.164	-0.024	134.0762	52	37.5	Lys-His
134.1002	283.164	-0.024	134.0762	15	58.6	Lys-His
205.1202	188.116	-0.0008	205.1194	64	42.1	Glycyl-L-norleucine
205.1202	204.075	-0.0383	205.0819	217	55.2	Gly-Glu
205.1202	408.237	0.0057	205.1259	140	13.6	Tyr-Val-Lys
257.1488	256.117	-0.0244	257.1244	96	47.9	Thr-His

257.1488	256.11	-0.0316	257.1172	8	100	Pterostilbene
257.1488	256.11	-0.0316	257.1172	50	100	Pterostilbene
149.0962	148.1	0.0111	149.1073	49	55.4	Nornicotine
149.0962	148.1	0.0111	149.1073	112	63.5	N-Benzylacetamide
149.0962	166.063	-0.0365	149.0597	99	74.1	Tropic acid
134.0898	135	-0.04	134.05	195	80.9	Adenine
134.0898	283.164	-0.0136	134.0762	50	36.9	Lys-His
134.0898	0	-0.01	134.08	194	50.5	L-O-Methylthreonine
149.1007	165.115	-0.0046	149.0961	38	64.3	(.+/-)-p-Methoxyamphetamine
149.1007	150	-0.05	149.05	94	59.3	D-(-)-Arabinose
149.0962	165.115	-0.0001	149.0961	8	100	(.+/-)-p-Methoxyamphetamine
149.0962	165.115	-0.0001	149.0961	80	84.5	(.+/-)-p-Methoxyamphetamine
164.0069	163.046	0.0459	164.0528	126	84.4	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	61	65.2	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	103	100	Pterine
164.0069	163.049	0.0498	164.0567	85	73	Pterine
164.0069	163	0.03	164.04	68	78.2	N-Acetyl-L-cysteine
164.0069	163	0.03	164.04	72	49.1	N-Acetyl-L-cysteine
164.0069	163.048	0.0484	164.0553	4	100	4-Hydroxy-L-glutamic acid
164.0069	163.046	0.0459	164.0528	75	78.9	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	60	48.3	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	20	100	Benzothiazole, 2,5-dimethyl-
164.0069	163.049	0.0498	164.0567	62	100	Pterine
211.1441	210.159	0.0225	211.1666	16	56	Altretamine
211.1441	420.223	-0.025	211.119	171	63	His-His-Lys
211.1441	210.126	-0.0112	211.1329	28	34.2	Jasmonic Acid
211.1441	0	-0.04	211.1	66	20.2	Sinapyl alcohol
205.1375	408.237	-0.0116	205.1259	97	23.8	Tyr-Val-Lys
205.1375	408.223	-0.018	205.119	116	26.2	Pro-His-Arg
205.1375	204.09	-0.0403	205.0972	216	73	Ethotoin
150.1003	167.095	-0.009	150.0913	76	70.9	Synephrine
150.1003	132.042	-0.0242	150.0761	65	22.5	Ethyl hydrogen malonate
150.1003	150.053	-0.0242	150.0761	81	52.2	D-(+)-Xylose
150.1003	150.053	-0.0242	150.0761	43	32.2	D-(+)-Xylose
276.1945	275.159	-0.0279	276.1666	138	62	Arg-Thr
276.1945	275.148	-0.0391	276.1554	42	100	Glu-Lys
276.1945	275.152	-0.0351	276.1594	108	81	Methylenedioxypropylvalerone
211.1441	0	-0.01	211.13	49	38.1	Jasmonic acid
211.1441	0	0.03	211.17	129	32.6	altretamine
211.1441	0	-0.04	211.1	65	72.2	Sinapyl alcohol
296.2263	295.178	-0.0407	296.1856	31	100	Esmolol
238.1427	0	-0.05	238.09	46	27.7	Biopterin
238.1427	237.092	-0.0434	238.0993	24	38.6	Ketamine
238.1427	237.092	-0.0434	238.0993	32	73.2	Ketamine

238.1427	237.103	-0.0319	238.1108	152	76.5	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.103	-0.0319	238.1108	38	100	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1427	237.136	0.0011	238.1438	44	41.9	Viloxazine
238.1427	0	-0.05	238.09	91	49.4	Biopterin
238.1427	474.234	-0.0185	238.1242	77	47	Trp-Asn-Arg
276.1945	275.159	-0.0279	276.1666	43	81.4	Thr-Arg
276.1945	319.133	-0.0438	276.1507	84	100	Norfloxacin
276.1945	275.159	-0.0279	276.1666	21	100	Arg-Thr
276.1945	275.152	-0.0351	276.1594	214	81.9	Homatropine
137.0555	136.039	-0.0097	137.0458	51	16.4	Allopurinol
137.0555	154.063	0.0042	137.0597	158	24.1	3-Hydroxy-4-methoxybenzyl alcohol
137.0555	136.039	-0.0097	137.0458	98	20.6	Hypoxanthine
137.0555	138.045	-0.0182	137.0373	121	23.9	Butylphosphonic acid
276.1945	275.148	-0.0391	276.1554	59	34.8	Glu-Lys
276.1945	275.152	-0.0351	276.1594	5	100	Homatropine
276.1945	275.148	-0.0391	276.1554	74	62.3	Glu-Lys
276.1945	275.159	-0.0279	276.1666	91	35	Thr-Arg
276.1945	275.163	-0.0238	276.1707	228	97	Physostigmine
276.1945	319.133	-0.0438	276.1507	69	52.2	Norfloxacin
276.1945	275.159	-0.0279	276.1666	124	30	Thr-Arg
393.3061	370.308	-0.0086	393.2975	83	80.2	Hexanedioic acid, bis(2- ethylhexyl) ester
393.3061	392.293	-0.0062	393.2999	43	100	Deoxycholic acid
393.3061	392.293	-0.0062	393.2999	12	57.9	Deoxycholic acid
115.0519	114.025	-0.0195	115.0324	37	36.4	Methimazole
115.0519	114.025	-0.0195	115.0324	72	43.9	Methimazole
115.0519	0	-0.02	115.03	8	27.3	Methimazole
164.0069	163.046	0.0459	164.0528	53	83.3	Benzothiazole, 2,5-dimethyl-
164.0069	163.046	0.0459	164.0528	78	53.3	Benzothiazole, 2,5-dimethyl-
164.0069	163	0.03	164.04	74	55.4	N-Acetyl-L-cysteine
164.0069	163.049	0.0498	164.0567	61	100	Pterine
205.1202	204.09	-0.023	205.0972	145	52.1	Fenozolone
205.1202	188.116	-0.0008	205.1194	79	82.4	Glycyl-L-norleucine
205.1202	204.072	-0.0408	205.0794	159	40.6	Levamisole
205.1202	408.237	0.0057	205.1259	208	65.3	Tyr-Val-Lys
164.0069	163.049	0.0498	164.0567	101	71.1	Pterine
164.0069	163.038	0.0386	164.0455	60	44.8	7-Nitroindazole
164.0069	163.048	0.0484	164.0553	117	100	4-Hydroxy-L-glutamic acid
164.0069	163.049	0.0498	164.0567	39	100	Pterine
205.1202	182.087	-0.0443	205.0759	181	39	Eflornithine
205.1202	204.075	-0.0383	205.0819	172	84.2	Gly-Glu
205.1202	204.075	-0.0383	205.0819	210	34.6	Gly-Glu

205.1202	204.072	-0.0408	205.0794	152	46.3	Tetramisole
266.1363	283.128	-0.0115	266.1248	83	86.6	His-Gln
266.1363	283.128	-0.0115	266.1248	76	70.1	His-Gln
266.1363	0	0	266.14	50	69.3	ANISOMYCIN
266.1363	265.147	0.0176	266.1539	116	94.2	Desmethyldoxepin
150.0831	167.095	0.0082	150.0913	18	57.3	Synephrine
150.0831	149.12	0.0446	150.1277	260	46.2	Methamphetamine
150.0831	149.12	0.0446	150.1277	94	34.6	Methamphetamine
150.0831	149.12	0.0446	150.1277	109	67.2	Methamphetamine
211.1441	210.116	-0.021	211.123	36	77.6	Naphtazoline
211.1441	420.223	-0.025	211.119	92	31.8	His-His-Lys
211.1441	0	-0.01	211.13	139	34.6	Jasmonic acid
211.1441	420.179	-0.0473	211.0968	123	28.9	Met-Asp-Arg
137.0514	137.071	0.0195	137.0709	32	6.2	1-Methylnicotinamide cation
137.0514	136.039	-0.0056	137.0458	236	71.3	Allopurinol
137.0514	138.045	-0.0141	137.0373	84	19.8	Butylphosphonic acid
137.0514	154.027	-0.0281	137.0233	108	92.3	Benzoic acid, 2,3-dihydroxy-
371.3164	370.308	-0.0008	371.3156	52	100	Hexanedioic acid, bis(2-ethylhexyl) ester
225.154	0	0	225.15	152	54.7	Methyl jasmonate
225.154	224.189	0.0422	225.1961	272	89	1,3-Dicyclohexylurea
225.154	0	0	225.15	147	64.9	Methyl jasmonate
225.154	0	0	225.15	138	100	Methyl jasmonate
419.2933	418.236	-0.0498	419.2435	171	100	Met-Ile-Arg
419.2933	418.236	-0.0498	419.2435	131	81.7	Met-Ile-Arg
419.2933	418.308	0.0223	419.3156	233	88	1,2-Benzenedicarboxylic acid, dinonyl ester
419.2933	418.308	0.0223	419.3156	129	78.2	1,2-Benzenedicarboxylic acid, dinonyl ester
257.1363	256.11	-0.0191	257.1172	96	47.6	Pterostilbene
257.1363	256.117	-0.0119	257.1244	118	23	His-Thr
257.1363	256.11	-0.0191	257.1172	193	100	Pterostilbene
276.1945	275.159	-0.0279	276.1666	111	39.2	Thr-Arg
276.1945	319.133	-0.0438	276.1507	69	32.9	Norfloxacin
276.1945	319.133	-0.0438	276.1507	68	64.7	Norfloxacin
276.1945	275.152	-0.0351	276.1594	173	82.2	Methylenedioxypropylvalerone
276.1945	275.167	-0.0198	276.1747	69	39.8	Cyclobenzaprine
276.1945	319.133	-0.0438	276.1507	70	49	Norfloxacin
276.1945	275.152	-0.0351	276.1594	169	77.8	Methylenedioxypropylvalerone
276.1945	275.152	-0.0351	276.1594	126	65.9	Methylenedioxypropylvalerone
176.1195	175	-0.05	176.07	194	61.5	1-Methoxy-3-carbaldehyde
176.1195	175.063	-0.0489	176.0706	116	80.7	3-Indoleacetic acid
150.1003	149.07	-0.0229	150.0774	188	70.8	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	209	68	Synephrine
150.1003	149.07	-0.0229	150.0774	92	84.7	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	79	34.5	Adenine, N6-methyl
276.1945	275.159	-0.0279	276.1666	139	58.6	Arg-Thr

276.1945	319.133	-0.0438	276.1507	150	75.6	Norfloxacin
276.1945	319.133	-0.0438	276.1507	149	77	Norfloxacin
276.1945	275.152	-0.0351	276.1594	150	44.3	Methylenedioxypropylvalerone
176.0975	175.121	0.0306	176.1281	152	100	Threonine, butyl ester
176.0975	175.121	0.0306	176.1281	192	74.9	Threonine, butyl ester
276.1945	275.159	-0.0279	276.1666	67	53	Thr-Arg
276.1945	275.152	-0.0351	276.1594	91	79.3	Methylenedioxypropylvalerone
276.1945	275.159	-0.0279	276.1666	86	71.3	Arg-Thr
276.1945	275.152	-0.0351	276.1594	136	62.7	Methylenedioxypropylvalerone
276.1945	275.163	-0.0238	276.1707	120	40.6	Physostigmine
276.1945	275.163	-0.0238	276.1707	121	58.6	Physostigmine
276.1945	0	-0.02	276.17	140	50.6	cyclobenzaprine
276.1945	275.152	-0.0351	276.1594	109	79.6	Methylenedioxypropylvalerone
150.1003	149.07	-0.0229	150.0774	241	91.3	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	288	65	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	94	46.5	Synephrine
150.1003	149.07	-0.0229	150.0774	60	79.9	Adenine, N6-methyl
238.1427	237.092	-0.0434	238.0993	210	87.6	Ketamine
238.1427	0	-0.05	238.09	158	45	Biopterin
238.1427	237.136	0.0011	238.1438	109	42.2	Viloxazine
238.1427	474.234	-0.0185	238.1242	167	54.3	Trp-Asn-Arg
150.1003	167.095	-0.009	150.0913	190	79.6	Synephrine
150.1003	149.07	-0.0229	150.0774	173	83.8	Adenine, N6-methyl
150.1003	149.07	-0.0229	150.0774	177	36.6	Adenine, N6-methyl
150.1003	167.095	-0.009	150.0913	172	56.5	Synephrine
283.1685	282.122	-0.0396	283.1289	124	30.4	Thr-Tyr
283.1685	282.122	-0.0396	283.1289	278	63.1	Tyr-Thr
283.1685	282.179	0.0179	283.1864	194	75	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	282.179	0.0179	283.1864	181	84.5	1,3-Bis(tris(hydroxymethyl)methylamino)propane
257.1185	256.117	0.0059	257.1244	85	55.3	Thr-His
257.1185	256.11	-0.0013	257.1172	135	72.6	Pterostilbene
257.1185	256.117	0.0059	257.1244	70	35.6	Thr-His
257.1185	256.11	-0.0013	257.1172	62	100	Pterostilbene
283.1685	282.179	0.0179	283.1864	169	100	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	282.122	-0.0396	283.1289	206	43.8	Thr-Tyr
283.1685	0	-0.02	283.15	190	44.1	Artemisinin
283.1685	0	-0.02	283.15	152	29.7	Artemisinin
371.3164	370.308	-0.0008	371.3156	26	100	Hexanedioic acid, bis(2-ethylhexyl) ester
150.0756	169.074	-0.0195	150.0561	235	86.1	DL-Norepinephrine
150.0756	149.07	0.0018	150.0774	67	55	Adenine, N6-methyl

150.0756	169.074	-0.0195	150.0561	232	41	DL-Norepinephrine
150.0756	167.058	-0.021	150.055	207	61.2	3-Methyl-2-nitrobenzyl alcohol
266.1481	265.158	0.0171	266.1652	96	56	Acridine Orange
266.1481	265.168	0.027	266.1751	103	45.1	Oxprenolol
266.1481	265.168	0.027	266.1751	96	100	Oxprenolol
266.1481	265.168	0.027	266.1751	93	45.5	Oxprenolol
205.1202	204.072	-0.0408	205.0794	151	38.3	Levamisole
205.1202	408.223	-0.001	205.119	147	37.3	Pro-His-Arg
205.1202	204.072	-0.0408	205.0794	383	51.3	Tetramisole
205.1202	204.09	-0.023	205.0972	205	96.3	Fenozolone
205.1202	222.1	-0.023	205.0972	201	68.9	Gly-Phe
205.1202	204.09	-0.023	205.0972	208	66.6	Fenozolone
205.1202	204.09	-0.023	205.0972	248	47.3	Fenozolone
428.2804	1284	-0.0503	428.2301	25	60.8	DRVYVHPFHL/3
310.1687	309.169	0.0074	310.1761	73	66.9	Tyr-Lys
310.1687	309.134	-0.0274	310.1413	162	72	Fluoxetine
310.1687	309.119	-0.043	310.126	62	51.2	10H-Benzo[4,5]cyclohepta[1,2-b]thiophen-10-one, 4,9-dihydro-4-(1-methyl-4-piperidinylidene)-
310.1687	309.134	-0.0274	310.1413	189	90.3	Fluoxetine
310.1846	309.169	-0.0085	310.1761	82	74.3	Tyr-Lys
310.1846	327.22	0.0319	310.2165	107	82.5	Butorphanol
310.1846	327.22	0.0319	310.2165	144	86.7	Butorphanol
310.1846	309.194	0.0167	310.2013	47	76.9	Metipranolol
266.1425	265.158	0.0227	266.1652	93	100	Acridine Orange
266.1425	0	0.03	266.17	131	100	antazoline
266.1425	265	-0.02	266.12	188	81.2	Thiamine hydrochloride
238.1311	237.092	-0.0318	238.0993	163	37.7	Ketamine
238.1311	215.091	-0.0513	238.0798	122	24.6	4-Ethyl-2E-(hydroxyimino)-5-nitro-3E-hexenamide
238.1311	237.103	-0.0203	238.1108	126	36.5	3-(Cyclohexylamino)-2-hydroxy 1-propanesulfonic acid
238.1311	237.092	-0.0318	238.0993	156	56.9	Ketamine
257.1363	256.117	-0.0119	257.1244	63	54.7	Thr-His
257.1363	256.117	-0.0119	257.1244	106	22.4	Thr-His
257.1363	256.117	-0.0119	257.1244	141	25.7	Thr-His
257.1363	256.11	-0.0191	257.1172	203	68.2	Pterostilbene
276.1945	275.148	-0.0391	276.1554	72	37.2	Glu-Lys
276.1945	275.152	-0.0351	276.1594	116	46.7	Methylenedioxypropylvalerone
276.1945	275.152	-0.0351	276.1594	123	40.5	Methylenedioxypropylvalerone
276.1945	275.152	-0.0351	276.1594	132	72.7	Methylenedioxypropylvalerone
276.1945	319.133	-0.0438	276.1507	115	39.1	Norfloxacin
276.1945	275.152	-0.0351	276.1594	221	90.1	Methylenedioxypropylvalerone

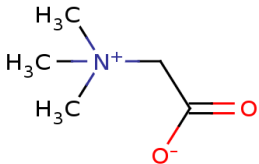
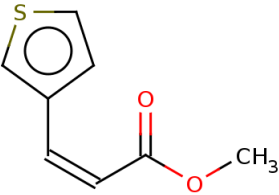
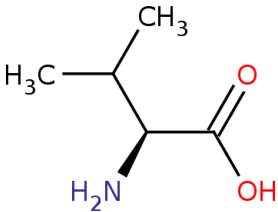
276.1945	275.163	-0.0238	276.1707	108	49.1	Physostigmine
276.1945	275.163	-0.0238	276.1707	140	81.2	Physostigmine
276.1945	275.159	-0.0279	276.1666	221	76.4	Arg-Thr
276.1945	275.159	-0.0279	276.1666	150	70.1	Arg-Thr
276.1945	275.152	-0.0351	276.1594	101	58.2	Methylenedioxypropylvalerone
276.1945	275.152	-0.0351	276.1594	212	78.4	Homatropine
310.154	309.169	0.0221	310.1761	111	100	Tyr-Lys
310.154	309.106	-0.0407	310.1133	122	100	(-)-N-Acetylneuraminic acid
310.154	309.106	-0.0407	310.1133	98	34	(-)-N-Acetylneuraminic acid
310.154	309.106	-0.0407	310.1133	59	55.4	(-)-N-Acetylneuraminic acid
150.1003	303.147	-0.009	150.0913	116	41.1	Cocaine
150.1003	149	-0.02	150.08	263	36.7	3-Methyladenine
150.1003	167.058	-0.045	150.055	322	73.5	3-Methyl-2-nitrobenzyl alcohol
150.1003	167.095	-0.009	150.0913	170	66.8	Synephrine
137.0419	136.039	0.0039	137.0458	176	31.3	Allopurinol
137.0419	0	0.03	137.07	100	16.6	PRALIDOXIME
137.0419	154.027	-0.0186	137.0233	195	61.9	Gentisic acid
137.0419	136.039	0.0039	137.0458	289	39.4	Hypoxanthine
131.082	0	0.05	131.13	316	42.3	Agmatine
131.082	130.027	-0.0481	131.0339	233	25.4	Butanedioic acid, methylene-
131.082	131.13	0.0476	131.1296	98	100	Chlormequat-d9
131.082	130.063	-0.0117	131.0703	67	55.4	4-Oxohexanoic acid
257.123	256.117	0.0014	257.1244	84	88.5	Thr-His
257.123	256.11	-0.0058	257.1172	194	93.2	Pterostilbene
257.123	256.117	0.0014	257.1244	259	28.3	His-Thr
257.123	256.117	0.0014	257.1244	165	48.3	Thr-His
150.0885	149.07	-0.0111	150.0774	289	92.5	Adenine, N6-methyl
150.0885	167.058	-0.034	150.055	307	75.3	3-Methyl-2-nitrobenzyl alcohol
150.0885	149.07	-0.0111	150.0774	255	50	Adenine, N6-methyl
150.0885	167.095	0.0028	150.0913	241	49.6	Synephrine
238.1427	237.136	0.0011	238.1438	124	50	Viloxazine
238.1427	474.234	-0.0185	238.1242	128	39.7	His-Tyr-Arg
238.1427	474.234	-0.0185	238.1242	224	41.4	Trp-Asn-Arg
238.1427	0	-0.05	238.09	291	91.2	Biopterin
257.1363	256.117	-0.0119	257.1244	175	62.3	Thr-His
257.1363	256.11	-0.0191	257.1172	97	50.9	Pterostilbene
257.1363	256.117	-0.0119	257.1244	236	65.3	Thr-His
131.0774	0	0.05	131.13	207	36.8	Agmatine
131.0774	130	0.05	131.13	54	39.3	Agmatine sulfate salt
131.0774	148.052	-0.0283	131.0491	82	100	trans-Cinnamic acid
150.0885	303.147	0.0028	150.0913	200	70.8	Cocaine
150.0885	303.147	0.0028	150.0913	242	55.4	Cocaine
150.0885	167.095	0.0028	150.0913	86	57.8	Synephrine
150.0885	149.07	-0.0111	150.0774	166	79.2	Adenine, N6-methyl

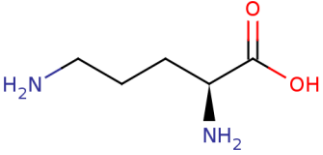
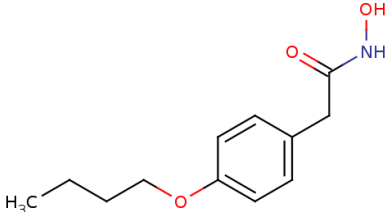
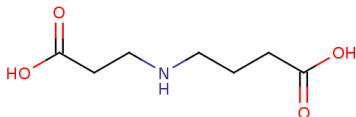
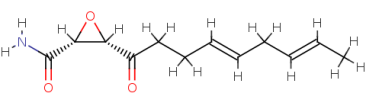
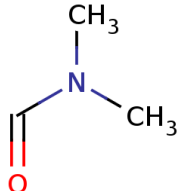
419.3108	418.308	0.0048	419.3156	205	100	1,2-Benzenedicarboxylic acid, dinonyl ester
150.0803	149.07	-0.0029	150.0774	195	70.8	Adenine, N6-methyl
150.0803	167.095	0.011	150.0913	279	92.3	Synephrine
150.0803	149.12	0.0474	150.1277	299	46	Methamphetamine
150.0803	149.07	-0.0029	150.0774	231	95.3	Adenine, N6-methyl
211.116	210.126	0.0169	211.1329	112	45.3	Jasmonic Acid
211.116	420.201	-0.0083	211.1077	89	33.7	PyroGlu-Tyr-Lys
211.116	420.223	0.003	211.119	225	55.5	His-His-Lys
211.116	0	-0.02	211.1	65	100	Sinapyl alcohol
205.1202	204.09	-0.023	205.0972	41	100	Fenozolone
205.1202	204.075	-0.0383	205.0819	207	27.5	Ala-Asp
205.1202	408.212	-0.0069	205.1133	199	22.1	Phe-Ser-Arg
205.1202	204.09	-0.023	205.0972	247	49.9	Fenozolone
176.1195	175.063	-0.0489	176.0706	100	43.7	3-Indoleacetic acid
176.1195	175	-0.05	176.07	124	76.2	1-Methoxy-3-carbaldehyde
176.1195	175.096	-0.017	176.103	85	44	L-Citrulline
176.1195	175	-0.05	176.07	98	70.2	1-Methoxy-3-carbaldehyde
205.1202	204.072	-0.0408	205.0794	161	54.8	Levamisole
205.1202	204.1	-0.013	205.107	270	53.2	1,6-Anhydro-b-D-glucose, permethyl-
205.1202	204.072	-0.0408	205.0794	337	44.8	Levamisole
205.1202	204.075	-0.0383	205.0819	79	100	Gly-Glu
205.1202	204.072	-0.0408	205.0794	210	51	Levamisole
205.1202	408.212	-0.0069	205.1133	244	49.8	Tyr-Ala-Arg
205.1202	204.072	-0.0408	205.0794	169	39.9	Tetramisole
176.0975	175	-0.03	176.07	125	54.6	1-Methoxy-3-carbaldehyde
176.0975	175	-0.03	176.07	46	79.3	1-Methoxy-3-carbaldehyde
176.0975	175	-0.03	176.07	96	40.6	1-Methoxy-3-carbaldehyde
176.0975	175.063	-0.0269	176.0706	225	56.7	3-Indoleacetic acid
283.1402	282.179	0.0462	283.1864	206	52.5	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1402	282.179	0.0462	283.1864	208	39.3	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1402	282.122	-0.0113	283.1289	238	42.1	Thr-Tyr
283.1402	0	0.01	283.15	192	32.9	Artemisinin
283.1685	282.179	0.0179	283.1864	191	52.7	1,3-Bis(tris(hydroxymethyl)methylamino)propane
283.1685	282.122	-0.0396	283.1289	270	63.7	Thr-Tyr
283.1685	282.122	-0.0396	283.1289	222	31.9	Thr-Tyr
283.1685	282.179	0.0179	283.1864	275	69	1,3-Bis(tris(hydroxymethyl)methylamino)propane
150.0756	167.095	0.0157	150.0913	154	58	Synephrine

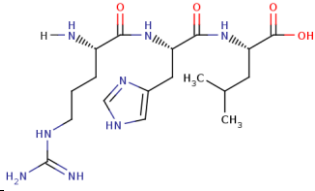
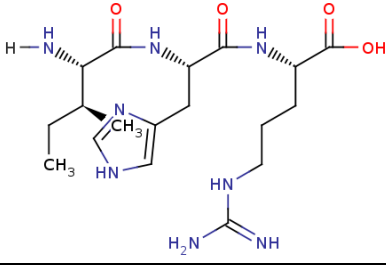
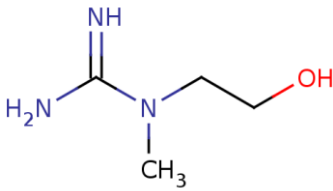
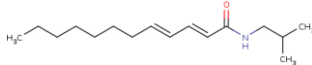
150.0756	149.07	0.0018	150.0774	236	61.8	Adenine, N6-methyl
150.0756	149.07	0.0018	150.0774	162	68.4	Adenine, N6-methyl
150.0756	167.095	0.0157	150.0913	311	78	Synephrine
205.1202	204.075	-0.0383	205.0819	76	100	Gly-Glu
205.1202	204.075	-0.0383	205.0819	173	82.6	Gly-Glu
205.1202	204.1	-0.013	205.107	118	33.8	1,6-Anhydro-b-D-glucose, permethyl-
205.1202	408.237	0.0057	205.1259	319	51.9	Tyr-Val-Lys
176.0975	175	-0.03	176.07	148	100	1-Methoxy-3-carbaldehyde
176.0975	175	-0.03	176.07	124	48	1-Methoxy-3-carbaldehyde
176.0975	175	-0.03	176.07	30	100	1-Methoxy-3-carbaldehyde
176.0975	175.111	0.0207	176.1182	43	100	Debrisoquin
276.1945	275.159	-0.0279	276.1666	135	43.3	Arg-Thr
276.1945	319.133	-0.0438	276.1507	182	86.1	Norfloxacin
276.1945	275.152	-0.0351	276.1594	172	94.6	Methylenedioxyprovalerone
276.1945	275.163	-0.0238	276.1707	153	80.3	Physostigmine
276.1945	319.133	-0.0438	276.1507	118	27.6	Norfloxacin
276.1945	275.159	-0.0279	276.1666	98	24.7	Thr-Arg
276.1945	275.148	-0.0391	276.1554	113	40.7	Glu-Lys
276.1945	275.152	-0.0351	276.1594	167	80.3	Methylenedioxyprovalerone
276.1945	275.152	-0.0351	276.1594	124	31.4	Methylenedioxyprovalerone
276.1945	275.159	-0.0279	276.1666	156	47	Arg-Thr
276.1945	275.152	-0.0351	276.1594	174	52.7	Homatropine
276.1945	275.152	-0.0351	276.1594	213	69.9	Homatropine
205.1202	204.075	-0.0383	205.0819	105	100	Gly-Glu

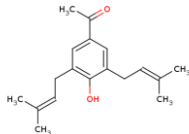
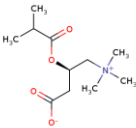
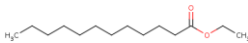
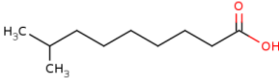
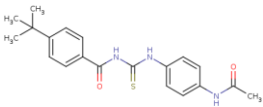
Table A13. List of non-volatile metabolites (LC/MS) for managed population animals with manually identified best tentative match(es) given for each compound. Samples collected in Dec 2011 from multiple animals were pooled. Experiment was conducted using lipids fraction protocol analysis on RP column in positive ion mode (refer to Materials and Methods section in the main text). All matches are tentative.

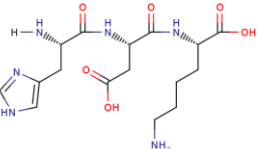
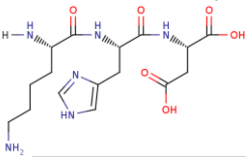
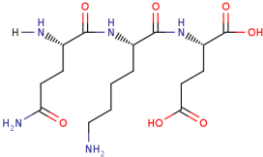
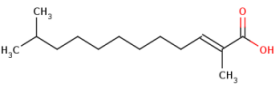
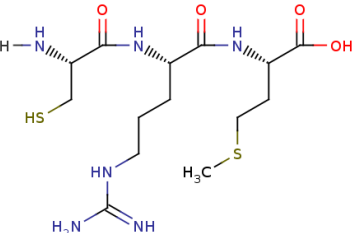
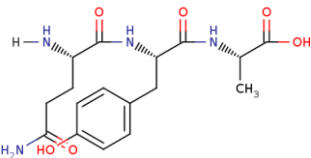
* For the compounds marked with an asterisk, the suggested chemical identity is highly tentative due to one or more of the following factors: an unexpected precursor; identified compound is not expected to be present in a marine environment; MS/MS is not available due to the low parent abundance and exact mass match is used for ID. In the latter case, the METLIN score is not available (N/A) and the Δ ppm from the expected mass is given instead.

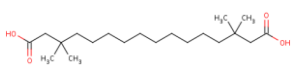
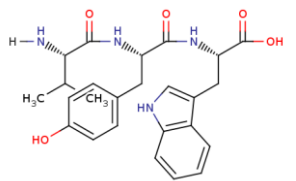
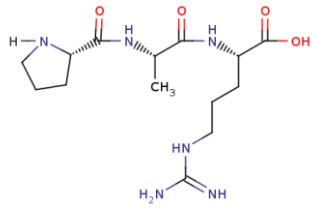
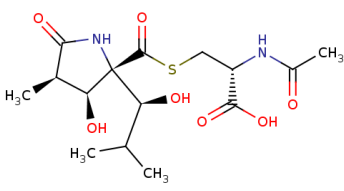
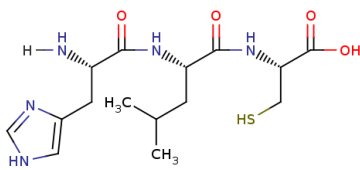
Name of Chemical	Precursor	Structure	METLIN Score	Precursor m/z:
Betaine	M+H		17-60	118.087
3-thio-pheneacrylic acid methyl ester*	M+NH4		39-44	186.059
L-Valine*	M+Na		0	140.069

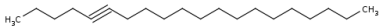
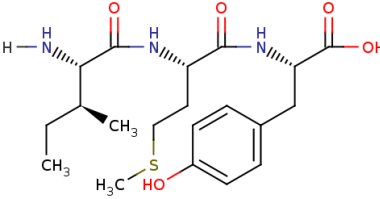
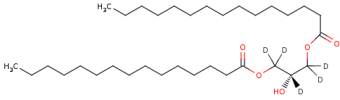
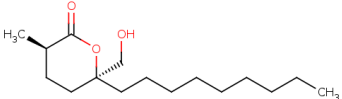
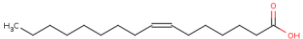
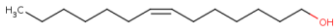
L-Ornithine	M+H-2H ₂ O		20	97.0773676 ; m/z of molecule: 97.0771
Unidentified Compound 1				144.983
Bufexamac	M+H		41-50	224.129
N-Carboxyethyl-γ-aminobutyric acid*	M+H-2H ₂ O		25	140.069
Cerulenin	M+H		52	224.129
Dimethylformamide	M+CH ₃ O H+H		20-29	106.087

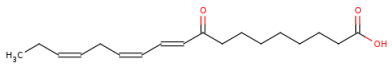
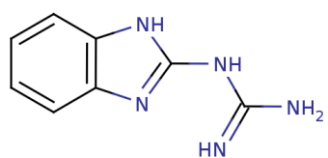
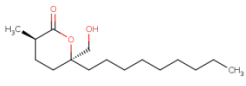
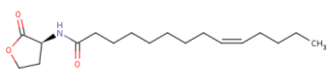
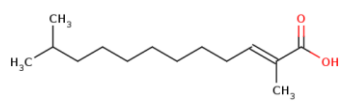
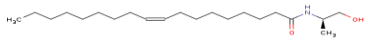
Arg His Leu	M+H+Na		52	224.129
Ile His Arg	M+H+Na		40	224.129
Unidentified Compound 2	M+2H		N/A Δ ppm=3	243.186
1-(2-hydroxyethyl)-1-methylguanidine*	M+H		12	118.096
Unidentified Compound 3				139.06
Dodeca-2(E),4(E)-dienoic acid isobutylamide*	M+H-2H ₂ O		21	216.205

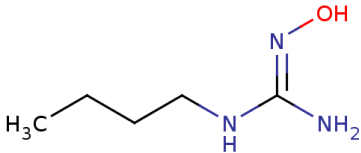
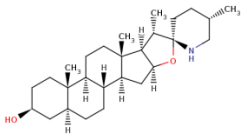
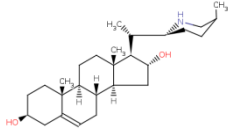
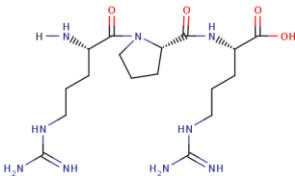
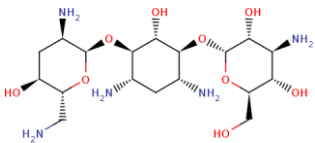
3,5-Diprenyl-4-hydroxyacetophenone, Lauric acid ethyl ester, or Isobutyryl carnitine*	Lauric acid ethyl ester (M+H); Isobutyryl carnitine (M+ACN+H) 3,5-Diprenyl-4-Hydroxyacetophenone (M+2Na-H)	 <p>3,5-DIPRENYL-4-HYDROXYACETOPHENONE</p>  <p>Isobutyryl carnitine</p>  <p>Lauric Acid ethyl ester</p>	Lauric acid ethyl ester score: 54; Isobutyryl carnitine score: 49 3,5-Diprenyl-4-Hydroxyacetophenone score: 39-44	273.178
8-methyl Nonanoic acid	M+Na		21-24	195.133
Unidentified Compound 4 (Possibly a phosphatidylcholine)				432.289
Tenovin-1	M+NH4		47-56	387.182

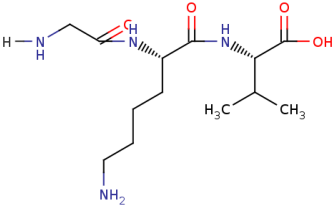
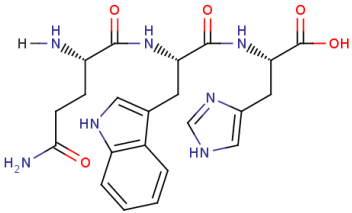
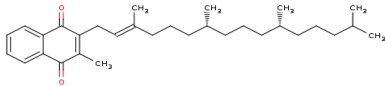
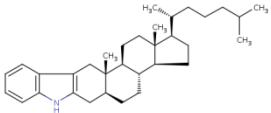
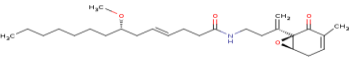
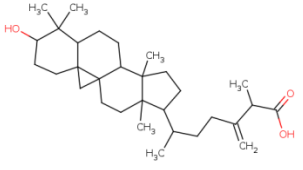
His Asp Lys or Lys His Asp*	M+CH3O H+H	 <p>His Asp Lys</p>  <p>Lys His Asp</p>	36	431.219
Gln Lys Glu	M+H		56	404.208
cis- Δ^2 -11-methyl- dodecenoic acid*	M+NH ₄		19-24	244.228
Cys Arg Met	M+H		55	409.163
Gln Tyr Ala	M+2Na-H		40	425.138

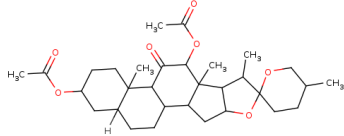
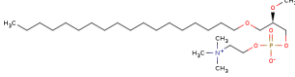
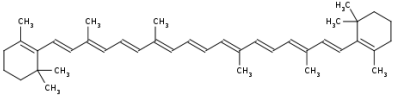
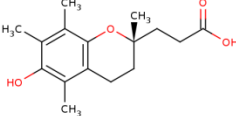
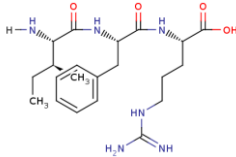
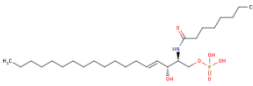
Medica 16	M+H		36-44	343.291
Val Tyr Trp	M+H-2H ₂ O		54	431.214
Pro Ala Arg	M+2Na-H		57	387.176
Unidentified Compound 5				118.082
Lactacystin*	M+CH ₃ O H+H		44	409.158
His Leu Cys	M+CH ₃ O H+H		61	404.202

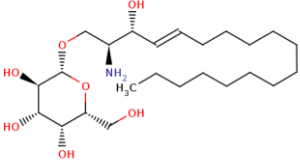
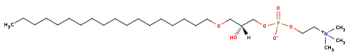
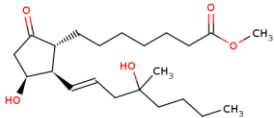
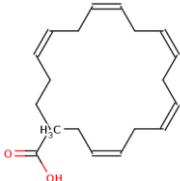



				
5-Eicosyne*	M+Na		N/A Δ ppm =2	301.286
				
Ile Met Tyr	M+NH4		39	443.235
Unidentified Molecule 6				285.291
				
DG(15:0/0:0/15:0) (d5)	M+Na		N/A Δ ppm=6	558.419
				
(-)-Malyngolide	M+NH4		44	288.26
				
cis-7-hexadecenoic acid	M+NH4		31	272.263
				
7Z-Tetradecen-1-ol*	M+NH4		N/A Δ ppm=19	230.252

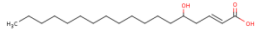
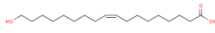

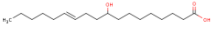
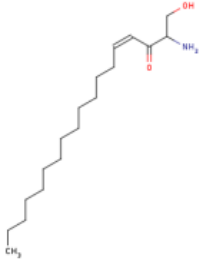
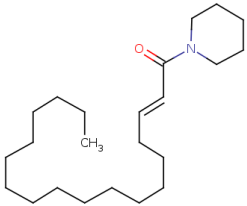
9-OxoOTrE	M+NH ₄		35	310.24
2-Benzimidazolylguanidine*	[M+H-2H ₂ O] ⁺		N/A Δppm=19	140.073
(-)-Malyngolide	M+NH ₄		41	288.255
N-cis-tetradec-9Z-enoyl-L-homoserine lactone	M+H		22	310.236
cis-Δ ² -11-methyl-dodecenoic acid	M+NH ₄		17	244.228
AM3102	M+H-2H ₂ O		17	304.302

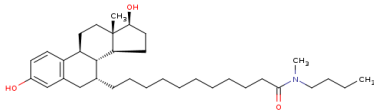
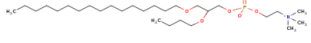
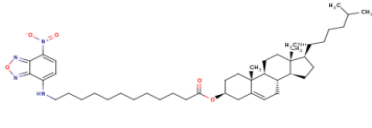
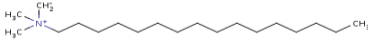
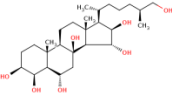
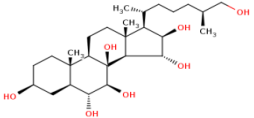
N-HBG*	M+ACN+ Na		29	195.124
Teinimine, Tomatidine, or Isomers*	M+H- 2H ₂ O	 <p style="text-align: center; border: 1px solid black; padding: 5px;">Tomatidine</p>  <p style="text-align: center; border: 1px solid black; padding: 5px;">Teinimine</p>	N/a Δ ppm=15	380.338
Arg Pro Arg*	M+CH ₃ O H+H		41	460.295
Tobramycin	M+ACN+ H		55	509.288

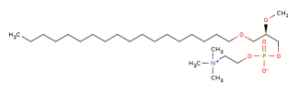
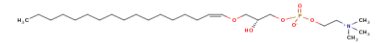
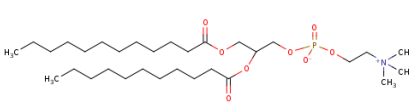
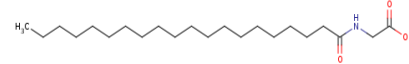
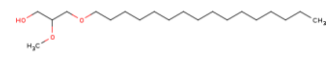
Gly Lys Val	M+H-2H ₂ O		38	267.174
Gln Trp His	M+NH ₄		43	487.233
Phylloquinone*	M+NH ₄		23	468.393
1'H-5alpha-cholest-2-eno[3,2-β]indole*	M+H-2H ₂ O		N/A Δppm=19	424.366
Malyngamide H	M+ACN+H		18	473.346
Ambolic acid*	M+ACN+H		N/A Δppm=15	512.418

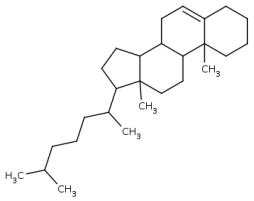
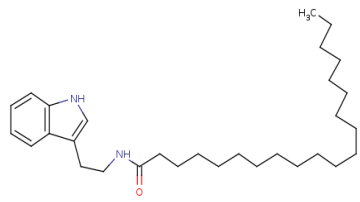
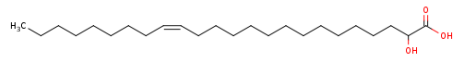
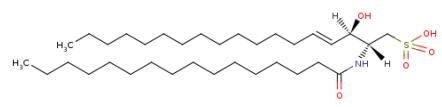
11-Ketorockogenin acetate*	M+2Na-H		15	575.285
2-O-methyl PAF C-18	M+CH3O H+H		17	556.443
β -Carotene	M+ACN+ Na		33	600.469
α -CEHC	M+H		31	279.163
Ile Phe Arg	M+H- 2H2O		37	399.254
C-8 Ceramide-1-phosphate*	M+H- H2O		14	488.36

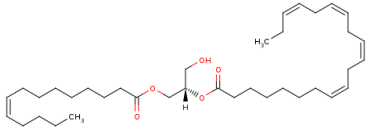
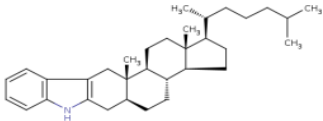
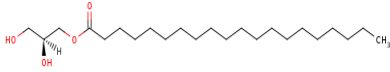

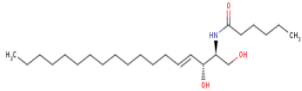
Psychosine*	M+H- H ₂ O		23	444.335
Lyso-PAF C-18*	M+Na		6	532.387
11β-Misoprostol	M+NH ₄		35	400.31
EPA	M+NH ₄		43	320.258
Eicosyne, Icosyne, or isomer of either*	M+ACN+ Na	 <div style="border: 1px solid black; padding: 5px; width: fit-content; margin: 10px auto;">3-Eicosyne</div>  <div style="border: 1px solid black; padding: 5px; width: fit-content; margin: 10px auto;">5-Eicosyne</div>  <div style="border: 1px solid black; padding: 5px; width: fit-content; margin: 10px auto;">9-Eicosyne</div>	N/A; Δppm=0	342.313

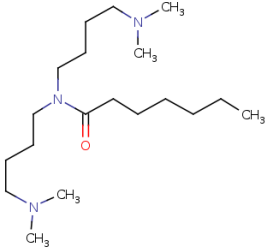
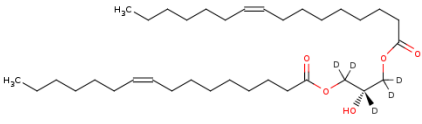
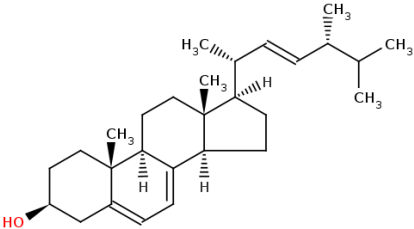
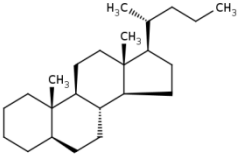
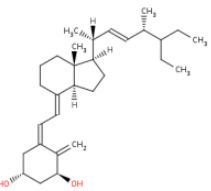
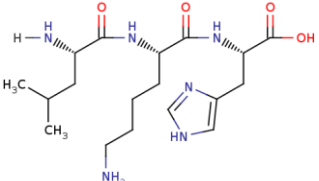
Possibly a fatty acid*	M+NH4	 <p data-bbox="683 275 1024 390">2-Octadecenoic acid, 5-hydroxy-</p>  <p data-bbox="675 554 1060 674">18-hydroxy-9Z-octadecenoic acid</p>  <p data-bbox="672 816 1027 932">17-hydroxy-9Z-octadecenoic acid</p>  <p data-bbox="660 1073 1023 1171">9-hydroxy-12-octadecenoic acid</p>	N/A; Δ ppm=6	316.287
3-ketosphingosine	M+H		21	298.276
Piperцитine*	M+H- H2O		N/a; Δ ppm=0	332.332

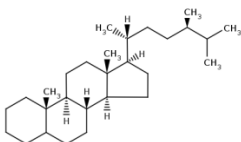
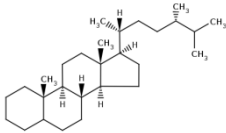
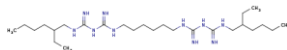
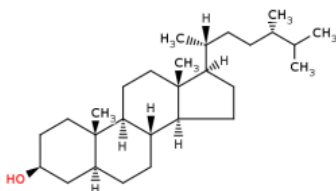
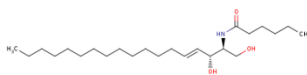
ICI 164384*	M+H		N/a; Δ ppm=7	526.43
PC(O-16:0/O-4:0)[U]*	M+CH ₃ O H+H		N/a; Δ ppm=0	570.45
3-dodecanoyl-NBD cholesterol	M+ACN+ Na		88	810.554
Cetrimonium	M+H		54	284.331
(25S)-5alpha-cholestan-3beta,4beta,6alpha,8beta,15alpha,16beta,26-heptol*	M+NH ₄	 <div data-bbox="657 1476 1088 1606" style="border: 1px solid black; padding: 5px; margin: 10px 0;"> <p>(25S)-5alpha-cholestan-3beta,4beta,6alpha,8beta,15alpha,16beta,26-heptol</p> </div>  <div data-bbox="673 1774 1047 1963" style="border: 1px solid black; padding: 5px; margin: 10px 0;"> <p>(25S)-5alpha-cholestan-3beta,6alpha,7beta,8beta,15alpha,16beta,26-heptol</p> </div>	N/A; Δ ppm=0	502.373

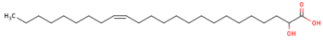
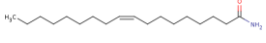
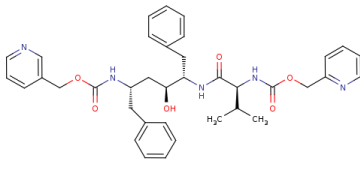
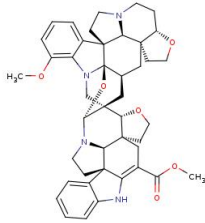
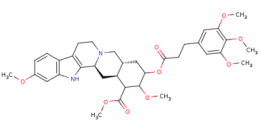
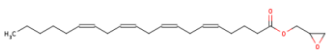
2-O-methyl PAF C-18	M+Na		16	546.4
PC(P-17:0/0:0)*	M+H-2H ₂ O		N/A; Δppm=14	458.347
PC(12:0/11:0)[U]*	M+H-H ₂ O		N/A; Δppm=12	590.426
Arachidoyl glycine*	M+CH ₃ O H+H		82	402.359
1-Hexadecyl-2-O-methyl-glycerol	M+ACN+H		53	372.35

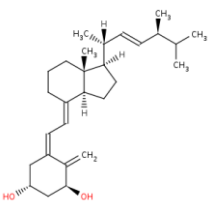
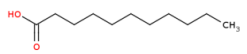
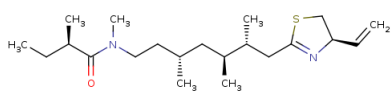
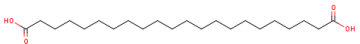
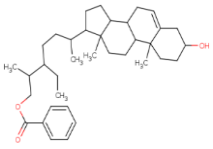
Cholest-5-ene*	M+H- H ₂ O		N/A Δ ppm=6	353.355
Nb- Arachidoyltryptamine *	M+ACN+ H		N/A Δ ppm=8	496.422
Unidentified Molecule 8				540.452
Unidentified Molecule 9				326.38
Hydroxynervonic acid*	M+ACN+ H		N/A Δ ppm=7	424.382
N-acyl capnines*	M+H- H ₂ O		N/A Δ ppm=3	584.473

DG(14:1(9Z)/20:4(8Z,11Z,14Z,17Z)/0:0)*	M+ACN+H		N/A Δ ppm=8	628.499
1'H-5alpha-cholest-2-eno[3,2-β]indole*	M+H-2H ₂ O		N/A Δ ppm=8	424.37
MG(20:0/0:0/0:0)*	M+ACN+H		N/a Δ ppm=3	428.375
N-stearoyl valine*	M+CH ₃ O H+H		N/a Δ ppm=4	416.375
C-6 Ceramide*	M+H		17	398.363
Unidentified Molecule 10				424.426

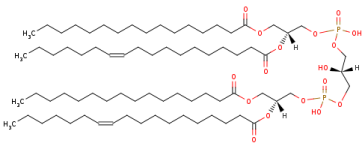
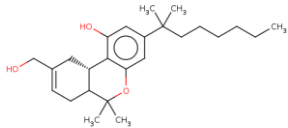
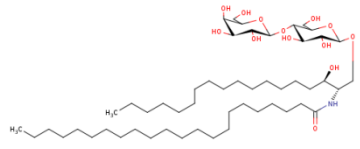
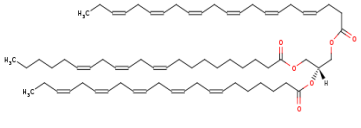
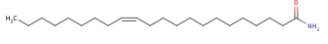
N-Heptanoylsolamine*	M+CH3O H+H		N/a Δ ppm=11	360.363
Possibly a diglyceride such as DG(16:1(9Z)/0:0/16:1(9Z)) (d5)*	M+H- H2O		N/a Δ ppm=15	542.442
Ergosterol*	M+ACN+ H		9	438.378
5-alpha-cholane*	M+ACN+ Na		N/A Δ ppm=22	394.353
26,27-Dihomo-1 α -hydroxyvitamin D2*	M+ACN+ H		N/A Δ ppm=11	482.405
Leu Lys His	M+H- H2O		33	379.239

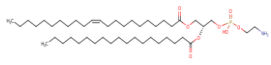
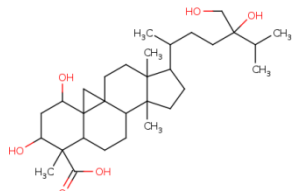
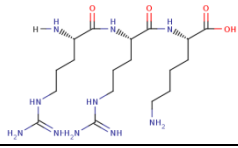
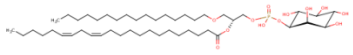
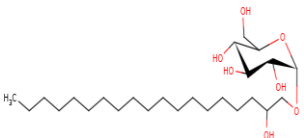
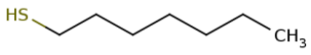
		 <p>Campestan skeleton</p>		
Campestan skeleton or Ergostan skeleton*	M+H-H ₂ O	 <p>Ergostan skeleton</p>	N/A Δppm=6	369.386
Alexidine*	M+ACN+H		N/A Δppm=13	550.495
Unidentified Molecule 11				452.459
ergostan-3β-ol*	M+H-H ₂ O		N/A Δppm=13	385.38
Unidentified Molecule 12				312.363
C-6 Ceramide	M+CH ₃ O H+H		18	430.39

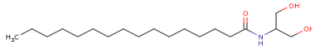
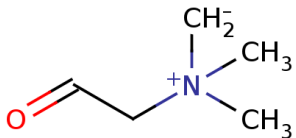
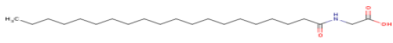
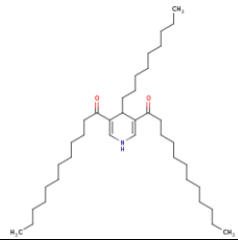
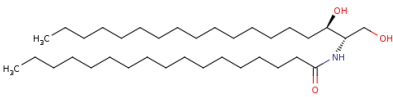
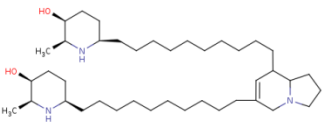
Hydroxynervonic acid*	M+NH ₄		N/A $\Delta\text{ppm}=2$	400.38
Oleamide	M+H		52	282.28
A 80987*	M+H		N/A Δppm $=5$	654.333
Amataine*	M+H-2H ₂ O		N/A Δppm $=2$	681.343
Dihydro isorescinnamine*	M+H		N/A Δppm $=7$	637.307
O-Arachidonoyl glycidol	M+H-H ₂ O		35	393.299

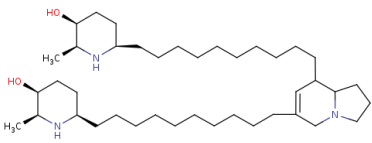
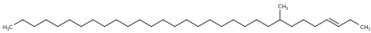
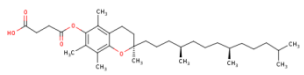
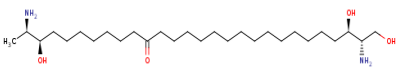
Doxercalciferol*	M+NH ₄		54	430.365
Undecanoic acid	M+ACN+H		45	228.196
Kalkitoxin	M+ACN+H		44	408.309
Unidentified Molecule 14				689.491
Unidentified Molecule 15				623.452
Unidentified Molecule 16				601.441
Docosanedioic acid*	M+H		N/A Δppm =2	371.316
(3b,24R,25x)-26-Benzoyloxystigmast-5-ene-3-ol*	M+H		N/A Δppm =25	535.401
Unidentified Molecule 17				615.456

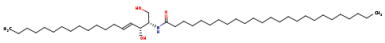
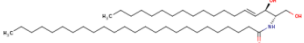
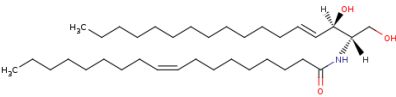
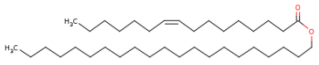
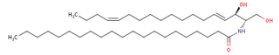
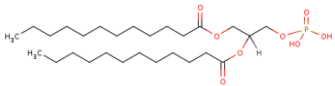
Val Leu Lys*	M+CH ₃ O H+H		29	391.286
9-Oxoasimicinone*	M+H		N/A Δppm =4	637.47
Possibly a glycoside such as Niazinin A or Eruberin B*	Niazinin A- M+NH ₄ ; Eruberin B- M+ACN+ Na	 <div style="border: 1px solid black; padding: 2px; display: inline-block; margin: 5px;">Niazinin A</div> <div style="border: 1px solid black; padding: 2px; display: inline-block; margin: 5px;">Eruberin B</div>	N/A Δppm =0	704.252
Unidentified Molecule 20				659.482
Parasiloxanthin*	M+Na		N/A Δppm =14	593.442
Possibly a phosphatidic acid such as PA(O- 16:0/20:5(5Z,8Z,11Z, 14Z,17Z))*	M+H		N/A Δppm =12	681.494
Unidentified Molecule 19				725.522

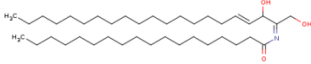
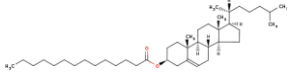
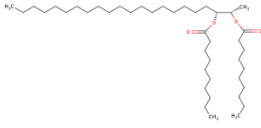
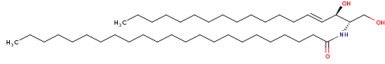
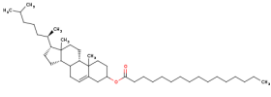
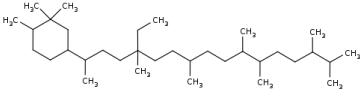
Possibly a cardiolipid such as CL(1'- [16:0/18:1(11Z)],3'- [16:0/18:1(11Z)])*	M+2H		N/A Δ ppm =0	703.509
Unidentified Molecule 20				571.432
Unidentified Molecule 21				549.419
Unidentified Molecule 22				368.428
HU-211	M+CH3O H+H		8	419.319
Unidentified Molecule 23				992.742
Lactosylceramide*	M+H		score: N/A Δ ppm=19	948.716
Unidentified Molecule 23				505.39
Possibly a triglyceride such as TG(22:3(10Z,13Z,16Z)/22:5(7Z,10Z,13Z,16 Z,19Z)/22:6(4Z,7Z,10 Z,13Z,16Z,19Z))[iso6] *	M+H+Na		score: N/A Δ ppm=9	527.403
13Z-Docosamide	M+H		37	338.342

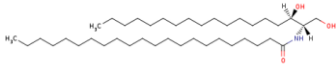
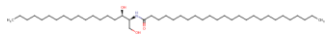
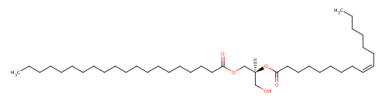

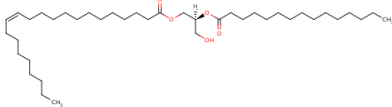
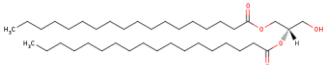
Possibly a phosphatidylethanolamine such as PE(22:1(11Z)/19:0)*	M+H		score: N/A Δ ppm=6	816.642
Cyclopassifloic acid B*	M+CH ₃ O H+H		score: N/A Δ ppm=2	553.408
Arg Arg Lys	M+H- H ₂ O		35	441.301
Possibly a phosphatidylinositols such as PI(O-16:0/22:2(13Z,16Z))*	M+H- H ₂ O		score: N/A Δ ppm=0	859.606
1-O-alpha-D-glucopyranosyl-1,2-nonadecandiol*	M+H		score: N/A Δ ppm=10	859.606
Heptane-1-thiol*	M+H- 2H ₂ O		score: N/A Δ ppm=5	97.0839

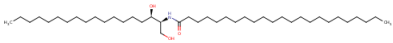
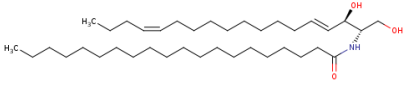
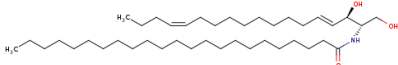
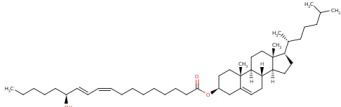
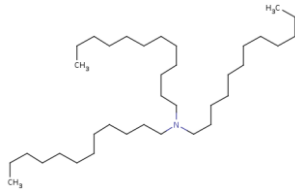
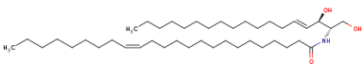
Palmitoyl serinol	M+ACN+ H		27	371.324
Betaine aldehyde	M+H- H2O		13-31	84.0822
Arachidoyl glycine	M+ACN+ Na		85	433.333
1,1'-(1,4-Dihydro-4-nonyl-3,5-pyridinediyl)bis[1-dodecanone]*	M+CH3O H+H		score: N/A Δ ppm =17	604.577
Unidentified Molecule 25				560.551
Cer(d18:0/17:0)*	M+CH3O H+H		score: N/A Δ ppm =15	586.568
Juliflorine*	M+H		score: N/A Δ ppm =0	630.593

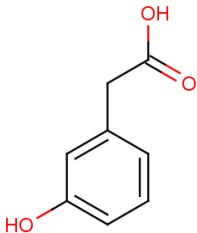
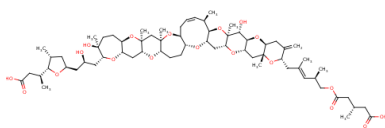
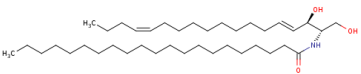
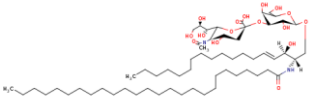
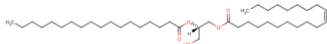
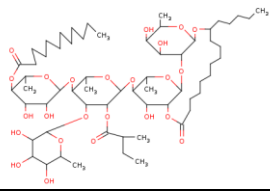
Juliflorine*	M+H- H2O		score: N/A Δ ppm =0	612.583
8-Methyl-3-hentriacontene*	M+NH4		score: N/A Δ ppm =2	466.536
Vitamin E succinate(Tocopherol succinate)	M+Na		score: N/A Δ ppm =11	553.393
Oceanin*	M+2Na-H		score: N/A Δ ppm =3	531.409
Unidentified Molecule 26				578.563

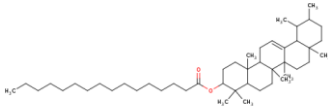
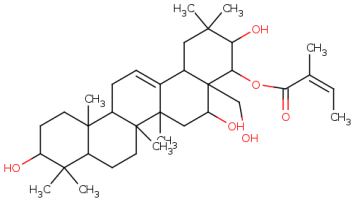
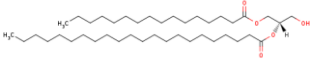
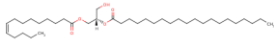
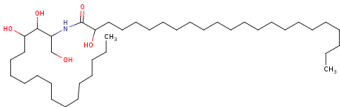
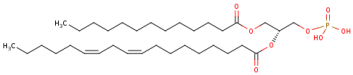
Possibly a Ceramide such as Ceramide (d18:1/25:0)*	M+2Na-H	 <p style="text-align: center; border: 1px solid black; padding: 5px;">Ceramide (d18:1/25:0)</p>  <p style="text-align: center; border: 1px solid black; padding: 5px;">Cer(d18:1/25:0)</p>	score: N/A Δ ppm =1	708.623
N-Oleoyl-D-erythro- sphingosine (C18:1 Ceramide)*	M+CH3O H+H		score: N/A Δ ppm =5	582.549
Heneicosanyl oleate*	M+ACN+ Na		score: N/A Δ ppm =9	612.563
Cer(d18:2/21:0)*	M+H		score: N/A Δ ppm =17	606.593
Unidentified Molecule 27				608.577
Phosphatidic acids similar to PA(12:0/12:0)[U]*	M+CH3O H+H		score: N/A Δ ppm =1	569.38

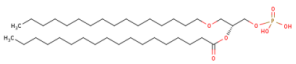
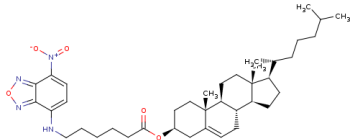
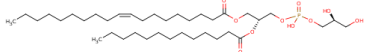
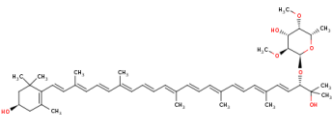
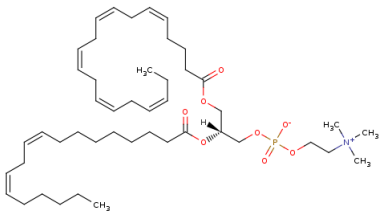
Hemsleyin imine A*	M+H-H ₂ O		score: N/A Δ ppm =19	588.583
Unidentified Molecule 28				632.609
14:0 Cholesteryl ester*	M+NH ₄		score: N/A Δ ppm =19	614.599
Unidentified Molecule 29				632.609
2S,3R-didecanoyl-docosane-2,3-diol*	M+H-H ₂ O		score: N/A Δ ppm =11	633.611
Cer(d18:1/23:0) due to large Δ ppm	M+Na		score: N/A Δ ppm =11	658.624
CE(16:0)*	M+NH ₄		score: N/A Δ ppm =15	642.629
Monocyclic botryococcane*	M+NH ₄		score: N/A Δ ppm =1	494.566

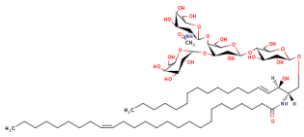
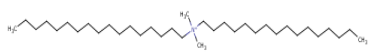
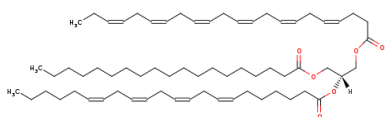
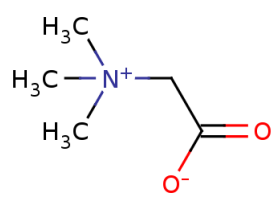
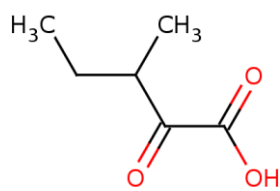
Cer(d18:0/22:0)*	M+Na		score: N/A Δ ppm =18	646.623
Cer(d18:0/25:0)*	M+Na		score: N/A Δ ppm =16	688.669
Unidentified Molecule 30				610.577
Diglycerides such as DG(20:0/16:1(9Z)/0:0)*	M+NH4		score: N/A Δ ppm =1	640.587
Unidentified Molecule 31				632.609
Ethylene glycol distearate*	M+ACN+H		score: N/A Δ ppm =1	636.59347 53, 636.60247 80
Possibly a Diglyceride such as DG(22:1(13Z)/15:0/0:0)*	M+NH4		score: N/A Δ ppm =21	654.589
Unidentified Molecule 32				632.609
Possibly a Diglyceride such as DG(18:0/18:0/0:0)*	M+ACN+H		score: N/A Δ ppm =0	666.603

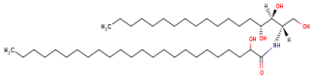
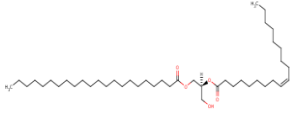
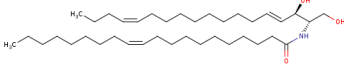
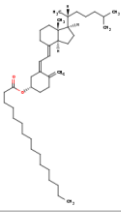
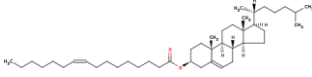
Cer(d18:0/23:0)*	M+Na		score: N/A Δ ppm =22	660.641
Cer(d18:2/20:0)*	M+CH3O H+H		score: N/A Δ ppm =0	624.593
Cer(d18:2/23:0)*	M+H		score: N/A Δ ppm =19	634.626
Cholesteryl ester such as 13(S)-HODE cholesteryl ester*	M+NH4		score: N/A Δ ppm =11	682.621
Tridodecylamine	M+H		score: N/A Δ ppm =1	522.598
Possibly a Ceramide such as Cer(d18:1/24:1(15Z))*	M+H		score: N/A Δ ppm =15	648.639

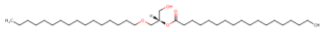
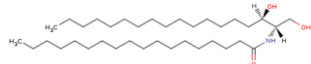
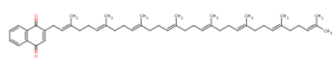
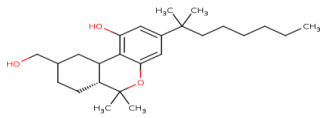
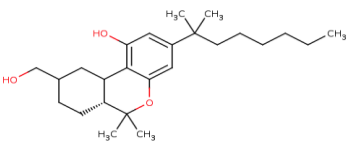
3-Hydroxyphenylacetic acid	M+NH4		72	170.079
Gambieric acid D*	M+NH4		score: N/A Δ ppm =13	1216.75
Cer(d18:2/21:0)*	M+CH3O H+H		score: N/A Δ ppm =0	638.609
NeuAc-alpha-2-3-gal-beta-cer(d18:1/26:0)*	M+ACN+ Na		score: N/A Δ ppm =11	1194.82
Possibly a Diglyceride such as DG(20:1(11Z)/18:0/0:0)*	M+NH4		score: N/A Δ ppm =0	668.619
Simonin III*	M+H- 2H2O		score: N/A Δ ppm =18	1215.75
Unidentified Molecule 33				664.623

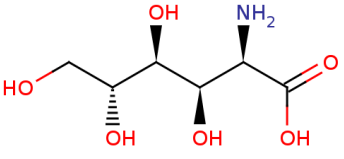
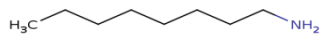
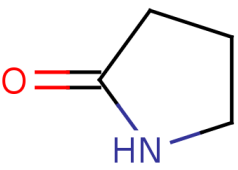
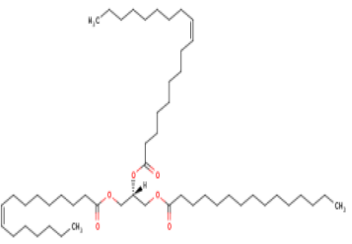
alpha-Amyrin palmitate*	M+H		score: N/A Δ ppm =5	665.627
22- Angeloylbarringtonen ol C*	M+H- 2H ₂ O		score: N/A Δ ppm =0	537.395
Possibly a Diglyceride such as DG(16:0/22:0/0:0)[iso 2]*	M+ACN+ H		score: N/A Δ ppm =2	694.633
Possibly a Diglyceride such as DG(14:1(9Z)/20:0/0:0)*	M+H- 2H ₂ O		score: N/A Δ ppm =8	559.515
N-(2R- Hydroxypentacosanoy l)-2S-amino-1,3S,4R- octadecanetriol*	M+H- 2H ₂ O		score: N/A Δ ppm =13	662.6542 969
Possibly a Phosphatidic acid such as PA(13:0/18:2(9Z,12Z))*	M+CH ₃ O H+H		score: N/A Δ ppm =5	663.456

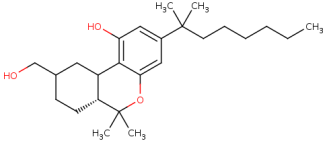
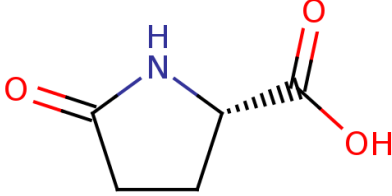
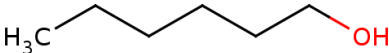
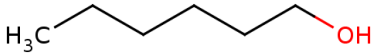
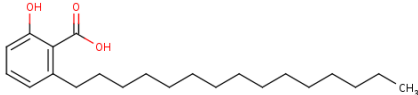
Possibly a Phosphatidic acid such as PA(O-16:0/18:0)*	M+2Na-H		score: N/A Δ ppm =3	707.494
3-hexanoyl-NBD Cholesterol	M+Na		33	685.437
Possibly a Phosphatidylglycerol such as PG(19:1(9Z)/13:0)*			score: N/A Δ ppm =8	721.508
(3R,2'S)-Myxol 2'-(2,4-di-O-methyl- α -L-fucoside)*	M+H		score: N/A Δ ppm =5	759.524
Possibly a Phosphatidylcholine such as PC(20:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))*	M+H-2H2O		score: N/A Δ ppm =0	768.533

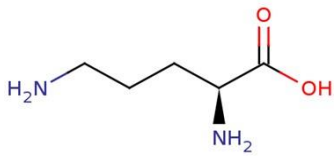
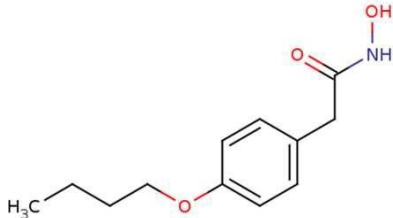
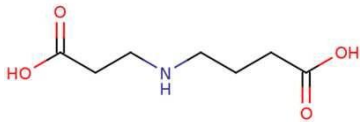
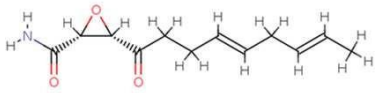
Gal-alpha1-3-(GalNAc-beta1-4)-Gal-beta1-4-Glc-beta-cer(d18:1/26:1(17Z))*	M+H-H ₂ O		score: N/A Δppm =6	1347.88
*Dimethyl dialkyl ammonium chloride	M+ACN+H		score: N/A Δppm =23	550.629
Possibly a Triglyceride such as TG(19:0/22:4(7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[is o6]*	M+H-2H ₂ O		score: N/A Δppm =4	961.806
Betaine	M+Na		40	140.069
2-oxo-3-methylvaleric acid	M+NH ₄		26-30	148.097

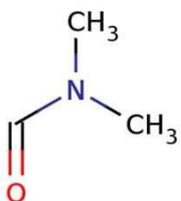
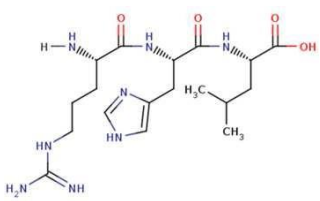
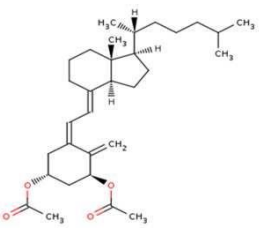
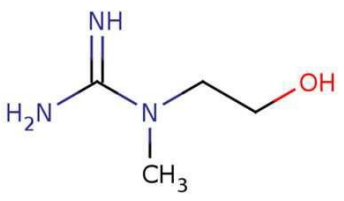
Possibly a Ceramide such as Cer(d18:1/24:1(15Z))*	M+H- H2O		score: N/A, Δ ppm=0	666.641
Possibly a Diglyceride uch as DG(22:0/18:1(9Z)/0:0)*	M+NH4		score: N/A, Δ ppm=1	696.651
Possibly a Ceramide such as Cer(d18:2/20:1)*	M+ACN+ H		score: N/A, Δ ppm=2	631.576
Vitamin D3 palmitate or 16:1 Cholesteryl ester*	M+H- 2H2O	 <div data-bbox="675 1654 987 1734" style="border: 1px solid black; padding: 5px; margin: 10px auto; width: fit-content;">Vitamin D3 palmitate</div>  <div data-bbox="704 1940 1016 2020" style="border: 1px solid black; padding: 5px; margin: 10px auto; width: fit-content;">16:1 Cholesteryl ester</div>	score: N/A, Δ ppm=12	587.549

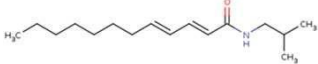
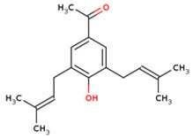
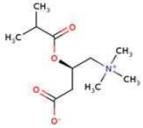
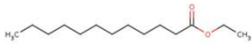
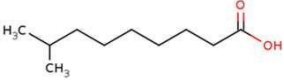
DG(16:0e/18:0/0:0)*	M+H- H2O		score: N/A, Δ ppm=19	565.567
Possibly a ceramide similar to Cer(d18:0/18:0)*	M+ACN+ H		score: N/A, Δ ppm=17	609.603
Unidentified Chemical 34				578.66
2- demethylmenaquinone -8 *	M+H		score: N/A, Δ ppm=3	703.547
HU210	M+H- H2O		2 – 21	371.297
HU210	M+H- H2O		2 – 9	371.293

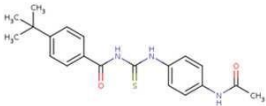
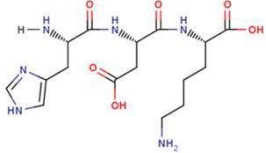

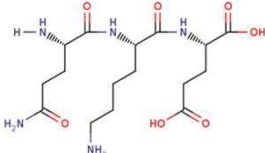
Glucosaminic acid	M+CH3O H+H	 <p>The structure shows a six-carbon chain with a carboxylic acid group at C1, an amino group at C2, and hydroxyl groups at C3, C4, and C5. The C4 hydroxyl group is on a dashed bond, while the others are on wedged bonds.</p>	5	228.107
Octylamine*	M+H	 <p>A straight-chain alkane with an amino group at the end, labeled with H₃C and NH₂.</p>	N/A Δ ppm=3	130.159
2-Pyrrolidinone	M+H	 <p>A five-membered ring containing one nitrogen atom and one carbonyl group.</p>	42	86.0616
Possibly a triglyceride such as TG(15:0/18:1(9Z))/16:1(9Z)[iso6]* based on exact mass match	M+Na	 <p>A glycerol backbone esterified with three fatty acid chains: one saturated (15:0), one monounsaturated (18:1(9Z)), and one saturated (16:1(9Z)).</p>	N/A Δ ppm=1	825.694

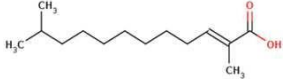
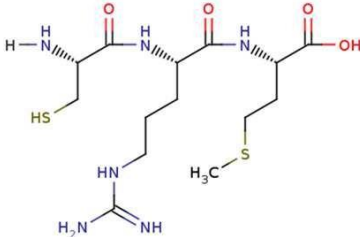
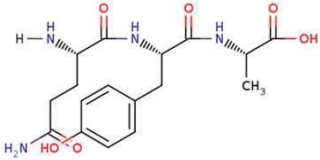
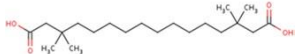
HU210*	M+H- H2O		H U 2 15	371.289
Pyroglutamic acid	M+ACN+ H		94	171.077
1-Hexanol	M+H		37	121.123
1-Hexanol	M+H		27	103.112
Anacardic acid	M+Na		6	371.257

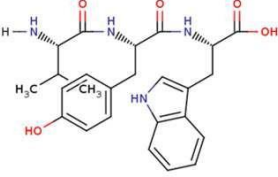
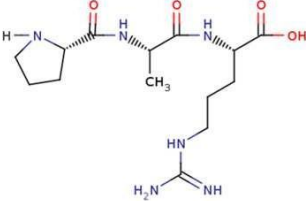
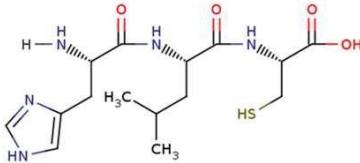
L-Ornithine	M+H-2H ₂ O		20	97.07736 76 ; m/z of molecule : 97.0771
Unidentified Compound 1				144.983
BUFEXAMAC	M+H		41-50	224.129
N-Carboxyethyl- γ -aminobutyric acid highly tentative	M+H-2H ₂ O		25	140.069
Cerulenin (doubtful due to ethylene oxide ring)	M+H		52	224.129


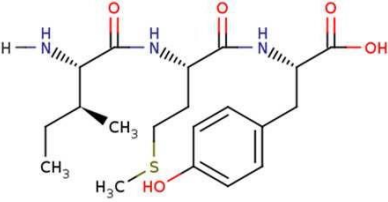
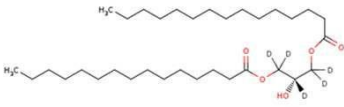
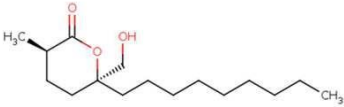
Dimethylformamide	M+CH ₃ OH+H		20-29	106.087
Arg His Leu	M+H+Na		52	224.129
Ile His Arg	M+H+Na	Previously Included	40	224.129
Unidentified Compound 2 (Perhaps 1-Hydroxyvitamin D3 diacetate or a chemical with similar structural motif)	M+2H		N/A Δppm=3	243.186
1-(2-hydroxyethyl)-1-methylguanidine highly tentative	M+H		12	118.096
Unidentified Compound 3				139.06

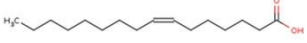
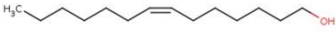
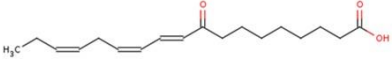
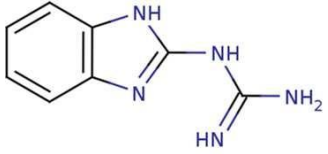
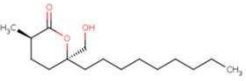
<p>*DODECA-2(E),4(E)-DIENOIC ACID ISOBUTYLAMIDE* Highly unlikely</p>	<p>M+H-2H₂O</p>		<p>21</p>	<p>216.205</p>
<p>All Tentative *3,5-DIPRENYL-4-HYDROXYACETOPHENONE, or Lauric Acid ethyl ester, or Isobutyryl carnitine* (results inconclusive to the most likely)</p>	<p>Lauric Acid ethyl ester (M+H); Isobutyryl carnitine(M+A CN+H)3,5-DIPRENYL-4-HYDROXYACETOPHENONE (M+2Na-H)</p>	 <p>3,5-DIPRENYL-4-HYDROXYACETOPHENONE</p>  <p>Isobutyryl carnitine</p>  <p>Lauric Acid ethyl ester</p>	<p>Lauric Acid ethyl ester score: 54; Isobutyryl carnitine score: 49 3,5-DIPRENYL-4-HYDROXYACETOPHENONE score: 39-44</p>	<p>273.178</p>
<p>8-methyl Nonanoic acid</p>	<p>M+Na</p>		<p>21-24</p>	<p>195.133</p>

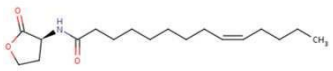
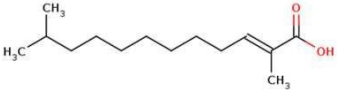
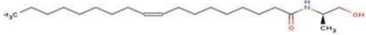
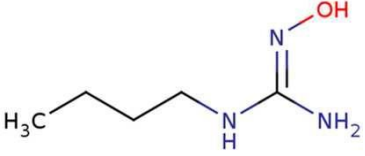
Unidentified Compound 4				432.289
Tenovin-1	M+NH ₄		47-56	387.182
His Asp Lys or Lys His Asp tentative	M+CH ₃ OH+H	 <p data-bbox="675 968 945 1016">His Asp Lys</p>  <p data-bbox="766 1188 1006 1236">Lys His Asp</p>	36	431.219
Gln Lys Glu	M+H		56	404.208

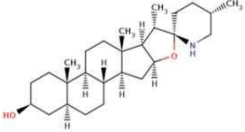
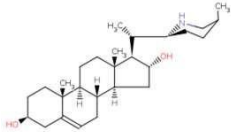
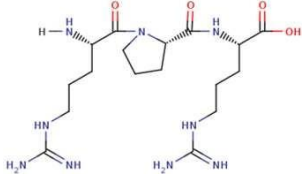
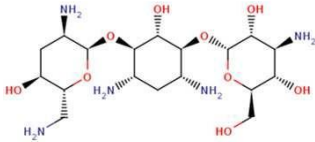
<p>*cis-Δ^2-11-methyl-Dodecenoic Acid* Highly tentative</p>	M+NH ₄		19-24	244.228
Cys Arg Met	M+H		55	409.163
Gln Tyr Ala	M+2Na-H		40	425.138
MEDICA 16	M+H		36-44	343.291

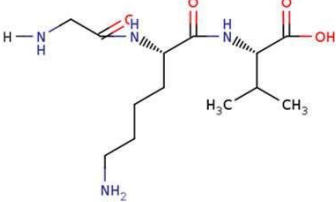
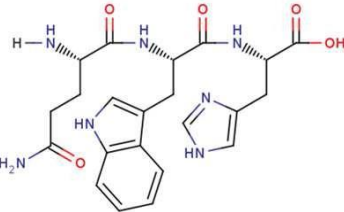
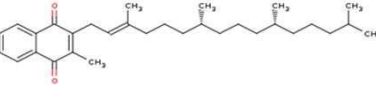
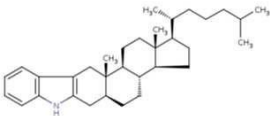

Val Tyr Trp	M+H-2H ₂)		54	431.214
Pro Ala Arg	M+2Na-H		57	387.176
Unidentified Compound 5				118.082
Lactacystin Tentative	M+CH ₃ OH+H	Previously Included	44	409.158
His Leu Cys	M+CH ₃ OH+H		61	404.202

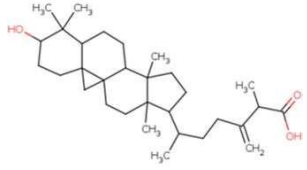
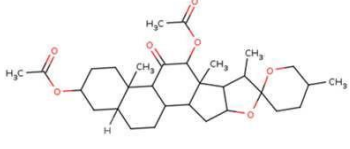
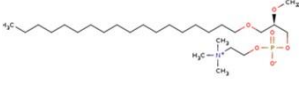
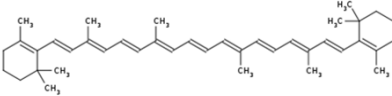
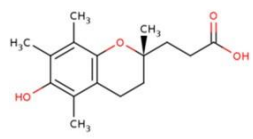
<p>*5-Eicosyne*</p> <p>Tentative due to exact match, not MS/MS</p>	<p>*M+Na*</p>		<p>N/A</p> <p>$\Delta\text{ppm} = 2$</p>	<p>301.286</p>
<p>Ile Met Tyr</p>	<p>M+NH4</p>		<p>39</p>	<p>443.235</p>
<p>Unidentified Molecule 6</p>				<p>285.291</p>
<p>DG(15:0/0:0/15:0) (d5)</p>	<p>M+Na</p>		<p>N/A</p> <p>$\Delta\text{ppm} = 6$</p>	<p>558.419</p>
<p>(-)-Malyngolide</p>	<p>M+NH4</p>		<p>44</p>	<p>288.26</p>

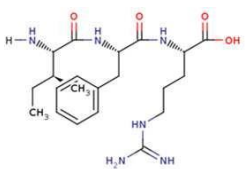

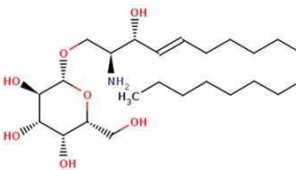
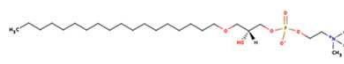
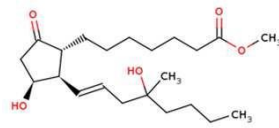
cis-7-Hexadecenoic Acid	M+NH ₄		31	272.263
7Z-Tetradecen-1-ol from exact mass match	M+NH ₄		N/A Δppm=1 9	230.252
9-OxoOTrE	M+NH ₄		35	310.24
2-Benzimidazolylguanine tentative because based on exact mass match	[M+H-2H ₂ O] ⁺		N/A Δppm=1 9	140.073
(-)-Malyngolide	M+NH ₄		41	288.255

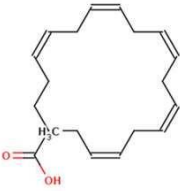



N-cis-tetradec-9Z-enoyl-L-Homoserine lactone(quorum sensing molecule)	M+H		22	310.236
cis-Δ ² -11-methyl-Dodecenoic Acid	M+NH ₄		17	244.228
AM3102	M+H-2H ₂ O		17	304.302
N-HBG tentative	M+ACN+Na		29	195.124





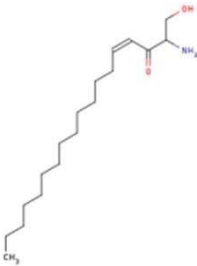
<p>*Teinimine, tomatidine, or isomers* based on exact mass not MS/MS</p>	<p>M+H-2H₂O</p>	<div style="text-align: center;">  <p>Tomatidine</p>  <p>Teinimine</p> </div>	<p>score: N/a Δppm=1 5</p>	<p>380.338</p>
<p>*Arg Pro Arg* tentative showing methanol but possible</p>	<p>M+CH₃OH+H</p>	<div style="text-align: center;">  </div>	<p>41</p>	<p>460.295</p>
<p>Tobramycin</p>	<p>M+ACN+H</p>	<div style="text-align: center;">  </div>	<p>55</p>	<p>509.288</p>

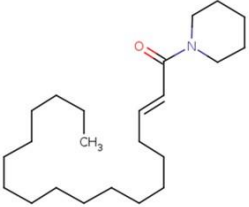
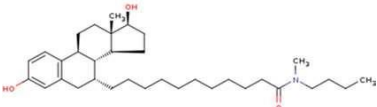
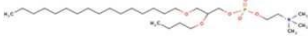
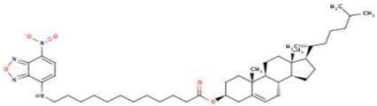
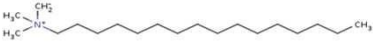
Gly Lys Val	M+H-2H ₂ O		38	267.174
Gln Trp His	M+NH ₄		43	487.233
Phylloquinone Highly tentative based on ammonia precursor	M+NH ₄		23	468.393
1'H-5alpha-Cholest- 2-eno[3,2-b]indole Highly tentative based on exact mass match	M+H-2H ₂ O		N/A Δppm=1 9	424.366
Malyngamide H	M+ACN+H		18	473.346

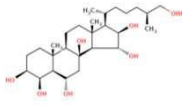
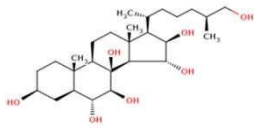
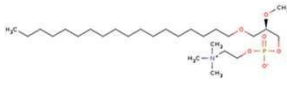

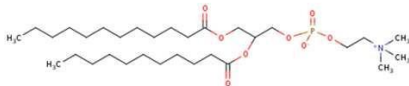
<p>*Ambolic Acid* HIGHLY tentative based on exact mass</p>	<p>M+ACN+H</p>		<p>N/A Δppm =15</p>	<p>512.418</p>
<p>*11-KETOROCKOGENIN ACETATE* Highly tentative based on Precursor requirements</p>	<p>M+2Na-H</p>		<p>15</p>	<p>575.285</p>
<p>2-O-methyl PAF C-18</p>	<p>M+CH3OH+H</p>		<p>17</p>	<p>556.443</p>
<p>β-Carotene</p>	<p>M+ACN+Na</p>		<p>33</p>	<p>600.469</p>
<p>α-CEHC</p>	<p>M+H</p>		<p>31</p>	<p>279.163</p>

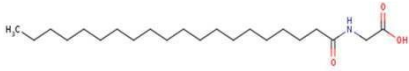
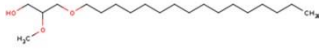
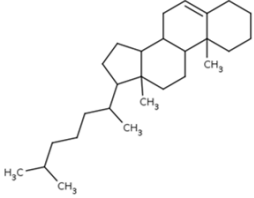
Ile Phe Arg	M+H-2H ₂ O		37	399.254
C-8 Ceramide-1-phosphate highly tentative, not a great msms comparison	M+H-H ₂ O		14	488.36
Psychosine tentative	M+H-H ₂ O		23	444.335
Lyso-PAFC-18 highly tentative based on low score a	M+Na		6	532.387
11β-Misoprostol	M+NH ₄		35	400.31

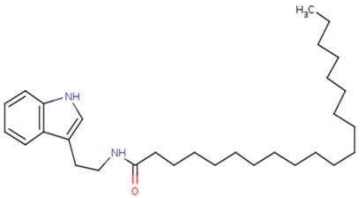
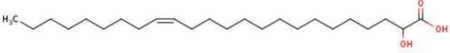
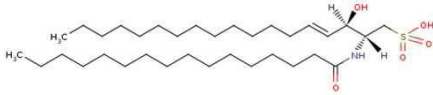
EPA	M+NH4		43	320.258
Eicosyne or Icosyne Isomers tentative based on exact mass match and precursor	M+ACN+Na	 <div data-bbox="678 764 1037 842" style="border: 1px solid black; padding: 5px; margin: 5px 0;">3-Eicosyne</div>  <div data-bbox="669 968 1024 1045" style="border: 1px solid black; padding: 5px; margin: 5px 0;">5-Eicosyne</div>  <div data-bbox="696 1171 1047 1249" style="border: 1px solid black; padding: 5px; margin: 5px 0;">9-Icosyne</div>	N/A; $\Delta\text{ppm}=0$	342.313

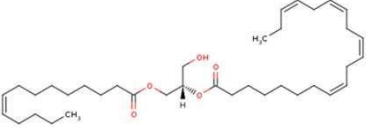
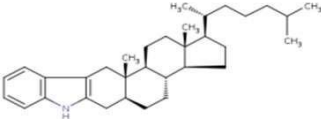
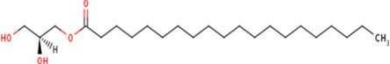

<p>*Various alkenoic acids with hydroxy substituents* Highly tentative based on exact match</p>	<p>M+NH4</p>	<div style="text-align: center;">  <p>2-Octadecenoic acid, 5-hydroxy-</p> </div> <div style="text-align: center;">  <p>18-hydroxy-9Z-octadecenoic acid</p> </div> <div style="text-align: center;">  <p>17-hydroxy-9Z-octadecenoic acid</p> </div> <div style="text-align: center;">  <p>9-hydroxy-12-octadecenoic acid</p> </div>	<p>N/A; Δppm=6</p>	<p>316.287</p>
<p>3-ketosphingosine</p>	<p>M+H</p>	<div style="text-align: center;">  </div>	<p>21 (chose because precursor is M+H and MS/MS graphs appear closer)</p>	<p>298.276</p>


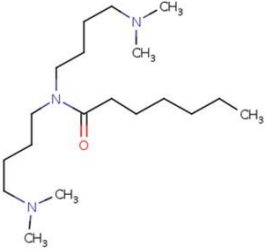
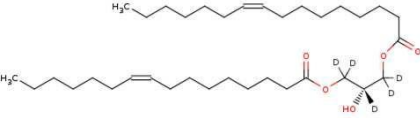
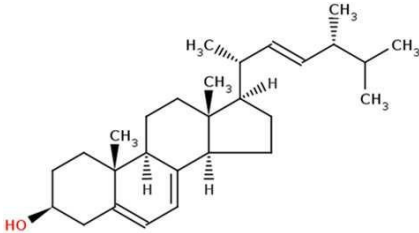
<p>*Piperidine* Tentative based on source of chemical and exact mass match not MS/MS</p>	M+H-H ₂ O		N/a; Δppm=0	332.332
<p>*ICI 164384* tentative based on exact mass match</p>	M+H		N/a; Δppm=7	526.43
<p>*PC(O-16:0/O-4:0)[U]* or similar chemicals, highly tentative based on exact match</p>	M+CH ₃ OH+H	 <p>The hydrocarbon chain off of the substituent ether has variable length</p>	N/a; Δppm=0	570.45
<p>3-dodecanoyl-NBD Cholesterol</p>	M+ACN+Na		88	810.554
<p>CETRIMONIUM</p>	M+H		54	284.331

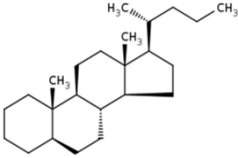
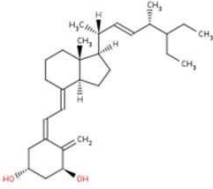
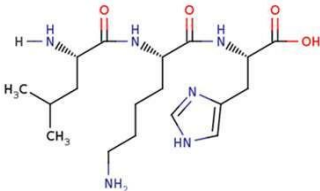
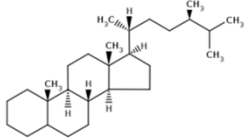
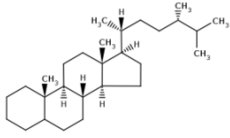
<p>*(25S)-5alpha-cholestan-3beta,4beta,6alpha,8beta,15alpha,16beta,26heptol*; *(25S)-5alpha-cholestan-3beta,6alpha,7beta,8beta,15alpha,16beta,26heptol* Both tentative based on exact mass match</p>	M+NH ₄	 <p>(25S)-5alpha-cholestan-3beta,4beta,6alpha,8beta,15alpha,16beta,26-heptol</p>  <p>(25S)-5alpha-cholestan-3beta,6alpha,7beta,8beta,15alpha,16beta,26-heptol</p>	N/A; Δppm=0	502.373
2-O-methyl PAF C-18	M+Na		16	546.4
PC(P-17:0/0:0) highly tentative based on exact match and closer chemicals by mass	M+H-2H ₂ O		N/A; Δppm=14	458.347
PC(12:0/11:0)[U] or a similar compound tentative based on exact mass match	M+H-H ₂ O		N/A; Δppm=12	590.426

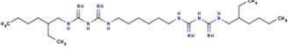
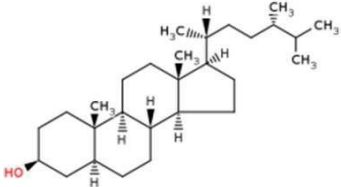
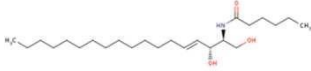
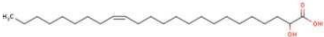
<p>*Arachidoyl glycine* tentative based on methanol precursor</p>	<p>M+CH₃OH+H</p>		<p>82</p>	<p>402.359</p>
<p>1-Hexadecyl-2-O- methyl-glycerol</p>	<p>M+ACN+H</p>		<p>53</p>	<p>372.35</p>
<p>*Cholest-5-ene* tentative based on exact match</p>	<p>M+H-H₂O</p>		<p>N/A Δppm=6</p>	<p>353.355</p>


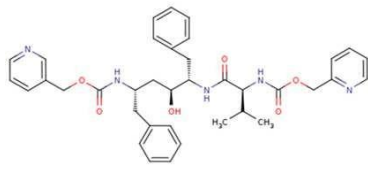
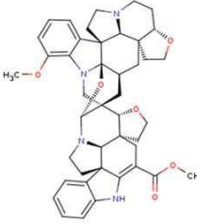
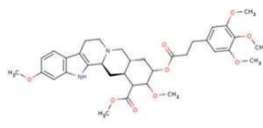

<p>*Nb- Arachidoyltryptamin e* tentative based on exact mass match</p>	<p>M+ACN+H</p>		<p>N/A Δppm=8</p>	<p>496.422</p>
<p>Unidentified Molecule 8</p>				<p>540.452</p>
<p>Unidentified Molecule 9</p>				<p>326.38</p>
<p>*Hydroxynervonic acid* tentative based on exact mass match</p>	<p>M+ACN+H</p>		<p>N/A Δppm=7</p>	<p>424.382</p>
<p>*N-acyl capnines* Highly tentative because sulfonolipid and minus water and exact mass match</p>	<p>M+H-H2O</p>		<p>N/A Δppm=3</p>	<p>584.473</p>

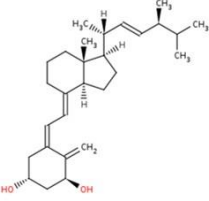
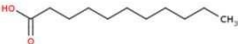
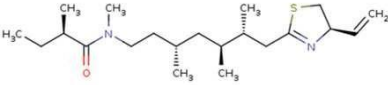

<p>*Diglycerides such as DG(14:1(9Z)/20:4(8Z,11Z,14Z,17Z)/0:0) * tentative based on exact match and precursor requires ACN to fit</p>	M+ACN+H		N/A $\Delta\text{ppm}=8$	628.499
<p>*1'H-5alpha-Cholest-2-eno[3,2-b]indole* tentative based on exact match; this chemical has shown up under a similar</p>	M+H-2H ₂ O		N/A $\Delta\text{ppm}=8$	424.37
<p>*Long Monoglycerides such as MG(20:0/0:0/0:0)*tentative based on exact match</p>	M+ACN+H		N/a $\Delta\text{ppm}=3$	428.375
<p>*N-stearoyl valine* tentative based on exact mass</p>	M+CH ₃ OH+H		N/a $\Delta\text{ppm}=4$	416.375

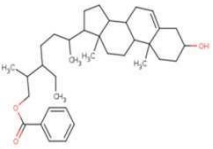
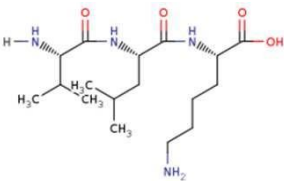
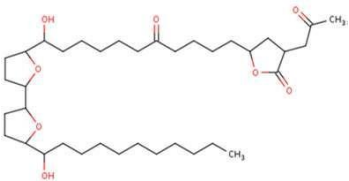
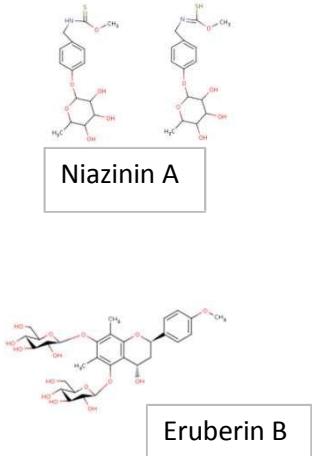
<p>*C-6 Ceramide* somewhat tentative due to lots of "noise" on MS/MS match</p>	M+H		17	398.363
Unidentified Molecule 10				424.426
<p>*N- Heptanoylsolamine* tentative based on exact match and known sources of the molecule</p>	M+CH ₃ OH+H		N/a Δppm=1 1	360.363
<p>Diglyceride such as DG(16:1(9Z)/0:0/16: 1(9Z)) (d5)* Tentative based on exact mass match and water loss</p>	M+H-H ₂ O		N/a Δppm=1 5	542.442
<p>*Ergosterol* tentative because not found in mammalian cells</p>	M+ACN+H		9	438.378

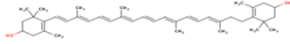
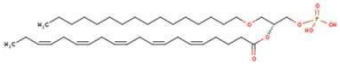
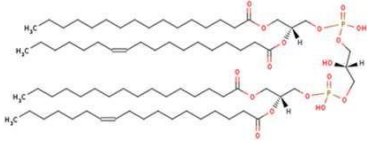
<p>*5-α-Cholane* tentative based on exact mass match and high ppm difference and precursor</p>	M+ACN+Na		N/A Δ ppm=2	394.353
<p>*26,27-Dihomo-1α-hydroxyvitamin D2* Tentative based on exact mass match and precursor with acetonitrile</p>	M+ACN+H		N/A Δ ppm=1	482.405
Leu Lys His	M+H-H2O		33	379.239
<p>*Campestane skeleton or Ergostane skeleton* Highly tentative due to the chemicals being "skeletons" and exact mass match and water loss</p>	M+H-H2O	 <div data-bbox="662 1293 954 1402" style="border: 1px solid black; padding: 5px; margin: 5px 0;">Campestane skeleton</div>  <div data-bbox="662 1577 987 1654" style="border: 1px solid black; padding: 5px; margin: 5px 0;">Ergostane skeleton</div>	N/A Δ ppm=6	369.386

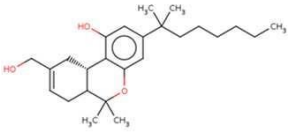
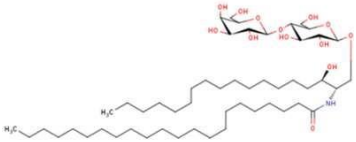
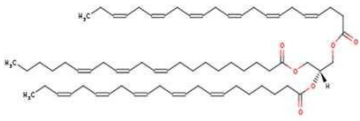
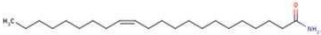
Alexidine Highly tentative due to exact match, precursor, and nature of chemical	M+ACN+H		N/A Δ ppm=1 3	550.495
Unidentified Molecule 11				452.459
ergostan-3 β -ol tentative due to exact mass match	M+H-H ₂ O		N/A Δ ppm=1 3	385.38
Unidentified Molecule 12				312.363
C-6 Ceramide	M+CH ₃ OH+H		18	430.39
Hydroxynervonic acid tentative based on exact mass match and precursor ion	M+NH ₄		N/A Δ ppm=2	400.38


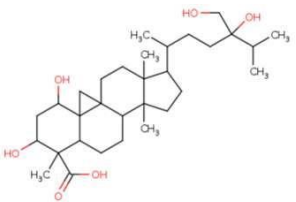
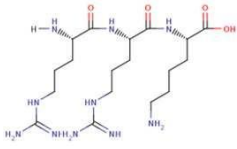
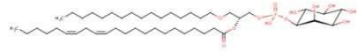
Oleamide	M+H		52	282.28
A 80987 Highly tentative due to exact mass match, especially with a high molecular mass like this	M+H		N/A $\Delta\text{ppm} = 5$	654.333
Amataine tentative based on exact mass search and water loss from precursor	M+H-2H ₂ O		N/A $\Delta\text{ppm} = 2$	681.343
Dihydro Isorescinnamine tentative based on exact match and known source of chemical	M+H		N/A $\Delta\text{ppm} = 7$	637.307
O-Arachidonoyl Glycidol	M+H-H ₂ O		35	393.299

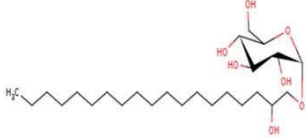
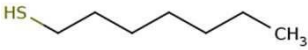

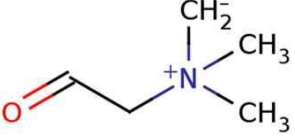

Doxercalciferol tentative based on ammonium in precursor and a much less busy MSMS graph	M+NH4		54	430.365
Undecanoic acid	M+ACN+H		45	228.196
Kalkitoxin	M+ACN+H		44	408.309
Unidentified Molecule 14				689.491
Unidentified Molecule 15				623.452
Unidentified Molecule 16				601.441
Docosanedioic acid Tentative based on exact mass match	M+H		N/A Δ ppm =2	371.316

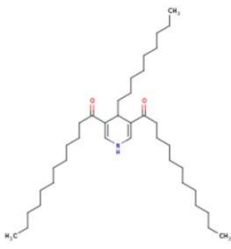
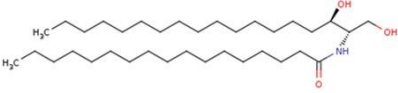
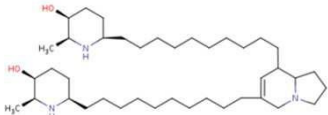
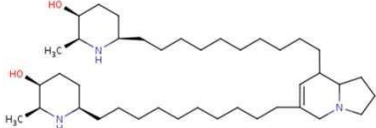
<p>*(3b,24R,25x)-26-Benzoyloxystigmast-5-ene-3-ol* Highly tentative based on exact mass match and high Δppm</p>	M+H		N/A Δ ppm =25	535.401
Unidentified Molecule 17				615.456
<p>*Val Leu Lys* tentative</p>	M+CH ₃ OH+H		29	391.286
<p>*9-Oxoasimicinone* Highly tentative based on exact mass match and known source of molecule</p>	M+H		N/A Δ ppm =4	637.47
<p>*Glycosides such as Niazinin A or Eruberin B* Highly tentative based on exact mass match and the precursors</p>	Niazinin A- M+NH ₄ ; Eruberin B- M+ACN+Na	 <p style="text-align: center;">Niazinin A</p> <p style="text-align: center;">Eruberin B</p>	N/A Δ ppm =0	704.252

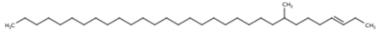
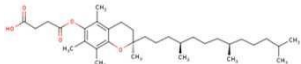
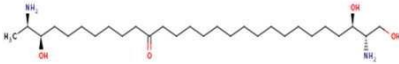
Unidentified Molecule 20				659.482
Parasiloxanthin Tentative due to exact mass match and precursor, chosen because it is a marine lipid and not a carotenoid	M+Na		N/A $\Delta\text{ppm} = 14$	593.442
Phosphatidic Acids similar to PA(O-16:0/20:5(5Z,8Z,11Z,14Z,17Z)) tentative based on exact mass match	M+H		N/A $\Delta\text{ppm} = 12$	681.494
Unidentified Molecule 19				725.522
Cardiolipins such as CL(1'-[16:0/18:1(11Z)],3'-[16:0/18:1(11Z)]) Tentative based on exact mass match	M+2H		N/A $\Delta\text{ppm} = 0$	703.509
Unidentified Molecule 20				571.432
Unidentified Molecule 21				549.419
Unidentified Molecule 22				368.428

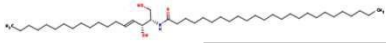

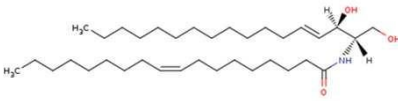
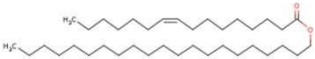

HU-211 Tentative identification based on low metlin score	M+CH ₃ OH+H		8	419.319
Unidentified Molecule 23				992.742
Lactosylceramide tentative based on exact mass match	M+H		score: N/A Δ ppm=1 9	948.716
Unidentified Molecule 23 *Maslinic Acid possible if precursor				505.39
Triglycerides similar to TG(22:3(10Z,13Z,16Z)/22:5(7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[iso6] Tentative based off of exact mass match	M+H+Na		score: N/A Δ ppm=9	527.403
13Z-Docosenamide	M+H		37	338.342

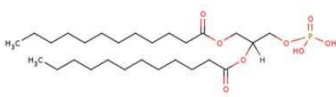
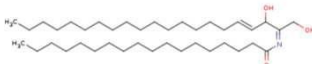
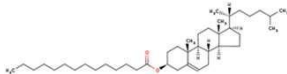

<p>*Phosphatidylethanol amines similar to PE(22:1(11Z)/19:0)* tentative based on exact mass match</p>	M+H		<p>score: N/A Δppm=6</p>	816.642
<p>*Cyclopassifloic acid B* tentative based on exact mass match and known sources of chemical</p>	M+CH ₃ OH+H		<p>score: N/A Δppm=2</p>	553.408
Arg Arg Lys	M+H-H ₂ O		35	441.301
<p>*Phosphatidylinositols similar to PI(O-16:0/22:2(13Z,16Z)) * tentative based on exact mass match</p>	M+H-H ₂ O		<p>score: N/A Δppm=0</p>	859.606


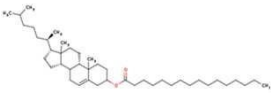
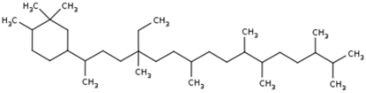
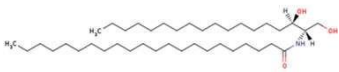
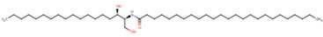
<p>*1-O-alpha-D-glucopyranosyl-1,2-nonadecandiol*</p> <p>Highly tentative based on exact mass match, chosen over closer compounds due to precursor and known sources of other chemicals, as well as chemical</p>	M+H		<p>score: N/A Δppm=1 0</p>	859.606
<p>*Heptane-1-thiol*</p> <p>tentative based on exact mass match and known sources of the chemical as well as the precursor</p>	M+H-2H ₂ O		<p>score: N/A Δppm=5</p>	97.0839
<p>Palmitoyl Serinol</p>	M+ACN+H		27	371.324
<p>Betaine Aldehyde</p>	M+H-H ₂ O		13-31	84.0822
<p>Arachidoyl glycine</p>	M+ACN+Na		85	433.333

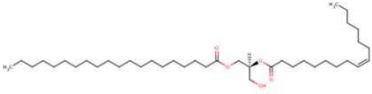

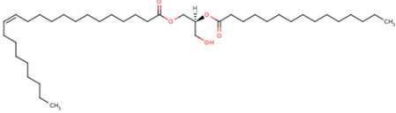
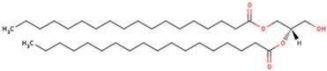
<p>*1,1'-(1,4-Dihydro-4-nonyl-3,5-pyridinediyl)bis[1-dodecanone]* tentative based on exact mass match</p>	<p>M+CH₃OH+H</p>		<p>score: N/A Δppm =17</p>	<p>604.577</p>
<p>Unidentified Molecule 25 (none of the exact mass results seemed plausible due to the precursors and high delta ppm)</p>				<p>560.551</p>
<p>*Cer(d18:0/17:0)* tentative based on exact mass match</p>	<p>M+CH₃OH+H</p>		<p>score: N/A Δppm =15</p>	<p>586.568</p>
<p>*Juliflorine* tentative based on exact mass match and known sources of chemical</p>	<p>M+H</p>		<p>score: N/A Δppm =0</p>	<p>630.593</p>
<p>*Juliflorine(different precursor)* tentative based on exact mass match and known sources of chemical</p>	<p>M+H-H₂O</p>		<p>score: N/A Δppm =0</p>	<p>612.583</p>

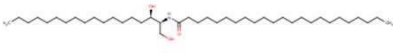
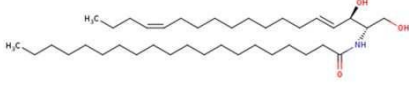
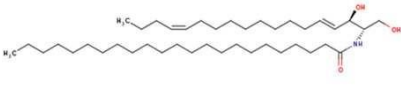
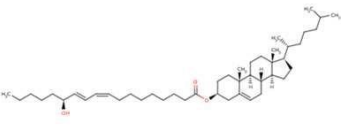
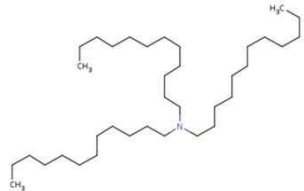
<p>*8-Methyl-3-hentriacontene* tentative based on exact mass match and ammonia precursor</p>	M+NH4		<p>score: N/A Δppm =2</p>	466.536
<p>*VITAMIN E SUCCINATE(TOCOPHEROL SUCCINATE)* tentative based on exact mass match, chosen over other possibilities due to known sources of the chemicals, and precursors</p>	M+Na		<p>score: N/A Δppm =11</p>	553.393
<p>*Oceanin* tentative based on exact mass match and numerous possible chemicals</p>	M+2Na-H		<p>score: N/A Δppm =3</p>	531.409
<p>Unidentified Molecule 26</p>				578.563

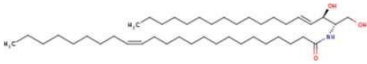
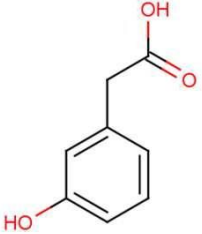
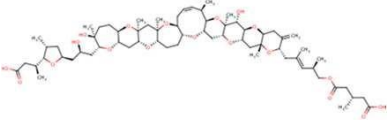

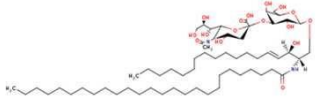
<p>*Ceramide similar to Ceramide (d18:1/25:0)* Highly tentative based on exact mass match, could also be a diglyceride</p>	<p>M+2Na-H</p>	 <p>Ceramide (d18:1/25:0)</p>  <p>Cer(d18:1/25:0)</p>	<p>score: N/A Δppm =1</p>	<p>708.623</p>
<p>*N-Oleoyl-D-erythro-Sphingosine (C18:1 Ceramide)* tentative</p>	<p>M+CH3OH+H</p>		<p>score: N/A Δppm =5</p>	<p>582.549</p>
<p>*Heneicosanyl oleate* tentative</p>	<p>M+ACN+Na</p>		<p>score: N/A Δppm =9</p>	<p>612.563</p>
<p>*Cer(d18:2/21:0)* tentative</p>	<p>M+H</p>		<p>score: N/A Δppm =17</p>	<p>606.593</p>

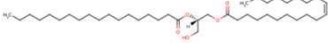
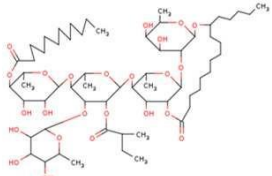
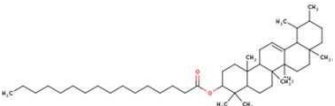
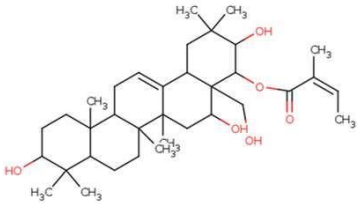
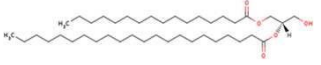
Unidentified Molecule 27				608.577
Phosphatidic Acids similar to PA(12:0/12:0)[U] tentative based on exact mass match	M+CH ₃ OH+H		score: N/A Δ ppm =1	569.38
Hemsleyin imine A tentative based on exact mass match and high Δ ppm	M+H-H ₂ O		score: N/A Δ ppm =19	588.583
Unidentified Molecule 28				632.609
14:0 Cholesteryl ester	M+NH ₄		score: N/A Δ ppm =19	614.599
Unidentified Molecule 29				632.609
2S,3R-didecanoyl-docosane-2,3-diol	M+H-H ₂ O		score: N/A Δ ppm =11	633.611

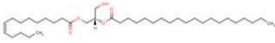
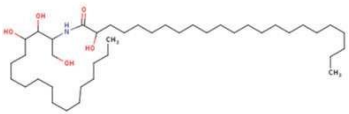
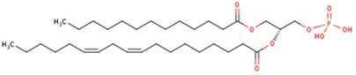

Cer(d18:1/23:0) tentative due to large Δ ppm	M+Na		score: N/A Δ ppm =11	658.624
CE(16:0) tentative due to exact mass match	M+NH4		score: N/A Δ ppm =15	642.629
Monocyclic botryococcane tentative due to exact mass match	M+NH4		score: N/A Δ ppm =1	494.566
Cer(d18:0/22:0) exact mass match	M+Na		score: N/A Δ ppm =18	646.623
Cer(d18:0/25:0) exact mass match	M+Na		score: N/A Δ ppm =16	688.669
Unidentified Molecule 30				610.577

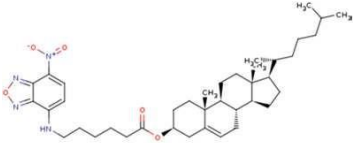
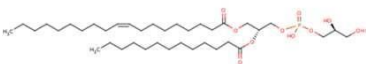
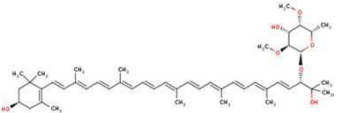
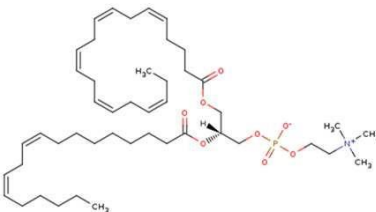
Diglycerides such as DG(20:0/16:1(9Z)/0:0) tentative based on exact mass match and precursor	M+NH4		score: N/A Δ ppm =1	640.587
Unidentified Molecule 31				632.609
Ethylene glycol distearate tentative based on exact mass match	M+ACN+H		score: N/A Δ ppm =1	636.5934 753, 636.6024 780
Diglycerides such as DG(22:1(13Z)/15:0/0:0) tentative based on exact mass match and high Δ ppm	M+NH4		score: N/A Δ ppm =21	654.589
Unidentified Molecule 32				632.609
Diglycerides such as DG(18:0/18:0/0:0) tentative based on exact mass match	M+ACN+H		score: N/A Δ ppm =0	666.603

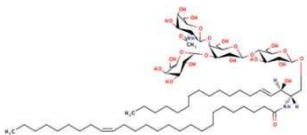
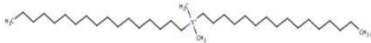
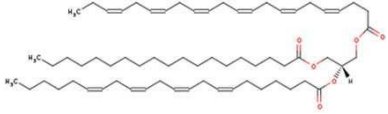
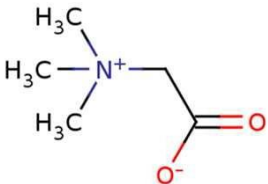
Cer(d18:0/23:0) tentative based on exact mass match	M+Na		score: N/A Δ ppm =22	660.641
Cer(d18:2/20:0) tentative based on exact mass match	M+CH ₃ OH+H		score: N/A Δ ppm =0	624.593
Cer(d18:2/23:0) tentative based on exact mass match	M+H		score: N/A Δ ppm =19	634.626
Cholesteryl ester such as 13(S)-HODE cholesteryl ester tentative based on exact mass match	M+NH ₄		score: N/A Δ ppm =11	682.621
Tridodecylamine	M+H		score: N/A Δ ppm =1	522.598

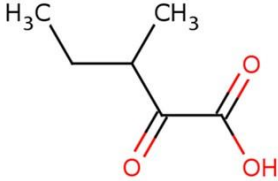
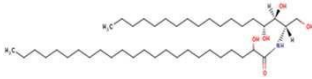
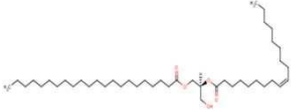
<p>*Ceramides similar to Cer(d18:1/24:1(15Z)) * tentative</p>	M+H		<p>score: N/A Δppm =15</p>	648.639
<p>3-Hydroxyphenylacetic acid</p>	M+NH4		72	170.079
<p>*Gambieric acid D* tentative based on exact mass match</p>	M+NH4		<p>score: N/A Δppm =13</p>	1216.75
<p>*Cer(d18:2/21:0)* tentative</p>	M+CH3OH+H		<p>score: N/A Δppm =0</p>	638.609
<p>*NeuAalpha2-3Galbeta-Cer(d18:1/26:0)* tentative</p>	M+ACN+Na		<p>score: N/A Δppm =11</p>	1194.82

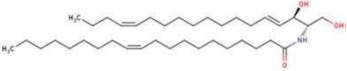
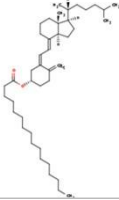
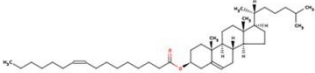

<p>*Diglyceride similar to DG(20:1(11Z)/18:0/0:0)* tentative</p>	M+NH4		<p>score: N/A Δppm =0</p>	668.619
<p>*Simonin III* tentative based on exact mass match</p>	M+H-2H2O		<p>score: N/A Δppm =18</p>	1215.75
<p>Unidentified Molecule 33</p>				664.623
<p>*alpha-Amyrin palmitate* tentative due to exact mass match</p>	M+H		<p>score: N/A Δppm =5</p>	665.627
<p>*22-Angeloylbarringtonol C* tentative due to exact mass match</p>	M+H-2H2O		<p>score: N/A Δppm =0</p>	537.395
<p>*Diglycerides such as DG(16:0/22:0/0:0)[iso2]* tentative due to exact mass match</p>	M+ACN+H		<p>score: N/A Δppm =2</p>	694.633

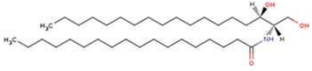
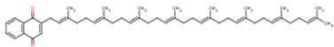
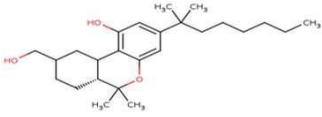
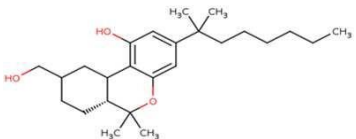
<p>*Diglycerides such as DG(14:1(9Z)/20:0/0:0)* tentative</p>	<p>M+H-2H₂O</p>		<p>score: N/A Δppm =8</p>	<p>559.515</p>
<p>*N-(2R-Hydroxypentacosanoyl)-2S-amino-1,3S,4R-octadecanetriol* tentative based on exact mass match</p>	<p>M+H-2H₂O</p>		<p>score: N/A Δppm =13</p>	<p>662.654 2969</p>
<p>*Phosphatidic Acids similar to PA(13:0/18:2(9Z,12Z)))* exact mass match</p>	<p>M+CH₃OH+H</p>		<p>score: N/A Δppm =5</p>	<p>663.456</p>
<p>*Phosphatidic Acids similar to PA(O-16:0/18:0)* exact mass match</p>	<p>M+2Na-H</p>		<p>score: N/A Δppm =3</p>	<p>707.494</p>

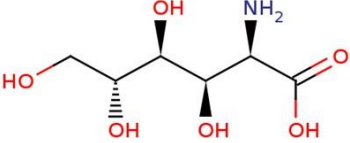

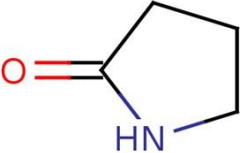
3-hexanoyl-NBD Cholesterol	M+Na		33	685.437
Phosphatidylglycerols similar to PG(19:1(9Z)/13:0)			score: N/A Δ ppm =8	721.508
(3R,2'S)-Myxol 2'- (2,4-di-O-methyl- α -L- fucoside) highly tentative due to exact mass match	M+H		score: N/A Δ ppm =5	759.524
Phosphatidylcholine s similar to PC(20:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))) tentative due to exact mass match	M+H-2H2O		score: N/A Δ ppm =0	768.533

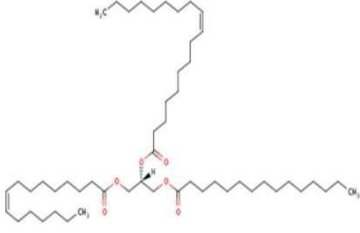
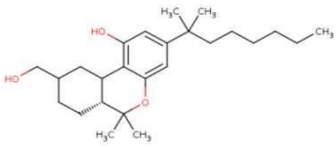
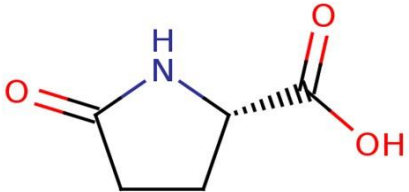
<p>3(GalNAcβ1-4)Galβ1-4Glcβ1-Cer(d18:1/26:1(17Z)) * highly tentative based on exact mass match</p>	M+H-H ₂ O		<p>score: N/A Δppm =6</p>	1347.88
<p>*Dimethyl dialkyl ammonium chloride* highly tentative based on exact mass match</p>	M+ACN+H		<p>score: N/A Δppm =23</p>	550.629
<p>*Triglycerides similar to TG(19:0/22:4(7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)))[iso6]* tentative based on exact mass match</p>	M+H-2H ₂ O		<p>score: N/A Δppm =4</p>	961.806
<p>Betaine(sodiated not protonated)</p>	M+Na		40	140.069

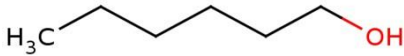
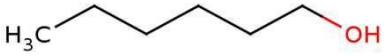
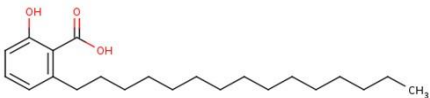
2-oxo-3-methylvaleric acid	M+NH4	 <p>The structure shows a five-carbon chain with a methyl group at the 3-position, a ketone group at the 2-position, and a carboxylic acid group at the 1-position. The methyl group is labeled H₃C and CH₃. The ketone and carboxylic acid groups are shown in red.</p>	26-30	148.097
*Ceramides similar to Cer(d18:1/24:1(15Z)) * tentative exact mass match	M+H-H2O	 <p>The structure shows a sphingosine backbone with a long-chain fatty acid (24:1(15Z)) and a sphingosine head group. The sphingosine head group is shown in red.</p>	score: N/A, Δppm=0	666.641
Diglycerides similar to DG(22:0/18:1(9Z)/0:0) tentative exact mass match	M+NH4	 <p>The structure shows a glycerol backbone with two long-chain fatty acids (22:0 and 18:1(9Z)) and a phosphate group. The phosphate group is shown in red.</p>	score: N/A, Δppm=1	696.651

<p>*Ceramide similar to Cer(d18:2/20:1)* tentative</p>	<p>M+ACN+H</p>		<p>score: N/A, Δppm=2</p>	<p>631.576</p>
<p>*Vitamin D3 palmitate or 16:1 Cholesteryl ester* tentative based on exact mass match</p>	<p>M+H-2H2O</p>	 <p>Vitamin D3 palmitate</p>  <p>16:1 Cholesteryl ester</p>	<p>score: N/A, Δppm=1 2</p>	<p>587.549</p>
<p>*DG(16:0e/18:0/0:0) *</p>	<p>M+H-H2O</p>		<p>score: N/A, Δppm=1 9</p>	<p>565.567</p>

ceramides similar to Cer(d18:0/18:0)	M+ACN+H		score: N/A, Δ ppm=1 7	609.603
Unidentified Chemical 34				578.66
2-demethylmenaquinone-8 * tentative based on exact mass match	M+H		score: N/A, Δ ppm=3	703.547
HU210	M+H-H2O		2 – 21	371.297
HU210	M+H-H2O		2 – 9	371.293

Glucosaminic acid	M+CH ₃ OH+H	 <p>The structure shows a six-carbon chain with a carboxylic acid group at C1, an amino group at C2, and hydroxyl groups at C3, C4, and C6. The hydroxyl groups at C3 and C4 are shown with dashed bonds, while the hydroxyl at C6 and the amino group at C2 are shown with wedged bonds.</p>	5	228.107
Octylamine tentative based on exact mass match	M+H	 <p>The structure shows a straight-chain alkane with a methyl group (H₃C) at one end and an amino group (NH₂) at the other, representing octylamine.</p>	N/A Δppm=3	130.159
2-Pyrrolidinone	M+H	 <p>The structure shows a five-membered ring containing one nitrogen atom and one carbonyl group (C=O) at the 2-position, representing 2-pyrrolidinone.</p>	42	86.0616

<p>*Triglycerides similar to TG(15:0/18:1(9Z)/16:1(9Z))[iso6]* based on exact mass match</p>	<p>M+Na</p>		<p>N/A Δppm=1</p>	<p>825.694</p>
<p>*HU210* tentative based on exact mass match</p>	<p>M+H-H₂O</p>		<p>15</p>	<p>371.289</p>
<p>Pyroglutamic Acid</p>	<p>M+ACN+H</p>		<p>94</p>	<p>171.077</p>

1-Hexanol	M+H		37	121.123
1-Hexanol	M+H		27	103.112
Anacardic Acid	M+Na		6	371.257