

Table S2

Possible metabolites	Formula	Ion type	Experimental mass	Theoretical mass	ppm
Succinic anhydride	C4H4O3	[M+H] ⁺	101.0236	101.02332	2.75
1-Aminocyclopropane-1-carboxylate, Hom	C4H7NO2	[M+H] ⁺	102.0551	102.05495	1.45
4-Hydroxybutanoic acid, (R)-3-Hydroxybut	C4H8O3	[M+H] ⁺	105.0548	105.05462	1.69
Cyclopentanone, 3-Methyl-2-butenal, Pren	C5H8O	[M+Na] ⁺	107.0469	107.04674	1.53
Nitrosobenzene, 3-Pyridinaldehyde, 6-Imin	C6H5NO	[M+H] ⁺	108.0447	108.04439	2.90
N-Methylaniline, ortho-Toluidine, Benzylam	C7H9N	[M+H] ⁺	108.0810	108.08077	2.11
Phenylhydrazine, Phenylenediamine, 1,2-Di	C6H8N2	[M+H] ⁺	109.0763	109.07602	2.59
Monomethyl sulfate	CH4O4S	[M+H] ⁺	112.9901	112.99031	-1.84
1-Pyrroline-2-carboxylate, (S)-1-Pyrroline	C5H7NO2	[M+H] ⁺	114.0552	114.05495	2.17
5,6-Dihydrouracil, 3-Cyano-L-alanine, N-N	C4H6N2O2	[M+H] ⁺	115.0504	115.05020	1.76
L-Aspartate 4-semialdehyde, 2-Amino-3- <i>o</i>	C4H7NO3	[M+H] ⁺	118.0500	118.04987	1.13
trans-1,2-Dichloroethene, cis-1,2-Dichloro	C2H2Cl2	[M+Na] ⁺	118.9427	118.94258	1.03
Succinate, Methylmalonate, Methyl oxalate	C4H6O4	[M+H] ⁺	119.0341	119.03389	1.79
Furfuryl alcohol	C5H6O2	[M+Na] ⁺	121.0261	121.02600	0.82
1-Phenylethylamine, N,N-Dimethylaniline, I	C8H11N	[M+H] ⁺	122.0964	122.09642	-0.18
Cyclohexanol, 4-Methylpentanal, Unsaturat	C6H12O	[M+Na] ⁺	123.0781	123.07804	0.52
2,4-Diaminotoluene, 2,5-Diaminotoluene	C7H10N2	[M+H] ⁺	123.0916	123.09167	-0.54
ortho-Anisidine, para-Anisidine	C7H9NO	[M+H] ⁺	124.0757	124.07569	0.10
2-Hydroxy-1,4-benzoquinone	C6H4O3	[M+H] ⁺	125.0235	125.02332	1.42
Prenol, Pentan-2-one, Cyclopentanol, 2-M	C5H10O	[M+K] ⁺	125.0365	125.03632	1.42
Pentanoate, 3-Methylbutanoic acid, 2-Met	C5H10O2	[M+Na] ⁺	125.0575	125.05730	1.59
Hydroxypyruvate, Malonate, 2-Hydroxy-3-	C3H4O4	[M+Na] ⁺	127.0004	127.00018	1.72
Melamine	C3H6N6	[M+H] ⁺	127.0730	127.07265	2.78
(S)-2,3,4,5-Tetrahydropyridine-2-carboxyl	C6H9NO2	[M+H] ⁺	128.0706	128.07060	-0.02
Coniine	C8H17N	[M+H] ⁺	128.1435	128.14337	1.00
D-Glycerate	C3H6O4	[M+Na] ⁺	129.0156	129.01583	-1.79
Aromatic aldehyde, Benzaldehyde	C7H6O	[M+Na] ⁺	129.0311	129.03109	0.11
(R,R)-Butane-2,3-diol, (S,S)-Butane-2,3-c	C4H10O2	[M+K] ⁺	"	129.03124	-1.07
Naphthalene, Azulene	C10H8	[M+H] ⁺	129.0702	129.06988	2.50
L-Lysine 1,6-lactam, D-2-Amino-hexano-	C6H12N2O	[M+H] ⁺	129.1023	129.10223	0.53
L-Pipecolate, 1-Aminocyclopentanecarbox	C6H11NO2	[M+H] ⁺	130.0863	130.08625	0.37
N-Methylhexanamide	C7H15NO	[M+H] ⁺	130.1227	130.12264	0.48
2,5-Dioxopentanoate, Itaconate, Mesacona	C5H6O4	[M+H] ⁺	131.0339	131.03389	0.10
2-Aminophenol, 4-Hydroxyaniline, Hydroxy	C6H7NO	[M+Na] ⁺	132.0421	132.04198	0.90
trans-1,3-Dichloropropene, cis-1,3-Dichlo	C3H4Cl2	[M+Na] ⁺	132.9582	132.95823	-0.20
Glutarate, 2-Acetolactate, Deoxyribonolact	C5H8O4	[M+H] ⁺	133.0496	133.04954	0.47
1,1-Diethyl-2-hydroxy-2-nitrosohydrazine	C4H10N3O2	[M+H] ⁺	133.0843	133.08457	-2.01
N-Hydroxy-L-valine	C5H11NO3	[M+H] ⁺	134.0811	134.08117	-0.50

(S)-Malate, (R)-Malate, Malate, 3-Dehydro	C4H6O5	[M+H] ⁺	135.0288	135.02880	-0.01
(-)-Ureidoglycolate, Ureidoglycolic acid	C3H6N2O4	[M+H] ⁺	135.0400	135.04003	-0.20
Cyclohexane-1,3-dione, cis-1,2-Dihydrobe	C6H8O2	[M+Na] ⁺	135.0418	135.04165	1.10
2-Phenylacetamide, Acetanilide, N-Benzylf	C8H9NO	[M+H] ⁺	136.0756	136.07569	-0.64
Amphetamine, Dextroamphetamine, 2,4,5-1	C9H13N	[M+H] ⁺	136.1121	136.11207	0.21
Bis(chloromethyl) ether, 1,2-Dichloroethan	C2H4Cl2O	[M+Na] ⁺	136.9531	136.95314	-0.31
2-Hydroxy-2,4-pentadienoate, cis-Acetyla	C5H6O3	[M+Na] ⁺	137.0209	137.02092	-0.12
2-Heptanone, Heptanal	C7H14O	[M+Na] ⁺	137.0937	137.09369	0.10
L-Aspartate 4-semialdehyde, 2-Amino-3-α	C4H7NO3	[M+Na] ⁺	140.0320	140.03181	1.35
S-Acetylthioethanolamine	C4H9NOS	[M+Na] ⁺	142.0300	142.02970	2.10
Ethosuximide, Hypoglycin, Arecaidine, Guva	C7H11NO2	[M+H] ⁺	142.0863	142.08625	0.34
Tropine, Pseudotropine, Hygrine, Pelletierin	C8H15NO	[M+H] ⁺	142.1226	142.12264	-0.26
Bis(2-chloroethyl)ether	C4H8Cl2O	[M+H] ⁺	143.0021	143.00250	-2.78
Phenylacetaldehyde, Styrene oxide, 4-Hyd	C8H8O	[M+Na] ⁺	143.0467	143.04674	-0.25
2-Hydroxymethylclavam	C6H9NO3	[M+H] ⁺	144.0656	144.06552	0.58
4-(Trimethylammonio)but-2-enoate, Stach	C7H13NO2	[M+H] ⁺	144.1019	144.10190	-0.01
(-)-Hygroline, Pseudoconhydrine, Conhydr	C8H17NO	[M+H] ⁺	144.1387	144.13829	2.87
Ethephon	C2H6ClO3P	[M+H] ⁺	144.9815	144.98159	-0.60
Erythritol, D-Threitol	C4H10O4	[M+Na] ⁺	145.0470	145.04713	-0.90
2-Naphthol, 1-Naphthol, (1R,2S)-Naphthale	C10H8O	[M+H] ⁺	145.0646	145.06479	-1.32
4-Acetamidobutanoate, 6-Amino-2-oxohe	C6H11NO3	[M+H] ⁺	146.0811	146.08117	-0.46
trans-1,4-Dichlorobutene	C4H6Cl2	[M+Na] ⁺	146.9739	146.97388	0.16
Coumarin	C9H6O2	[M+H] ⁺	147.0440	147.04406	-0.39
L-Lysine, D-Lysine, (3S)-3,6-Diaminohexa	C6H14N2O2	[M+H] ⁺	147.1129	147.11280	0.70
N-Methyl-N'-nitro-N-nitrosoguanidine	C2H5N5O3	[M+H] ⁺	148.0462	148.04650	-2.01
Fagomine, N-Hydroxy-L-isoleucine	C6H13NO3	[M+H] ⁺	148.0968	148.09682	-0.11
Actinidine	C10H13N	[M+H] ⁺	148.1119	148.11207	-1.16
1,2,3-Trihydroxybenzene, Phloroglucinol, T	C6H6O3	[M+Na] ⁺	149.0208	149.02092	-0.78
Toluene-cis-dihydrodiol, 1-Cyclohexeneca	C7H10O2	[M+Na] ⁺	149.0573	149.05730	-0.01
L-Methionine, D-Methionine, Methionine, F	C5H11NO2S	[M+H] ⁺	150.0586	150.05832	1.85
D-Cathinone, 3-Phenylpropionaldoxim	C9H11NO	[M+H] ⁺	150.0915	150.09134	1.09
Dihydro-4,4-dimethyl-2,3-Furandione, Dihy	C6H8O3	[M+Na] ⁺	151.0365	151.03657	-0.44
(+)-Norephedrine, N-Methyltyramine, N-Me	C9H13NO	[M+H] ⁺	152.1070	152.10699	0.09
5-Aminolevulinic acid, cis-4-Hydroxy-L-prolin	C5H9NO3	[M+Na] ⁺	154.0476	154.04746	0.90
Diethylphosphoric acid	C4H11O4P	[M+H] ⁺	155.0467	155.04677	-0.48
Cinnamaldehyde, Indanone, 2-Indanone, At	C9H8O	[M+Na] ⁺	"	155.04674	-0.23
Hexanoic acid, 4-Hydroxyhexan-3-one, tra	C6H12O2	[M+K] ⁺	"	155.04689	-1.21
1-tert-Butoxy-2-propanol	C7H16O2	[M+Na] ⁺	155.1039	155.10425	-2.26
N-Hydroxy-L-valine	C5H11NO3	[M+Na] ⁺	156.0634	156.06311	1.85
(S)-Malate, (R)-Malate, Malate, 3-Dehydro	C4H6O5	[M+Na] ⁺	157.0108	157.01075	0.34

Indan-1-ol, Cinnamyl alcohol, Phenylacetone	C9H10O	[M+Na]+	157.0625	157.06239	0.73
2-Butoxyethanol	C6H14O2	[M+K]+	"	157.06254	-0.24
1-Naphthaldehyde, 2-Naphthaldehyde	C11H8O	[M+H]+	157.0647	157.06479	-0.59
2-Methylcholine	C6H16NO	[M+K]+	157.0867	157.08634	2.27
(2-Naphthyl)methanol, 1-Hydroxymethylna	C11H10O	[M+H]+	159.0804	159.08044	-0.26
N-Nitrosodi-n-butylamine	C8H18N2O	[M+H]+	159.1496	159.14918	2.63
5-Acetamidopentanoate, (-)-Betonicine, 3	C7H13NO3	[M+H]+	160.0968	160.09682	-0.11
3-Methoxybenzyl alcohol, 4-Hydroxypheny	C8H10O2	[M+Na]+	161.0572	161.05730	-0.63
Naphthalene-1,2-diol, 2-Formyl-1-indanon	C10H8O2	[M+H]+	161.0596	161.05971	-0.66
Ethyl (R)-3-hydroxyhexanoate, Ethyl (S)-3	C8H16O3	[M+H]+	161.1171	161.11722	-0.76
L-2-Amino adipate, N-Methyl-L-glutamate	C6H11NO4	[M+H]+	162.0761	162.07608	0.11
L-Carnitine, (S)-Carnitine	C7H15NO3	[M+H]+	162.1125	162.11247	0.20
2,3,5-Trihydroxytoluene, Gentisyl alcohol, 4	C7H8O3	[M+Na]+	163.0365	163.03657	-0.40
Lichenin, (R)-3,3-Dimethylmalate, 3-Ethylm	C6H10O5	[M+H]+	163.0604	163.06010	1.83
cis-1,2-Dihydro-3-ethylcatechol, 2-Propy	C8H12O2	[M+Na]+	163.0730	163.07295	0.30
gamma-Coniceine	C8H15N	[M+K]+	164.0836	164.08360	-0.02
Tropine, Pseudotropine, Hygrine, Pelletierin	C8H15NO	[M+Na]+	164.1048	164.10458	1.33
Bis(2-chloroethyl)ether	C4H8Cl2O	[M+Na]+	164.9845	164.98444	0.35
4-Oxocyclohexanecarboxylate	C7H10O3	[M+Na]+	165.0522	165.05222	-0.10
Phenylpyruvate, 4-Coumarate, trans-2-Hy	C9H8O3	[M+H]+	165.0546	165.05462	-0.13
L-Rhamnose, 2-Deoxy-D-glucose, L-Rham	C6H12O5	[M+H]+	165.0757	165.07575	-0.32
4-(Trimethylammonio)but-2-enoate, Stach	C7H13NO2	[M+Na]+	166.0837	166.08385	-0.88
(-)-Hygroline, Pseudoconhydrine, Conhydr	C8H17NO	[M+Na]+	166.1200	166.12023	-1.39
2,3-Dimethylmaleate, Triacetate, Methylita	C6H8O4	[M+Na]+	167.0315	167.03148	0.11
4-Acetamidobutanoate, 6-Amino-2-oxohe	C6H11NO3	[M+Na]+	168.0627	168.06311	-2.45
Ethyl isovalerate, Isoamyl acetate, Heptan	C7H14O2	[M+K]+	169.0627	169.06254	0.96
Octane-1,8-diol, Ethohexadiol, 1,2-Octane	C8H18O2	[M+Na]+	169.1200	169.11990	0.59
Piperidione	C9H15NO2	[M+H]+	170.1177	170.11755	0.87
Oxalureate	C3H4N2O4	[M+K]+	170.9805	170.98026	1.42
D-Arabinono-1,4-lactone, 2-Dehydro-3-de	C5H8O5	[M+Na]+	171.0262	171.02640	-1.15
3,4-Dihydroxyphenylethyleneglycol, 1,6-Dih	C8H10O4	[M+H]+	171.0652	171.06519	0.08
4-Isopropylbenzaldehyde, Anethole, Estrag	C10H12O	[M+Na]+	171.0778	171.07804	-1.38
1-tert-Butoxy-2-propanol	C7H16O2	[M+K]+	"	171.07819	-2.27
Metronidazole	C6H9N3O3	[M+H]+	172.0720	172.07166	1.99
D-Cathinone, 3-Phenylpropionaldoxim	C9H11NO	[M+Na]+	172.0729	172.07328	-2.21
D-Ribose, D-Xylose, D-Arabinose, L-Arab	C5H10O5	[M+Na]+	173.0418	173.04205	-1.42
Dipropyl disulfide	C6H14S2	[M+Na]+	173.0427	173.04291	-1.23
Tris(1-aziridinyl)phosphine oxide	C6H12N3OP	[M+H]+	174.0795	174.07906	2.50
N-Acetyl-L-leucine, Swainsonine	C8H15NO3	[M+H]+	174.1125	174.11247	0.19
Menadiol, 1,8-Dihydroxy-3-methylnaphthal	C11H10O2	[M+H]+	175.0753	175.07536	-0.33

Echinorine	C11H12NO	[M+H] ⁺	175.0990	175.09916	-0.93
N-Acetylornithine, N5-Ethyl-L-glutamine	C7H14N2O3	[M+H] ⁺	175.1079	175.10771	1.07
L-Arginine, D-Arginine, Amino acid(Arg-)	C6H14N4O2	[M+H] ⁺	175.1187	175.11894	-1.35
Calystegin B2	C7H13NO4	[M+H] ⁺	176.0917	176.09173	-0.18
L-Cladinosose, Metaldehyde	C8H16O4	[M+H] ⁺	177.1126	177.11214	2.61
(-)-Menthone, Borneol, Geraniol, (+)-Borne	C10H18O	[M+Na] ⁺	177.1249	177.12499	-0.49
Retronecine, Arecoline, Heliotridine, Scopo	C8H13NO2	[M+Na] ⁺	178.0836	178.08385	-1.38
Anthopleurine	C7H15NO4	[M+H] ⁺	178.1073	178.10738	-0.46
Vermelone, Coniferyl aldehyde, 3-Acetyl-6	C10H10O3	[M+H] ⁺	179.0702	179.07027	-0.40
Digitalose, D-Thevetose	C7H14O5	[M+H] ⁺	179.0912	179.09140	-1.13
(-)-Menthol, (+)-Neomenthol, beta-Citron	C10H20O	[M+Na] ⁺	179.1405	179.14064	-0.76
Homostachydrine, Lentiginosine, Tranexam	C8H15NO2	[M+Na] ⁺	180.0993	180.09950	-1.09
2-Isopropylmaleate, (1S,4S)-4-Hydroxy-3-	C7H10O4	[M+Na] ⁺	181.0470	181.04713	-0.72
Nonanoic acid	C9H18O2	[M+Na] ⁺	181.1197	181.11990	-1.11
5-Acetamidopentanoate, (-)-Betonicine, 3	C7H13NO3	[M+Na] ⁺	182.0787	182.07876	-0.34
2-Oxadipate, 3-Oxadipate, 3D-(3,5/4)-T	C6H8O5	[M+Na] ⁺	183.0266	183.02640	1.11
3-(4-Hydroxyphenyl)lactate, (R)-3-(4-Hyd	C9H10O4	[M+H] ⁺	183.0653	183.06519	0.62
Diisopropyl sulfate	C6H14O4S	[M+H] ⁺	183.0686	183.06856	0.23
Mannitol, D-Sorbitol, D-Iditol, L-Iditol, Gala	C6H14O6	[M+H] ⁺	183.0862	183.08632	-0.64
3-Dehydrocarnitine	C7H14NO3	[M+Na] ⁺	"	183.08659	-2.11
4-Nitrosobiphenyl	C12H9NO	[M+H] ⁺	184.0753	184.07569	-2.10
Acetyltropine, Acetylpsuedotropine	C10H17NO2	[M+H] ⁺	184.1332	184.13320	-0.01
Dibenzothiophene	C12H8S	[M+H] ⁺	185.0420	185.04195	0.28
Lichenin, (R)-3,3-Dimethylmalate, 3-Ethylm	C6H10O5	[M+Na] ⁺	"	185.04205	-0.25
cis-1,2-Dihydronaphthalene-1,2-diol, (1S,2	C10H10O2	[M+Na] ⁺	185.0572	185.05730	-0.55
Choline phosphate, 7-Methyl-2-hydroxy-6	C5H15NO4P	[M+H] ⁺	185.0808	185.08114	-1.86
Hydronitroxide radical	C12H10NO	[M+H] ⁺	185.0833	185.08351	-1.15
Octane-1,8-diol, Ethohexadiol, 1,2-Octane	C8H18O2	[M+K] ⁺	185.0936	185.09384	-1.29
Trientine	C6H18N4	[M+K] ⁺	185.1160	185.11629	-1.56
5-exo-Hydroxy-1,2-campholide, 1,6,6-Trim	C10H16O3	[M+H] ⁺	185.1172	185.11722	-0.12
Otonecine, Ecgonine, Pseudoecgonine	C9H15NO3	[M+H] ⁺	186.1125	186.11247	0.18
L-Rhamnose, 2-Deoxy-D-glucose, L-Rham	C6H12O5	[M+Na] ⁺	187.0578	187.05770	0.56
Undecanoic acid	C11H22O2	[M+H] ⁺	187.1692	187.16926	-0.30
6-Acetamido-3-oxohexanoate, 6-Acetamid	C8H13NO4	[M+H] ⁺	188.0917	188.09173	-0.17
n-Decanohydroxamic acid	C10H21NO2	[M+H] ⁺	188.1645	188.16450	-0.01
6-Methylmercaptapurine	C6H6N4S	[M+Na] ⁺	189.0208	189.02052	1.47
D-Xylonate, L-Arabinonate, D-Arabinonate	C5H10O6	[M+Na] ⁺	189.0374	189.03696	2.32
3-(2-Hydroxyphenyl)propanoate, Tropate,	C9H10O3	[M+Na] ⁺	189.0524	189.05222	0.97
2-Oxosuberate	C8H12O5	[M+H] ⁺	189.0759	189.07575	0.78
cis-2,3-Dihydro-2,3-dihydroxybiphenyl, Bu	C12H12O2	[M+H] ⁺	189.0908	189.09101	-1.09

10-Hydroxydecanoic acid, 6-Hydroxy-3,7-Phensuximide, 6,7-Dimethoxyisoquinoline, Castanospermine, (2S)-2-[[1-(R)-Carboxy EPTC, 8-Methylthiooctanaldoxime	C10H20O3	[M+H] ⁺	189.1485	189.14852	-0.12
Zoxazolamine	C11H11NO2	[M+H] ⁺	190.0857	190.08625	-2.90
D-Mycnose	C8H15NO4	[M+H] ⁺	190.1074	190.10738	0.09
Thymyl acetate, Senkyunolide, Sedanonic acid	C9H19NOS	[M+H] ⁺	190.1261	190.12601	0.48
2-Anthramine	C7H5CIN2O	[M+Na] ⁺	190.9982	190.99825	-0.28
3-Dehydroshikimate, 5-Dehydroshikimate, 7-Carboxy-7-carbaguanine	C8H16O5	[M+H] ⁺	193.1073	193.10705	1.28
Capillone	C12H16O2	[M+H] ⁺	193.1223	193.12231	-0.04
Nonane-4,6-dione, Chalcogran, gamma-No	C14H11N	[M+H] ⁺	194.0966	194.09642	0.92
Caffeine	C7H8O5	[M+Na] ⁺	195.0264	195.02640	0.02
(-)-Menthol, (+)-Neomenthol, beta-Citrene	C7H6N4O3	[M+H] ⁺	195.0507	195.05125	-2.83
Decanoic acid, p-Menthane-3,8-diol, Isoam Shikimate, (2S)-2-Isopropyl-3-oxosuccinat	C12H12O	[M+Na] ⁺	195.0781	195.07804	0.33
N-Formimino-L-glutamate, Formylisoglutam	C9H16O2	[M+K] ⁺	"	195.07819	-0.45
Ethyl 3-oxohexanoate, 3-Oxovalproic acid, 4-Hydroxy-9-fluorenone, 6,7-Benzocouma	C8H10N4O2	[M+H] ⁺	195.0878	195.08764	0.84
(Indol-3-yl)acetamide, Indole-3-acetaldehy	C10H20O	[M+K] ⁺	195.1142	195.11457	-1.91
Suberic acid, Dimethyl adipate, 2-Propylglu	C10H20O2	[M+Na] ⁺	195.1358	195.13555	1.28
2,3-Dihydroxy-p-cumate, Phlorisobutyroph	C7H10O5	[M+Na] ⁺	197.0423	197.04205	1.29
Echinorine	C6H10N2O4	[M+Na] ⁺	197.0534	197.05327	0.65
trans-4-Hydroxystilbene, cis-Stilbene oxid	C8H14O3	[M+K] ⁺	197.0579	197.05745	2.27
N-Methyltryptamine, Gramine, alpha-Methy	C13H8O2	[M+H] ⁺	197.0601	197.05971	1.99
N-Nitrosodi-n-butylamine	C10H10N2O	[M+Na] ⁺	197.0683	197.06853	-1.15
2-Amino-5-phosphopentanoic acid, FR 900	C8H14O4	[M+Na] ⁺	197.0783	197.07843	-0.66
Indole-3-acetate, NH2Mec, N-Acetyloxy	C10H12O4	[M+H] ⁺	197.0809	197.08084	0.32
5-Acetamidopentanoate, (-)-Betonicine, 3	C11H12NO	[M+Na] ⁺	"	197.08111	-1.05
3-Propylmalate, alpha-Isopropylmalate, (R)	C14H12O	[M+H] ⁺	197.0958	197.09609	-1.48
cis-2,3-Dihydroxy-2,3-dihydro-p-cumate,	C11H14N2	[M+Na] ⁺	197.1048	197.10491	-0.56
Methacholine	C8H18N2O	[M+K] ⁺	"	197.10506	-1.33
2-Amino-3-methylimidazo[4,5-f]quinoline,	C5H12NO5P	[M+H] ⁺	198.0527	198.05258	0.59
Methacholine	C10H9NO2	[M+Na] ⁺	"	198.05255	0.78
2-Amino-3-methylimidazo[4,5-f]quinoline,	C7H13NO3	[M+K] ⁺	"	198.05270	0.01
Hercynine	C7H12O5	[M+Na] ⁺	199.0576	199.05770	-0.48
(-)-Menthyl acetate, Citronellyl acetate, N	C10H14O4	[M+H] ⁺	199.0966	199.09649	0.57
Cycluron	C8H18NO2	[M+K] ⁺	"	199.09691	-1.55
Dimaprit	C11H10N4	[M+H] ⁺	199.0973	199.09781	-2.55
D-Glucono-1,5-lactone, 2-Dehydro-3-deo	C8H18NO2	[M+K] ⁺	"	199.09691	1.97
	C11H10N4	[M+H] ⁺	199.0980	199.09781	0.97
	C9H16N3O2	[M+H] ⁺	199.1314	199.13152	-0.59
	C12H22O2	[M+H] ⁺	199.1689	199.16926	-1.79
	C11H22N2O	[M+H] ⁺	199.1806	199.18048	0.59
	C6H15N3S	[M+K] ⁺	200.0614	200.06181	-2.07
	C6H10O6	[M+Na] ⁺	201.0366	201.03696	-1.80

Digitalose, D-Thevetose	C7H14O5	[M+Na]+	201.0732	201.07335	-0.73
Carnitine	C7H16NO3	[M+K]+	201.0758	201.07617	-1.86
Simazine	C7H12ClN5	[M+H]+	202.0855	202.08538	0.59
alpha,beta-Didehydrotryptophan, Vasicinon	C11H10N2O2	[M+H]+	203.0820	203.08150	2.48
Diethyl 2-methyl-3-oxosuccinate	C9H14O5	[M+H]+	203.0913	203.09140	-0.50
Metamitron	C10H10N4O	[M+H]+	203.0922	203.09272	-2.57
Diisopropyl phosphate	C6H15O4P	[M+Na]+	205.0602	205.06002	0.89
Cyromazine	C6H10N6	[M+K]+	"	205.05983	1.81
5-Oxo-1,2-campholide, Iridotrial, 2-Oxo-de	C10H14O3	[M+Na]+	205.0836	205.08352	0.41
2-Oxo-8-methylthiooctanoic acid	C9H16O3S	[M+H]+	205.0888	205.08929	-2.40
1,2-Dihydrostilbene	C14H14	[M+Na]+	205.0985	205.09877	-1.32
Diethyl (2R,3R)-2-methyl-3-hydroxysuccin	C9H16O5	[M+H]+	205.1069	205.10705	-0.74
N-Acetyl-D-fucosamine, N-Acetyl-D-quin	C8H15NO5	[M+H]+	206.1025	206.10230	0.98
Acetylropine, Acetylpsuedotropine	C10H17NO2	[M+Na]+	206.1153	206.11515	0.75
Pantothenol	C9H19NO4	[M+H]+	206.1386	206.13868	-0.40
beta-Carboline	C11H8N2	[M+K]+	207.0321	207.03190	0.98
Benzyl 2-methyl-3-oxobutanoate, p-Metho	C12H14O3	[M+H]+	207.1013	207.10157	-1.31
Ibuprofen, Plastoquinol-1	C13H18O2	[M+H]+	207.1379	207.13796	-0.28
Bis(2-chloro-1-methylethyl)ether	C6H12Cl2O	[M+K]+	208.9897	208.98968	0.10
N-Nitrosoguvacoline	C7H10N2O3	[M+K]+	209.0322	209.03229	-0.44
6-endo-Hydroxycineole, (E)-3,7-Dimethylo	C10H18O2	[M+K]+	209.0935	209.09384	-1.62
Benzyl (2R,3S)-2-methyl-3-hydroxybutano	C12H16O3	[M+H]+	209.1170	209.11722	-1.06
Undecanoic acid	C11H22O2	[M+Na]+	209.1515	209.15120	1.43
2-Oxosuberate	C8H12O5	[M+Na]+	211.0576	211.05770	-0.45
Sinapyl alcohol, Phlorisovalerophenone, Mu	C11H14O4	[M+H]+	211.0969	211.09649	1.96
10-Hydroxydecanoic acid, 6-Hydroxy-3,7-	C10H20O3	[M+Na]+	211.1308	211.13047	1.58
(-)-Jasmonic acid, (+)-7-Isojasmonic acid	C12H18O3	[M+H]+	211.1335	211.13287	2.97
Indospicine	C7H15N3O2	[M+K]+	212.0801	212.07957	2.48
3-Dehydroquinate, 4-Hydroxy-4-methyl-2	C7H10O6	[M+Na]+	213.0369	213.03696	-0.29
(R)-3-((R)-3-Hydroxybutanoyloxy)butanoa	C8H14O5	[M+Na]+	213.0735	213.07335	0.72
Propyl cinnamate, Precocene I, 3-Dimethy	C12H14O2	[M+Na]+	213.0890	213.08860	1.87
5-Methoxytryptamine, N-Methylserotonin,	C11H14N2O	[M+Na]+	213.1000	213.09983	0.82
Muscarine	C9H20NO2	[M+K]+	213.1126	213.11256	0.20
Cucurbitic acid, Putaminoxin, Traumatina, 12-	C12H20O3	[M+H]+	213.1484	213.14852	-0.57
Ephedroxane	C11H13NO2	[M+Na]+	214.0833	214.08385	-2.55
Quinate, 2D-5-O-Methyl-2,3,5/4,6-pentah	C7H12O6	[M+Na]+	215.0526	215.05261	-0.05
CAI-1, Tridecanoic acid	C13H26O2	[M+H]+	215.2004	215.20056	-0.73
2-Amino-9,10-epoxy-8-oxodecanoic acid	C10H17NO4	[M+H]+	216.1230	216.12303	-0.15
Ethyl 3-(N-butylacetamido)propionate	C11H21NO3	[M+H]+	216.1595	216.15942	0.38
gamma-L-Glutamyl-D-alanine	C8H14N2O5	[M+H]+	219.0971	219.09754	-2.02

Coryneine	C11H18NO2	[M+Na] ⁺	219.1226	219.12297	-1.69
D-Lysopine	C9H18N2O4	[M+H] ⁺	219.1339	219.13393	-0.12
Ethyl(E,Z)-decadienoate, (1S,2R,4S)-(-)-B	C12H20O2	[M+Na] ⁺	219.1357	219.13555	0.68
Pantothenate	C9H17NO5	[M+H] ⁺	220.1179	220.11795	-0.21
N-Acetyl-D-glucosamine, N-Acetyl-D-ma	C8H15NO6	[M+H] ⁺	222.0977	222.09721	2.20
1-Guanidino-1-deoxy-scyllo-inositol	C7H15N3O5	[M+H] ⁺	222.1088	222.10844	1.63
Buthionine sulfoximine	C8H18N2O3S	[M+H] ⁺	223.1114	223.11108	1.42
Diethyl 2-methyl-3-oxosuccinate	C9H14O5	[M+Na] ⁺	225.0733	225.07335	-0.20
Tremetone	C13H14O2	[M+Na] ⁺	225.0887	225.08860	0.44
10-Oxodecanoate, (3R)-6-Hydroxy-3-isop	C10H18O3	[M+K] ⁺	"	225.08875	-0.24
Flavanone, Isoflavanone, (2S)-Flavanone, 2	C15H12O2	[M+H] ⁺	225.0909	225.09101	-0.48
Dinotefuran	C7H14N4O3	[M+Na] ⁺	225.0960	225.09580	0.91
3-o-Ethyl-L-ascorbic acid	C8H12O6	[M+Na] ⁺	227.0525	227.05261	-0.49
4'-Hydroxy-3'-prenylacetophenone, Plasto	C13H16O2	[M+Na] ⁺	227.1042	227.10425	-0.22
10-Hydroxydecanoic acid, 6-Hydroxy-3,7-	C10H20O3	[M+K] ⁺	"	227.10440	-0.89
Butopyronoxyl	C12H18O4	[M+H] ⁺	227.1278	227.12779	0.06
Tetrahomomethionine	C9H19NO2S	[M+Na] ⁺	228.1030	228.10287	0.58
Acanthiifoline, 2,6-Dihydroxy-N-methylmy	C10H12N2O2	[M+K] ⁺	231.0527	231.05303	-1.42
Dehydrocostus lactone, Eremanthin, Dehyd	C15H18O2	[M+H] ⁺	231.1386	231.13796	2.78
O-Butanoylcarnitine, N(alpha)-t-Butoxyca	C11H21NO4	[M+H] ⁺	232.1544	232.15433	0.29
Sinapyl alcohol, Phlorisovalerophenone, Mu	C11H14O4	[M+Na] ⁺	233.0789	233.07843	2.01
Lidocaine, Angustifoline	C14H22N2O	[M+H] ⁺	235.1807	235.18048	0.93
5,6,7-Trimethoxycoumarin, Orthosporin	C12H12O5	[M+H] ⁺	237.0758	237.07575	0.20
(-)-Menthyl acetate, Citronellyl acetate, N	C12H22O2	[M+K] ⁺	237.1248	237.12514	-1.43
Bombykal	C16H28O	[M+H] ⁺	237.2212	237.22129	-0.39
2-Amino-9,10-epoxy-8-oxodecanoic acid	C10H17NO4	[M+Na] ⁺	238.1046	238.10498	-1.58
Ethyl 3-(N-butylacetamido)propionate	C11H21NO3	[M+Na] ⁺	238.1414	238.14136	0.16
D-erythro-1-(Imidazol-4-yl)glycerol 3-pho	C6H11N2O6P	[M+H] ⁺	239.0434	239.04274	2.74
Dihydroclavaminic acid, Alanylclavam	C8H12N2O4	[M+K] ⁺	239.0434	239.04286	2.27
Felbamate	C11H14N2O4	[M+H] ⁺	239.1021	239.10263	-2.20
Atractylone, Furanodiene	C15H20O	[M+Na] ⁺	239.1410	239.14064	1.52
Dodecanoic acid	C12H24O2	[M+K] ⁺	"	239.14079	0.89
Pirimicarb	C11H18N4O2	[M+H] ⁺	239.1500	239.15024	-0.99
Centarol, Daucol, Debneyol, Seiricardine A	C15H26O2	[M+H] ⁺	239.2004	239.20056	-0.66
O-Propanoylcarnitine	C10H19NO4	[M+Na] ⁺	240.1203	240.12063	-1.36
Pyrene, Fluoranthene	C16H10	[M+K] ⁺	241.0418	241.04141	1.63
Hexadecanal, 1,2-Epoxyhexadecane	C16H32O	[M+H] ⁺	241.2524	241.25259	-0.80
Mefenamic acid, N-Methylflindersine, 6-(1,	C15H15NO2	[M+H] ⁺	242.1170	242.11755	-2.28
(R)-(Homo)2-citrate, 1-Hydroxypentane-1	C8H12O7	[M+Na] ⁺	243.0476	243.04753	0.30
Oblongolide, Glutinosone	C14H20O2	[M+Na] ⁺	243.1356	243.13555	0.20

2-trans,6-trans-Farnesal, alpha-Santalol, l	C15H24O	[M+Na]+	243.1716	243.17194	-1.38
Falcarinone, Dehydrofalcarinol	C17H22O	[M+H]+	243.1744	243.17434	0.24
Pentadecanoic acid, 12-Methyltetradecano	C15H30O2	[M+H]+	243.2318	243.23186	-0.23
Biotin amide	C10H17N3O2S	[M+H]+	244.1111	244.11141	-1.28
6-Acetyl-D-glucose	C8H14O7	[M+Na]+	245.0633	245.06318	0.51
Rishitin, Isokobusone, Kobusone	C14H22O2	[M+Na]+	245.1507	245.15120	-2.04
Arnebinol, Geranylbenzoquinone	C16H20O2	[M+H]+	245.1541	245.15361	2.01
Neostigmine	C12H19N2O2	[M+Na]+	246.1337	246.13387	-0.67
(6S,9R)-Vomifoliol, (+/-)-6-Hydroxy-3-oxo	C13H20O3	[M+Na]+	247.1302	247.13047	-1.08
Geranylhydroquinone	C16H22O2	[M+H]+	247.1692	247.16926	-0.23
Yellow AB	C16H13N3	[M+H]+	248.1188	248.11821	2.37
Prometon, Terbumeton, Secbumeton	C10H19N5O	[M+Na]+	248.1485	248.14816	1.37
5-Hydroxyindoleacetyl glycine	C12H12N2O4	[M+H]+	249.0863	249.08698	-2.72
Sterol, 3beta-Hydroxysterol, Heptadecatrie	C17H28O	[M+H]+	249.2206	249.22129	-2.78
Benzoin, Pinosylvil, (+)-cis-3,4-Dihydroph	C14H12O2	[M+K]+	251.0466	251.04689	-1.15
Tetradecanoic acid	C14H28O2	[M+Na]+	251.1979	251.19815	-1.00
Methyl farnesoate	C16H26O2	[M+H]+	251.2005	251.20056	-0.23
(+)-12-(2-Cyclopenten-1-yl)-2-dodecano	C17H30O	[M+H]+	251.2368	251.23694	-0.57
Pumiliotoxin 251D	C16H29NO	[M+H]+	252.2323	252.23219	0.45
Dehydrocostus lactone, Eremanthin, Dehyd	C15H18O2	[M+Na]+	253.1204	253.11990	1.97
3-Oxododecanoic acid	C12H22O3	[M+K]+	"	253.12005	1.37
Hydnocarpic acid	C16H28O2	[M+H]+	253.2160	253.21621	-0.82
Diclomezine	C11H8Cl2N2O	[M+H]+	255.0081	255.00864	-2.11
Enecalinal, Mexicanin E	C14H16O3	[M+Na]+	255.0994	255.09917	0.92
Ferimzone	C15H18N4	[M+H]+	255.1600	255.16041	-1.60
(R)-(Homo)3-citrate, 1-Hydroxyhexane-1,2	C9H14O7	[M+Na]+	257.0625	257.06318	-2.63
Phenolic steroid, 3-Deoxyestradiol	C18H24O	[M+H]+	257.1899	257.18999	-0.36
5,6,7-Trimethoxycoumarin, Orthosporin	C12H12O5	[M+Na]+	259.0578	259.05770	0.40
(2E,6E)-Farnesol, (2Z,6E)-Farnesol, (-)-alp	C15H26O	[M+K]+	261.1621	261.16152	2.21
Yellow OB	C17H15N3	[M+H]+	262.1338	262.13386	-0.24
Zinnimidine, Cochlearine, cis-1,3,4,6,7,11b-	C15H19NO3	[M+H]+	262.1434	262.14377	-1.40
6,8-Dimethyl-6,7-didehydroergoline	C16H19N2	[M+Na]+	"	262.14404	-2.43
Virol B	C17H26O2	[M+H]+	263.2004	263.20056	-0.60
4-Chlorochalcone	C15H11ClO	[M+Na]+	265.0387	265.03906	-1.37
Clofibrate	C12H15ClO3	[M+Na]+	265.0596	265.06019	-2.24
Dehydrojuvabione, 5-Hydroxy-1-(4-hydrox	C16H24O3	[M+H]+	265.1797	265.17982	-0.46
2-N-Undecyltetrahydrothiophene	C15H30S	[M+Na]+	265.1963	265.19604	0.97
Heptadecatrienoic acid	C17H28O2	[M+H]+	265.2160	265.21621	-0.78
Mirtazapine, Brevicolline, Acridine orange	C17H19N3	[M+H]+	266.1644	266.16516	-2.86
Apraclonidine	C9H10Cl2N4	[M+Na]+	267.0181	267.01746	2.41

2-Methyl-4-chlorophenoxybutyric acid	C11H13ClO3	[M+K] ⁺	"	267.01848	-1.43
Nevirapine, SB 200646, Vasconine	C15H14N4O	[M+H] ⁺	267.1248	267.12402	2.91
Mukaadial, Rugosal A, Zinniol, Xanthoxic ac	C15H22O4	[M+H] ⁺	267.1593	267.15909	0.80
Allopumiliotoxin 267A	C16H29NO2	[M+H] ⁺	268.2272	268.22710	0.37
8-Azaadenosine	C9H12N6O4	[M+H] ⁺	269.0996	269.09926	1.27
3-Methoxyestra-1,3,5(10),16-tetraene, 4-[C19H24O	[M+H] ⁺	269.1898	269.18999	-0.71
omega-Cyclohexylundecanoic acid, 9E-Hep	C17H32O2	[M+H] ⁺	269.2475	269.24751	-0.03
Octadecanal	C18H36O	[M+H] ⁺	269.2839	269.28389	0.03
Estrone, Hexestrol, Trenbolone, 17beta-Dih	C18H22O2	[M+H] ⁺	271.1700	271.16926	2.74
Aphylline, Lupanine, Matrine, Isomatrine, 17	C15H24N2O	[M+Na] ⁺	271.1785	271.17808	1.56
Leontiformine, Retamine	C15H26N2O	[M+Na] ⁺	273.1934	273.19373	-1.19
Hexadecasphinganine	C16H35NO2	[M+H] ⁺	274.2741	274.27405	0.18
Nandrolone, Cinmethylin, 17beta-Hydroxye	C18H26O2	[M+H] ⁺	275.2009	275.20056	1.25
Homatropine, Annotine, Annotinine, Norhyo	C16H21NO3	[M+H] ⁺	276.1588	276.15942	-2.23
Felbamate	C11H14N2O4	[M+K] ⁺	277.0588	277.05851	1.05
Biotin sulfone	C10H16N2O5S	[M+H] ⁺	277.0859	277.08526	2.30
3-beta-D-Galactosyl-sn-glycerol, 2-(beta	C9H18O8	[M+Na] ⁺	"	277.08939	-1.77
3-Deoxyestrone, 4-(1-Ethyl-2-phenylbuty	C18H22O	[M+Na] ⁺	277.1564	277.15629	0.41
Centarol, Daucol, Debneyol, Seiricardine A	C15H26O2	[M+K] ⁺	"	277.15644	-0.14
Hexadecenal, Bombykol	C16H30O	[M+K] ⁺	277.1927	277.19282	-0.44
Stearidonic acid, Kinoprene	C18H28O2	[M+H] ⁺	277.2164	277.21621	0.70
Fluorofelbamate	C11H13FN2O4	[M+Na] ⁺	279.0754	279.07515	0.90
Phenylgalactoside, Aryl beta-D-glucoside,	C12H16O6	[M+Na] ⁺	279.0843	279.08391	1.39
2-N-Dodecyltetrahydrothiophene	C16H32S	[M+Na] ⁺	279.2115	279.21169	-0.69
Hexadecanoic acid	C16H32O2	[M+Na] ⁺	279.2295	279.22945	0.18
Cicutoxin, Enanthotoxin	C17H22O2	[M+Na] ⁺	281.1511	281.15120	-0.36
Dibutyl adipate, Diisobutyl adipate	C14H26O4	[M+Na] ⁺	281.1719	281.17233	-1.53
p-Nitrophenyl-O-ethyl ethylphosphonate,	C10H14NO5P	[M+Na] ⁺	282.0504	282.05018	0.79
Falcarindiol, Virol A	C17H24O2	[M+Na] ⁺	283.1666	283.16685	-0.89
2S-Hydroxytetradecanoic acid	C14H28O3	[M+K] ⁺	"	283.16700	-1.42
(9Z)-Octadecenoic acid, (9E)-Octadeceno	C18H34O2	[M+H] ⁺	283.2633	283.26316	0.50
Tris(2-chloroethyl)phosphate	C6H12Cl3O4P	[M+H] ⁺	284.9609	284.96116	-0.91
Thiometon	C6H15O2PS3	[M+K] ⁺	284.9609	284.96034	1.97
Retinol, 11-cis-Retinol, Ferruginol, Kaur-16	C20H30O	[M+H] ⁺	287.2368	287.23694	-0.49
Allopumiliotoxin 267A	C16H29NO2	[M+Na] ⁺	290.2089	290.20905	-0.50
Capsi-amide	C17H35NO	[M+Na] ⁺	292.2613	292.26108	0.75
Methyl palmitate	C17H34O2	[M+Na] ⁺	293.2453	293.24510	0.68
2-N-Dodecyltetrahydrothiophene	C16H32S	[M+K] ⁺	295.1851	295.18563	-1.79