

Table S1

Possible metabolites	Formula	Ion type	Experimental mass	Theoretical mass	Δ ppm
alpha-(Methylenecyclopropyl)glycine, L-Ba	C6H9NO2	[M+Na] ⁺	150.0524	150.05255	-0.97
1,2-Dichloropropane	C3H6Cl2	[M+K] ⁺	150.9480	150.94781	1.23
Barbiturate, 1-Methylparabanic acid	C4H4N2O3	[M+Na] ⁺	151.0118	151.01141	2.61
N-Methylantranilamide, N,N-Dimethyl-4- <i>l</i>	C8H10N2O	[M+H] ⁺	151.0863	151.08658	-1.87
6-Imino-5-oxocyclohexa-1,3-dienecarboxy	C7H5NO3	[M+H] ⁺	152.0344	152.03422	1.20
Hypotaurocyamine	C3H9N3O2S	[M+H] ⁺	152.0488	152.04881	-0.09
Carbon tetrachloride	CCl4	[M+H] ⁺	152.8823	152.88269	-2.54
Xanthine, Alloxanthine	C5H4N4O2	[M+H] ⁺	153.0406	153.04069	-0.57
Tetraethylammonium	C8H20N	[M+Na] ⁺	153.1486	153.14879	-1.25
4,6-Diamino-5-formamidopyrimidine	C5H7N5O	[M+H] ⁺	154.0722	154.07232	-0.76
3-(N-Nitrosomethylamino)propionaldehyde	C4H8N2O2	[M+K] ⁺	155.0215	155.02173	-1.47
Glycylglycine, D-Asparagine, N-Carbamoyl	C4H8N2O3	[M+Na] ⁺	155.0429	155.04271	1.25
3-Nitroacrylate	C3H3NO4	[M+K] ⁺	155.9697	155.96936	2.16
2-Amino-3-oxobutanoate, L-Aspartate 4-	C4H7NO3	[M+K] ⁺	156.0061	156.00575	2.26
N-Methylethanolamine phosphate, D-1-An	C3H10NO4P	[M+H] ⁺	156.0418	156.04202	-1.40
4-Hydroxyphenylacetone nitrile, (S)-Mandelor	C8H7NO	[M+Na] ⁺	156.0418	156.04198	-1.16
4-Chlorobenzoate, 2-Chlorobenzoate	C7H5ClO2	[M+H] ⁺	157.0047	157.00509	-2.45
S,S-Dimethyl-beta-propiothetin	C5H10O2S	[M+Na] ⁺	157.0297	157.02937	2.09
Thio-THIP	C6H8N2OS	[M+H] ⁺	157.0427	157.04300	-1.93
4-Chloronitrobenzene, 2-Chloronitrobenze	C6H4ClNO2	[M+H] ⁺	158.0006	158.00033	1.71
L-Homoserine, L-Threonine, D-Threonine,	C4H9NO3	[M+K] ⁺	158.0213	158.02140	-0.62
Dextroamphetamine, Amphetamine, 2,4,5- <i>l</i>	C9H13N	[M+Na] ⁺	158.0939	158.09402	-0.73
S-Methyl-1-thio-D-glycerate	C4H8O3S	[M+Na] ⁺	159.0086	159.00864	-0.23
4-Fluoro-L-threonine	C4H8FNO3	[M+Na] ⁺	160.0381	160.03804	0.38
5-Chloro-1,2,4-trihydroxybenzene, 6-Chlo	C6H5ClO3	[M+H] ⁺	160.9998	161.00000	-1.24
Salicylaldehyde, 3-Hydroxybenzaldehyde, 4	C7H6O2	[M+K] ⁺	160.9998	160.99994	-0.86
1-Methyl-1,6-dihydropyridine-2-carbaldox	C7H10N2O	[M+Na] ⁺	161.0685	161.06853	-0.16
Pinidine	C9H17N	[M+Na] ⁺	162.1251	162.12532	-1.33
7-Mercaptoheptanoic acid	C7H14O2S	[M+H] ⁺	163.0785	163.07873	-1.40
Carbamoyl phosphate	CH4NO5P	[M+Na] ⁺	163.9721	163.97193	1.05
2-Thiophenesulfonamide	C4H5NO2S2	[M+H] ⁺	163.9831	163.98344	-2.10
Nornitrogen mustard	C4H9Cl2N	[M+Na] ⁺	164.0002	164.00042	-1.35
2-Aminomuconate semialdehyde, 6-Oxo-1	C6H7NO3	[M+Na] ⁺	164.0316	164.03181	-1.29
Tiopronin, Acetylcysteine	C5H9NO3S	[M+H] ⁺	164.0378	164.03759	1.29
(+)-N-Methylconiine	C9H19N	[M+Na] ⁺	164.1412	164.14097	1.43
Chloral hydrate	C2H3Cl3O2	[M+H] ⁺	164.9268	164.92714	-2.07
5-Hydroxymethyluracil, 4-Imidazolone-5-a	C5H6N2O3	[M+Na] ⁺	165.0274	165.02706	2.08
5-Tetrazolyl-glycine	C3H5N5O2	[M+Na] ⁺	166.0336	166.03353	0.45

1,3-Dichloro-2-propanol	C3H6Cl2O	[M+K] ⁺	166.9431	166.94273	2.22
Ethephon	C2H6ClO3P	[M+Na] ⁺	166.9631	166.96353	-2.58
alpha-Amino-gamma-cyanobutanoate, gar	C5H8N2O2	[M+K] ⁺	167.0218	167.02173	0.43
Azulene, Naphthalene	C10H8	[M+K] ⁺	167.0260	167.02576	1.45
Fluorene, 1-Phenyl-5-heptene-1,3-diyne	C13H10	[M+H] ⁺	167.0852	167.08553	-1.96
Butyro-betaine	C8H18NO	[M+Na] ⁺	167.1283	167.12806	1.46
Cyanuric acid	C3H3N3O3	[M+K] ⁺	167.9809	167.98059	1.86
2-Mercaptobenzothiazole	C7H5NS2	[M+H] ⁺	167.9940	167.99361	2.30
Taurocyamine	C3H9N3O3S	[M+H] ⁺	168.0438	168.04373	0.43
Phosphoenolpyruvate, 3-Phosphonopyruva	C3H5O6P	[M+H] ⁺	168.9892	168.98965	-2.69
4-Fluorocyclohexadiene-cis,cis-1,2-diol, 1	C6H7FO2	[M+K] ⁺	169.0060	169.00617	-0.98
1,2-Dinitrobenzene	C6H4N2O4	[M+H] ⁺	169.0243	169.02438	-0.46
N-Cyclopropylammelide	C6H8N4O2	[M+H] ⁺	169.0722	169.07199	1.26
Thiomorpholine 3-carboxylate	C5H9NO2S	[M+Na] ⁺	170.0242	170.02462	-2.45
Phosphodimethylethanolamine	C4H12NO4P	[M+H] ⁺	170.0574	170.05767	-1.58
2-Indanone oxime, 3-Methyloxindole	C9H9NO	[M+Na] ⁺	//	170.05763	-1.36
(3R)-beta-Leucine, 6-Aminohexanoate, L-	C6H13NO2	[M+K] ⁺	//	170.05778	-2.25
Trichloroethanol	C2H3Cl3O	[M+Na] ⁺	170.9143	170.91417	0.76
Glycerone phosphate, D-Glyceraldehyde 3	C3H7O6P	[M+H] ⁺	171.0050	171.00530	-1.78
Dodecane	C12H26	[M+H] ⁺	171.2108	171.21073	0.43
N-(Carboxyaminoethyl)urea, (S)-Ureidogl	C3H7N3O3	[M+K] ⁺	172.0121	172.01189	1.23
Nitrogen mustard N-oxide	C5H11Cl2NO	[M+H] ⁺	172.0291	172.02904	0.33
Metronidazole	C6H9N3O3	[M+H] ⁺	172.0714	172.07166	-1.49
(-)-Ureidoglycolate, Ureidoglycolic acid	C3H6N2O4	[M+K] ⁺	172.9963	172.99591	2.27
Glycerol 1-phosphate, sn-Glycerol 3-phos	C3H9O6P	[M+H] ⁺	173.0211	173.02095	0.84
Piperonal, 2-Carboxybenzaldehyde, alpha-(	C8H6O3	[M+Na] ⁺	//	173.02092	1.06
1-Deoxy-D-xylulose, (R)-2,3-Dihydroxy-3	C5H10O4	[M+K] ⁺	//	173.02107	0.18
L-Capreomycin	C6H12N4O2	[M+H] ⁺	173.1031	173.10329	-1.08
Proxan	C4H8OS2	[M+K] ⁺	174.9645	174.96482	-1.80
Hypoxanthine	C5H4N4O	[M+K] ⁺	175.0013	175.00165	-2.02
Isoniazid	C6H7N3O	[M+K] ⁺	176.0221	176.02206	0.24
1-Methylnicotinamide, Pralidoxime	C7H9N2O	[M+K] ⁺	176.0346	176.03464	-0.22
Canavanine	C5H12N4O3	[M+H] ⁺	177.0981	177.09820	-0.58
Serotonin, N-Hydroxyl-tryptamine	C10H12N2O	[M+H] ⁺	177.1027	177.10223	2.64
N-Methylethanolamine phosphate, D-1-An	C3H10NO4P	[M+Na] ⁺	178.0238	178.02396	-0.92
L-Hypoglycin, Ethosuximide, Arecaidine, G	C7H11NO2	[M+K] ⁺	180.0425	180.04213	2.04
N-Acetylisoniazid	C8H9N3O2	[M+H] ⁺	180.0772	180.07674	2.54
Buformin	C6H15N5	[M+Na] ⁺	180.1223	180.12195	1.97
2-Methylnaphthalene, 1-Methylnaphthalen	C11H10	[M+K] ⁺	181.0412	181.04141	-1.15
1,10-Phenanthroline	C12H8N2	[M+H] ⁺	181.0764	181.07602	2.12

3-Chlorocatechol, 4-Chlorocatechol, Chlor	C6H5ClO2	[M+K]+	182.9611	182.96097	0.73
3D-(3,5/4)-Trihydroxycyclohexane-1,2-dic	C6H8O5	[M+Na]+	183.0266	183.02640	1.11
Fluoren-9-ol, Benzophenone, Xanthan, Car	C13H10O	[M+H]+	183.0800	183.08044	-2.41
Methacholine	C8H18NO2	[M+Na]+	183.1232	183.12297	1.25
3,4-Dichloroaniline, 2,4-Dichloroaniline, 2,5	C6H5Cl2N	[M+Na]+	183.9692	183.96912	0.42
Trientine	C6H18N4	[M+K]+	185.1161	185.11629	-1.02
L-Serine O-sulfate	C3H7NO6S	[M+H]+	186.0064	186.00668	-1.52
4-Chlorophenoxyacetate	C8H7ClO3	[M+H]+	187.0162	187.01565	2.94
2-Amino-4-chloro-4-pentenoic acid	C5H8ClNO2	[M+K]+	187.9877	187.98751	1.01
1,1,2,2-Tetrachloroethane, 1,1,1,2-Tetrach	C2H2Cl4	[M+Na]+	188.8801	188.88028	-0.97
Propamocarb, N6,N6,N6-Trimethyl-L-lysine	C9H20N2O2	[M+H]+	189.1599	189.15975	0.81
2,6-Dichlorobenzamide	C7H5Cl2NO	[M+H]+	189.9816	189.98209	-2.59
Taurocyamine	C3H9N3O3S	[M+Na]+	190.0260	190.02567	1.73
3-(Hydroxyphosphoryl)pyruvate	C3H5O5P	[M+K]+	190.9505	190.95062	-0.63
Xanthine, Alloxanthine	C5H4N4O2	[M+K]+	190.9966	190.99657	0.17
1,2-Dinitrobenzene	C6H4N2O4	[M+Na]+	191.0064	191.00632	0.41
3,4-Dihydroxymandelaldehyde, (R)-4-Hydro	C8H8O4	[M+Na]+	191.0312	191.03148	-1.47
4-Nitroquinoline N-oxide	C9H6N2O3	[M+H]+	191.0452	191.04511	0.46
Cyclo(deltaAla-L-Val), Pyridoxamine, 4-Ph	C8H12N2O2	[M+Na]+	191.0793	191.07909	1.09
Prothiocarb	C8H18N2OS	[M+H]+	191.1211	191.12125	-0.80
L-Cysteate	C3H7NO5S	[M+Na]+	191.9939	191.99371	0.98
Phosphodimethylethanolamine	C4H12NO4P	[M+Na]+	192.0399	192.03961	1.49
O-Oxalylhomoserine, Isosorbide mononitrat	C6H9NO6	[M+H]+	192.0501	192.05026	-0.84
4-(beta-Acetylaminoethyl)imidazole, 2,4-D	C7H11N3O	[M+K]+	192.0538	192.05336	2.30
Nitrogen mustard N-oxide	C5H11Cl2NO	[M+Na]+	194.0108	194.01099	-0.96
2-Formyloxymethylclavam, AminoDHS, 2,3,	C7H9NO4	[M+Na]+	194.0426	194.04238	1.15
Deisopropylhydroxyatrazine	C5H9N5O	[M+K]+	194.0439	194.04385	0.27
4-Imidazolone-5-propanoate, (S)-3-(Imida	C6H8N2O3	[M+K]+	195.0168	195.01664	0.81
Sulfanilamide	C6H8N2O2S	[M+Na]+	195.0197	195.01986	-0.83
4-Chloronitrobenzene, 2-Chloronitrobenze	C6H4ClNO2	[M+K]+	195.9562	195.95621	-0.06
Allidochlor	C8H12ClNO	[M+Na]+	196.0503	196.04996	1.74
alpha-[3-(Nitrosoamino)propyl]-3-pyridine	C9H13N3O2	[M+H]+	196.1075	196.10804	-2.76
1-Hydroxymethylnaphthalene, (2-Naphthyl	C11H10O	[M+K]+	197.0361	197.03632	-1.13
Phosphoguanidinoacetate	C3H8N3O5P	[M+H]+	198.0271	198.02742	-1.64
Indole-3-acetaldehyde, 3-Methyl-quinolin-	C10H9NO	[M+K]+	198.0312	198.03157	-1.86
Pargyline	C11H13N	[M+K]+	198.0679	198.06795	-0.27
5-Chloro-1,2,4-trihydroxybenzene, 6-Chlo	C6H5ClO3	[M+K]+	198.9554	198.95588	-2.42
2,6-Dichloro-para-phenylenediamine, Sodi	C6H6Cl2N2	[M+Na]+	198.9798	198.98002	-1.09
Hydralazine	C8H8N4	[M+K]+	199.0380	199.03804	-0.19
Nitrofurazone, 2,4-Dinitrophenylhydrazine	C6H6N4O4	[M+H]+	199.0463	199.04617	0.67

D-Alanyl-D-serine	C6H12N2O4	[M+Na] ⁺	199.0689	199.06892	-0.11
4,4'-Methylenedianiline, Tacrine, N-(Pheny	C13H14N2	[M+H] ⁺	199.1232	199.12297	1.17
N-Formyl-L-aspartate	C5H7NO5	[M+K] ⁺	199.9952	199.99558	-1.89
Dihomomethionine	C7H15NO2S	[M+Na] ⁺	200.0719	200.07157	1.66
Umbelliferone	C9H6O3	[M+K] ⁺	200.9951	200.99485	1.23
Methomyl	C5H10N2O2S	[M+K] ⁺	201.0090	201.00945	-2.23
3,6,8-Trimethylallantoin	C7H12N4O3	[M+H] ⁺	201.0984	201.09820	0.98
Memantine, Rimantadine	C12H21N	[M+Na] ⁺	202.1569	202.15662	1.40
2-Dehydro-D-xylionate	C5H8O6	[M+K] ⁺	202.9955	202.99525	1.24
S-Methyl-L-methionine	C6H14NO2S	[M+K] ⁺	203.0377	203.03768	0.10
Dinotefuran	C7H14N4O3	[M+H] ⁺	203.1141	203.11385	1.22
(3Z,6Z,9Z)-3,6,9-Dodecatrien-1-ol	C12H20O	[M+Na] ⁺	203.1403	203.14064	-1.65
2-Methylthiobenzothiazole	C8H7NS2	[M+Na] ⁺	203.9913	203.99121	0.45
4-Methylthiobutylthiohydroximate	C5H11NOS2	[M+K] ⁺	//	203.99136	-0.29
3-Methylguanine, 7-Methylguanine	C6H7N5O	[M+K] ⁺	204.0287	204.02820	2.46
Triacanthine, N6-(delta2-Isopentenyl)-ade	C10H13N5	[M+H] ⁺	204.1246	204.12435	1.21
Dicyclohexylamine	C12H23N	[M+Na] ⁺	204.1725	204.17227	1.15
Diisopropyl sulfate	C6H14O4S	[M+Na] ⁺	205.0505	205.05050	-0.01
Levamisole	C11H12N2S	[M+H] ⁺	205.0795	205.07939	0.55
Mipafox	C6H16FN2OP	[M+Na] ⁺	205.0876	205.08764	-0.20
Diethyl (2S,3R)-2-methyl-3-hydroxysuccir	C9H16O5	[M+H] ⁺	205.1068	205.10705	-1.23
Ethambutol	C10H24N2O2	[M+H] ⁺	205.1910	205.19105	-0.23
2,4-Dinitroaniline	C6H5N3O4	[M+Na] ⁺	206.0169	206.01722	-1.53
3-Methoxyanthranilate, 3-Hydroxy-4-metf	C8H9NO3	[M+K] ⁺	206.0214	206.02140	0.01
6-Hydroxykynurenate, Xanthurenic acid, 6-	C10H7NO4	[M+H] ⁺	206.0442	206.04478	-2.82
N-Cyclopropylammeline	C6H9N5O	[M+K] ⁺	//	206.04385	1.71
Choline sulfate	C5H13NO4S	[M+Na] ⁺	206.0460	206.04575	1.23
Chlorphentermine	C10H14ClN	[M+Na] ⁺	206.0703	206.07069	-1.91
Phosphoenolpyruvate, 3-Phosphonopyruva	C3H5O6P	[M+K] ⁺	206.9451	206.94554	-2.10
Desflurane	C3H2F6O	[M+K] ⁺	206.9638	206.96414	-1.65
Urate	C5H4N4O3	[M+K] ⁺	206.9912	206.99148	-1.37
L-3,4-Dihydroxybutan-2-one 4-phosphate	C4H9O6P	[M+Na] ⁺	207.0026	207.00290	-1.44
MTIC	C5H8N6O	[M+K] ⁺	207.0388	207.03909	-1.42
Indolylmethylthiohydroximate	C10H10N2OS	[M+H] ⁺	207.0585	207.05865	-0.74
Chamazulene	C14H16	[M+Na] ⁺	207.1147	207.11442	1.35
L-Cysteate	C3H7NO5S	[M+K] ⁺	207.9679	207.96765	1.21
o-Chloroacetanilide, 4-Chloroacetanilide	C8H8ClNO	[M+K] ⁺	207.9928	207.99260	0.98
O-Phospho-D-serine, O-Phospho-L-serin	C3H8NO6P	[M+Na] ⁺	207.9981	207.99814	-0.21
Arenaine, Alchornine	C11H17N3O	[M+H] ⁺	208.1441	208.14443	-1.57
4-Chlorophenylacetate	C8H7ClO2	[M+K] ⁺	208.9767	208.97662	0.40

Thiourocanic acid	C6H6N2O2S	[M+K] ⁺	208.9782	208.97815	0.24
Propylthiouracil	C7H10N2OS	[M+K] ⁺	209.0150	209.01453	2.23
Psoralen, Angelicin	C11H6O3	[M+Na] ⁺	209.0207	209.02092	-1.03
cis-1,2-Dihydroxy-4-methylcyclohexa-3,5	C8H10O4	[M+K] ⁺	//	209.02107	-1.76
Epibatidine	C11H13ClN2	[M+H] ⁺	209.0835	209.08400	-2.37