

Electronic Supplementary Information for “A practical approach to detect unique metabolic patterns for personalized medicine”

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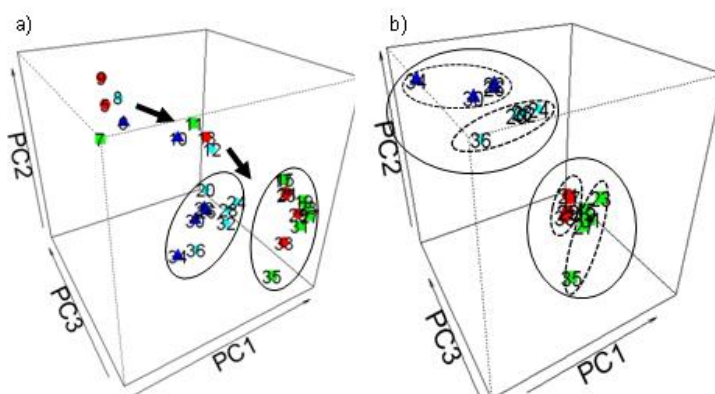


Fig S-1 a) Initial PCA analysis shows separation by run-time and column. Plasma was collected from 4 individuals, identified by colors, and run in 6 replicates on 2 columns. Results show a need for an 8 to 10 run wash-in period and a strong separation by column. b) After wash-in analyses were removed from the analysis, PCA shows a strong separation by column, indicated by solid circles, with a secondary separation by individual, indicated by broken circles.

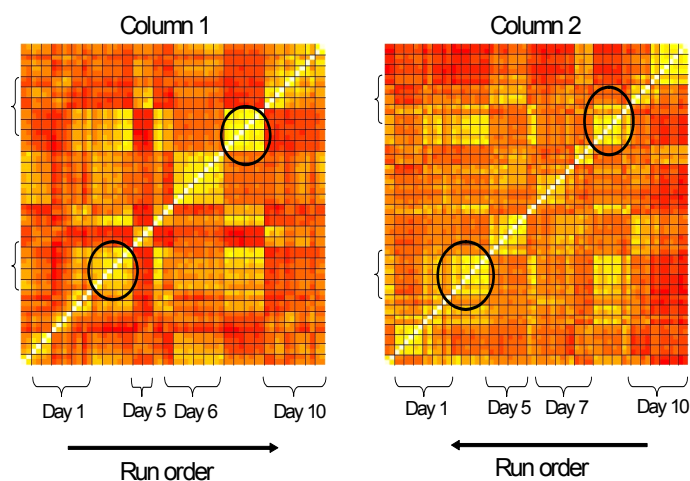


Fig S-2 Correlation analysis shows experimental results obtained from each column gives the same experimental answer. Plasma from a previously described experiment²¹ was run using the described LC-FTMS method. Samples were run in duplicate on each of 2 columns in reverse order. Correlation analysis using R software showed that neither column nor run order had large effects on correlation patterns. Some differences are apparent but these appear to be due to lost data for one of the columns.

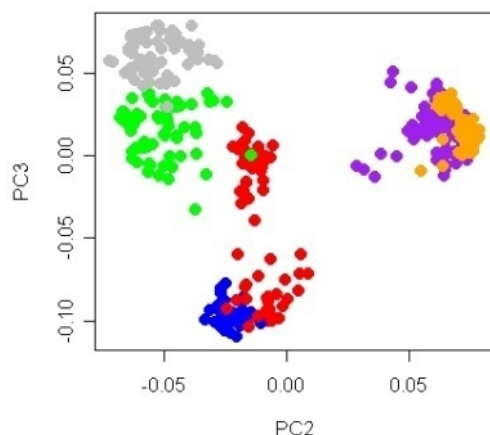


Fig S-3 Intra-individual variation is smaller than inter-individual variation even with variable dietary intake. Plasma was collected from 6 individuals on different chemically defined diets as described previously.²¹ Briefly, 34 samples were collected from each individual over a 10-day time course and included fasting and postprandial samples with a nutritionally complete and a nutritionally deficient diet. The metabolic profile was analyzed for each sample and PCA analysis done to visualize the results. Projections including PC1 (not shown) also separated grey and green and red and blue, but individuals represented by purple and gold were still close.

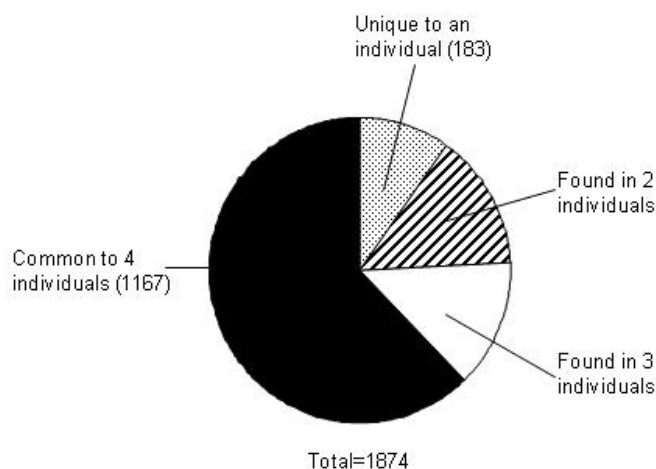


Fig S-4. Inter-individual comparison of LC-FTMS metabolic profiles of human plasma. To obtain a sample reflective of real variability in humans, plasma samples were collected from 4 healthy individuals (1 male, 3 females) without control of diet or other lifestyle factors. Following analysis by LC-FTMS, feature profiles were compared among individuals. Results showed that among the features detected, most were common to all individuals and only 10% were found in only one subject. Thus, even without control for diet or other factors, the predominance of m/z features detected by the LC-FTMS method were common among individuals.

Table S-1 Endogenous metabolism database

Metabolite	Elemental formula	Precise Mass	M + 1H	10ppm-	10ppm+
acetaldehyde	C2 H4 O	44.0262	45.0335	45.0330	45.0339
formate	C H2 O2	46.0055	47.0127	47.0123	47.0132
ethanol	C2 H6 O	46.0419	47.0491	47.0487	47.0496
2-propyn-1-al	C3 H2 O	54.0106	55.0178	55.0173	55.0184
acrolein	C3 H4 O	56.0262	57.0335	57.0329	57.0341
2-propyn-1-ol	C3 H4 O	56.0262	57.0335	57.0329	57.0341
acetone	C3 H6 O	58.0419	59.0491	59.0485	59.0497
propanal	C3 H6 O	58.0419	59.0491	59.0485	59.0497
acetamide	C2 H5 N O	59.0371	60.0444	60.0438	60.0450
guanidine	C H5 N3	59.0483	60.0556	60.0550	60.0562
trimethylamine	C3 H9 N	59.0735	60.0808	60.0802	60.0814
acetic acid	C2 H4 O2	60.0211	61.0284	61.0278	61.0290
glycolaldehyde	C2 H4 O2	60.0211	61.0284	61.0278	61.0290
urea	C H4 N2 O	60.0324	61.0396	61.0390	61.0402
1-propanol	C3 H8 O	60.0575	61.0648	61.0642	61.0654
2-propanol	C3 H8 O	60.0575	61.0648	61.0642	61.0654
carbamate	C H3 N O2	61.0164	62.0236	62.0230	62.0243
ethanolamine	C2 H7 N O	61.0528	62.0600	62.0594	62.0607
carbonic acid	C H2 O3	62.0004	63.0077	63.0070	63.0083
ethylene glycol	C2 H6 O2	62.0368	63.0440	63.0434	63.0447
aminoimidazole	C3 H5 N2	69.0453	70.0525	70.0518	70.0532
propynoate	C3 H2 O2	70.0055	71.0127	71.0120	71.0135
3-butyrol	C4 H6 O	70.0419	71.0491	71.0484	71.0498
methylglyoxal	C3 H4 O2	72.0211	73.0284	73.0277	73.0291
butyraldehyde	C4 H8 O	72.0575	73.0648	73.0641	73.0655
aminoacetone	C3 H7 N O	73.0528	74.0600	74.0593	74.0608
methylguanidine	C2 H7 N3	73.0640	74.0713	74.0705	74.0720
glyoxylic acid	C2 H2 O3	74.0004	75.0077	75.0069	75.0084
hydroxyacetone	C3 H6 O2	74.0368	75.0440	75.0433	75.0448
lactaldehyde	C3 H6 O2	74.0368	75.0440	75.0433	75.0448
propanoate	C3 H6 O2	74.0368	75.0440	75.0433	75.0448
1-butanol	C4 H10 O	74.0732	75.0804	75.0797	75.0812
1,3-diaminopropane	C3 H10 N2	74.0844	75.0917	75.0909	75.0924
glycine	C2 H5 N O2	75.0320	76.0393	76.0385	76.0401
1-amino-propan-2-ol	C3 H9 N O	75.0684	76.0757	76.0749	76.0764
trimethylamine N-oxide	C3 H9 N O	75.0684	76.0757	76.0749	76.0764
glycolate	C2 H4 O3	76.0160	77.0233	77.0225	77.0241
1,2-propandiol	C3 H8 O2	76.0524	77.0597	77.0589	77.0605
cysteamine	C2 H7 N S	77.0299	78.0372	78.0364	78.0380

piperidine	C5 H9 N	83.0735	84.0808	84.0799	84.0816
imidazolone	C3 H4 N2 O	84.0324	85.0396	85.0388	85.0405
3-butynoate	C4 H6 O2	86.0368	87.0440	87.0432	87.0449
2-aminoacrylate	C3 H5 N O2	87.0320	88.0393	88.0384	88.0402
4-aminobutyraldehyde	C4 H9 N O	87.0684	88.0757	88.0748	88.0766
pyruvic acid	C3 H4 O3	88.0160	89.0233	89.0224	89.0242
malonate semialdehyde	C3 H4 O3	88.0160	89.0233	89.0224	89.0242
acetoin	C4 H8 O2	88.0524	89.0597	89.0588	89.0606
butyric acid	C4 H8 O2	88.0524	89.0597	89.0588	89.0606
α -alanine	C3 H7 NO2	89.0477	90.0549	90.0540	90.0558
β -alanine	C3 H7 NO2	89.0477	90.0549	90.0540	90.0558
sarcosine	C3 H7 N O2	89.0477	90.0549	90.0540	90.0558
oxalic acid	C2 H2 O4	89.9953	91.0026	91.0017	91.0035
lactic acid	C3 H6 O3	90.0317	91.0390	91.0380	91.0399
3-hydroxypropionate	C3 H6 O3	90.0317	91.0390	91.0380	91.0399
glyceraldehyde	C3 H6 O3	90.0317	91.0390	91.0380	91.0399
glycerone	C3 H6 O3	90.0317	91.0390	91.0380	91.0399
2,3 butanediol	C4 H10 O2	90.0681	91.0753	91.0744	91.0763
3-amino-isobutyrate	C4 H9 N O2	91.0633	92.0706	92.0697	92.0715
glycerol	C3 H8 O3	92.0473	93.0546	93.0537	93.0555
isocaproic aldehyde	C6 H12 O	100.0888	101.0961	101.0951	101.0971
putrescine	C4 H12 N2	100.1000	101.1073	101.1063	101.1083
1-aminocyclopropane-1-carboxylate	C4 H7 N O2	101.0477	102.0549	102.0539	102.0560
acetoacetic acid	C4 H6 O3	102.0317	103.0390	103.0379	103.0400
2-oxo-butyrate	C4 H6 O3	102.0317	103.0390	103.0379	103.0400
methylmalonate semialdehyde	C4 H6 O3	102.0317	103.0390	103.0379	103.0400
succinate semialdehyde	C4 H6 O3	102.0317	103.0390	103.0379	103.0400
formiminoglycine	C3 H6 N2 O2	102.0429	103.0502	103.0492	103.0512
betaine aldehyde	C5 H12 N O	102.0919	103.0992	103.0981	103.1002
cadaverine	C5 H14 N2	102.1157	103.1230	103.1219	103.1240
β -amino-isobutyric acid	C4 H9 N O2	103.0633	104.0706	104.0696	104.0716
4-amino-butyrate	C4 H9 N O2	103.0633	104.0706	104.0696	104.0716
dimethylglycine	C4 H9 N O2	103.0633	104.0706	104.0696	104.0716
□□□□□□□□□□□□□□□□□□□□	C4 H9 N O2	103.0633	104.0706	104.0696	104.0716
hydroxypyruvate	C3 H4 O4	104.0109	105.0182	105.0172	105.0193
malonate	C3 H4 O4	104.0109	105.0182	105.0172	105.0193
tartronate semialdehyde	C3 H4 O4	104.0109	105.0182	105.0172	105.0193
2-hydroxybutyrate	C4 H8 O3	104.0473	105.0546	105.0536	105.0557
3-hydroxybutyric acid	C4 H8 O3	104.0473	105.0546	105.0536	105.0557
3-hydroxyisobutyrate	C4 H8 O3	104.0473	105.0546	105.0536	105.0557
4-hydroxybutyrate	C4 H8 O3	104.0473	105.0546	105.0536	105.0557
choline	C5 H14 N O	104.1075	105.1148	105.1138	105.1159
serine	C3 H7 N O3	105.0426	106.0499	106.0488	106.0509

diethanolamine	C4 H11 N O2	105.0790	106.0862	106.0852	106.0873
glycerate	C3 H6 O4	106.0266	107.0339	107.0328	107.0349
nicotinamide	C6 H6 N2 O	106.0531	107.0604	107.0593	107.0614
hypotaurine	C2 H7 N O2 S	109.0197	110.0270	110.0259	110.0281
catechol	C6 H6 O2	109.0289	110.0362	110.0351	110.0373
2-aminophenol	C6 H7 N O	109.0528	110.0600	110.0589	110.0611
pyrrole-2-carboxylate	C5 H4 N O2	110.0242	111.0315	111.0304	111.0326
1,4-benzenediol	C6 H6 O2	110.0368	111.0440	111.0429	111.0452
pyrocatechol	C6 H6 O2	110.0368	111.0440	111.0429	111.0452
imidazole-4-acetaldehyde	C5 H6 N2 O	110.0480	111.0553	111.0542	111.0564
2,5-dihydroxy-pyridine	C5 H5 N O2	111.0320	112.0393	112.0382	112.0404
cytosine	C4 H5 N3 O	111.0432	112.0505	112.0494	112.0516
histamine	C5 H9 N3	111.0796	112.0869	112.0858	112.0880
uracil	C4 H4 N2 O2	112.0273	113.0345	113.0334	113.0357
5-amino-4-imidazole carboxylate	C4 H5 N2 O2	113.0351	114.0424	114.0412	114.0435
1-pyrroline 2-carboxylate	C5 H7 N O2	113.0477	114.0549	114.0538	114.0561
1-pyrroline-5-carboxylate	C5 H7 N O2	113.0477	114.0549	114.0538	114.0561
creatinine	C4 H7 N3 O	113.0589	114.0662	114.0650	114.0673
acetylenedicarboxylate	C4 H2 O4	113.9953	115.0026	115.0014	115.0037
2-oxo-pent-4-enoate	C5 H6 O3	114.0317	115.0390	115.0378	115.0401
5,6-dihydrouracil	C4 H6 N2 O2	114.0429	115.0502	115.0490	115.0513
allyl sulfide	C6 H10 S	114.0503	115.0576	115.0564	115.0587
maleamate	C4 H5 N O3	115.0269	116.0342	116.0330	116.0354
proline	C5 H9 N O2	115.0633	116.0706	116.0694	116.0718
fumaric acid	C4 H4 O4	116.0109	117.0182	117.0170	117.0194
maleate	C4 H4 O4	116.0109	117.0182	117.0170	117.0194
2-oxoisovalerate	C5 H8 O3	116.0473	117.0546	117.0534	117.0558
glutarate semialdehyde	C5 H8 O3	116.0473	117.0546	117.0534	117.0558
5-aminopentanamide	C5 H12 N2 O	116.0950	117.1022	117.1011	117.1034
2-aminoacetoacetate	C4 H7 N O3	117.0426	118.0499	118.0487	118.0510
aspartate-4-semialdehyde	C4 H7 N O3	117.0426	118.0499	118.0487	118.0510
guanidinoacetate	C3 H7 N3 O2	117.0538	118.0611	118.0599	118.0623
indole	C8 H7 N	117.0578	118.0651	118.0639	118.0663
5-aminovalerate	C5 H11 N O2	117.0790	118.0862	118.0851	118.0874
succinic acid	C4 H6 O4	118.0266	119.0339	119.0327	119.0351
methylmalonate	C4 H6 O4	118.0266	119.0339	119.0327	119.0351
N-methylhydantoin	C3 H6 N2 O2	118.0378	119.0451	119.0439	119.0463
2,4-diaminobutanoate	C4 H10 N2 O2	118.0742	119.0815	119.0803	119.0827
betaine	C5 H12 N O2	118.0868	119.0941	119.0929	119.0953
homoserine	C4 H9 N O3	119.0582	120.0655	120.0643	120.0667
threonine	C4 H9 N O3	119.0582	120.0655	120.0643	120.0667
3-mercaptopyruvate	C3 H4 O3 S	119.9881	120.9954	120.9942	120.9966
3-(methylthio) propionic acid	C4 H8 O2 S	120.0245	121.0318	121.0306	121.0330

N-carbanoylsarcosine	C3 H8 N2 O3	120.0535	121.0607	121.0595	121.0620
pehnylacetalddehyde	C8 H8 O	120.0575	121.0648	121.0636	121.0660
3-mercaptolactate	C3 H5 O3 S	120.9959	122.0032	122.0020	122.0044
cysteine	C3 H7 N O2 S	121.0197	122.0270	122.0258	122.0282
phenylethylamine	C8 H11 N	121.0891	122.0964	122.0952	122.0976
phenylethylalcohol	C8 H10 O	122.0732	123.0804	123.0792	123.0817
niacin	C6 H5 N O2	123.0320	124.0393	124.0381	124.0405
methylimidazole acetaldehyde	C6 H8 N2 O	124.0637	125.0709	125.0697	125.0722
glutaric acid	C5 H8 O4	124.0749	125.0822	125.0809	125.0834
taurine	C2 H7 N O3 S	125.0146	126.0219	126.0207	126.0232
5-methylcytosine	C5 H7 N3 O	125.0589	126.0662	126.0649	126.0674
N-methylhistamine	C6 H11 N3	125.0953	126.1026	126.1013	126.1038
formyl phosphate	C H3 O5 P	125.9712	126.9785	126.9772	126.9798
imidazole acetic acid	C5 H6 N2 O2	126.0429	127.0502	127.0489	127.0515
thymine	C5 H6 N2 O2	126.0429	127.0502	127.0489	127.0515
4-amino-4-imidazolecarboxamide	C4 H6 N4 O	126.0541	127.0614	127.0601	127.0627
cholesten-3-on	C8 H14 O	126.1045	127.1117	127.1105	127.1130
ethanolamine phosphate	C2 H8 N O4 P	127.0155	128.0227	128.0214	128.0240
2,3,4,5-tetrahydropyridine-3-carboxylate	C6 H9 N O2	127.0633	128.0706	128.0693	128.0719
piperideine-2-carboxylate	C6 H9 N O2	127.0633	128.0706	128.0693	128.0719
barbiturate	C4 H4 N2 O3	128.0222	129.0294	129.0282	129.0307
5,6-dihydrothymine	C5 H8 N2 O2	128.0586	129.0658	129.0645	129.0671
1-pyrroline-3-hydroxy-5-carboxylate	C5 H7 N O3	129.0426	130.0499	130.0486	130.0512
1-pyrroline-4-hydroxy-2-carboxylate	C5 H7 N O3	129.0426	130.0499	130.0486	130.0512
4-oxoproline	C5 H7 N O3	129.0426	130.0499	130.0486	130.0512
α-ketoisocaproic acid	C6 H9 O3	129.0552	130.0624	130.0611	130.0637
N4-acetylaminobutanal	C6 H11 N O2	129.0790	130.0862	130.0849	130.0875
pipecolate	C6 H11 N O2	129.0790	130.0862	130.0849	130.0875
4-guanidinobutanal	C5 H11 N3 O	129.0902	130.0975	130.0962	130.0988
itaconate	C5 H6 O4	130.0266	131.0339	131.0326	131.0352
2-oxoglutarate semialdehyde	C5 H6 O4	130.0266	131.0339	131.0326	131.0352
citraconate	C5 H6 O4	130.0266	131.0339	131.0326	131.0352
mesaconate	C5 H6 O4	130.0266	131.0339	131.0326	131.0352
2-oxo-3-methylvalerate	C6 H10 O3	130.0630	131.0703	131.0689	131.0716
2-oxo-isocaproate	C6 H10 O3	130.0630	131.0703	131.0689	131.0716
3-oxo-4-methylpentanoic acid	C6 H10 O3	130.0630	131.0703	131.0689	131.0716
N-acetylputrescine	C6 H14 N2 O	130.1106	131.1179	131.1166	131.1192
agmatine	C5 H14 N4	130.1218	131.1291	131.1278	131.1304
4-trimethylammonibutanal	C7 H16 N O +	130.1232	131.1305	131.1291	131.1318
coprostanol	C8 H18 O	130.1358	131.1430	131.1417	131.1443
2-oxosuccinamate	C4 H5 N O4	131.0218	132.0291	132.0278	132.0304
hydroxyproline	C5 H9 N O3	131.0582	132.0655	132.0642	132.0668
2-oxo-5-aminovalerate	C5 H9 N O3	131.0582	132.0655	132.0642	132.0668

4-hydroxyglutamate semialdehyde	C5 H9 N O3	131.0582	132.0655	132.0642	132.0668
5-aminolevulinate	C5 H9 N O3	131.0582	132.0655	132.0642	132.0668
glutamate-1-semialdehyde	C5 H9 N O3	131.0582	132.0655	132.0642	132.0668
glutamate-5-semialdehyde	C5 H9 N O3	131.0582	132.0655	132.0642	132.0668
creatine	C4 H9 N3 O2	131.0695	132.0767	132.0754	132.0781
isoleucine	C6 H13 N O2	131.0946	132.1019	132.1006	132.1032
leucine	C6 H13 N O2	131.0946	132.1019	132.1006	132.1032
norleucine	C6 H13 N O2	131.0946	132.1019	132.1006	132.1032
β-leucine	C6 H13 N O2	131.0946	132.1019	132.1006	132.1032
N-carbamoylputrescine	C5 H13 N3 O	131.1058	132.1131	132.1118	132.1144
oxalacetic acid	C4 H4 O5	132.0059	133.0131	133.0118	133.0145
2-hydroxyethylenedicarboxylate	C4 H4 O5	132.0059	133.0131	133.0118	133.0145
trans-2,3-epoxysuccinate	C4 H4 O5	132.0059	133.0131	133.0118	133.0145
oxalureate	C3 H4 N2 O4	132.0171	133.0244	133.0230	133.0257
2-acetolactate	C5 H8 O4	132.0422	133.0495	133.0482	133.0508
4-hydroxy-2-oxovalerate	C5 H8 O4	132.0422	133.0495	133.0482	133.0508
glutarate	C5 H8 O4	132.0422	133.0495	133.0482	133.0508
asparagine	C4 H8 N2 O3	132.0535	133.0607	133.0594	133.0621
3-ureidopropionate	C4 H8 N2 O3	132.0535	133.0607	133.0594	133.0621
gly-gly		132.0535	133.0607	133.0594	133.0621
ornithine	C5 H12 N2 O2	132.0899	133.0971	133.0958	133.0985
aspartic acid	C4 H7 N O4	133.0375	134.0448	134.0434	134.0461
ureidoglycine	C3 H7 N3 O3	133.0487	134.0560	134.0547	134.0573
indoxyl	C8 H7 N O	133.0528	134.0600	134.0587	134.0614
malic acid	C4 H6 O5	134.0215	135.0288	135.0274	135.0301
3-dehydro threonate	C4 H6 O5	134.0215	135.0288	135.0274	135.0301
ureidoglycolate	C3 H6 N2 O4	134.0327	135.0400	135.0387	135.0414
2,3-dihydroxyisovalerate	C5 H10 O4	134.0579	135.0652	135.0638	135.0665
deoxyribose	C5 H10 O4	134.0579	135.0652	135.0638	135.0665
acetanilide	C8 H8 N O	134.0606	135.0679	135.0665	135.0692
picolinate	C7 H5 N O2	135.0320	136.0393	136.0379	136.0407
homocysteine	C4 H9 N O2 S	135.0354	136.0427	136.0413	136.0440
4-chlorophenylacetate	C8 H7 O2 Cl	135.0446	136.0519	136.0505	136.0532
adenine	C5 H5 N5	135.0545	136.0618	136.0604	136.0631
phenylacetamide	C8 H9 N O	135.0684	136.0757	136.0743	136.0770
threonate	C4 H8 O5	136.0372	137.0444	137.0431	137.0458
hypoxanthine	C5 H4 N4 O	136.0385	137.0458	137.0444	137.0471
phenylacetic acid	C8 H8 O2	136.0524	137.0597	137.0583	137.0611
4-hydroxyphenylacetaldehyde	C8 H8 O2	136.0524	137.0597	137.0583	137.0611
4-aminobenzoate	C7 H7 N O2	137.0477	138.0549	138.0536	138.0563
anthranilate	C7 H7 N O2	137.0477	138.0549	138.0536	138.0563
tyramine	C8 H11 N O	137.0841	138.0913	138.0900	138.0927
acetyl-P	C2 H3 O5 P	137.9712	138.9785	138.9771	138.9799

4-hydroxybenzoate	C7 H6 O3	138.0317	139.0390	139.0376	139.0403
gentisate aldehyde	C7 H6 O3	138.0317	139.0390	139.0376	139.0403
urocanate	C6 H6 N2 O2	138.0429	139.0502	139.0488	139.0516
4-hydroxyphenylethanol	C8 H10 O2	138.0681	139.0753	139.0740	139.0767
O-phosphoethanolamine	C2 H6 N O4 P	139.0029	140.0101	140.0087	140.0115
6-hydroxy-nicotinate	C6 H5 N O3	139.0269	140.0342	140.0328	140.0356
histidinal	C6 H9 N3 O	139.0745	140.0818	140.0804	140.0832
methylimidazoleacetic acid	C6 H8 N2 O2	140.0586	141.0658	141.0644	141.0672
carbamoyl phosphate	C H4 N O5 P	140.9821	141.9894	141.9880	141.9908
histidinol	C6 H11 N3 O	141.0902	142.0975	142.0961	142.0989
coenzyme M	C2 H6 O3 S2	141.9758	142.9831	142.9817	142.9845
3-oxoadipate-enol-lactone	C6 H6 O4	142.0266	143.0339	143.0324	143.0353
muconate	C6 H6 O4	142.0266	143.0339	143.0324	143.0353
5-methyl-barbiturate	C5 H6 N2 O3	142.0378	143.0451	143.0437	143.0465
imidazolone acetate	C5 H6 N2 O3	142.0378	143.0451	143.0437	143.0465
2-methyleneglutarate	C6 H8 O4	144.0422	145.0495	145.0481	145.0510
dimethylmaleate	C6 H8 O4	144.0422	145.0495	145.0481	145.0510
methylitaconate	C6 H8 O4	144.0422	145.0495	145.0481	145.0510
ectoine	C6 H12 N2 O2	144.0899	145.0971	145.0957	145.0986
4-guanidinobutanamide	C5 H12 N4 O	144.1011	145.1084	145.1069	145.1098
2-oxo-glutamamate	C5 H7 N O4	145.0375	146.0448	146.0433	146.0462
4-oxoglutamamate	C5 H7 N O4	145.0375	146.0448	146.0433	146.0462
2-amino-5-oxohexanoate	C6 H11 N O3	145.0739	146.0812	146.0797	146.0826
2-aminoadipate 6-semialdehyde	C6 H11 N O3	145.0739	146.0812	146.0797	146.0826
2-oxo-6-aminocaproate	C6 H11 N O3	145.0739	146.0812	146.0797	146.0826
4-acetamidobutanoate	C6 H11 N O3	145.0739	146.0812	146.0797	146.0826
5-amino-3-oxohexanoic acid	C6 H11 N O3	145.0739	146.0812	146.0797	146.0826
4-guanidinobutyrate	C5 H11 N3 O2	145.0851	146.0924	146.0909	146.0938
3,6-diaminohexonate	C6 H13 N2 O2	145.0977	146.1050	146.1035	146.1064
spermidine	C7 H19 N3	145.1579	146.1652	146.1637	146.1666
2-oxoglutaric acid	C5 H6 O5	146.0215	147.0288	147.0273	147.0302
erythroascorbate	C5 H6 O5	146.0215	147.0288	147.0273	147.0302
methyloxaloacetate	C5 H6 O5	146.0215	147.0288	147.0273	147.0302
oxoglutaric acid	C5 H6 O5	146.0215	147.0288	147.0273	147.0302
4,5-dihydro-orotate	C4 H6 N2 O4	146.0327	147.0400	147.0385	147.0415
adipic acid	C6 H10 O4	146.0579	147.0652	147.0637	147.0666
2-aceto-2-hydroxybutyrate	C6 H10 O4	146.0579	147.0652	147.0637	147.0666
2-dehydropantoate	C6 H10 O4	146.0579	147.0652	147.0637	147.0666
glutamine	C5 H10 N2 O3	146.0691	147.0764	147.0749	147.0779
3-ureido-isobutyrate	C5 H10 N2 O3	146.0691	147.0764	147.0749	147.0779
gly-ala		146.0691	147.0764	147.0749	147.0779
lysine	C6 H14 N2 O2	146.1055	147.1128	147.1113	147.1143
3,5-diaminohexonate	C6 H14 N2 O2	146.1055	147.1128	147.1113	147.1143

δ1-piperideine-2-carboxylate	C6 H14 N2 O2	146.1055	147.1128	147.1113	147.1143
4-trimethylammoniumbutanoate	C7 H16 N O2 +	146.1181	147.1254	147.1239	147.1268
acetylcholine	C7 H16 N O2 +	146.1181	147.1254	147.1239	147.1268
indole-5,6-quinone	C8 H5 N O2	147.0320	148.0393	148.0378	148.0408
glutamic acid	C5 H9 N O4	147.0531	148.0604	148.0589	148.0619
2-oxo-4-hydroxy-5-amino-valerate	C5 H9 N O4	147.0531	148.0604	148.0589	148.0619
3-methylaspartate	C5 H9 N O4	147.0531	148.0604	148.0589	148.0619
isoglutamate	C5 H9 N O4	147.0531	148.0604	148.0589	148.0619
O-acetylserine	C5 H9 N O4	147.0531	148.0604	148.0589	148.0619
2-hydroxy-3-oxosuccinate	C4 H4 O6	148.0008	149.0080	149.0065	149.0095
dihydrofumarate	C4 H4 O6	148.0008	149.0080	149.0065	149.0095
4-methylthio-2-oxobutanoic acid	C5 H8 O3 S	148.0194	149.0267	149.0252	149.0282
2-dehydro-3-deoxy arabionate	C5 H8 O5	148.0372	149.0444	149.0429	149.0459
2-dehydro-3-deoxy xylonate	C5 H8 O5	148.0372	149.0444	149.0429	149.0459
2-hydroxyglutarate	C5 H8 O5	148.0372	149.0444	149.0429	149.0459
2-methylmalate	C5 H8 O5	148.0372	149.0444	149.0429	149.0459
arabino-1,5-lactone	C5 H8 O5	148.0372	149.0444	149.0429	149.0459
arabinono-1,4-lactone	C5 H8 O5	148.0372	149.0444	149.0429	149.0459
citramalate	C5 H8 O5	148.0372	149.0444	149.0429	149.0459
erythro-3-methylmalate	C5 H8 O5	148.0372	149.0444	149.0429	149.0459
threo-3-methylmalate	C5 H8 O5	148.0372	149.0444	149.0429	149.0459
xylonolactone	C5 H8 O5	148.0372	149.0444	149.0429	149.0459
trans-cinnamate	C9 H8 O2	148.0524	149.0597	149.0582	149.0612
2,3-dihydroxy-3-methylvalerate	C6 H12 O4	148.0735	149.0808	149.0793	149.0823
mevalonate	C6 H12 O4	148.0735	149.0808	149.0793	149.0823
pantoate	C6 H12 O4	148.0735	149.0808	149.0793	149.0823
2-formylaminobenzaldehyde	C8 H7 N O2	149.0477	150.0549	150.0534	150.0564
5,6-dihydroxyindole	C8 H7 N O2	149.0477	150.0549	150.0534	150.0564
dihydroxyindole	C8 H7 N O2	149.0477	150.0549	150.0534	150.0564
methionine	C5 H11 N O2 S	149.0510	150.0583	150.0568	150.0598
triethanolamine	C6 H15 N O3	149.1052	150.1125	150.1110	150.1140
tartrate	C4 H6 O6	150.0164	151.0237	151.0222	151.0252
guanine	C5 H4 N5 O	150.0416	151.0488	151.0473	151.0503
arabinose	C5 H10 O5	150.0528	151.0601	151.0586	151.0616
lyxose	C5 H10 O5	150.0528	151.0601	151.0586	151.0616
ribose	C5 H10 O5	150.0528	151.0601	151.0586	151.0616
ribulose	C5 H10 O5	150.0528	151.0601	151.0586	151.0616
xylose	C5 H10 O5	150.0528	151.0601	151.0586	151.0616
xylulose	C5 H10 O5	150.0528	151.0601	151.0586	151.0616
phenylpropanoate	C9 H10 O2	150.0681	151.0753	151.0738	151.0769
acetaminophen	C8 H9 N O2	151.0633	152.0706	152.0691	152.0721
4-hydroxyphenylacetaldehyde-oxime	C8 H9 N O2	151.0633	152.0706	152.0691	152.0721
N-methyltyramine	C9 H13 N O	151.0997	152.1070	152.1055	152.1085

3-sulfinylpyruvate	C3 H4 O5 S	151.9779	152.9852	152.9837	152.9867
xanthine	C5 H4 N4 O2	152.0334	153.0407	153.0391	153.0422
cystamine	C4 H12 N2 S2	152.0442	153.0515	153.0499	153.0530
2-hydroxyphenylacetate	C8 H8 O3	152.0473	153.0546	153.0531	153.0561
3,4-dihydroxyphenylacetaldehyde	C8 H8 O3	152.0473	153.0546	153.0531	153.0561
3-hydroxyphenylacetate	C8 H8 O3	152.0473	153.0546	153.0531	153.0561
4-hydroxyphenylacetate	C8 H8 O3	152.0473	153.0546	153.0531	153.0561
arabitol	C5 H12 O5	152.0685	153.0757	153.0742	153.0773
ribitol	C5 H12 O5	152.0685	153.0757	153.0742	153.0773
xylitol	C5 H12 O5	152.0685	153.0757	153.0742	153.0773
thiocysteine	C3 H7 N O2 S2	152.9918	153.9991	153.9975	154.0006
3-sulfinoalanine	C3 H7 N O4 S	153.0096	154.0168	154.0153	154.0184
3-hydroxyanthranilate	C7 H7 N O3	153.0426	154.0499	154.0483	154.0514
dopamine	C8 H11 N O2	153.0790	154.0862	154.0847	154.0878
4-(β -acetylaminoethyl) imidazole	C7 H11 N3 O	153.0902	154.0975	154.0959	154.0990
propionyl phosphate	C3 H7 O5 P	154.0025	155.0098	155.0083	155.0114
3,4-dihydroxybenzoate	C7 H6 O4	154.0266	155.0339	155.0323	155.0354
imidazol-5-yl-pyruvate	C6 H6 N2 O3	154.0378	155.0451	155.0435	155.0466
N-methylethanolamine phosphate	C3 H10 N O4 P	155.0342	156.0414	156.0399	156.0430
2,5-dihydroxybenzoate	C7 H7 O4	155.0344	156.0417	156.0401	156.0433
histidine	C6 H9 N3 O2	155.0695	156.0767	156.0752	156.0783
2-phosphoglycolate	C2 H5 O6 P	155.9818	156.9891	156.9875	156.9906
methyl-CoM	C3 H8 O3 S2	155.9915	156.9987	156.9972	157.0003
orotic acid	C5 H4 N2 O4	156.0171	157.0244	157.0228	157.0259
5-ureido-4-imidazole carboxylate	C5 H6 N3 O3	156.0409	157.0482	157.0466	157.0497
4-imidazolone-5-propionate	C6 H8 N2 O3	156.0535	157.0607	157.0592	157.0623
imidazole lactate	C6 H8 N2 O3	156.0535	157.0607	157.0592	157.0623
3-indoleacetonitrile	C10 H8 N2	156.0687	157.0760	157.0744	157.0776
2-amino-muconate	C6 H7 N O4	157.0375	158.0448	158.0432	158.0463
2-hydroxymuconate	C6 H6 O5	158.0215	159.0288	159.0272	159.0304
4-methylene-2-oxoglutarate	C6 H6 O5	158.0215	159.0288	159.0272	159.0304
5-oxohex-2-enedioate	C6 H6 O5	158.0215	159.0288	159.0272	159.0304
allantoin	C4 H6 N4 O3	158.0440	159.0512	159.0496	159.0528
dimethylcitrate	C7 H10 O4	158.0579	159.0652	159.0636	159.0668
4-methylene glutamine	C6 H10 N2 O3	158.0691	159.0764	159.0748	159.0780
4-methylene glutamate	C6 H9 N O4	159.0531	160.0604	160.0588	160.0620
valine	C5 H11 N O2	159.0882	160.0955	160.0939	160.0971
5-acetamidopentanoate	C7 H13 N O3	159.0895	160.0968	160.0952	160.0984
2,3-diketo 4-dexoy-epi-inositol	C6 H8 O5	160.0372	161.0444	161.0428	161.0460
2-oxoadipate	C6 H8 O5	160.0372	161.0444	161.0428	161.0460
3,5/4-trihydroxycyclohexa-1,2-dione	C6 H8 O5	160.0372	161.0444	161.0428	161.0460
3-oxo-adipate	C6 H8 O5	160.0372	161.0444	161.0428	161.0460
5-dehydro-4-deoxy-D-glucuronate	C6 H8 O6	160.0372	161.0444	161.0428	161.0460

N-formiminoaspartate	C5 H8 N2 O4	160.0484	161.0557	161.0540	161.0573
allantoate	C4 H8 N4 O3	160.0596	161.0669	161.0653	161.0685
glycerol 3-P	C3 H9 O6 P	160.0621	161.0693	161.0677	161.0709
3-methyladipic acid	C7 H12 O4	160.0735	161.0808	161.0792	161.0824
indole acetaldehyde	C10 H10 N O	160.0762	161.0835	161.0819	161.0851
N-γ-acetyldiaminobutyrate	C6 H12 N2 O3	160.0848	161.0920	161.0904	161.0937
ala-ala		160.0848	161.0920	161.0904	161.0937
tryptamine	C10 H12 N2	160.1000	161.1073	161.1057	161.1089
N-formyl aspartate	C5 H7 N O5	161.0324	162.0397	162.0381	162.0413
4,6-dihydroxyquinoline	C9 H7 N O2	161.0477	162.0549	162.0533	162.0566
4,8-dihydroxyquinoline	C9 H7 N O2	161.0477	162.0549	162.0533	162.0566
α-aminoadipic acid	C6 H11 N O4	161.0688	162.0761	162.0744	162.0777
4-methyl glutamate	C6 H11 N O4	161.0688	162.0761	162.0744	162.0777
N-methyl glutamate	C6 H11 N O4	161.0688	162.0761	162.0744	162.0777
O-acetyl homoserine	C6 H11 N O4	161.0688	162.0761	162.0744	162.0777
indole-3-ethanol	C10 H11 N O	161.0841	162.0913	162.0897	162.0930
4-hydroxy-2-oxoglutarate	C5 H6 O6	162.0164	163.0237	163.0221	163.0253
1,2-dihydroxy-5-(methylthio) pent-1-en-3-one	C6 H10 O3 S	162.0351	163.0423	163.0407	163.0440
2,3-dimethylmalate	C6 H10 O5	162.0528	163.0601	163.0584	163.0617
2-ethylmalate	C6 H10 O5	162.0528	163.0601	163.0584	163.0617
3-ethylmalate	C6 H10 O5	162.0528	163.0601	163.0584	163.0617
rhamno-1,4-lactone	C6 H10 O5	162.0528	163.0601	163.0584	163.0617
gly-ser		162.0640	163.0713	163.0697	163.0729
safrole	C10 H10 O2	162.0681	163.0753	163.0737	163.0770
□□□□□□□□□□□□□□	C6 H14 N2 O3	162.1004	163.1077	163.1061	163.1093
N6-hydroxylysine	C6 H14 N2 O3	162.1004	163.1077	163.1061	163.1093
carnitine	C7 H16 N O3	162.1130	163.1203	163.1186	163.1219
nicotine	C10 H14 N2	162.1157	163.1230	163.1213	163.1246
N-acetylcysteine	C5 H9 N O3 S	163.0303	164.0376	164.0359	164.0392
erythro-4-hydroxyglutamate	C5 H9 N O5	163.0480	164.0553	164.0537	164.0570
3-methyldioxyindole	C9 H9 N O2	163.0633	164.0706	164.0690	164.0722
parapyruvate	C6 H8 O6	164.0321	165.0393	165.0377	165.0410
2-hydroxy-3-phenylpropenoate	C9 H8 O3	164.0473	165.0546	165.0530	165.0563
cinnamatedihydrodiol	C9 H8 O3	164.0473	165.0546	165.0530	165.0563
p-coumaric acid	C9 H8 O3	164.0473	165.0546	165.0530	165.0563
o-coumaric acid	C9 H8 O3	164.0473	165.0546	165.0530	165.0563
phenylpyruvate	C9 H8 O3	164.0473	165.0546	165.0530	165.0563
trans-3-hydroxycinnamate	C9 H8 O3	164.0473	165.0546	165.0530	165.0563
fuculose	C6 H12 O5	164.0685	165.0757	165.0741	165.0774
rhamnofuranose	C6 H12 O5	164.0685	165.0757	165.0741	165.0774
rhamnose	C6 H12 O5	164.0685	165.0757	165.0741	165.0774
rhamnulose	C6 H12 O5	164.0685	165.0757	165.0741	165.0774
formylanthranilate	C8 H7 N O3	165.0426	166.0499	166.0482	166.0515

methionine sulfoxide	C5 H11 N O3 S	165.0459	166.0532	166.0516	166.0549
phenylalanine	C9 H11 N O2	165.0790	166.0862	166.0846	166.0879
hordenine	C10 H15 N O	165.1154	166.1226	166.1210	166.1243
terephthalic acid	C8 H6 O4	166.0266	167.0339	167.0322	167.0355
arabinonate	C5 H10 O6	166.0477	167.0550	167.0533	167.0567
lyxonate	C5 H10 O6	166.0477	167.0550	167.0533	167.0567
xylonate	C5 H10 O6	166.0477	167.0550	167.0533	167.0567
2-hydroxyphenylpropanoate	C9 H10 O3	166.0630	167.0703	167.0686	167.0719
3-hydroxyphenylpropanoate	C9 H10 O3	166.0630	167.0703	167.0686	167.0719
3-methoxy-4-hydroxyphenylacetaldehyde	C9 H10 O3	166.0630	167.0703	167.0686	167.0719
phenylpropanoate-dihydrodiol	C9 H10 O3	166.0630	167.0703	167.0686	167.0719
pyridoxal	C8 H9 N O3	167.0582	168.0655	168.0638	168.0672
3-methoxyanthranilate	C8 H9 N O3	167.0582	168.0655	168.0638	168.0672
3-methoxytyramine	C9 H13 N O2	167.0946	168.1019	168.1002	168.1036
3-sulfopyruvate	C3 H4 O6 S	167.9728	168.9801	168.9784	168.9818
2-phosphoglycerate	C3 H5 O6 P	167.9818	168.9891	168.9874	168.9908
3-phosphoglycerate	C3 H5 O6 P	167.9818	168.9891	168.9874	168.9908
glyceraldehyde 3-P	C3 H5 O6 P	167.9818	168.9891	168.9874	168.9908
phosphoenolpyruvate	C3 H5 O6 P	167.9818	168.9891	168.9874	168.9908
butyryl-P	C4 H9 O5 P	168.0182	169.0255	169.0238	169.0272
uric acid	C5 H4 N4 O3	168.0283	169.0356	169.0339	169.0373
3,4-dihydroxymandelaldehyde	C8 H8 O4	168.0422	169.0495	169.0478	169.0512
3,4-dihydroxyphenylacetate	C8 H8 O4	168.0422	169.0495	169.0478	169.0512
homogentisate	C8 H8 O4	168.0422	169.0495	169.0478	169.0512
pyridoxamine	C8 H12 N2 O2	168.0899	169.0971	169.0954	169.0988
cysteic acid	C3 H7 N O5 S	169.0045	170.0117	170.0100	170.0134
2,3-dihydrodipicolinate	C7 H7 N O4	169.0375	170.0448	170.0431	170.0465
phosphodimethylethanolamine	C4 H12 N O4 P	169.0498	170.0571	170.0554	170.0588
pyridoxine	C8 H11 N O3	169.0739	170.0812	170.0795	170.0829
norepinephrine	C8 H11 N O3	169.0739	170.0812	170.0795	170.0829
3-methylhistidine	C7 H11 N3 O2	169.0851	170.0924	170.0907	170.0941
N-methylhistidine	C7 H11 N3 O2	169.0851	170.0924	170.0907	170.0941
glycerone phosphate	C3 H7 O6 P	169.9974	171.0047	171.0030	171.0064
thiourocanic acidq	C6 H6 N2 O2 S	170.0150	171.0223	171.0205	171.0240
3,4-dihydroxyphenylethyleneglycol	C8 H10 O4	170.0579	171.0652	171.0635	171.0669
2,3,4,5-tetrahydrodipicolinate	C7 H9 N O4	171.0531	172.0604	172.0587	172.0621
2-oxohept-3-enedioate	C7 H8 O5	172.0372	173.0444	173.0427	173.0462
hydantoin propionate	C6 H8 N2 O4	172.0484	173.0557	173.0539	173.0574
gly-pro		172.0848	173.0920	173.0903	173.0938
N-acetylglutamate semialdehyde	C7 H11 N O4	173.0688	174.0761	174.0743	174.0778
2-oxoarginine	C6 H11 N3 O3	173.0800	174.0873	174.0856	174.0890
aconitic acid	C6 H6 O6	174.0164	175.0237	175.0219	175.0254
dehydroascorbate	C6 H6 O6	174.0164	175.0237	175.0219	175.0254

shikimate	C7 H10 O5	174.0528	175.0601	175.0583	175.0618
N-forminoglutamate	C6 H10 N2 O4	174.0640	175.0713	175.0696	175.0731
indole-3-acetaldoxime	C10 H10 N2 O	174.0793	175.0866	175.0848	175.0883
indole-3-acetamide	C10 H10 N2 O	174.0793	175.0866	175.0848	175.0883
N-acetylornithine	C7 H14 N2 O3	174.1004	175.1077	175.1059	175.1094
arginine	C6 H14 N4 O2	174.1117	175.1189	175.1172	175.1207
N-methyltryptamine	C11 H14 N2	174.1157	175.1230	175.1212	175.1247
monodehydroascorbate	C6 H7 O6	175.0242	176.0315	176.0298	176.0333
2-amino-3-oxoadipate	C6 H9 N O5	175.0480	176.0553	176.0536	176.0571
N-acetylaspartate	C6 H9 N O5	175.0480	176.0553	176.0536	176.0571
N-formyl glutamate	C6 H9 N O5	175.0480	176.0553	176.0536	176.0571
indolyl-3-acetic acid	C10 H9 N O2	175.0633	176.0706	176.0688	176.0724
3-indoleglycolaldehyde	C10 H9 N O2	175.0633	176.0706	176.0688	176.0724
5-hydroxyindole acetaldehyde	C10 H9 N O2	175.0633	176.0706	176.0688	176.0724
N-acetyloxyindolyl	C10 H9 N O2	175.0633	176.0706	176.0688	176.0724
citrulline	C6 H13 N3 O3	175.0957	176.1029	176.1012	176.1047
ascorbic acid	C6 H8 O6	176.0321	177.0393	177.0376	177.0411
2-dehydro-glucono-1,5-lactone	C6 H8 O6	176.0321	177.0393	177.0376	177.0411
2-hydroxy-3-oxoadipate	C6 H8 O6	176.0321	177.0393	177.0376	177.0411
4,6-dihydroxy-2,5-dioxohexanoate	C6 H8 O6	176.0321	177.0393	177.0376	177.0411
galacturonolactone	C6 H8 O6	176.0321	177.0393	177.0376	177.0411
glucuronolactone	C6 H8 O6	176.0321	177.0393	177.0376	177.0411
xylo-hexulonolactone	C6 H8 O6	176.0321	177.0393	177.0376	177.0411
carbamyiaspartic acid	C5 H8 N2 O5	176.0433	177.0506	177.0488	177.0523
2-isopropylmalate	C7 H12 O5	176.0685	177.0757	177.0740	177.0775
2-propylmalate	C7 H12 O5	176.0685	177.0757	177.0740	177.0775
3-carboxy-3-hydroxyisocaproate	C7 H12 O5	176.0685	177.0757	177.0740	177.0775
3-isopropylmalate	C7 H12 O5	176.0685	177.0757	177.0740	177.0775
3-propylmalate	C7 H12 O5	176.0685	177.0757	177.0740	177.0775
gly-thr		176.0797	177.0870	177.0852	177.0887
ala-ser		176.0797	177.0870	177.0852	177.0887
serotonin	C10 H12 N2 O	176.0950	177.1022	177.1005	177.1040
N-formyl methionine	C6 H11 N O3 S	177.0459	178.0532	178.0514	178.0550
4-hydroxy-4-methylglutamate	C6 H11 N O5	177.0637	178.0710	178.0692	178.0728
cysteinylglycine	C5 H10 N2 O3 S	178.0412	179.0485	179.0467	179.0503
gly-cys		178.0412	179.0485	179.0467	179.0503
2-dehydro-3-deoxy-galactonate	C6 H10 O6	178.0477	179.0550	179.0532	179.0568
2-dehydro-3-deoxygluconate	C6 H10 O6	178.0477	179.0550	179.0532	179.0568
2-dehydro-3-deoxy-rhamnonate	C6 H10 O6	178.0477	179.0550	179.0532	179.0568
2-dehydro-glucose	C6 H10 O6	178.0477	179.0550	179.0532	179.0568
2-dexoy-5-keto gluconic acid	C6 H10 O6	178.0477	179.0550	179.0532	179.0568
2-inosose	C6 H10 O6	178.0477	179.0550	179.0532	179.0568

3-keto-β-galactose	C6 H10 O6	178.0477	179.0550	179.0532	179.0568
galactono-1,4-lactone	C6 H10 O6	178.0477	179.0550	179.0532	179.0568
glucono-1,5-lactone	C6 H10 O6	178.0477	179.0550	179.0532	179.0568
gulono-1,4-lactone	C6 H10 O6	178.0477	179.0550	179.0532	179.0568
quinolinate	C8 H5 N O4	179.0218	180.0291	180.0273	180.0309
cysteine (S-carboxymethyl)	C5 H9 N O4 S	179.0252	180.0325	180.0307	180.0343
hippuric acid	C9 H9 N O3	179.0582	180.0655	180.0637	180.0673
glucosamine	C6 H13 N O5	179.0793	180.0866	180.0848	180.0884
2-hydroxy-3-(4-hydroxyphenyl) propenoate	C9 H8 O4	180.0422	181.0495	181.0477	181.0513
4-hydroxyphenylpyruvate	C9 H8 O4	180.0422	181.0495	181.0477	181.0513
trans-2,3-dihydroxycinnamate	C9 H8 O4	180.0422	181.0495	181.0477	181.0513
5-methylthio ribose	C6 H12 O4 S	180.0456	181.0529	181.0511	181.0547
galactose	C6 H12 O6	180.0634	181.0706	181.0688	181.0724
glucose	C6 H12 O6	180.0634	181.0706	181.0688	181.0724
inositol	C6 H12 O6	180.0634	181.0706	181.0688	181.0724
fructose	C6 H12 O6	180.0634	181.0706	181.0688	181.0724
fuconate	C6 H12 O6	180.0634	181.0706	181.0688	181.0724
mannose	C6 H12 O6	180.0634	181.0706	181.0688	181.0724
mesoinositol	C6 H12 O6	180.0634	181.0706	181.0688	181.0724
rhamnonate	C6 H12 O6	180.0634	181.0706	181.0688	181.0724
sorbose	C6 H12 O6	180.0634	181.0706	181.0688	181.0724
tagatose	C6 H12 O6	180.0634	181.0706	181.0688	181.0724
theophylline	C7 H8 N4 O2	180.0647	181.0720	181.0702	181.0738
3-hydroxykynurenamine	C9 H12 N2 O2	180.0899	181.0971	181.0953	181.0989
5-hydroxykynurenamine	C9 H12 N2 O2	180.0899	181.0971	181.0953	181.0989
4-hydroxymandelonitrile	C8 H7 N O4	181.0375	182.0448	182.0429	182.0466
tyrosine	C9 H11 N O3	181.0739	182.0812	182.0793	182.0830
β-tyrosine	C9 H11 N O3	181.0739	182.0812	182.0793	182.0830
O-phosphocholine	C5 H13 N O4 P	182.0576	183.0649	183.0631	183.0668
2,3-dihydroxyphenylpropanoate	C9 H10 O4	182.0579	183.0652	183.0633	183.0670
3-methoxy-4-hydroxyphenylacetate	C9 H10 O4	182.0579	183.0652	183.0633	183.0670
3-methoxy-4-hydroxyphenylglycolaldehyde	C9 H10 O4	182.0579	183.0652	183.0633	183.0670
4-hydroxyphenyllactate	C9 H10 O4	182.0579	183.0652	183.0633	183.0670
homovanillate	C9 H10 O4	182.0579	183.0652	183.0633	183.0670
galactitol	C6 H14 O6	182.0790	183.0863	183.0845	183.0881
mannitol	C6 H14 O6	182.0790	183.0863	183.0845	183.0881
sorbitol	C6 H14 O6	182.0790	183.0863	183.0845	183.0881
saccharin	C7 H5 N O3 S	182.9990	184.0063	184.0044	184.0081
piperidine-2,6-dicarboxylate	C8 H9 N O4	183.0531	184.0604	184.0586	184.0623
colinephosphoric acid	C5 H14 N O4 P	183.0655	184.0727	184.0709	184.0746
epinephrine	C9 H13 N O3	183.0895	184.0968	184.0950	184.0986
normetanephrine	C9 H13 N O3	183.0895	184.0968	184.0950	184.0986
3-P-hydroxypyruvate	C3 H5 O7 P	183.9767	184.9840	184.9821	184.9858

5-hydroxyisourate	C5 H4 N4 O4	184.0232	185.0305	185.0286	185.0323
3,4-dihydroxymandelate	C8 H8 O5	184.0372	185.0444	185.0426	185.0463
phosphorylcholine	C5 H15 N O4 P	184.0733	185.0806	185.0787	185.0824
3-methoxy-4-hydroxyphenylethyleneglycol	C9 H12 O4	184.0735	185.0808	185.0790	185.0827
3-P-serine	C3 H8 N O6 P	185.0083	186.0156	186.0138	186.0175
2-amino-3-carboxy-muconate semialdehyde	C7 H7 N O5	185.0324	186.0397	186.0378	186.0415
3-fumarylpyruvate	C7 H6 O6	186.0164	187.0237	187.0218	187.0256
ala-pro		186.1004	187.1077	187.1058	187.1096
thiohistidine	C6 H9 N3 O2 S	187.0415	188.0488	188.0469	188.0507
2-oxo-6-acetoamidocaproate	C8 H13 N O4	187.0844	188.0917	188.0898	188.0936
N2-acetylamino adipate semialdehyde	C8 H13 N O4	187.0844	188.0917	188.0898	188.0936
3-dehydroshikimate	C7 H8 O6	188.0321	189.0393	189.0374	189.0412
But-2-ene-1,2,3-tricarboxylate	C7 H8 O6	188.0321	189.0393	189.0374	189.0412
homo-cis-aconitate	C7 H8 O6	188.0321	189.0393	189.0374	189.0412
hyp-gly		188.0797	189.0870	189.0851	189.0888
N-acetyl-lysine	C8 H16 N2 O3	188.1161	189.1233	189.1215	189.1252
gly-leu		188.1161	189.1233	189.1215	189.1252
gly-ile		188.1161	189.1233	189.1215	189.1252
n,n-dimethyltryptamine	C12 H16 N2	188.1313	189.1386	189.1367	189.1405
N6,N6,N6-trimethyllysine	C9 H20 N2 O2 +	188.1525	189.1597	189.1578	189.1616
isocitric acid	C6 H5 O7	189.0035	190.0108	190.0089	190.0127
kynurenate	C10 H7 N O3	189.0426	190.0499	190.0480	190.0518
N-acetylisatin	C10 H7 N O3	189.0426	190.0499	190.0480	190.0518
2-amino-6-oxoheptanedioate	C7 H11 N O5	189.0637	190.0710	190.0691	190.0729
N-acetyl-glutamate	C7 H11 N O5	189.0637	190.0710	190.0691	190.0729
gly-gly-gly		189.0749	190.0822	190.0803	190.0841
gly-asn		189.0749	190.0822	190.0803	190.0841
oxalosuccinate	C6 H6 O7	190.0113	191.0186	191.0167	191.0205
2,4-dihydroxyhept-2-enedioate	C7 H10 O6	190.0477	191.0550	191.0531	191.0569
2-hydroxyhepta-2,4-dienedioate	C7 H10 O6	190.0477	191.0550	191.0531	191.0569
3-dehydroquinate	C7 H10 O6	190.0477	191.0550	191.0531	191.0569
N-carbamylglutamate	C6 H10 N2 O5	190.0589	191.0662	191.0643	191.0681
gly-asp		190.0589	191.0662	191.0643	191.0681
2,6-diaminoheptanedioate	C7 H14 N2 O4	190.0953	191.1026	191.1007	191.1045
ala-thr		190.0953	191.1026	191.1007	191.1045
N-(ω)-hydroxyarginine	C6 H14 N4 O3	190.1066	191.1138	191.1119	191.1157
5-methoxytryptamine	C11 H14 N2 O	190.1106	191.1179	191.1160	191.1198
N-methylserotonin	C11 H14 N2 O	190.1106	191.1179	191.1160	191.1198
5-hydroxy-indole acetate	C10 H9 N O3	191.0582	192.0655	192.0636	192.0674
citric acid	C6 H8 O7	192.0270	193.0342	193.0323	193.0362
2,3-dioxogulonate	C6 H8 O7	192.0270	193.0342	193.0323	193.0362
2-dehydro-3-deoxy-D-glucarate	C6 H8 O7	192.0270	193.0342	193.0323	193.0362

4,5,6-trihydroxy-2,3-dioxohexanoate	C6 H8 O7	192.0270	193.0342	193.0323	193.0362
5-dehydro-4-deoxy-D-glucarate	C6 H8 O7	192.0270	193.0342	193.0323	193.0362
ala-cys		192.0568	193.0641	193.0622	193.0660
quinat	C7 H12 O6	192.0634	193.0706	193.0687	193.0726
ser-ser		192.0746	193.0819	193.0799	193.0838
O-acetylcarnitine	C8 H18 N O4	192.1236	193.1308	193.1289	193.1328
5,6-dihydroxyindole-2-carboxylate	C9 H7 N O4	193.0375	194.0448	194.0428	194.0467
L-dopachrome	C9 H7 N O4	193.0375	194.0448	194.0428	194.0467
homocysteine (S-carboxymethyl)	C6 H11 N O4 S	193.0409	194.0481	194.0462	194.0501
phenylacetyl glycine	C10 H11 N O3	193.0739	194.0812	194.0792	194.0831
2-dehydro-gluconate	C6 H10 O7	194.0426	195.0499	195.0479	195.0518
3-dehydro-L-gulonate	C6 H10 O7	194.0426	195.0499	195.0479	195.0518
fructuronate	C6 H10 O7	194.0426	195.0499	195.0479	195.0518
galacturonate	C6 H10 O7	194.0426	195.0499	195.0479	195.0518
glucuronate	C6 H10 O7	194.0426	195.0499	195.0479	195.0518
1-O-methyl-myo-inositol	C7 H14 O6	194.0790	195.0863	195.0843	195.0882
3-O-methyl-myo-inositol	C7 H14 O6	194.0790	195.0863	195.0843	195.0882
caffeine	C8 H10 N4 O2	194.0804	195.0876	195.0857	195.0896
2-carboxy-2,3-dihydro-5,6-dihydroxyindole	C9 H9 N O4	195.0531	196.0604	196.0585	196.0624
dopaquinone	C9 H9 N O4	195.0531	196.0604	196.0585	196.0624
glucosaminat	C6 H13 N O6	195.0743	196.0815	196.0796	196.0835
3-(3,4-dihydroxyphenyl) pyruvat	C9 H8 O5	196.0372	197.0444	197.0425	197.0464
altronate	C6 H12 O7	196.0583	197.0655	197.0636	197.0675
galactonat	C6 H12 O7	196.0583	197.0655	197.0636	197.0675
gluconat	C6 H12 O7	196.0583	197.0655	197.0636	197.0675
gulonat	C6 H12 O7	196.0583	197.0655	197.0636	197.0675
mannonat	C6 H12 O7	196.0583	197.0655	197.0636	197.0675
tagaturonat	C6 H10 O7	196.0583	197.0655	197.0636	197.0675
guanidino-acetat-P	C3 H8 N3 O5 P	197.0196	198.0268	198.0249	198.0288
dihydroxy-phenylalanine	C9 H11 N O4	197.0688	198.0761	198.0741	198.0780
L-Dopa	C9 H11 N O4	197.0688	198.0761	198.0741	198.0780
N-hydroxytyrosine	C9 H11 N O4	197.0688	198.0761	198.0741	198.0780
metanephrine	C10 H15 N O3	197.1052	198.1125	198.1105	198.1144
erythrose 4--P	C4 H7 O7 P	197.9924	198.9996	198.9976	199.0016
O-phosphohomoserine	C4 H9 N O6 P	198.0162	199.0234	199.0215	199.0254
3-(3,4-dihydroxyphenyl) lactate	C9 H10 O5	198.0528	199.0601	199.0581	199.0621
3-methoxy-4-hydroxymandelat	C9 H10 O5	198.0528	199.0601	199.0581	199.0621
hercynine	C9 H16 N3 O2	198.1242	199.1315	199.1295	199.1335
2-hydroxy-5-carboxymethylmuconat	C8 H8 O6	200.0321	201.0393	201.0373	201.0413
4-maleylacetoacetat	C8 H8 O6	200.0321	201.0393	201.0373	201.0413
S-sulfocysteine	C3 H7 N O5 S2	200.9765	201.9838	201.9818	201.9858
5-hydroxy-2-oxo-4-ureido-2,5-dihydro-1H-imidazole-5-carboxylate	C5 H6 N4 O5	202.0338	203.0411	203.0390	203.0431

ser-pro		202.0953	203.1026	203.1006	203.1046
hyp-ala		202.0953	203.1026	203.1006	203.1046
ala-leu		202.1317	203.1390	203.1370	203.1410
ala-ile		202.1317	203.1390	203.1370	203.1410
spermine	C10 H26 N4	202.2157	203.2230	203.2210	203.2250
8-methoxykynurenate	C11 H9 N O3	203.0582	204.0655	204.0635	204.0675
N2-acetylaminoadipate	C8 H13 N O5	203.0793	204.0866	204.0846	204.0887
gly-gly-ala		203.0906	204.0979	204.0958	204.0999
gly-gln		203.0906	204.0979	204.0958	204.0999
ala-asn		203.0906	204.0979	204.0958	204.0999
gly-lys		203.1270	204.1342	204.1322	204.1363
oxaloglutarate	C7 H8 O7	204.0270	205.0342	205.0322	205.0363
1,4-dihydroxy-2-naphthoate	C11 H8 O4	204.0422	205.0495	205.0475	205.0516
indole pyruvate	C11H10 N O3	204.0661	205.0733	205.0713	205.0754
gly-glu		204.0746	205.0819	205.0798	205.0839
ala-asp		204.0746	205.0819	205.0798	205.0839
tryptophan	C11 H12 N2 O2	204.0899	205.0971	205.0951	205.0992
N6-acetyl-N6-hydroxylysine	C8 H16 N2 O4	204.1110	205.1183	205.1162	205.1203
bufotenine	C12 H16 N2 O	204.1263	205.1335	205.1315	205.1356
6-methoxykynurenate	C10 H7 N O4	205.0375	206.0448	206.0427	206.0468
thioctic acid amide	C8 H15 N O S2	205.0595	206.0668	206.0647	206.0688
5-methoxyindoleacetate	C11 H11 N O3	205.0739	206.0812	206.0791	206.0832
pantothenol	C9 H19 N O4	205.1314	206.1387	206.1366	206.1407
3-hydroxy-N6,N6,N6-trimethyllysine	C9 H21 N2 O3 +	205.1552	206.1625	206.1604	206.1645
3-oxolomalate	C6 H6 O8	206.0062	207.0135	207.0114	207.0156
2-methylcitrate	C7 H10 O7	206.0426	207.0499	207.0478	207.0520
homocitrate	C7 H10 O7	206.0426	207.0499	207.0478	207.0520
homoisocitrate	C7 H10 O7	206.0426	207.0499	207.0478	207.0520
lipoic acid	C8 H14 O2 S2	206.0435	207.0508	207.0487	207.0529
xanthurenate	C10 H8 N O4	206.0453	207.0526	207.0505	207.0547
gly-met		206.0725	207.0798	207.0777	207.0818
ser-thr		206.0902	207.0975	207.0954	207.0996
ibuprofen	C13 H18 O2	206.1307	207.1379	207.1359	207.1400
2-formaminobenzoylacetate	C10 H9 N O4	207.0531	208.0604	208.0583	208.0625
4-(2-aminophenyl)-2,4-dioxobutanoate	C10 H9 N O4	207.0531	208.0604	208.0583	208.0625
indole acetate	C10 H9 N O2	207.0531	208.0604	208.0583	208.0625
dihydrolipoamide	C8 H17 N O S2	207.0751	208.0824	208.0803	208.0845
N-acetylphenylalanine	C11 H13 N O3	207.0895	208.0968	208.0947	208.0989
ser-cys		208.0518	209.0590	209.0569	209.0611
dihydrolipoic acid	C8 H16 O2 S2	208.0592	209.0664	209.0643	209.0685
formyl-5-hydroxykynurenamine	C10 H12 N2 O3	208.0848	209.0920	209.0900	209.0941
kynurenine	C10 H12 N2 O3	208.0848	209.0920	209.0900	209.0941

4-hydroxyphenylacetyl glycine	C10 H11 N O4	209.0688	210.0761	210.0740	210.0782
galactarate	C6 H10 O8	210.0375	211.0448	211.0427	211.0469
glucarate	C6 H10 O8	210.0375	211.0448	211.0427	211.0469
creatine-P	C4 H10 N3 O5 P	211.0352	212.0425	212.0404	212.0446
5-(2'-formylethyl)-4,6-dihydroxypicolinate	C9 H9 N O5	211.0480	212.0553	212.0532	212.0574
4-aspartyl-P	C4 H7 N O7 P	211.9954	213.0027	213.0006	213.0048
isophenoxazine	C12 H8 N2 O2	212.0586	213.0658	213.0637	213.0680
gly-his		212.0909	213.0982	213.0961	213.1003
pro-pro		212.1161	213.1233	213.1212	213.1255
indoxylsulfuric acid	C8 H7 N O4 S	213.0096	214.0168	214.0147	214.0190
1-deoxy xylulose 5-phosphate	C5 H11 O7 P	214.0237	215.0309	215.0288	215.0331
2-deoxyribose 1-phosphate	C5 H11 O7 P	214.0237	215.0309	215.0288	215.0331
2-deoxy-ribose-5-phosphate	C5 H11 O7 P	214.0237	215.0309	215.0288	215.0331
glutamyl-P	C4 H10 N O7 P	215.0189	216.0262	216.0240	216.0283
glycero-3-phosphoethanolamine	C5 H14 N O6 P	215.0553	216.0626	216.0604	216.0647
5-carboxy-2-oxohept-3-enedioate	C8 H8 O7	216.0270	217.0342	217.0321	217.0364
5-carboxymethyl-2-hydroxymuconate	C8 H8 O7	216.0270	217.0342	217.0321	217.0364
gly-val		216.1096	217.1169	217.1147	217.1191
pro-thr		216.1110	217.1183	217.1161	217.1204
3-methylindolepyruvate	C12 H11 N O3	217.0739	218.0812	218.0790	218.0833
gly-ala-ala		217.1062	218.1135	218.1113	218.1157
ala-gln		217.1062	218.1135	218.1113	218.1157
ala-lys		217.1426	218.1499	218.1477	218.1521
pro-cys		218.0725	219.0798	219.0776	219.0820
ala-glu		218.0902	219.0975	219.0953	219.0997
hyp-ser		218.0902	219.0975	219.0953	219.0997
N-acetylserotonin	C12 H14 N2 O2	218.1055	219.1128	219.1106	219.1150
lysopine	C9 H18 N2 O4	218.1266	219.1339	219.1317	219.1361
ser-leu		218.1266	219.1339	219.1317	219.1361
ser-ile		218.1266	219.1339	219.1317	219.1361
histidinol-P	C6 H10 N3 O4 P	219.0403	220.0476	220.0454	220.0498
5-hydroxyindolepyruvate	C11 H9 N O4	219.0531	220.0604	220.0582	220.0626
O-succinylhomoserine	C8 H13 N O6	219.0743	220.0815	220.0793	220.0837
gly-gly-ser		219.0855	220.0928	220.0906	220.0950
ser-asn		219.0855	220.0928	220.0906	220.0950
pantothenic acid	C9 H17 N O5	219.1106	220.1179	220.1157	220.1201
imidazole acetol-P	C6 H9 N2 O5 P	220.0243	221.0316	221.0294	221.0338
ser-asp		220.0695	221.0768	221.0746	221.0790
N-acetylmannosamine	C8 H15 N O6	220.0821	221.0894	221.0871	221.0916
5-hydroxytryptophan	C11 H12 N2 O3	220.0848	221.0920	221.0898	221.0943
N-formulkynurenine	C11 H12 N2 O4	220.0848	221.0920	221.0898	221.0943
ala-met		220.0881	221.0954	221.0932	221.0976

thr-thr		220.1059	221.1132	221.1110	221.1154
7,8-dihydroxykynurenate	C10 H7 N O5	221.0324	222.0397	222.0375	222.0419
6-hydroxyindolelactate	C11 H11 N O4	221.0688	222.0761	222.0738	222.0783
indolyl-3-lactic acid	C11 H11 N O4	221.0688	222.0761	222.0738	222.0783
N-acetyl glucosamine	C8 H15 N O6	221.0899	222.0972	222.0950	222.0994
2-succinylbenzoate	C11 H10 O5	222.0528	223.0601	223.0578	223.0623
cystathionine	C7 H14 N2 O4 S	222.0674	223.0747	223.0724	223.0769
thr-cys		222.0674	223.0747	223.0724	223.0769
gly-phe		222.1004	223.1077	223.1055	223.1099
4-(2-amino-3-hydroxyphenyl)-2,4-dioxobutanoate	C10 H9 N O5	223.0480	224.0553	224.0531	224.0576
4(2-amino-5-hydroxyphenyl)-2,4-dioxobutanoate	C10 H9 N O5	223.0480	224.0553	224.0531	224.0576
7,8-dihydro-7,8-dihydroxykynurenate	C10 H9 N O5	223.0480	224.0553	224.0531	224.0576
cys-cys		224.0289	225.0362	225.0339	225.0384
3-hydroxy-kynurenine	C10 H12 N2 O4	224.0797	225.0870	225.0847	225.0892
5-hydroxykynurenine	C10 H12 N2 O4	224.0797	225.0870	225.0847	225.0892
chorismate	C10 H10 O6	226.0477	227.0550	227.0527	227.0573
isochorismate	C10 H10 O6	226.0477	227.0550	227.0527	227.0573
prephenate	C10 H10 O6	226.0477	227.0550	227.0527	227.0573
porphobilinogen	C10 H14 N2 O4	226.0953	227.1026	227.1003	227.1049
carosine	C9 H14 N4 O3	226.1066	227.1138	227.1116	227.1161
ala-his		226.1066	227.1138	227.1116	227.1161
serine phosphoethanolamine	C5 H13 N2 O6 P	227.0427	228.0500	228.0477	228.0523
5-(2'-carboxyethyl)-4,6-dihydroxypicolinate	C9 H9 N O6	227.0430	228.0502	228.0480	228.0525
stizolobinate	C9 H9 N O6	227.0430	228.0502	228.0480	228.0525
2'-deoxy-cytidine	C9 H13 N3 O4	227.0906	228.0979	228.0956	228.1001
(4-aminophenyl)-1,2,3,4-tetrahydroxypentane	C11 H17 N O4	227.1157	228.1230	228.1207	228.1253
ribose 5-P	C5 H9 O8 P	228.0029	229.0102	229.0079	229.0125
ribulose 5-P	C5 H9 O8 P	228.0029	229.0102	229.0079	229.0125
xylulose 5-P	C5 H9 O8 P	228.0029	229.0102	229.0079	229.0125
deoxyuridine	C9 H12 N2 O5	228.0746	229.0819	229.0796	229.0842
hyp-pro		228.1110	229.1183	229.1160	229.1205
pro-leu		228.1474	229.1546	229.1524	229.1569
pro-ile		228.1474	229.1546	229.1524	229.1569
4-(alanin-3-yl)-2-hydroxy-cis,cis-muconate 6-semialdehyde	C9 H11 N O6	229.0586	230.0659	230.0636	230.0682
5-(alanin-3-yl)-2-hydroxy-cis,cis-muconate 6-semialdehyde	C9 H11 N O6	229.0586	230.0659	230.0636	230.0682
ergothioneine	C9 H15 N3 O2 S	229.0885	230.0958	230.0935	230.0981
gly-gly-pro		229.1062	230.1135	230.1112	230.1158
pro-asn		229.1062	230.1135	230.1112	230.1158
ribose 1-phosphate	C5 H11 O8 P	230.0186	231.0258	231.0235	231.0282
xylulose 1-P	C5 H11 O8 P	230.0186	231.0258	231.0235	231.0282

α-xylose 1-phosphate	C5 H11 O8 P	230.0186	231.0258	231.0235	231.0282
pro-asp		230.0902	231.0975	231.0952	231.0998
ala-val		230.1253	231.1326	231.1302	231.1349
N-succinylglutamate 5-semialdehyde	C9 H13 N O6	231.0743	232.0815	232.0792	232.0839
ala-ala-ala		231.1219	232.1292	232.1268	232.1315
gly-arg		231.1331	232.1404	232.1381	232.1427
ribitol-5-phosphate	C5 H13 O8 P	232.0342	233.0415	233.0392	233.0438
N2-succinylornithine	C9 H16 N2 O5	232.1059	233.1132	233.1108	233.1155
N6-acetyl-2,6-diaminoheptanedioate	C9 H16 N2 O5	232.1059	233.1132	233.1108	233.1155
hyp-thr		232.1059	233.1132	233.1108	233.1155
melatonin	C13 H16 N2 O2	232.1212	233.1284	233.1261	233.1308
thr-leu		232.1423	233.1496	233.1472	233.1519
thr-ile		232.1423	233.1496	233.1472	233.1519
gly-gly-thr		233.1011	234.1084	234.1061	234.1108
gly-ala-ser		233.1011	234.1084	234.1061	234.1108
ser-gln		233.1011	234.1084	234.1061	234.1108
thr-asn		233.1011	234.1084	234.1061	234.1108
ser-lys		233.1375	234.1448	234.1425	234.1471
hyp-cys		234.0674	235.0747	235.0723	235.0770
ser-glu		234.0852	235.0924	235.0901	235.0948
thr-asp		234.0852	235.0924	235.0901	235.0948
cys-leu		234.1038	235.1111	235.1087	235.1134
cys-ile		234.1038	235.1111	235.1087	235.1134
gly-gly-cys		235.0626	236.0699	236.0676	236.0723
cys-asn		235.0626	236.0699	236.0676	236.0723
D-erythro-imidazole-glycerol-P	C6 H9 N2 O6 P	236.0192	237.0265	237.0241	237.0289
cys-asp		236.0467	237.0539	237.0516	237.0563
formylkynurenine	C11 H12 N2 O4	236.0797	237.0870	237.0846	237.0893
ser-met		236.0831	237.0903	237.0880	237.0927
ala-phe		236.1161	237.1233	237.1210	237.1257
6-pyruvoyltetrahydropterin	C9 H11 N5 O3	237.0862	238.0934	238.0911	238.0958
erythro-1-(imidazol-4-yl) glycerol 3-phosphate	C6 H11 N2 O6 P	238.0349	239.0422	239.0398	239.0446
gly-tyr		238.0953	239.1026	239.1002	239.1050
5-P-β-ribosylamine	C6 H10 N O7 P	239.0189	240.0262	240.0238	240.0286
cystine	C6 H12 N2 O4 S2	240.0238	241.0311	241.0287	241.0335
homocarnosine	C10 H16 N4 O3	240.1222	241.1295	241.1271	241.1319
anserine	C10 H16 N4 O3	240.1222	241.1295	241.1271	241.1319
16-hexadecanal	C16 H32 O	240.2453	241.2526	241.2502	241.2550
diphosphoglyceric acid	C3 H3 O10 P2	241.0006	242.0079	242.0055	242.0103
5,6,7,8-tetrahydrobiopterin	C9 H15 N5 O3	241.1175	242.1247	242.1223	242.1272
2,3-diketo-5-methylthiopentyl-1-phosphate	C6 H11 O6 S P	242.0008	243.0081	243.0057	243.0105
2-hydroxy-3-keto-5-methylthiopentyl-1-phosphate	C6 H11 O6 S P	242.0008	243.0081	243.0057	243.0105

5-phosphono-oxy-lysine	C6 H15 N2 O6 P	242.0662	243.0735	243.0710	243.0759
thymidine	C10 H14 N2 O5	242.0902	243.0975	243.0951	243.0999
ser-his		242.1015	243.1087	243.1063	243.1112
16-hexadecanol	C16 H34 O	242.2610	243.2682	243.2658	243.2707
cytidine	C9 H13 N3 O5	243.0855	244.0928	244.0903	244.0952
gly-ala-pro		243.1219	244.1292	244.1267	244.1316
pro-gln		243.1219	244.1292	244.1267	244.1316
pro-lys		243.1583	244.1655	244.1631	244.1680
fucose-1P	C6 H13 O8 P	244.0342	245.0415	245.0390	245.0439
fuculose-1P	C6 H13 O8 P	244.0342	245.0415	245.0390	245.0439
mevalonate-5-P	C6 H13 O8 P	244.0342	245.0415	245.0390	245.0439
rhamnulose-1P	C6 H13 O8 P	244.0342	245.0415	245.0390	245.0439
pseudouridine	C9 H12 N2 O6	244.0695	245.0768	245.0743	245.0792
uridine	C9 H12 N2 O6	244.0695	245.0768	245.0743	245.0792
biotin	C10 H16 N2 O3 S	244.0881	245.0954	245.0930	245.0979
pro-glu		244.1059	245.1132	245.1107	245.1156
hyp-hyp		244.1059	245.1132	245.1107	245.1156
hyp-leu		244.1423	245.1496	245.1471	245.1520
hyp-ile		244.1423	245.1496	245.1471	245.1520
leu-leu		244.1787	245.1859	245.1835	245.1884
leu-ile		244.1787	245.1859	245.1835	245.1884
ile-ile		244.1787	245.1859	245.1835	245.1884
hyp-asn		245.1011	246.1084	246.1060	246.1109
gly-gly-leu		245.1375	246.1448	246.1423	246.1473
gly-gly-ile		245.1375	246.1448	246.1423	246.1473
leu-asn		245.1375	246.1448	246.1423	246.1473
ile-asn		245.1375	246.1448	246.1423	246.1473
ala-arg		245.1488	246.1560	246.1536	246.1585
dimethylallyl-PP	C5 H12 O7 P2	246.0047	247.0120	247.0095	247.0144
isopentenyl-PP	C5 H12 O7 P2	246.0047	247.0120	247.0095	247.0144
phosphatidyl glycerol	C6 H15 O8 P	246.0499	247.0571	247.0547	247.0596
hyp-asp		246.0852	247.0924	247.0900	247.0949
gly-gly-asn		246.0964	247.1037	247.1012	247.1061
asn-asn		246.0964	247.1037	247.1012	247.1061
pro-met		246.1038	247.1111	247.1086	247.1135
ser-val		246.1202	247.1275	247.1250	247.1299
leu-asp		246.1215	247.1288	247.1263	247.1313
ile-asp		246.1215	247.1288	247.1263	247.1313
octopine	C9 H18 N4 O4	246.1328	247.1400	247.1376	247.1425
2-C-methyl erythritol 4-phosphate	C5 H13 O9 P	247.0213	248.0286	248.0261	248.0311
N-succinylglutamate	C9 H13 N O7	247.0692	248.0764	248.0740	248.0789
gly-gly-asp		247.0804	248.0877	248.0852	248.0902

asn-asp		247.0804	248.0877	248.0852	248.0902
gly-ala-thr		247.1168	248.1241	248.1216	248.1265
ala-ala-ser		247.1168	248.1241	248.1216	248.1265
thr-gln		247.1168	248.1241	248.1216	248.1265
thr-lys		247.1532	248.1605	248.1580	248.1629
asp-asp		248.0644	249.0717	249.0692	249.0742
5-hydroxyindoleacetyl glycine	C12 H12 N2 O4	248.0797	249.0870	249.0845	249.0894
thr-glu		248.1008	249.1081	249.1056	249.1106
6-hydroxymelatonin	C13 H16 N2 O3	248.1161	249.1233	249.1209	249.1258
abscisic aldehyde	C15 H20 O3	248.1412	249.1485	249.1460	249.1510
linatine	C10 H7 N3 O5	249.0385	250.0458	250.0433	250.0483
gly-ala-cys		249.0783	250.0856	250.0831	250.0881
cys-gln		249.0783	250.0856	250.0831	250.0881
6-S-Acetyldihydrolipoamide	C10 H19 N O2 S2	249.0857	250.0930	250.0905	250.0955
gly-ser-ser		249.0960	250.1033	250.1008	250.1058
cys-lys		249.1147	250.1220	250.1195	250.1245
cys-glu		250.0623	251.0696	251.0671	251.0721
γ-glutamylcysteine	C8 H14 N2 O5 S	250.0623	251.0696	251.0671	251.0721
thr-met		250.0987	251.1060	251.1035	251.1085
abscisic alcohol	C15 H22 O3	250.1569	251.1642	251.1616	251.1667
xanthoxin	C15 H22 O3	250.1569	251.1642	251.1616	251.1667
deoxyadenosine	C10 H13 N5 O3	251.1018	252.1091	252.1066	252.1116
shikimate-5-P	C7 H9 O8 P	252.0029	253.0102	253.0077	253.0127
cys-met		252.0602	253.0675	253.0650	253.0700
5-hydroxy-N-formylkynurenine	C11 H12 N2 O5	252.0746	253.0819	253.0793	253.0844
deoxyinosine	C10 H12 N4 O4	252.0858	253.0931	253.0906	253.0956
ala-tyr		252.1110	253.1183	253.1157	253.1208
ser-phe		252.1110	253.1183	253.1157	253.1208
pro-his		252.1222	253.1295	253.1270	253.1320
5-(3'-carboxy-3'-oxopropenyl)-4,6-dihydroxypicolinate	C10 H7 N O7	253.0222	254.0295	254.0270	254.0320
N-acetyl-glutamyl-P	C7 H12 N O7 P	253.0346	254.0418	254.0393	254.0444
cysteine-homocystein disulfide	C7 H14 N2 O4 S2	254.0395	255.0467	255.0442	255.0493
arginine-P	C6 H15 N4 O5 P	254.0774	255.0847	255.0821	255.0872
galactosylglycerol	C9 H18 O8	254.1001	255.1074	255.1049	255.1100
5-(3'-carboxy-3'-oxopropyl)-4,6-dihydroxypicolinate	C10 H9 N O7	255.0379	256.0451	256.0426	256.0477
2-amino-4-hydroxy-6-(erythro)-trihydroxypropyl-dihydropteridine	C9 H13 N5 O4	255.0967	256.1040	256.1014	256.1066
2-dehydro-3-deoxy-6-P-gluconate	C6 H9 O9 P	255.9978	257.0051	257.0025	257.0077
6-P glucono-1,5-lactone	C6 H9 O9 P	255.9978	257.0051	257.0025	257.0077
thr-his		256.1171	257.1244	257.1218	257.1270
pro-val		256.1409	257.1482	257.1456	257.1508

palmitic acid	C16 H32 O2	256.2402	257.2475	257.2449	257.2501
glucosamine 6-P	C6 H12 N O8 P	257.0295	258.0367	258.0342	258.0393
ala-ala-pro		257.1375	258.1448	258.1422	258.1474
2-dehydro-3-dexoy galactonate 6-P	C6 H11 O9 P	258.0135	259.0208	259.0182	259.0233
2-deoxy-5-keto gluconic acid 6-phosphate	C6 H11 O9 P	258.0135	259.0208	259.0182	259.0233
3-oxo-6-P-hexulose	C6 H11 O9 P	258.0135	259.0208	259.0182	259.0233
fructose 6-P	C6 H11 O9 P	258.0135	259.0208	259.0182	259.0233
galactose 1-P	C6 H11 O9 P	258.0135	259.0208	259.0182	259.0233
glucose 1-P	C6 H11 O9 P	258.0135	259.0208	259.0182	259.0233
glucose 6-P	C6 H11 O9 P	258.0135	259.0208	259.0182	259.0233
inositol 1-P	C6 H11 O9 P	258.0135	259.0208	259.0182	259.0233
Mannose 6-P	C6 H11 O9 P	258.0135	259.0208	259.0182	259.0233
β-fructose 1-P	C6 H11 O9 P	258.0135	259.0208	259.0182	259.0233
cys-his		258.0786	259.0859	259.0833	259.0885
(1-ribosylimidazole)-4-acetate	C10 H14 N2 O6	258.0852	259.0924	259.0898	259.0950
1-glycero-3-phosphocholine	C8 H21 N O6 P	258.1101	259.1173	259.1148	259.1199
S-methyl-5-thioribulose 1-phosphate	C6 H13 O7 S P	259.0036	260.0108	260.0082	260.0134
glucosamine 1-phosphate	C6 H14 N O8 P	259.0451	260.0524	260.0498	260.0550
gly-ser-pro		259.1168	260.1241	260.1215	260.1267
hyp-gln		259.1168	260.1241	260.1215	260.1267
gly-ala-leu		259.1532	260.1605	260.1579	260.1631
gly-ala-ile		259.1532	260.1605	260.1579	260.1631
leu-gln		259.1532	260.1605	260.1579	260.1631
ile-gln		259.1532	260.1605	260.1579	260.1631
hyp-lys		259.1532	260.1605	260.1579	260.1631
leu-lys		259.1896	260.1968	260.1942	260.1994
ile-lys		259.1896	260.1968	260.1942	260.1994
S-methyl-5-thioribose 1-phosphate	C6 H13 O7 S P	260.0114	261.0187	261.0160	261.0213
arabino-3-hexulose 6-phosphate	C6 H13 O9 P	260.0291	261.0364	261.0338	261.0390
inositol 3-phosphate	C6 H13 O9 P	260.0291	261.0364	261.0338	261.0390
inositol 4-phosphate	C6 H13 O9 P	260.0291	261.0364	261.0338	261.0390
tagatose 6-phosphate	C6 H13 O9 P	260.0291	261.0364	261.0338	261.0390
hyp-glu		260.1008	261.1081	261.1055	261.1107
gly-gly-gln		260.1120	261.1193	261.1167	261.1219
gly-ala-asn		260.1120	261.1193	261.1167	261.1219
asn-gln		260.1120	261.1193	261.1167	261.1219
thr-val		260.1358	261.1431	261.1405	261.1457
leu-glu		260.1372	261.1445	261.1419	261.1471
ile-glu		260.1372	261.1445	261.1419	261.1471
gly-gly-lys		260.1484	261.1557	261.1531	261.1583
asn-lys		260.1484	261.1557	261.1531	261.1583
gly-gly-glu		261.0960	262.1033	262.1007	262.1059
gly-ala-asp		261.0960	262.1033	262.1007	262.1059

asn-glu		261.0960	262.1033	262.1007	262.1059
asp-gln		261.0960	262.1033	262.1007	262.1059
gly-try		261.1186	262.1259	262.1232	262.1285
ala-ala-thr		261.1324	262.1397	262.1371	262.1423
asp-lys		261.1324	262.1397	262.1371	262.1423
ser-arg		261.1437	262.1509	262.1483	262.1536
1,3-diphosphoglycerate	C3 H4 O10 P2	261.9268	262.9341	262.9315	262.9367
2,3-diphosphoglycerate	C3 H4 O10 P2	261.9268	262.9341	262.9315	262.9367
1-hydroxy-2-methyl-2butenyl 4-diphosphate	C5 H12 O8 P2	261.9996	263.0069	263.0042	263.0095
galactitol 1-phosphate	C6 H15 O9 P	262.0448	263.0521	263.0494	263.0547
asp-glu		262.0801	263.0873	263.0847	263.0900
cys-val		262.0974	263.1046	263.1020	263.1073
hyp-met		262.0987	263.1060	263.1033	263.1086
pro-phe		262.1317	263.1390	263.1364	263.1416
leu-met		262.1351	263.1424	263.1397	263.1450
ile-met		262.1351	263.1424	263.1397	263.1450
gly-gly-met		263.0939	264.1012	264.0986	264.1039
ala-ala-cys		263.0939	264.1012	264.0986	264.1039
asn-met		263.0939	264.1012	264.0986	264.1039
gly-ser-thr		263.1117	264.1190	264.1163	264.1216
ala-ser-ser		263.1117	264.1190	264.1163	264.1216
asp-met		264.0780	265.0852	265.0826	265.0879
thiamine	C12 H16 N4 O S	264.1045	265.1117	265.1091	265.1144
formyl-N-acetyl-5-methoxykynurenamine	C13 H16 N2 O4	264.1110	265.1183	265.1156	265.1209
phenylacetylglutamine	C13 H16 N2 O4	264.1110	265.1183	265.1156	265.1209
gly-ser-cys		265.0732	266.0805	266.0778	266.0831
thr-phe		266.1266	267.1339	267.1312	267.1366
xanthoxic acid	C15 H22 O4	266.1518	267.1591	267.1564	267.1617
S-ribosyl homocysteine	C9 H17 N O6 S	267.0776	268.0849	268.0822	268.0876
neuraminic acid	C9 H17 N O8	267.0954	268.1027	268.1000	268.1053
deoxyguanosine	C10 H13 N5 O4	267.0967	268.1040	268.1013	268.1067
homocystine	C8 H16 N2 O4 S2	268.0551	269.0624	269.0597	269.0651
inosine	C10 H12 N4 O5	268.0807	269.0880	269.0853	269.0907
xanthosine	C10 H12 N4 O5	268.0807	269.0880	269.0853	269.0907
cys-phe		268.0881	269.0954	269.0927	269.0981
ser-tyr		268.1059	269.1132	269.1105	269.1159
hyp-his		268.1171	269.1244	269.1217	269.1271
leu-his		268.1535	269.1608	269.1581	269.1635
ile-his		268.1535	269.1608	269.1581	269.1635
N-acetylglutamate 5-phosphate	C7 H12 N O8 P	269.0295	270.0367	270.0340	270.0394
gly-gly-his		269.1124	270.1196	270.1169	270.1223
asn-his		269.1124	270.1196	270.1169	270.1223

pro-gly-pro		269.1375	270.1448	270.1421	270.1475
genistein	C15 H10 O5	270.0528	271.0601	271.0574	271.0628
lombricine	C6 H15 N4 O6 P	270.0723	271.0796	271.0769	271.0823
asp-his		270.0964	271.1037	271.1009	271.1064
estrone	C18 H22 O2	270.1620	271.1692	271.1665	271.1720
retinol	C20 H30 O	270.2348	271.2420	271.2393	271.2447
pro-arg		271.1644	272.1717	272.1690	272.1744
Galacturonate 1-P	C6 H9 O10 P	271.9927	273.0000	272.9973	273.0027
glucuronate 1-P	C6 H9 O10 P	271.9927	273.0000	272.9973	273.0027
arbutin	C12 H16 O7	272.0896	273.0968	273.0941	273.0996
hyp-val		272.1358	273.1431	273.1404	273.1458
leu-val		272.1722	273.1795	273.1768	273.1822
ile-val		272.1722	273.1795	273.1768	273.1822
estradiol-17β	C18 H24 O2	272.1776	273.1849	273.1822	273.1876
gly-gly-val		273.1311	274.1384	274.1356	274.1411
asn-val		273.1311	274.1384	274.1356	274.1411
gly-pro-thr		273.1324	274.1397	274.1370	274.1425
ala-ser-pro		273.1324	274.1397	274.1370	274.1425
ala-ala-leu		273.1688	274.1761	274.1734	274.1788
ala-ala-ile		273.1688	274.1761	274.1734	274.1788
6-phospho-2-dehydrogluconate	C6 H11 O10 P	274.0084	275.0157	275.0129	275.0184
β-arabinose 1-phosphate	C6 H11 O10 P	274.0084	275.0157	275.0129	275.0184
asp-val		274.1151	275.1224	275.1196	275.1251
N2-succinylarginine	C10 H18 N4 O5	274.1277	275.1350	275.1322	275.1377
gly-ala-gln		274.1277	275.1350	275.1322	275.1377
ala-ala-asn		274.1277	275.1350	275.1322	275.1377
gln-gln		274.1277	275.1350	275.1322	275.1377
gly-ala-lys		274.1641	275.1713	275.1686	275.1741
gln-lys		274.1641	275.1713	275.1686	275.1741
lys-lys		274.2005	275.2077	275.2050	275.2105
3-dehydro gulonate 6-phosphate	C6 H12 O10 P	275.0162	276.0235	276.0207	276.0262
6-P-gluconate	C6 H12 O10 P	275.0162	276.0235	276.0207	276.0262
gly-pro-cys		275.0939	276.1012	276.0985	276.1040
gly-ala-glu		275.1117	276.1190	276.1162	276.1217
ala-ala-asp		275.1117	276.1190	276.1162	276.1217
gln-glu		275.1117	276.1190	276.1162	276.1217
ala-try		275.1342	276.1415	276.1388	276.1443
gly-ser-leu		275.1481	276.1554	276.1526	276.1581
gly-ser-ile		275.1481	276.1554	276.1526	276.1581
lys-glu		275.1481	276.1554	276.1526	276.1581
thr-arg		275.1593	276.1666	276.1638	276.1694
glu-glu		276.0957	277.1030	277.1002	277.1058

gly-ser-asn		276.1069	277.1142	277.1114	277.1170
saccharopine	C11 H20 N2 O6	276.1321	277.1394	277.1366	277.1421
gly-ser-asp		277.0910	278.0982	278.0955	278.1010
gly-ala-met		277.1096	278.1169	278.1141	278.1197
gln-met		277.1096	278.1169	278.1141	278.1197
S-(2-methylpropanoyl)-dihydrolipoamide	C12 H23 N O2 S2	277.1170	278.1243	278.1215	278.1271
cys-arg		277.1208	278.1281	278.1253	278.1309
gly-thr-thr		277.1273	278.1346	278.1318	278.1374
ala-ser-thr		277.1273	278.1346	278.1318	278.1374
lys-met		277.1460	278.1533	278.1505	278.1560
2-C-methyl erythritol 2,4-cyclodiphosphate	C5 H12 O9 P2	277.9945	279.0018	278.9990	279.0046
glu-met		278.0936	279.1009	279.0981	279.1037
α-ribazole	C14 H18 N2 O4	278.1266	279.1339	279.1311	279.1367
pro-tyr		278.1266	279.1339	279.1311	279.1367
hyp-phe		278.1266	279.1339	279.1311	279.1367
pantetheine	C11 H22 N2 O4 S	278.1300	279.1373	279.1345	279.1401
leu-phe		278.1630	279.1703	279.1675	279.1731
ile-phe		278.1630	279.1703	279.1675	279.1731
crepenynate	C18 H30 O2	278.2246	279.2318	279.2291	279.2346
γ-linolenic acid	C18 H30 O2	278.2246	279.2318	279.2291	279.2346
gly-thr-cys		279.0889	280.0961	280.0933	280.0989
ala-ser-cys		279.0889	280.0961	280.0933	280.0989
ser-ser-ser		279.1066	280.1139	280.1111	280.1167
gly-gly-phe		279.1219	280.1292	280.1264	280.1320
asn-phe		279.1219	280.1292	280.1264	280.1320
met-met		280.0915	281.0988	281.0960	281.1016
asp-phe		280.1059	281.1132	281.1104	281.1160
9-cis,11-trans-octadecadienoate	C18 H32 O2	280.2402	281.2475	281.2447	281.2503
linoleic acid	C18 H32 O2	280.2402	281.2475	281.2447	281.2503
gly-cys-cys		281.0504	282.0576	282.0548	282.0605
4-hydroxyphenylacetylglutamine	C13 H15 N O6	281.0899	282.0972	282.0944	282.1000
indican	C13 H16 N O6	282.0977	283.1050	283.1022	283.1078
thr-tyr		282.1215	283.1288	283.1260	283.1316
cis-vaccenate	C18 H34 O2	282.2559	283.2631	283.2603	283.2660
N2-acetylaminoadipyl-γ-phosphate	C8 H14 N O8 P	283.0451	284.0524	284.0495	284.0552
guanosine	C10 H13 N5 O5	283.0916	284.0989	284.0961	284.1017
gly-ala-his		283.1280	284.1353	284.1325	284.1381
gln-his		283.1280	284.1353	284.1325	284.1381
ala-pro-pro		283.1532	284.1605	284.1576	284.1633
lys-his		283.1644	284.1717	284.1688	284.1745
5-P ribosylglycinamide (GAR)	C7 H13 N2 O8 P	284.0404	285.0476	285.0448	285.0505
cys-tyr		284.0831	285.0903	285.0875	285.0932

glu-his		284.1120	285.1193	285.1165	285.1222
11-cis-retinal	C20 H28 O	284.2140	285.2213	285.2184	285.2241
all-trans-retinal	C20 H28 O	284.2140	285.2213	285.2184	285.2241
gly-pro-leu		285.1688	286.1761	286.1732	286.1790
gly-pro-ile		285.1688	286.1761	286.1732	286.1790
7P-2-dehydro-3-dexoyarabionheptonate	C7 H11 O10 P	286.0084	287.0157	287.0128	287.0185
(3-indolyl)-glycerol-P	C11 H13 N O6 P	286.0475	287.0547	287.0519	287.0576
salicin	C13 H18 O7	286.1052	287.1125	287.1096	287.1154
met-his		286.1099	287.1172	287.1143	287.1201
gly-pro-asn		286.1277	287.1350	287.1321	287.1378
16 α -hydroxyestrone	C18 H22 O3	286.1569	287.1642	287.1613	287.1670
2-hydroxyestrone	C18 H22 O3	286.1569	287.1642	287.1613	287.1670
androst-4-ene-3,17-dione	C19 H26 O2	286.1933	287.2005	287.1977	287.2034
all-trans-retinol	C20 H30 O	286.2297	287.2369	287.2341	287.2398
indoleglycerol	C11 H14 N O6 P	287.0553	288.0626	288.0597	288.0654
gly-pro-asp		287.1117	288.1190	288.1161	288.1219
gly-ala-val		287.1467	288.1540	288.1511	288.1569
gln-val		287.1467	288.1540	288.1511	288.1569
ala-pro-thr		287.1481	288.1554	288.1525	288.1582
hyp-arg		287.1593	288.1666	288.1637	288.1695
lys-val		287.1831	288.1904	288.1875	288.1933
leu-arg		287.1957	288.2030	288.2001	288.2059
ile-arg		287.1957	288.2030	288.2001	288.2059
dehydroepiandrosterone	C19 H27 O2	287.2011	288.2084	288.2055	288.2113
2-dehydro-3-deoxy-arabino-heptonate 7-phosphate	C7 H13 O10 P	288.0240	289.0313	289.0284	289.0342
glu-val		288.1308	289.1380	289.1351	289.1409
ala-ala-gln		288.1433	289.1506	289.1477	289.1535
gly-gly-arg		288.1546	289.1618	289.1589	289.1647
asn-arg		288.1546	289.1618	289.1589	289.1647
2-hydroxyestradiol-17 β	C18 H24 O3	288.1725	289.1798	289.1769	289.1827
6 β -hydroxyestradiol-17 β	C18 H24 O3	288.1725	289.1798	289.1769	289.1827
estriol	C18 H24 O3	288.1725	289.1798	289.1769	289.1827
ala-ala-lys		288.1797	289.1870	289.1841	289.1899
3 β ,17 β -dihydroxyandrost-5-ene	C19 H28 O2	288.2089	289.2162	289.2133	289.2191
5 β -androstane-3,17-dione	C19 H28 O2	288.2089	289.2162	289.2133	289.2191
androstanedione	C19 H28 O2	288.2089	289.2162	289.2133	289.2191
testosterone	C19 H28 O2	288.2089	289.2162	289.2133	289.2191
N-succinyl-2-amino-6-oxopimelate	C11 H15 N O8	289.0797	290.0870	290.0841	290.0899
cys-ala-pro		289.1096	290.1169	290.1140	290.1198
ala-ala-glu		289.1273	290.1346	290.1317	290.1375
ser-ser-pro		289.1273	290.1346	290.1317	290.1375
asp-arg		289.1386	290.1459	290.1430	290.1488

gly-thr-leu		289.1637	290.1710	290.1681	290.1739
gly-thr-ile		289.1637	290.1710	290.1681	290.1739
ala-ser-leu		289.1637	290.1710	290.1681	290.1739
ala-ser-ile		289.1637	290.1710	290.1681	290.1739
sedoheptulose 7-P	C7 H15 O10 P	290.0397	291.0470	291.0441	291.0499
N-succinyl-2,6-diaminopimelate	C11 H18 N2 O7	290.1114	291.1186	291.1157	291.1215
arginosuccinic acid	C10 H18 N4 O6	290.1226	291.1299	291.1270	291.1328
N-(arginino) succinate	C10 H18 N4 O6	290.1226	291.1299	291.1270	291.1328
gly-ser-gln		290.1226	291.1299	291.1270	291.1328
gly-thr-asn		290.1226	291.1299	291.1270	291.1328
ala-ser-asn		290.1226	291.1299	291.1270	291.1328
met-val		290.1287	291.1359	291.1330	291.1388
gly-ser-lys		290.1590	291.1663	291.1633	291.1692
2-methoxyestradiol-17β	C18 H26 O3	290.1882	291.1955	291.1925	291.1984
3α-hydroxy-5β-androstan-17-one	C19 H30 O2	290.2246	291.2318	291.2289	291.2348
5β-dihydrotestosterone	C19 H30 O2	290.2246	291.2318	291.2289	291.2348
androstanolone	C19 H30 O2	290.2246	291.2318	291.2289	291.2348
Androstenediol	C19 H30 O2	290.2246	291.2318	291.2289	291.2348
gly-ser-glu		291.1066	292.1139	292.1110	292.1168
gly-thr-asp		291.1066	292.1139	292.1110	292.1168
ala-ser-asp		291.1066	292.1139	292.1110	292.1168
gly-cys-leu		291.1252	292.1325	292.1296	292.1354
gly-cys-ile		291.1252	292.1325	292.1296	292.1354
ala-ala-met		291.1252	292.1325	292.1296	292.1354
ser-try		291.1292	292.1364	292.1335	292.1394
S-(2-methylbutanoyl)-dihydrolipoamide	C13 H25 N O2 S2	291.1327	292.1399	292.1370	292.1429
S-(3-methylbutanoyl)-dihydrolipoamide	C13 H25 N O2 S2	291.1327	292.1399	292.1370	292.1429
ala-thr-thr		291.1430	292.1503	292.1474	292.1532
gly-cys-asn		292.0841	293.0914	293.0884	293.0943
his-his		292.1284	293.1356	293.1327	293.1386
5-phosphoribosyl-5-aminoimidazole	C8 H12 N3 O7 P	293.0407	294.0480	294.0450	294.0509
2-amino-4-hydroxy-6-hydroxymethyl- dihydropteridine-PP	C7 H11 N5 O8	293.0607	294.0680	294.0650	294.0709
gly-cys-asp		293.0681	294.0754	294.0725	294.0783
ala-thr-cys		293.1045	294.1118	294.1088	294.1147
gly-ser-met		293.1045	294.1118	294.1088	294.1147
ser-ser-thr		293.1223	294.1295	294.1266	294.1325
gly-ala-phe		293.1375	294.1448	294.1419	294.1477
gln-phe		293.1375	294.1448	294.1419	294.1477
lys-phe		293.1739	294.1812	294.1783	294.1841
hyp-tyr		294.1215	295.1288	295.1259	295.1318
glu-phe		294.1215	295.1288	295.1259	295.1318

leu-tyr		294.1579	295.1652	295.1623	295.1682
ile-tyr		294.1579	295.1652	295.1623	295.1682
13-oxoODE	C18 H30 O3	294.2195	295.2268	295.2238	295.2297
9-oxoODE	C18 H30 O3	294.2195	295.2268	295.2238	295.2297
aminoimidazole ribotide	C8 H14 N3 O7 P	295.0563	296.0636	296.0607	296.0666
ala-cys-cys		295.0660	296.0733	296.0703	296.0763
ser-ser-cys		295.0838	296.0910	296.0881	296.0940
gly-gly-tyr		295.1168	296.1241	296.1211	296.1270
asn-tyr		295.1168	296.1241	296.1211	296.1270
asp-tyr		296.1008	297.1081	297.1051	297.1110
met-phe		296.1194	297.1267	297.1237	297.1297
his-val		296.1471	297.1543	297.1514	297.1573
10-EpOME	C18 H32 O3	296.2351	297.2424	297.2394	297.2454
12-EpOME	C18 H32 O3	296.2351	297.2424	297.2394	297.2454
13-HODE	C18 H32 O3	296.2351	297.2424	297.2394	297.2454
9-HODE	C18 H32 O3	296.2351	297.2424	297.2394	297.2454
thromboxane	C20 H40 O	296.3079	297.3152	297.3122	297.3182
methylthioadenosine	C11 H15 N5 O3 S	297.0895	298.0968	298.0938	298.0998
ala-ala-his		297.1437	298.1509	298.1480	298.1539
tuberculoaterate	C19 H38 O2	298.2872	299.2944	299.2915	299.2974
N-acetyl glucosamine 1-P	C8 H14 N O9 P	299.0400	300.0473	300.0443	300.0503
N-acetyl glucosamine 6-P	C8 H14 N O9 P	299.0400	300.0473	300.0443	300.0503
4-P-pantothenate	C9 H18 N O8	299.0764	300.0837	300.0807	300.0867
gly-ser-his		299.1229	300.1302	300.1272	300.1332
ser-pro-pro		299.1481	300.1554	300.1524	300.1584
leu-ala-pro		299.1845	300.1918	300.1888	300.1948
ile-ala-pro		299.1845	300.1918	300.1888	300.1948
3-dehydrosphinganine	C18 H37 N O2	299.2824	300.2897	300.2867	300.2927
spingosine	C18 H37 N O2	299.2824	300.2897	300.2867	300.2927
cinnavalinate	C14 H8 N2 O6	300.0382	301.0455	301.0425	301.0485
salidroside	C14 H20 O7	300.1209	301.1281	301.1251	301.1312
gly-pro-gln		300.1433	301.1506	301.1476	301.1536
ala-pro-asn		300.1433	301.1506	301.1476	301.1536
val-val		300.1658	301.1731	301.1701	301.1761
16 α -hydroxyandrost-4-ene-3,17-dione	C19 H24 O3	300.1725	301.1798	301.1768	301.1828
19-oxo-androst-4-ene-3,17-dione	C19 H24 O3	300.1725	301.1798	301.1768	301.1828
2-methoxyestrone	C19 H24 O3	300.1725	301.1798	301.1768	301.1828
adrenosterone	C19 H24 O3	300.1725	301.1798	301.1768	301.1828
andrenosterone	C19 H24 O3	300.1725	301.1798	301.1768	301.1828
gly-pro-lys		300.1797	301.1870	301.1840	301.1900
retinoate	C20 H28 O2	300.2089	301.2162	301.2132	301.2192
gly-pro-glu		301.1273	302.1346	302.1316	302.1376

ala-pro-asp		301.1273	302.1346	302.1316	302.1376
pro-try		301.1499	302.1572	302.1541	302.1602
ala-ala-val		301.1624	302.1697	302.1666	302.1727
gly-leu-leu		301.2001	302.2074	302.2044	302.2104
gly-leu-ile		301.2001	302.2074	302.2044	302.2104
gly-ile-ile		301.2001	302.2074	302.2044	302.2104
sphinganine	C18 H39 N O2	301.2981	302.3053	302.3023	302.3084
his-phe		302.1379	303.1451	303.1421	303.1482
leu-gly-asn		302.1590	303.1663	303.1632	303.1693
ile-gly-asn		302.1590	303.1663	303.1632	303.1693
gly-ala-arg		302.1702	303.1775	303.1745	303.1805
gln-arg		302.1702	303.1775	303.1745	303.1805
11 β -hydroxyandrost-4-ene-3,17-dione	C19 H26 O3	302.1882	303.1955	303.1924	303.1985
16 α -hydroxydehydroepiandrosterone	C19 H26 O3	302.1882	303.1955	303.1924	303.1985
19-hydroxyandrost-4-ene-3,17-dione	C19 H26 O3	302.1882	303.1955	303.1924	303.1985
19-oxo-testosterone	C19 H26 O3	302.1882	303.1955	303.1924	303.1985
7 α -hydroxyandrostenedione	C19 H26 O3	302.1882	303.1955	303.1924	303.1985
testololactone	C19 H26 O3	302.1882	303.1955	303.1924	303.1985
lys-arg		302.2066	303.2139	303.2108	303.2169
eicosapentaenoic acid	C20 H30 O2	302.2246	303.2318	303.2288	303.2349
retinyl ester	C20 H30 O2	302.2246	303.2318	303.2288	303.2349
cyclic GMP	C10 H12 N2 O7 P	303.0376	304.0449	304.0419	304.0479
gly-asn-asn		303.1178	304.1251	304.1221	304.1282
gly-pro-met		303.1252	304.1325	304.1295	304.1356
ser-gly-val		303.1416	304.1489	304.1459	304.1520
ser-pro-thr		303.1430	304.1503	304.1472	304.1533
leu-gly-asp		303.1430	304.1503	304.1472	304.1533
ile-gly-asp		303.1430	304.1503	304.1472	304.1533
glu-arg		303.1542	304.1615	304.1585	304.1645
ala-thr-leu		303.1794	304.1867	304.1836	304.1897
ala-thr-ile		303.1794	304.1867	304.1836	304.1897
gly-asn-asp		304.1019	305.1091	305.1061	305.1122
Nopaline	C11 H20 N4 O6	304.1382	305.1455	305.1425	305.1486
gly-thr-gln		304.1382	305.1455	305.1425	305.1486
ala-ser-gln		304.1382	305.1455	305.1425	305.1486
ala-thr-asn		304.1382	305.1455	305.1425	305.1486
gly-thr-lys		304.1746	305.1819	305.1789	305.1850
ala-ser-lys		304.1746	305.1819	305.1789	305.1850
19-hydroxytestosterone	C19 H28 O3	304.2038	305.2111	305.2081	305.2142
7 α -hydroxytestosterone	C19 H28 O3	304.2038	305.2111	305.2081	305.2142
arachidonic acid	C20 H32 O2	304.2402	305.2475	305.2444	305.2505
cyclic CMP	C9 H12 N3 O7 P	305.0407	306.0480	306.0449	306.0510

gly-asp-asp		305.0859	306.0931	306.0901	306.0962
cys-ser-pro		305.1045	306.1118	306.1087	306.1148
gly-thr-glu		305.1223	306.1295	306.1265	306.1326
ala-ser-glu		305.1223	306.1295	306.1265	306.1326
ala-thr-asp		305.1223	306.1295	306.1265	306.1326
ala-cys-leu		305.1409	306.1482	306.1451	306.1512
ala-cys-ile		305.1409	306.1482	306.1451	306.1512
thr-try		305.1448	306.1521	306.1490	306.1551
met-arg		305.1521	306.1594	306.1563	306.1625
ser-ser-leu		305.1586	306.1659	306.1629	306.1690
ser-ser-ile		305.1586	306.1659	306.1629	306.1690
cyclic UMP	C9 H11 N2 O8 P	306.0247	307.0320	307.0289	307.0351
gly-cys-gln		306.0998	307.1070	307.1040	307.1101
ala-cys-asn		306.0998	307.1070	307.1040	307.1101
ser-ser-asn		306.1175	307.1248	307.1217	307.1278
gly-cys-lys		306.1361	307.1434	307.1403	307.1465
val-phe		306.1566	307.1639	307.1608	307.1669
corrinoid	C19 H22 N4	306.1844	307.1917	307.1886	307.1948
8,11,14-icosatrienoate	C20 H34 O2	306.2559	307.2631	307.2601	307.2662
3-iodotyrosine	C9 H10 N O3 I	306.9700	307.9772	307.9742	307.9803
dCMP	C9 H14 N3 O7 P	307.0563	308.0636	308.0605	308.0667
glutathione	C10 H17 N3 O6 S	307.0838	308.0910	308.0880	308.0941
gly-cys-glu		307.0838	308.0910	308.0880	308.0941
ala-cys-asp		307.0838	308.0910	308.0880	308.0941
S-succinylidihydrolipoamide	C12 H21 N O4 S2	307.0912	308.0985	308.0954	308.1015
ser-ser-asp		307.1015	308.1088	308.1057	308.1119
cys-try		307.1063	308.1136	308.1105	308.1167
gly-thr-met		307.1202	308.1274	308.1244	308.1305
ala-ser-met		307.1202	308.1274	308.1244	308.1305
ser-thr-thr		307.1379	308.1452	308.1421	308.1483
ala-ala-phe		307.1532	308.1605	308.1574	308.1635
dUMP	C9 H14 N2 O8 P	309.0482	310.0555	310.0524	310.0586
cys-gly-met		309.0817	310.0889	310.0858	310.0920
ser-thr-cys		309.0994	310.1067	310.1036	310.1098
sialate	C11 H19 N O9	309.1059	310.1132	310.1101	310.1163
gly-ala-tyr		309.1324	310.1397	310.1366	310.1428
gly-ser-phe		309.1324	310.1397	310.1366	310.1428
gln-tyr		309.1324	310.1397	310.1366	310.1428
gly-pro-his		309.1437	310.1509	310.1478	310.1540
pro-pro-pro		309.1688	310.1761	310.1730	310.1792
lys-tyr		309.1688	310.1761	310.1730	310.1792

ribose-1,5-bisphosphate	C5 H12 O11 P2	309.9843	310.9916	310.9885	310.9947
ribulose 1,5-bisphosphate	C5 H12 O11 P2	309.9843	310.9916	310.9885	310.9947
glu-tyr		310.1165	311.1237	311.1206	311.1268
ser-cys-cys		311.0609	312.0682	312.0651	312.0713
dhurrin	C14 H17 N O7	311.1005	312.1077	312.1046	312.1109
taxiphyllin	C14 H17 N O7	311.1005	312.1077	312.1046	312.1109
his-arg		311.1705	312.1778	312.1747	312.1809
met-tyr		312.1144	313.1216	313.1185	313.1248
phe-phe		312.1474	313.1546	313.1515	313.1578
11-hydroperoxyoctadeca-9,12-dienoic acid	C18 H32 O4	312.2300	313.2373	313.2342	313.2404
12,13-epoxy-9-hydroxy-10-octadecenoate	C18 H32 O4	312.2300	313.2373	313.2342	313.2404
13-hydroperoxyoctadeca-9,11-dienoic acid	C18 H32 O4	312.2300	313.2373	313.2342	313.2404
7,8-DiHODE	C18 H32 O4	312.2300	313.2373	313.2342	313.2404
8-HPODE	C18 H32 O4	312.2300	313.2373	313.2342	313.2404
9,10-12,13-diepoxyoctadecanoate	C18 H32 O4	312.2300	313.2373	313.2342	313.2404
9,10-epoxy-13-hydroxy-11-octadecenoate	C18 H32 O4	312.2300	313.2373	313.2342	313.2404
9-HPODE	C18 H32 O4	312.2300	313.2373	313.2342	313.2404
phytanic acid	C20 H40 O2	312.3028	313.3101	313.3070	313.3132
5-phosphoribosyl-N-formylglycinamide	C8 H16 N3 O8 P	313.0669	314.0742	314.0710	314.0773
gly-thr-his		313.1386	314.1459	314.1427	314.1490
ala-ser-his		313.1386	314.1459	314.1427	314.1490
gly-pro-val		313.1624	314.1697	314.1665	314.1728
pro-pro-thr		313.1637	314.1710	314.1679	314.1742
5'-phosphoribosyl-N-formylglycinamide	C8 H15 N2 O9 P	314.0509	315.0582	315.0550	315.0613
geranyl-PP	C10 H20 O7 P2	314.0673	315.0746	315.0714	315.0777
7,8-dihydropteroate	C14 H14 N6 O3	314.1127	315.1200	315.1168	315.1231
ala-pro-gln		314.1590	315.1663	315.1631	315.1694
lys-ala-pro		314.1954	315.2026	315.1995	315.2058
progesterone	C21 H30 O2	314.2246	315.2318	315.2287	315.2350
12,13-DHOME	C18 H34 O4	314.2457	315.2530	315.2498	315.2561
9,10-DHOME	C18 H34 O4	314.2457	315.2530	315.2498	315.2561
adenosine	C10 H13 N5 O4	315.0814	316.0887	316.0856	316.0919
cys-gly-his		315.1001	316.1074	316.1042	316.1105
pro-pro-cys		315.1252	316.1325	316.1294	316.1357
ala-pro-glu		315.1430	316.1503	316.1471	316.1534
leu-ser-pro		315.1794	316.1867	316.1835	316.1898
ile-ser-pro		315.1794	316.1867	316.1835	316.1898
val-arg		315.1893	316.1965	316.1934	316.1997
ala-leu-leu		315.2158	316.2231	316.2199	316.2262
ala-leu-ile		315.2158	316.2231	316.2199	316.2262
ala-ile-ile		315.2158	316.2231	316.2199	316.2262
5β-pregnane-3,20-dione	C21 H31 O2	315.2324	316.2397	316.2365	316.2428

ser-pro-asn		316.1382	317.1455	317.1423	317.1487
gly-leu-gln		316.1746	317.1819	317.1787	317.1851
gly-ile-gln		316.1746	317.1819	317.1787	317.1851
ala-leu-asn		316.1746	317.1819	317.1787	317.1851
ala-ile-asn		316.1746	317.1819	317.1787	317.1851
ala-ala-arg		316.1859	317.1931	317.1900	317.1963
15-deoxy- δ -12,14-prostoglandin J2	C20 H28 O3	316.2038	317.2111	317.2079	317.2143
gly-leu-lys		316.2110	317.2183	317.2151	317.2215
gly-ile-lys		316.2110	317.2183	317.2151	317.2215
20 α -hydroxy-4-pregnen-3-one	C21 H32 O2	316.2402	317.2475	317.2443	317.2507
pregnenolone	C21 H32 O2	316.2402	317.2475	317.2443	317.2507
ser-pro-asp		317.1223	318.1295	318.1264	318.1327
gly-asn-gln		317.1335	318.1408	318.1376	318.1439
ala-asn-asn		317.1335	318.1408	318.1376	318.1439
ala-pro-met		317.1409	318.1482	318.1450	318.1514
hyp-try		317.1448	318.1521	318.1489	318.1553
gly-thr-val		317.1573	318.1646	318.1614	318.1678
ala-ser-val		317.1573	318.1646	318.1614	318.1678
gly-leu-glu		317.1586	318.1659	318.1627	318.1691
gly-ile-glu		317.1586	318.1659	318.1627	318.1691
pro-thr-thr		317.1586	318.1659	318.1627	318.1691
ala-leu-asp		317.1586	318.1659	318.1627	318.1691
ala-ile-asp		317.1586	318.1659	318.1627	318.1691
asn-gly-lys		317.1699	318.1772	318.1740	318.1803
leu-try		317.1812	318.1885	318.1853	318.1917
ile-try		317.1812	318.1885	318.1853	318.1917
3 α -hydroxy-5 β -pregnan-20-one	C21 H33 O2	317.2480	318.2553	318.2521	318.2585
phytosphingosine	C18 H39 N O3	317.2930	318.3003	318.2971	318.3034
gly-asn-glu		318.1175	319.1248	319.1216	319.1280
gly-asp-gln		318.1175	319.1248	319.1216	319.1280
ala-asn-asp		318.1175	319.1248	319.1216	319.1280
his-tyr		318.1328	319.1400	319.1369	319.1432
gly-gly-try		318.1400	319.1473	319.1441	319.1505
asn-try		318.1400	319.1473	319.1441	319.1505
ala-thr-gln		318.1539	319.1612	319.1580	319.1644
asp-gly-lys		318.1539	319.1612	319.1580	319.1644
gly-ser-arg		318.1651	319.1724	319.1692	319.1756
ala-thr-lys		318.1903	319.1976	319.1944	319.2007
12-oxoETE	C20 H30 O3	318.2195	319.2268	319.2236	319.2299
15-oxoicosa-5,8,11,13-tetraeonic acid	C20 H30 O3	318.2195	319.2268	319.2236	319.2299
5-oxoETE	C20 H30 O3	318.2195	319.2268	319.2236	319.2299
leukotriene A4	C20 H30 O3	318.2195	319.2268	319.2236	319.2299
gly-asp-glu		319.1015	320.1088	320.1056	320.1120

ala-asp-asp		319.1015	320.1088	320.1056	320.1120
gly-cys-val		319.1188	320.1261	320.1229	320.1293
pro-thr-cys		319.1202	320.1274	320.1242	320.1306
asp-try		319.1241	320.1313	320.1281	320.1345
ala-thr-glu		319.1379	320.1452	320.1420	320.1484
phe-gly-pro		319.1532	320.1605	320.1573	320.1637
leu-gly-met		319.1565	320.1638	320.1606	320.1670
ile-gly-met		319.1565	320.1638	320.1606	320.1670
ser-thr-leu		319.1743	320.1816	320.1784	320.1848
ser-thr-ile		319.1743	320.1816	320.1784	320.1848
ala-cys-gln		320.1154	321.1227	321.1195	321.1259
gly-asn-met		320.1154	321.1227	321.1195	321.1259
ser-ser-gln		320.1332	321.1404	321.1372	321.1436
ser-thr-asn		320.1332	321.1404	321.1372	321.1436
ala-cys-lys		320.1518	321.1591	321.1559	321.1623
ser-ser-lys		320.1695	321.1768	321.1736	321.1800
11,12-EET	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
11-HETE	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
12-HETE	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
14,15-EET	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
15-hydroxy-5,8,11-cis-13-trans- eicosatetraenoate	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
16-HETE	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
19-HETE	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
20-HETE	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
5,6-EET	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
5-hydroxyeicosatetraenoate	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
8,9-EET	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
8-HETE	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
9-HETE	C20 H32 O3	320.2351	321.2424	321.2392	321.2456
pro-cys-cys		321.0817	322.0889	322.0857	322.0922
ala-cys-glu		321.0994	322.1067	322.1035	322.1099
gly-asp-met		321.0994	322.1067	322.1035	322.1099
S-glutaryl dihydro lipamide	C13 H23 N O4 S2	321.1068	322.1141	322.1109	322.1173
ser-ser-glu		321.1172	322.1244	322.1212	322.1277
ser-thr-asp		321.1172	322.1244	322.1212	322.1277
ala-thr-met		321.1358	322.1431	322.1399	322.1463
ser-cys-leu		321.1358	322.1431	322.1399	322.1463
ser-cys-ile		321.1358	322.1431	322.1399	322.1463
thr-thr-thr		321.1536	322.1608	322.1576	322.1641
phe-arg		321.1801	322.1873	322.1841	322.1906
pregnenediol	C21 H37 O2	321.2793	322.2866	322.2834	322.2898
1-carbosyvinyl-3-P-shikimate	C10 H11 O10 P	322.0084	323.0157	323.0124	323.0189

thymidine monophosphate (TMP)	C10 H15 N2 O8 P	322.0560	323.0633	323.0601	323.0665
ser-cys-asn		322.0947	323.1019	323.0987	323.1052
N-pantothenoyl-cysteine	C12 H22 N2 O6 S	322.1198	323.1271	323.1239	323.1303
val-tyr		322.1515	323.1588	323.1555	323.1620
cytidine monophosphate (CMP)	C9 H14 N3 O8 P	323.0513	324.0585	324.0553	324.0618
ser-cys-asp		323.0787	324.0860	324.0827	324.0892
ala-cys-met		323.0973	324.1046	324.1014	324.1078
ser-ser-met		323.1151	324.1223	324.1191	324.1256
thr-thr-cys		323.1151	324.1223	324.1191	324.1256
ala-ala-tyr		323.1481	324.1554	324.1521	324.1586
ala-ser-phe		323.1481	324.1554	324.1521	324.1586
thr-gly-phe		323.1481	324.1554	324.1521	324.1586
ala-pro-his		323.1593	324.1666	324.1634	324.1698
mevalonate-5-PP	C6 H14 O11 P2	324.0000	325.0073	325.0040	325.0105
O5-(1-carboxyvinyl)-3-phosphoshikimate	C10 H13 O10 P	324.0240	325.0313	325.0281	325.0346
pseudouridine 5'-phosphate	C9 H13 N2 O9 P	324.0353	325.0425	325.0393	325.0458
uridine monophosphate (UMP)	C9 H13 N2 O9 P	324.0353	325.0425	325.0393	325.0458
urothione	C11 H11 N5 O3 S2	325.0303	326.0376	326.0343	326.0408
thr-cys-cys		325.0766	326.0839	326.0806	326.0871
N-glycoloyl-neuraminic acid	C11 H19 N O10	325.1008	326.1081	326.1049	326.1114
gly-cys-phe		325.1096	326.1169	326.1136	326.1201
gly-ser-tyr		325.1273	326.1346	326.1314	326.1379
leu-gly-his		325.1750	326.1822	326.1790	326.1855
ile-gly-his		325.1750	326.1822	326.1790	326.1855
pro-pro-leu		325.2001	326.2074	326.2041	326.2107
pro-pro-ile		325.2001	326.2074	326.2041	326.2107
gly-asn-his		326.1338	327.1411	327.1378	327.1444
pro-pro-asn		326.1590	327.1663	327.1630	327.1695
2,3-dinor-8-iso prostaglandin F2 α	C18 H30 O5	326.2093	327.2166	327.2133	327.2198
homophytanic acid	C21 H42 O2	326.3185	327.3257	327.3225	327.3290
cys-cys-cys		327.0381	328.0454	328.0421	328.0486
gly-asp-his		327.1178	328.1251	328.1218	328.1284
pro-pro-asp		327.1430	328.1503	328.1470	328.1536
ala-thr-his		327.1542	328.1615	328.1582	328.1648
val-ala-pro		327.1780	328.1853	328.1820	328.1886
cyclic AMP	C10 H11 N5 O6 P	328.0441	329.0514	329.0481	329.0547
phe-tyr		328.1423	329.1496	329.1463	329.1528
gly-pro-arg		328.1859	329.1931	329.1898	329.1964
2,3-dinor-8-iso prostaglandin F1 α	C18 H32 O5	328.2250	329.2322	329.2289	329.2355
ala-cys-his		329.1157	330.1230	330.1197	330.1263

ser-ser-his		329.1335	330.1408	330.1375	330.1441
gly-leu-val		329.1937	330.2010	330.1977	330.2043
gly-ile-val		329.1937	330.2010	330.1977	330.2043
pro-thr-leu		329.1950	330.2023	330.1990	330.2056
pro-thr-ile		329.1950	330.2023	330.1990	330.2056
asn-gly-val		330.1525	331.1598	331.1565	331.1631
ser-pro-gln		330.1539	331.1612	331.1579	331.1645
pro-thr-asn		330.1539	331.1612	331.1579	331.1645
ala-leu-gln		330.1903	331.1976	331.1942	331.2009
ala-ile-gln		330.1903	331.1976	331.1942	331.2009
lys-ser-pro		330.1903	331.1976	331.1942	331.2009
arg-arg		330.2127	331.2200	331.2167	331.2233
11-dexsycorticosterone	C21 H30 O3	330.2195	331.2268	331.2234	331.2301
11 β -hydroxyprogesterone	C21 H30 O3	330.2195	331.2268	331.2234	331.2301
17 α -hydroxyprogesterone	C21 H30 O3	330.2195	331.2268	331.2234	331.2301
ala-leu-lys		330.2267	331.2339	331.2306	331.2373
ala-ile-lys		330.2267	331.2339	331.2306	331.2373
9,10,13-TriHOME	C18 H34 O5	330.2406	331.2479	331.2446	331.2512
9,10-dihydroxy-12,13-epoxyoctadecanoate	C18 H34 O5	330.2406	331.2479	331.2446	331.2512
9,12,13-TriHOME	C18 H34 O5	330.2406	331.2479	331.2446	331.2512
inosine-5-phosphate	C10 H13 N4 O7 P	331.0438	332.0510	332.0477	332.0544
dAMP	C10 H14 N5 O6 P	331.0676	332.0748	332.0715	332.0782
asp-gly-val		331.1366	332.1438	332.1405	332.1472
ser-pro-glu		331.1379	332.1452	332.1419	332.1485
pro-thr-asp		331.1379	332.1452	332.1419	332.1485
gly-gln-gln		331.1491	332.1564	332.1531	332.1597
ala-asn-gln		331.1491	332.1564	332.1531	332.1597
pro-cys-leu		331.1565	332.1638	332.1605	332.1671
pro-cys-ile		331.1565	332.1638	332.1605	332.1671
ala-thr-val		331.1729	332.1802	332.1769	332.1835
ala-leu-glu		331.1743	332.1816	332.1783	332.1849
ala-ile-glu		331.1743	332.1816	332.1783	332.1849
gly-gln-lys		331.1855	332.1928	332.1895	332.1961
ala-asn-lys		331.1855	332.1928	332.1895	332.1961
ser-leu-leu		331.2107	332.2180	332.2146	332.2213
ser-leu-ile		331.2107	332.2180	332.2146	332.2213
ser-ile-ile		331.2107	332.2180	332.2146	332.2213
gly-lys-lys		331.2219	332.2292	332.2259	332.2325
dIMP	C10 H13 N4 O7 P	332.0516	333.0589	333.0555	333.0622
cys-pro-asn		332.1154	333.1227	333.1193	333.1260
gly-gln-glu		332.1332	333.1404	333.1371	333.1438
ala-asn-glu		332.1332	333.1404	333.1371	333.1438

