

Supplementary Table S4

Metabolites	Mass (m/z)	LogFoldChange	LinearFoldChange
(-)-Epinephrine	166.0853	-0.69593	0.617312574
(-)-N-Acetylneuraminic acid	310.1119	0.504788	1.41891531
(-)-Verbenone	151.0482	-0.28233	0.822260654
(.+/-)-17-Hydroxy-4Z,7Z,10Z,13Z,15E,19Z-docosahexaenoic acid	327.2164	-0.23159	0.851696137
(.+/-)-4-Hydroxy-5E,7Z,10Z,13Z,16Z,19Z-docosahexaenoic acid	327.2184	-0.20485	0.867627713
(.+/-)-7-Hydroxy-4Z,8E,10Z,13Z,16Z,19Z-docosahexaenoic acid	326.2122	0.118286	1.085444587
(.+/-)-8-Hydroxy-4Z,6E,10Z,13Z,16Z,19Z-docosahexaenoic acid	326.232	-0.23782	0.848023305
(.+/-)-9-Hydroxy-5Z,7E,11Z,14Z,17Z-eicosapentaenoic acid	301.1426	-0.67049	0.628293616
(+)-2,5-epi-Gonithalesdiol	249.1442	0.259613	1.197157154
(+/-)-2-cis-4-trans-Abcisic acid	247.0775	-0.47302	0.720454715
(+/-)-11-Hydroxy-5Z,8Z,12E,14Z,17Z-eicosapentaenoic acid	301.2161	-0.26933	0.829703641
(+/-)-16(17)-Epoxy-4Z,7Z,10Z,13Z,19Z-docosapentaenoic acid	327.2164	0.105306	1.075722283
(3-Carboxypropyl)trimethylammonium cation	146.1176	0.516383	1.430365115
(7,7-Dimethyl-2-oxonorbornan-1-yl)methanesulfonic acid	231.0279	0.393862	1.313905839
(R)-(+)-Citronellic acid	171.063	-0.36092	0.778667754
(R)-Butaprost	358.2954	0.3476	1.272442412
(Z,E)-Tetradeca-9,12-dienol	210.0884	-0.24627	0.843075586
Bisabolol	223.0273	-0.29711	0.813881082
CMBHC	136.0622	0.391139	1.311428184
Guanidinoglutamic acid	189.1354	-0.52365	0.695609695
Hydroxyisocaproic acid	155.0417	0.444073	1.360439559
Estradiol	289.1439	-0.1741	0.88632189
Estradiol 17-propionate	347.1273	-0.48352	0.715228345
Estradiol 3-benzoate	253.1431	-0.29305	0.816174161
Nicotinamide adenine dinucleotide	664.1174	-0.62518	0.648339755
17-6-Ketoprostaglandin F1.alpha.	367.0421	-0.33153	0.794695716
6 Testosterone enanthate	269.1355	-0.21134	0.863734513
3 Arachidonic acid	305.1966	0.272443	1.207851433
3 Arachidonic acid ethyl ester	333.2884	0.463242	1.378636827
1-(2-Hydroxyethyl)-2-hydroxymethyl-5-nitroimidazole	188.0664	0.255187	1.193490377
1-(4-Methoxyphenyl)piperazine	191.9827	-0.7364	0.600233289
1,11-Undecanedicarboxylic acid	226.1784	-0.29387	0.815710978
1,2-Benzenedicarboxylic acid	149.0233	-0.34485	0.787391961
1,2-Diamino-2-methylpropane	72.0835	0.249036	1.188413143
1,2-Dilinoleoyl-sn-glycero-3-phospho-(1'-rac-glycerol)	507.2734	0.179674	1.132628182
1,2-Dipalmitoleoyl-sn-glycero-3-phosphoethanolamine	686.0449	-0.23436	0.850064308
1,3-Dicyclohexylurea	225.1939	-0.08764	0.941063452
1,5-Diaminonaphthalene	158.0412	0.489038	1.403508337
1,6-Anhydro-2,3-O-isopropylidene-.beta.-D-mannopyranose	203.0878	0.09438	1.067606135
10(S),17(S)-DiHDoHE	343.2082	-0.35898	0.779716145
11,15-Dioxo-9S-hydroxy-5Z-prostenoic acid	352.3053	-0.31746	0.802479289
11.alpha.-Hydroxyprogesterone	331.2646	-0.14071	0.907069939
11.beta.,17.alpha.,20.beta.,21-Tetrahydroypregn-4-en-3-one	365.2785	0.38489	1.305760421

11-.beta.-Hydroxyandrosterone	288.2903	0.146188	1.106641852
11.beta.-Prostaglandin E2	335.2222	-0.30685	0.808405632
11-Dehydrothromboxane B2	367.2681	-0.19453	0.873854665
11-Deoxyprostaglandin E1	303.1997	0.220565	1.165189823
11-Deoxyprostaglandin F1.alpha.	339.2528	0.281069	1.215094943
11-Nor-.DELTA.9-tetrahydrocannabinol-9-carboxylic acid-d3	329.1606	0.232764	1.17508406
11-Oxo-15S-hydroxy-5Z,9,13E-prostatrienoic acid	317.2682	-0.21675	0.860499251
11S-Hydroxy-5Z,8Z,12E,14Z-eicosatetraenoic acid	304.1857	0.649628	1.568764096
12(13)-Epoxy-9Z-octadecenoic acid	278.2474	-0.20832	0.865543587
12(S)-HpEPE	317.2667	-0.23745	0.848240383
12-Ketodeoxycholic acid	373.2574	-0.30313	0.810491839
13(S)-HODE methyl ester	261.1109	-0.3355	0.792508971
13(S)-HODE-biotin	259.1429	-0.62132	0.650074098
13,14-Dehydro-15-cyclohexyl Carbaprostacyclin	328.1847	-0.48043	0.716765954
13,14-Dihydro-15-ketoprostaglandin F2.alpha. isopropyl ester	202.1076	-0.54706	0.684411727
13,14-Dihydro-15-keto-tetranor prostaglandin F1.beta.	283.1813	-0.29915	0.81273387
13,14-Dihydro-16,16-difluoroprostaglandin J2	355.2437	0.206942	1.154239236
14(15)-EET ethanolamide	345.1051	1.247207	2.373814099
14,15-EE-(5Z)-E	325.2375	-0.15694	0.896928227
14,15-EE-(8Z)-E	307.2269	0.166886	1.122632787
15(R),19(R)-Hydroxyprostaglandin F1.alpha.	353.2298	-0.28065	0.823218504
15(R)-15-Methylprostaglandin D2	348.2107	-0.19848	0.871465401
15(R)-15-Methylprostaglandin F2.alpha. methyl ester	365.2325	-0.28121	0.822900516
15(R)-Methylprostaglandin A2	331.2488	-0.18094	0.882129578
15(S)-15-Methylprostaglandin E2	348.2734	0.200422	1.149034019
15(S)-HpEDE	322.2745	0.276466	1.211223849
15(S)-HpEPE	317.2697	-0.19356	0.874444882
15-HEDE	237.1499	-0.23366	0.850474031
15-Ketofluprostenol	421.229	-0.26788	0.830541854
15-Ketoilprost	341.2342	0.199355	1.148184756
15-Ketoprostaglandin E1	353.2323	-0.29006	0.817866143
15-Ketoprostaglandin E2	332.2164	0.167566	1.123161918
15S-Hydroxy-8Z,11Z,13E-eicosatrienoic acid	287.2373	0.35293	1.277151872
16,16-Dimethylprostaglandin D2	362.2366	0.747176	1.678504002
16,16-Dimethylprostaglandin F2.alpha.	365.2324	-0.30427	0.809850664
16-Phenoxy tetranor prostaglandin F2.alpha. methyl amide	337.1066	-0.3806	0.768119126
16-Phenyl tetranor prostaglandin F2.alpha.	355.2488	0.219134	1.164034496
17.alpha.-Hydroxypregnenolone	315.1826	-0.2273	0.854232654
17.alpha.-Methyltestosterone	285.2066	-0.43409	0.740159136
17-Keto-(7Z,10Z,13Z,15E,19Z)-docosapentaenoic acid	327.2626	0.108354	1.077997475
17-Octadecynoic acid	299.2594	-0.24962	0.841117061
17-Phenoxy trinor prostaglandin F2.alpha. ethyl amide	351.1772	-0.27063	0.828956328
17-Phenyl trinor prostaglandin E2	367.2712	-0.16136	0.894179203
17-trans-Prostaglandin E3	333.2066	0.140089	1.101973452
17-Trifluoromethylphenyl trinor prostaglandin F2.alpha.	361.1462	-0.26304	0.833331086
17-Trifluoromethylphenyl trinor prostaglandin F2.alpha. isopropyl ester	481.2811	-0.30422	0.809881045
19(20)-EpDPE	327.2192	-0.25012	0.840828994

19(R)-Hydroxyprostaglandin B2	333.2077	-0.37607	0.770531827
1H-1,2,4-Triazol-3-amine	86.0986	0.391874	1.312096755
1-Hexadecanoyl-2-sn-glycero-3-phosphate	393.241	-0.32209	0.799907728
1-Hexadecanoyl-sn-glycerol	331.0795	0.247965	1.187531166
1'-Hydroxymidazolam .beta.-D-glucuronide	518.1122	-0.76818	0.587157263
1-Methylnicotinamide cation	137.0721	-1.20277	0.434439805
1-Octadecanoyl-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosph	341.1984	-0.29493	0.81511247
1-Octadecanoyl-sn-glycero-3-phospho-(1'-myo-inositol)	599.3201	0.653142	1.572589388
1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phospho-(1'-rac-glycerol)	367.2105	-0.37558	0.770795874
1-Pentadecanoyl-sn-glycero-3-phosphocholine	269.2097	0.115891	1.083644418
2-(4-Ethoxyphenyl)-4-oxo-4H-chromen-3-yl 4-bromobenzenesulfonate	280.9072	-0.16825	0.889923483
2,3-Dihydroxynaphthalene	161.0309	0.206122	1.153583177
2,4,7,9-Tetramethyl-5-decyne-4,7-diol	243.1946	0.195366	1.14501478
2,5-Dimethoxycinnamic acid	191.9819	0.110146	1.079337649
2,6-Di-tert-butyl-4-hydroxymethylphenol	219.1008	-0.36399	0.777010545
2,6-Xylidine	122.0978	0.331383	1.258218676
20a,20b-Dihomo-9-oxo-11R,15S-dihydroxy-5Z,13E-prostadienoic acid	327.2329	0.278292	1.212758571
20-HETE ethanolamide	345.1031	1.19521	2.289782046
20-Hydroxycholesterol	384.2911	-0.28938	0.818254
24S-Hydroxycholesterol	384.2989	-0.1954	0.873332486
26-Hydroxycholesterol-(25R)	302.1383	-0.40265	0.756466517
2-Amino-1-phenylethanol	120.0807	0.279527	1.213797004
2-Butanone, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	195.1378	0.137103	1.099695015
2-Butenoic acid, 3-methyl-	100.112	-0.36623	0.775808052
2'-Deoxyadenosine 5'-monophosphate	332.0747	0.448528	1.364647508
2'-Deoxyuridine 5'-monophosphate	352.0588	0.615633	1.532229846
2-Ethylhexanal	129.0399	2.008423	4.023421427
2-Fluoropalmitic acid	275.1389	-0.634	0.644387318
2-Keto-D-gluconic acid	174.9581	-0.21564	0.861164457
2-Methoxyestrone	283.1779	0.131162	1.095175663
2-Oxazolidinone, 3-amino-5-(4-morpholinylmethyl)-	203.1425	0.440225	1.356815545
3,2',4',5'-Tetramethoxyflavone	343.0324	-0.31256	0.805212802
3,3',7,8-Tetramethoxyflavone	344.1055	-0.49426	0.709924274
3,4,5-Trimethoxyamphetamine	226.1793	-0.29145	0.817082791
3,4,5-Trimethoxycinnamic acid	239.1564	-0.33383	0.7934254
3',4'-Dimethoxy-3-hydroxy-6-methylflavone	314.1003	-0.43249	0.740979682
3,5,7,3',4'-Pentahydroxyflavanone	305.1606	-0.25236	0.839522169
3,5-Dihydroxybenzyl alcohol	141.0912	-0.15927	0.895475931
3',5'-Dihydroxyflavone	255.1161	-0.22816	0.853720663
3,6,2',4'-Tetrahydroxyflavone	288.2164	-0.70178	0.614812674
3,6-Dimethyl-4-methoxycoumarin	205.085	-0.4109	0.75215436
3,7-Dihydroxy-12-oxocholanoic acid	387.2	0.241846	1.182504874
3,7-Dihydroxy-3',4'-dimethoxyflavone	314.0867	-0.29348	0.815929561
3,7-Dimethyl-9-(2,6,6-trimethylcyclohex-1-enyl)nona-2,4,6,8-tetraenoi	282.9071	1.547706	2.923518139
3.alpha.,7.alpha.,12.alpha.-Trihydroxycholestanoic acid	413.2652	0.28155	1.215500154
3.beta.-14,16.beta.-Trihydroxy-5.beta.-bufa-20,22-dienolide	349.1848	0.160134	1.11739065
3-[(3-Cholamidopropyl)dimethylammonio]-1-propanesulfonate	615.4043	0.358055	1.281696569

3-Dehydroquinic acid	189.094	-0.42729	0.743655043
3-Hydroxy-3-(2-(2-hydroxyphenyl)-2-oxoethyl)-1,3-dihydro-2H-indol-2-	283.2629	-0.17177	0.887752248
3-Hydroxy-3-methylglutaric acid	185.1146	0.358703	1.282272705
3-Hydroxy-6,2',4'-trimethoxyflavone	329.1976	0.499296	1.413523954
3-Hydroxy-7,3',4',5'-tetramethoxyflavone	359.109	0.527459	1.441388141
3-Hydroxy-7,8,2'-trimethoxyflavone	329.197	0.439902	1.356511862
3-Hydroxy-7,8,3'-trimethoxyflavone	330.129	-0.33251	0.79415273
3'-Hydroxy-D-sepiapterin	253.2135	-0.2336	0.85050779
3-Indoleacetic acid	176.0702	-0.28459	0.820975308
3-Methoxyprostaglandin F1.alpha.	369.2652	-0.1578	0.896389711
3-Ureidopropionic acid	132.0306	1.331854	2.517258716
4,5-Dehydrodocosaehaenoic Acid	327.2511	-0.13473	0.910842861
4',7-Dimethoxy-8-methylisoflavone	297.0823	0.214533	1.160328654
4,7-Dimethyl-3-(4-methoxyphenyl)coumarin	281.2206	-0.12332	0.918072451
4-Androsten-3.alpha.-ol-17-one	271.1866	-0.42546	0.744602398
4-Androstene-3,17-dione	309.2407	0.170373	1.125349046
4-Hydrazinobenzenesulfonic acid	81.033	0.694498	1.618321155
4'-Hydroxy-6-methylflavone	251.1853	-0.35665	0.780977686
4-Hydroxyhexenal	114.0921	-0.45086	0.731604426
4-Imidazolecarboxaldehyde	112.0507	-0.17867	0.883517723
5-(3,5-Dimethoxybenzylidene)-2-thioxo-1,3-thiazolidin-4-one	283.0143	0.460032	1.375572087
5(6)-EpETE methyl ester	315.1346	-0.22267	0.85697711
5-(Galactosylhydroxy)-L-lysine	325.1614	0.46883	1.383986401
5(S),14(R)-Lipoxin B4	352.3369	-0.28393	0.821353002
5(S),6(R),15(R)-Lipoxin A4	334.183	-0.45999	0.7269897
5(Z),8(Z),11(Z)-Eicosatrienoic acid methyl ester	321.1299	-0.37621	0.770457156
5,16-Pregnadien-3.beta.-ol-20-one	315.1851	-0.19919	0.871038092
5,6-DiHETE	318.2268	-0.31712	0.802670252
5,7-Dimethoxy-4-methylcoumarin	222.1149	0.119599	1.086432895
5.alpha.-Hydroxy-6-ketocholesterol	418.2804	-0.18389	0.880327113
5.alpha.-Pregnan-3.alpha.-ol-11,20-dione	314.2682	0.403082	1.32232957
5-Aminolevulinic acid	114.0926	-0.4898	0.712122896
5-Aminouracil	129.0545	-0.77798	0.583183684
5-Aminovaleric acid	100.0773	-0.45806	0.727963143
5-Androsten-3.beta.-ol-17-one	271.19	-0.1153	0.923189554
5-Hydroxyflavone	239.0776	-0.28894	0.818500775
5-Pregnen-3.beta.-ol-20-one	299.2579	-0.29466	0.815265268
5S-Hydroxy-6E,8Z,11Z-eicosatrienoic acid	305.2477	0.304143	1.234684687
5-trans U-44069	332.2173	0.105124	1.075587113
5-trans-Prostaglandin F2.alpha.	337.2381	-0.26808	0.830423241
6,7,3',4'-Tetramethoxyisoflavone	344.2398	-0.22477	0.855731842
6,7-Dihydroxycoumarin-4-acetic acid	237.1483	-0.19639	0.872733007
6,7-Dimethoxy-4-ethylcoumarin	236.2226	0.08678	1.061997443
6.beta.-Hydroxytestosterone	304.1756	-0.20958	0.864790896
6.beta.-Testosterone enanthate	399.2515	-0.36378	0.777128212
6-Ketoprostaglandin E1	351.0986	0.249684	1.188946804
6-Ketoprostaglandin F1.alpha.	353.2328	-0.28412	0.821242869

7,8,2'-Trihydroxyflavone	268.1893	-0.44659	0.733775438
7,8,3',4'-Tetrahydroxyflavone	285.1181	-0.24344	0.844728719
7,8,4'-Trimethoxyisoflavone	314.0957	-0.46082	0.726573141
7.alpha.,27-Dihydroxycholesterol	441.2371	-0.32492	0.798342853
7-Aminonitrazepam	253.007	-0.32514	0.79822124
7-Dimethylamino-4-methylcoumarin	205.1198	0.103799	1.074599311
7-Hydroxy-3-methylflavone	253.2167	-0.21716	0.860255756
7-Keto-8-aminopelargonic acid	185.0576	0.282947	1.216677338
7-Methoxy-4-methylcoumarin	190.012	0.164213	1.120554417
7-Methoxycoumarin-4-acetic acid	236.1647	-0.29525	0.814930555
8(9)-EET ethanolamide	345.1075	0.351126	1.275555724
8(S),15(S)-DiHETE	273.1103	-0.31246	0.805266236
8,11,14-Eicosatriynoic acid	299.2192	-0.20395	0.868169756
8-Chloro-1-octanol	165.0757	-1.41591	0.374772546
9(11),(5.alpha.)-Androsten-3.beta.-ol-17-one	288.2151	0.120867	1.087387963
9(11),(5.beta.)-Pregnen-3,20-dione	316.2843	0.430577	1.347772794
9,11-Didehydrooestriol	269.2106	-0.15993	0.895070014
9,11-Dioxo-15S-hydroxy-5Z,13E-prostadienoic acid	315.1562	0.186965	1.138366041
9-Hydroxy-5Z,7E,11Z,14Z-eicosatetraenoic acid	302.2314	-0.35079	0.784156327
9-Octadecenamide, (Z)-	282.2794	0.143457	1.10454892
9-Oxo-11R,15S,20-trihydroxy-5Z,13E-prostadienoic acid	351.2188	-0.22838	0.853595461
9-Oxo-15S-hydroxy-10Z,13E-prostadienoic acid-cyclo[8S,12S]	319.1899	-0.20002	0.870540114
9-Oxo-15S-hydroxy-5Z,10Z,13E,17Z-prostatetraenoic acid	315.1938	-0.23356	0.850532325
9-Oxo-15S-hydroxy-5Z,8(12),13E,17Z-prostatetraenoic acid	333.2066	-0.2624	0.833702744
9S,11,15S-Trihydroxythrombox-13E-enoic acid	300.1509	0.102429	1.073579304
9S,11R,15S-Trihydroxy-13E-prostaenoic acid	337.1063	-0.25245	0.839469818
9S,11R,15S-Trihydroxy-20a,20b-dihomo-5Z,13E-prostadienoic acid	365.1389	-0.30615	0.808796977
9S,11R-Dihydroxy-15-oxoprostanoic acid	304.1161	0.250799	1.189865923
9S,11R-Epidioxy-15S-hydroperoxy-5Z,13E-prostadienoic acid	355.2488	-0.3447	0.787470785
9S,15S-Dihydroxy-11-oxothromboxa-5Z,13E,17Z-trienoic acid	349.2001	-0.31162	0.80573697
9S,15S-Dihydroxy-5Z,13E-prostadienoic acid	319.2281	0.321258	1.24941923
Acetyl-DL-carnitine	204.1231	1.028072	2.039297405
Acipimox	110.0717	0.920628	1.892938798
Acitretin	309.2054	0.211104	1.157573345
Adenosine 5'-triphosphate	347.0279	0.650691	1.5699199
Adenylyl(3'-5')cytidine	573.1467	0.352391	1.276674861
Alpinetin	167.1168	-0.51542	0.699591256
Amodiaquin	357.1041	0.499386	1.413611848
Androst-4-en-3-one, 17- (1-oxopropoxy)-, (17.beta.)-	289.1069	-0.5285	0.693276531
Androstane-3,17-diol, (3.alpha.,5.alpha.,17.beta.)-	274.1841	-0.4482	0.732954631
Arachidonoyl amide	305.1278	-0.28125	0.822877896
Arachidonoyl-1-thioglycerol	305.2474	0.297192	1.228750575
Araguspongin B	236.1638	-0.29756	0.813626481
Atenolol	267.1686	-0.72709	0.60412292
Azelaic acid	188.1275	0.246407	1.186249492
Batyl alcohol	345.1045	1.21884	2.327594903
Bavachinin	321.1317	-0.53996	0.687789229

Beclomethasone	337.106	0.136935	1.099566346
Benzenamine, N,N-dimethyl-	122.097	0.29673	1.228357321
Benzeneethanol, 2-hydroxy-	120.0804	0.278609	1.213025028
Benzoic acid, 4-hydroxy-	121.0424	-0.35234	0.783314463
Benzyl butyl phthalate	313.1444	-0.25054	0.840583375
Bicyclo[2.2.1]heptane-2-methanol	109.1022	-0.35364	0.782608853
Bilobalide	308.2268	-0.15799	0.896269924
Bimatoprost diethylamide	335.221	0.433678	1.350672836
Bimatoprost isopropyl ester	353.2286	-0.28956	0.818150153
Biotin	245.1003	-0.55708	0.679678235
Bisphenol A bis(2,3-dihydroxypropyl) ether	394.2235	0.125055	1.090549202
Bolasterone	299.2582	-0.28887	0.818543598
Boldenone	269.2102	-0.20304	0.868720218
Budesonide	430.2672	-0.19052	0.876292493
Buflomedil	309.2434	0.119898	1.086658406
Calcipotriol	394.2968	0.353256	1.277440069
Cantharidin	197.1525	-0.31309	0.804914041
Carbaprostacyclin	315.2545	0.198327	1.147367424
Carboxyibuprofen	219.1345	-0.30324	0.810430106
CAY10410	301.0049	-0.34181	0.789050386
Ceftriaxone	555.0539	0.563386	1.477733195
Cholest-5-ene-3.beta.,22(S)-diol	384.0351	-0.38229	0.767219592
Cholest-5-ene-3.beta.,4.beta.-diol	384.2965	-0.37866	0.769153419
Cholesta-4,6-dien-3-one	383.3333	-0.24658	0.84289253
Cholesta-5,7-dien-3-ol, (3.beta.)-	384.2203	-0.17593	0.885194063
Cholic acid	373.2006	-0.35265	0.783143417
Ciprofibrate	270.1632	0.446367	1.362604542
cis-10-Heptadecenoic acid	269.2478	-0.11487	0.923464375
cis-4,10,13,16-Docosatetraenoic acid	333.2798	0.343253	1.268614081
cis-4,7,10,13,16,19-Docosahexaenoic acid	329.2477	0.285096	1.218491299
cis-5,8,11,14-Eicosatetraenoic acid	305.2473	0.301153	1.232128548
cis-5,8,11-Eicosatrienoic acid	329.2333	-0.30313	0.81049002
cis-7,10,13,16-Docosatetraenoic acid	333.2985	0.417179	1.335313608
cis-7-Hexadecenoic acid methyl ester	269.2105	-0.22713	0.854329859
cis-Vaccenic acid	283.1873	-0.24343	0.844737365
Clasto-lactacystin .beta.-lactone	234.9814	-0.45118	0.731444958
Coenzyme Q1	251.1606	-0.10803	0.927852041
Colchicine	399.1746	-0.09282	0.937689595
Conjugated linoleic acid (9E,11E)	263.2367	0.350374	1.274891136
Corilagin	317.1142	0.126165	1.091388953
Cortisone	343.1739	-0.35786	0.780322537
Cuminaldehyde	149.0595	0.145857	1.106387652
Cyclopentasiloxane, decamethyl-	371.1036	0.604143	1.520075758
Cyclopropanecarboxylic acid, 1-amino-	102.056	0.200515	1.14910885
Cytidine	243.1094	0.338912	1.264802763
Cytidine 5'-diphosphocholine	489.1148	0.456924	1.372612095
Cytosine	112.0869	2.758718	6.767946234

D-(-)-Ribose	133.0328	0.245407	1.185426902
D-(+)-Mannose	360.1523	-0.3051	0.809388384
D-(+)-Trehalose	325.1136	-0.7178	0.608022545
Decapropylene glycol monobutyl ether	656.0063	-0.56069	0.677976624
D-erythro-C18-Sphingosine	283.1033	-0.24654	0.84291363
Desogestrel	311.2205	-0.1739	0.886440236
Dexpanthenol	206.1383	0.404715	1.323827309
D-Fructose 1,6-bisphosphate	217.0682	0.411462	1.330032569
D-Glucosyl-.beta.1-1'-D-erythro-sphingosine	253.2631	-0.20572	0.867107125
D-Glucuronic acid	177.0064	-0.60978	0.65529877
Dibutyl adipate	259.1905	0.347112	1.272012021
Dihydroartemisinin	267.1233	-0.15718	0.896779228
Dihydrouracil	229.1293	-0.48614	0.7139311
Dimethipin	210.1149	-0.58997	0.664357432
Dimethylfraxetin	175.0213	-0.27433	0.8268323
Dimetridazole	141.0664	0.484636	1.399232356
Dinitramine	323.0554	0.403292	1.322522085
Dinor-12-oxophytodienoic Acid	265.2152	-0.23901	0.847324327
DL-2,3-Diaminopropionic acid	88.0408	0.237997	1.179354504
DL-Arginine	175.1192	-1.82168	0.282891387
DL-Lysine, 5-hydroxy-	163.1087	0.43827	1.354978911
DL-Methionine	150.0589	0.27154	1.207095486
D-Mannitol	183.0864	-0.55954	0.678519624
D-myo-Inositol-4-phosphate	261.0378	-0.21796	0.859782382
Docosahexaenoic acid ethyl ester	357.2783	-0.29848	0.81310659
Docosatetraenoyl ethanolamide	357.2754	-0.16479	0.892056183
Dodecanedioic acid	213.1487	-0.28715	0.819518156
Dodecanoic acid	182.9631	-0.28555	0.820431404
Donepezil	380.2232	0.387812	1.308407852
D-Psicose	181.0836	0.599726	1.515428461
D-Pyroglutamic acid	130.0504	0.351383	1.275782869
D-Quinovose	163.026	0.434899	1.351816119
D-Sorbitol	183.0859	-0.91104	0.531802483
Dulcitol	165.0883	-0.91104	0.531802483
Eicosapentaenoic acid ethyl ester	331.0807	-1.01091	0.496232399
Eicosapentaenoyl ethanolamide	345.1025	1.203022	2.302214873
Enrofloxacin	332.1394	-0.71899	0.607521217
ent-Corey PG-Lactone diol	250.1784	-0.13524	0.910516173
Enterodiol	303.1777	0.363013	1.286108709
Enterolactone	281.2954	-0.28436	0.821104518
Erythromycin	716.4658	-0.89672	0.537105621
Estriol	253.2157	-0.43341	0.740509725
Estrone	271.225	-0.30631	0.808706039
Ethidimuron	114.0911	0.275015	1.210006344
Ethyl 7-hydroxycoumarin-4-carboxylate	207.1112	-0.29677	0.814072538
Fenthion sulfoxide	262.1414	-0.24936	0.841270637
Finasteride	318.1706	-0.62237	0.649601842

Flumethasone pivalate	374.2129	0.400661	1.320112978
Fluocinolone acetonide	337.1043	-0.22161	0.857607551
Fluorometholone	341.1858	0.344399	1.269622138
Flurandrenolide	341.2666	-0.20184	0.869441017
Fluvastatin	395.2404	-0.31295	0.804993627
Formestane	285.0943	0.331581	1.258391879
Fumonisin B2	337.2701	0.315407	1.244362526
Gemfibrozil	250.1779	0.28849	1.221360899
Genistein	271.1889	-0.09252	0.93788573
Glucoheptonic acid	225.0569	-0.45036	0.731860292
Glycan Chitobiose	288.0789	0.287377	1.220419665
Glycan Lacto-N-biose	384.1512	0.378231	1.299747378
Glycan Le-X Trisaccharide	530.2123	-0.33512	0.79271594
Glycan N-Acetylglucosamine	384.1537	0.540337	1.454312042
Glycerol 1-stearate	359.3162	0.199149	1.148021002
Glycodeoxycholic acid	414.3026	0.410291	1.328953976
Glycoursodeoxycholic acid	432.3114	0.358235	1.28185649
Glycyl-L-norleucine	189.0726	-0.3638	0.7771176
Granisetron	139.1226	-0.5033	0.705492992
Guanidinosuccinic acid	176.0663	0.704691	1.62979528
Heptadecanoyl ethanolamide	297.1687	0.923122	1.896213697
Heptadecaspheing-4-enine	269.2108	-0.29865	0.81301101
Heptapropylene glycol	425.3125	-0.21541	0.861303409
Hexapropylene glycol	367.2702	-0.1954	0.873329435
Hydrocortisone	363.2155	0.645643	1.564436932
Hydromorphone	286.1416	-1.13594	0.455038628
I-BOP	351.0973	-0.41737	0.748787133
Iloprost	325.1992	-0.24255	0.845250694
Indole-3-pyruvic acid	203.035	-0.28962	0.818115778
Inosine, 2'-deoxy-	270.108	-0.22885	0.853313799
iPF2.alpha.-IV	336.2079	0.270775	1.206455983
Isopentenyl pyrophosphate	251.1278	-0.13509	0.910615352
Isopimaric acid	285.094	0.284677	1.218137678
Isosorbide	147.0637	-1.08546	0.471243596
Jasmonic acid	211.1323	-0.38596	0.765267823
Ketogluconic acid methyl ester	209.1376	0.19051	1.141167054
L-(+)-Gulose	181.0842	0.600081	1.51580196
L-Arabinitol	175.1443	-0.58322	0.66747388
L-Arginine	175.1191	0.257923	1.195756113
L-Asparagine	116.0348	0.233449	1.175642324
Latrunculin B	359.1082	-0.38585	0.765328048
L-Canavanine	159.0272	-0.24754	0.842331522
L-Carnitine	162.1116	2.307592	4.95056078
L-Citrulline	176.104	0.473771	1.388734623
Leukotriene B3	275.1952	-0.0921	0.938158485
Leukotriene B4	319.2253	-0.27272	0.827759134
Leukotriene D4 methyl ester	391.0128	-0.21641	0.860706803

L-Fucitol	167.0902	-0.42174	0.746524488
L-Glutamine	130.0507	-0.3603	0.779005057
Linoleic acid	281.2462	-0.83702	0.559797643
L-Isoleucine	132.1031	0.442983	1.359411934
L-Lysine	130.0867	0.230535	1.173269588
L-Methionine	150.0581	0.273507	1.208742917
Lobeline	109.0771	0.96451	1.95140099
Loratadine	383.1535	-0.31883	0.801719342
L-Pipecolic acid	130.0868	0.231304	1.173895775
L-Proline	116.0349	0.234184	1.176241178
Lysine, butyl ester	204.1345	1.502619	2.83356705
Maltitol	345.139	-0.69134	0.61928047
Mefluidide	136.0482	2.299376	4.922447927
Mesterolone	305.1965	-0.10917	0.927120479
Methimazole	116.0349	0.234184	1.176241178
Methyl .beta.-D-galactopyranoside	195.1218	-0.2113	0.863760753
Methyl 7-hydroxycoumarin-4-acetate	234.9496	-0.21688	0.860421502
Methyl jasmonate	175.0404	-0.29773	0.813531464
Methyl myristoleate	241.1787	-0.21065	0.864146908
Methylprednisolone succinate	339.2698	0.256753	1.194786759
Mifepristone	413.2668	0.226104	1.169671671
Misoprostol, free acid	351.2083	-0.2532	0.839035549
Mono-2-ethylhexyl phthalate	277.1805	-0.20793	0.865778748
Monoerucin	321.1327	-0.2104	0.864295773
Monolinolenin (9c,12c,15c)	261.1364	0.268455	1.204517109
Mononervonin (15c)	404.2689	0.168021	1.123515968
Mono-n-octyl phthalate	277.1797	-0.19656	0.872627215
Myristic acid alkyne	109.1019	-0.16034	0.894816743
Myristoleic acid	227.1634	-0.21956	0.858829671
N-(11R,15S-Dihydroxy-9-oxo-5Z,13E-prostadienoyl)-ethanolamine	377.3244	0.223166	1.167292568
N-(8Z,11Z,14Z-Eicosatrienoyl)ethanolamine	331.2249	0.186609	1.138085312
N(G),N(G')-Dimethyl-L-arginine	225.184	-0.40444	0.755527025
N.alpha.-(tert-Butoxycarbonyl)-L-Histidine	255.1468	0.499554	1.41377666
N.alpha.-Acetyl-L-lysine	189.1225	-0.50491	0.70470386
N.epsilon.-Acetyl-L-lysine	189.1233	-0.53878	0.688350955
N.epsilon.-Methyl-L-lysine	161.1291	0.788162	1.726873279
N1-Acetylspermine	266.1525	-0.53541	0.689961069
N-3-Oxododecanoyl-L-homoserine lactone	197.1509	-0.30831	0.807587944
N-3-Oxotetradec-7Z-enoyl-L-homoserine lactone	205.0864	-0.36358	0.777230962
N-Acetyl-D-glucosamine	204.0874	0.592792	1.508162481
N-Acetyl-D-glucosamine 6-phosphate	324.0456	0.377806	1.299364752
N-Acetyl-D-lactosamine	384.1507	0.375071	1.296903413
N-Acetyl-D-mannosamine	204.0862	0.590771	1.506050935
N-Acetylglucosaminylasparagine	336.1418	0.262326	1.199411085
N-Acetyl-L-aspartic acid	176.0553	0.714219	1.640594617
N-Acetylneuraminic Acid, 2,3-Dehydro-2-deoxy-	274.0927	0.460783	1.376288821
Nalbuphine	357.1515	0.607253	1.523355382

Nandrolone	257.1359	-0.32238	0.799748661
N-Cyclohexanecarbonylpentadecylamine	338.0669	-0.24536	0.843605488
Nicotine	163.1233	-0.33407	0.793296626
Nicotinic acid adenine dinucleotide	664.1226	-0.63388	0.644441821
Nilotinib	266.1485	0.949144	1.930726746
Nis(monooleoylglycero)phosphate (S,R Isomer)	441.0468	0.228464	1.171586949
N-Methyl-D-aspartic acid	148.062	0.341304	1.266901277
N-Methyl-D-glucamine	129.0398	2.022194	4.062009388
N-Methylnicotinic acid cation	138.0552	0.658217	1.578131024
N-n-Butylpropionamide	130.1597	-0.43616	0.739097966
Nobiletin	403.2416	0.459866	1.375414312
Nonapropylene glycol	541.3982	-0.25074	0.840467467
Nonapropylene glycol monobutyl ether	597.9586	-0.55849	0.679012629
Norcodeine	267.1351	-0.33799	0.791142135
Norethindrone	299.2003	-0.32049	0.800795318
N-Undecanoyl-L-homoserine lactone	253.2144	-0.2185	0.859457639
O-2545	275.1714	-0.27794	0.824768358
Octadec-9-enoic acid butyl ester	265.2536	-0.48096	0.716499495
Ofloxacin	362.1523	-1.80456	0.286268524
o-Phenylenediamine	110.0275	0.474867	1.389790095
Oxycodone	316.113	-0.35501	0.781862803
Palitantin	254.1381	-0.34596	0.78678379
Palmitamide	256.2644	0.198392	1.147418877
Palmitoylcarnitine	400.3418	0.470091	1.385196747
Peimisine	427.1943	-0.27005	0.829293673
Pentadecanoic acid	225.1499	-0.15095	0.900657224
Pentadecanoic acid, 14-methyl-	257.1373	-0.30774	0.807905448
Phenol, 4-(2-aminoethyl)-	120.081	0.305825	1.236125735
Phenol, o-amino-	110.0276	0.47538	1.390284807
Phenprobamate	179.0747	-0.36381	0.777109705
Phosphoric acid	116.035	0.231345	1.173928566
Phthalic anhydride	149.0233	-0.35849	0.779983107
Phytanic acid	110.0098	0.139552	1.101562773
Phytomonic acid	298.2752	-0.14687	0.903205067
Phytosphingosine	281.2489	-0.213	0.862742003
Piceatannol	245.0993	-0.52769	0.693662736
Pinolenic acid	278.2489	-0.19671	0.872536026
Pinolenic acid methyl ester	261.1107	-0.35095	0.784069423
PIT-1	336.211	0.370614	1.292903221
Prednisone	341.2685	-0.24469	0.843999345
Pregabalin	160.133	1.486973	2.803002974
Prostaglandin A1 methyl ester	274.1459	-0.29084	0.817426123
Prostaglandin A2 methyl ester	331.0988	-0.73782	0.599644892
Prostaglandin D1 alcohol	322.97	0.277254	1.211886019
Prostaglandin E1	338.0489	0.131203	1.095206764
Prostaglandin E1 alcohol	305.2456	0.275199	1.210161384
Prostaglandin E1 ethanolamide	379.1916	-0.37958	0.768659641

Prostaglandin E2 p-benzamidophenyl ester	281.2206	-0.28133	0.822830876
Prostaglandin F2.alpha.	335.2222	0.426283	1.34376698
Prostaglandin F2.alpha. 1,9-lactone	319.2253	-0.10765	0.92809839
Prostaglandin F2.alpha. Alcohol	305.1598	-0.0869	0.941544104
Prostaglandin F2.alpha. isopropyl ester	301.14	-0.24495	0.843844297
Prostaglandin H2	335.1201	-0.31079	0.806198067
Prostaglandin K1	289.0419	0.291506	1.223916951
Pterostilbene	257.2103	-0.20662	0.866562605
p-Toluenesulfonic acid	173.0784	-0.31451	0.804123501
Purmorphamine	262.1656	0.113433	1.081799272
Pyridoxamine	169.0576	-0.17513	0.885690513
Quinestrol	296.1549	-0.13399	0.91130894
Quinine	325.1898	-0.18642	0.878781822
Resveratrol	229.1411	-0.25741	0.836588934
Retinoic acid	301.1401	-0.24343	0.844737365
Ricinoleic acid methyl ester	295.1897	-0.17928	0.883145294
Ropinirole	261.1288	-0.42037	0.747234919
S-1 Methanandamide	345.1035	1.172781	2.254459135
Sclerotiorin	373.1989	-0.38378	0.766428995
Sebacic acid monomethyl ester	199.1696	-0.3834	0.766626304
Sepiapterin	239.1563	-0.30069	0.811866579
Serotonin	177.1021	0.288466	1.221341298
Sinapyl alcohol	211.0587	0.110146	1.079337649
S-Lactoylglutathione	402.1067	0.353149	1.277346115
Stearidonic acid	277.2164	-0.21823	0.859618911
Stearidonic acid ethyl ester	305.128	-0.21639	0.860717927
Stearidonic acid methyl ester	291.2557	-0.31297	0.804982944
Sucrose	325.1144	-0.39276	0.761671679
Taurine	376.0528	1.80208	3.487225477
Tauroursodeoxycholic acid	500.3075	-0.25555	0.837666242
Testosterone	289.2116	-0.10556	0.929444168
Tetradecanedioic acid	241.1044	-0.34144	0.789253278
Tetradecanoyl coenzyme A	160.0628	-0.13937	0.907914686
Tetrazepam	288.1908	0.154736	1.113217972
Thiothixene	429.2392	-0.15116	0.900523212
Tibolone	313.2378	-0.18149	0.881789054
trans-.DELTA.2-11-Methyldodecenoic Acid	214.18	-0.25997	0.835103305
trans-13-Octadecenoic acid	283.2617	-0.2467	0.842822723
trans-4-(Aminomethyl)cyclohexanecarboxylic acid	158.1172	-0.18165	0.881691567
trans-8, trans-10-Dodecadien-1-ol	183.0859	-0.34346	0.788150846
trans-Androsterone	273.1717	0.163251	1.119807553
trans-Cinnamic acid	131.05	-0.47143	0.72124701
trans-Traumatic acid	227.1292	-0.48702	0.71349906
Tributyl phosphate	533.3385	0.297426	1.228950179
Trinexapac-ethyl	253.2129	-0.22412	0.856115472
Tris(2-butoxyethyl) phosphate	399.2519	0.877343	1.836989259
Troxol	250.1792	-0.44725	0.733440081

Tryptamine	321.905	0.234598	1.176578508
Undecanedioic acid	217.1035	-0.37147	0.772994471
Uracil	113.0349	0.727677	1.655970056
Ureidosuccinic acid	176.0557	0.638042	1.556215741
Uridine, 5-methyl-	281.2479	0.140241	1.102089304
Zearalenone	301.1397	-0.71891	0.607557086