

Aldehydes

1	4-hydroxybenzaldehyde	HMDB0011718
2	trans-2-Hexenal	HMDB0031496
3	Glyoxylic Acid	HMDB0000119
4	4-Hydroxynonenal	HMDB0004362

Alkaloids and Derivatives

1	Piperine	HMDB0029377
2	Trigonelline	HMDB0000875
3	caffeine	HMDB0001847

Phenolic acids

1	4-Hydroxyphenylacetic acid	HMDB0000020
2	3,5-dihydroxybenzoic acid	HMDB0013677
3	p-coumaric acid	HMDB0002035
4	Ferulic acid	HMDB0000954
5	Ferulic Acid 4-glucuronide	HMDB0041733
6	3,4-Dihydroxybutyric acid	HMDB0000337
7	4-Hydroxybenzoic acid	HMDB0000500
8	3-Hydroxyphenylacetic acid	HMDB0000440
9	2-Hydroxyphenylacetic acid	HMDB0000669
10	3,4-Dihydroxyphenylacetic acid	HMDB0001336
11	Vanillic acid	HMDB0000913
12	Vanillic acid	HMDB0000484
13	Syringic acid	HMDB0002085
14	Avenanthramide A	HMDB0038577
15	o-coumaric acid	HMDB0002641
16	4-Pyridoxic Acid	HMDB0000017

Amino acids and Derivatives

1	5-Aminovaleric acid	HMDB0003355
2	Ectonine	HMDB0240650
3	Alliin	HMDB0301759
4	4-Oxo-L-Proline	HMDB0246561
5	Nicotinic Acid	HMDB0003269
6	S-Allylcysteine	HMDB0034323
7	2-Methylbutyrylglycine	HMDB0000339
8	5-Hydroxylysine	HMDB0000450
9	Methylhistidine	HMDB0000479
10	Ergothioneine	HMDB0003045

Fatty Acids and Derivatives

1	gamma-Linolenic acid	HMDB0003073
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Amino acids and Derivatives

1	3-Aminobutyric acid	HMDB0031654
2	Beta-Leucine	HMDB0003640
3	3-MethoxyTyrosine	HMDB0001434
4	Formiminoglutamic acid	HMDB0000854
5	3-Hydroxyhippuric acid	HMDB0006116
6	S-phenylmercapturic acid	HMDB0042011
7	N1-Acetyl-Lysine + N6-Acetyl-Lysine	HMDB0000206
8	N1-Acetyl-Lysine	HMDB0000446
9	N-Acetyl-Histidine	HMDB0032055
10	N-Acetyl-Arginine	HMDB0004620
11	3-Aminoisobutyric acid	HMDB0003911
12	Dimethylglycine	HMDB0000092
13	N-Acetyl-Asparagine	HMDB0006028
14	N-Acetyl-Serine	HMDB0002931
15	N-Acetyl-Glutamine	HMDB0006029
16	N-Acetyl-Glycine	HMDB0000532
17	5-Oxoproline	HMDB0000267
18	N-Methyl-Aspartic acid	HMDB0002393
19	N-Acetyl-Alanine	HMDB0000766
20	N-Acetyl-Proline	HMDB0094701
21	p-Hydroxyhippuric acid	HMDB0013678
22	N-Acetyl-Tyrosine	HMDB0000866
23	N-Acetyl-Valine	HMDB0011757
24	5-Aminolevulinic Acid	HMDB0001149
25	N-Acetyl-Methionine	HMDB0011745
26	Tiglylglycine	HMDB0000959
27	Phenylacetylglutamine	HMDB0006344
28	N-Acetyl-Aspartic acid	HMDB0000812
29	N-Acetyl-Isoleucine	HMDB0061684
30	N-Acetyl-Glutamic acid	HMDB0001138
31	N-Acetyl-Leucine	HMDB0011756
32	AABA	HMDB0000452
33	ADMA	HMDB0001539
34	Ala	HMDB0000161
35	alpha-Aminoadipic acid	HMDB0000510
36	Arg	HMDB0000517
37	Asn	HMDB0000168
38	Asp	HMDB0000191
39	beta-Alanine	HMDB0000056
40	cis-4-Hydroxyproline	HMDB0240251

41	Citrulline	HMDB0000904
42	Cystathionine	HMDB0000099
43	GABA	HMDB0000112
44	Gln	HMDB0000641
45	Glu	HMDB0000148
46	Gly	HMDB0000123
47	His	HMDB0000177
48	Homoarginine	HMDB0000670
49	Homocitrulline	HMDB0000679
50	Homocysteine	HMDB0000742
51	Ile	HMDB0000172
52	Leu	HMDB0000687
53	Lys	HMDB0000182
54	Met	HMDB0000696
55	Methionine sulfoxide	HMDB0002005
56	N2-Acetyl-Orn	HMDB0003357
57	Nitro-Tyr	HMDB0001904
58	Orn	HMDB0000214
59	Phe	HMDB0000159
60	Pro	HMDB0000162
61	Sarcosine	HMDB0000271
62	Ser	HMDB0000187
63	Thr	HMDB0000167
64	trans-4-Hydroxyproline	HMDB0000725
65	Tyr	HMDB0000158
66	Val	HMDB0000883
67	2-Aminopimelic acid	HMDB0034252
68	Proline betaine	HMDB0004827

Bile Acids

1	Taurolithocholic acid 3-sulfate	HMDB0002580
2	Muricholic acid	HMDB0000364+HMDB0000506+ HMDB0000415
3	Chenodeoxycholic acid	HMDB0000518
4	Deoxycholic acid	HMDB0000626
5	Tauromuricholic acid	HMDB0000932
6	Tauroursodeoxycholic acid	HMDB0000874
7	taurocholic acid	HMDB0000036
8	taurochenodeoxycholic acid	HMDB0000951
9	Taurodeoxycholic acid	HMDB0000896
10	Glycocholic acid	HMDB0000138
11	Taurolithocholic acid	HMDB0000722
12	Cholic acid	HMDB0000619
13	Ursodeoxycholic acid	HMDB0000946

14	Hyodeoxycholic acid	HMDB0000733
15	Glycochenodeoxycholic Acid	NA
16	Glycodeoxycholic acid	NA
17	Glycolithocholic acid	HMDB0000698
18	Lithocholic acid	HMDB0000761

Biogenic Amines

1	N1-Acetylspermine	HMDB0001186
2	1,3-Diaminopropane	HMDB0000002
3	3-Methoxytyramine	HMDB0000022
4	Agmatine	HMDB0001432
5	Cadaverine	HMDB0002322
6	Diacetylspermine	HMDB0002172
7	Dimethylamine	HMDB0000087
8	Ethanolamine	HMDB0000149
9	Histamine	HMDB0000870
10	Methylamine	HMDB0000164
11	N1-Acetylspermidine	HMDB0001276
12	N-Acetylputrescine	HMDB0002064
13	Phenylethylamine	HMDB0012275
14	Putrescine	HMDB0001414
15	Spermidine	HMDB0001257
16	Spermine	HMDB0001256
17	Trimethylamine	HMDB0000906
18	Tyramine	HMDB0000306
19	Creatinine	HMDB0000562
20	TMAO	HMDB0000925

Catecholamines and Derivatives

1	DOPA	HMDB0000181
2	Dopamine	HMDB0000073
3	Epinephrine	HMDB0000068
4	Norepinephrine	HMDB0000216
5	Hydroxytyrosol	HMDB0005784
6	Dopamine 3-O-sulfate	HMDB0006275
7	Metanephrine	HMDB0004063

Dipeptides

1	Cyclo(L-Pro-L-Val)	HMDB0240493
2	Anserine	HMDB0000194
3	Glycyl-Glycine	HMDB0011733
4	Glycylvaline	HMDB0028854

5	Phenylalanylglycine	HMDB0028995
6	Glycylleucine	HMDB0000759
7	Aspartylleucine	HMDB0028757
8	enterolactone	HMDB0006101
9	Carnosine	HMDB0000033

Drugs, Pollutants, Food Additives, and Toxic Compounds

1	Ethylparaben	HMDB0032573
2	Ibuprofen	HMDB0001925
3	Cotinine	HMDB0001046

Fatty Acids and Derivatives

1	3-Hydroxy propionic acid	HMDB0000700
2	2-hydroxymethylbutanoic acid	
3	Azelaic acid	HMDB0000784
4	Itaconic acid	HMDB0002092
5	Adipic acid	HMDB0000448
6	Citraconic acid	HMDB0000634
7	3-Methylglutaric acid	HMDB0000752
8	Pimelic acid	HMDB0000857
9	3-Methylglutaconic acid	HMDB0000522
10	3-Methylvaleric acid	HMDB0033774
11	2-Isopropylmalic acid	HMDB0000402
12	Heptanoic acid	HMDB0000666
13	Pelargonic acid	HMDB0000847
14	Undecylenic acid	HMDB0033724
15	Capric acid	HMDB0000511
16	Undecylic acid	HMDB0000947
17	Tridecylic acid	HMDB0000910
18	cis-8, 11, 14-Eicosatrienoic acid	HMDB0002925
19	Erucic acid	HMDB0002068
20	Behenic acid	HMDB0000944
21	Butyric acid + Isobutyric acid	HMDB0000039
22	2-Hydroxy-3-methylvaleric acid+2-hydroxy-4-methylpentanoic acid	HMDB0000317+HMDB0000624
23	3-Hydroxypentanoic acid	HMDB0000531
24	3-Hydroxysebacic acid	HMDB0000350
25	2-oxovaleric acid	HMDB0001865
26	Docosahexaenoic acid	HMDB0002183
27	Myristic acid	HMDB0000806
28	Palmitoleic acid	HMDB0003229
29	Linoleic acid	HMDB0000673
30	alpha-linolenic acid	HMDB0001388
31	Pentadecylic acid	HMDB0000826
32	Palmitic acid	HMDB0000220

33	Margaric acid	HMDB0002259
34	Pristanic acid	HMDB0000795
35	Phytanic acid	HMDB0000801
36	Propionic acid	HMDB0000237
37	Isovaleric acid	HMDB0000718
38	Lactic acid	HMDB0000190
39	3-Hydroxyisobutyric acid	HMDB0000336
40	2-Hydroxyisobutyric acid	HMDB0000729
41	3-Hydroxyisovaleric acid	HMDB0000754
42	2-Hydroxybutyric acid	HMDB0000008
43	3-(3-Hydroxyphenyl)-3-hydroxypropanoic acid	HMDB0002643
44	2-Hydroxy-2-methylbutyric acid	HMDB0001987
45	Tartaric acid	HMDB0000956
46	2-Hydroxyisovaleric acid	HMDB0000407
47	Homovanillic acid	HMDB0000118
48	Valeric acid	HMDB0000892
49	Caproic acid	HMDB0000535
50	4-Hydroxybutyric acid	HMDB0000710
51	4-Acetamidobutyric acid	HMDB0003681
52	3-Hydroxyglutaric acid	HMDB0000428
53	Glutaconic Acid	HMDB0000620
54	methylsuccinic acid	HMDB0001844
55	Suberic Acid	HMDB0000893
56	2-Methylglutaric acid	HMDB0000422
57	Malic acid	HMDB0000156
58	Malonic acid	HMDB0000691
59	Succinic acid	HMDB0000254
60	Glutaric acid	HMDB0000661
61	Methylmalonic acid	HMDB0000202
62	Fumaric acid	HMDB0000134
63	3-Hydroxyhexanedioic Acid	HMDB0000345
64	Caprylic acid	HMDB0000482

Indole Derivatives

1	1H-Indole-4-carboxaldehyde	HMDB0341228
2	indole-3-carboxaldehyde	HMDB0029737
3	5,6-Dimethoxyindole-2-Carboxylic Acid	HMDB0001253
4	Indoxyl glucoside	HMDB0061755
5	5-Hydroxyindoleacetic acid	HMDB0000763
6	Indoxyl glucuronide	HMDB0010319
7	Indolelactic acid	HMDB0000671
8	Indole-3-carboxylic acid	HMDB0003320
9	3-Indoleacetic acid	HMDB0000197

10	Indole-3-propionic acid	HMDB0002302
11	Indole	HMDB0000738
12	Indole-3-acetamide	HMDB0029739

Ketone and Keto acids

1	3-Methyl-2-oxovaleric acid	HMDB0000491
2	beta-Hydroxypyruvic acid	HMDB0001352
3	Phenylpyruvic acid	HMDB0000205
4	2-Ketobutyric acid	HMDB0000005
5	3-Hydroxybutyric acid	HMDB0000011
6	2-oxoadipic acid	HMDB0000225
7	Acetoacetic acid	HMDB0000060
8	alpha-Ketoglutaric acid	HMDB0000208
9	Pyruvic acid	HMDB0000243
10	2-oxoisocaproic acid	HMDB0000695
11	alpha-Ketoisovaleric acid	HMDB0000019

Nucleo Bases and Nucleosides

1	1-Methyluric acid	HMDB0003099
2	1,3-Dimethyluric Acid	HMDB0001857
3	Guanidine	HMDB0001842
4	ADMA+SDMA	HMDB0001539+HMDB0003334
5	Total MethylXanthine	HMDB0001886
6	Xanthine	HMDB0000292
7	Xanthosine	HMDB0000299
8	Cyclic AMP	HMDB0000058
9	5-Methyluridine	HMDB0000884
10	7-Methylguanine	HMDB0000897
11	Adenine	HMDB0000034
12	Adenosine	HMDB0000050
13	Cytidine	HMDB0000089
14	Cytosine	HMDB0000630
15	Deoxyadenosine	HMDB0000101
16	Deoxycytidine	HMDB0000014
17	Deoxyguanosine	HMDB0000085
18	Deoxyinosine	HMDB0000071
19	Deoxyuridine	HMDB0000012
20	Guanine	HMDB0000132
21	Guanosine	HMDB0000133
22	Hypoxanthine	HMDB0000157
23	Inosine	HMDB0000195
24	Thymidine	HMDB0000273
25	Thymine	HMDB0000262
26	Uracil	HMDB0000300

27	Uridine	HMDB0000296
28	1-Methylguanosine	HMDB0001563
29	1-Methylinosine	HMDB0002721
30	Uric acid	HMDB0000289
31	Theobromine	HMDB0002825
32	3-Methyladenine	HMDB0011600

Organic Acids		
1	Hydrocinnamic Acid+2-Phenylpropionic acid	HMDB0000764+HMDB0011743
2	Imidazoleacetic Acid	HMDB0002024
3	Betaine	HMDB0000043
4	Pipelic acid	HMDB0000070
5	N-Acetylneuraminic Acid	HMDB0000230
6	Erythronic acid	HMDB0000613
7	Urocanic Acid	HMDB0000301
8	Ureidopropionic acid	HMDB0000026
9	Glycolic acid	HMDB0000115
10	Mandelic Acid	HMDB0000703
11	Citramalic acid	HMDB0000426
12	Anthranilic acid	HMDB0001123
13	Monobutyl-Phthalate	HMDB0013247
14	Guanidoacetic acid	HMDB0000128
15	Guanidinopropionic acid	HMDB0013222
16	Argininic acid	HMDB0003148
17	Threonic acid	HMDB0000943
18	Glyceric acid	HMDB0000139
19	Shikimic acid	HMDB0003070
20	Orotic acid	HMDB0000226
21	Hippuric acid	HMDB0000714
22	2-hydroxyglutaric acid	HMDB0059655
23	Benzoic acid	HMDB0001870
24	Maleic acid	HMDB0000176
25	Phenylacetic acid	HMDB0000209
26	Ethylmalonic acid	HMDB0000622
27	Salicylic acid	HMDB0001895
28	3-Methyladipic acid	HMDB0000555
29	Isocitric acid	HMDB0000193
30	2,5-Furandicarboxylic acid	HMDB0004812
31	Citric acid	HMDB0000094
32	cis-Aconitic acid	HMDB0000072
33	Quinaldic acid	HMDB0000842
34	4-Hydroxyphenylpyruvic acid	HMDB0000707
35	3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid	HMDB0061112

36	Creatine	HMDB0000064
37	Cinnabarinic acid	HMDB0004078
38	Quinoline-4-carboxylic acid	HMDB0257047
39	Caffeic acid	HMDB0001964

Others

1	Sulforaphane	HMDB0005792
2	4-Coumaryl alcohol	HMDB0003654
3	Homovanillyl alcohol	HMDB0038925
4	4-Methylcatechol	HMDB0000873
5	Urolithin B	HMDB0013696
6	4-Hydroxybenzophenone	HMDB0240708
7	Triclocarban	HMDB0240702
8	Nudifloramide	HMDB0004193
9	Urea	HMDB0000294

Polyphenol and Isoflavones

1	Resveratrol	HMDB0003747
2	Daidzein	HMDB0003312
3	Phloretin	HMDB0003306
4	Naringenin	HMDB0002670
5	Genistein	HMDB0003217
6	Hesperetin	HMDB0005782
7	Cyanidin-3-Glucoside	HMDB0030684
8	Capsaicin	HMDB0002227
9	Dihydroisoferulic acid	NA

Steroids and Hormones

1	Estrone sulfate	HMDB0001425
2	Abscisic acid	HMDB0036093
3	Solanidine	HMDB0003236
4	Solanine	HMDB0034202

Sugars, Sugar and acids and Sugar alcohols

1	N-acetylgalactosamine+n-Acetylglucosamine	HMDB0000803+HMDB0000042
2	Gluconic Acid+Galactonic acid	HMDB0000625+HMDB0000565
3	Ribonic acid+Xylonic acid	HMDB0000867+HMDB0059750
4	quinic acid	HMDB0003072
5	Glucose	HMDB0000122
6	Pentose (Arabinose+Ribose+Xylose+Xylulose)	HMDB0029942+HMDB0000283+ HMDB0000098+HMDB0001644
7	Fucose	HMDB0029196

8	Pinitol	HMDB0034219
9	Glucuronic acid	HMDB0000127
10	L-Iduronic Acid	HMDB0002704
11	Lactose	HMDB0000186
12	Maltose	HMDB0000163
13	Mannose	HMDB0000169
14	D-Psicose	HMDB0250793
15	Fructose	HMDB0000660
16	Ethyl glucuronide	HMDB0010325
17	Glucose	HMDB0000122
18	3-Deoxyglucosone	HMDB0005876

Sulfates

1	Ferulic Acid 4-Sulfate	HMDB0029200
2	Indoxyl sulfate	HMDB0000682
3	p-Cresol sulfate	HMDB0011635
4	4-Ethylphenyl sulfate	HMDB0062551
5	Taurine	HMDB0000251

Trp-Kyn Pathway Metabolites

1	N'-FormylKynurenine	HMDB0060485
2	Kynurenic acid	HMDB0000715
3	N-Acetyl-Tryptophan	HMDB0013713
4	Picolinic acid	HMDB0002243
5	Quinolinic acid	HMDB0000232
6	5-Methoxytryptamine	HMDB0004095
7	Kynurenine	HMDB0000684
8	Serotonin	HMDB0000259
9	Trp	HMDB0000929
10	Tryptamine	HMDB0000303

Vitamins and Derivatives

1	Pantothenic acid	HMDB0000210
2	Nicotinic acid	HMDB0001488
3	1-Methylnicotinamide	HMDB0000699
4	Choline	HMDB0000097
5	Nicotinamide ribotide	HMDB0000229
6	α-Tocopherol	HMDB0001893

Drugs, pollutants, food additives and toxic compounds

1	Butyl Paraben	HMDB0032575
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Alkaloids and derivatives

1	Allantoin	HMDB0000462
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Acylcarnitines

1	C0	HMDB0000062
2	C10	HMDB0000651
3	C10:1	HMDB0013205
4	C10:1-2OH	
5	C10:2	HMDB0241102, HMDB0241094
6	C10:3	
7	C10:3:DC	
8	C10:DC-OH	
9	C10-2OH	
10	C11:1	
11	C11:2	
12	C11:3	
13	C11:DC	
14	C12	HMDB0002250
15	C12:1	HMDB0013326
16	C12:3	
17	C12:4	
18	C12-2OH	
19	C12DC	HMDB0013327
20	C13	
21	C13:1	
22	C13:2	
23	C13:3	
24	C13:4	
25	C14	HMDB0005066
26	C14:1	HMDB0002014
27	C14:1OH	HMDB0013330
28	C14:2	HMDB0013331
29	C14:2OH	HMDB0013332
30	C14:3	
31	C14:3OH	
32	C14:DC	
33	C14DC	
34	C16	HMDB0000222
35	C16:1	HMDB0013207
36	C16:1OH	HMDB0013333
37	C16:2	HMDB0013334
38	C16:2OH	HMDB0013335
39	C16:3	

40	C16:4	
41	C16:5	
42	C16DC	
43	C16OH	HMDB0013336
44	C18	HMDB0000848
45	C18:1	HMDB0006464
46	C18:1OH	HMDB0013340
47	C18:2	HMDB0006469
48	C2	HMDB0000201
49	C3	HMDB0000824
50	C3:1	HMDB0013124
51	C3OH	HMDB0013125
52	C4	HMDB0002013
53	C4:1	HMDB0013126
54	C4OH	HMDB0013127
55	C5	HMDB0013128
56	C5:1	HMDB0002366
57	C5:1DC	HMDB0013129
58	C5DC	HMDB0013130
59	C5MDC	HMDB0000552
60	C5OH	HMDB0013132
61	C6	HMDB0000756
62	C6:1	HMDB0013161
63	C6:2	
64	C6:3	
65	C7:1	
66	C7:2	
67	C7DC	HMDB0013328
68	C8	HMDB0000791
69	C8:1	
70	C8:2	
71	C8:DC	
72	C9	HMDB0006320
73	C9:1	
74	C9:1:DC	
75	C9:2	
76	C9:3	
77	C9:4	
78	C9:5	
79	C9:DC	
80	C9-2OH	
81	Benzoylcarnitine	HMDB0240664
82	Phenylacetylcarnitine	HMDB0341372
83	Phenylbutyrylcarnitine	
84	Phenylbutyrylcarnitine	

85	Phenylvalerylcarnitine	
86	Phenylvalerylcarnitine	

Phosphatidylcholines

1	LysoPC a C14:0	HMDB0010379
2	LysoPC a C16:0	HMDB0010382
3	LysoPC a C16:1	HMDB0010383
4	LysoPC a C17:0	HMDB0012108
5	LysoPC a C18:0	HMDB0010384, HMDB0011128
6	LysoPC a C18:1	HMDB0002815, HMDB0010385
7	LysoPC a C18:2	HMDB0010386
8	LysoPC a C20:3	HMDB0010393, HMDB0010394
9	LysoPC a C20:4	HMDB0010395, HMDB0010396
10	LysoPC a C24:0	HMDB0010405
11	LysoPC a C26:0	HMDB0029205
12	LysoPC a C26:1	HMDB0029220
13	LysoPC a C28:0	HMDB0029206
14	LysoPC a C28:1	HMDB0029221
15	PC aa C24:0	HMDB0341514
16	PC aa C26:0	HMDB0341515
17	PC aa C28:1	HMDB0007867, HMDB0007899
18	PC aa C30:0	HMDB0007869, HMDB0007934, HMDB0007965
19	PC aa C32:0	HMDB0000564, HMDB0007871, HMDB0008031
20	PC aa C32:1	HMDB0007904, HMDB0007969, HMDB0008001, HMDB0008032,
21	PC aa C32:2	HMDB0007874, HMDB0008002
22	PC aa C32:3	HMDB0007907, HMDB0008131, HMDB0008163, HMDB0008196
23	PC aa C34:1	HMDB0007971, HMDB0007972, HMDB0008003, HMDB0008035,
24	PC aa C34:2	HMDB0007973, HMDB0008004, HMDB0008005, HMDB0008068,
25	PC aa C34:3	HMDB0007913, HMDB0007974, HMDB0007975, HMDB0008006,
26	PC aa C34:4	HMDB0007914, HMDB0007915, HMDB0007976, HMDB0008007,
27	PC aa C36:0	HMDB0007886, HMDB0007977
28	PC aa C36:1	HMDB0007978, HMDB0008010, HMDB0008037, HMDB0008038,
29	PC aa C36:2	HMDB0007920, HMDB0007979, HMDB0008011, HMDB0008039,
30	PC aa C36:3	HMDB0007981, HMDB0008012, HMDB0008040, HMDB0008041,

31	PC aa C36:4	HMDB0007983, HMDB0008013, HMDB0008014, HMDB0008042,
32	PC aa C36:5	HMDB0007922, HMDB0007984, HMDB0008015, HMDB0008016,
33	PC aa C36:6	HMDB0008690, HMDB0007892
34	PC aa C38:0	HMDB0007893, HMDB0007985
35	PC aa C38:1	HMDB0007986, HMDB0008018, HMDB0008044, HMDB0008076,
36	PC aa C38:3	HMDB0008047, HMDB0008078, HMDB0008111, HMDB0008144,
37	PC aa C38:4	HMDB0008049, HMDB0008079, HMDB0008080, HMDB0008112,
38	PC aa C38:5	HMDB0008021, HMDB0008050, HMDB0008081, HMDB0008082,
39	PC aa C38:6	HMDB0007991, HMDB0008083
40	PC aa C40:1	HMDB0007993, HMDB0008052
41	PC aa C40:2	HMDB0008688, HMDB0008276
42	PC aa C40:3	HMDB0008151, HMDB0008183, HMDB0008216, HMDB0008277,
43	PC aa C40:4	HMDB0008184, HMDB0008217, HMDB0008249, HMDB0008279,
44	PC aa C40:5	HMDB0008087, HMDB0008120, HMDB0008185, HMDB0008218,
45	PC aa C40:6	
46	PC aa C42:0	HMDB0008058, HMDB0008282, HMDB0008537, HMDB0008760
47	PC aa C42:1	HMDB0008124, HMDB0008283, HMDB0008315, HMDB0008538,
48	PC aa C42:2	HMDB0008157, HMDB0008284, HMDB0008316, HMDB0008348,
49	PC aa C42:4	HMDB0008256, HMDB0008285, HMDB0008350, HMDB0008382,
50	PC aa C42:5	HMDB0008287, HMDB0008318, HMDB0008383, HMDB0008415,
51	PC aa C42:6	HMDB0008320, HMDB0008351, HMDB0008448, HMDB0008481,
52	PC ae C30:0	HMDB0013341
53	PC ae C30:1	HMDB0013402, HMDB0013403
54	PC ae C30:2	HMDB0013410
55	PC ae C32:1	HMDB0013404
56	PC ae C32:2	HMDB0013411
57	PC ae C34:0	HMDB0013405
58	PC ae C34:1	HMDB0013412, HMDB0013424, HMDB0013426
59	PC ae C34:2	HMDB0011151

60	PC ae C34:3	HMDB0013413
61	PC ae C36:0	HMDB0013406, HMDB0013417
62	PC ae C36:1	HMDB0013414, HMDB0013427
63	PC ae C36:2	HMDB0013418, HMDB0013428
64	PC ae C36:3	HMDB0013425, HMDB0013429, HMDB0039527
65	PC ae C36:4	HMDB0013407, HMDB0013435
66	PC ae C36:5	HMDB0013415, HMDB0039528
67	PC ae C38:0	HMDB0013408, HMDB0013419
68	PC ae C38:1	HMDB0013416, HMDB0013430
69	PC ae C38:2	HMDB0013431, HMDB0013436
70	PC ae C38:3	HMDB0013439, HMDB0013440
71	PC ae C38:4	HMDB0013420
72	PC ae C38:5	HMDB0013432
73	PC ae C38:6	HMDB0013409
74	PC ae C40:1	HMDB0013433
75	PC ae C40:2	HMDB0013437
76	PC ae C40:3	HMDB0013445, HMDB0013446
77	PC ae C40:4	HMDB0013442
78	PC ae C40:5	HMDB0013444
79	PC ae C40:6	HMDB0013422
80	PC ae C42:0	HMDB0013423, HMDB0013443
81	PC ae C42:1	HMDB0013434, HMDB0013447
82	PC ae C42:2	HMDB0013438
83	PC ae C42:3	HMDB0013458, HMDB0013459
84	PC ae C42:4	HMDB0013448, HMDB0013454
85	PC ae C42:5	HMDB0013451
86	PC ae C44:3	HMDB0013449, HMDB0013452
87	PC ae C44:4	HMDB0013453, HMDB0013455, HMDB0013460
88	PC ae C44:5	HMDB0013456
89	PC ae C44:6	HMDB0013450, HMDB0013457

Sphingomyelins

1	SM C16:0	HMDB0010169
2	SM C16:1	HMDB0240613
3	SM C18:0	HMDB0001348
4	SM C18:1	HMDB0012100, HMDB0012101
5	SM C20:2	HMDB0013465
6	SM C24:0	HMDB0011697
7	SM C24:1	HMDB0012107
8	SM C26:0	HMDB0011698
9	SM C26:1	HMDB0013461
10	SM(OH) C14:1	HMDB0013462

11	SM(OH) C16:1	HMDB0013463
12	SM(OH) C22:1	HMDB0013466
13	SM(OH) C22:2	HMDB0013467
14	SM(OH) C24:1	HMDB0013469

Ceramides

1	Cer(d16:1/18:0)	HMDB0341516
2	Cer(d16:1/20:0)	HMDB0341517
3	Cer(d16:1/22:0)	HMDB0240682
4	Cer(d16:1/24:0)	HMDB0341518
5	Cer(d18:1/16:0)	HMDB0004949
6	Cer(d18:1/18:0)	HMDB0004950
7	Cer(d18:1/22:0)	HMDB0004952
8	Cer(d18:1/23:0)	HMDB0000950
9	Cer(d18:1/24:0)	HMDB0004956
10	Cer(d18:1/24:1)	HMDB0004953
11	Cer(d18:1/25:0)	HMDB0004957
12	Cer(d18:2/22:0)	HMDB0341519
13	Cer(d18:2/24:0)	HMDB0341520
14	Cer(d18:2/24:1)	HMDB0240680
15	Cer(d18:0/20:0)	HMDB0011764
16	Cer(d18:0/22:0)	HMDB0011765
17	Cer(d18:0/24:0)	HMDB0011768
18	Cer(d18:0/24:1)	HMDB0011769

Cholesterol esters

1	CE(14:0)	HMDB0006725
2	CE(14:1)	HMDB0010367
3	CE(15:0)	HMDB0060057
4	CE(15:1)	HMDB0060056
5	CE(16:0)	HMDB0000885
6	CE(16:1)	HMDB0000658
7	CE(17:0)	HMDB0060059
8	CE(17:1)	HMDB0060060
9	CE(18:0)	HMDB0010368
10	CE(18:1)	HMDB0000918
11	CE(18:2)	HMDB0000610
12	CE(18:3)	HMDB0010369
13	CE(20:0)	HMDB0006740
14	CE(20:1)	HMDB0005193
15	CE(20:3)	HMDB0006736
16	CE(20:4)	HMDB0006726
17	CE(20:5)	HMDB0006731
18	CE(22:0)	HMDB0006727

19	CE(22:1)	HMDB0010372
20	CE(22:2)	HMDB0006737
21	CE(22:5)	HMDB0010374
22	CE(22:6)	HMDB0245627

Hexylceramides

1	Hex2Cer(d18:1/14:0)	HMDB0341522
2	Hex2Cer(d18:1/16:0)	HMDB0006750
3	Hex2Cer(d18:1/18:0)	HMDB0011591
4	Hex2Cer(d18:1/20:0)	HMDB0011593
5	Hex2Cer(d18:1/22:0)	HMDB0011594
6	Hex2Cer(d18:1/24:0)	HMDB0011595
7	Hex2Cer(d18:1/24:1)	HMDB04872
8	Hex3Cer(d18:1/16:0)	HMDB0004879
9	Hex3Cer(d18:1/18:0)	HMDB0004880
10	Hex3Cer(d18:1/24:1)	HMDB0004883
11	Hex3Cer(d18:1 22:0)	HMDB0004882
12	HexCer(d16:1/22:0)	HMDB0341523
13	HexCer(d18:1/16:0)	HMDB0004971
14	HexCer(d18:1/18:0)	HMDB0004972
15	HexCer(d18:1/18:1)	HMDB0004970
16	HexCer(d18:1/20:0)	HMDB0004973
17	HexCer(d18:1/22:0)	HMDB0004974
18	HexCer(d18:1/23:0)	HMDB0341524
19	HexCer(d18:1/24:0)	HMDB0004978
20	HexCer(d18:1/24:1)	HMDB0004975
21	HexCer(d18:1/26:0)	HMDB0004977
22	HexCer(d18:1/26:1)	HMDB0004976
23	HexCer(d18:2/16:0)	HMDB0341525
24	HexCer(d18:2/18:0)	HMDB0341526
25	HexCer(d18:2/20:0)	HMDB0341527
26	HexCer(d18:2/22:0)	HMDB0341528
27	HexCer(d18:2/23:0)	HMDB0341529
28	HexCer(d18:2/24:0)	HMDB0341530

Diacylglycerols

1	DAG(14:0_14:0)	
2	DAG(14:0_15:0)	
3	DAG(14:0_16:0)	
4	DAG(14:0_16:1)	
5	DAG(14:0_17:0)	
6	DAG(14:0_18:0)	
7	DAG(14:0_18:1)	HMDB0007014
8	DAG(14:0_18:2)	HMDB0007016

9	DAG(14:0_18:3)	
10	DAG(14:0_19:0)	
11	DAG(14:0_20:0)	HMDB0007020
12	DAG(14:0_20:1)	
13	DAG(14:0_20:2)	
14	DAG(14:0_20:3)	
15	DAG(14:0_20:4)	
16	DAG(14:0_20:5)	
17	DAG(14:0_22:4)	
18	DAG(14:0_22:5)	
19	DAG(14:0_22:6)	
20	DAG(15:0_15:0)	
21	DAG(15:0_16:0)	
22	DAG(15:0_16:1)	
23	DAG(15:0_17:0)	
24	DAG(15:0_18:0)	
25	DAG(15:0_18:1)	
26	DAG(15:0_18:2)	
27	DAG(15:0_18:3)	
28	DAG(15:0_19:0)	
29	DAG(15:0_20:0)	
30	DAG(15:0_20:1)	
31	DAG(15:0_20:2)	
32	DAG(15:0_20:3)	
33	DAG(15:0_20:4)	
34	DAG(15:0_20:5)	
35	DAG(15:0_22:4)	
36	DAG(15:0_22:5)	
37	DAG(15:0_22:6)	
38	DAG(16:0_16:0)	HMDB0007098
39	DAG(16:0_16:1)	HMDB0007099
40	DAG(16:0_17:0)	
41	DAG(16:0_18:0)	
42	DAG(16:0_18:1)	HMDB0007101
43	DAG(16:0_18:2)	HMDB0007103
44	DAG(16:0_18:3)	
45	DAG(16:0_19:0)	
46	DAG(16:0_20:0)	HMDB0007107
47	DAG(16:0_20:1)	
48	DAG(16:0_20:2)	
49	DAG(16:0_20:3)	
50	DAG(16:0_20:4)	
51	DAG(16:0_20:5)	
52	DAG(16:0_22:4)	
53	DAG(16:0_22:5)	

54	DAG(16:0_22:6)	
55	DAG(16:1_16:1)	
56	DAG(16:1_17:0)	
57	DAG(16:1_18:0)	
58	DAG(16:1_18:1)	HMDB0007130
59	DAG(16:1_18:2)	HMDB0007132
60	DAG(16:1_18:3)	
61	DAG(16:1_19:0)	
62	DAG(16:1_20:0)	HMDB0007136
63	DAG(16:1_20:1)	
64	DAG(16:1_20:2)	
65	DAG(16:1_20:3)	
66	DAG(16:1_20:4)	
67	DAG(16:1_20:5)	
68	DAG(16:1_22:4)	
69	DAG(16:1_22:5)	
70	DAG(16:1_22:6)	
71	DAG(17:0_17:0)	
72	DAG(17:0_18:0)	
73	DAG(17:0_18:1)	HMDB0295723
74	DAG(17:0_18:2)	
75	DAG(17:0_18:3)	
76	DAG(17:0_19:0)	
77	DAG(17:0_20:0)	
78	DAG(17:0_20:1)	
79	DAG(17:0_20:2)	
80	DAG(17:0_20:3)	
81	DAG(17:0_20:4)	
82	DAG(17:0_20:5)	
83	DAG(17:0_22:4)	
84	DAG(17:0_22:5)	
85	DAG(17:0_22:6)	
86	DAG(18:0_18:0)	
87	DAG(18:0_18:1)	
88	DAG(18:0_18:2)	
89	DAG(18:0_18:3)	
90	DAG(18:0_19:0)	
91	DAG(18:0_20:0)	HMDB0007165
92	DAG(18:0_20:1)	
93	DAG(18:0_20:2)	
94	DAG(18:0_20:3)	
95	DAG(18:0_20:4)	
96	DAG(18:0_20:5)	
97	DAG(18:0_22:4)	
98	DAG(18:0_22:5)	

99	DAG(18:0_22:6)	
100	DAG(18:1_18:1)	HMDB0007188
101	DAG(18:1_18:2)	HMDB0007190
102	DAG(18:1_18:3)	HMDB0007191
103	DAG(18:1_19:0)	
104	DAG(18:1_20:0)	
105	DAG(18:1_20:1)	
106	DAG(18:1_20:2)	
107	DAG(18:1_20:3)	HMDB0007197
108	DAG(18:1_20:4)	HMDB0007199
109	DAG(18:1_20:5)	
110	DAG(18:1_22:4)	
111	DAG(18:1_22:5)	
112	DAG(18:1_22:6)	HMDB0007208
113	DAG(18:2_18:2)	HMDB0007248
114	DAG(18:2_18:3)	
115	DAG(18:2_19:0)	
116	DAG(18:2_20:0)	
117	DAG(18:2_20:1)	
118	DAG(18:2_20:2)	
119	DAG(18:2_20:3)	
120	DAG(18:2_20:4)	
121	DAG(18:2_20:5)	
122	DAG(18:2_22:4)	
123	DAG(18:2_22:5)	
124	DAG(18:2_22:6)	
125	DAG(18:3_18:3)	
126	DAG(18:3_19:0)	
127	DAG(18:3_20:0)	
128	DAG(18:3_20:1)	
129	DAG(18:3_20:2)	
130	DAG(18:3_20:3)	
131	DAG(18:3_20:4)	
132	DAG(18:3_20:5)	
133	DAG(18:3_22:4)	
134	DAG(18:3_22:5)	
135	DAG(18:3_22:6)	
136	DAG(19:0_19:0)	
137	DAG(19:0_20:0)	
138	DAG(19:0_20:1)	
139	DAG(19:0_20:2)	
140	DAG(19:0_20:3)	
141	DAG(19:0_20:4)	
142	DAG(19:0_20:5)	
143	DAG(19:0_22:4)	

144	DAG(19:0_22:5)	
145	DAG(19:0_22:6)	
146	DAG(20:0_20:0)	
147	DAG(20:0_20:1)	
148	DAG(20:0_20:2)	
149	DAG(20:0_20:3)	
150	DAG(20:0_20:4)	
151	DAG(20:0_20:5)	
152	DAG(20:0_22:4)	
153	DAG(20:0_22:5)	
154	DAG(20:0_22:6)	
155	DAG(20:1_20:1)	
156	DAG(20:1_20:2)	
157	DAG(20:1_20:3)	
158	DAG(20:1_20:4)	
159	DAG(20:1_20:5)	
160	DAG(20:1_22:4)	
161	DAG(20:1_22:5)	
162	DAG(20:1_22:6)	
163	DAG(20:2_20:2)	
164	DAG(20:2_20:3)	
165	DAG(20:2_20:4)	
166	DAG(20:2_20:5)	
167	DAG(20:2_22:4)	
168	DAG(20:2_22:5)	
169	DAG(20:2_22:6)	
170	DAG(20:3_20:3)	
171	DAG(20:3_20:4)	
172	DAG(20:3_20:5)	
173	DAG(20:3_22:4)	
174	DAG(20:3_22:5)	
175	DAG(20:3_22:6)	
176	DAG(20:4_20:4)	
177	DAG(20:4_20:5)	
178	DAG(20:4_22:4)	
179	DAG(20:4_22:5)	
180	DAG(20:4_22:6)	
181	DAG(20:5_20:5)	
182	DAG(20:5_22:4)	
183	DAG(20:5_22:5)	
184	DAG(20:5_22:6)	
185	DAG(22:4_22:4)	
186	DAG(22:4_22:5)	
187	DAG(22:4_22:6)	
188	DAG(22:5_22:5)	

189	DAG(22:5_22:6)	
190	DAG(22:6_22:6)	

Triacylglycerols		
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1	TAG(40:0_FA14:0)	
2	TAG(40:0_FA16:0)	
3	TAG(42:0_FA14:0)	
4	TAG(42:0_FA16:0)	
5	TAG(42:1_FA14:0)	
6	TAG(42:1_FA16:0)	
7	TAG(42:1_FA16:1)	
8	TAG(42:1_FA18:1)	
9	TAG(42:2_FA18:2)	
10	TAG(44:0_FA14:0)	
11	TAG(44:0_FA16:0)	
12	TAG(44:0_FA18:0)	
13	TAG(44:1_FA14:0)	
14	TAG(44:1_FA16:0)	
15	TAG(44:1_FA16:1)	
16	TAG(44:1_FA18:1)	
17	TAG(44:2_FA14:0)	
18	TAG(44:2_FA16:0)	
19	TAG(44:2_FA16:1)	
20	TAG(44:2_FA18:1)	
21	TAG(44:2_FA18:2)	
22	TAG(44:3_FA18:2)	
23	TAG(45:0_FA14:0)	
24	TAG(45:0_FA16:0)	
25	TAG(45:1_FA16:0)	
26	TAG(45:1_FA18:1)	
27	TAG(46:0_FA14:0)	
28	TAG(46:0_FA16:0)	
29	TAG(46:0_FA18:0)	
30	TAG(46:1_FA14:0)	
31	TAG(46:1_FA16:0)	
32	TAG(46:1_FA16:1)	
33	TAG(46:1_FA18:0)	
34	TAG(46:1_FA18:1)	
35	TAG(46:2_FA14:0)	
36	TAG(46:2_FA16:0)	
37	TAG(46:2_FA16:1)	
38	TAG(46:2_FA18:1)	
39	TAG(46:2_FA18:2)	
40	TAG(46:3_FA14:0)	

41	TAG(46:3_FA16:0)	
42	TAG(46:3_FA16:1)	
43	TAG(46:3_FA18:1)	
44	TAG(46:3_FA18:2)	
45	TAG(46:3_FA18:3)	
46	TAG(46:4_FA18:2)	
47	TAG(47:0_FA14:0)	
48	TAG(47:0_FA16:0)	
49	TAG(47:0_FA17:0)	
50	TAG(47:1_FA14:0)	
51	TAG(47:1_FA16:0)	
52	TAG(47:1_FA16:1)	
53	TAG(47:1_FA17:0)	
54	TAG(47:1_FA18:1)	
55	TAG(47:2_FA14:0)	
56	TAG(47:2_FA16:1)	
57	TAG(47:2_FA18:1)	
58	TAG(47:2_FA18:2)	
59	TAG(48:0_FA14:0)	
60	TAG(48:0_FA16:0)	
61	TAG(48:0_FA18:0)	
62	TAG(48:1_FA14:0)	
63	TAG(48:1_FA16:0)	
64	TAG(48:1_FA16:1)	
65	TAG(48:1_FA18:0)	
66	TAG(48:1_FA18:1)	
67	TAG(48:2_FA14:0)	
68	TAG(48:2_FA16:0)	
69	TAG(48:2_FA16:1)	
70	TAG(48:2_FA18:0)	
71	TAG(48:2_FA18:1)	
72	TAG(48:2_FA18:2)	
73	TAG(48:3_FA14:0)	
74	TAG(48:3_FA16:0)	
75	TAG(48:3_FA16:1)	
76	TAG(48:3_FA18:1)	
77	TAG(48:3_FA18:2)	
78	TAG(48:3_FA18:3)	
79	TAG(48:4_FA14:0)	
80	TAG(48:4_FA16:0)	
81	TAG(48:4_FA16:1)	
82	TAG(48:4_FA18:1)	
83	TAG(48:4_FA18:2)	
84	TAG(48:4_FA18:3)	
85	TAG(48:4_FA20:4)	

86	TAG(48:5_FA18:2)	
87	TAG(48:5_FA18:3)	
88	TAG(49:0_FA16:0)	
89	TAG(49:0_FA17:0)	
90	TAG(49:0_FA18:0)	
91	TAG(49:1_FA14:0)	
92	TAG(49:1_FA16:0)	
93	TAG(49:1_FA16:1)	
94	TAG(49:1_FA17:0)	
95	TAG(49:1_FA18:1)	
96	TAG(49:2_FA14:0)	
97	TAG(49:2_FA16:0)	
98	TAG(49:2_FA16:1)	
99	TAG(49:2_FA17:0)	
100	TAG(49:2_FA18:1)	
101	TAG(49:2_FA18:2)	
102	TAG(49:3_FA16:0)	
103	TAG(49:3_FA16:1)	
104	TAG(49:3_FA18:2)	
105	TAG(49:3_FA18:3)	
106	TAG(50:0_FA14:0)	
107	TAG(50:0_FA16:0)	
108	TAG(50:0_FA18:0)	
109	TAG(50:1_FA14:0)	
110	TAG(50:1_FA16:0)	
111	TAG(50:1_FA16:1)	
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120	TAG(50:2_FA18:2)	
121	TAG(50:2_FA20:2)	
122	TAG(50:3_FA14:0)	
123	TAG(50:3_FA16:0)	
124	TAG(50:3_FA16:1)	
125	TAG(50:3_FA18:0)	
126	TAG(50:3_FA18:1)	
127	TAG(50:3_FA18:2)	
128	TAG(50:3_FA18:3)	
129	TAG(50:3_FA20:3)	
130	TAG(50:4_FA14:0)	

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135	TAG(50:4_FA18:3)	
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141	TAG(50:5_FA18:1)	
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143	TAG(50:5_FA18:3)	
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148	TAG(51:0_FA17:0)	
149	TAG(51:0_FA18:0)	
150	TAG(51:1_FA16:0)	
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260	TAG(54:1_FA20:1)	
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345	TAG(56:3_FA18:2)	
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399	TAG(56:8_FA22:5)	
400	TAG(56:8_FA22:6)	

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404	TAG(56:9_FA22:6)	
405	TAG(57:10_FA22:6)	
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407	TAG(57:3_FA18:2)	
408	TAG(58:10_FA18:2)	
409	TAG(58:10_FA20:4)	
410	TAG(58:10_FA20:5)	
411	TAG(58:10_FA22:5)	
412	TAG(58:10_FA22:6)	
413	TAG(58:2_FA18:1)	
414	TAG(58:3_FA18:1)	
415	TAG(58:5_FA18:1)	
416	TAG(58:6_FA16:0)	
417	TAG(58:6_FA18:0)	
418	TAG(58:6_FA18:1)	
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421	TAG(58:6_FA22:5)	
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423	TAG(58:7_FA18:0)	
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431	TAG(58:8_FA18:2)	
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439	TAG(58:9_FA22:5)	
440	TAG(58:9_FA22:6)	
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442	TAG(60:10_FA22:6)	
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444	TAG(60:11_FA22:6)	
445	TAG(60:12_FA22:6)	

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