

Supplementary Table 1. List of endogenous metabolites included in the study

Metabolite	Super pathway	Sub pathway	Compound ID	PubChem	KEGG	HMDB
1-methyl-4-imidazoleacetate	Amino Acid	Histidine Metabolism	32350	75810	C05828	HMDB02820
1-methylhistidine	Amino Acid	Histidine Metabolism	30460	92105	C01152	HMDB00001
2-aminoadipate	Amino Acid	Lysine Metabolism	6146	469	C00956	HMDB00510
2-aminobutyrate	Amino Acid	Glutathione Metabolism	42374	439691	C02261	HMDB00650
2-hydroxy-3-methylvalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	36746	164623	NA	HMDB00317
2-hydroxybutyrate/2-hydroxyisobutyrate	Amino Acid	Glutathione Metabolism	52281	NA	NA	NA
2-hydroxyphenylacetate	Amino Acid	Tyrosine Metabolism	1432	11970	C05852	HMDB00669
2-methylbutyrylcarnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	45095	6426901	NA	HMDB00378
2-oxoarginine*	Amino Acid	Urea cycle; Arginine and Proline Metabolism	55072	558	C03771	HMDB04225
3-(4-hydroxyphenyl)lactate	Amino Acid	Tyrosine Metabolism	32197	9378	C03672	HMDB00755
3-hydroxy-2-ethylpropionate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	32397	188979	NA	HMDB00396
3-hydroxyisobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1549	87	C06001	HMDB00336
3-indoxyl sulfate	Amino Acid	Tryptophan Metabolism	27672	10258	NA	HMDB00682
3-methoxytyramine sulfate	Amino Acid	Tyrosine Metabolism	44618	NA	NA	NA
3-methoxytyrosine	Amino Acid	Tyrosine Metabolism	12017	1670	NA	HMDB01434
3-methyl-2-oxobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	44526	49	C00141	HMDB00019
3-methyl-2-oxovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	15676	47	C00671	HMDB03736
3-methylglutaconate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	38667	1551553	NA	HMDB00522
3-methylglutaryl carnitine (2)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	46548	128145	NA	HMDB00552
3-methylhistidine	Amino Acid	Histidine Metabolism	15677	64969	C01152	HMDB00479
4-acetamidobutanoate	Amino Acid	Polyamine Metabolism	1558	18189	C02946	HMDB03681
4-hydroxyglutamate	Amino Acid	Glutamate Metabolism	40499	439902	C03079	HMDB01344
4-hydroxyphenylpyruvate	Amino Acid	Tyrosine Metabolism	1669	979	C01179	HMDB00707
4-methyl-2-oxopentanoate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	22116	70	C00233	HMDB00695
5-methylthioadenosine (MTA)	Amino Acid	Polyamine Metabolism	1419	439176	C00170	HMDB01173
5-oxoproline	Amino Acid	Glutathione Metabolism	1494	7405	C01879	HMDB00267
6-oxopiperidine-2-carboxylate	Amino Acid	Lysine Metabolism	43231	3014237	NA	HMDB61705
alanine	Amino Acid	Alanine and Aspartate Metabolism	1126	5950	C00041	HMDB00161
alpha-hydroxyisocaproate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	22132	83697	C03264	HMDB00746
alpha-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	33937	99823	NA	HMDB00407
alpha-ketobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	4968	58	C00109	HMDB00005

argininate*	Amino Acid	Urea cycle; Arginine and Proline Metabolism	57461	160437	NA	HMDB03148
arginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1638	232	C00062	HMDB00517
asparagine	Amino Acid	Alanine and Aspartate Metabolism	512	6267	C00152	HMDB00168
aspartate	Amino Acid	Alanine and Aspartate Metabolism	443	5960	C00049	HMDB00191
beta-citrylglutamate	Amino Acid	Glutamate Metabolism	54923	72715786	C20775	NA
beta-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	12129	69362	NA	HMDB00754
betaine	Amino Acid	Glycine, Serine and Threonine Metabolism	3141	247	C00719	HMDB00043
C-glycosyltryptophan	Amino Acid	Tryptophan Metabolism	48782	10981970	NA	NA
carboxyethyl-GABA	Amino Acid	Glutamate Metabolism	40007	2572	NA	HMDB02201
citrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	2132	9750	C00327	HMDB00904
creatine	Amino Acid	Creatine Metabolism	27718	586	C00300	HMDB00064
creatinine	Amino Acid	Creatine Metabolism	513	588	C00791	HMDB00562
cys-gly, oxidized	Amino Acid	Glutathione Metabolism	18368	333293	NA	NA
cystathionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	15705	439258	C02291	HMDB00099
cysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1868	5862	C00097	HMDB00574
cysteine s-sulfate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	22176	115015	C05824	HMDB00731
cysteine sulfinic acid	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	37443	109	C00606	HMDB00996
cysteine-glutathione disulfide	Amino Acid	Glutathione Metabolism	35159	4247235	NA	HMDB00656
cysteinylglycine	Amino Acid	Glutathione Metabolism	35637	439498	C01419	HMDB00078
cystine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	56	67678	C00491	HMDB00192
dimethylarginine (SDMA + ADMA)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	36808	123831	C03626	HMDB01539
dimethylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	5086	673	C01026	HMDB00092
dopamine 3-O-sulfate	Amino Acid	Tyrosine Metabolism	48407	122136	C13690	HMDB06275
ethylmalonate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	15765	11756	NA	HMDB00622
formiminoglutamate	Amino Acid	Histidine Metabolism	43493	439233	C00439	HMDB00854
gentisate	Amino Acid	Tyrosine Metabolism	18280	3469	C00628	HMDB00152
glutamate	Amino Acid	Glutamate Metabolism	57	611	C00025	HMDB00148
glutamine	Amino Acid	Glutamate Metabolism	53	5961	C00064	HMDB00641
glutaryl carnitine (C5-DC)	Amino Acid	Lysine Metabolism	44664	71464488	NA	HMDB13130
glycine	Amino Acid	Glycine, Serine and Threonine Metabolism	58	750	C00037	HMDB00123
guanidinoacetate	Amino Acid	Creatine Metabolism	43802	763	C00581	HMDB00128
histidine	Amino Acid	Histidine Metabolism	59	6274	C00135	HMDB00177
homoarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	22137	9085	C01924	HMDB00670

homocitrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	22138	65072	C02427	HMDB00679
hydantoin-5-propionic acid	Amino Acid	Histidine Metabolism	40473	782	C05565	HMDB01212
hypotaurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	590	107812	C00519	HMDB00965
imidazole lactate	Amino Acid	Histidine Metabolism	15716	440129	C05568	HMDB02320
indole-3-carboxylic acid	Amino Acid	Tryptophan Metabolism	38116	69867	C19837	HMDB03320
indoleacetate	Amino Acid	Tryptophan Metabolism	27513	802	C00954	HMDB00197
indoleacetylglutamine	Amino Acid	Tryptophan Metabolism	42087	25200879	NA	HMDB13240
indolelactate	Amino Acid	Tryptophan Metabolism	18349	92904	C02043	HMDB00671
indolepropionate	Amino Acid	Tryptophan Metabolism	32405	3744	NA	HMDB02302
isobutyrylcarnitine (C4)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	33441	168379	NA	HMDB00736
isobutyrylglycine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	35437	10855600	NA	HMDB00730
isoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1125	6306	C00407	HMDB00172
isovalerate (i5:0)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	44656	10430	C08262	HMDB00718
isovalerylcarnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	34407	6426851	NA	HMDB00688
isovalerylglycine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	35107	546304	NA	HMDB00678
kynurenate	Amino Acid	Tryptophan Metabolism	1417	3845	C01717	HMDB00715
kynurenine	Amino Acid	Tryptophan Metabolism	15140	161166	C00328	HMDB00684
leucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	60	5246661	NA	NA
lysine	Amino Acid	Lysine Metabolism	1301	5962	C00047	HMDB00182
methionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1302	6137	C00073	HMDB00696
methionine sulfone	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	44878	69961	NA	NA
methionine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	18374	158980	C02989	HMDB02005
methylsuccinate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	15745	10349	NA	HMDB01844
N-acetyl-1-methylhistidine*	Amino Acid	Histidine Metabolism	43255	193270	NA	NA
N-acetylalanine	Amino Acid	Alanine and Aspartate Metabolism	1585	88064	C02847	HMDB00766
N-acetylarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	33953	67427	C02562	HMDB04620
N-acetylasparagine	Amino Acid	Alanine and Aspartate Metabolism	33942	99715	NA	HMDB06028
N-acetylaspartate (NAA)	Amino Acid	Alanine and Aspartate Metabolism	22185	65065	C01042	HMDB00812
N-acetylcarnosine	Amino Acid	Histidine Metabolism	43488	9903482	NA	HMDB12881
N-acetylcitrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	48434	656979	C15532	HMDB00856
N-acetylglutamate	Amino Acid	Glutamate Metabolism	15720	70914	C00624	HMDB01138
N-acetylglutamine	Amino Acid	Glutamate Metabolism	33943	182230	C02716	HMDB06029
N-acetylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	27710	10972	NA	HMDB00532

N-acetylhistidine	Amino Acid	Histidine Metabolism	33946	75619	C02997	HMDB32055
N-acetylisoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	33967	2802421	NA	HMDB61684
N-acetylleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1587	70912	C02710	HMDB11756
N-acetylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1589	448580	C02712	HMDB11745
N-acetylphenylalanine	Amino Acid	Phenylalanine Metabolism	33950	74839	C03519	HMDB00512
N-acetylputrescine	Amino Acid	Polyamine Metabolism	37496	122356	C02714	HMDB02064
N-acetylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	37076	65249	NA	HMDB02931
N-acetyltaurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	48187	159864	NA	NA
N-acetylthreonine	Amino Acid	Glycine, Serine and Threonine Metabolism	33939	152204	NA	NA
N-acetyltryptophan	Amino Acid	Tryptophan Metabolism	33959	700653	C03137	HMDB13713
N-acetyltyrosine	Amino Acid	Tyrosine Metabolism	32390	68310	NA	HMDB00866
N-acetylvaline	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1591	66789	NA	HMDB11757
N-delta-acetylornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	43249	9920500	NA	NA
N-formylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	2829	439750	C03145	HMDB01015
N-methylproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	37431	557	NA	NA
N2-acetyllysine	Amino Acid	Lysine Metabolism	36751	92907	C12989	HMDB00446
N2,N5-diacetylornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	43591	10398396	NA	NA
N6-acetyllysine	Amino Acid	Lysine Metabolism	36752	92832	C02727	HMDB00206
N6,N6,N6-trimethyllysine	Amino Acid	Lysine Metabolism	1498	440120	C03793	HMDB01325
ornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1493	6262	C00077	HMDB03374
p-cresol glucuronide*	Amino Acid	Tyrosine Metabolism	48841	154035	NA	HMDB11686
phenol sulfate	Amino Acid	Tyrosine Metabolism	32553	74426	C02180	HMDB60015
phenylalanine	Amino Acid	Phenylalanine Metabolism	64	6140	C00079	HMDB00159
phenyllactate (PLA)	Amino Acid	Phenylalanine Metabolism	22130	3848	C05607	HMDB00779
phenylpyruvate	Amino Acid	Phenylalanine Metabolism	566	997	C00166	HMDB00205
pipecolate	Amino Acid	Lysine Metabolism	1444	849	C00408	HMDB00070
pro-hydroxy-pro	Amino Acid	Urea cycle; Arginine and Proline Metabolism	35127	11673055	NA	HMDB06695
proline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1898	145742	C00148	HMDB00162
pyroglutamine*	Amino Acid	Glutamate Metabolism	46225	134508	NA	NA
S-adenosylhomocysteine (SAH)	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	42382	439155	C00021	HMDB00939
S-methylcysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	39592	24417	NA	HMDB02108
S-methylcysteine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	43378	82142	NA	HMDB29432
S-methylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	38127	458	C05319	HMDB38670

sarcosine	Amino Acid	Glycine, Serine and Threonine Metabolism	1516	1088	C00213	HMDB00271
serine	Amino Acid	Glycine, Serine and Threonine Metabolism	1648	5951	C00065	HMDB00187
serotonin	Amino Acid	Tryptophan Metabolism	2342	5202	C00780	HMDB00259
spermidine	Amino Acid	Polyamine Metabolism	485	1102	C00315	HMDB01257
taurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	2125	1123	C00245	HMDB00251
threonine	Amino Acid	Glycine, Serine and Threonine Metabolism	1284	6288	C00188	HMDB00167
thyroxine	Amino Acid	Tyrosine Metabolism	2761	5819	C01829	HMDB01918
tiglylcarnitine (C5:1-DC)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	35428	22833596	NA	HMDB02366
trans-4-hydroxyproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	32306	5810	C01157	HMDB00725
tryptophan	Amino Acid	Tryptophan Metabolism	54	6305	C00078	HMDB00929
tryptophan betaine	Amino Acid	Tryptophan Metabolism	37097	442106	C09213	HMDB61115
tyramine O-sulfate	Amino Acid	Tyrosine Metabolism	48408	153005	NA	HMDB06409
tyrosine	Amino Acid	Tyrosine Metabolism	1299	6057	C00082	HMDB00158
urea	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1670	1176	C00086	HMDB00294
valine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1649	6287	C00183	HMDB00883
vanillactate	Amino Acid	Tyrosine Metabolism	54910	160637	NA	HMDB00913
vanillylmandelate (VMA)	Amino Acid	Tyrosine Metabolism	1567	1245	C05584	HMDB00291
xanthurenate	Amino Acid	Tryptophan Metabolism	15679	5699	C02470	HMDB00881
1,5-anhydroglucitol (1,5-AG)	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	20675	64960	C07326	HMDB02712
arabitol/xylitol	Carbohydrate	Pentose Metabolism	48885	6912	C01904	NA
arabonate/xylonate	Carbohydrate	Pentose Metabolism	48255	NA	NA	NA
erythronate*	Carbohydrate	Aminosugar Metabolism	42420	2781043	NA	HMDB00613
fructose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	48195	5984	C00095	HMDB00660
glucose	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	20488	79025	C00031	HMDB00122
glucuronate	Carbohydrate	Aminosugar Metabolism	15443	444791	C00191	HMDB00127
glycerate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	1572	752	C00258	HMDB00139
lactate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	527	612	C00186	HMDB00190
maltose	Carbohydrate	Glycogen Metabolism	15586	10991489	C00208	HMDB00163
maltotriose	Carbohydrate	Glycogen Metabolism	44688	439586	C01835	HMDB01262
mannitol/sorbitol	Carbohydrate	Fructose, Mannose and Galactose Metabolism	46142	5780	C00794	HMDB00247
mannose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	48153	18950	C00159	HMDB00169
N-acetylglucosamine/N-acetylgalactosamine	Carbohydrate	Aminosugar Metabolism	46539	24139	NA	HMDB00215
N-acetylneuraminate	Carbohydrate	Aminosugar Metabolism	32377	439197	C00270	HMDB00230

pyruvate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	42582	1060	C00022	HMDB00243
ribitol	Carbohydrate	Pentose Metabolism	15772	6912	C00474	HMDB00508
ribonate	Carbohydrate	Pentose Metabolism	27731	5460677	C01685	HMDB00867
1-methylnicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	27665	10129985	C02918	HMDB00699
alpha-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	1561	14985	C02477	HMDB01893
beta-cryptoxanthin	Cofactors and Vitamins	Vitamin A Metabolism	57591	6384256	NA	HMDB33844
bilirubin (E,E)*	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	32586	5315454	NA	NA
bilirubin (E,Z or Z,E)*	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	47886	5799469	NA	HMDB00488
bilirubin (Z,Z)	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	43807	5280352	C00486	HMDB00054
biliverdin	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	2137	5353439	C00500	HMDB01008
gamma-CEHC	Cofactors and Vitamins	Tocopherol Metabolism	44876	133098	NA	HMDB01931
gamma-tocopherol/beta-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	52473	NA	NA	NA
gulonate*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	46957	9794176	C00257	HMDB03290
N1-Methyl-2-pyridone-5-carboxamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	40469	69698	C05842	HMDB04193
nicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	594	936	C00153	HMDB01406
oxalate (ethanedioate)	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	20694	971	C00209	HMDB02329
pantothenate	Cofactors and Vitamins	Pantothenate and CoA Metabolism	1508	6613	C00864	HMDB00210
pyridoxate	Cofactors and Vitamins	Vitamin B6 Metabolism	31555	6723	C00847	HMDB00017
quinolinate	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	1899	1066	C03722	HMDB00232
retinol (Vitamin A)	Cofactors and Vitamins	Vitamin A Metabolism	1806	445354	C00473	HMDB00305
threonate	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	27738	151152	C01620	HMDB00943
trigonelline (N'-methylnicotinate)	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	32401	5570	C01004	HMDB00875
2-methylcitrate/homocitrate	Energy	TCA Cycle	52282	NA	NA	NA
aconitate [cis or trans]	Energy	TCA Cycle	46173	NA	NA	NA
alpha-ketoglutarate	Energy	TCA Cycle	528	51	C00026	HMDB00208
citrate	Energy	TCA Cycle	1564	311	C00158	HMDB00094
malate	Energy	TCA Cycle	1303	525	C00149	HMDB00156
phosphate	Energy	Oxidative Phosphorylation	42109	1061	C00009	HMDB01429
succinate	Energy	TCA Cycle	1437	1110	C00042	HMDB00254
succinylcarnitine (C4-DC)	Energy	TCA Cycle	37058	71464481	NA	HMDB61717
1-(1-enyl-oleoyl)-GPE (P-18:1)*	Lipid	Lysoplasmalogen	44621	NA	NA	NA
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*	Lipid	Plasmalogen	52689	NA	NA	HMDB11220
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	Lipid	Plasmalogen	52673	NA	NA	HMDB11352

1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	Lipid	Plasmalogen	52682	NA	NA	HMDB11211
1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*	Lipid	Plasmalogen	52677	NA	NA	HMDB11343
1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	Lipid	Plasmalogen	52478	NA	NA	NA
1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*	Lipid	Plasmalogen	52713	NA	NA	HMDB11207
1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*	Lipid	Plasmalogen	52716	11146967	NA	HMDB11206
1-(1-enyl-palmitoyl)-GPC (P-16:0)*	Lipid	Lysoplasmalogen	52474	10917802	NA	HMDB10407
1-(1-enyl-palmitoyl)-GPE (P-16:0)*	Lipid	Lysoplasmalogen	39270	NA	NA	NA
1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	Lipid	Plasmalogen	52475	9547058	NA	HMDB05779
1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)*	Lipid	Plasmalogen	52748	NA	NA	HMDB11376
1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	Lipid	Plasmalogen	52614	NA	NA	HMDB11375
1-(1-enyl-stearoyl)-GPE (P-18:0)*	Lipid	Lysoplasmalogen	39271	NA	NA	NA
1-arachidonoyl-GPC (20:4n6)*	Lipid	Lysophospholipid	33228	NA	C05208	HMDB10395
1-arachidonoyl-GPE (20:4n6)*	Lipid	Lysophospholipid	35186	42607465	NA	HMDB11517
1-arachidonoyl-GPI (20:4)*	Lipid	Lysophospholipid	34214	NA	NA	HMDB61690
1-arachidonylglycerol (20:4)	Lipid	Monoacylglycerol	34397	5282281	C13857	HMDB11549
1-dihomo-linolenylglycerol (20:3)	Lipid	Monoacylglycerol	48341	NA	NA	NA
1-docosahexaenoylglycerol (22:6)	Lipid	Monoacylglycerol	35153	NA	NA	HMDB11587
1-lignoceroyl-GPC (24:0)	Lipid	Lysophospholipid	49617	NA	NA	HMDB10405
1-linolenoyl-GPC (18:3)*	Lipid	Lysophospholipid	45951	NA	NA	HMDB10388
1-linolenoylglycerol (18:3)	Lipid	Monoacylglycerol	34393	53480978	NA	HMDB11569
1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)*	Lipid	Phosphatidylcholine (PC)	52710	NA	NA	HMDB08147
1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)*	Lipid	Phosphatidylcholine (PC)	53176	NA	NA	HMDB08141
1-linoleoyl-GPC (18:2)	Lipid	Lysophospholipid	34419	11988421	C04100	HMDB10386
1-linoleoyl-GPE (18:2)*	Lipid	Lysophospholipid	36600	52925130	NA	HMDB11507
1-linoleoyl-GPG (18:2)*	Lipid	Lysophospholipid	54885	NA	NA	NA
1-linoleoyl-GPI (18:2)*	Lipid	Lysophospholipid	36594	NA	NA	NA
1-linoleoylglycerol (18:2)	Lipid	Monoacylglycerol	27447	5283469	NA	NA
1-oleoyl-2-linoleoyl-GPE (18:1/18:2)*	Lipid	Phosphatidylethanolamine (PE)	52687	9546753	NA	HMDB05349
1-oleoyl-GPC (18:1)	Lipid	Lysophospholipid	48258	16081932	NA	HMDB02815
1-oleoyl-GPE (18:1)	Lipid	Lysophospholipid	35628	9547071	NA	HMDB11506
1-oleoyl-GPI (18:1)*	Lipid	Lysophospholipid	36602	NA	NA	NA
1-oleoylglycerol (18:1)	Lipid	Monoacylglycerol	21184	5283468	NA	HMDB11567
1-palmitoleoyl-GPC (16:1)*	Lipid	Lysophospholipid	33230	24779461	NA	HMDB10383

1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	Lipid	Phosphatidylcholine (PC)	52462	10747814	NA	HMDB07982
1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*	Lipid	Phosphatidylethanolamine (PE)	52464	9546800	NA	HMDB05323
1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*	Lipid	Phosphatidylinositol (PI)	52467	NA	NA	HMDB09789
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	Lipid	Phosphatidylcholine (PC)	42446	5287971	NA	HMDB07973
1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	Lipid	Phosphatidylethanolamine (PE)	42449	9546747	NA	HMDB05322
1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)	Lipid	Phosphatidylinositol (PI)	52450	NA	NA	HMDB09784
1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	Lipid	Phosphatidylcholine (PC)	52461	6436017	NA	HMDB07972
1-palmitoyl-2-oleoyl-GPE (16:0/18:1)	Lipid	Phosphatidylethanolamine (PE)	19263	5283496	NA	HMDB05320
1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*	Lipid	Phosphatidylinositol (PI)	52669	NA	NA	HMDB09783
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*	Lipid	Phosphatidylcholine (PC)	52470	NA	NA	HMDB07969
1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	Lipid	Phosphatidylcholine (PC)	52616	NA	NA	HMDB07970
1-palmitoyl-GPC (16:0)	Lipid	Lysophospholipid	33955	86554	NA	HMDB10382
1-palmitoyl-GPE (16:0)	Lipid	Lysophospholipid	35631	9547069	NA	HMDB11503
1-palmitoyl-GPG (16:0)*	Lipid	Lysophospholipid	45970	3300276	NA	NA
1-palmitoyl-GPI (16:0)	Lipid	Lysophospholipid	35305	NA	NA	HMDB61695
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	Lipid	Phosphatidylcholine (PC)	42450	16219824	NA	HMDB08048
1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	Lipid	Phosphatidylethanolamine (PE)	52447	5289133	NA	HMDB09003
1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	Lipid	Phosphatidylinositol (PI)	52449	NA	NA	HMDB09815
1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*	Lipid	Phosphatidylcholine (PC)	52452	NA	NA	HMDB08039
1-stearoyl-2-linoleoyl-GPE (18:0/18:2)*	Lipid	Phosphatidylethanolamine (PE)	52446	9546749	NA	HMDB08994
1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	Lipid	Phosphatidylinositol (PI)	52468	NA	NA	HMDB09809
1-stearoyl-2-oleoyl-GPC (18:0/18:1)	Lipid	Phosphatidylcholine (PC)	52438	NA	NA	HMDB08038
1-stearoyl-2-oleoyl-GPE (18:0/18:1)	Lipid	Phosphatidylethanolamine (PE)	42448	NA	NA	HMDB08993
1-stearoyl-2-oleoyl-GPS (18:0/18:1)	Lipid	Phosphatidylserine (PS)	19265	9547087	NA	HMDB10163
1-stearoyl-GPC (18:0)	Lipid	Lysophospholipid	33961	497299	NA	HMDB10384
1-stearoyl-GPE (18:0)	Lipid	Lysophospholipid	42398	9547068	NA	HMDB11130
1-stearoyl-GPI (18:0)	Lipid	Lysophospholipid	19324	NA	NA	HMDB61696
1,2-dilinoleoyl-GPC (18:2/18:2)	Lipid	Phosphatidylcholine (PC)	52603	5288075	NA	HMDB08138
1,2-dipalmitoyl-GPC (16:0/16:0)	Lipid	Phosphatidylcholine (PC)	19130	452110	NA	HMDB00564
10-heptadecenoate (17:1n7)	Lipid	Long Chain Fatty Acid	33971	5312435	NA	HMDB60038
10-nonadecenoate (19:1n9)	Lipid	Long Chain Fatty Acid	33972	5312513	NA	HMDB13622
10-undecenoate (11:1n1)	Lipid	Medium Chain Fatty Acid	32497	14891	C13910	HMDB33724
12-HETE	Lipid	Eicosanoid	37536	5312983	NA	HMDB06111

14-HDoHE/17-HDoHE	Lipid	Fatty Acid, Monohydroxy	53034	NA	NA	NA
15-methylpalmitate (i17:0)	Lipid	Fatty Acid, Branched	38768	17903417	NA	NA
16-hydroxypalmitate	Lipid	Fatty Acid, Monohydroxy	39609	10466	C18218	HMDB06294
16a-hydroxy DHEA 3-sulfate	Lipid	Androgenic Steroids	38168	NA	NA	NA
17-methylstearate (i19:0)	Lipid	Fatty Acid, Branched	38296	3083779	NA	HMDB37397
2-aminoheptanoate	Lipid	Fatty Acid, Amino	43761	227939	NA	NA
2-aminooctanoate	Lipid	Fatty Acid, Amino	43343	69522	NA	HMDB00991
2-arachidonoylglycerol (20:4)	Lipid	Monoacylglycerol	19266	5282280	C13856	HMDB04666
2-hydroxydecanoate	Lipid	Fatty Acid, Monohydroxy	42489	21488	NA	NA
2-hydroxyglutarate	Lipid	Fatty Acid, Dicarboxylate	37253	43	C02630	HMDB00606
2-hydroxyoctanoate	Lipid	Fatty Acid, Monohydroxy	22036	94180	NA	HMDB02264
2-hydroxypalmitate	Lipid	Fatty Acid, Monohydroxy	35675	92836	NA	HMDB31057
2-hydroxystearate	Lipid	Fatty Acid, Monohydroxy	17945	69417	C03045	NA
2-linoleoylglycerol (18:2)	Lipid	Monoacylglycerol	32506	5365676	NA	HMDB11538
2-oleoylglycerol (18:1)	Lipid	Monoacylglycerol	21232	5319879	NA	HMDB11537
2-palmitoleoyl-GPC (16:1)*	Lipid	Lysophospholipid	47118	NA	NA	HMDB10383
2-palmitoyl-GPC (16:0)*	Lipid	Lysophospholipid	35253	15061532	NA	HMDB61702
2-stearoyl-GPE (18:0)*	Lipid	Lysophospholipid	41220	NA	NA	HMDB11129
21-hydroxypregnenolone disulfate	Lipid	Pregnenolone Steroids	46115	134595	NA	NA
3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)	Lipid	Fatty Acid, Dicarboxylate	31787	123979	NA	HMDB61112
3-hydroxy-3-methylglutarate	Lipid	Mevalonate Metabolism	531	1662	C03761	HMDB00355
3-hydroxybutyrate (BHBA)	Lipid	Ketone Bodies	542	441	C01089	HMDB00357
3-hydroxydecanoate	Lipid	Fatty Acid, Monohydroxy	22053	26612	NA	HMDB02203
3-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	53230	151492	NA	NA
3-hydroxylaurate	Lipid	Fatty Acid, Monohydroxy	32457	94216	NA	HMDB00387
3-hydroxyoctanoate	Lipid	Fatty Acid, Monohydroxy	22001	26613	NA	HMDB01954
3-hydroxysebacate	Lipid	Fatty Acid, Monohydroxy	31943	3017884	NA	HMDB00350
3-methyladipate	Lipid	Fatty Acid, Dicarboxylate	36749	12292	NA	HMDB00555
3beta-hydroxy-5-cholestenoate	Lipid	Sterol	54805	165511	C17333	NA
3beta,7alpha-dihydroxy-5-cholestenoate	Lipid	Sterol	36803	3081084	C17335	NA
4-cholesten-3-one	Lipid	Sterol	38125	91477	C00599	HMDB00921
5-dodecenoate (12:1n7)	Lipid	Medium Chain Fatty Acid	33968	5312378	NA	HMDB00529
5-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	31938	170748	NA	HMDB00525

5alpha-androstan-3alpha,17beta-diol monosulfate (1)	Lipid	Androgenic Steroids	37186	NA	NA	NA
5alpha-androstan-3beta,17alpha-diol disulfate	Lipid	Androgenic Steroids	37187	NA	NA	NA
5alpha-androstan-3beta,17beta-diol disulfate	Lipid	Androgenic Steroids	37190	242332	C12525	HMDB00493
5alpha-androstan-3beta,17beta-diol monosulfate (2)	Lipid	Androgenic Steroids	37192	NA	NA	NA
5alpha-pregnan-3beta,20alpha-diol disulfate	Lipid	Progestin Steroids	37198	NA	NA	NA
5alpha-pregnan-3beta,20alpha-diol monosulfate (2)	Lipid	Progestin Steroids	37200	NA	NA	NA
5alpha-pregnan-3beta,20beta-diol monosulfate (1)	Lipid	Progestin Steroids	37196	NA	NA	NA
7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)	Lipid	Sterol	36776	3081085	C17337	HMDB12458
9-hydroxystearate	Lipid	Fatty Acid, Monohydroxy	47120	9570127	NA	HMDB61661
acetylcarnitine (C2)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	32198	1	C02571	HMDB00201
adrenate (22:4n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	32980	5497181	C16527	HMDB02226
andro steroid monosulfate C19H28O6S (1)*	Lipid	Androgenic Steroids	32827	NA	C04555	HMDB02759
androstenediol (3alpha, 17alpha) monosulfate (2)	Lipid	Androgenic Steroids	37207	NA	NA	NA
androstenediol (3alpha, 17alpha) monosulfate (3)	Lipid	Androgenic Steroids	37209	NA	NA	NA
androstenediol (3beta,17beta) disulfate (1)	Lipid	Androgenic Steroids	37202	87120982	C04295	HMDB03818
androstenediol (3beta,17beta) disulfate (2)	Lipid	Androgenic Steroids	37203	87120982	C04295	HMDB03818
androstenediol (3beta,17beta) monosulfate (1)	Lipid	Androgenic Steroids	37211	13847309	NA	HMDB03818
androstenediol (3beta,17beta) monosulfate (2)	Lipid	Androgenic Steroids	37210	NA	NA	NA
androsterone sulfate	Lipid	Androgenic Steroids	31591	159663	NA	HMDB02759
arachidate (20:0)	Lipid	Long Chain Fatty Acid	1118	10467	C06425	HMDB02212
arachidonate (20:4n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	1110	444899	C00219	HMDB01043
arachidonoylcarnitine (C20:4)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57518	NA	NA	NA
arachidonoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	53261	NA	NA	NA
azelate (C9-DC)	Lipid	Fatty Acid, Dicarboxylate	18362	2266	C08261	HMDB00784
behenoyl dihydrosphingomyelin (d18:0/22:0)*	Lipid	Dihydrosphingomyelins	57331	NA	NA	HMDB12091
behenoyl sphingomyelin (d18:1/22:0)*	Lipid	Sphingomyelins	48492	NA	NA	HMDB12103
behenoylcarnitine (C22)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57514	NA	NA	NA
beta-sitosterol	Lipid	Sterol	27414	222284	C01753	HMDB00852
butyrylcarnitine (C4)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	32412	439829	C02862	HMDB02013
campesterol	Lipid	Sterol	33997	173183	C01789	HMDB02869
caprate (10:0)	Lipid	Medium Chain Fatty Acid	1642	2969	C01571	HMDB00511
caproate (6:0)	Lipid	Medium Chain Fatty Acid	32489	8892	C01585	HMDB00535
caprylate (8:0)	Lipid	Medium Chain Fatty Acid	32492	379	C06423	HMDB00482

carnitine	Lipid	Carnitine Metabolism	15500	10917	C00318	HMDB00062
ceramide (d18:1/14:0, d16:1/16:0)*	Lipid	Ceramides	57432	NA	NA	NA
ceramide (d18:1/17:0, d17:1/18:0)*	Lipid	Ceramides	57434	NA	NA	NA
ceramide (d18:1/20:0, d16:1/22:0, d20:1/18:0)*	Lipid	Ceramides	57440	NA	NA	NA
ceramide (d18:2/24:1, d18:1/24:2)*	Lipid	Ceramides	57443	NA	NA	NA
cerotylcarnitine (C26)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57516	NA	NA	HMDB06347
chenodeoxycholate	Lipid	Primary Bile Acid Metabolism	1563	10133	C02528	HMDB00518
cholate	Lipid	Primary Bile Acid Metabolism	22842	221493	C00695	HMDB00619
cholesterol	Lipid	Sterol	63	11025495	C00187	HMDB00067
choline	Lipid	Phospholipid Metabolism	15506	305	C00114	HMDB00097
choline phosphate	Lipid	Phospholipid Metabolism	34396	1014	C00588	HMDB01565
cis-4-decenoylcarnitine (C10:1)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	38178	NA	NA	NA
cortisol	Lipid	Corticosteroids	1712	5754	C00735	HMDB00063
cortisone	Lipid	Corticosteroids	1769	222786	C00762	HMDB02802
decanoylcarnitine (C10)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	33941	10245190	NA	HMDB00651
dehydroisoandrosterone sulfate (DHEA-S)	Lipid	Androgenic Steroids	32425	12594	C04555	HMDB01032
deoxycarnitine	Lipid	Carnitine Metabolism	36747	134	C01181	HMDB01161
deoxycholate	Lipid	Secondary Bile Acid Metabolism	1114	222528	C04483	HMDB00626
dihomo-linoleate (20:2n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	17805	6439848	C16525	HMDB05060
dihomo-linolenate (20:3n3 or n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	35718	5280581	C03242	HMDB02925
dihomo-linolenoyl-choline	Lipid	Fatty Acid Metabolism (Acyl Choline)	53262	NA	NA	NA
dihomo-linolenoylcarnitine (C20:3n3 or 6)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57521	NA	NA	NA
dihomo-linoleoylcarnitine (C20:2)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57520	NA	NA	NA
docosadienoate (22:2n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	32415	5282807	C16533	HMDB61714
docosahexaenoate (DHA; 22:6n3)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	44675	445580	C06429	HMDB02183
docosahexaenoylcarnitine (C22:6)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57523	NA	NA	NA
docosahexaenoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	53263	NA	NA	NA
docosapentaenoate (n3 DPA; 22:5n3)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	32504	6441454	C16513	HMDB06528
docosapentaenoate (n6 DPA; 22:5n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	37478	6441454	C16513	HMDB01976
docosapentaenoylcarnitine (C22:5n3)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57529	NA	NA	NA
dodecanedioate (C12-DC)	Lipid	Fatty Acid, Dicarboxylate	32388	12736	C02678	HMDB00623
eicosanodioate (C20-DC)	Lipid	Fatty Acid, Dicarboxylate	39831	75502	NA	NA
eicosapentaenoate (EPA; 20:5n3)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	18467	446284	C06428	HMDB01999

eicosapentaenoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	53258	NA	NA	NA
eicosenoate (20:1)	Lipid	Long Chain Fatty Acid	33587	5282768	C16526	HMDB02231
eicosenoylcarnitine (C20:1)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57519	NA	NA	NA
epiandrosterone sulfate	Lipid	Androgenic Steroids	33973	9929317	NA	NA
erucate (22:1n9)	Lipid	Long Chain Fatty Acid	1552	5281116	C08316	HMDB02068
etiocholanolone glucuronide	Lipid	Androgenic Steroids	47112	270605	NA	HMDB04484
glutarate (C5-DC)	Lipid	Fatty Acid, Dicarboxylate	396	743	C00489	HMDB00661
glycerol	Lipid	Glycerolipid Metabolism	15122	753	C00116	HMDB00131
glycerol 3-phosphate	Lipid	Glycerolipid Metabolism	43847	754	C00093	HMDB00126
glycerophosphoethanolamine	Lipid	Phospholipid Metabolism	37455	123874	C01233	HMDB00114
glycerophosphoinositol*	Lipid	Phospholipid Metabolism	47155	167572	NA	NA
glycerophosphorylcholine (GPC)	Lipid	Phospholipid Metabolism	15990	71920	C00670	HMDB00086
glycochenodeoxycholate	Lipid	Primary Bile Acid Metabolism	32346	12544	C05466	HMDB00637
glycochenodeoxycholate glucuronide (1)	Lipid	Primary Bile Acid Metabolism	52983	NA	NA	NA
glycochenodeoxycholate sulfate	Lipid	Primary Bile Acid Metabolism	52974	NA	NA	NA
glycocholate	Lipid	Primary Bile Acid Metabolism	18476	10140	C01921	HMDB00138
glycocholate sulfate*	Lipid	Secondary Bile Acid Metabolism	32599	NA	NA	NA
glycodeoxycholate	Lipid	Secondary Bile Acid Metabolism	18477	3035026	C05464	HMDB00631
glycodeoxycholate sulfate	Lipid	Secondary Bile Acid Metabolism	52975	NA	NA	NA
glycolithocholate sulfate*	Lipid	Secondary Bile Acid Metabolism	32620	72222	C11301	HMDB02639
glycosyl ceramide (d18:1/20:0, d16:1/22:0)*	Lipid	Hexosylceramides (HCER)	57595	NA	NA	NA
glycosyl ceramide (d18:2/24:1, d18:1/24:2)*	Lipid	Hexosylceramides (HCER)	57453	NA	NA	NA
glycosyl-N-behenoyl-sphingadienine (d18:2/22:0)*	Lipid	Hexosylceramides (HCER)	57421	NA	NA	NA
glycosyl-N-nervonoyl-sphingosine (d18:1/24:1)*	Lipid	Hexosylceramides (HCER)	57369	NA	NA	NA
glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	Lipid	Hexosylceramides (HCER)	53013	NA	NA	NA
glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	Lipid	Hexosylceramides (HCER)	52234	NA	NA	NA
glycoursodeoxycholate	Lipid	Secondary Bile Acid Metabolism	39379	12310288	NA	HMDB00708
hexadecanedioate (C16-DC)	Lipid	Fatty Acid, Dicarboxylate	35678	10459	C19615	HMDB00672
hexanoylcarnitine (C6)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	32328	6426853	NA	HMDB00705
hexanoylglutamine	Lipid	Fatty Acid Metabolism (Acyl Glutamine)	54907	NA	NA	NA
hexanoylglycine	Lipid	Fatty Acid Metabolism(Acyl Glycine)	35436	99463	NA	HMDB00701
isoursodeoxycholate	Lipid	Secondary Bile Acid Metabolism	57577	127601	C17662	HMDB00686
lactosyl-N-nervonoyl-sphingosine (d18:1/24:1)*	Lipid	Lactosylceramides (LCER)	57370	NA	NA	NA

lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)	Lipid	Lactosylceramides (LCER)	53010	NA	NA	NA
laurate (12:0)	Lipid	Medium Chain Fatty Acid	1645	3893	C02679	HMDB00638
laurylcarnitine (C12)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	34534	10427569	NA	HMDB02250
lignoceroyl sphingomyelin (d18:1/24:0)	Lipid	Sphingomyelins	57330	NA	NA	NA
lignoceroylcarnitine (C24)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57515	NA	NA	NA
linoleate (18:2n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	1105	5280450	C01595	HMDB00673
linolenate [alpha or gamma; (18:3n3 or 6)]	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	34035	5280934	C06426	HMDB03073
linolenoylcarnitine (C18:3)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57511	NA	NA	NA
linoleoyl ethanolamide	Lipid	Endocannabinoid	52608	5283446	NA	HMDB12252
linoleoyl-arachidonoyl-glycerol (18:2/20:4) [1]*	Lipid	Diacylglycerol	54955	NA	NA	HMDB07257
linoleoyl-arachidonoyl-glycerol (18:2/20:4) [2]*	Lipid	Diacylglycerol	54956	NA	NA	HMDB07257
linoleoyl-docosahexaenoyl-glycerol (18:2/22:6) [2]*	Lipid	Diacylglycerol	54950	NA	NA	HMDB07266
linoleoyl-linoleoyl-glycerol (18:2/18:2) [1]*	Lipid	Diacylglycerol	54968	NA	NA	HMDB07248
linoleoylcarnitine (C18:2)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	46223	6450015	NA	HMDB06469
linoleoylcholine*	Lipid	Fatty Acid Metabolism (Acyl Choline)	57463	NA	NA	NA
maleate	Lipid	Fatty Acid, Dicarboxylate	20676	444266	C01384	HMDB00176
margarate (17:0)	Lipid	Long Chain Fatty Acid	1121	10465	NA	HMDB02259
margaroylcarnitine (C17)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57512	NA	NA	HMDB06210
myo-inositol	Lipid	Inositol Metabolism	1124	892	C00137	HMDB00211
myristate (14:0)	Lipid	Long Chain Fatty Acid	1365	11005	C06424	HMDB00806
myristoleate (14:1n5)	Lipid	Long Chain Fatty Acid	32418	5281119	C08322	HMDB02000
myristoleoylcarnitine (C14:1)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	48182	90659872	NA	NA
myristoyl dihydrosphingomyelin (d18:0/14:0)*	Lipid	Dihydrosphingomyelins	57365	NA	NA	HMDB12085
myristoylcarnitine (C14)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	33952	6426854	NA	HMDB05066
N-behenoyl-sphingadienine (d18:2/22:0)*	Lipid	Ceramides	57372	NA	NA	NA
N-palmitoyl-sphinganine (d18:0/16:0)	Lipid	Dihydroceramides	52604	5283572	NA	HMDB11760
N-palmitoyl-sphingosine (d18:1/16:0)	Lipid	Ceramides	44877	5283564	NA	HMDB04949
N-palmitoylglycine	Lipid	Fatty Acid Metabolism(Acyl Glycine)	42092	151008	NA	HMDB13034
N-stearoyl-sphingosine (d18:1/18:0)*	Lipid	Ceramides	54979	5283565	NA	HMDB04950
nervonoylcarnitine (C24:1)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57531	NA	NA	NA
nonadecanoate (19:0)	Lipid	Long Chain Fatty Acid	1356	12591	C16535	HMDB00772
octadecanedioate (C18-DC)	Lipid	Fatty Acid, Dicarboxylate	36754	70095	NA	HMDB00782
octanoylcarnitine (C8)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	33936	123701	C02838	HMDB00791

oleate/vaccenate (18:1)	Lipid	Long Chain Fatty Acid	52285	NA	NA	NA
oleoyl-arachidonoyl-glycerol (18:1/20:4) [1]*	Lipid	Diacylglycerol	54960	NA	NA	HMDB07228
oleoyl-arachidonoyl-glycerol (18:1/20:4) [2]*	Lipid	Diacylglycerol	54961	NA	NA	HMDB07228
oleoyl-linoleoyl-glycerol (18:1/18:2) [1]	Lipid	Diacylglycerol	46798	NA	NA	HMDB07219
oleoyl-linoleoyl-glycerol (18:1/18:2) [2]	Lipid	Diacylglycerol	46799	NA	NA	HMDB07219
oleoyl-oleoyl-glycerol (18:1/18:1) [1]*	Lipid	Diacylglycerol	54945	NA	NA	HMDB07218
oleoyl-oleoyl-glycerol (18:1/18:1) [2]*	Lipid	Diacylglycerol	54946	NA	NA	HMDB07218
oleoylcarnitine (C18:1)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	35160	6441392	NA	HMDB05065
oleoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	53260	NA	NA	NA
palmitate (16:0)	Lipid	Long Chain Fatty Acid	1336	985	C00249	HMDB00220
palmitoleate (16:1n7)	Lipid	Long Chain Fatty Acid	33447	445638	C08362	HMDB03229
palmitoleoyl-linoleoyl-glycerol (16:1/18:2) [1]*	Lipid	Diacylglycerol	54967	NA	NA	HMDB07132
palmitoleoylcarnitine (C16:1)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	53223	71464547	NA	NA
palmitoleoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	53257	NA	NA	NA
palmitoyl dihydrosphingomyelin (d18:0/16:0)*	Lipid	Dihydrosphingomyelins	52434	9939965	NA	NA
palmitoyl sphingomyelin (d18:1/16:0)	Lipid	Sphingomyelins	37506	9939941	NA	NA
palmitoyl-arachidonoyl-glycerol (16:0/20:4) [2]*	Lipid	Diacylglycerol	54958	NA	NA	HMDB07112
palmitoyl-linoleoyl-glycerol (16:0/18:2) [1]*	Lipid	Diacylglycerol	52633	9543695	NA	HMDB07103
palmitoyl-linoleoyl-glycerol (16:0/18:2) [2]*	Lipid	Diacylglycerol	52634	NA	NA	HMDB07103
palmitoyl-oleoyl-glycerol (16:0/18:1) [2]*	Lipid	Diacylglycerol	54942	NA	C13861	HMDB07102
palmitoylcarnitine (C16)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	44681	461	C02990	HMDB00222
palmitoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	52944	151731	NA	NA
pentadecanoate (15:0)	Lipid	Long Chain Fatty Acid	1361	13849	C16537	HMDB00826
phosphoethanolamine	Lipid	Phospholipid Metabolism	1600	1015	C00346	HMDB00224
pregnenediol-3-glucuronide	Lipid	Progesterin Steroids	40708	123796	NA	HMDB10318
pregnenediol disulfate (C21H34O8S2)*	Lipid	Pregnenolone Steroids	32562	NA	NA	NA
pregnenediol sulfate (C21H34O5S)*	Lipid	Pregnenolone Steroids	32619	NA	NA	NA
pregnenolone sulfate	Lipid	Pregnenolone Steroids	38170	105074	NA	HMDB00774
propionylcarnitine (C3)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	32452	107738	C03017	HMDB00824
propionylglycine	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	31932	98681	NA	HMDB00783
sebacate (C10-DC)	Lipid	Fatty Acid, Dicarboxylate	32398	5192	C08277	HMDB00792
sphinganine	Lipid	Sphingolipid Synthesis	17769	3126	C00836	HMDB00269
sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*	Lipid	Sphingomyelins	52433	NA	NA	NA

sphingomyelin (d17:2/16:0, d18:2/15:0)*	Lipid	Sphingomyelins	57483	NA	NA	NA
sphingomyelin (d18:0/18:0, d19:0/17:0)*	Lipid	Dihydrosphingomyelins	57473	NA	NA	HMDB12087
sphingomyelin (d18:0/20:0, d16:0/22:0)*	Lipid	Dihydrosphingomyelins	57476	NA	NA	NA
sphingomyelin (d18:1/14:0, d16:1/16:0)*	Lipid	Sphingomyelins	42463	11433862	NA	HMDB12097
sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)	Lipid	Sphingomyelins	52615	NA	NA	NA
sphingomyelin (d18:1/18:1, d18:2/18:0)	Lipid	Sphingomyelins	37529	6443882	NA	HMDB12101
sphingomyelin (d18:1/19:0, d19:1/18:0)*	Lipid	Sphingomyelins	57475	NA	NA	NA
sphingomyelin (d18:1/20:0, d16:1/22:0)*	Lipid	Sphingomyelins	48490	NA	NA	HMDB12102
sphingomyelin (d18:1/20:1, d18:2/20:0)*	Lipid	Sphingomyelins	48491	NA	NA	NA
sphingomyelin (d18:1/20:2, d18:2/20:1, d16:1/22:2)*	Lipid	Sphingomyelins	57481	NA	NA	NA
sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*	Lipid	Sphingomyelins	52495	NA	NA	NA
sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*	Lipid	Sphingomyelins	48493	NA	NA	HMDB12104
sphingomyelin (d18:1/22:2, d18:2/22:1, d16:1/24:2)*	Lipid	Sphingomyelins	57477	NA	NA	NA
sphingomyelin (d18:1/24:1, d18:2/24:0)*	Lipid	Sphingomyelins	47153	NA	NA	HMDB12107
sphingomyelin (d18:1/25:0, d19:0/24:1, d20:1/23:0, d19:1/24:0)*	Lipid	Sphingomyelins	57478	NA	NA	NA
sphingomyelin (d18:2/14:0, d18:1/14:1)*	Lipid	Sphingomyelins	47154	NA	NA	NA
sphingomyelin (d18:2/16:0, d18:1/16:1)*	Lipid	Sphingomyelins	42459	NA	NA	NA
sphingomyelin (d18:2/18:1)*	Lipid	Sphingomyelins	57474	NA	NA	NA
sphingomyelin (d18:2/21:0, d16:2/23:0)*	Lipid	Sphingomyelins	57480	NA	NA	NA
sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*	Lipid	Sphingomyelins	52435	NA	NA	NA
sphingomyelin (d18:2/23:1)*	Lipid	Sphingomyelins	57482	NA	NA	NA
sphingomyelin (d18:2/24:1, d18:1/24:2)*	Lipid	Sphingomyelins	52437	NA	NA	NA
sphingomyelin (d18:2/24:2)*	Lipid	Sphingomyelins	57479	NA	NA	NA
sphingosine	Lipid	Sphingosines	17747	5353955	C00319	HMDB00252
sphingosine 1-phosphate	Lipid	Sphingosines	34445	5283560	C06124	HMDB00277
stearate (18:0)	Lipid	Long Chain Fatty Acid	1358	5281	C01530	HMDB00827
stearidonate (18:4n3)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	33969	5312508	C16300	HMDB06547
stearoyl sphingomyelin (d18:1/18:0)	Lipid	Sphingomyelins	19503	6453725	C00550	HMDB01348
stearoyl-arachidonoyl-glycerol (18:0/20:4) [1]*	Lipid	Diacylglycerol	57450	NA	NA	NA
stearoyl-arachidonoyl-glycerol (18:0/20:4) [2]*	Lipid	Diacylglycerol	57449	NA	NA	NA
stearoylcarnitine (C18)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	34409	6426855	NA	HMDB00848
stearoylcholine*	Lipid	Fatty Acid Metabolism (Acyl Choline)	57464	NA	NA	NA
taurochenodeoxycholate	Lipid	Primary Bile Acid Metabolism	18494	387316	C05465	HMDB00951

taurocholate sulfate	Lipid	Secondary Bile Acid Metabolism	32807	NA	NA	NA
taurodeoxycholate	Lipid	Secondary Bile Acid Metabolism	12261	2733768	C05463	HMDB00896
tauroolithocholate 3-sulfate	Lipid	Secondary Bile Acid Metabolism	36850	440071	C03642	HMDB02580
tetradecanedioate (C14-DC)	Lipid	Fatty Acid, Dicarboxylate	35669	13185	NA	HMDB00872
tricosanoyl sphingomyelin (d18:1/23:0)*	Lipid	Sphingomyelins	52436	NA	NA	HMDB12105
trimethylamine N-oxide	Lipid	Phospholipid Metabolism	40406	1145	C01104	HMDB00925
ursodeoxycholate	Lipid	Secondary Bile Acid Metabolism	1605	31401	C07880	HMDB00946
ximenoylcarnitine (C26:1)*	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	57517	NA	NA	NA
2'-deoxyuridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	1412	13712	C00526	HMDB00012
2'-O-methylcytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	57554	150971	NA	NA
3-ureidopropionate	Nucleotide	Pyrimidine Metabolism, Uracil containing	3155	111	C02642	HMDB00026
5-methyluridine (ribothymidine)	Nucleotide	Pyrimidine Metabolism, Uracil containing	35136	445408	NA	HMDB00884
5,6-dihydrothymine	Nucleotide	Pyrimidine Metabolism, Thymine containing	1418	93556	C00906	HMDB00079
7-methylguanine	Nucleotide	Purine Metabolism, Guanine containing	35114	11361	C02242	HMDB00897
adenine	Nucleotide	Purine Metabolism, Adenine containing	554	190	C00147	HMDB00034
adenosine	Nucleotide	Purine Metabolism, Adenine containing	555	60961	C00212	HMDB00050
allantoin	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	1107	204	C02350	HMDB00462
beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	55	239	C00099	HMDB00056
cytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	514	6175	C00475	HMDB00089
dihydroorotate	Nucleotide	Pyrimidine Metabolism, Orotate containing	601	648	C00337	HMDB03349
guanine	Nucleotide	Purine Metabolism, Guanine containing	32352	764	C00242	HMDB00132
hypoxanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	3127	790	C00262	HMDB00157
inosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	1123	6021	C00294	HMDB00195
N-acetyl-beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	37432	76406	C01073	NA
N1-methyladenosine	Nucleotide	Purine Metabolism, Adenine containing	15650	27476	C02494	HMDB03331
N1-methylinosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	48351	65095	NA	HMDB02721
N2,N2-dimethylguanosine	Nucleotide	Purine Metabolism, Guanine containing	35137	92919	NA	HMDB04824
N6-carbamoylthreonyladenosine	Nucleotide	Purine Metabolism, Adenine containing	35157	161466	NA	HMDB41623
N6-succinyladenosine	Nucleotide	Purine Metabolism, Adenine containing	48130	165243	NA	HMDB00912
orotate	Nucleotide	Pyrimidine Metabolism, Orotate containing	1505	967	C00295	HMDB00226
orotidine	Nucleotide	Pyrimidine Metabolism, Orotate containing	35172	92751	NA	HMDB00788
pseudouridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	33442	15047	C02067	HMDB00767
uracil	Nucleotide	Pyrimidine Metabolism, Uracil containing	605	1174	C00106	HMDB00300

urate	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	1604	1175	C00366	HMDB00289
uridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	606	6029	C00299	HMDB00296
xanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	3147	1188	C00385	HMDB00292
4-hydroxyphenylacetylglutamine	Peptide	Acetylated Peptides	55017	NA	NA	NA
gamma-glutamylalanine	Peptide	Gamma-glutamyl Amino Acid	37063	440103	NA	HMDB29142
gamma-glutamylglutamine	Peptide	Gamma-glutamyl Amino Acid	2730	150914	C05283	HMDB11738
gamma-glutamylglycine	Peptide	Gamma-glutamyl Amino Acid	33949	165527	NA	HMDB11667
gamma-glutamylhistidine	Peptide	Gamma-glutamyl Amino Acid	18245	7017195	NA	NA
gamma-glutamylisoleucine*	Peptide	Gamma-glutamyl Amino Acid	34456	14253342	NA	HMDB11170
gamma-glutamylleucine	Peptide	Gamma-glutamyl Amino Acid	18369	151023	NA	HMDB11171
gamma-glutamylmethionine	Peptide	Gamma-glutamyl Amino Acid	44872	7009567	NA	HMDB29155
gamma-glutamylphenylalanine	Peptide	Gamma-glutamyl Amino Acid	33422	111299	NA	HMDB00594
gamma-glutamylthreonine	Peptide	Gamma-glutamyl Amino Acid	33364	76078708	NA	HMDB29159
gamma-glutamyltryptophan	Peptide	Gamma-glutamyl Amino Acid	33947	3989307	NA	HMDB29160
gamma-glutamyltyrosine	Peptide	Gamma-glutamyl Amino Acid	2734	94340	NA	HMDB11741
gamma-glutamylvaline	Peptide	Gamma-glutamyl Amino Acid	43829	7015683	NA	HMDB11172
isoleucylglycine	Peptide	Dipeptide	40008	342532	NA	HMDB28907
phenylacetylglutamine	Peptide	Acetylated Peptides	35126	92258	C04148	HMDB06344

Legend: ID – identifier, NA – not available, PubChem – identifier on the library of the National Center for Biotechnology Information (<https://pubchem.ncbi.nlm.nih.gov/>), KEGG – identifier on the Kyoto Encyclopedia of Genes and Genomes (<https://www.genome.jp/kegg/compound/>), HMDB – identifier based on the human metabolome database (<https://hmdb.ca/>)