

Compound (Metabolite)	KEGG ID	HMDB ID	PubChem	CAS	METABOLIC PATHWAY
Trimethylamine (TMA)	C00565	HMDB00906	1146	75-50-3	Microbial metabolism
Ethanolamine	C00189	HMDB00149	700	141-43-5	Glycerophospholipid modification/metabolism
Aminoacetone	C01888	HMDB02134	215	298-08-8	Amino acids metabolism/Gly, Ser, Thr
1-methylguanidine	C02294	HMDB01522	10111	471-29-4	Amino acid metabolism/Arg
Glycine (Gly)	C00037	HMDB00123	750	56-40-6	Amino Acid
Trimethylamine-N-oxide (TMAO)	C01104	HMDB00925	1145	1184-78-7	Gut flora metabolism / Redox
Putrescine	C00134	HMDB01414	1045	110-60-1	Polyamine metabolism
beta-Alanine	C00099	HMDB00056	239	107-95-9	Beta Amino Acid
Alanine (Ala)	C00041	HMDB00161	5950	56-41-7	Amino Acid
Sarcosine	C00213	HMDB00271	3513	107-97-1	Amino Acid
Betaine Aldehyde	C00576	HMDB01252	249	7418-61-3	Amino acids metabolism/Gly, Ser, Thr
Cadaverine	C01672	HMDB02322	273	462-94-2	Amino Acid
3-Aminoisobutyrate	C03284	HMDB03911	64956	144-90-1	Amino acids metabolism/Ile, Leu, Val
Choline	C00114	HMDB00097	305	62-49-7	Vitamins
Dimethylglycine	C01026	HMDB00092	673	1118-68-9	Vitamins
L-2-aminobutyric acid	C02356	HMDB00452	80283	1492-24-6	Amino acid metabolism/Met, Ser, Thr
2-aminoisobutyric acid	C03665	HMDB01906	6119	62-57-7	Nucleotide/Pyrimidine metabolism
Serine (Ser)	C00065	HMDB00187	5951	56-45-1	Amino Acid
Hypotaurine	C00519	HMDB00965	107812	300-84-5	Amino acids metabolism/Sulfur metabolism
Cytosine (Cyt)	C00380	HMDB00630	597	71-30-7	Nucleotide
Histamine	C00388	HMDB00870	774	51-45-6	Nucleotide
Creatinine	C00791	HMDB00562	588	60-27-5	Amino acids metabolism/Arg, Gly
5,6-dihydrouracil	C00429	HMDB00076	649	504-07-4	Nucleotide/Pyrimidine metabolism
Proline (Pro)	C00148	HMDB00162	145742	147-85-3	Amino Acid
5-Aminovalerate	C00431	HMDB03355	138	660-88-8	Amino Acid
Betaine	C00719	HMDB00043	247	107-43-7	Amino acids metabolism/Gly, Ser, Thr
Valine (Val)	C00183	HMDB00883	6287	72-18-4	Amino Acid
Indole	C00463	HMDB00738	798	120-72-9	Amino acids metabolism/Phe, Tyr, Trp
Threonine (Thr)	C00188	HMDB00167	6288	72-19-5	Amino Acid
Cysteine (Cys)	C00097	HMDB00574	5862	52-90-4	Amino Acid
Niacinamide	C00153	HMDB01406	936	98-92-0	Vitamins
Taurine (Tau)	C00245	HMDB00251	1123	107-35-7	Amino acids metabolism/Sulfur metabolism
1-Methylhistamine	C05127	HMDB00898	3614	501-75-7	Amino acid metabolism/His
Imidazoleacetic acid	C02835	HMDB02024	96215	645-65-8	Amino acids metabolism/His
5,6-dihydrothymine	C00906	HMDB00079	93556	696-04-8	Nucleotide/Pyrimidine metabolism
Pyroglutamic Acid	C01879	HMDB00267	7405	98-79-3	Amino acids/Glu
Pipecolate	C00408	HMDB00070	6931663	3105-95-1	Amino Acid
Agmatine	C00179	HMDB01432	199	2482-00-0	Polyamine metabolism

N-acetylputrescine	C02714	HMDB02064	122356	18233-70-0	Polyamine metabolism
Creatine	C00300	HMDB00064	586	57-00-1	Amino acids metabolism/Arg, Gly
Hydroxyproline	C01015	HMDB00725	5810	51-35-4	Amino acid metabolism/Pro
Aminolevulinate	C00430	HMDB01149	137	106-60-5	Amino acids metabolism/Gly, Ser, Thr
D-Norleucine	N/A	N/A	456468	327-56-0	Unnatural Amino acid
Leucine (Leu)	C00123	HMDB00687	6106	61-90-5	Amino acid
allo-isoleucine	C21096	HMDB00557	99288	1509-34-8	Isoleucine derivative
isoLeucine (isoLeu)	C00407	HMDB00172	791	73-32-5	Amino Acid
Ornithine	C01602	HMDB03374	6262	3184-13-2	Urea cycle
Asparagine (Asp)	C00152	HMDB00168	6267	70-47-3	Amino Acid
Aspartic Acid	C00049	HMDB00191	5960	56-84-8	Amino Acid
Homocysteine	C00155	HMDB00742	778	454-29-5	Amino acid metabolism/Cys, Met
S-methyl-L-cysteine	N/A	HMDB02108	24417	1187-84-4	Amino acid metabolism/Cys
1-methylnicotinamide	C02918	HMDB00699	457	3106-60-3	Nicotinate and nicotinamide metabolism
Tyramine	C00483	HMDB00306	5610	51-67-2	Amino Acid
4-aminobenzoic acid	C00568	HMDB01392	978	150-13-0	Benzoate degradation
Trigonelline	C01004	HMDB00875	5570	535-83-1	Nicotinate and nicotinamide metabolism
1-Methylimidazoleacetic acid	C05828	HMDB02820	75810	2625-49-2	Amino acid metabolism/His
Imidazole propionate	C20522	HMDB02271	70630	1074-59-5	Amino acids metabolism/His
Spermidine	C00315	HMDB01257	1102	124-20-9	Polyamine metabolism
4-guanidinobutanoate	C01035	HMDB03464	5000	463-00-3	Amino acid metabolism/Arg
Acetylcholine	C01996	HMDB00895	187	60-32-1	Lipids/phospholipids, ligand
Glutamine (Glu)	C00303	HMDB00641	5961	56-85-9	Amino Acid
Lysine (Lys)	C00047	HMDB00182	5962	56-87-1	Amino Acid
Deoxycarnitine	C01181	HMDB01161	725	6249-56-5	Lipids/phospholipids, ligand
Glutamic acid (Glu A)	C00025	HMDB03339	611	56-86-0	Amino Acid
Methionine (Met)	C01733	HMDB00696	6137	63-68-3	Amino Acid
Guanine	C00242	HMDB00132	764	73-40-5	Nucleotide/Purine metabolism
Cystamine	N/A	N/A	2915	51-85-4	Amino acids metabolism/Cys
Histidine (His)	C00768	HMDB00177	6274	5934-29-2	Amino Acid
Serotonin	C00780	HMDB00259	5202	50-67-9	Amino acid metabolism/Trp
Tryptamine	C00398	HMDB00303	1150	61-54-1	Amino Acid
Carnitine	C00487	HMDB00062	2724480	541-15-1	Amino acids metabolism/Lys
Phenylalanine	C02057	HMDB00159	6140	63-91-2	Amino Acid
Methionine sulfoxide	N/A	HMDB02005	847	62697-73-8	Methionine oxidative stress product
Epinephrine	C00788	HMDB00068	5816	51-43-4	Amino Acid metabolism/Tyr,ligand
7-methylguanine	C02242	HMDB00897	11361	578-76-7	Methylated nucleoside
Normetanephrine	C05589	HMDB00819	1237	97-31-4	Amino Acid metabolism/Tyr,ligand
Taurocyamine	C01959	HMDB03584	68340	543-18-0	Amino acids metabolism/Sulfur metabolism

Pyridoxamine (Vitamin B6)	C00534	HMDB01431	1052	85-87-0	Vitamins
1/3-Methylhistidine	C01152	HMDB00001	4381	368-16-1	Amino acid metabolism/His
Norepinephrine	C00547	HMDB00216	439260	51-41-2	Amino Acid metabolism/Trp
n-glycylproline	N/A	HMDB00721	3013625	704-15-4	Collagen degradation
Arginine	C00062	HMDB00517	232	1119-34-2	Amino Acid
N-acetyl-L-ornithine	C00437	HMDB03357	439232	1572591	Acetylated amino acid/Orn
Cotinine	N/A	HMDB01046	408	486-56-6	Nicotine Metabolism
CysteinylGlycine (Cys-Gly)	C01419	HMDB28775	439498	19246-18-5	Amino acids degradation
Gluconolactone	C00198	HMDB00150	7027	90-80-2	Sugars
Glucosamine	C00329	HMDB06479	439213	3416-24-8	Amino sugar and nucleotide sugar metabolism
Theobromine	C07480	HMDB02825	5429	83-67-0	Caffeine metabolism/Cocoa biomarker
1,7-dimethylxanthine	C13747	HMDB01860	4687	611-56-6	Caffeine Metabolism
Tyrosine (Tyr)	C00082	HMDB00158	6057	60-18-4	Amino Acid
Se-methylselenocysteine	C05689	HMDB04113	147004	26046-90-2	Selenium amino acids
Phosphorylcholine	C00588	HMDB01565	1014	626852	Fatty acid metabolism
N6-acetyl-L-lysine	C02727	HMDB00206	92832	692-04-6	Acetylated amino acid/Leu
Homoarginine	C01924	HMDB00670	9085	156-86-5	Urea cycle/Ornithine metabolite
N6,N6,N6-trimethyl-L-lysine	C03793	HMDB01325	6992003	19253-88-4	Amino acid metabolism/Leu
Homocitrulline	C02427	HMDB00679	65072	1190-49-4	Urea cycle/Ornithine metabolite
Caffeine	C07481	HMDB01847	2519	58-08-2	Caffeine metabolism
Salicylurate	C07588	HMDB00840	10253	487-54-7	Amino acid metabolism/Gly
DL-DOPA (3,4-Dihydroxy-DL-phenylalanine)	C00355	HMDB00609	836	63-84-3	Amino acid metabolism/Tyr
Selenomethionine	C05335	HMDB03966	15103	3211-76-5	Selenium amino acids
N(G),N(G)-dimethylarginine (ADMA)	C03626	HMDB01539	123831	30315-93-6	Methylated amino acid/Arg
N(G),N(G')-dimethylarginine (SDMA)	N/A	HMDB03334	169148	30344-004	Methylated amino acid/Arg
Spermine	C00750	HMDB01256	1103	71-44-3	Polyamine metabolism
3-Indolebutyric acid	C11284	HMDB02096	8617	133-32-4	Tryptophan cycle
Acetylcarnitine	C02571	HMDB00201	5567	3040-38-8	Fatty acid Oxidation
Tryptophan (Try)	C00078	HMDB00929	6305	73-22-3	Tryptophan Cycle
L-Kynurenine	C00328	HMDB00684	161166	343-65-7	Tryptophan Cycle
Phosphocreatine	C02305	HMDB01511	9548602	67-07-2	Amino acid metabolism/Arg, Pro
N-acetyl-L-arginine	N/A	HMDB04620	67427	155-84-0	Acetylated amino acid/Arg
Carnosine	C00386	HMDB00033	439224	305-84-0	Amino acids metabolism/His
2'-deoxycytidine	C00881	HMDB00014	13711	951-77-9	Nucleotide/Pyrimidine metabolism
2'-Deoxyuridine	C00526	HMDB00012	13712	951-78-0	Nucleotide/Pyrimidine metabolism
Biopterin	C06313	HMDB00468	445040	22150-76-1	Folate Biosynthesis Pathway/Pterin Synthesis
Anserine	C01262	HMDB00194	112072	584-85-0	Amino acids metabolism/His
Cystine	C00491	HMDB00192	67678	56-89-3	Amino acids metabolism
Cytidine	C00475	HMDB00089	6175	65-46-3	Nucleotide/Pyrimidine metabolism

Uridine	C00299	HMDB00296	6029	58-96-8	Nucleotide/Pyrimidine metabolism
Isovalerylcarnitine	C20826	HMDB00688	6426851	31023-24-2	Acyl carnitine
Neopterin	C05926	HMDB00845	4455	2009-64-5	Folate Biosynthesis Pathway/Pterin Synthesis
Glycerophosphocholine	C00670	HMDB00086	71920	28319-77-9	Lipids/phospholipids, ligand
5-methylcytidine	N/A	HMDB00982	92918	2140-61-6	Modified nucleoside
Phosphotyrosine	C06501	HMDB06049	30819	N/A	Amino acids metabolism
Succinylcarnitine	N/A	HMDB61717	71464481	256928-74-2	Fatty acid metabolism
Thiamine (Vitamin B1)	C00378	HMDB00235	1130	59-43-8	Vitamins
2,3-diphosphoglyceric acid	C01159	HMDB01294	186004	138-81-8	Glycolysis
Deoxyguanosine	C00330	HMDB00085	187790	961-07-9	Nucleotide/Purine metabolism
Adenosine	C00212	HMDB00050	60961	58-61-7	Nucleotide/Purine metabolism
Retinol (Vitamin A)	C19962	HMDB00305	9904001	68-26-8	Vitamins
Inosine	C00294	HMDB00195	6021	58-63-9	Nucleotide/Purine metabolism
Glutaryl carnitine	N/A	HMDB13130	71317118	102636-82-8	Acyl carnitine
1-Methyladenosine	C02494	HMDB03331	27476	15763-06-1	Nucleotide/Purine metabolism
6-methyladenosine	N/A	HMDB04044	102175	1867-73-8	Methylated nucleoside
Guanosine	C00387	HMDB00133	6802	118-00-3	Nucleotide/Purine metabolism
Retinal	C00376	HMDB01358	6436079	116-31-4	Vitamins
Argininosuccinate	C03406	HMDB00052	16950	2387-71-5	Amino acid metabolism/Arg
5'-methylthioadenosine	C00170	HMDB01173	439176	2457-80-9	Amino acid metabolism/Cys, Met
N2,N2-Dimethylguanosine	N/A	HMDB04824	92919	2140-67-2	Nucleotide/Purine metabolism
Uridine 5'-monophosphate (UMP)	C00105	HMDB0000288	101543	3387-36-8	Nucleotide/Pyrimidine metabolism
Adenosine-3'-5'-cyclic monophosphate (cAMP)	C00575	HMDB00058	6076	60-92-4	Secondary messenger and regulator
Guanosine-5'-monophosphate (GMP)	C00144	HMDB01397	6804	85-32-5	Nucleotide/Purine metabolism
Riboflavin (Vitamin B2)	C00255	HMDB00244	493570	83-88-5	Vitamin
S-adenosyl-L-homocysteine (SAH)	C00021	HMDB0000939	439155	979-92-0	Amino acid metabolism/Cys, Met
Cholecalciferol (Vitamin D3)	C05443	HMDB00876	5280795	67-97-0	Vitamins
Ergocalciferol (Vitamin D2)	C05441	HMDB00900	5280793	50-14-6	Vitamins
S-adenosyl-L-methionine (SAM)	C00019	HMDB01185	16757548	485-80-3	Amino acid metabolism/Arg, Cys, Met, Pro
Cytidine 5'-diphosphate (CDP)	C00112	HMDB01546	6132	63-38-7	Nucleotide/Pyrimidine metabolism
Thiamine pyrophosphate	C00068	HMDB0001372	9068	154-87-0	Coenzyme
Folic Acid	C00504	HMDB00121	6037	59-30-3	One carbon pool by folate
Vitamin K1	C02059	HMDB03555	5280483	12001-79-5	Vitamins
Biliverdin	C00500	HMDB01008	5353439	114-25-0	Hemoglobin metabolism
Nicotinamide adenine dinucleotide (NAD)	C00003	HMDB00902	5893	53-84-9	Coenzyme
Nicotinamide adenine dinucleotide reduced (NADH)	C00004	HMDB01487	439153	606-68-8	Coenzyme
Methylcobalamin (Vitamin B12)	C06453	HMDB02274	10898559	13422-55-4	Coenzyme/Vitamin
Cyanocobalamin (Vitamin B12)	C05776	HMDB00607	5311498	68-19-9	Vitamins
tinamide adenine dinucleotide phosphate reduced (NAI	C00005	HMDB00221	5884	53-57-6	Coenzyme

Thyroxine	C01829	HMDB00248	5819	51-48-9	Hormone and Amino acid metabolism/Tyr
Flavin Adenine Dinucleotide (FAD)	C00016	HMDB01248	643975	146-14-5	Coenzyme
Adenosylcobalamin	C00194	HMDB02086	70678541	13870-90-1	Vitamins
Ubiquinol (Q10)	C11378	HMDB13111	9962735	5677-55-4	Coenzyme
Malondialdehyde	C19440	HMDB06112	10964	542-78-9	Oxidative Damage
Glycolic acid	C03547	HMDB00115	757	79-14-1	Glyoxylate and dicarboxylate metabolism
Pyruvate	C00022	HMDB00243	1060	127-17-3	Glycolysis/amino acids metabolism
Lactate	C00186	HMDB00190	612	79-33-4	Glycolysis/TCA
Glyceraldehyde	C02426	HMDB01051	751	56-82-6	Sugar
3-hydroxypropionic acid	C01013	HMDB00700	68152	503-66-2	Amino acids
isoValeric Acid	C08262	HMDB00718	10461	503-74-2	Amino Acid
Acetoacetate	C00164	HMDB00060	96	541-50-4	Ketone
4-oxobutanoate	C00232	HMDB0001259	9543238	13865-19-5	protein degradation & absorption/Amino Acid/Ketone metabolism
2-oxobutyrate	C00109	HMDB00005	58	600-18-0	Amino acid metabolism/Cys, Gly, Ile, Leu, Met, Ser, Thr, Val
Malonic Acid	C00383	HMDB00691	867	141-82-2	TCA Cycle
3-Hydroxybutyric Acid (3HBA)	C01089	HMDB00357	441	625-72-9	TCA Cycle
2-hydroxyisobutyrate	N/A	HMDB00729	11671	594-61-4	Amino acid metabolism/Thr
2-hydroxybutyrate	C05984	HMDB00008	11266	600-15-7	Amino acid metabolism/Thr, Met
Glycerate	C00258	HMDB00139	752	600-19-1	Amino Acid metabolism/Gly, Ser
Uracil	C00106	HMDB00300	1174	66-22-8	Nucleotide/Pyrimidine metabolism
Fumaric Acid	C00122	HMDB00134	444972	100-17-8	TCA Cycle
Maleic Acid	C01384	HMDB00176	444266	110-16-7	TCA Cycle
N-Acetyl-L-glycine	N/A	HMDB00532	10972	543-24-8	Amino Acid metabolism
Guanidinoacetate	C00581	HMDB00128	763	352-97-6	Amino Acid metabolism/Gly, Ser, Thr
2-hydroxyisovaleric acid	N/A	HMDB00407	99823	4026-18-0	Amino Acid metabolism/Ile, Leu, Val
Succinate	C00042	HMDB00254	1110	110-15-6	TCA Cycle
Methylmalonate	C02170	HMDB00202	487	516-05-2	Vitamins
3-Hydroxyisovaleric Acid	N/A	HMDB00754	69362	625-08-1	Amino Acid
Erythrose	C01796	HMDB02649	439574	1758-51-6	Sugar
Threitol	C16884	HMDB04136	169019	2418-52-2	Sugar metabolism
Nicotinate (Niacin)	C00253	HMDB01488	938	59-67-6	Nicotinate and nicotinamide metabolism
Picolinic Acid	C10164	HMDB0002243	1018	98-98-6	Tryptophan Cycle
Thymine	C00178	HMDB00262	1135	65-71-4	Nucleotide/Pyrimidine metabolism
Citraconic Acid	C02226	HMDB00634	643798	498-23-7	Amino Acid metabolism/Ile, Leu, Val
2-oxoisocaproic acid	C00233	HMDB00695	3527278	816-66-0	Amino Acid metabolism/Ile, Leu, Val
Itaconic acid	C00490	HMDB02092	811	97-65-4	Glyoxylate and dicarboxylate metabolism
N-acetyl-L-alanine	N/A	HMDB00766	88064	97-69-8	Acetylated amino acid/Ala
Methylsuccinate	C08645	HMDB01844	10349	498-21-5	Amino acid metabolism/Ile
D-Leucic Acid	C03264	HMDB00624	439960	20312-37-2	Amino Acid metabolism/Leu

Glutaric Acid	C00489	HMDB00661	743	110-94-1	Amino Acids/Lys, Trp, fatty acids
Oxaloacetate	C00036	HMDB00223	970	328-42-7	TCA Cycle
Ethylmalonic acid	N/A	HMDB00622	11756	601-75-2	Fatty acid metabolism
N-carbamoyl-B-alanine	C02642	HMDB00026	111	462-88-4	Urea cycle
Malate	C00149	HMDB00156	525	6915-15-7	TCA Cycle
Adenine	C00147	HMDB00034	190	73-24-5	Nucleotide/Purine metabolism
Allopurinol	D00224	HMDB14581	2094	315-30-0	Nucleotide metabolism (Drug)
Hypoxanthine	C00262	HMDB00157	790	68-94-0	Nucleotide
Phenylacetic acid	N/A	HMDB00209	999	103-82-2	Amino acid metabolism/Phe
Erythronic acid	N/A	HMDB00613	2781043	488-16-4	Sugar metabolism
Threonic acid	C01620	HMDB00943	151152	3909-12-4	Ascorbate metabolism
Anthranilate	C00108	HMDB01123	227	118-92-3	Amino Acid metabolism/Phe, Trp, Tyr
4-hydroxybenzoic acid	C00156	HMDB00500	135	99-96-7	Amino acid metabolism/Phe
Acetylphosphate	C00227	HMDB01494	186	590-54-5	Amino acids metabolism/Sulfur metabolism
Phosphoethanolamine	C00346	HMDB00224	1015	1071-23-4	Glycerophospholipid/Sphingolipid modification/metabolism
N-isobutyrylglycine	N/A	HMDB00730	10855600	15926-18-8	Fatty acid metabolism
Adipic Acid	C06104	HMDB00448	196	124-04-9	Caprolactam degradation
3-methylglutaric acid	N/A	HMDB00752	12284	626-51-7	Amino acid metabolite/Leu
Alpha-Ketoglutaric Acid	C00026	HMDB00208	51	328-50-7	TCA Cycle
2-methylglutaric acid	N/A	HMDB00422	12046	617-62-9	TCA Cycle
Mevalonate	C00418	HMDB00227	449	150-97-0	Terpenoid backbone biosynthesis
2-Hydroxyglutarate	C02630	HMDB59655	43	63512-50-5	Amino-acid metabolism & Glycine/Serine/Threonine metabolism
Citramalic Acid	C00815	HMDB0000426	1081	6236-09-5	TCA Cycle
L-Tartaric acid	C00898	HMDB59916	444305	87-69-4	Glyoxylate and dicarboxylate metabolism
Xylose	C00181	HMDB00098	644160	25990-60-7	Sugar
Alpha-ketophenylacetic acid	N/A	HMDB0001587	11915	611-73-4	Benzoate degradation and amino acid metabolism/Phe
Hydrocinnamic acid	C05629	HMDB00764	107	501-52-0	Amino acid metabolism/Phe
Oxypurinol	C07599	HMDB00786	4644	2465-59-0	Nucleotide metabolism
Xanthine	C00385	HMDB00292	1188	69-89-6	Nucleotide
(R)-2-Hydroxy-2-phenylacetic acid (R-mandelic acid)	C01983	HMDB62635	11914	611-71-2	Benzoate degradation
(S)-2-Hydroxy-2-phenylacetate (L-mandelic acid)	C01984	HMDB00703	439616	17199-29-0	Adrenaline Metabolism
Arabitol	C01904	HMDB00568	94154	488-82-4	Sugar metabolism
3-hydroxyphenylacetic acid	C05593	HMDB00440	12122	621-37-4	Amino acid metabolism/Phe, Tyr
4-hydroxyphenylacetic acid	C00642	HMDB60390	127	156-38-7	Amino acid metabolism/Phe, Tyr
3-hydroxyanthranilate	C00632	HMDB01476	86	548-93-6	Amino Acid metabolism/Trp
Dopamine	C03758	HMDB00073	681	62-31-7	Adrenaline Metabolism
2,3-dihydroxybenzoic acid (2-pyrocatechuic acid)	C00196	HMDB00397	19	303-38-8	Benzoate degradation
Gentisate	C00628	HMDB00152	3469	490-79-9	Amino acid metabolism/Tyr and benzoate degradation
Orotic acid	C00295	HMDB00226	967	50887-69-9	Nucleotide/Pyrimidine metabolism

Allantoin	C01551	HMDB00462	204	97-59-6	Nucleotide Degredation
N-isovaleryl glycine	N/A	HMDB00678	546304	16284-60-9	Fatty acid metabolism
2-Amino adipate	C00956	HMDB00510	469	542-32-5	Amino acid metabolism/Lys
Indole-3-carboxylic acid	C19837	HMDB03320	69867	771-50-6	Tryptophan cycle
Indole-2-carboxylic acid	N/A	HMDB02285	72899	1477-50-5	Amino acids metabolism/Trp
3-Hydroxymethylglutaric acid	C03761	HMDB00355	1662	503-49-1	Amino acid metabolism/Leu
Phenylpyruvic acid (PPA)	C00166	HMDB00205	997	156-06-9	Amino acids metabolism/Phe
3-hydroxycinnamic acid	C12621	HMDB01713	637541	588-30-7	Amino acid metabolism/Phe
4-hydroxycinnamic acid (p-coumaric acid)	C00811	HMDB02035	637542	7400-08-0	Amino Acid metabolism/Phe, Tyr
Xylonate	C05411	HMDB60256	6971043	4172-44-5	Sugar metabolism
Phenyllactic acid	N/A	HMDB00779	3848	828-01-3	Amino acid metabolism/Phe
3-(4-hydroxyphenyl)propionate	C01744	HMDB02199	10394	501-97-3	Amino acid metabolism/Tyr
Quinolinic Acid	C03722	HMDB0000232	1066.0	89-00-9	Tryptophan Cycle
Phosphoenolpyruvic Acid (PEP)	C00074	HMDB00263	1005	138-08-9	Glycolysis
Homogentisate	C00544	HMDB00130	780	451-13-8	Amino acid metabolism/Tyr
Urate	C00366	HMDB00289	1175	69-93-2	Nucleotide/Purine metabolism
Dihydroxyacetone phosphate (DHAP)	C00111	HMDB01473	668	57-04-5	Glycolysis/phospholipid
D-Glyceraldehyde-3-phosphate (D-GA3P)	C00661	HMDB01112	729	142-10-9	Glycolysis/Glycogenesis
Glycerol-3-Phosphate	C00093	HMDB00126	754	29849-82-9	Lipids/Glycerollipid
trans-Aconitate	C02341	HMDB00958	444212	4023-65-8	C5-branched dibasic acid metabolism
Shikimic Acid	C00493	HMDB03070	8742	138-59-0	Amino acid metabolism/Phe, Trp, Tyr
cis-Aconitate	C00417	HMDB00072	643757	585-84-2	TCA Cycle
Suberic acid	C08278	HMDB00893	10457	505-48-6	Fatty acid metabolism
Indole-3-Acetic Acid	C00954	HMDB00197	802	87-51-4	Amino acids metabolism/Trp
Citrulline	C00327	HMDB00904	833	372-75-8	Urea Cycle
N-acetylaspartate	C01042	HMDB00812	65065	997-55-7	Neuropeptide, acetylated amino acids
Ascorbic Acid (Vit. C)	C00072	HMDB00044	54670067	50-81-7	Vitamin, Cofactor
2-isopropylmalate	C02504	HMDB00402	5280523	3237-44-3	Amino Acid metabolism/Ile, Leu, Val
3-isopropylmalate	C04411	HMDB12156	5462261	921-28-8	Amino acids metabolism/Ile, Leu, Val
N-formyl-L-methionine	C03145	HMDB01015	439750	4289-98-9	Amino acid metabolism/Met
Hippuric Acid	C01586	HMDB00714	4741	495-69-2	Amino acid metabolism/Phe
Inositol	C00137	N/A	892	87-89-8	Glucose/inositol metabolism
Glucose	C00031	HMDB00122	79025	50-99-7	Glycolysis/sugar
Mannose	C00159	HMDB00169	3459	3458-28-4	Sugar/Galactose Metabolism
Fructose	C00095	HMDB00660	5984	57-48-7	Sugar
4-Hydroxyphenylpyruvate	C01179	HMDB00707	979	156-39-8	Amino Acid metabolism/Phe, Tyr
Theophylline	C07130	HMDB01889	2153	58-55-9	Caffeine metabolism
Sorbitol	C00794	HMDB00247	107428	6706-59-8	Sugar
Homovanillate	C05582	HMDB00118	1738	306-08-1	Amino acid metabolism/Tyr, ligand

Mannitol	C00392	HMDB00765	6251	69-65-8	Sugar metabolism
4-Pyridoxic acid (Vitamin B6)	C00847	HMDB00017	6723	82-82-6	Vitamins
Phosphoserine	C01005	HMDB00272	68841	407-41-0	Amino acid metabolism/Ser
2-Phosphoglyceric Acid	C00597	HMDB00362	59	2553-59-5	Glycolosis
3-Phosphoglyceric Acid	C00197	HMDB00807	724	820-11-1	Glycolosis
Azelaic Acid	C08261	HMDB00784	10460	123-99-9	Fatty Acids and Conjugates
N-acetyl-L-glutamine	N/A	HMDB06029	25561	2490-97-3	Acetylated amino acid/Gln
Kynurenate	C01717	HMDB00715	3845	492-27-3	Amino acid metabolism/Trp
N-acetyl-L-glutamate	C00624	HMDB01138	70914	1188-37-0	Acetylated amino acid/Glu
Indole-3-propionate	N/A	HMDB02302	3744	830-96-6	Tryptophan cycle
5-hydroxy-indole-3-acetic acid	C05635	HMDB00763	1826	54-16-0	Amino Acid metabolism/Trp
N-acetyl-L-methionine	C02712	HMDB11745	448580	65-82-7	Acetylated amino acid/Met
Citric Acid	C00158	HMDB00094	311	77-92-9	TCA Cycle
Glucuronate	C00191	HMDB00127	444791	1700908	Amino sugar and nucleotide sugar metabolism
4-hydroxy-3-nitrophenylacetate	N/A	HMDB62403	447364	N/A	Nitrotyrosine metabolism
Vanilmandelic acid	C05584	HMDB00291	1245	55-10-7	Amino acid metabolism/Tyr
Erythrose-4-phosphate	C00279	HMDB01321	122357	585-18-2	Pentose phosphate pathway
Cysteine-s-sulfate	C05824	HMDB00731	115015	1637-71-4	Amino acid metabolism/Cys, Met
Indolepyruvic acid	C00331	HMDB60484	803	35656-49-6	Amino acids metabolism/Trp
Xanthurenic acid	C02470	HMDB00881	5699	59-00-7	Amino acids metabolism
Indolelactic acid	C02043	HMDB00671	92904	1821-52-9	Amino acids metabolism/Trp
N-acetyl-L-phenylalanine	C03519	HMDB00512	74839	2018-61-3	Acetylated amino acid/Phe
3-indoxyl sulfate	N/A	HMDB00682	10258	487-94-5	Amino Acid metabolism/Trp
Pantothenate	C00864	HMDB00210	6613	137-08-6	Amino acid metabolism/alanine, CoA
Cystathionine	C00542	HMDB00099	439258	56-88-2	Amino acids metabolism/Cys
N-acetyl-L-tyrosine	N/A	HMDB00866	68310	537-55-3	Acetylated amino acid/Tyr
Myristic Acid	C06424	HMDB0000806	11005	544-63-8	Fatty acid metabolism
Ribose-5-Phosphate	C00117	HMDB01548	439167	3615-55-2	Pentose phosphate pathway
Ribulose 5-phosphate	C00199	HMDB00618	439184	4151-19-3	Pentose phosphate pathway
Melatonin	C01598	HMDB01389	896	73-31-4	Neuroactive ligand
Tetrahydrobiopterin	C00272	HMDB00027	1125	17528-72-2	Folate Biosynthesis Pathway/Pterin Synthesis
Thymidine	C00214	HMDB00273	5789	50-89-5	Nucleotide/Pyrimidine metabolism
Pseudouridine	C02067	HMDB00767	15047	1445-07-4	Nucleotide/Pyrimidine metabolism
Biotin	C00120	HMDB00030	171548	58-85-5	Vitamins
N-acetyl-L-tryptophan	N/A	HMDB13713	700653	1218-34-4	Acetylated amino acid/Trp
Pyridoxal-5-Phosphate	C00018	HMDB01491	1051	54-47-7	Vitamins/B6
Palmitic Acid	C00249	HMDB0000220	985	57-10-3	Fatty acid metabolism
5-methyluridine	N/A	HMDB00884	445408	1463-10-1	Methylated nucleoside
5-hydroxymethyl-2'-deoxyuridine	N/A	N/A	91541	5116-24-5	Modified nucleoside

Glucosamine-6-phosphate	C00352	HMDB0001254	439217	9013-10-9	Amino sugar and nucleotide sugar metabolism
Glucose-6-phosphate (G6P)	C00092	HMDB01401	5958	56-73-5	Glycolosis/PPP
Fructose-1-phosphate (F1P)	C01094	HMDB01076	10400369	15978-08-2	Glycolosis
Fructose-6-phosphate (F6P)	C00085	HMDB00124	69507	643-13-0	Glycolosis
Glucose-1-phosphate (G1P)	C00103	HMDB01586	439165	59-56-3	Glycolysis
Phenylacetylglutamine	C04148	HMDB06344	92258	28047-15-6	Amino acid metabolism/Phe
MOPEG Sulfate	N/A	HMDB00559	4183	3415-67-6	Amino Acid metabolism/Tyr
Margaric Acid	N/A	HMDB02259	10465	506-12-7	Fatty acid metabolism
6-phosphogluconic acid	N/A	HMDB0001316	91493	921-62-0	Pentose phosphate pathway
Linolenic Acid	C06427	HMDB01388	5280934	463-40-1	Fatty acid metabolism
Linoleic Acid	C01595	HMDB00673	5280450	60-33-3	Fatty acid metabolism
Xanthosine	C01762	HMDB00299	64959	146-80-5	Nucleotide/Purine metabolism
Sedoheptulose 7-phosphate	C00281	HMDB01068	22833559	2646-35-7	Pentose phosphate pathway
Retinoic acid	C00777	HMDB01852	444795	302-79-4	Vitamins
N-acetylaspartylglutamate	C12270	HMDB01067	188803	3106-85-2	Neuropeptide, acetylated amino acids
Arachidonate	C00219	HMDB60102	444899	6610-25-9	Lipids/phospholipids, ligand
Deoxycytidylic acid (DCMP)	C00239	HMDB01202	13945	1032-65-1	Nucleotide/pyrimidine
Reduced glutathione	C00051	HMDB00125	124886	70-18-8	Oxidative Damage
Deoxyuridylic acid (DUMP)	C00365	HMDB01409	65063	964-26-1	Nucleotide/pyrimidine
N-acetylneuraminate	C00270	HMDB00230	445063	131-48-6	Sugars
Geranyl Pyrophosphate	C00341	HMDB01285	445995	763-10-0	Ubiquinone and other terpenoid-quinone biosynthesis
D-Thymidine monophosphate (DTMP)	C00364	HMDB01227	3655	365-07-1	Nucleic Acid
Thymidine-5-phosphate (DTMP)	C00364	HMDB01227	9700	365-07-1	Nucleotide/pyrimidine
Cytidine-5'-monophosphate (CMP)	C00055	HMDB00095	7058165	63-37-6	Nucleotide/Pyrimidine metabolism
Fructose-1,6-bisphosphate (F16BP)	C00354	HMDB01058	172313	488-69-7	Glycolysis
Fructose-2,6-bisphosphate (F26BP)	C00665	HMDB01047	105021	79082-92-1	Glycolosis
Glucose-1,6-bisphosphate (G16BP)	C01231	HMDB03514	82400	10139-18-1	Glycolysis/Glycogenesis
Lactose	C00243	HMDB00186	84571	63-42-3	Sugar/Galactose
Sucrose	C00089	HMDB00258	5988	57-50-1	Sugar
Guanosine-3,5-cyclic monophosphate (cGMP)	C00942	HMDB01314	24316	7665-99-8	Nucleotide/Purine metabolism
Gibberellin	C01699	HMDB03559	9819600	77-06-5	Diterpenoid biosynthesis
Adenosine monophosphate (AMP)	C00020	HMDB00045	15938965	149022-20-8	Nucleotide
Inosine monophosphate (IMP)	C00130	HMDB00175	8582	131-99-7	Nucleotide/Purine metabolism
Prostaglandin E2	C00584	HMDB01220	5280360	363-24-6	Lipids/Arachidonic acid metabolism
Cortisol	C00735	HMDB14879	5754	50-23-7	Steroid
2-Deoxycytidine Diphosphate (DCDP)	C00705	HMDB01245	150855	800-73-7	Nucleotide/Pyrimidine metabolism
Deoxycytidine 5'-diphosphate (DCDP)	C00705	HMDB01245	150855	800-73-7	Nucleotide/Pyrimidine metabolism
Phosphoribosyl pyrophosphate (PRPP)	C00119	HMDB00280	7339	7540-64-9	Nucleotide/Purine metabolism
Deoxycholic acid	C04483	HMDB00626	222528	83-44-3	Bile acid

Chenodeoxycholate	C02528	HMDB00518	10133	474-25-9	Bile acid metabolism
Uridine diphosphate (UDP)	C00015	HMDB00295	6031	21931-53-3	Nucleotide/Pyrimidine metabolism
beta-muricholic acid	C17726	HMDB00865	119473	39016-49-4	Bile acid biosynthesis
Cholic acid	C00695	HMDB00619	221493	81-25-4	Bile acid
gamma-tocopherol	C02483	HMDB01492	92729	54-28-4	Ubiquinone and other terpenoid-quinone biosynthesis
Adenosine diphosphate (ADP)	C00008	HMDB01341	6022	20398-34-9	Nucleotide/Purine metabolism
alpha-tocopherol (Vitamin E)	C02477	HMDB01893	14985	59-02-9	Vitamins
Guanosine-5-diphosphate (GDP)	C00035	HMDB01201	8977	43139-22-6	Nucleotide/Purine metabolism
Glycochenodeoxycholate	C05466	HMDB00637	22833540	640-79-9	Bile acid metabolism
Adenylosuccinate	C03794	HMDB00536	195	19046-78-7	Nucleotide/Purine metabolism
Glycocholate	C01921	HMDB00138	23617285	475-31-0	Bile acid metabolism
Cholesteryl sulfate	C18043	HMDB00653	65076	1256-86-6	Steroids
Deoxycytidine triphosphate (dCTP)	C00458	HMDB0000288	65091	9024-87-7	Nucleotide/Pyrimidine metabolism
Deoxyuridine-3-phosphate (DUTP)	C00460	HMDB01191	65070	1173-82-6	Nucleotide/pyrimidine
Thymidine 5'-triphosphate (TTP)	C00459	HMDB0001342	64968	365-08-2	Nucleotide/Pyrimidine metabolism
Cytidine-5'-triphosphate (CTP)	C00063	HMDB00082	6176	65-47-4	Nucleotide/Pyrimidine metabolism
Adenosine-3-triphosphate (ATP)	C00002	HMDB00538	5957	51963-61-2	Nucleotide
Phosphoadenosine phosphosulfate	C00053	HMDB01134	10214	482-67-7	Sulfur metabolism
Tauro-alpha-muricholic acid	N/A	N/A	1.02E+08	25613-05-2	Bile acid
Tauro-beta-muricholic acid	N/A	HMDB00932	168408	25696-60-0	Bile acid
Taurocholate	C05122	HMDB00036	6675	81-24-3	Conjugated bile acid biosynthesis
Guanosine-5-triphosphate (GTP)	C00044	HMDB01273	6830	373-49-9	Nucleotide/Purine metabolism
UDP-Glucose	C00029	HMDB00286	53477679	133-89-1	Glycogen metabolism
Uridine diphosphate-N-acetylglucosamine (UDP-GlcNAc)	C00043	HMDB00290	445675	528-04-1	Amino sugar and nucleotide sugar metabolism
Oxidized glutathione	C00127	HMDB03337	975	27025-41-8	Oxidative Damage
Nicotinamide adenine dinucleotide phosphate (NADP)	C00006	HMDB00217	5886	53-59-8	Coenzyme