

Metabolite	MOLECULAR_FORMULA	KEGG ID	CAS	HMDB/YMDB ID
1,3-DIAMINOPROPANE	C3H10N2	C00986	109-76-2	HMDB00002
10-HYDROXYDECANOATE	C10H20O3	C02774	1679-53-4	-
1-AMINOCYCLOPROPANECARBOXYLATE	C4H7NO2	C01234	22059-21-8	HMDB36458
1-METHYLADENOSINE	C11H15N5O4	C02494	15763-06-1	HMDB03331
1-METHYL-L-HISTIDINE	C7H11N3O2	C01152	332-80-9	HMDB00001
1-METHYLNICOTINAMIDE	C7H9N2O	C02918	1005-24-9	HMDB00699
2',4'-DIHYDROXYACETOPHENONE	C8H8O3	C03663	89-84-9	HMDB29659
2,4-DIHYDROXYPTERIDINE	C6H4N4O2	C03212	487-21-8	-
2-AMINOISOBUTYRATE	C4H9NO2	C03665	62-57-7	HMDB01906
2-HYDROXYPYRIDINE	C5H5NO	C02502	142-08-5	HMDB13751
3,5-DIIODO-L-THYRONINE	C15H13I2NO4		1041-01-6	HMDB00582
3,5-DIIODO-L-TYROSINE	C9H9I2NO3	C01060	18835-59-1	HMDB03474
3-AMINO-5-HYDROXYBENZOATE	C7H7NO3	C12107	76045-71-1	-
3-HYDROXYBENZOATE	C7H6O3	C00587	99-06-9	HMDB02466
3-HYDROXYMETHYLGLUTARATE	C6H10O5	C03761	503-49-1	HMDB00355
3-METHOXYTYRAMINE	C9H13NO2	C05587	1477-68-5	HMDB00022
3-METHOXYTYROSINE	C10H13NO4		300-48-1	HMDB01434
3-METHYL-2-OXINDOLE	C9H9NO		1504-06-9	-
3-METHYLADENINE	C6H7N5	C00913	5142-23-4	HMDB11600
3-METHYLHISTAMINE	C6H11N3		36475-47-5	HMDB01861
3-NITRO-L-TYROSINE	C9H10N2O5		621-44-3	-
4-ACETAMIDOBUTANOATE	C6H11NO3	C02946	3025-96-5	HMDB03681
4-AMINOBENZOATE	C7H7NO2	C00568	150-13-0	HMDB01392
4-GUANIDINOBUTANOATE	C5H11N3O2	C01035	463-00-3	HMDB03464
4-HYDROXYBENZOATE	C7H6O3	C00156	99-96-7	HMDB00500
4-IMIDAZOLEACETATE	C5H6N2O2	C02835	3251-69-2	HMDB02024
4-PYRIDOXATE	C8H9NO4	C00847	82-82-6	HMDB00017
4-QUINOLINECARBOXYLATE	C10H7NO2	C06414	486-74-8	-
5-AMINOLEVULINATE	C5H9NO3	C00430	5451-09-2	HMDB01149
5-AMINOPENTANOATE	C5H11NO2	C00431	660-88-8	HMDB03355
5'-DEOXYADENOSINE	C10H13N5O3	C05198	4754-39-6	HMDB01983
5-HYDROXYLYSINE	C6H14N2O3	C16741	13204-98-3	HMDB00450
5-METHYLCYTOSINE	C5H7N3O	C02376	58366-64-6	HMDB02894
6-CARBOXYHEXANOATE	C7H12O4	C02656	111-16-0	HMDB00857

6-HYDROXYNICOTINATE	C6H5NO3	C01020	5006-66-6	HMDB02658
ACETYLCHOLINE	C7H16NO2	C01996	60-31-1	HMDB00895
ADENINE	C5H5N5	C00147	73-24-5	HMDB00034
ADENOSINE	C10H13N5O4	C00212	58-61-7	HMDB00050
ADENOSINE 2',3'-CYCLIC PHOSPHATE	C10H12N5O6P	C02353	37063-35-7	HMDB11616
AGMATINE SULFATE	C5H14N4	C00179	2482-00-0	HMD01432
ALANINE	C3H7NO2	C00041	56-41-7	HMDB00161
AMINOADIPATE	C6H11NO4	C00956	542-32-5	HMDB00510
AMINOISOBUTANOATE	C4H9NO2	C05145	144-90-1	HMDB03911
ANSERINE	C10H16N4O3	C01262	10030-52-1	HMDB00194
ARGININE	C6H14N4O2	C00062	1119-34-2	HMDB00517
ASPARTATE	C4H7NO4	C00402	1783-96-6	HMDB06483
AZELATE	C9H16O4	C08261	123-99-9	HMDB00784
BENZOATE	C7H6O2	C00180	532-32-1	HMDB01870
BIOTIN	C10H16N2O3S	C00120	58-85-5	HMDB00030
CADAVERINE	C5H14N2	C01672	1476-39-7	HMDB02322
CAFFEATE	C9H8O4	C01481	331-39-5	HMDB01964
CAFFEINE	C8H10N4O2	C07481	58-08-2	HMDB01847
CARNOSINE	C9H14N4O3	C00386	305-84-0	HMDB00033
CHOLINE	C5H14NO	C00114	123-41-1	HMDB00097
CITICOLINE	C14H26N4O11P2	C00307	33818-15-4	HMDB01413
CITRULLINE	C6H13N3O3	C00327	372-75-8	HMDB00904
CORTISOL	C21H30O5	C00735	50-23-7	HMDB00063
CORTISOL 21-ACETATE	C23H32O6	C02821	50-03-3	-
CREATINE	C4H9N3O2	C00300	57-00-1	HMDB00064
CREATININE	C4H7N3O	C00791	60-27-5	HMDB00562
CYCLIC AMP	C10H12N5O6P	C00575	37839-81-9	HMDB00058
CYCLIC GMP	C10H12N5O7P	C00942	40732-48-7	HMDB01314
CYSTATHIONINE	C7H14N2O4S	C02291	56-88-2	HMDB00099
CYSTINE	C6H12N2O4S2	C01420	56-89-3	HMDB00192
CYTIDINE	C9H13N3O5	C00475	65-46-3	HMDB00089
CYTIDINE MONOPHOSPHATE	C9H14N3O8P	C00055	63-37-6	HMDB00095
CYTOSINE	C4H5N3O	C00380	71-30-7	HMDB00630
DEOXYADENOSINE	C10H13N5O3	C00559	16373-93-6	HMDB00101
DEOXYCARNITINE	C7H15NO2	C01181	6249-56-5	HMDB01161

DEOXYCYTIDINE	C9H13N3O4	C00881	951-77-9	HMDB00014
DEOXYGUANOSINE	C10H13N5O4	C00330	961-07-9	HMDB00085
DETHIOBIOTIN	C10H18N2O3	C01909	533-48-2	HMDB03581
DIAMINOPIMELATE	C7H14N2O4	C00666	583-93-7	HMDB01370
DOPAMINE	C8H11NO2	C03758	62-31-7	HMDB00073
EPINEPHRINE	C9H13NO3	C00788	51-43-4	HMDB00068
ETHYL 3-INDOLEACETATE	C12H13NO2		778-82-5	-
FERULATE	C10H10O4	C01494	1135-24-6	HMDB00954
GAMMA-AMINOBUTYRATE	C4H9NO2	C00334	56-12-2	HMDB00112
GLUTAMATE	C5H9NO4	C00025	56-86-0	HMDB00148
GLUTAMINE	C5H10N2O3	C00064	56-85-9	HMDB00641
GLUTARYLCARNITINE	C12H21NO6		102636-82-8	HMDB13130
GLUTATHIONE REDUCED	C10H17N3O6S	C00051	70-18-8	HMDB00125
GLYCOCHOLATE	C26H43NO6	C01921	475-31-0	HMDB00138
GUANIDINOACETATE	C3H7N3O2	C00581	352-97-6	HMDB00128
GUANIDINOSUCCINATE	C5H9N3O4	C03139	6133-30-8	HMDB03157
GUANINE	C5H5N5O	C00242	73-40-5	HMDB00132
GUANOSINE	C10H13N5O5	C00387	118-00-3	HMDB00133
HIPPURATE	C9H9NO3	C01586	495-69-2	HMDB00714
HISTAMINE	C5H9N3	C00388	56-92-8	HMDB00870
HISTIDINE	C6H9N3O2	C00135	5934-29-2	HMDB00177
HISTIDINOL	C6H11N3O	C00860	1596-64-1	HMDB03431
HOMOCYSTEINE	C4H9NO2S	C00155	454-29-5	HMDB00742
HOMOCYSTEINE THIOLACTONE	C4H7NOS		31828-68-9	HMDB02287
HOMOCYSTINE	C8H16N2O4S2	C01817	462-10-2	HMDB00575
HYPOXANTHINE	C5H4N4O	C00262	68-94-0	HMDB00157
INDOLE-3-ACETAMIDE	C10H10N2O	C02693	879-37-8	HMDB29739
INDOLE-3-ACETATE	C10H9NO2	C00954	87-51-4	HMDB00197
INDOLE-3-ETHANOL	C10H11NO	C00955	526-55-6	HMDB03447
INDOLE-3-METHYL ACETATE	C11H11NO2		1912-33-0	HMDB29738
INDOLEACETALDEHYDE	C10H9NO	C00637	20095-27-6	HMDB01190
INOSINE	C10H12N4O5	C00294	58-63-9	HMDB00195
ISOLEUCINE	C6H13NO2	C00407	73-32-5	HMDB00172
ITACONATE	H-H2O	C5H6O4	C00490	97-65-4
KYNURENATE	C10H7NO3	C01717	492-27-3	HMDB00715

KYNURENINE	C10H12N2O3	C00328	343-65-7	HMDB00684
LAUROYL CARNITINE	C19H37NO4		25518-54-1	HMDB02250
L-CARNITINE	C7H15NO3	C00318	6645-46-1	HMDB00062
L-DOPA	C9H11NO4	C00355	59-92-7	HMDB00181
LEUCINE	C6H13NO2	C00123	328-39-2	HMDB00687
LIPOAMIDE	C8H15NOS2	C00248	940-69-2	HMDB00962
L-TRYPTOPHANAMIDE	C11H13N3O	C00977	5022-65-1	HMDB13318
LUMICHROME	C12H10N4O2	C01727	1086-80-2	-
LYSINE	C6H14N2O2	C00047	56-87-1	HMDB00182
MELATONIN	C13H16N2O2	C01598	73-31-4	HMDB01389
METHIONINE	C5H11NO2S	C00073	63-68-3	HMDB00696
METHIONINE SULFOXIMINE	C5H12N2O3S	C03510	15985-39-4	HMDB29430
METHYLGUANIDINE	C2H7N3	C02294	22661-87-6	HMDB01522
METHYLTHIOADENOSINE	C11H15N5O3S	C00170	2457-80-9	HMDB01173
N,N,N-TRIMETHYLLYSINE	C9H20N2O2	C03793	55528-53-5	HMDB01325
N,N-DIMETHYL-ARGININE	C8H18N4O2	C03626	220805-22-1	HMDB01539
N1-ACETYLSPERMINE	C12H28N4O	C02567	77928-70-2	HMDB01186
N6-(DELTA2-ISOPENTENYL)-ADENINE	C10H13N5	C04083	2365-40-4	-
N-ACETYLLEUCINE	C8H15NO3	C02710	1188-21-2	HMDB11756
N-ACETYLMETHIONINE	C7H13NO3S	C02712	1115-47-5	HMDB11745
N-ACETYLPHENYLALANINE	C11H13NO3	C03519	2018-61-3	HMDB00512
N-ACETYLPROLINE	C7H11NO3		68-95-1	-
N-ACETYLPUTRESCINE	C6H14N2O	C02714	18233-70-0	HMDB02064
N-ACETYLTRYPTOPHAN	C13H14N2O3		87-32-1	-
N-ALPHA-ACETYLLYSINE	C8H16N2O3	C12989	1946-82-3	HMDB00446
N-FORMYL-L-METHIONINE	C6H11NO3S	C03145	4289-98-9	HMDB01015
NICOTINAMIDE	C6H6N2O	C00153	98-92-0	HMDB01406
NICOTINAMIDE MONONUCLEOTIDE	C11H15N2O8P	C00455	1094-61-7	HMDB00229
NICOTINATE	C6H5NO2	C00253	59-67-6	HMDB01488
N-METHYLGLUTAMATE	C6H11NO4	C01046	6753-62-4	-
N-METHYLTRYPTAMINE	C11H14N2	C06213	61-49-4	HMDB04370
NORMETANEPHRINE	C9H13NO3	C05589	1011-74-1	HMDB00819
NORVALINE	C5H11NO2	C01799	6600-40-4	HMDB13716
O-ACETYLCARNITINE	C9H17NO4	C02571	5080-50-2	HMDB00201
OPHTHALMATE	C11H19N3O6	C21016	495-27-2	HMDB05765

ORNITHINE	C5H12N2O2	C00077	3184-13-2	HMDB00214
O-SUCCINYL-HOMOSERINE	C8H13NO6	C01118	1492-23-5	YMDB00917
OXOPROLINE	C5H7NO3	C01879	4042-36-8	HMDB00805
PANTOTHENATE	C9H17NO5	C00864	137-08-6	HMDB00210
PARAXANTHINE	C7H8N4O2	C13747	611-59-6	HMDB01860
PHENYLALANINE	C9H11NO2	C02057	63-91-2	HMDB00159
PHENYLETHANOLAMINE	C8H11NO	C02735	7568-93-6	HMDB01065
PHOSPHORYLCHOLINE	C5H14NO4P	C00588	72556-74-2	HMDB01565
PICOLINATE	C6H5NO2	C10164	98-98-6	HMDB02243
PIPECOLATE	C6H11NO2	C00408	535-75-1	HMDB00070
P-OCTOPAMINE	C8H11NO2	C04227	770-05-8	HMDB04825
PROLINE	C5H9NO2	C16435	147-85-3	HMDB00162
PTERIN	C6H5N5O	C00715	2236-60-4	HMDB00802
PURINE	C5H4N4	C15587	120-73-0	HMDB01366
PUTRESCINE	C4H12N2	C00134	110-60-1	HMDB01414
PYRIDOXAL	C8H9NO3	C00250	65-22-5	HMDB01545
PYRIDOXAMINE	C8H12N2O2	C00534	524-36-7	HMDB01431
PYRIDOXINE	C8H11NO3	C00314	65-23-6	HMDB00239
PYROGLUTAMATE	C5H7NO3	C01879	98-79-3	HMDB00267
PYRROLE-2-CARBOXYLATE	C5H5NO2	C05942	634-97-9	HMDB04230
RIBOFLAVIN	C17H20N4O6	C00255	83-88-5	HMDB00244
S-ADENOSYLHOMOCYSTEINE	C14H20N6O5S	C00021	979-92-0	HMDB00939
S-ADENOSYLMETHIONINE	C15H22N6O5S	C00019	17176-17-9	HMDB01185
SALICYLAMIDE	C7H7NO2		65-45-2	HMDB15687
SALSOLINOL	C10H13NO2	C09642	59709-57-8	HMDB42012
S-CARBOXYMETHYLCYSTEINE	C5H9NO4S	C03727	638-23-3	HMDB29415
SEBACATE	C10H18O4	C08277	111-20-6	HMDB00792
SELENOCYSTAMINE	C4H12N2Se2		3542-13-0	-
SELENOMETHIONINE	C5H11NO2Se	C05335	1464-42-2	HMDB03966
SERINE	C3H7NO3	C00065	56-45-1	HMDB00187
S-HEXYL-GLUTATHIONE	C16H29N3O6S	C02886	24425-56-7	-
SORBATE	C6H8O2		24634-61-5	YMDB01784
SPERMIDINE	C7H19N3	C00315	334-50-9	HMDB01257
SPERMINE	C10H26N4	C00750	306-67-2	HMDB01256
THEOBROMINE	C7H8N4O2	C07480	83-67-0	HMDB02825

THEOPHYLLINE	C7H8N4O2	C07130	58-55-9	HMDB01889
THIAMINE	C12H17N4OS	C00378	67-03-8	HMDB00235
THIAMINE MONOPHOSPHATE	C12H17N4O4PS	C01081	273724-21-3	HMDB02666
THIOPURINE S-METHYLETHER	C6H6N4S	C16614	50-66-8	HMDB60412
THREONINE	C4H9NO3	C00188	72-19-5	HMDB00167
THYMIDINE	C10H14N2O5	C00214	50-89-5	HMDB00273
THYMINE	C5H6N2O2	C00178	65-71-4	HMDB00262
THYROTROPIN RELEASING HORMONE	C16H22N6O4	C03958	24305-27-9	HMDB60080
TRIGONELLINE	C7H7NO2	C01004	6138-41-6	HMDB00875
TRIMETHYLAMINE	C3H9N	C00565	593-81-7	HMDB00906
TRYPTAMINE	C10H12N2	C00398	61-54-1	HMDB00303
TRYPTOPHAN	C11H12N2O2	C00078	73-22-3	HMDB00929
TYRAMINE	C8H11NO	C00483	51-67-2	HMDB00306
TYROSINE	C9H11NO3	C01536	60-18-4	HMDB00158
UROCANATE	C6H6N2O2	C00785	104-98-3	HMDB00301
VALINE	C5H11NO2	C16436	72-18-4	HMDB00883
XANTHOSINE	C10H12N4O6	C01762	5968-90-1	HMDB00299