

No.	Metabolites	KEGG ID	Plasma	Serum	CSF	Cortex	Hippocampus	Striatum	Thalamus + Midbrain	White matter	Whole Brain tissue	Pineal body ,Olfactory bulb	Reference
1	2-Hydroxybutyric acid	C05984			√								[45, 65]
2	3,4-dihydroxyphenylacetic acid (DOPAC)	C01161				√	√	√	√				[48]
3	3-Hydroxybutanoic acid	C01089			√								[45]
4	3-Hydroxyisovalerate	C20827			√								[45]
5	3-hydroxypropyl mercapturic acid	No KEGG ID				√	√	√		√			[46, 83]
6	3-methoxy-4-hydroxyphenylglycol(HMPG)	C05583				√	√	√		√			[48]
7	5-hydroxyindoleacetic acid (5-HIAA)	C05635				√	√	√	√				[48]
8	6-Deoxy-6-[18F]Fluoro-L-Ascorbic Acid	No KEGG ID										√	[82]
9	Acetate	C00033			√						√		[45, 47, 50]
10	Acetone	C00207			√								[45]
11	ADP	C00008				√		√					[46]
12	Alanine	C01401	√	√	√	√	√						[43, 45, 46, 50]
13	Alpha-2-Ketoisovaleric acid	C00141			√								[45]
14	alpha-D-Glucose	C00267									√		[45, 50]
15	Aminoguanidine	No KEGG ID									√		[85]
16	AMP	C00020				√		√					[46]
17	Arginine	C02385				√		√					[47]
18	Ascorbate	C00072				√		√			√		[46]
19	Aspartate	C16433 <sup>#</sup>		√		√		√			√		[43, 46, 50, 51,52]
20	ATP	C00002				√		√			√		[46]



45	Glycerol	C00116		√							[45]
46	Glycerophosphoricacid	C00093			√		√				[46]
47	Glycine	C00037	√	√						√	[45, 47, 51]
48	GMP	C00144			√		√				[46]
49	Guanosine	C00387			√		√				[46]
50	Histidine	C00768 <sup>#</sup>			√		√			√	[46]
51	Homocysteine	C05330 <sup>#</sup>	√								[43]
52	Homovanillicacid (HVA)	C05582			√	√	√	√			[48]
53	Isoleucine	C16434 <sup>#</sup>	√		√					√	[44]
54	Lactate	C01432 <sup>#</sup>		√	√	√	√	√		√	[47, 49, 52, 62, 63]
55	Leucine	C16439 <sup>#</sup>	√		√						[44]
56	leukotriene C4	C02166								√	[84]
57	Lysine	C16440 <sup>#</sup>			√						[44]
58	L-Malate	C00149			√		√			√	[46, 50]
59	Malonate	C00383	√								[47]
60	L-Methionine	C00073	√								[43]
61	Myo-Inositol	C00137		√	√	√	√				[49, 50, 62]
62	N-acetylaspartate (NAA)	C01042	√		√	√	√	√	√	√	[46, 49, 52, 62-64]
63	N-Acetylaspartylglutamate (NAAG)	No KEGG ID			√		√			√	[46, 81]
64	NAD+	C00003			√		√				[46]
65	neu5Ac	C00270			√		√				[46]
66	NG-nitro-L-arginine methyl nester	No KEGG ID					√				[80]

67	Nicotinuric acid	C05380			√		√			[50]
68	Norepinephrine (NE)	C00547			√	√	√	√		[48]
69	Ornithine	C01602 <sup>#</sup>	√							[47]
70	Oxaloacetate	C00036		√						[45]
71	PE	No KEGG ID			√		√			[46]
72	PEP	C00074			√		√			[46]
73	Phenylalanine	C02057 <sup>#</sup>	√		√		√			[44, 46]
74	polyamines	No KEGG ID			√	√			√	[86]
75	prostaglandin E2	C00584							√	[84]
76	pseudouridine	C02067			√		√			[46]
77	putrescine	C00134			√	√			√	[66, 87]
78	Pyruvate	C00022	√	√						[45, 47]
79	Ribose 5-phosphate	C00117			√		√			[46]
80	L-Serine	C00065	√	√						[45, 47]
81	Serotonin(5-HT)	C00780			√	√	√	√		[48, 59, 60]
82	spermidine	C00315			√	√			√	[66, 88]
83	spermine	C00750			√	√			√	[66, 88]
84	Succinate	C00042	√						√	[50]
85	Taurine	C00245			√		√		√	[46, 50, 51, 57]
86	L-Threonine	C00188	√							[47]
87	D-Threonine	C00820	√							[47]
88	L-Tryptophan	C00078	√		√	√				[43, 46]
89	Tryptophan	C00806 <sup>#</sup>	√		√	√				[43, 46]
90	L-Tyrosine	C00082	√		√		√			[43, 45, 46]

91	D-Tyrosine	C06420 <sup>#</sup>	√	√	√		[43, 45, 46]
92	UDP	C00015		√	√	√	[46, 50]
93	UDP-glucose	C00029		√	√		[46]
94	UMP	C00105		√	√		[46]
95	Uracil	C00106		√	√	√	[46, 50]
96	Uridine	C00299		√	√		[46]
97	UTP	C00075				√	[50]
98	Valine	C16436 <sup>#</sup>	√	√	√		[44, 47]
99	Xanthine	C00385		√	√	√	[46, 50]
100	γ-Hydroxybutyrate	C00989			√		[65]
101	sulfatide (d18:1-C24h:0)	No KEGG ID				√	[66]
102	PC 32:0	No KEGG ID		√	√	√	[67]
103	PC 34:1	No KEGG ID		√	√	√	[67]
104	PC 36:4	No KEGG ID		√	√	√	[67]
105	SM 18:0	No KEGG ID		√	√	√	[67]
106	LPC 16:0	No KEGG ID		√	√	√	[67]
107	LPC 18:1	No KEGG ID		√	√	√	[67]
108	LPC 18:0	No KEGG ID		√	√	√	[67]

109	PC 34:0	No KEGG ID	√	√	√	[67]
110	PC 36:1	No KEGG ID	√	√	√	[67]
111	PC 40:6	No KEGG ID	√	√	√	[67]
112	Ceramide 18:0-H2O	No KEGG ID	√	√	√	[67]
113	PC 16:0/16:0	No KEGG ID	√	√	√	[67]
114	PC 16:0/18:1	No KEGG ID	√	√	√	[67]
115	PC 16:0/18:0	No KEGG ID	√	√	√	[67]
116	PC 16:0/20:4	No KEGG ID	√	√	√	[67]
117	PC 18:0/18:1	No KEGG ID	√	√	√	[67]
118	PC 16:0/22:6	No KEGG ID	√	√	√	[67]
119	PC 18:0/20:4	No KEGG ID	√	√	√	[67]
120	PC 18:0/22:6	No KEGG ID	√	√	√	[67]

**C00000<sup>#</sup>, lacked pathway annotation in KEGG**