

No.	BIOCHEMICAL	SUPER_PATHWAY	SUB_PATHWAY	KEGG	Group.HMDB	T_Stat_D_V s_Sham	Pval.T	Qval.T
1	kynurenate	Amino acid	Tryptophan metabolism	C01717	HMDB00715	4.69	0.00655	0.0204
2	3-phenylpropionate (hydrocinnamate)	Amino acid	Phenylalanine & tyrosine metabolism	C05629	HMDB00764	3.12	0.01438	0.0324
3	N-acetylphenylalanine	Amino acid	Phenylalanine & tyrosine metabolism	C03519	HMDB00512	2.71	0.02664	0.0491
4	citrulline	Amino acid	Urea cycle; arginine-, proline-, metabolism	C00327	HMDB00904	-2.61	0.03093	0.0533
5	N-acetylglycine	Amino acid	Glycine, serine and threonine metabolism		HMDB00532	-2.70	0.02710	0.0491
6	cysteine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	C00097	HMDB00574	-2.74	0.04197	0.0657
7	tryptophan	Amino acid	Tryptophan metabolism	C00078	HMDB00929	-2.94	0.02213	0.0426
8	cysteine-glutathione disulfide	Amino acid	Glutathione metabolism		HMDB00656	-2.97	0.02230	0.0435
9	3-methyl-2-oxovalerate	Amino acid	Valine, leucine and isoleucine metabolism	C00671	HMDB03736	-3.29	0.01860	0.0388
10	p-cresol sulfate	Amino acid	Phenylalanine & tyrosine metabolism	C01468	HMDB11635	-3.34	0.01318	0.0306
11	3-(4-hydroxyphenyl)propionate	Amino acid	Phenylalanine & tyrosine metabolism	C01744	HMDB02199	-3.39	0.01635	0.0353
12	hydroxyproline	Amino acid	Urea cycle; arginine-, proline-, metabolism	C01157	HMDB00725	-3.81	0.00620	0.0202
13	4-methyl-2-oxopentanoate	Amino acid	Valine, leucine and isoleucine metabolism	C00233	HMDB00695	-3.86	0.00607	0.0202
14	glutamine	Amino acid	Glutamate metabolism	C00064	HMDB00641	-3.97	0.00713	0.0214
15	kynurenine	Amino acid	Tryptophan metabolism	C00328	HMDB00684	-4.08	0.00499	0.0196
16	N-formylmethionine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	C03145	HMDB01015	-4.11	0.00925	0.0253
17	homocitrulline	Amino acid	Urea cycle; arginine-, proline-, metabolism	C02427	HMDB00679	-4.84	0.00322	0.0137
18	phenylacetyl glycine	Amino acid	Phenylalanine & tyrosine metabolism	C05598	HMDB00821	-5.39	0.00107	0.0086
19	2-oxoadipate	Amino acid	Lysine metabolism	C00322	HMDB00225	-6.80	0.00164	0.0105
20	ribitol	Carbohydrate	Nucleotide sugars, pentose metabolism	C00474	HMDB00508	-2.54	0.03967	0.0634
21	arabinose	Carbohydrate	Nucleotide sugars, pentose metabolism	C00216	HMDB00646	-2.98	0.02243	0.0435
22	ribose	Carbohydrate	Nucleotide sugars, pentose metabolism	C00121	HMDB00283	-4.24	0.00287	0.0133
23	mannose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	C00159	HMDB00169	-4.37	0.00278	0.0133
24	trigonelline (N'-methylnicotinate)	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	C01004	HMDB00875	5.64	0.00052	0.0060
25	alpha-ketoglutarate	Energy	Krebs cycle	C00026	HMDB00208	-2.86	0.02580	0.0485
26	citrate	Energy	Krebs cycle	C00158	HMDB00094	-3.46	0.01554	0.0345
27	caprate (10:0)	Lipid	Medium chain fatty acid	C01571	HMDB00511	6.93	0.00012	0.0033
28	pinitol	Lipid	Inositol metabolism	C03844		5.50	0.00161	0.0105
29	12-HETE	Lipid	Eicosanoid		HMDB06111	3.10	0.01874	0.0388
30	sebacate (decanedioate)	Lipid	Fatty acid, dicarboxylate	C08277	HMDB00792	3.04	0.02719	0.0491
31	myristoleate (14:1n5)	Lipid	Long chain fatty acid	C08322	HMDB02000	-2.46	0.03928	0.0634
32	stearate (18:0)	Lipid	Long chain fatty acid	C01530	HMDB00827	-2.60	0.03464	0.0577
33	palmitate (16:0)	Lipid	Long chain fatty acid	C00249	HMDB00220	-2.62	0.03408	0.0574
34	azelate (nonanedioate; C9)	Lipid	Fatty acid, dicarboxylate	C08261	HMDB00784	-2.69	0.02753	0.0491
35	1-heptadecanoyl-GPC (17:0)	Lipid	Lysolipid		HMDB12108	-2.70	0.02861	0.0504
36	3-hydroxydecanoate	Lipid	Fatty acid, monohydroxy		HMDB02203	-2.74	0.04495	0.0689
37	myristate (14:0)	Lipid	Long chain fatty acid	C06424	HMDB00806	-2.89	0.02596	0.0485
38	hexanoylglycine (C6)	Lipid	Fatty acid metabolism		HMDB00701	-2.92	0.02179	0.0434
39	2-hydroxystearate	Lipid	Fatty acid, monohydroxy	C03045		-2.95	0.03560	0.0587
40	1-palmitoylplasmenylethanolamine*	Lipid	Lysolipid			-3.06	0.01763	0.0375
41	carnitine	Lipid	Carnitine metabolism	C00318		-3.16	0.01410	0.0323
42	stearidonate (18:4n3)	Lipid	Long chain fatty acid	C16300	HMDB06547	-3.27	0.01170	0.0285
43	palmitoylcarnitine (C16)	Lipid	Carnitine metabolism	C02990	HMDB00222	-3.32	0.01067	0.0271
44	hexanoylcarnitine (C6)	Lipid	Carnitine metabolism		HMDB00705	-3.41	0.00923	0.0253
45	2-docosahexaenoyl-GPC* (22:6)*	Lipid	Lysolipid			-3.42	0.01587	0.0348
46	1-oleoyl-GPC (18:1)	Lipid	Lysolipid			-3.68	0.00665	0.0204
47	campesterol	Lipid	Sterol/Steroid	C01789	HMDB02869	-3.69	0.00909	0.0253
48	2-hydroxypalmitate	Lipid	Fatty acid, monohydroxy			-3.73	0.01030	0.0268
49	2-arachidonoyl-GPC* (20:4)*	Lipid	Lysolipid			-3.86	0.00568	0.0200
50	oleate (18:1n9)	Lipid	Long chain fatty acid	C00712	HMDB00207	-3.88	0.00500	0.0196
51	hydroxybutyrylcarnitine*	Lipid	Fatty acid metabolism (also BCAA metabolism)		HMDB13127	-3.90	0.00809	0.0239
52	arachidonate (20:4n6)	Lipid	Long chain fatty acid	C00219	HMDB01043	-3.97	0.00641	0.0204
53	docosapentaenoate (n6 DPA; 22:5n6)	Lipid	Essential fatty acid	C16513	HMDB13123	-3.97	0.00562	0.0200
54	1-linoleoyl-GPC (18:2)	Lipid	Lysolipid	C04100		-4.02	0.01114	0.0275
55	deoxycarnitine	Lipid	Carnitine metabolism	C01181	HMDB01161	-4.06	0.00870	0.0252
56	2-palmitoyl-GPE* (16:0)*	Lipid	Lysolipid			-4.13	0.00959	0.0258
57	oleoylcarnitine (C18)	Lipid	Carnitine metabolism		HMDB05065	-4.40	0.00311	0.0136
58	1-arachidonoyl-GPC* (20:4)*	Lipid	Lysolipid	C05208		-4.48	0.00266	0.0133
59	1-linoleoyl-GPI* (18:2)*	Lipid	Lysolipid			-4.56	0.00186	0.0110
60	3-hydroxyoctanoate	Lipid	Fatty acid, monohydroxy		HMDB01954	-4.61	0.00175	0.0107
61	1-myristoyl-GPC (14:0)	Lipid	Lysolipid		HMDB10379	-4.61	0.00574	0.0200
62	hexadecanedioate (C16)	Lipid	Fatty acid, dicarboxylate		HMDB00672	-4.83	0.00198	0.0112
63	1-palmitoleoyl-GPC* (16:1)*	Lipid	Lysolipid			-4.91	0.00118	0.0088
64	1-palmitoyl-GPE (16:0)	Lipid	Lysolipid		HMDB11503	-4.93	0.00535	0.0200
65	octadecanedioate (C18)	Lipid	Fatty acid, dicarboxylate		HMDB00782	-5.09	0.00256	0.0133
66	10-heptadecenoate (17:1n7)	Lipid	Long chain fatty acid			-5.10	0.00129	0.0090
67	dihomolinoleate (20:2n6)	Lipid	Long chain fatty acid	C16525		-5.20	0.00083	0.0075
68	octanoylcarnitine (C8)	Lipid	Carnitine metabolism	C02838	HMDB00791	-5.45	0.00094	0.0080
69	margarate (17:0)	Lipid	Long chain fatty acid		HMDB02259	-5.46	0.00070	0.0067
70	1-arachidonoyl-GPI* (20:4)*	Lipid	Lysolipid			-5.57	0.00054	0.0060
71	1-stearoyl-GPI (18:0)	Lipid	Lysolipid			-5.64	0.00064	0.0065
72	10-nonadecenoate (19:1n9)	Lipid	Long chain fatty acid			-5.98	0.00121	0.0088
73	1-eicosatrienoyl-GPC* (20:3)*	Lipid	Lysolipid			-6.86	0.00015	0.0033
74	eicosapentaenoate (EPA; 20:5n3)	Lipid	Essential fatty acid	C06428	HMDB01999	-7.00	0.00013	0.0033
75	docosapentaenoate (DPA; 22:5n3)	Lipid	Essential fatty acid	C16513	HMDB01976	-7.04	0.00026	0.0039
76	acetylcarnitine (C2)	Lipid	Carnitine metabolism	C02571	HMDB00201	-7.12	0.00022	0.0037
77	1-docosahexaenoyl-GPC* (22:6)*	Lipid	Lysolipid			-7.13	0.00020	0.0037
78	dihomolinolenate (20:3n3 or 3n6)	Lipid	Essential fatty acid	C03242	HMDB02925	-7.77	0.00052	0.0060
79	mead acid (20:3n9)	Lipid	Long chain fatty acid		HMDB10378	-7.88	0.00006	0.0029

80	1-arachidonoyl-GPE* (20:4)*	Lipid	Lysolipid		HMDB11517	-8.22	0.00004	0.0029
81	docosahexaenoate (DHA; 22:6n3)	Lipid	Essential fatty acid	C06429	HMDB02183	-8.28	0.00032	0.0045
82	1-oleoyl-GPE (18:1)	Lipid	Lysolipid		HMDB11506	-11.91	0.00001	0.0016
83	uracil	Nucleotide	Pyrimidine metabolism, uracil containing	C00106	HMDB00300	3.43	0.01295	0.0306
84	cytidine	Nucleotide	Pyrimidine metabolism, cytidine containing	C00475	HMDB00089	-2.75	0.04293	0.0665
85	pseudouridine	Nucleotide	Pyrimidine metabolism, uracil containing	C02067	HMDB00767	-2.87	0.03359	0.0572
86	allantoin	Nucleotide	Purine metabolism, urate metabolism	C02350	HMDB00462	-3.04	0.03019	0.0526
87	TDTEDKGEFLSEGGGV*	Peptide	Fibrinogen cleavage peptide			2.43	0.04181	0.0657
88	alanylalanine	Peptide	Dipeptide	C00993	HMDB03459	-2.87	0.02500	0.0479
89	gamma-glutamylmethionine	Peptide	gamma-glutamyl			-3.42	0.01003	0.0265
90	gamma-glutamylvaline	Peptide	gamma-glutamyl		HMDB11172	-3.82	0.00552	0.0200
91	gamma-glutamylleucine	Peptide	gamma-glutamyl		HMDB11171	-3.88	0.00484	0.0196
92	gamma-glutamylisoleucine*	Peptide	gamma-glutamyl		HMDB11170	-4.07	0.01202	0.0288
93	carnosine	Peptide	Dipeptide derivative	C00386	HMDB00033	-4.24	0.01077	0.0271
94	gamma-glutamylglutamine	Peptide	gamma-glutamyl		HMDB11738	-4.62	0.00277	0.0133
95	prolylhydroxyproline	Peptide	Dipeptide		HMDB06695	-8.23	0.00010	0.0033
96	hippurate	Xenobiotics	Benzoate metabolism	C01586	HMDB00714	3.94	0.00601	0.0202
97	catechol sulfate	Xenobiotics	Benzoate metabolism	C00090		2.89	0.02046	0.0418
98	EDTA	Xenobiotics	EDTA	C00284		2.59	0.03770	0.0615
99	ethyl glucuronide	Xenobiotics	Detoxification metabolism			-4.49	0.00211	0.0116
100	ergothioneine	Xenobiotics	Food component/Plant	C05570	HMDB03045	-4.84	0.00308	0.0136