

Host-Microbe Metabolomics Facility (DFI - HMMF)

Panel 1: Bile Acid Panel

Compound Number	Compound name	Data Provided		PubChemID	HMDB ID (if available)	Molecular Formula	Molecular Weight
		Quantified (y/n)	Normalized Relative Abundance (y/n)				
1	12-oxochenodeoxycholic acid	y	y	94235	HMDB0000400	C24H38O5	406.27192
2	3-oxocholic acid	y	y	5283956	HMDB0000502	C24H38O5	406.27192
3	3-oxolithocholic acid	y	y	5283906	NA	C24H38O3	374.2821
4	7-oxodeoxycholic acid	y	y	188292	HMDB0000391	C24H38O5	406.27192
5	allocholic acid	y	y	160636	HMDB0000505	C24H40O5	408.28757
6	alloisolithocholic acid	y	y	94228	HMDB0000713	C24H40O3	376.29775
7	alpha-muricholic acid	y	y	5283852	HMDB0000506	C24H40O5	408.28757
8	beta-muricholic acid	y	y	5283853	HMDB0000415	C24H40O5	408.28757
9	chenodeoxycholic acid	y	y	10133	HMDB0000518	C24H40O4	392.29266
10	cholic acid	y	y	221493	HMDB0000619	C24H40O5	408.28757
11	deoxycholic acid	y	y	222528	HMDB0000626	C24H40O4	392.29266
12	glycochenodeoxycholic acid	y	y	12544	HMDB0000637	C26H43NO5	449.31412
13	glycocholic acid	y	y	10140	HMDB0000138	C26H43NO6	465.30904
14	glycodeoxycholic acid	y	y	3035026	HMDB0242414	C26H43NO5	449.31412
15	glycolithocholic acid	y	y	115245	HMDB0000698	C26H43NO4	433.31921
16	glycoursodeoxycholic acid	y	y	12310288	HMDB0000708	C26H43NO5	449.31412
17	isochenodeoxycholic acid	y	y	164673	HMDB0000361	C24H40O4	392.29266
18	isodeoxycholic acid	y	y	160530	HMDB0000438	C24H40O4	392.29266
19	isolithocholic acid	y	y	164853	HMDB0000717	C24H40O3	376.29775
20	lithocholic acid	y	y	9903	HMDB0000761	C24H40O3	376.29775
21	taurochenodeoxycholic acid	y	y	387316	HMDB0000951	C26H45NO6S	499.29676
22	taurocholic acid	y	y	6675	HMDB0000036	C26H45NO7S	515.29167
23	taurodeoxycholic acid	y	y	2733768	HMDB0000896	C26H45NO6S	499.29676
24	tauroolithocholic acid	y	y	439763	HMDB0000722	C26H45NO5S	483.30184
25	tauroursodeoxycholic acid	y	y	9848818	HMDB0000874	C26H45NO6S	499.29676
26	ursodeoxycholic acid	y	y	31401	HMDB0000946	C24H40O4	392.29266
27	12-beta-hydroxyisocholic acid		y	5283869	NA	C24H40O5	408.28757
28	12-epideoxycholic acid		y	5283831	HMDB0000411	C24H40O4	392.29266
29	12-oxolithocholic acid		y	3080612	HMDB0000328	C24H38O4	390.27701
30	3-12-dioxo-5beta-cholanoic acid		y	94248	NA	C24H36O4	388.26136
31	3-7-dioxo-5beta-cholanoic acid		y	94192	NA	C24H36O4	388.26136
32	3-deoxycholic acid		y	164672	HMDB00002536	C24H40O4	392.29266
33	3-epicholic acid		y	5283870	HMDB0000419	C24H40O5	408.28757
34	3-oxochenodeoxycholic acid		y	5283932	HMDB0000503	C24H38O5	406.27192
35	3-oxodeoxycholic acid		y	160738	HMDB0062742	C24H38O5	406.27192
36	6-oxolithocholic acid		y	164960	NA	C24H38O4	390.27701
37	7-12-dioxolithocholic acid		y	3080560	NA	C24H36O5	404.25627
38	7-oxolithocholic acid		y	444262	HMDB0000467	C24H38O4	390.27701
39	allolithocholic acid		y	5283803	HMDB0000381	C24H40O3	376.29775
40	beta-hyodeoxycholic acid		y	5283822	HMDB0000664	C24H40O4	392.29266
41	chenodeoxycholic acid-3-sulfate		y	21252312	HMDB0002586	C24H40O7S	472.24947
42	chenodeoxycholic acid-7-sulfate		y	21252308	HMDB0002522	C24H40O7S	472.24947
43	cholonic acid		y	92997	HMDB0000308	C24H38O3	374.2821
44	cholic acid-3-sulfate		y	465402	NA	C24H40O8S	488.24439
45	cholic acid-7-sulfate		y	459070	HMDB0002421	C24H40O8S	488.24439
46	dehydrocholic acid		y	6674	HMDB0304121	C24H34O5	402.24062
47	deoxycholic acid-3-sulfate		y	22833601	HMDB0002504	C24H40O7S	472.24947
48	gamma-muricholic acid		y	92805	HMDB0000760	C24H40O5	408.28757
49	glyco-beta muricholic acid		y	137333454	HMDB0341323	C26H43NO6	465.30904
50	glyco-gamma muricholic acid		y	NA	NA	C26H43NO6	465.30904
51	glyco-omega muricholic acid		y	NA	NA	C26H43NO6	465.30904
52	glycochenodeoxycholic acid-3-sulfate		y	21125002	HMDB0002497	C26H43NO8S	529.27094
53	glycodehydrocholic acid		y	13955640	NA	C26H37NO6	459.26209
54	glycodeoxycholic acid-3-sulfate		y	101602538	HMDB0341325	C26H43NO8S	529.27094
55	glycohyodeoxycholic acid		y	114611	HMDB0304944	C26H43NO5	449.31412
56	glycolithocholic acid-3-sulfate		y	72222	HMDB0002639	C26H43NO7S	513.27602
57	hyodeoxycholic acid		y	5283820	HMDB0000733	C24H40O4	392.29266
58	isoursodeoxycholic acid		y	127601	HMDB0000686	C24H40O4	392.29266
59	lithocholic acid-3-sulfate		y	451489	NA	C24H40O6S	456.25456
60	murideoxycholic acid		y	5283821	HMDB0246318	C24H40O4	392.29266
61	omega-muricholic acid		y	5283851	HMDB0000364	C24H40O5	408.28757
62	tauro-alpha muricholic acid		y	101657566	HMDB0258742	C26H45NO7S	515.29167
63	tauro-beta muricholic acid		y	21124703	HMDB0000932	C26H45NO7S	515.29167
64	tauro-gamma muricholic acid		y	11954195	HMDB0011637	C26H45NO7S	515.29167
65	tauro-omega muricholic acid		y	118703092	NA	C26H45NO7S	515.29167
66	taurocholic acid-3-sulfate		y	14454428	HMDB0002581	C26H45NO10S2	595.24849
67	taurohyodeoxycholic acid		y	119046	NA	C26H45NO6S	499.29676
68	ursocholic acid		y	122340	HMDB0000917	C24H40O5	408.28757
69	ursodeoxycholic acid-3-sulfate		y	9826093	HMDB0002642	C24H40O7S	472.24947

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Panel 2: PFBB(SCFA) Panel

Compound Number	Compound name	Data Provided		PubChemID	HMDB_ID (if available)	Molecular Formula	Molecular Weight
		Quantified (y/n)	Normalized Relative Abundance (y/n)				
1	5-aminovalerate	y	y	138	HMDB0003355	C5H11NO2	117.15
2	acetate	y	y	176	HMDB0000042	C2H4O2	60.05
3	butyrate	y	y	264	HMDB0000039	C4H8O2	88.11
4	glycine	y	y	750	HMDB0000123	C2H5NO2	75.07
5	proline	y	y	145742	HMDB0000162	C5H9NO2	115.13
6	propionate	y	y	1032	HMDB0000237	C3H6O2	74.08
7	succinate	y	y	1110	HMDB0000254	C4H6O4	118.09
8	tyramine	y	y	5610	HMDB0000306	C8H11NO	137.18
9	2-methylbutyrate		y	8314	HMDB0002176	C5H10O2	102.13
10	3-aminoisobutyrate		y	64956	HMDB0003911	C4H9NO2	103.12
11	4-methylvalerate		y	12587	HMDB0000689	C6H12O2	116.16
12	alanine		y	5950	HMDB0000161	C3H7NO2	89.09
13	aspartic acid		y	5960	HMDB0000191	C4H7NO4	133.1
14	benzoic acid		y	243	HMDB0001870	C7H6O2	122.12
15	catechol		y	289	HMDB0000957	C6H6O2	110.11
16	crotonic acid		y	637090	HMDB0010720	C4H6O2	86.09
17	cysteine		y	5862	HMDB0000574	C3H7NO2S	121.16
18	desaminotyrosine		y	10394	HMDB0002199	C9H10O3	166.17
19	dopamine		y	681	HMDB0000073	C8H11NO2	153.18
20	glutamic acid		y	33032	HMDB0000148	C5H9NO4	147.13
21	hexanoate		y	8892	HMDB0000535	C6H12O2	116.16
22	histamine		y	774	HMDB0000870	C5H9N3	111.15
23	hydrocinnamic acid		y	107	HMDB0000764	C9H10O2	150.17
24	indole-3-acetate		y	802	HMDB0000197	C10H9NO2	175.18
25	indole-3-carboxaldehyde		y	10256	HMDB0029737	C9H7NO	145.16
26	indole-3-propionate		y	3744	HMDB0002302	C11H11NO2	189.21
27	isobutyrate		y	6590	HMDB0001873	C4H8O2	88.11
28	isoleucine		y	6306	HMDB0000172	C6H13NO2	131.17
29	isovalerate		y	10430	HMDB0000718	C5H10O2	102.13
30	itaconic acid		y	811	HMDB0002092	C5H6O4	130.1
31	leucine		y	6106	HMDB0000687	C6H13NO2	131.17
32	lysine		y	5962	HMDB0000182	C6H14N2O2	146.19
33	methionine		y	6137	HMDB0000696	C5H11NO2S	149.21
34	p-cresol		y	2879	HMDB0001858	C7H8O	108.14
35	palmitic acid		y	985	HMDB0000220	C16H32O2	256.42
36	phenol		y	996	HMDB0000228	C6H6O	94.11
37	phenylacetate		y	999	HMDB0000209	C8H8O2	136.15
38	phenylalanine		y	6140	HMDB0000159	C9H11NO2	165.19
39	serine		y	5951	HMDB0000187	C3H7NO3	105.09
40	synephrine		y	7172	HMDB0004826	C9H13NO2	167.2
41	threonine		y	6288	HMDB0000167	C4H9NO3	119.12
42	toluic acid		y	7470	HMDB0029635	C8H8O2	136.15
43	trans-indole-3-acrylate		y	5375048	HMDB0000734	C11H9NO2	187.19
44	tryptamine		y	1150	HMDB0000303	C10H12N2	160.22
45	tryptophan		y	6305	HMDB0000929	C11H12N2O2	204.22
46	tyrosine		y	6057	HMDB0000158	C9H11NO3	181.19
47	valerate		y	7991	HMDB0000892	C5H10O2	102.13
48	valine		y	6287	HMDB0000883	C5H11NO2	117.15
49	vanillin		y	1183	HMDB0012308	C8H8O3	152.15

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Panel 3: Tryptophan(Indole), B Vitamins, Neurotransmitter Panel

Compound Number	Compound name	Data Provided		PubChemID	HMDB_ID (if available)	Molecular Formula	Molecular Weight
		Quantified (y/n)	Normalized Relative Abundance (y/n)				
1	5-hydroxyindoleacetate	y	y	1826	HMDB0000763	C10H9NO3	191.18
2	anthranilic acid	y	y	227	HMDB0001123	C7H7NO2	137.14
3	desaminotyrosine	y	y	10394	HMDB0002199	C9H10O3	166.17
4	indole-3-acetamide	y	y	397	HMDB0029739	C10H10N2O	174.2
5	indole-3-acrylic acid	y	y	5375048	HMDB0000734	C11H9NO2	187.19
6	indole-3-carboxaldehyde	y	y	10256	HMDB0029737	C9H7NO	145.16
7	indole-3-lactate	y	y	92904	NULL	C11H11NO3	205.21
8	indole-3-propionate	y	y	3744	HMDB0002302	C11H11NO2	189.21
9	kynurenic acid	y	y	3845	HMDB0000715	C10H7NO3	189.17
10	melatonin	y	y	896	HMDB0001389	C13H16N2O2	232.28
11	niacin	y	y	938	HMDB0001488	C6H5NO2	123.11
12	phenylalanine	y	y	6140	HMDB0000159	C9H11NO2	165.19
13	serotonin	y	y	5202	HMDB0000259	C10H12N2O	176.21
14	tryptamine	y	y	1150	HMDB0000303	C10H12N2	160.22
15	tryptophan	y	y	6305	HMDB0000929	C11H12N2O2	204.22
16	tyrosine	y	y	6057	HMDB0000158	C9H11NO3	181.19
17	3-hydroxyanthranilic acid		y	86	HMDB0001476	C7H7NO3	153.14
18	5-hydroxy-L-tryptophan		y	439280	HMDB0000472	C11H12N2O3	220.22
19	biotin		y	171548	HMDB0000030	C10H16N2O3S	244.31
20	dopamine		y	681	HMDB0000073	C8H11NO2	153.18
21	epinephrine		y	5816	HMDB0000068	C9H13NO3	183.2
22	folic acid		y	135398658	HMDB0000121	C19H19N7O6	441.4
23	glycine		y	750	HMDB0000123	C2H5NO2	75.07
24	indole		y	798	HMDB0000738	C8H7N	117.15
25	indole-3-acetate		y	802	HMDB0000197	C10H9NO2	175.18
26	indole-3-pyruvate		y	803	HMDB0060484	C11H9NO3	203.19
27	kynurenine		y	846	HMDB0250769	C10H12N2O3	208.21
28	methylserotonin		y	150885	HMDB0004369	C11H14N2O	190.24
29	n-acetylserotonin		y	903	HMDB0001238	C12H14N2O2	218.25
30	pantothenic acid		y	6613	HMDB0000210	C9H17NO5	219.23
31	picolinic acid		y	1018	HMDB0002243	C6H5NO2	123.11
32	pre-q1		y	136229764	NULL	C7H11Cl2N5O	252.1
33	pyridoxal phosphate		y	1051	HMDB0001491	C8H10NO6P	247.14
34	queuine		y	135398670	NULL	C12H15N5O3	277.28
35	quinolinic acid		y	1066	HMDB0000232	C7H5NO4	167.12
36	tryptophol		y	10685	HMDB0003447	C10H11NO	161.2

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Panel 4: TMS - MOX Panel (4 pages)

Compound Number	Compound name	Normalized Relative Abundance (y/n)	PubChemID	HMDB_ID (if available)	Molecular Formula	Molecular Weight
1	1-2-propanediol	y	1030	NULL	C3H8O2	76.09
2	12-ketolithocholic acid	y	3080612	HMDB0000328	C24H38O4	390.6
3	2-3-butanediol	y	225936	HMDB0033007	C4H10O2	90.12
4	2-aminobutyrate	y	6657	HMDB0245013	C4H9NO2	103.12
5	2-deoxy-ribose	y	5460005	NULL	C5H10O4	134.13
6	2-hydroxy-3-methylbutyrate	y	99823	HMDB0000407	C5H10O3	118.13
7	2-hydroxybutyrate	y	11266	NULL	C4H8O3	104.1
8	2-hydroxyhexanoate	y	99824	HMDB0001624	C6H12O3	132.16
9	2-hydroxyisocaproic acid	y	92779	HMDB0000665	C6H12O3	132.16
10	2-keto-gluconic acid	y	102424	NULL	C6H10O7	194.14
11	3-(3-hydroxyphenyl)propionate	y	91	HMDB0000375	C9H10O3	166.17
12	3-4-dihydroxyphenylacetate	y	547	HMDB0001336	C8H8O4	168.15
13	3-aminoisobutyrate	y	64956	HMDB0003911	C4H9NO2	103.12
14	3-epideoxycholic acid	y	160530	HMDB0000438	C24H40O4	392.6
15	3-hydroxybutyrate	y	441	NULL	C4H8O3	104.1
16	3-ketolithocholic acid	y	5283906	NULL	C24H38O3	374.6
17	3-oxodeoxycholic acid	y	160738	HMDB0062742	C24H38O4	390.6
18	4-ethylphenol	y	31242	HMDB0029306	C8H10O	122.16
19	4-hydroxyphenylacetic acid	y	127	HMDB0000020	C8H8O3	152.15
20	4-hydroxyphenyllactate	y	9378	HMDB0000755	C9H10O4	182.17
21	4-methylvalerate	y	12587	HMDB0000689	C6H12O2	116.16
22	5-aminovalerate	y	138	HMDB0003355	C5H11NO2	117.15
23	5-hydroxylysine	y	3032849	HMDB0000450	C6H14N2O3	162.19
24	5-oxoproline	y	7405	HMDB0000267	C5H7NO3	129.11
25	7-ketolithocholic acid	y	444262	NULL	C24H38O4	390.6
26	alanine	y	5950	HMDB0000161	C3H7NO2	89.09
27	allocholic acid	y	160636	HMDB0000505	C24H40O5	408.6
28	allosolicholic acid	y	94228	HMDB0000713	C24H40O3	376.6
29	allolithocholic acid	y	5283803	NULL	C24H40O3	376.6
30	allose	y	439507	NULL	C6H12O6	180.16
31	alpha-ketobutyric acid	y	58	HMDB0000005	C4H6O3	102.09
32	alpha-ketoglutaric acid	y	51	HMDB0000208	C5H6O5	146.1
33	alpha-muricholic acid	y	5283852	HMDB0000506	C24H40O5	408.6
34	aminocaproic acid	y	564	HMDB0001901	C6H13NO2	131.17
35	arabinose	y	439195	NULL	C5H10O5	150.13
36	asparagine	y	6267	HMDB0000168	C4H8N2O3	132.12
37	aspartic acid	y	5960	HMDB0000191	C4H7NO4	133.1
38	benzoic acid	y	243	HMDB0001870	C7H6O2	122.12
39	beta-muricholic acid	y	5283853	HMDB0000415	C24H40O5	408.6
40	cadaverine	y	273	HMDB0002322	C5H14N2	102.18
41	caffeic acid	y	689043	HMDB0001964	C9H8O4	180.16
42	caffeine	y	2519	HMDB0001847	C8H10N4O2	194.19
43	catechol	y	289	HMDB0000957	C6H6O2	110.11
44	cellobiose	y	10712	HMDB0000055	C12H22O11	342.3
45	chlorogenic acid	y	1794427	HMDB0003164	C16H18O9	354.31
46	cholesterol	y	5997	HMDB0000067	C27H46O	386.7
47	cholic acid	y	221493	HMDB0000619	C24H40O5	408.6
48	cis-aconitic acid	y	643757	HMDB0000072	C6H6O6	174.11
49	cis-oleic acid	y	445639	HMDB0000207	C18H34O2	282.5
50	citric acid	y	311	HMDB0000094	C6H8O7	192.12

51	coprostanol	y	221122	HMDB0000577	C27H48O	388.7
52	coprostanone	y	92128	HMDB0000871	C27H46O	386.7
53	creatine	y	586	HMDB0000064	C4H9N3O2	131.13
54	creatinine	y	588	NULL	C4H7N3O	113.12
55	cysteine	y	5862	HMDB0000574	C3H7NO2S	121.16
56	cystine	y	67678	HMDB0000192	C6H12N2O4S2	240.3
57	decanoic acid	y	2969	HMDB0000511	C10H20O2	172.26
58	deoxycarnitine	y	725	HMDB0001161	C7H15NO2	145.2
59	deoxycholic acid	y	222528	HMDB0000626	C24H40O4	392.6
60	desaminotyrosine	y	10394	HMDB0002199	C9H10O3	166.17
61	dihydrocaffeic acid	y	348154	HMDB0000423	C9H10O4	182.17
62	dihydrocholesterol	y	6665	HMDB0000908	C27H48O	388.7
63	dihydroferulic acid	y	14340	HMDB0062121	C10H12O4	196.2
64	dihydroresveratrol	y	185914	HMDB0240498	C14H14O3	230.26
65	dihydrosinapic acid	y	84681	HMDB0041727	C11H14O5	226.23
66	dihydrotestosterone	y	10635	HMDB0002961	C19H30O2	290.4
67	dodecanoic acid	y	3893	HMDB0000638	C12H24O2	200.32
68	dopamine	y	681	HMDB0000073	C8H11NO2	153.18
69	dulcitol	y	11850	HMDB0000107	C6H14O6	182.17
70	elaidic acid	y	637517	HMDB0000573	C18H34O2	282.5
71	erythronic acid	y	2781043	HMDB0000613	C4H8O5	136.1
72	ethanolamine	y	700	HMDB0000149	C2H7NO	61.08
73	fructose	y	2723872	NULL	C6H12O6	180.16
74	fucose	y	17106	NULL	C6H12O5	164.16
75	fumaric acid	y	444972	HMDB0000134	C4H4O4	116.07
76	gabapentim-lactam	y	47457	HMDB0247166	C9H15NO	153.22
77	gabapentin	y	3446	HMDB0005015	C9H17NO2	171.24
78	galactose	y	6036	NULL	C6H12O6	180.16
79	gamma-aminobutyric acid	y	119	HMDB0000112	C4H9NO2	103.12
80	gamma-muricholic acid	y	92805	NULL	C24H40O5	408.6
81	gluconic acid	y	10690	HMDB0000625	C6H12O7	196.16
82	glucose	y	5793	HMDB0304632	C6H12O6	180.16
83	glutamic acid	y	33032	HMDB0000148	C5H9NO4	147.13
84	glutamine	y	5961	HMDB0000641	C5H10N2O3	146.14
85	glutaric acid	y	743	HMDB0000661	C5H8O4	132.11
86	glycerol	y	753	HMDB0000131	C3H8O3	92.09
87	glycine	y	750	HMDB0000123	C2H5NO2	75.07
88	glycodeoxycholic acid	y	3035026	NULL	C26H43NO5	449.6
89	glycolic acid	y	757	HMDB0000115	C2H4O3	76.05
90	hexanoate	y	8892	HMDB0000535	C6H12O2	116.16
91	histamine	y	774	HMDB0000870	C5H9N3	111.15
92	histidine	y	6274	HMDB0000177	C6H9N3O2	155.15
93	hydrocinnamic acid	y	107	HMDB0000764	C9H10O2	150.17
94	hyodeoxycholic acid	y	5283820	NULL	C24H40O4	392.6
95	imidazoleacetate	y	96215	HMDB0002024	C5H6N2O2	126.11
96	imidazolepropionate	y	70630	HMDB0002271	C6H8N2O2	140.14
97	indole	y	798	HMDB0000738	C8H7N	117.15
98	indole-3-acetamide	y	397	HMDB0029739	C10H10N2O	174.2
99	indole-3-acetate	y	802	HMDB0000197	C10H9NO2	175.18
100	indole-3-acrylate	y	5375048	HMDB0000734	C11H9NO2	187.19
101	indole-3-carboxaldehyde	y	10256	HMDB0029737	C9H7NO	145.16
102	indole-3-lactate	y	92904	NULL	C11H11NO3	205.21
103	indole-3-propionate	y	3744	HMDB0002302	C11H11NO2	189.21
104	indole-3-pyruvate	y	803	HMDB0060484	C11H9NO3	203.19
105	isocitric acid	y	1198	HMDB0000193	C6H8O7	192.12
106	isodeoxycholic acid	y	164672	HMDB0002536	C24H40O4	392.6
107	isoleucine	y	6306	HMDB0000172	C6H13NO2	131.17
108	isolithocholic acid	y	164853	HMDB0000717	C24H40O3	376.6
109	itaconic acid	y	811	HMDB0002092	C5H6O4	130.1
110	lactic acid	y	612	NULL	C3H6O3	90.08
111	lactose	y	6134	HMDB0041627	C12H22O11	342.3
112	lactulose	y	11333	HMDB0000740	C12H22O11	342.3
113	leucine	y	6106	HMDB0000687	C6H13NO2	131.17

114	linoleic acid	y	5280450	HMDB0000673	C18H32O2	280.4
115	lithocholic acid	y	9903	HMDB0000761	C24H40O3	376.6
116	lysine	y	5962	HMDB0000182	C6H14N2O2	146.19
117	m-coumaric acid	y	637541	HMDB0001713	C9H8O3	164.16
118	maleic acid	y	444266	HMDB0000176	C4H4O4	116.07
119	malic acid	y	525	NULL	C4H6O5	134.09
120	malonic acid	y	867	HMDB0000691	C3H4O4	104.06
121	maltitol	y	493591	HMDB0002928	C12H24O11	344.31
122	maltose	y	6255	NULL	C12H22O11	342.3
123	mannitol	y	6251	HMDB0000765	C6H14O6	182.17
124	mannose	y	18950	NULL	C6H12O6	180.16
125	melatonin	y	896	HMDB0001389	C13H16N2O2	232.28
126	melibiose	y	440658	NULL	C12H22O11	342.3
127	meso-erythritol	y	222285	HMDB0002994	C4H10O4	122.12
128	methionine	y	6137	HMDB0000696	C5H11NO2S	149.21
129	methionine sulfoxide	y	847	HMDB0250776	C5H11NO3S	165.21
130	methylsuccinate	y	10349	NULL	C5H8O4	132.11
131	myo-inositol	y	892	HMDB0000211	C6H12O6	180.16
132	myristic acid	y	11005	HMDB0000806	C14H28O2	228.37
133	n-acetyl-glucosamine	y	439174	HMDB0000215	C8H15NO6	221.21
134	niacin	y	938	HMDB0001488	C6H5NO2	123.11
135	o-phosphorylethanolamine	y	1015	HMDB0000224	C2H8NO4P	141.06
136	octanoic acid	y	379	HMDB0000482	C8H16O2	144.21
137	octopamine	y	4581	NULL	C8H11NO2	153.18
138	ornithine	y	6262	HMDB0000214	C5H12N2O2	132.16
139	oxalic acid	y	971	HMDB0002329	C2H2O4	90.03
140	oxaloacetate	y	970	HMDB0000223	C4H4O5	132.07
141	p-coumaric acid	y	637542	HMDB0002035	C9H8O3	164.16
142	p-cresol	y	2879	HMDB0001858	C7H8O	108.14
143	p-toluic acid	y	7470	HMDB0029635	C8H8O2	136.15
144	palmitic acid	y	985	HMDB0000220	C16H32O2	256.42
145	pantothenic acid	y	6613	HMDB0000210	C9H17NO5	219.23
146	phenethylamine	y	1001	HMDB0012275	C8H11N	121.18
147	phenylacetate	y	999	HMDB0000209	C8H8O2	136.15
148	phenylalanine	y	6140	HMDB0000159	C9H11NO2	165.19
149	phenyllactate	y	3848	HMDB0000779	C9H10O3	166.17
150	phenylpyruvate	y	997	HMDB0000205	C9H8O3	164.16
151	picolinic acid	y	1018	HMDB0002243	C6H5NO2	123.11
152	pinitol	y	164619	HMDB0034219	C7H14O6	194.18
153	proline	y	145742	HMDB0000162	C5H9NO2	115.13
154	proline	y	145742	HMDB0000162	C5H9NO2	115.13
155	psicose	y	90008	NULL	C6H12O6	180.16
156	putrescine	y	1045	HMDB0001414	C4H12N2	88.15
157	pyruvic acid	y	1060	HMDB0000243	C3H4O3	88.06
158	quinic acid	y	6508	HMDB0003072	C7H12O6	192.17
159	quinolinic acid	y	1066	HMDB0000232	C7H5NO4	167.12
160	raffinose	y	439242	HMDB0003213	C18H32O16	504.4
161	resveratrol	y	445154	HMDB0003747	C14H12O3	228.24
162	rhamnose	y	25310	HMDB0000849	C6H12O5	164.16
163	ribose	y	10975657	NULL	C5H10O5	150.13
164	rosmarinic acid	y	5281792	HMDB0003572	C18H16O8	360.3
165	serine	y	5951	HMDB0000187	C3H7NO3	105.09
166	shikimic acid	y	8742	HMDB0003070	C7H10O5	174.15
167	sinapic acid	y	637775	HMDB0032616	C11H12O5	224.21
168	sorbitol	y	5780	HMDB0000247	C6H14O6	182.17
169	sorbose	y	6904	NULL	C6H12O6	180.16
170	stearic acid	y	5281	HMDB0000827	C18H36O2	284.5
171	succinate	y	1110	HMDB0000254	C4H6O4	118.09
172	sucrose	y	5988	HMDB0000258	C12H22O11	342.3
173	tartaric acid	y	875	HMDB0062642	C4H6O6	150.09
174	taurine	y	1123	HMDB0000251	C2H7NO3S	125.15
175	testosterone	y	6013	HMDB0000234	C19H28O2	288.4
176	threitol	y	169019	HMDB0004136	C4H10O4	122.12

177	threonine	y	6288	HMDB0000167	C4H9NO3	119.12
178	trans-4-hydroxyproline	y	5810	HMDB0000725	C5H9NO3	131.13
179	trans-cinnamic acid	y	444539	HMDB0000930	C9H8O2	148.16
180	trans-ferulic acid	y	445858	HMDB0000954	C10H10O4	194.18
181	trans-ferulic acid	y	445858	HMDB0000954	C10H10O4	194.18
182	tryptamine	y	1150	HMDB0000303	C10H12N2	160.22
183	tryptophan	y	6305	HMDB0000929	C11H12N2O2	204.22
184	tryptophol	y	10685	HMDB0003447	C10H11NO	161.2
185	tyramine	y	5610	HMDB0000306	C8H11NO	137.18
186	tyrosine	y	6057	HMDB0000158	C9H11NO3	181.19
187	tyrosol	y	10393	HMDB0004284	C8H10O2	138.16
188	uracil	y	1174	HMDB0000300	C4H4N2O2	112.09
189	urea	y	1176	HMDB0000294	CH4N2O	60.056
190	urocanic acid	y	736715	HMDB0000301	C6H6N2O2	138.12
191	ursodeoxycholic acid	y	31401	HMDB0000946	C24H40O4	392.6
192	valerate	y	7991	HMDB0000892	C5H10O2	102.13
193	valine	y	6287	HMDB0000883	C5H11NO2	117.15
194	vanillin	y	1183	HMDB0012308	C8H8O3	152.15
195	xylose	y	135191	HMDB0000098	C5H10O5	150.13