

Host-Microbe Metabolomics Facility (DFI - HMMF)

Bile Acid Panel

Panel	Compound name	Data Provided		PubChemID	HMDB_ID if available)	Molecular Formula	Molecular Weight
		Quantified (y/n)	Normalized Relative Abundance (y/n)				
Bile-acid	3-oxolithocholic acid	y	y	5283906	NULL	C24H38O3	374.6
Bile-acid	allocholic acid	y	y	160636	HMDB0000505	C24H40O5	408.6
Bile-acid	allosolithocholic acid	y	y	94228	HMDB0000713	C24H40O3	376.6
Bile-acid	alpha-muricholic acid	y	y	5283852	HMDB0000506	C24H40O5	408.6
Bile-acid	beta-muricholic acid	y	y	5283853	HMDB0000415	C24H40O5	408.6
Bile-acid	chenodeoxycholic acid	y	y	10133	HMDB0000518	C24H40O4	392.6
Bile-acid	cholic acid	y	y	221493	HMDB0000619	C24H40O5	408.6
Bile-acid	deoxycholic acid	y	y	222528	HMDB0000626	C24H40O4	392.6
Bile-acid	glycochenodeoxycholic acid	y	y	12544	HMDB0000637	C26H43NO5	449.6
Bile-acid	glycocholic acid	y	y	10140	HMDB0000138	C26H43NO6	465.6
Bile-acid	isodeoxycholic acid	y	y	160530	HMDB0000438	C24H40O4	392.6
Bile-acid	lithocholic acid	y	y	9903	HMDB0000761	C24H40O3	376.6
Bile-acid	taurochenodeoxycholic acid	y	y	387316	HMDB0000951	C26H45NO6S	499.7
Bile-acid	taurocholic acid	y	y	6675	HMDB0000036	C26H45NO7S	515.7
Bile-acid	ursocholic acid	y	y	122340	HMDB0000917	C24H40O5	408.6
Bile-acid	ursodeoxycholic acid	y	y	31401	HMDB0000946	C24H40O4	392.6
Bile-acid	12-oxochenodeoxycholic acid		y	94235	HMDB0000400	C24H38O5	406.6
Bile-acid	12-oxolithocholic acid		y	3080612	HMDB0000328	C24H38O4	390.6
Bile-acid	3-deoxycholic acid		y	164672	HMDB0002536	C24H40O4	392.6
Bile-acid	3-epicholic acid		y	5283870	HMDB0000419	C24H40O5	408.6
Bile-acid	3-oxochenodeoxycholic acid		y	5283932	HMDB0000503	C24H38O4	390.6
Bile-acid	3-oxocholic acid		y	5283956	HMDB0000502	C24H38O5	406.6
Bile-acid	3-oxodeoxycholic acid		y	160738	HMDB0062742	C24H38O4	390.6
Bile-acid	6-oxolithocholic acid		y	164960	NULL	C24H38O4	390.6
Bile-acid	7-12-dioxolithocholic acid		y	3080560	NULL	C24H36O5	404.5
Bile-acid	7-oxodeoxycholic acid		y	188292	HMDB0000391	C24H38O5	406.6
Bile-acid	7-oxolithocholic acid		y	444262	NULL	C24H38O4	390.6
Bile-acid	allolithocholic acid		y	5283803	NULL	C24H40O3	376.6
Bile-acid	gamma-muricholic acid		y	92805	NULL	C24H40O5	408.6
Bile-acid	glycodehydrocholic acid		y	13955640	NULL	C26H37NO6	459.6
Bile-acid	glycodeoxycholic acid		y	3035026	NULL	C26H43NO5	449.6
Bile-acid	glycohyodeoxycholic acid		y	114611	NULL	C26H43NO5	449.6
Bile-acid	glycolithocholic acid		y	115245	HMDB0000698	C26H43NO4	433.6
Bile-acid	glycoursodeoxycholic acid		y	12310288	HMDB0000708	C26H43NO5	449.6
Bile-acid	hyodeoxycholic acid		y	5283820	NULL	C24H40O4	392.6
Bile-acid	isolithocholic acid		y	164853	HMDB0000717	C24H40O3	376.6
Bile-acid	omega-muricholic acid		y	5283851	HMDB0000364	C24H40O5	408.6
Bile-acid	tauro-alpha-muricholic acid		y	168408	HMDB0000932	C26H45NO7S	515.7
Bile-acid	tauro-beta-muricholic acid		y	168408	HMDB0000932	C26H45NO7S	515.7
Bile-acid	taurodeoxycholic acid		y	2733768	HMDB0000896	C26H45NO6S	499.7
Bile-acid	taurohyodeoxycholic acid		y	119046	NULL	C26H45NO6S	499.7
Bile-acid	taurolithocholic acid		y	439763	HMDB0000722	C26H45NO5S	483.7
Bile-acid	tauroursodeoxycholic acid		y	9848818	NULL	C26H45NO6S	499.7

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PFBBR(SCFA) Panel

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

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Tryptophan(Indole) Panel

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

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TMS - MOX Panel (4 pages)

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

TMS-MOX	cis-oleic acid	y	445639	HMDB0000207	C18H34O2	282.5
TMS-MOX	citric acid	y	311	HMDB0000094	C6H8O7	192.12
TMS-MOX	coprostanol	y	221122	HMDB0000577	C27H48O	388.7
TMS-MOX	coprostanone	y	92128	HMDB0000871	C27H46O	386.7
TMS-MOX	creatine	y	586	HMDB0000064	C4H9N3O2	131.13
TMS-MOX	creatinine	y	588	NULL	C4H7N3O	113.12
TMS-MOX	cysteine	y	5862	HMDB0000574	C3H7NO2S	121.16
TMS-MOX	cystine	y	67678	HMDB0000192	C6H12N2O4S2	240.3
TMS-MOX	decanoic acid	y	2969	HMDB0000511	C10H20O2	172.26
TMS-MOX	deoxycarnitine	y	725	HMDB0001161	C7H15NO2	145.2
TMS-MOX	deoxycholic acid	y	222528	HMDB0000626	C24H40O4	392.6
TMS-MOX	desaminotyrosine	y	10394	HMDB0002199	C9H10O3	166.17
TMS-MOX	dihydrocaffeic acid	y	348154	HMDB0000423	C9H10O4	182.17
TMS-MOX	dihydrocholesterol	y	6665	HMDB0000908	C27H48O	388.7
TMS-MOX	dihydroferulic acid	y	14340	HMDB0062121	C10H12O4	196.2
TMS-MOX	dihydroresveratrol	y	185914	HMDB0240498	C14H14O3	230.26
TMS-MOX	dihydrosinapic acid	y	84681	HMDB0041727	C11H14O5	226.23
TMS-MOX	dihydrotestosterone	y	10635	HMDB0002961	C19H30O2	290.4
TMS-MOX	dodecanoic acid	y	3893	HMDB0000638	C12H24O2	200.32
TMS-MOX	dopamine	y	681	HMDB0000073	C8H11NO2	153.18
TMS-MOX	dulcitol	y	11850	HMDB0000107	C6H14O6	182.17
TMS-MOX	elaidic acid	y	637517	HMDB0000573	C18H34O2	282.5
TMS-MOX	erythronic acid	y	2781043	HMDB0000613	C4H8O5	136.1
TMS-MOX	ethanolamine	y	700	HMDB0000149	C2H7NO	61.08
TMS-MOX	fructose	y	2723872	NULL	C6H12O6	180.16
TMS-MOX	fucose	y	17106	NULL	C6H12O5	164.16
TMS-MOX	fumaric acid	y	444972	HMDB0000134	C4H4O4	116.07
TMS-MOX	gabapentim-lactam	y	47457	HMDB0247166	C9H15NO	153.22
TMS-MOX	gabapentin	y	3446	HMDB0005015	C9H17NO2	171.24
TMS-MOX	galactose	y	6036	NULL	C6H12O6	180.16
TMS-MOX	gamma-aminobutyric acid	y	119	HMDB0000112	C4H9NO2	103.12
TMS-MOX	gamma-muricholic acid	y	92805	NULL	C24H40O5	408.6
TMS-MOX	gluconic acid	y	10690	HMDB0000625	C6H12O7	196.16
TMS-MOX	glucose	y	5793	HMDB0304632	C6H12O6	180.16
TMS-MOX	glutamic acid	y	33032	HMDB0000148	C5H9NO4	147.13
TMS-MOX	glutamine	y	5961	HMDB0000641	C5H10N2O3	146.14
TMS-MOX	glutaric acid	y	743	HMDB0000661	C5H8O4	132.11
TMS-MOX	glycerol	y	753	HMDB0000131	C3H8O3	92.09
TMS-MOX	glycine	y	750	HMDB0000123	C2H5NO2	75.07
TMS-MOX	glycodeoxycholic acid	y	3035026	NULL	C26H43NO5	449.6
TMS-MOX	glycolic acid	y	757	HMDB0000115	C2H4O3	76.05
TMS-MOX	hexanoate	y	8892	HMDB0000535	C6H12O2	116.16
TMS-MOX	histamine	y	774	HMDB0000870	C5H9N3	111.15
TMS-MOX	histidine	y	6274	HMDB0000177	C6H9N3O2	155.15
TMS-MOX	hydrocinnamic acid	y	107	HMDB0000764	C9H10O2	150.17
TMS-MOX	hyodeoxycholic acid	y	5283820	NULL	C24H40O4	392.6
TMS-MOX	imidazoleacetate	y	96215	HMDB0002024	C5H6N2O2	126.11
TMS-MOX	imidazolepropionate	y	70630	HMDB0002271	C6H8N2O2	140.14
TMS-MOX	indole	y	798	HMDB0000738	C8H7N	117.15
TMS-MOX	indole-3-acetamide	y	397	HMDB0029739	C10H10N2O	174.2
TMS-MOX	indole-3-acetate	y	802	HMDB0000197	C10H9NO2	175.18
TMS-MOX	indole-3-acrylate	y	5375048	HMDB0000734	C11H9NO2	187.19
TMS-MOX	indole-3-carboxaldehyde	y	10256	HMDB0029737	C9H7NO	145.16
TMS-MOX	indole-3-lactate	y	92904	NULL	C11H11NO3	205.21
TMS-MOX	indole-3-propionate	y	3744	HMDB0002302	C11H11NO2	189.21
TMS-MOX	indole-3-pyruvate	y	803	HMDB0060484	C11H9NO3	203.19
TMS-MOX	isocitric acid	y	1198	HMDB0000193	C6H8O7	192.12
TMS-MOX	isodeoxycholic acid	y	164672	HMDB0002536	C24H40O4	392.6
TMS-MOX	isoleucine	y	6306	HMDB0000172	C6H13NO2	131.17
TMS-MOX	isolithocholic acid	y	164853	HMDB0000717	C24H40O3	376.6
TMS-MOX	itaconic acid	y	811	HMDB0002092	C5H6O4	130.1

TMS-MOX	lactic acid	y	612	NULL	C3H6O3	90.08
TMS-MOX	lactose	y	6134	HMDB0041627	C12H22O11	342.3
TMS-MOX	lactulose	y	11333	HMDB0000740	C12H22O11	342.3
TMS-MOX	leucine	y	6106	HMDB0000687	C6H13NO2	131.17
TMS-MOX	linoleic acid	y	5280450	HMDB0000673	C18H32O2	280.4
TMS-MOX	lithocholic acid	y	9903	HMDB0000761	C24H40O3	376.6
TMS-MOX	lysine	y	5962	HMDB0000182	C6H14N2O2	146.19
TMS-MOX	m-coumaric acid	y	637541	HMDB0001713	C9H8O3	164.16
TMS-MOX	maleic acid	y	444266	HMDB0000176	C4H4O4	116.07
TMS-MOX	malic acid	y	525	NULL	C4H6O5	134.09
TMS-MOX	malonic acid	y	867	HMDB0000691	C3H4O4	104.06
TMS-MOX	maltitol	y	493591	HMDB0002928	C12H24O11	344.31
TMS-MOX	maltose	y	6255	NULL	C12H22O11	342.3
TMS-MOX	mannitol	y	6251	HMDB0000765	C6H14O6	182.17
TMS-MOX	mannose	y	18950	NULL	C6H12O6	180.16
TMS-MOX	melatonin	y	896	HMDB0001389	C13H16N2O2	232.28
TMS-MOX	melibiose	y	440658	NULL	C12H22O11	342.3
TMS-MOX	meso-erythritol	y	222285	HMDB0002994	C4H10O4	122.12
TMS-MOX	methionine	y	6137	HMDB0000696	C5H11NO2S	149.21
TMS-MOX	methionine sulfoxide	y	847	HMDB0250776	C5H11NO3S	165.21
TMS-MOX	methylsuccinate	y	10349	NULL	C5H8O4	132.11
TMS-MOX	myo-inositol	y	892	HMDB0000211	C6H12O6	180.16
TMS-MOX	myristic acid	y	11005	HMDB0000806	C14H28O2	228.37
TMS-MOX	n-acetyl-glucosamine	y	439174	HMDB0000215	C8H15NO6	221.21
TMS-MOX	niacin	y	938	HMDB0001488	C6H5NO2	123.11
TMS-MOX	o-phosphorylethanolamine	y	1015	HMDB0000224	C2H8NO4P	141.06
TMS-MOX	octanoic acid	y	379	HMDB0000482	C8H16O2	144.21
TMS-MOX	octopamine	y	4581	NULL	C8H11NO2	153.18
TMS-MOX	ornithine	y	6262	HMDB0000214	C5H12N2O2	132.16
TMS-MOX	oxalic acid	y	971	HMDB0002329	C2H2O4	90.03
TMS-MOX	oxaloacetate	y	970	HMDB0000223	C4H4O5	132.07
TMS-MOX	p-coumaric acid	y	637542	HMDB0002035	C9H8O3	164.16
TMS-MOX	p-cresol	y	2879	HMDB0001858	C7H8O	108.14
TMS-MOX	p-toluic acid	y	7470	HMDB0029635	C8H8O2	136.15
TMS-MOX	palmitic acid	y	985	HMDB0000220	C16H32O2	256.42
TMS-MOX	pantothenic acid	y	6613	HMDB0000210	C9H17NO5	219.23
TMS-MOX	phenethylamine	y	1001	HMDB0012275	C8H11N	121.18
TMS-MOX	phenylacetate	y	999	HMDB0000209	C8H8O2	136.15
TMS-MOX	phenylalanine	y	6140	HMDB0000159	C9H11NO2	165.19
TMS-MOX	phenyllactate	y	3848	HMDB0000779	C9H10O3	166.17
TMS-MOX	phenylpyruvate	y	997	HMDB0000205	C9H8O3	164.16
TMS-MOX	picolinic acid	y	1018	HMDB0002243	C6H5NO2	123.11
TMS-MOX	pinitol	y	164619	HMDB0034219	C7H14O6	194.18
TMS-MOX	proline	y	145742	HMDB0000162	C5H9NO2	115.13
TMS-MOX	proline	y	145742	HMDB0000162	C5H9NO2	115.13
TMS-MOX	psicose	y	90008	NULL	C6H12O6	180.16
TMS-MOX	putrescine	y	1045	HMDB0001414	C4H12N2	88.15
TMS-MOX	pyruvic acid	y	1060	HMDB0000243	C3H4O3	88.06
TMS-MOX	quinic acid	y	6508	HMDB0003072	C7H12O6	192.17
TMS-MOX	quinolinic acid	y	1066	HMDB0000232	C7H5NO4	167.12
TMS-MOX	raffinose	y	439242	HMDB0003213	C18H32O16	504.4
TMS-MOX	resveratrol	y	445154	HMDB0003747	C14H12O3	228.24
TMS-MOX	rhamnose	y	25310	HMDB0000849	C6H12O5	164.16
TMS-MOX	ribose	y	10975657	NULL	C5H10O5	150.13
TMS-MOX	rosmarinic acid	y	5281792	HMDB0003572	C18H16O8	360.3
TMS-MOX	serine	y	5951	HMDB0000187	C3H7NO3	105.09
TMS-MOX	shikimic acid	y	8742	HMDB0003070	C7H10O5	174.15
TMS-MOX	sinapic acid	y	637775	HMDB0032616	C11H12O5	224.21
TMS-MOX	sorbitol	y	5780	HMDB0000247	C6H14O6	182.17
TMS-MOX	sorbose	y	6904	NULL	C6H12O6	180.16
TMS-MOX	stearic acid	y	5281	HMDB0000827	C18H36O2	284.5

TMS-MOX	succinate	y	1110	HMDB0000254	C4H6O4	118.09
TMS-MOX	sucrose	y	5988	HMDB0000258	C12H22O11	342.3
TMS-MOX	tartaric acid	y	875	HMDB0062642	C4H6O6	150.09
TMS-MOX	taurine	y	1123	HMDB0000251	C2H7NO3S	125.15
TMS-MOX	testosterone	y	6013	HMDB0000234	C19H28O2	288.4
TMS-MOX	threitol	y	169019	HMDB0004136	C4H10O4	122.12
TMS-MOX	threonine	y	6288	HMDB0000167	C4H9NO3	119.12
TMS-MOX	trans-4-hydroxyproline	y	5810	HMDB0000725	C5H9NO3	131.13
TMS-MOX	trans-cinnamic acid	y	444539	HMDB0000930	C9H8O2	148.16
TMS-MOX	trans-ferulic acid	y	445858	HMDB0000954	C10H10O4	194.18
TMS-MOX	trans-ferulic acid	y	445858	HMDB0000954	C10H10O4	194.18
TMS-MOX	tryptamine	y	1150	HMDB0000303	C10H12N2	160.22
TMS-MOX	tryptophan	y	6305	HMDB0000929	C11H12N2O2	204.22
TMS-MOX	tryptophol	y	10685	HMDB0003447	C10H11NO	161.2
TMS-MOX	tyramine	y	5610	HMDB0000306	C8H11NO	137.18
TMS-MOX	tyrosine	y	6057	HMDB0000158	C9H11NO3	181.19
TMS-MOX	tyrosol	y	10393	HMDB0004284	C8H10O2	138.16
TMS-MOX	uracil	y	1174	HMDB0000300	C4H4N2O2	112.09
TMS-MOX	urea	y	1176	HMDB0000294	CH4N2O	60.056
TMS-MOX	urocanic acid	y	736715	HMDB0000301	C6H6N2O2	138.12
TMS-MOX	ursodeoxycholic acid	y	31401	HMDB0000946	C24H40O4	392.6
TMS-MOX	valerate	y	7991	HMDB0000892	C5H10O2	102.13
TMS-MOX	valine	y	6287	HMDB0000883	C5H11NO2	117.15
TMS-MOX	vanillin	y	1183	HMDB0012308	C8H8O3	152.15
TMS-MOX	xylose	y	135191	HMDB0000098	C5H10O5	150.13