

Table S1. Fold Changes of Qualified Metabolites

Fold Change: Cases of WTC-LI/Control	
	<1
	>1

Super Pathway	Sub Pathway	Metabolite	Comp ID	KEGG	HMDB	PubChem	WTC-LI Control	CAS	Retention Index	Mass
Amino Acid	Alanine and Aspartate Metabolism	asparagine	512	C00152	HMDB00168	6267		70-47-3	1225	133.06
		aspartate	443	C00049	HMDB00191	5960		56-84-8	1165	134.04
		N-acetylalanine	1585	C02847	HMDB00766	88064		97-69-8	861.2	130.05
		N-acetylasparagine	33942		HMDB06028	99715		4033-40-3	785	175.07
		N-acetylaspartate (NAA)	22185	C01042	HMDB00812	65065		997-55-7;997-55-7	880	176.06
	Creatine Metabolism	creatine	27718	C00300	HMDB00064	586		57-00-1	1947	132.08
		creatinine	513	C00791	HMDB00562	588		60-27-5	2055	114.07
		guanidinoacetate	43802	C00581	HMDB00128	763		352-97-6	1937	118.06
	Glutamate Metabolism	beta-citrylglutamate	54923					73590-26-8	900	322.08
		glutamate	57	C00025	HMDB00148	611		56-86-0	1500	148.06
		glutamate, gamma-methyl ester	33487			68662		1499-55-4	2170	162.08
		glutamine	53	C00064	HMDB00641	5961		56-85-9	1291	147.08
		N-acetyl-aspartyl-glutamate (NAAG)	35665	C12270	HMDB01067	5255		3106-85-2	1035	305.1
		N-acetylglutamate	15720	C00624	HMDB01138	70914		8/3/17	1050	190.07
		N-acetylglutamine	33943	C02716	HMDB06029	182230		2490-97-3	2140	187.07
		pyroglutamine*	46225			134508		2353-44-8	1900	129.07
	Glutathione Metabolism	5-oxoproline	1494	C01879	HMDB00267	7405		98-79-3	738.5	128.04
	Glycine, Serine and Threonine Metabolism	allo-threonine	15142	C05519	HMDB04041	99289		28954-12-3	2511.1	118.05
		betaine	3141	C00719	HMDB00043	247		107-43-7	1064	118.09
		dimethylglycine	5086	C01026	HMDB00092	673		1118-68-9	1104	104.07
		glycine	58	C00037	HMDB00123	750		56-40-6	1375	76.04
		N-acetylglycine	27710		HMDB00532	10972		543-24-8	731	116.04
		N-acetylserine	37076		HMDB02931	65249		97-14-3	2000	146.05
N-acetylthreonine		33939			152204		17093-74-2	821.6	160.06	

	sarcosine	1516	C00213	HMDB00271	1088		107-97-1	1280	90.05
	serine	1648	C00065	HMDB00187	5951		56-45-1	1239	106.05
	threonine	1284	C00188	HMDB00167	6288		72-19-5	1514	120.07
Guanidino and Acetamido Metabolism	4-guanidinobutanoate	15681	C01035	HMDB03464	500		463-003;463-00-3	2320	146.09
Histidine Metabolism	1-methylhistidine	30460	C01152	HMDB00001	92105		332-80-9	2755	170.09
	1-methylimidazoleacetate	32350	C05828	HMDB02820	75810		2625-49-2	2064	141.07
	3-methylhistidine	15677	C01152	HMDB00479	64969		368-16-1	906.3	168.08
	histidine	59	C00135	HMDB00177	6274		5934-29-2	755.9	154.06
	hydantoin-5-propionic acid	40473	C05565	HMDB01212	782		5624-26-0	2080	171.04
	imidazole lactate	15716	C05568	HMDB02320	440129		14403-45-3	2040	157.06
	imidazole propionate	40730		HMDB02271	70630		1074-59-5	2263	141.07
Leucine, Isoleucine and Valine Metabolism	2-hydroxy-3-methylvalerate	36746		HMDB00317	164623		488-15-3	1800	131.07
	2-methylbutyrylcarnitine (C5)	45095		HMDB00378	6426901		31023-25-3	3035	246.17
	3-hydroxy-2-ethylpropionate	32397		HMDB00396	188979		4374-62-3	975	117.06
	3-hydroxyisobutyrate	1549	C06001	HMDB00336	87		2068-83-9	1619	103.04
	3-methyl-2-oxobutyrate	44526	C00141	HMDB00019	49		3715-29-5	1465	115.04
	3-methyl-2-oxovalerate	15676	C00671	HMDB03736	47		1460-34-0;51829-07-3	2064.2	129.06
	3-methylglutaconate	38667		HMDB00522	1551553		5746-90-7	2579.6	143.03
	4-methyl-2-oxopentanoate	22116	C00233	HMDB00695	70		816-66-0	2170	129.06
	alpha-hydroxyisocaproate	22132	C03264	HMDB00746	83697		10303-64-7	1840	131.07
	alpha-hydroxyisovalerate	33937		HMDB00407	99823		600-37-3	1126	117.06
	beta-hydroxyisovalerate	12129		HMDB00754	69362		625-08-1	1027	117.06
	ethylmalonate	15765		HMDB00622	11756		601-75-2	2785	131.03
	isobutyrylcarnitine	33441		HMDB00736	168379		25518-49-4	2810	232.15
	isobutyrylglycine	35437		HMDB00730	10855600		15926-18-8	1420	144.07
	isoleucine	1125	C00407	HMDB00172	6306		73-32-5	2800	132.1
	isovalerylcarnitine	34407		HMDB00688	6426851		31023-24-2	3085	246.17
	isovalerylglycine	35107		HMDB00678	546304		16284-60-9	1950	158.08
	leucine	60	C00123	HMDB00687	6106		61-90-5	2864	132.1
	methylsuccinate	15745		HMDB01844	10349		498-21-5	2800	131.03
	N-acetylisoleucine	33967			2802421		3077-46-1	2325	172.1
N-acetylleucine	1587	C02710	HMDB11756	70912		1188-21-2	2400	172.1	

	N-acetylvaline	1591		HMDB11757	66789		96-81-1	1704	158.08
	valine	1649	C00183	HMDB00883	6287		72-18-4	2479	118.09
Lysine Metabolism	2-aminoadipate	6146	C00956	HMDB00510	469		542-32-5;1118-90-7	3500	160.06
	5-hydroxylysine	15685	C16741	HMDB00450	1029		13204-98-3	2790	163.11
	6-oxopiperidine-2-carboxylate	43231			3014237		34622-39-4	1432	144.07
	glutarate (pentanedioate)	396	C00489	HMDB00661	743		110-94-1	2900	131.03
	glutaryl carnitine (C5)	44664		HMDB13130	71464488		102636-82-8	2393	276.14
	lysine	1301	C00047	HMDB00182	5962		56-87-1	2850	147.11
	N2-acetyllysine	36751	C12989	HMDB00446	92907		1946-82-3	3372.6	187.11
	N6-acetyllysine	36752	C02727	HMDB00206	92832		692-04-6	1059	187.11
	N6,N6,N6-trimethyllysine	1498	C03793	HMDB01325	440120		23284-33-5	2825	189.16
	pipecolate	1444	C00408	HMDB00070	849		4043-87-2	2200	130.09
Methionine, Cysteine, SAM and Taurine Metabolism	2-aminobutyrate	42374	C02261	HMDB00650	439691		1492-24-6	2059	104.07
	2-hydroxybutyrate/2-hydroxyisobutyrate	52281						1258	103.04
	cysteine	1868	C00097	HMDB00574	5862		52-90-4;56-89-3	1488	122.03
	cysteine s-sulfate	22176	C05824	HMDB00731	115015		1637-71-4	565	201.98
	cysteine sulfinic acid	37443	C00606	HMDB00996	109		207121-48-0	597	154.02
	cystine	56	C00491	HMDB00192	67678		56-89-3	2000	241.03
	hypotaurine	590	C00519	HMDB00965	107812		300-84-5	724	110.03
	lanthionine	42002			0		8/2/83	1730	209.06
	methionine	1302	C00073	HMDB00696	6137		63-68-3	2526	150.06
	methionine sulfone	44878			69961		820-10-0	1250	182.05
	methionine sulfoxide	18374	C02989	HMDB02005	158980		3226-65-1	1272	166.05
	N-acetylmethionine	1589	C02712	HMDB11745	448580		65-82-7	1787	190.05
	N-acetyltaurine	48187			159864			600	168.03
	N-formylmethionine	2829	C03145	HMDB01015	439750		4289-98-9	1543.8	176.04
	S-adenosylhomocysteine (SAH)	42382	C00021	HMDB00939	439155		979-92-0	1832.4	383.11
	S-methylcysteine	39592		HMDB02108	24417		1187-84-4	880	134.03
taurine	2125	C00245	HMDB00251	1123		107-35-7	690	124.01	
Phenylalanine and Tyrosine Metabolism	2-hydroxyphenylacetate	1432	C05852	HMDB00669	11970		614-75-5	858.6	151.04
	3-(4-hydroxyphenyl)lactate	32197	C03672	HMDB00755	9378		6482-98-0	1379	181.05
	3-methoxytyrosine	12017		HMDB01434	1670		300-48-1	1606	210.08
	3-phenylpropionate (hydrocinnamate)	15749	C05629	HMDB00764	107		501-52-0	2860	149.06
	4-hydroxyphenylpyruvate	1669	C01179	HMDB00707	979		156-39-8	1690.1	179.03

	5-bromotryptophan	53242			96735			3525	280.99
	dopamine sulfate (2)	48407						1556.2	232.03
	gentisate	18280	C00628	HMDB00152	3469		490-79-9	905	153.02
	N-acetylphenylalanine	33950	C03519	HMDB00512	74839		2018-61-3	2597	206.08
	N-acetyltyrosine	32390		HMDB00866	68310		537-55-3	1680	222.08
	p-cresol sulfate	36103	C01468	HMDB11635	4615423		3233-57-7	2890	187.01
	p-cresol-glucuronide*	48841		HMDB11686	154035		17680-99-8	2420	283.08
	phenol sulfate	32553	C02180	HMDB60015	74426		937-34-8	2156	172.99
	phenylalanine	64	C00079	HMDB00159	6140		63-91-2	2878	166.09
	phenyllactate (PLA)	22130	C05607	HMDB00779	3848		828-01-3	2208	165.06
	phenylpyruvate	566	C00166	HMDB00205	997		156-06-9	845	163.04
	thyroxine	2761	C01829	HMDB01918	5819		51-48-9	4808	775.68
	tyrosine	1299	C00082	HMDB00158	6057		60-18-4	2430	182.08
	vanillylmandelate (VMA)	1567	C05584	HMDB00291	1245		55-10-7	941	197.05
Polyamine Metabolism	4-acetamidobutanoate	1558	C02946	HMDB03681	18189		3025-96-5	1350	146.08
	acisoga	43258			129397		106692-36-8	1813	185.13
	N-acetylputrescine	37496	C02714	HMDB02064	122356		18233-70-0	2230	131.12
	N(4)-acetylspermidine	32356			128317		66039-56-3	3095	188.18
	spermidine	485	C00315	HMDB01257	1102		124-20-9	3355	146.17
Tryptophan Metabolism	3-indoxyl sulfate	27672		HMDB00682	10258		2642-37-7	2222.2	212
	5-hydroxyindoleacetate	437	C05635	HMDB00763	1826		54-16-0	1510.2	190.05
	C-glycosyltryptophan	48782			10981970		180509-18-6	1777	365.14
	indoleacetate	27513	C00954	HMDB00197	802		6505-45-9	2850	176.07
	indolelactate	18349	C02043	HMDB00671	92904		832-97-3	2286	204.07
	indolepropionate	32405		HMDB02302	3744		830-96-6	3205	190.09
	kynurenate	1417	C01717	HMDB00715	3845		492-27-3	2224	188.04
	kynurenine	15140	C00328	HMDB00684	161166		2922-83-0	2739	209.09
	N-acetyltryptophan	33959	C03137	HMDB13713	700653		1218-34-4	2630	245.09
	picolinate	1512	C10164	HMDB02243	1018		98-98-6	910	124.04
	serotonin	2342	C00780	HMDB00259	5202		153-98-0	2550	177.1
	thioprolin	53231			0		34592-47-4	1250	134.03
	tryptophan	54	C00078	HMDB00929	6305		73-22-3	2986	205.1
tryptophan betaine	37097	C09213	HMDB61115	442106		20671-76-5	2673	247.14	
	2-oxoarginine*	55072		HMDB04225	558		10/4/15	963	172.07

Urea cycle; Arginine and Proline Metabolism	arginine	1638	C00062	HMDB00517	232		1119-34-2	2825	175.12	
	dimethylarginine (SDMA + ADMA)	36808	C03626	HMDB01539	123831		102783-24-4	2850	203.15	
	homoarginine	22137	C01924	HMDB00670	9085		156-86-5	2882	189.13	
	homocitrulline	22138	C02427	HMDB00679	65072		1190-49-4	1908	190.12	
	N-acetylarginine	33953	C02562	HMDB04620	67427		155-84-0	2245	217.13	
	N-acetylcitrulline	48434	C15532	HMDB00856	656979		33965-42-3	940	216.1	
	N-acetylproline	34387			322640		1074-79-9	1695	158.08	
	N-delta-acetylornithine	43249			9920500			858	173.09	
	N-methylproline	37431			557		475-11-6	1335	130.09	
	N-monomethylarginine	43586	C03884	HMDB29416	132862		53308-83-1	2845	189.13	
	ornithine	1493	C00077	HMDB03374	6262		3184-13-2	2800	133.1	
	pro-hydroxy-pro	35127		HMDB06695	11673055		18684-24-7	2128	229.12	
	proline	1898	C00148	HMDB00162	145742		147-85-3	1603	116.07	
	trans-4-hydroxyproline	32306	C01157	HMDB00725	5810		51-35-4	1064	132.07	
	urea	1670	C00086	HMDB00294	1176		57-13-6	700	121.07	
Carbohydrate	Advanced Glycation End-product	N6-carboxymethyllysine	36713				4/3/46	2500	205.12	
	Aminosugar Metabolism	erythronate*	42420		HMDB00613	2781043		88759-55-1	2186	135.03
		glucuronate	15443	C00191	HMDB00127	444791		207300-70-7	3233.3	193.04
		N-acetylglucosamine/N-acetylgalactosamine	46539						715	222.1
		N-acetylneuraminate	32377	C00270	HMDB00230	439197		131-48-6	660	310.11
	Disaccharides and Oligosaccharides	sucrose	1519	C00089	HMDB00258	5988		57-50-1	3092	387.11
	Fructose, Mannose and Galactose Metabolism	fructose	48195	C00095	HMDB00660	5984		57-48-7	2022.2	225.06
		galactitol (dulcitol)	1117	C01697	HMDB00107	11850		608-66-2	2309.7	181.07
		galactonate	27719	C00880	HMDB00565	128869		299-28-5	3085	195.05
		mannitol/sorbitol	46142	C01507	HMDB00247	5780			2260	181.07
		mannose	48153	C00159	HMDB00169	18950		3458-28-4	2200	225.06
	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	1,5-anhydroglucitol (1,5-AG)	20675	C07326	HMDB02712	64960		154-58-5	802	163.06
		glucose	48152	C00031	HMDB00122	79025		50-99-7	2342	225.06
		glycerate	1572	C00258	HMDB00139	752		600-19-1	2070.4	105.02

Cofactors and Vitamins		lactate	527	C00186	HMDB00190	612		79-33-4	681.6	89.02	
		pyruvate	48990	C00022	HMDB00243	1060		127-17-3	1083	87.01	
	Pentose Metabolism		arabitol/xylitol	48885						1932.4	151.06
			arabonate/xylonate	48255						2664.6	165.04
			ribitol	15772	C00474	HMDB00508	6912		488-81-3	1789.6	151.06
			ribonate	27731	C01685	HMDB00867	5460677		8/3/36	2425	165.04
			ribose	1471	C00121	HMDB00283	5779		50-69-1	1508.2	195.05
			ribulose/xylulose	54671						1400	195.05
	Ascorbate and Aldarate Metabolism		gulonate*	46957		HMDB03290	9794176		20246-53-1	2750	195.05
			oxalate (ethanedioate)	20694	C00209	HMDB02329	971		144-62-7	603	88.99
			threonate	27738	C01620	HMDB00943	151152		70753-61-6	2384	135.03
	Hemoglobin and Porphyrin Metabolism		bilirubin (E,E)*	32586			5315454		114-25-0	4294	583.26
			bilirubin (Z,Z)	43807	C00486	HMDB00054	5280352		635-65-4	1840	585.27
			biliverdin	2137	C00500	HMDB01008	5353439		55482-27-4;55482-27-4	1016	583.26
	Nicotinate and Nicotinamide Metabolism		1-methylnicotinamide	27665	C02918	HMDB00699	10129985		1005-24-9	1940	137.07
			N1-Methyl-2-pyridone-5-carboxamide	40469	C05842	HMDB04193	69698		701-44-0	1250	153.07
			nicotinamide	594	C00153	HMDB01406	936		98-92-0	1942	123.06
quinolinate			1899	C03722	HMDB00232	1066		89-00-9	3000	166.01	
trigonelline (N'-methylnicotinate)			32401	C01004	HMDB00875	5570		535-83-1	1388	138.05	
Pantothenate and CoA Metabolism		pantothenate	1508	C00864	HMDB00210	6613		137-08-6	1498.7	218.1	
		Tocopherol Metabolism		alpha-tocopherol	1561	C02477	HMDB01893	14985		59-02-9;10191-41-0	2522
gamma-CEHC	44876				HMDB01931	133098		178167-75-4	3843	263.13	
gamma-tocopherol/beta-tocopherol	52473								2384	416.36	
Vitamin A Metabolism		retinol (Vitamin A)	1806	C00473	HMDB00305	445354		68-26-8	1636	269.23	
Vitamin B6 Metabolism		pyridoxate	31555	C00847	HMDB00017	6723		82-82-6	2185	182.05	
Energy	TCA Cycle	2-methylcitrate/homocitrate	52282						575	205.04	
		aconitate [cis or trans]	46173	C00417	HMDB00072				580	173.01	

		alpha-ketoglutarate	528	C00026	HMDB00208	51	305-72-6;328-50-7;22202-68-2	2700	145.01	
		citraconate/glutaconate	47076					2600	129.02	
		citrate	1564	C00158	HMDB00094	311	77-92-9	582	191.02	
		fumarate	1643	C00122	HMDB00134	444972	100-17-8	3084	115	
		isocitrate	12110	C00311	HMDB00193	1198	20226-99-7	773	210.06	
		malate	1303	C00149	HMDB00156	525	6915-15-7	615.6	133.01	
		succinate	1437	C00042	HMDB00254	1110	110-15-6	3149	117.02	
Lipid	Carnitine Metabolism	carnitine	15500	C00318	HMDB00062	10917	461-05-2	1978	162.11	
		deoxycarnitine	36747	C01181	HMDB01161	134	6249-56-5	2052	146.12	
		diacylglycerol (16:1/18:2 [2], 16:0/18:3 [1])*	54966						2733	608.52
		linoleoyl-arachidonoyl-glycerol (18:2/20:4) [1]*	54955						2566	658.54
		linoleoyl-arachidonoyl-glycerol (18:2/20:4) [2]*	54956						2624	658.54
		linoleoyl-linolenoyl-glycerol (18:2/18:3) [1]*	54963						2426	632.52
		linoleoyl-linolenoyl-glycerol (18:2/18:3) [2]*	54964						2478	632.52
		linoleoyl-linoleoyl-glycerol (18:2/18:2) [1]*	54968						2689	634.54
		oleoyl-arachidonoyl-glycerol (18:1/20:4) [2]*	54961						2990	660.56
		oleoyl-linolenoyl-glycerol (18:1/18:3) [2]*	54970						2819	634.54
		oleoyl-linoleoyl-glycerol (18:1/18:2) [1]	46798					106292-55-1	3115	636.56
		oleoyl-linoleoyl-glycerol (18:1/18:2) [2]	46799					104346-53-4	3223	636.56
		oleoyl-oleoyl-glycerol (18:1/18:1) [1]*	54945						3571	638.57
		oleoyl-oleoyl-glycerol (18:1/18:1) [2]*	54946						3695	638.57
		palmitoleoyl-linoleoyl-glycerol (16:1/18:2) [1]*	54967						2664	608.52
		palmitoleoyl-oleoyl-glycerol (16:1/18:1) [1]*	52632		HMDB07131	9543694			3035	610.54
		palmitoleoyl-oleoyl-glycerol (16:1/18:1) [2]*	52631						3154	610.54
		palmitoyl-arachidonoyl-glycerol (16:0/20:4) [1]*	54957						2916	634.54
		palmitoyl-arachidonoyl-glycerol (16:0/20:4) [2]*	54958						3015	634.54
		palmitoyl-linoleoyl-glycerol (16:0/18:2) [1]*	52633			9543695			3080	610.54
		palmitoyl-linoleoyl-glycerol (16:0/18:2) [2]*	52634						3197	610.54
		palmitoyl-oleoyl-glycerol (16:0/18:1) [1]*	54943						3562	612.56
		palmitoyl-oleoyl-glycerol (16:0/18:1) [2]*	54942						3695	612.56
		stearoyl-linoleoyl-glycerol (18:0/18:2) [1]*	54948						3650	638.57
		stearoyl-linoleoyl-glycerol (18:0/18:2) [2]*	54947						3762	638.57
		Eicosanoid	12-HETE	37536		HMDB06111	5312983	71030-37-0;73837-14-6	5326	319.23

	9-HETE	46301		HMDB10222	5312978			5341	319.23
	leukotriene B4	37530	C02165	HMDB01085	5280492		71160-24-2	5186	335.22
Endocannabinoid	linoleoyl ethanolamide	52608		HMDB12252	5283446		68171-52-8	6150	322.28
	oleoyl ethanolamide	38102		HMDB02088	5283454		11-58-0;111-58-0	6400	324.29
	palmitoyl ethanolamide	38165	C16512	HMDB02100	4671		544-31-0	6300	298.28
Fatty Acid Metabolism (Acyl Choline)	palmitoylcholine	52944			151731			1482	342.34
Fatty Acid Metabolism (also BCAA Metabolism)	butyrylcarnitine	32412	C02862	HMDB02013	439829		25576-40-3	2860	232.15
	methylmalonate (MMA)	1496	C02170	HMDB00202	487		516-05-2	3078.4	117.02
	propionylcarnitine	32452	C03017	HMDB00824	107738		17298-37-2	2590	218.14
	propionylglycine	31932		HMDB00783	98681		21709-90-0	1502.5	130.05
Fatty Acid Metabolism(Acyl Carnitine)	3-hydroxybutyrylcarnitine (1)	43264		HMDB13127	53481617			2400	248.15
	acetylcarnitine	32198	C02571	HMDB00201	1		5080-50-2	2282	204.12
	cis-4-decenoyl carnitine	38178					98930-66-6	1057	314.23
	decanoylcarnitine	33941		HMDB00651	10245190		1492-27-9	1130	316.25
	hexanoylcarnitine	32328		HMDB00705	6426853		6920-35-0	3308	260.19
	linoleoylcarnitine*	46223		HMDB06469	6450015		36816-10-1	1430	424.34
	myristoleoylcarnitine*	48182					889848-55-9	1316	370.29
	myristoylcarnitine	33952		HMDB05066	53477791		18822-89-4	1350	372.31
	octanoylcarnitine	33936	C02838	HMDB00791	123701		3671-77-0	950	288.22
	oleoylcarnitine	35160		HMDB05065	0		38677-66-6	1423	426.36
	palmitoleoylcarnitine*	53223						1357	398.33
	palmitoylcarnitine	44681	C02990	HMDB00222	461		6865-14-1	1425	400.34
stearoylcarnitine	34409		HMDB00848	6426855		18822-91-8	1485	428.37	
Fatty Acid Metabolism(Acyl Glycine)	N-palmitoylglycine	42092			151008		2441-41-0	5580	312.25
Fatty Acid Synthesis	malonate	15872	C00383	HMDB00691	867		141-82-2;26522-22-85-0	3447	103
Fatty Acid, Amino	2-aminoheptanoate	43761			227939		1115-90-8	3160	146.12
	2-aminooctanoate	43343		HMDB00991	69522		644-90-6	3385	158.12

Fatty Acid, Branched	13-methylmyristate	38293			151014		2485-71-4	5499	241.22
	15-methylpalmitate	38768			17903417			5695	269.25
	17-methylstearate	38296			3083779		2724-59-6	5993	297.28
Fatty Acid, Dicarboxylate	2-hydroxyglutarate	37253	C02630	HMDB00606	43		40951-21-1	3352.8	147.03
	3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)	31787		HMDB61112	123979		86879-39-2	2840	239.09
	3-methylglutarate/2-methylglutarate	54676						2832	145.05
	adipate	21134	C06104	HMDB00448	196		124-04-9	3000	145.05
	azelate (nonanedioate)	18362	C08261	HMDB00784	2266		123-99-9	1276	187.1
	docosadioate	39837			244872		505-56-6	5291.8	369.3
	dodecanedioate	32388	C02678	HMDB00623	12736		693-23-2	2990	229.14
	eicosanodioate	39831			75502		2424-92-2	5200.9	341.27
	hexadecanedioate	35678	C19615	HMDB00672	10459		505-54-4	4615	285.21
	maleate	20676	C01384	HMDB00176	444266		110-16-7	2510	115
	octadecanedioate	36754		HMDB00782	70095		871-70-5	5043	313.24
	sebacate (decanedioate)	32398	C08277	HMDB00792	5192		111-20-6	1788	201.11
	suberate (octanedioate)	15730	C08278	HMDB00893	10457		505-48-6	804.3	173.08
	tetradecanedioate	35669		HMDB00872	13185		821-38-5	4000	257.18
Fatty Acid, Dihydroxy	12,13-DiHOME	38395	C14829	HMDB04705	10236635		263399-35-5	5137	313.24
	9,10-DiHOME	38399	C14828	HMDB04704	9966640		263399-34-4	5180	313.24
Fatty Acid, Keto	1-dihomo-linoleoylglycerol (20:2)	35103						6800	307.26
Fatty Acid, Monohydroxy	13-HODE + 9-HODE	37752			43013			5275	295.23
	16-hydroxypalmitate	39609	C18218	HMDB06294	10466		506-13-8	5236.2	271.23
	2-hydroxydecanoate	42489			21488		5393-81-7	4840	187.13
	2-hydroxylaurate	52916			97783		2984-55-6	5211	215.17
	2-hydroxyoctanoate	22036		HMDB02264	94180		617-73-2	3736.8	159.1
	2-hydroxypalmitate	35675		HMDB31057	92836		764-67-0	5511.2	271.23
	2-hydroxystearate	17945	C03045		69417		629-22-1	5695	299.26
	3-hydroxydecanoate	22053		HMDB02203	26612		5561-87-5	4634.7	187.13
	3-hydroxyhexanoate	53230			151492		10191-24-9	1725	131.07
	3-hydroxylaurate	32457		HMDB00387	94216		53941-38-1	5175	215.17
	3-hydroxyoctanoate	22001		HMDB01954	26613		88930-08-9	3446	159.1
	3-hydroxystearate	52938			5282907		45261-96-9	5674	299.26

Glycerolipid Metabolism	glycerol	15122	C00116	HMDB00131	753		56-81-5	758	91.04
	glycerol 3-phosphate	43847	C00093	HMDB00126	754		29849-82-9	580	173.02
Inositol Metabolism	myo-inositol	1124	C00137	HMDB00211	892		87-89-8	3506.3	225.06
Ketone Bodies	3-hydroxybutyrate (BHBA)	542	C01089	HMDB00357	441		625-72-9	1443.3	103.04
Long Chain Fatty Acid	10-heptadecenoate (17:1n7)	33971		HMDB60038	5312435		29743-97-3	5555	267.23
	10-nonadecenoate (19:1n9)	33972		HMDB13622	5312513		73033-09-7	5780	295.26
	arachidate (20:0)	1118	C06425	HMDB02212	10467		506-30-9	6295	311.3
	eicosenoate (20:1)	33587		HMDB02231	5282768			5950	309.28
	erucate (22:1n9)	1552	C08316	HMDB02068	5281116		112-86-7	6355.6	337.31
	margarate (17:0)	1121		HMDB02259	10465		506-12-7	5731	269.25
	myristate (14:0)	1365	C06424	HMDB00806	11005		544-63-8	5440	227.2
	myristoleate (14:1n5)	32418	C08322	HMDB02000	5281119		544-64-9	5346.9	225.19
	nonadecanoate (19:0)	1356	C16535	HMDB00772	12591		646-30-0	6068	297.28
	oleate/vaccenate (18:1)	52285						5655	281.25
	palmitate (16:0)	1336	C00249	HMDB00220	985		57-10-3	5618	255.23
	palmitoleate (16:1n7)	33447	C08362	HMDB03229	445638		373-49-9	5475	253.22
	pentadecanoate (15:0)	1361	C16537	HMDB00826	13849		1002-84-2;10002-84-2	5521	241.22
stearate (18:0)	1358	C01530	HMDB00827	5281		57-11-4	5872	283.26	
Lysolipid	1-arachidonoyl-GPA (20:4)	46325					799268-65-8	5499	457.24
	1-arachidonoyl-GPC (20:4n6)*	33228	C05208	HMDB10395				1460	544.34
	1-arachidonoyl-GPE (20:4n6)*	35186		HMDB11517	42607465			1450	502.29
	1-arachidonoyl-GPI (20:4)*	34214		HMDB61690				5482	619.29
	1-linolenoyl-GPC (18:3)*	45951						1422	518.32
	1-linoleoyl-GPA (18:2)*	52690		HMDB07856				5483	433.24
	1-linoleoyl-GPC (18:2)	34419	C04100	HMDB10386	11988421			1465	520.34
	1-linoleoyl-GPE (18:2)*	36600		HMDB11507	52925130			1482	478.29
	1-linoleoyl-GPI (18:2)*	36594						5494	595.29
	1-oleoyl-GPA (18:1)	36812			5497152		325465-93-8	1635	437.27
	1-oleoyl-GPC (18:1)	48258		HMDB02815	16081932		19420-56-5	1540	522.36

	1-oleoyl-GPE (18:1)	35628		HMDB11506	9547071		89576-29-4	1554	480.31
	1-oleoyl-GPI (18:1)*	36602						5599	597.3
	1-palmitoleoyl-GPC (16:1)*	33230		HMDB10383	24779461			1450	494.32
	1-palmitoyl-GPA (16:0)	34428	C04036	HMDB00327	6419701		17618-08-5	5600	409.24
	1-palmitoyl-GPC (16:0)	33955		HMDB10382	86554		17364-16-8	1525	496.34
	1-palmitoyl-GPE (16:0)	35631		HMDB11503	9547069		53862-35-4	1544	454.29
	1-palmitoyl-GPI (16:0)*	35305		HMDB61695				5564	571.29
	1-stearoyl-GPE (18:0)	42398		HMDB11130	9547068		69747-55-3	1626	482.32
	1-stearoyl-GPI (18:0)	19324		HMDB61696			796963-93-4	1700	601.33
	2-palmitoleoyl-GPC (16:1)*	35819						1425	494.32
	2-palmitoyl-GPC (16:0)*	35253		HMDB61702	15061532			1505	496.34
	2-stearoyl-GPE (18:0)*	41220						6350	480.31
Lysoplasmalogen	1-(1-enyl-oleoyl)-GPE (P-18:1)*	44621						1566	464.31
	1-(1-enyl-palmitoyl)-GPC (P-16:0)*	52474			10917802			1547	480.34
	1-(1-enyl-palmitoyl)-GPE (P-16:0)*	39270						1558	438.3
	1-(1-enyl-stearoyl)-GPE (P-18:0)*	39271						1649	466.33
Medium Chain Fatty Acid	10-undecenoate (11:1n1)	32497					1333-28-4	5085.8	183.14
	5-dodecenoate (12:1n7)	33968		HMDB00529	5312378		2430-94-6	5224	197.15
	caprate (10:0)	1642	C01571	HMDB00511	2969		112-37-8	5090.7	171.14
	laurate (12:0)	1645	C02679	HMDB00638	3893		143-07-7	5300	199.17
	undecanoate (11:0)	12067	C17715	HMDB00947	8180		334-48-5	5219.2	185.15
Mevalonate Metabolism	3-hydroxy-3-methylglutarate	531	C03761	HMDB00355	1662		503-49-1	2700	161.05
Monoacylglycerol	1-arachidonylglycerol (20:4)	34397	C13857	HMDB11572	5282281		35474-99-8	6250	303.23
	1-dihomo-linolenylglycerol (20:3)	48341						6220	305.25
	1-docosahexaenoylglycerol (22:6)	35153		HMDB11587				6150	309.22
	1-linoleoylglycerol (18:2)	27447			5283469		2277-28-3	6477	279.23
	1-myristoylglycerol (14:0)	35625	C01885	HMDB11561	79050		75685-84-6	6353.3	227.2
	1-oleoylglycerol (18:1)	21184		HMDB11567	5283468		111-03-5	6500	281.25
	1-palmitoleoylglycerol (16:1)*	52431						6094	253.22
	1-palmitoylglycerol (16:0)	21127		HMDB31074	14900		542-44-9	6400	255.23
	1-pentadecanoylglycerol (15:0)	47898			190750		104140-07-0	6200	241.22
	2-arachidonoylglycerol (20:4)	19266	C13856	HMDB04666	5282280		53847-30-6	6170	303.23

	2-linoleoylglycerol (18:2)	32506		HMDB11538	5365676		3443-82-1	6250	279.23
	2-oleoylglycerol (18:1)	21232			5319879		3443-84-3	6300	281.25
	2-palmitoylglycerol (16:0)	33419		HMDB11533	123409		23470-00-0	6300	255.23
Phospholipid Metabolism	1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)*	52710						1969	806.57
	1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)*	53176						1939	780.55
	1-oleoyl-2-linoleoyl-GPC (18:1/18:2)*	52453						2165	784.59
	1-oleoyl-2-linoleoyl-GPE (18:1/18:2)*	52687		HMDB05349	9546753			2270	742.54
	1-palmitoleoyl-2-linoleoyl-GPC (16:1/18:2)*	52683						2003	756.55
	1-palmitoyl-2-alpha-linolenoyl-GPC (16:0/18:3n3)*	52684						2034	756.55
	1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	52462			10747814		35418-58-7	2091	782.57
	1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*	52464		HMDB05323	9546800			2198	740.52
	1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*	52467						2567	876.56
	1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	42449		HMDB05322	9546747			2275	716.52
	1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)	52450						2730	852.56
	1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	52461			6436017		26853-31-6;26853-31-6	2358	760.59
	1-palmitoyl-2-oleoyl-GPE (16:0/18:1)	19263		HMDB05320	5283496		26662-94-2	2509	718.54
	1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*	52669						3140	854.58
	1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*	52470						2160	732.55
	1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	52616					59403-51-9	2653	762.6
	1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	42450			16219824		35418-59-8	2300	810.6
	1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	52447			5289133			2424	768.55
	1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	52449						3000	904.59
	1-stearoyl-2-linoleoyl-GPE (18:0/18:2)*	52446			9546749			2522	744.55
	1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	52468						3185	880.59
	1-stearoyl-2-oleoyl-GPC (18:0/18:1)	52438					56421-10-4	2644	788.62
	1-stearoyl-2-oleoyl-GPE (18:0/18:1)	42448						2858	746.57
	1-stearoyl-2-oleoyl-GPI (18:0/18:1)*	52726						3711	882.61
	1,2-dilinoeoyl-GPC (18:2/18:2)	52603			5288075		998-06-1	2006	782.57
	1,2-dilinoeoyl-GPE (18:2/18:2)*	53174			9546812			2083	740.52
	1,2-dioleoyl-GPC (18:1/18:1)*	52457			10350317		4235-95-4	2346	786.6
	1,2-dioleoyl-GPE (18:1/18:1)	52609			9546757		5/1/04	2485	744.55
	1,2-dipalmitoyl-GPC (16:0/16:0)	19130		HMDB00564	452110		63-89-8	2365	734.57
	arachidonoylcholine	53261						1390	390.34

	choline	15506	C00114	HMDB00097	305		67-48-1	1961	104.11
	choline phosphate	34396	C00588	HMDB01565	1014		72556-74-2	700	184.07
	dihomo-linolenoyl-choline	53262						1424	392.35
	docosahexaenoylcholine	53263						1378	414.34
	glycerophosphoethanolamine	37455	C01233	HMDB00114	123874		33049-08-0	659	216.06
	glycerophosphoinositol*	47155					16824-65-0	3850	333.06
	glycerophosphorylcholine (GPC)	15990	C00670	HMDB00086	71920		28319-77-9	672	258.11
	oleoylcholine	53260						1449	368.35
	palmitoleoylcholine	53257						1385	340.32
	trimethylamine N-oxide	40406	C01104	HMDB00925	1145		1184-78-7	2100	76.08
Plasmalogen	1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*	52689						2154	766.57
	1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	52673						2270	724.53
	1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	52682						2226	742.57
	1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*	52677						2351	700.53
	1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	52478						2443	744.59
	1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)*	52477						2600	702.54
	1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*	52713						2218	716.56
	1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*	52716			11146967			2454	718.57
	1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	52475		HMDB05779	9547058			2511	752.56
	1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)*	52748						2633	728.56
1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	52614					144371-68-6	2950	730.57	
Polyunsaturated Fatty Acid (n3 and n6)	adrenate (22:4n6)	32980	C16527	HMDB02226	5497181		2091-25-0	5678	331.26
	arachidonate (20:4n6)	1110	C00219	HMDB01043	444899		506-32-1	5535	303.23
	dihomo-linoleate (20:2n6)	17805	C16525	HMDB05060	6439848		2091-39-6	5730	307.26
	dihomo-linolenate (20:3n3 or n6)	35718	C03242	HMDB02925	5280581		17046-59-2	5596	305.25
	docosadienoate (22:2n6)	32415	C16533	HMDB61714	5282807		7370-49-2	6034	335.3
	docosahexaenoate (DHA; 22:6n3)	44675	C06429	HMDB02183	445580		6217-54-5	5525	327.23
	docosapentaenoate (n3 DPA; 22:5n3)	32504	C16513	HMDB01976	6441454		2234-74-4	5571	329.25
	docosapentaenoate (n6 DPA; 22:5n6)	37478	C16513	HMDB01976	6441454		25182-74-5	5624.5	329.25
	eicosapentaenoate (EPA; 20:5n3)	18467	C06428	HMDB01999	446284		10-2005-9;10417-94-4	5450	301.22
	linoleate (18:2n6)	1105	C01595	HMDB00673	5280450		60-33-3	5535	279.23
	linolenate [alpha or gamma; (18:3n3 or 6)]	34035	C06426	HMDB03073	5280934			5450	277.22
	mead acid (20:3n9)	35174		HMDB10378	5312531		20590-32-3	5650	305.25

	stearidonate (18:4n3)	33969	C16300	HMDB06547	5312508		111174-40-4	5395	275.2
Primary Bile Acid Metabolism	chenodeoxycholate	1563	C02528	HMDB00518	10133		474-24-9;474-25-9	5264	391.29
	cholate	22842	C00695	HMDB00619	221493		81-25-4	5165	407.28
	glycochenodeoxycholate	32346	C05466	HMDB00637	12544		16564-43-5	5236.1	448.31
	glycochenodeoxycholate sulfate	52974						4820	263.63
	glycocholate	18476	C01921	HMDB00138	10140		475-31-0;863-57-0	5163	464.3
	taurochenodeoxycholate	18494	C05465	HMDB00951	387316		6009-98-9	5250	498.29
Secondary Bile Acid Metabolism	deoxycholate	1114	C04483	HMDB00626	222528		83-44-3	5294	391.29
	glycocholate sulfate*	32599						4750	254.62
	glycodeoxycholate	18477	C05464	HMDB00631	3035026		360-65-6	5281	448.31
	glycodeoxycholate sulfate	52975						4875	263.63
	glycolithocholate sulfate*	32620	C11301	HMDB02639	72222		15324-64-8	5011	255.63
	glycoursodeoxycholate	39379		HMDB00708	12310288		64480-66-6	5033	448.31
	taurocholate sulfate	32807						4750	279.61
	taurodeoxycholate	12261	C05463	HMDB00896	2733768		207737-97-1	5257.4	498.29
	tauroolithocholate 3-sulfate	36850	C03642	HMDB02580	440071		64936-83-0	5026.7	280.62
	ursodeoxycholate	1605	C07880	HMDB00946	31401		128-13-2	5055	391.29
Sphingolipid Metabolism	behenoyl dihydrosphingomyelin (d18:0/22:0)*	57331						3150	789.68
	behenoyl sphingomyelin (d18:1/22:0)*	48492						3083	787.67
	glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	53013						2623	700.57
	glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	52234						3053	728.6
	lactosyl-N-nervonoyl-sphingosine (d18:1/24:1)*	57370						3778	972.73
	lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)	53010					4201-62-1	2527	862.63
	lignoceroyl sphingomyelin (d18:1/24:0)	57330					60037-60-7	3437	815.7
	myristoyl dihydrosphingomyelin (d18:0/14:0)*	57365						2060	677.56
	N-behenoyl-sphingadienine (d18:2/22:0)*	57372						3911	620.6
	N-palmitoyl-sphinganine (d18:0/16:0)	52604		HMDB11760	5283572		5966-29-0	3090	540.54
	N-palmitoyl-sphingosine (d18:1/16:0)	44877		HMDB04949	5283564		24696-26-2	2893	538.52
	N-stearoyl-sphingosine (d18:1/18:0)*	54979		HMDB04950	5283565		104404-17-3	3392	566.55
	palmitoyl dihydrosphingomyelin (d18:0/16:0)*	52434			9939965			2290	705.59
	palmitoyl sphingomyelin (d18:1/16:0)	37506			9939941		6254-89-3	2168	703.57
	sphinganine	17769	C00836	HMDB00269	3126		3102-56-5	1413	302.31
	sphinganine-1-phosphate	52605		HMDB01383	520		19794-97-9	1431	382.27

	sphingomyelin (d18:1/14:0, d16:1/16:0)*	42463			11433862		1998	675.54
	sphingomyelin (d18:1/15:0, d16:1/17:0)*	52433				121999-58-4	2082	689.56
	sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)	52615				121999-64-2	2312	717.59
	sphingomyelin (d18:1/18:1, d18:2/18:0)	37529			6443882	108392-10-5	2167	729.59
	sphingomyelin (d18:1/20:0, d16:1/22:0)*	48490					2685	759.64
	sphingomyelin (d18:1/20:1, d18:2/20:0)*	48491				222403-67-0	2383	757.62
	sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*	52495					2793	773.65
	sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*	48493					2666	785.65
	sphingomyelin (d18:1/24:1, d18:2/24:0)*	47153				94359-13-4	3033	813.68
	sphingomyelin (d18:2/14:0, d18:1/14:1)*	47154					1860	673.53
	sphingomyelin (d18:2/16:0, d18:1/16:1)*	42459					2002	701.56
	sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*	52435					2845	799.67
	sphingomyelin (d18:2/24:1, d18:1/24:2)*	52437					2635	811.67
	sphingosine	17747	C00319	HMDB00252	5353955	123-78-4	1393	300.29
	sphingosine 1-phosphate	34445	C06124	HMDB00277	5283560	26993-30-6	1850	378.24
	stearoyl sphingomyelin (d18:1/18:0)	19503	C00550	HMDB01348	6453725	85187-10-6;85187-10-6	2400	731.61
	tricosanoyl sphingomyelin (d18:1/23:0)*	52436					3200	801.68
Steroid	16a-hydroxy DHEA 3-sulfate	38168					4240	383.15
	21-hydroxypregnenolone disulfate	46115	C05485	HMDB04026	134595	1164-98-3	3935	245.07
	4-androsten-3alpha,17alpha-diol monosulfate (2)	37207					4712	369.17
	4-androsten-3alpha,17alpha-diol monosulfate (3)	37209					5180	369.17
	4-androsten-3beta,17beta-diol disulfate (1)	37202	C04295	HMDB03818	10634		3740	224.06
	4-androsten-3beta,17beta-diol disulfate (2)	37203	C04295	HMDB03818	10634		4065	224.06
	4-androsten-3beta,17beta-diol monosulfate (1)	37211		HMDB03818		521-17-5	4500	369.17
	4-androsten-3beta,17beta-diol monosulfate (2)	37210					4500	369.17
	5alpha-androstan-3alpha,17beta-diol monosulfate (1)	37186					4925	371.19
	5alpha-androstan-3beta,17beta-diol disulfate	37190	C12525	HMDB00493	242332	571-20-0	3880	225.07
	5alpha-androstan-3beta,17beta-diol monosulfate (2)	37192					4685	371.19
	5alpha-pregnan-3beta,20alpha-diol disulfate	37198					3962	239.09
	5alpha-pregnan-3beta,20alpha-diol monosulfate (2)	37200					5060	399.22
	5alpha-pregnan-3beta,20beta-diol monosulfate (1)	37196					5180	399.22
	andro steroid monosulfate (1)*	32827	C04555	HMDB02759			3871	383.15

		androsterone sulfate	31591		HMDB02759	159663		2479-86-9	5022	369.17	
		cortisol	1712	C00735	HMDB00063	5754		50-23-7	4713.2	361.2	
		cortisone	1769	C00762	HMDB02802	222786		53-06-5	4572.5	359.19	
		dehydroisoandrosterone sulfate (DHEA-S)	32425	C04555	HMDB01032	12594		651-48-9	4745	367.16	
		epiandrosterone sulfate	33973	C07635	HMDB00365			22229-22-7	4855	369.17	
		etiocholanolone glucuronide	47112					9/3/02	4915	465.25	
		pregn steroid monosulfate*	32619					1247-64-9	5000	397.21	
		pregnen-diol disulfate*	32562						3868	238.08	
		pregnenolone sulfate	38170		HMDB00774	105074		1247-64-9	5100	395.19	
	Sterol	3-hydroxy-5-cholestenoic acid	54805					6561-58-6	5398	415.32	
		4-cholesten-3-one	38125	C00599	HMDB00921	91477		601-57-0	2520	385.35	
		7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)	36776	C17337	HMDB12458	3081085		115538-85-7	5288.1	429.3	
		cholesterol	63	C00187	HMDB00067	11025495		57-88-5	2707	369.35	
	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	allantoin	1107	C02350	HMDB00462	204		97-59-6	1672	157.04
			hypoxanthine	3127	C00262	HMDB00157	790		68-94-0	1291.2	135.03
			inosine	1123	C00294	HMDB00195	6021		58-63-9	1602.1	267.07
			N1-methylinosine	48351		HMDB02721	65095		20245-33-4	1430	283.1
urate			1604	C00366	HMDB00289	1175		69-93-2;120K5305	757.1	167.02	
xanthine			3147	C00385	HMDB00292	1188		69-89-6	1032	153.04	
Purine Metabolism, Adenine containing		N1-methyladenosine	15650	C02494	HMDB03331	27476		15763-06-1	2120	282.12	
		N6-carbamoylthreonyladenosine	35157		HMDB41623	161466		24719-82-2	2164	411.13	
Purine Metabolism, Guanine containing		7-methylguanine	35114	C02242	HMDB00897	11361		578-76-7	2175	166.07	
Pyrimidine Metabolism, Orotate containing		orotate	1505	C00295	HMDB00226	967		50887-69-9	1638.1	155.01	
		orotidine	35172	C01103	HMDB00788	92751		314-50-1	2250	287.05	
Pyrimidine Metabolism, Thymine containing		3-aminoisobutyrate	1566	C05145	HMDB03911	64956		10569-72-9;214139-20-5	2215	104.07	
		5,6-dihydrothymine	1418	C00906	HMDB00079	93556		696-04-8	1280	129.07	
Pyrimidine Metabolism, Uracil containing		3-ureidopropionate	3155	C02642	HMDB00026	111		462-88-4	875	133.06	
		5-methyluridine (ribothymidine)	35136		HMDB00884	445408		1463-10-1	1778.1	257.08	
		beta-alanine	55	C00099	HMDB00056	239		56-41-7;107-95-9	1905	90.05	
		N-acetyl-beta-alanine	37432	C01073		76406		3025-95-4	773	130.05	
	pseudouridine	33442	C02067	HMDB00767	15047		1445-07-4	1100	243.06		
	uridine	606	C00299	HMDB00296	6029		58-96-8	1457.6	243.06		

Peptide	Acetylated Peptides	phenylacetylglutamate	52925		HMDB59772	11579826		1630	264.09	
		phenylacetylglutamine	35126	C04148	HMDB06344	92258		28047-15-6	2330	263.1
	Dipeptide	glycylvaline	18357		HMDB28854	97417		1963-21-9	2734	175.11
		histidylalanine	42027			351667		16874-75-2	3014	227.11
		leucylalanine	40010			259321		7298-84-2	2801	203.14
		leucylglutamine*	53061			4305457			1965	258.15
		leucylglycine	40045			79070		686-50-0	2778	189.12
		phenylalanylglycine	41370			98207		721-90-4	2462	221.09
		prolylglycine	40703			0		2578-57-6	2136	173.09
		threonylphenylalanine	31530			0		16875-27-7	2322	265.12
		valylglutamine	42079			5253209		42854-54-6	2295	246.14
		valylglycine	40475		HMDB29127	136487		686-43-1	1506	173.09
		valylleucine	39994		HMDB29131	352039		22906-55-4	3138	231.17
	Dipeptide Derivative	N-acetylcarnosine	43488		HMDB12881	9903482		56353-15-2	2141	269.12
	Gamma-glutamyl Amino Acid	gamma-glutamyl-alpha-lysine	55015			65254			2784	276.16
		gamma-glutamyl-epsilon-lysine	33934		HMDB03869	0		17105-15-6	2717	276.16
		gamma-glutamylalanine	37063		HMDB29142	440103		5875-41-2	1986	219.1
		gamma-glutamylglutamate	36738	C05282	HMDB11737	92865		1116-22-9	1775	277.1
		gamma-glutamylglutamine	2730	C05283	HMDB11738	150914		10148-81-9	1430	276.12
		gamma-glutamylglycine	33949		HMDB11667	165527		1948-29-4	1535	205.08
gamma-glutamylhistidine		18245			7017195		37460-15-4	2740	285.12	
gamma-glutamylisoleucine*		34456		HMDB11170	14253342			2940	261.14	
gamma-glutamylleucine		18369		HMDB11171	151023		2566-39-4	2991	261.14	
gamma-glutamylmethionine		44872		HMDB29155	7009567		17663-87-5	2640	279.1	
gamma-glutamylphenylalanine		33422		HMDB00594	111299		7432-24-8	2992	295.13	
gamma-glutamylserine		54914					5875-35-4	1351	235.09	
gamma-glutamylthreonine		33364		HMDB29159			5652-48-2	1750	249.11	
gamma-glutamyltyrosine		2734		HMDB11741	94340		7432-23-7	1240	309.11	
gamma-glutamylvaline	43829		HMDB11172	7015683		2746-34-1	2700	247.13		

Xenobiotics

Bacterial/Fungal	tartrate (hydroxymalonate)	20693	C02287	HMDB35227	45		80-69-3	610	119
Benzoate Metabolism	2-hydroxyhippurate (salicylurate)	18281	C07588	HMDB00840	10253		487-54-7	2184	194.05
	3-hydroxyhippurate	39600		HMDB06116	450268		1637-75-8	1687	194.05
	3-methoxycatechol sulfate (1)	48763						2163	219
	3-methyl catechol sulfate (1)	46165						2790	203
	4-ethylphenylsulfate	36099	C13637				123-07-9	3580	201.02
	4-hydroxyhippurate	35527		HMDB13678	151012		2482-25-9	1475	194.05
	4-methylcatechol sulfate	46146						2665	203
	4-vinylphenol sulfate	36098	C05627	HMDB04072	6426766		2628-17-3	3320	199.01
	benzoate	15778	C00180	HMDB01870	243		65-85-0	1750	121.03
	catechol sulfate	35320	C00090	HMDB59724	3083879		4918-96-1	1906	188.99
	hippurate	15753	C01586	HMDB00714	464		495-69-2	2106.9	178.05
	methyl-4-hydroxybenzoate sulfate	48429						2873	231
	O-methylcatechol sulfate	46111			22473			2344	203
Chemical	1,2,3-benzenetriol sulfate (2)	48762						1709	204.98
	2-aminophenol sulfate	43266		HMDB61116	181670			1677	188
	2-pyrrolidinone	31675		HMDB02039	12025		616-45-5	1262	86.06
	3-hydroxypyridine sulfate	48448					1955-23-3	1595.5	173.99
	4-hydroxychlorothalonil	48441			34217		28343-61-5	4427	244.91
	6-hydroxyindole sulfate	48698						2498	212
	dimethyl sulfone	43424	C11142	HMDB04983	6213		67-71-0	832	95.02
	N-methylpipercolate	47101			0		41447-17-0	1932	144.1
	O-sulfo-L-tyrosine	45413			514186			990	260.02
	succinimide	41888	C07273		11439		123-56-8	2155	116.04
	sulfate*	46960	C00059	HMDB01448	1118		14808-79-8	616	96.96
Drug	hydroquinone sulfate	35322	C00530	HMDB02434	161220		123-31-9	1395	188.99
	salicylate	1515	C00805	HMDB01895	338		69-72-7	802	137.02
Food Component/Plant	2-keto-3-deoxy-gluconate	48141		HMDB01353	161227		17510-99-5	1900	177.04
	2,3-dihydroxyisovalerate	38276	C04039	HMDB12141	677		1756-18-9	1050	133.05
	4-allylphenol sulfate	37181						3805	213.02
	alliin	41494	C08265	HMDB33592	87310		556-27-4	1470	178.05
	dihydroferulic acid	40481			14340		1135-23-5	1928	195.07

	ergothioneine	37459	C05570	HMDB03045	3032311		58511-63-0	850	230.1
	erythritol	20699	C00503	HMDB02994	222285		149-32-6	1491	167.06
	gluconate	587	C00257	HMDB00625	10690		527-07-1	2922	195.05
	homostachydrine*	33009	C08283	HMDB33433	441447		1195-94-4	1750	158.12
	methyl glucopyranoside (alpha + beta)	46144						1070	193.07
	methyl indole-3-acetate	1584		HMDB29738	74706		1912-33-0	3339	190.09
	N-(2-furoyl)glycine	31536		HMDB00439	21863		5657-19-2;5657-19-2	1525.8	168.03
	phytanate	598	C01607		26840		14721-66-5	5908	311.3
	piperine	33935	C03882	HMDB29377	638024		94-62-2	1168	286.14
	quininate	18335	C00296	HMDB03072	6508		77-95-2	2432.9	191.06
	S-allylcysteine	43239			98280		21593-77-1	2690	162.06
	stachydrine	34384	C10172	HMDB04827	115244		4136-37-2	1440	144.1
	thymol sulfate	36095	C09908	HMDB01878			89-83-8	4410	229.05
Xanthine Metabolism	1-methylurate	34395	C16359	HMDB03099	69726		708-79-2	1900	181.04
	1,3-dimethylurate	32391		HMDB01857	70346		944-73-0	1671.4	195.05
	1,7-dimethylurate	34400	C16356	HMDB11103	91611		33868-03-0	1578.6	195.05
	5-acetylamino-6-amino-3-methyluracil	34424	C16366	HMDB04400	88299		1196153-01-1	1710	197.07
	7-methylurate	39598			69160		612-37-3	1138	181.04
	7-methylxanthine	34390	C16353	HMDB01991	68374		552-62-5	1350	167.06
	caffeine	569	C07481	HMDB01847	2519		58-08-2	2106	195.09
	paraxanthine	18254	C13747	HMDB01860	4687		611-59-6	2279	179.06
	theobromine	18392	C07480	HMDB02825	5429		83-67-0	1600	181.07
	theophylline	18394	C07130	HMDB01889	2153		58-55-9	1870	181.07