

Metabolomic Changes associated with IDH3 α ex

Heat map of statistically significant biochemicals profiled in this study.

Comparison groups significantly different:



$p \leq 0.05$, group means fold of change ≥ 1.00

$p \leq 0.05$, group means fold of change < 1.00

Comparison groups tr



$0.05 < p < 0$

$0.05 < p < 0$

Pathway Sort Order	Super Pathway	Sub Pathway	Biochemical Name
1		Glycine, Serine and Threonine Metabolism	glycine
2			N-acetylglycine
6			betaine
9			serine
10			N-acetylserine
16			threonine
17			N-acetylthreonine
28		Alanine and Aspartate Metabolism	alanine
30			N-acetylalanine
34			aspartate
35			N-acetylaspartate (NAA)
38			asparagine
39			N-acetylasparagine
40			glutamate
41		glutamine	
42		N-acetylglutamate	
43		N-acetylglutamine	
48		glutamate, gamma-methyl ester	

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Glutamate Metabolism	pyroglutamine*
	N-acetyl-aspartyl-glutamate (NAAG)
	beta-citrylglutamate
	gamma-aminobutyrate (GABA)
	N-methyl-GABA
	S-1-pyrroline-5-carboxylate
Histidine Metabolism	histidine
	1-methylhistidine
	3-methylhistidine
	N-acetylhistidine
	imidazole propionate
	imidazole lactate
	carnosine
	4-imidazoleacetate
Lysine Metabolism	lysine
	N2-acetyllysine
	N6-acetyllysine
	N6,N6,N6-trimethyllysine
	5-(galactosylhydroxy)-L-lysine
	2-aminoadipate
	pipecolate
	5-aminovalerate
	N-trimethyl 5-aminovalerate
Phenylalanine Metabolism	phenylalanine
	N-acetylphenylalanine
	phenyllactate (PLA)
Tyrosine Metabolism	tyrosine
	4-hydroxyphenylpyruvate
	3-(4-hydroxyphenyl)lactate
	phenol sulfate
	o-Tyrosine
	O-methyltyrosine
	N-formylphenylalanine

201		tryptophan
208		C-glycosyltryptophan
212		kynurenine
225		serotonin
232		indolelactate
248		leucine
249		N-acetylleucine
251		4-methyl-2-oxopentanoate
259		isovalerylcarnitine (C5)
266		beta-hydroxyisovalerate
269	Amino Acid	3-methylglutaconate
282		isoleucine
284		N-acetylisoleucine
285		3-methyl-2-oxovalerate
286		alpha-hydroxyisovalerate
288		2-methylbutyrylcarnitine (C5)
290		tiglylcarnitine (C5:1-DC)
295		ethylmalonate
296		methylsuccinate
302		valine
303		N-acetylvaline
305		3-methyl-2-oxobutyrate
308		isobutyrylcarnitine (C4)
310		3-hydroxyisobutyrate
314		methionine
315		N-acetylmethionine
316		N-formylmethionine
318		methionine sulfone
319		methionine sulfoxide
320		N-acetylmethionine sulfoxide
324		S-adenosylmethionine (SAM)
325		S-adenosylhomocysteine (SAH)
326		homocysteine

329		cystathionine
331		cysteine
332		N-acetylcysteine
337		cystine
342		hypotaurine
343		taurine
344		N-acetyltaurine
348		3-sulfo-L-alanine
350		arginine
351		argininosuccinate
354		ornithine
358		citrulline
360		homocitrulline
361		proline
364	Urea cycle; Arginine and Proline Metabolism	dimethylarginine (SDMA + ADMA)
365		N-acetylarginine
368		N-delta-acetylornithine
372		trans-4-hydroxyproline
374		pro-hydroxy-pro
377		N-methylproline
379		N-monomethylarginine
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384	Creatine Metabolism	creatine
385		creatinine
391	Polyamine Metabolism	putrescine
392		spermidine
399		N1,N12-diacetylspermine
400		5-methylthioadenosine (MTA)
401		N-acetylputrescine
407		(N(1) + N(8))-acetylspermidine
409	Guanidino and Acetamido Metabolism	4-guanidinobutanoate
412		glutathione, reduced (GSH)
413		glutathione, oxidized (GSSG)

415			cysteine-glutathione disulfide		
416		Glutathione Metabolism	S-methylglutathione		
418			cysteinylglycine		
420			5-oxoproline		
423			2-hydroxybutyrate/2-hydroxyisobutyrate		
428			4-hydroxy-nonenal-glutathione		
433				gamma-glutamylcysteine	
434		Gamma-glutamyl Amino Acid	gamma-glutamylglutamate		
435			gamma-glutamylglutamine		
436			gamma-glutamylglycine		
438			gamma-glutamylisoleucine*		
439			gamma-glutamylleucine		
441			gamma-glutamyl-epsilon-lysine		
442			gamma-glutamylmethionine		
443			gamma-glutamylphenylalanine		
444			gamma-glutamylthreonine		
446			gamma-glutamyltyrosine		
447			gamma-glutamylvaline		
448			gamma-glutamyl-2-aminobutyrate		
589	Peptide		Dipeptide	glycylisoleucine	
590				glycylleucine	
600		glycylvaline			
624		isoleucylglycine			
642		leucylglycine			
693		phenylalanylglycine			
711		prolylglycine			
752		threonylphenylalanine			
778		tyrosylglycine			
795		valylglycine			
798		valylleucine			
808				leucylglutamine*	
871				Acetylated Peptides	phenylacetylglycine
882					glucose

883		glucose 6-phosphate
884		glucose 1-phosphate
889		fructose 1,6-diphosphate/glucose 1,6-diphosphate/myo-inositol
891		dihydroxyacetone phosphate (DHAP)
895	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	2-phosphoglycerate
896		3-phosphoglycerate
897		phosphoenolpyruvate (PEP)
898		pyruvate
899		lactate
902		glycerate
905		6-phosphogluconate
908		ribose 1-phosphate
909	Pentose Phosphate Pathway	5-phosphoribosyl diphosphate (PRPP)
910		sedoheptulose-7-phosphate
912		ribulose/xylulose 5-phosphate
916		ribose
917		ribitol
918		ribonate
939	Pentose Metabolism	arabitol/xylitol
941		arabonate/xylonate
942		sedoheptulose
943		ribulonate/xylulonate*
956	Disaccharides and Oligosaccharides	lactose
991		fructose
996		mannitol/sorbitol
997		mannose
998	Fructose, Mannose and Galactose Metabolism	mannose-6-phosphate
1007		galactitol (dulcitol)
1008		galactose 1-phosphate
1021		UDP-glucose
1025		UDP-galactose
1026		UDP-glucuronate
1028	Nucleotide Sugar	guanosine 5'-diphospho-fucose

Carbohydrate

1032			UDP-N-acetylglucosamine/galactosamine
1033			cytidine 5'-monophospho-N-acetylneuraminic acid
1044		Aminosugar Metabolism	glucuronate
1048			N-acetylglucosamine 6-phosphate
1049			N-acetyl-glucosamine 1-phosphate
1055			N-acetylneuraminate
1066			N-acetylglucosaminylasparagine
1067			erythronate*
1069			N-acetylglucosamine/N-acetylgalactosamine
1074	Energy	TCA Cycle	citrate
1076			aconitate [cis or trans]
1078			isocitrate
1079			isocitric lactone
1080			alpha-ketoglutarate
1082			succinylcarnitine (C4-DC)
1083			succinate
1084			fumarate
1085			malate
1095			2-methylcitrate/homocitrate
1097		Oxidative Phosphorylation	acetylphosphate
1099			phosphate
1124		Medium Chain Fatty Acid	laurate (12:0)
1125			5-dodecanoate (12:1n7)
1127		Long Chain Fatty Acid	myristate (14:0)
1128			myristoleate (14:1n5)
1131			pentadecanoate (15:0)
1132			palmitate (16:0)
1133			palmitoleate (16:1n7)
1135			margarate (17:0)
1136			10-heptadecenoate (17:1n7)
1138			stearate (18:0)
1140			oleate/vaccenate (18:1)
1147			nonadecanoate (19:0)

1148		10-nonadecenoate (19:1n9)
1151		arachidate (20:0)
1154		eicosenoate (20:1)
1158		behenate (22:0)*
1159		erucate (22:1n9)
1165	Polyunsaturated Fatty Acid (n3 and n6)	heneicosapentaenoate (21:5n3)
1170		stearidonate (18:4n3)
1171		eicosapentaenoate (EPA; 20:5n3)
1172		docosapentaenoate (n3 DPA; 22:5n3)
1173		docosahexaenoate (DHA; 22:6n3)
1177		nisinate (24:6n3)
1178		linoleate (18:2n6)
1180		linolenate [alpha or gamma; (18:3n3 or 6)]
1182		dihomo-linolenate (20:3n3 or n6)
1183		arachidonate (20:4n6)
1184		adrenate (22:4n6)
1185		docosapentaenoate (n6 DPA; 22:5n6)
1186		docosadienoate (22:2n6)
1187		dihomo-linoleate (20:2n6)
1188		linoelaidate (tr 18:2n6)
1189		mead acid (20:3n9)
1190		docosatrienoate (22:3n6)*
1241	Fatty Acid, Branched	13-methylmyristate (i15:0)
1244		15-methylpalmitate (i17:0)
1247		17-methylstearate (i19:0)
1257	Fatty Acid, Dicarboxylate	glutarate (C5-DC)
1261		2-hydroxyglutarate
1268		maleate
1336	Fatty Acid Metabolism (also BCAA Metabolism)	butyrylcarnitine (C4)
1339		propionylcarnitine (C3)
1342		methylmalonate (MMA)
1362		acetylcarnitine (C2)
1364		3-hydroxybutyrylcarnitine (1)

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	3-hydroxybutyrylcarnitine (2)
	valerylcarnitine (C5)
	hexanoylcarnitine (C6)
	octanoylcarnitine (C8)
	decanoylcarnitine (C10)
	5-dodecenoylcarnitine (C12:1)
	laurylcarnitine (C12)
	myristoylcarnitine (C14)
	palmitoylcarnitine (C16)
	palmitoleoylcarnitine (C16:1)*
	stearoylcarnitine (C18)
	linoleoylcarnitine (C18:2)*
	linolenoylcarnitine (C18:3)*
	oleoylcarnitine (C18:1)
	myristoleoylcarnitine (C14:1)*
	arachidoylcarnitine (C20)*
	arachidonoylcarnitine (C20:4)
	behenoylcarnitine (C22)*
	dihomo-linoleoylcarnitine (C20:2)*
	eicosenoylcarnitine (C20:1)*
	docosatrienoylcarnitine (C22:3)*
	docosapentaenoylcarnitine (C22:5n3)*
	lignoceroylcarnitine (C24)*
	margaroylcarnitine (C17)*
	nervonoylcarnitine (C24:1)*
	deoxycarnitine
	carnitine
	3-hydroxybutyrate (BHBA)
	oleoylcholine
	2-hydroxynervonate*
	2-hydroxypalmitate
	3-hydroxydecanoate
	3-hydroxylaurate
Fatty Acid Metabolism(Acyl Carnitine)	
Carnitine Metabolism	
Ketone Bodies	
Fatty Acid Metabolism (Acyl Choline)	
Fatty Acid, Monohydroxy	

1458		3-hydroxymyristate
1459		3-hydroxypalmitate
1489		3-hydroxystearate
1588	Endocannabinoid	oleoyl ethanolamide
1591		palmitoyl ethanolamide
1596		arachidonoyl ethanolamide
1599		N-oleoyltaurine
1600		N-stearoyltaurine
1601		N-palmitoyltaurine
1612		palmitoleoyl ethanolamide*
1620	Inositol Metabolism	myo-inositol
1621		chiro-inositol
1629		inositol 1-phosphate (I1P)
1649	Phospholipid Metabolism	choline
1650		choline phosphate
1651		cytidine 5'-diphosphocholine
1653		glycerophosphorylcholine (GPC)
1655		phosphoethanolamine
1656		cytidine-5'-diphosphoethanolamine
1657		glycerophosphoethanolamine
1658		glycerophosphoserine*
1659		glycerophosphoinositol*
1676	Phosphatidylcholine (PC)	1-myristoyl-2-palmitoyl-GPC (14:0/16:0)
1680		1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)*
1689		1,2-dipalmitoyl-GPC (16:0/16:0)
1690		1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*
1694		1-palmitoyl-2-stearoyl-GPC (16:0/18:0)
1699		1-palmitoyl-2-oleoyl-GPC (16:0/18:1)
1704		1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)
1714		1-palmitoleoyl-2-oleoyl-GPC (16:1/18:1)*
1718		1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)*
1724		1-palmitoyl-2-dihomo-linolenoyl-GPC (16:0/20:3n3 or 6)*
1732		1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)

1748		1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)
1762		1-stearoyl-2-oleoyl-GPC (18:0/18:1)
1768		1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*
1771		1,2-dioleoyl-GPC (18:1/18:1)
1774		1-oleoyl-2-linoleoyl-GPC (18:1/18:2)*
1776		1,2-dilinoleoyl-GPC (18:2/18:2)
1784		1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)
1792		1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)*
1797		1-stearoyl-2-docosahexaenoyl-GPC (18:0/22:6)
1800		1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)*
1808		1,2-dipalmitoyl-GPE (16:0/16:0)*
1813		1-palmitoyl-2-stearoyl-GPE (16:0/18:0)*
1816		1-palmitoyl-2-oleoyl-GPE (16:0/18:1)
1817		1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)
1820		1-palmitoleoyl-2-oleoyl-GPE (16:1/18:1)*
1826		1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*
1830		1-palmitoyl-2-docosahexaenoyl-GPE (16:0/22:6)*
1831		1-stearoyl-2-oleoyl-GPE (18:0/18:1)
1839		1,2-dioleoyl-GPE (18:1/18:1)
1841		1-oleoyl-2-linoleoyl-GPE (18:1/18:2)*
1850		1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)
1851		1-oleoyl-2-arachidonoyl-GPE (18:1/20:4)*
1866		1-stearoyl-2-docosahexaenoyl-GPE (18:0/22:6)*
1868		1-oleoyl-2-docosahexaenoyl-GPE (18:1/22:6)*
1878		1-palmitoyl-2-oleoyl-GPS (16:0/18:1)
1883		1-stearoyl-2-oleoyl-GPS (18:0/18:1)
1889		1-stearoyl-2-arachidonoyl-GPS (18:0/20:4)
1894		1,2-dipalmitoyl-GPG (16:0/16:0)
1899		1-palmitoyl-2-oleoyl-GPG (16:0/18:1)
1904		1-stearoyl-2-oleoyl-GPG (18:0/18:1)
1906		1,2-dioleoyl-GPG (18:1/18:1)
1908		1,2-dipalmitoyl-GPI (16:0/16:0)*
1912		1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*
	Phosphatidylethanolamine (PE)	
	Phosphatidylserine (PS)	
	Phosphatidylglycerol (PG)	

1920	Lipid	Phosphatidylinositol (PI)	1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*	
1925			1-stearoyl-2-oleoyl-GPI (18:0/18:1)*	
1928			1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	
1930			1,2-dioleoyl-GPI (18:1/18:1)	
1943			1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	
1947			1-oleoyl-2-arachidonoyl-GPI (18:1/20:4) *	
1966		Lysophospholipid		1-palmitoyl-GPC (16:0)
1967				2-palmitoyl-GPC (16:0)*
1968				1-palmitoleoyl-GPC (16:1)*
1969				2-palmitoleoyl-GPC (16:1)*
1973				1-stearoyl-GPC (18:0)
1975				1-oleoyl-GPC (18:1)
1978				1-linoleoyl-GPC (18:2)
2005				1-lignoceroyl-GPC (24:0)
2011				1-palmitoyl-GPE (16:0)
2016				1-stearoyl-GPE (18:0)
2017				2-stearoyl-GPE (18:0)*
2018				1-oleoyl-GPE (18:1)
2020				1-linoleoyl-GPE (18:2)*
2027				1-arachidonoyl-GPE (20:4n6)*
2034	1-palmitoyl-GPS (16:0)*			
2035	1-stearoyl-GPS (18:0)*			
2036	1-oleoyl-GPS (18:1)			
2040	1-palmitoyl-GPG (16:0)*			
2042	1-stearoyl-GPG (18:0)			
2044	1-oleoyl-GPG (18:1)*			
2046	1-linoleoyl-GPG (18:2)*			
2047	1-palmitoyl-GPI (16:0)			
2050	1-stearoyl-GPI (18:0)			
2052	1-oleoyl-GPI (18:1)*			
2054	1-linoleoyl-GPI (18:2)*			
2058	1-arachidonoyl-GPI (20:4)*			
2128		Glycolipid Metabolism	galactosylglycerol*	

2151		1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)*
2152		1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*
2153		1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*
2154		1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*
2155		1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*
2157		1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*
2159		1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)
2163		1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*
2164		1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*
2168		1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*
2181		1-(1-enyl-palmitoyl)-GPC (P-16:0)*
2182		1-(1-enyl-palmitoyl)-GPE (P-16:0)*
2184		1-(1-enyl-oleoyl)-GPE (P-18:1)*
2186		1-(1-enyl-stearoyl)-GPE (P-18:0)*
2187		1-(1-enyl-oleoyl)-2-oleoyl-GPE (P-18:1/18:1)*
2189		glycerol
2190		glycerol 3-phosphate
2195		glycerophosphoglycerol
2196		1-myristoylglycerol (14:0)
2198		1-pentadecanoylglycerol (15:0)
2199		1-palmitoylglycerol (16:0)
2200		1-palmitoleoylglycerol (16:1)*
2201		1-margaroylglycerol (17:0)
2203		1-oleoylglycerol (18:1)
2204		1-linoleoylglycerol (18:2)
2208		1-dihomo-linolenylglycerol (20:3)
2209		1-arachidonylglycerol (20:4)
2212		1-docosahexaenoylglycerol (22:6)
2213		2-myristoylglycerol (14:0)
2214		2-palmitoylglycerol (16:0)
2215		2-palmitoleoylglycerol (16:1)*
2217		2-oleoylglycerol (18:1)
2218		2-linoleoylglycerol (18:2)
	Plasmalogen	
	Lysoplasmalogen	
	Glycerolipid Metabolism	
	Monoacylglycerol	

2219		2-arachidonoylglycerol (20:4)
2221		2-docosahexaenoylglycerol (22:6)*
2223		diacylglycerol (12:0/18:1, 14:0/16:1, 16:0/14:1) [1]*
2224		diacylglycerol (12:0/18:1, 14:0/16:1, 16:0/14:1) [2]*
2225		diacylglycerol (14:0/18:1, 16:0/16:1) [1]*
2226		diacylglycerol (14:0/18:1, 16:0/16:1) [2]*
2227		diacylglycerol (16:1/18:2 [2], 16:0/18:3 [1])*
2234		palmitoyl-myristoyl-glycerol (16:0/14:0) [1]*
2235		palmitoyl-myristoyl-glycerol (16:0/14:0) [2]
2238		palmitoyl-palmitoyl-glycerol (16:0/16:0) [1]*
2239		palmitoyl-palmitoyl-glycerol (16:0/16:0) [2]*
2240		palmitoleoyl-palmitoleoyl-glycerol (16:1/16:1) [2]*
2241		palmitoyl-oleoyl-glycerol (16:0/18:1) [1]*
2242		palmitoyl-oleoyl-glycerol (16:0/18:1) [2]*
2244		palmitoyl-linoleoyl-glycerol (16:0/18:2) [2]*
2245		palmitoyl-linolenoyl-glycerol (16:0/18:3) [2]*
2246		palmitoleoyl-oleoyl-glycerol (16:1/18:1) [1]*
2247		palmitoleoyl-oleoyl-glycerol (16:1/18:1) [2]*
2249		palmitoyl-dihomo-linolenoyl-glycerol (16:0/20:3n3 or 6) [2]*
2250		palmitoyl-arachidonoyl-glycerol (16:0/20:4) [1]*
2251		palmitoyl-arachidonoyl-glycerol (16:0/20:4) [2]*
2258		oleoyl-oleoyl-glycerol (18:1/18:1) [1]*
2259		oleoyl-oleoyl-glycerol (18:1/18:1) [2]*
2261		oleoyl-linoleoyl-glycerol (18:1/18:2) [1]
2262		oleoyl-linoleoyl-glycerol (18:1/18:2) [2]
2272		stearoyl-arachidonoyl-glycerol (18:0/20:4) [1]*
2273		stearoyl-arachidonoyl-glycerol (18:0/20:4) [2]*
2275		oleoyl-arachidonoyl-glycerol (18:1/20:4) [2]*
2279		stearoyl-docosahexaenoyl-glycerol (18:0/22:6) [2]*
2304		sphinganine
2306		3-ketosphinganine
2308		N-palmitoyl-sphinganine (d18:0/16:0)
2309		N-palmitoyl-sphingadienine (d18:2/16:0)*
	Diacylglycerol	

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Sphingolipid Metabolism

N-behenoyl-sphingadienine (d18:2/22:0)*
myristoyl dihydrosphingomyelin (d18:0/14:0)*
palmitoyl dihydrosphingomyelin (d18:0/16:0)*
behenoyl dihydrosphingomyelin (d18:0/22:0)*
palmitoyl sphingomyelin (d18:1/16:0)
stearoyl sphingomyelin (d18:1/18:0)
behenoyl sphingomyelin (d18:1/22:0)*
tricosanoyl sphingomyelin (d18:1/23:0)*
lignoceroyl sphingomyelin (d18:1/24:0)
sphingomyelin (d18:1/14:0, d16:1/16:0)*
sphingomyelin (d18:2/14:0, d18:1/14:1)*
sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*
sphingomyelin (d18:2/16:0, d18:1/16:1)*
sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)
sphingomyelin (d18:1/18:1, d18:2/18:0)
sphingomyelin (d18:1/20:0, d16:1/22:0)*
sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*
sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*
sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*
sphingomyelin (d18:1/24:1, d18:2/24:0)*
sphingomyelin (d18:2/24:1, d18:1/24:2)*
sphingosine
phytosphingosine
sphingomyelin (d18:2/23:1)*
sphingomyelin (d18:2/24:2)*
sphingomyelin (d18:1/25:0, d19:0/24:1, d20:1/23:0, d19:1/24:0)
sphingomyelin (d18:1/22:2, d18:2/22:1, d16:1/24:2)*
sphingomyelin (d18:0/20:0, d16:0/22:0)*
sphingomyelin (d18:0/18:0, d19:0/17:0)*
sphingomyelin (d17:2/16:0, d18:2/15:0)*
sphingomyelin (d18:1/19:0, d19:1/18:0)*
heptadecasphingosine (d17:1)
hexadecasphingosine (d16:1)*

2361		N-palmitoyl-heptadecasphingosine (d17:1/16:0)*	
2362		N-stearoyl-sphinganine (d18:0/18:0)*	
2363		sphingadienine	
2373		glycosyl-N-nervonoyl-sphingadienine (d18:2/24:1)*	
2405	Ceramides	N-palmitoyl-sphingosine (d18:1/16:0)	
2407		N-stearoyl-sphingosine (d18:1/18:0)*	
2408		N-stearoyl-sphingadienine (d18:2/18:0)*	
2410		ceramide (d16:1/24:1, d18:1/22:1)*	
2411		ceramide (d18:1/14:0, d16:1/16:0)*	
2412		ceramide (d18:1/17:0, d17:1/18:0)*	
2414		ceramide (d18:2/24:1, d18:1/24:2)*	
2415		glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	
2416		glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	
2417		glycosyl-N-arachidoyl-sphingosine (d18:1/20:0)*	
2419		glycosyl-N-behenoyl-sphingadienine (d18:2/22:0)*	
2422		glycosyl-N-stearoyl-sphinganine (d18:0/18:0)*	
2425		lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)	
2429		glycosyl ceramide (d16:1/24:1, d18:1/22:1)*	
2431		glycosyl ceramide (d18:1/23:1, d17:1/24:1)*	
2439	Mevalonate Metabolism	3-hydroxy-3-methylglutarate	
2454	Sterol	cholesterol	
2497		7-hydroxycholesterol (alpha or beta)	
3266	Purine Metabolism, (Hypo)Xanthine/Inosine containing	inosine 5'-monophosphate (IMP)	
3267		inosine	
3268		hypoxanthine	
3269		xanthine	
3271		xanthosine	
3275		2'-deoxyinosine	
3277		urate	
3278		allantoin	
3283			adenosine 5'-diphosphate (ADP)
3284			adenosine 5'-monophosphate (AMP)
3286		adenosine 2'-monophosphate (2'-AMP)	

3287	Nucleotide	Purine Metabolism, Adenine containing	adenosine 3',5'-cyclic monophosphate (cAMP)
3290			adenylosuccinate
3291			adenosine
3292			adenine
3293			1-methyladenine
3307			N6-carbamoylthreonyladenosine
3309			2'-deoxyadenosine 5'-diphosphate
3310			2'-deoxyadenosine 5'-monophosphate
3315			diadenosine triphosphate
3316			N6-succinyladenosine
3318		Purine Metabolism, Guanine containing	guanosine 5'- diphosphate (GDP)
3319			guanosine 5'- monophosphate (5'-GMP)
3324			guanosine
3325			guanine
3327			7-methylguanine
3341		2'-deoxyguanosine	
3345		Pyrimidine Metabolism, Orotate containing	orotate
3347			orotidine
3350		Pyrimidine Metabolism, Uracil containing	uridine 5'-triphosphate (UTP)
3351			uridine 5'-diphosphate (UDP)
3352			uridine 5'-monophosphate (UMP)
3357			uridine
3358			uracil
3359			pseudouridine
3360			5,6-dihydrouridine
3362			5-methyluridine (ribothymidine)
3373			2'-deoxyuridine
3376			3-ureidopropionate
3377		beta-alanine	
3382		Pyrimidine Metabolism, Cytidine containing	cytidine diphosphate
3383			cytidine 5'-monophosphate (5'-CMP)
3387			cytidine
3395			2'-deoxycytidine 5'-monophosphate

3398			2'-O-methylcytidine	
3403			thymidine 5'-monophosphate	
3407		Pyrimidine Metabolism, Thymine containing	thymidine	
3408			thymine	
3412		Purine and Pyrimidine Metabolism	methylphosphate	
3420	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	nicotinamide	
3422			nicotinamide ribonucleotide (NMN)	
3424			nicotinamide adenine dinucleotide (NAD+)	
3425			nicotinamide adenine dinucleotide reduced (NADH)	
3432			1-methylnicotinamide	
3437			trigonelline (N'-methylnicotinate)	
3441			adenosine 5'-diphosphoribose (ADP-ribose)	
3445			Riboflavin Metabolism	flavin adenine dinucleotide (FAD)
3446				flavin mononucleotide (FMN)
3447			Pantothenate and CoA Metabolism	pantothenate
3449		phosphopantetheine		
3450		3'-dephosphocoenzyme A		
3452		coenzyme A		
3454			pantetheine	
3460		Ascorbate and Aldarate Metabolism	threonate	
3464			gulonate*	
3466		Tocopherol Metabolism	alpha-tocopherol	
3482		Biotin Metabolism	biotin	
3486		Folate Metabolism	5-methyltetrahydrofolate (5MeTHF)	
3491		Pterin Metabolism	pterin	
3503		Hemoglobin and Porphyrin Metabolism	bilirubin (Z,Z)	
3515		Thiamine Metabolism	thiamin (Vitamin B1)	
3523		Vitamin A Metabolism	retinol (Vitamin A)	
3537		Vitamin B6 Metabolism	pyridoxine (Vitamin B6)	
3539			pyridoxamine	
3540			pyridoxamine phosphate	
3541			pyridoxal phosphate	
3542			pyridoxal	

3545	Xenobiotics	Benzoate Metabolism	hippurate
3577			O-methylcatechol sulfate
3612			p-cresol sulfate
3774		Food Component/Plant	gluconate
3793			beta-guanidinopropanoate
3845			ergothioneine
3847			erythritol
3871			homostachydrine*
3906			N-glycolylneuraminate
3961			stachydrine
4217		Drug - Antibiotic	penicillin G
4478		Drug - Other	S-carboxymethyl-L-cysteine
4518		Chemical	sulfate*
4521			O-sulfo-L-tyrosine
4539			2-aminophenol sulfate
4596			lanthionine
4611			phenol red
4623			succinimide
4655	thioprolin		

pression in NHAs

ending towards significant difference:

1.10, group means fold of change ≥ 1.00

1.10, group means fold of change < 1.00

Platform	Comp ID	KEGG	HMDB	PUBCHEM
LC/MS pos early	58	C00037	HMDB00123	750
LC/MS pos early	27710		HMDB00532	10972
LC/MS pos early	3141	C00719	HMDB00043	247
LC/MS pos early	1648	C00065	HMDB00187	5951
LC/MS pos early	37076		HMDB02931	65249
LC/MS pos early	1284	C00188	HMDB00167	6288
LC/MS neg	33939			152204
LC/MS pos early	1126	C00041	HMDB00161	5950
LC/MS neg	1585	C02847	HMDB00766	88064
LC/MS pos early	443	C00049	HMDB00191	5960
LC/MS polar	22185	C01042	HMDB00812	65065
LC/MS pos early	512	C00152	HMDB00168	6267
LC/MS pos early	33942		HMDB06028	99715
LC/MS pos early	57	C00025	HMDB00148	611
LC/MS pos early	53	C00064	HMDB00641	5961
LC/MS pos early	15720	C00624	HMDB01138	70914
LC/MS pos early	33943	C02716	HMDB06029	182230
LC/MS pos early	33487		HMDB61715	68662

Fold of Change		Statistical Values			
Welch's Two-Sample t-Test - Bradford Protein Normalized					
IDH3A KO CTRL KO	OE 6 OE CTRL	IDH3A KO CTRL KO		OE 6 OE CTRL	
		p-value	q-value	p-value	q-value
2.33	0.40	0.0001	0.0001	0.0014	0.0021
0.79	1.07	0.1748	0.0472	0.6842	0.2450
1.59	1.21	0.0030	0.0014	0.0347	0.0236
1.88	0.69	0.0008	0.0005	0.0134	0.0112
0.74	0.99	0.1225	0.0346	0.9449	0.3111
3.02	0.60	0.0000	0.0000	0.0008	0.0013
0.81	0.75	0.0744	0.0226	0.0068	0.0068
1.09	0.77	0.4183	0.1031	0.0582	0.0352
0.84	0.72	0.1151	0.0329	0.0206	0.0159
3.82	0.44	0.0000	0.0000	0.0000	0.0001
1.62	0.67	0.0068	0.0029	0.0137	0.0115
1.55	0.74	0.0034	0.0016	0.0027	0.0035
0.74	1.43	0.1044	0.0302	0.0085	0.0082
2.01	0.38	0.0004	0.0003	0.0001	0.0002
8.41	0.27	0.0000	0.0000	0.0000	0.0000
0.71	0.46	0.0696	0.0215	0.0002	0.0005
1.27	0.73	0.1319	0.0367	0.0938	0.0516
2.89	0.52	0.0001	0.0001	0.0270	0.0196

LC/MS pos early	46225			134508	0.50	2.14	0.0011	0.0007	0.0001	0.0003
LC/MS pos early	35665	C12270	HMDB01067	5255	0.35	1.06	0.0001	0.0001	0.5322	0.2075
LC/MS neg	54923	C20775		72715786	1.27	0.98	0.0840	0.0251	0.8908	0.3005
LC/MS pos early	1416	C00334	HMDB00112	119	4.51	0.65	0.0000	0.0000	0.0002	0.0005
LC/MS pos early	39577	C15987		70703	9.55	1.83	0.0002	0.0001	0.0043	0.0048
LC/MS pos early	42370	C04322	HMDB01301	1196	1.60	0.31	0.0919	0.0271	0.0286	0.0201
LC/MS neg	59	C00135	HMDB00177	6274	2.49	0.71	0.0001	0.0001	0.0063	0.0065
LC/MS pos early	30460	C01152	HMDB00001	92105	5.00	0.59	0.0000	0.0000	0.0005	0.0010
LC/MS neg	15677	C01152	HMDB00479	64969	4.88	0.53	0.0000	0.0000	0.0004	0.0008
LC/MS pos early	33946	C02997	HMDB32055	75619	0.95	1.02	0.6693	0.1560	0.7856	0.2725
LC/MS pos early	40730		HMDB02271	70630	1.90	0.50	0.0000	0.0001	0.0001	0.0003
LC/MS pos early	15716	C05568	HMDB02320	440129	0.20	6.33	0.0000	0.0000	0.0000	0.0000
LC/MS pos early	1768	C00386	HMDB00033	439224	1.28	0.86	0.0363	0.0123	0.0941	0.0516
LC/MS pos early	32349	C02835	HMDB02024	96215	1.47	0.75	0.0048	0.0022	0.0337	0.0232
LC/MS pos early	1301	C00047	HMDB00182	5962	1.09	0.94	0.4843	0.1177	0.6737	0.2430
LC/MS polar	36751	C12989	HMDB00446	92907	0.37	1.34	0.0008	0.0005	0.0242	0.0180
LC/MS polar	36752	C02727	HMDB00206	92832	0.33	2.73	0.0076	0.0032	0.0521	0.0320
LC/MS pos early	1498	C03793	HMDB01325	440120	0.55	1.34	0.0002	0.0002	0.0835	0.0472
LC/MS pos early	43582				2.24	0.75	0.0000	0.0001	0.0338	0.0232
LC/MS polar	6146	C00956	HMDB00510	469	1.34	1.17	0.1934	0.0518	0.3254	0.1397
LC/MS pos early	1444	C00408	HMDB00070	849	1.26	1.33	0.0721	0.0221	0.0709	0.0417
LC/MS pos early	18319	C00431	HMDB03355	138	8.32	0.50	0.0000	0.0000	0.0000	0.0001
LC/MS pos early	57687				1.42	1.18	0.0215	0.0078	0.0935	0.0516
LC/MS pos early	64	C00079	HMDB00159	6140	2.05	0.73	0.0001	0.0001	0.0210	0.0161
LC/MS neg	33950	C03519	HMDB00512	74839	1.25	0.79	0.0171	0.0064	0.0069	0.0069
LC/MS neg	22130	C05607	HMDB00779	3848	1.03	2.51	0.8897	0.1981	0.0086	0.0083
LC/MS pos early	1299	C00082	HMDB00158	6057	2.26	0.77	0.0000	0.0000	0.0282	0.0200
LC/MS neg	1669	C01179	HMDB00707	979	0.83	1.02	0.7209	0.1671	0.8657	0.2933
LC/MS neg	32197	C03672	HMDB00755	9378	0.25	6.09	0.0000	0.0000	0.0000	0.0000
LC/MS neg	32553	C02180	HMDB60015	74426	0.42	1.50	0.0006	0.0004	0.0002	0.0005
LC/MS pos early	43392		HMDB06050	91482	2.04	0.91	0.0060	0.0026	0.8488	0.2896
LC/MS pos early	37451		HMDB14903	76957	2.04	0.56	0.0027	0.0013	0.0100	0.0091
LC/MS neg	48433			759256	0.93	0.83	0.8663	0.1942	0.2771	0.1227

LC/MS pos early	54	C00078	HMDB00929	6305	2.05	0.77	0.0000	0.0000	0.0100	0.0091
LC/MS neg	48782			10981970	1.30	0.80	0.0674	0.0209	0.0298	0.0208
LC/MS pos early	15140	C00328	HMDB00684	161166	6.91	0.39	0.0000	0.0000	0.0000	0.0001
LC/MS pos early	2342	C00780	HMDB00259	5202	13.13	0.19	0.0000	0.0000	0.0000	0.0001
LC/MS neg	18349	C02043	HMDB00671	92904	0.14	12.18	0.0000	0.0000	0.0000	0.0001
LC/MS pos early	60	C00123	HMDB00687	6106	2.42	0.72	0.0000	0.0000	0.0077	0.0075
LC/MS neg	1587	C02710	HMDB11756	70912	1.33	0.63	0.0230	0.0082	0.0003	0.0007
LC/MS neg	22116	C00233	HMDB00695	70	7.38	0.49	0.0001	0.0001	0.0473	0.0298
LC/MS pos early	34407		HMDB00688	6426851	1.21	0.81	0.1922	0.0515	0.0549	0.0333
LC/MS polar	12129		HMDB00754	69362	2.33	0.44	0.0006	0.0004	0.0012	0.0019
LC/MS polar	57747		HMDB00522	1551553	0.69	0.54	0.0083	0.0034	0.0001	0.0004
LC/MS pos early	1125	C00407	HMDB00172	6306	2.61	0.64	0.0000	0.0000	0.0049	0.0053
LC/MS neg	33967		HMDB61684	2802421	1.49	0.69	0.0028	0.0014	0.0006	0.0010
LC/MS neg	15676	C00671	HMDB03736	47	10.46	0.46	0.0001	0.0001	0.0329	0.0228
LC/MS polar	46537		HMDB00407	99823	0.81	1.57	0.3464	0.0878	0.0018	0.0024
LC/MS pos early	45095		HMDB00378	6426901	0.85	1.61	0.3704	0.0928	0.0003	0.0006
LC/MS pos early	35428		HMDB02366	22833596	0.78	1.23	0.0335	0.0114	0.0164	0.0132
LC/MS polar	15765		HMDB00622	11756	0.80	0.41	0.0713	0.0219	0.0000	0.0001
LC/MS polar	15745		HMDB01844	10349	0.42	0.92	0.0007	0.0004	0.3560	0.1506
LC/MS pos early	1649	C00183	HMDB00883	6287	3.04	0.62	0.0000	0.0000	0.0001	0.0003
LC/MS neg	1591		HMDB11757	66789	0.84	0.91	0.0664	0.0206	0.1905	0.0918
LC/MS polar	44526	C00141	HMDB00019	49	9.91	0.44	0.0000	0.0000	0.0526	0.0322
LC/MS pos early	33441		HMDB00736	168379	6.17	1.37	0.0000	0.0000	0.0271	0.0196
LC/MS polar	1549	C06001	HMDB00336	87	1.55	0.46	0.1178	0.0335	0.0351	0.0237
LC/MS pos early	1302	C00073	HMDB00696	6137	2.63	0.65	0.0000	0.0000	0.0153	0.0124
LC/MS neg	1589	C02712	HMDB11745	448580	0.95	0.99	0.6295	0.1478	0.6750	0.2430
LC/MS neg	2829	C03145	HMDB01015	439750	0.46	0.64	0.0000	0.0000	0.0002	0.0005
LC/MS pos early	44878			69961	2.76	0.75	0.0000	0.0000	0.0223	0.0168
LC/MS pos early	18374	C02989	HMDB02005	158980	1.34	0.92	0.0334	0.0114	0.3816	0.1582
LC/MS pos early	45428			193368	0.41	1.46	0.0000	0.0001	0.0798	0.0454
LC/MS pos early	15915	C00019	HMDB01185	34756	1.34	0.58	0.0992	0.0290	0.0013	0.0020
LC/MS neg	42382	C00021	HMDB00939	439155	0.61	1.17	0.0135	0.0053	0.1700	0.0853
LC/MS pos early	15128	C00155	HMDB00742	778	0.28	1.00	0.0000	0.0000	0.9609	0.3153

LC/MS pos early	15705	C02291	HMDB00099	439258	2.29	1.33	0.0002	0.0001	0.0428	0.0275
LC/MS pos early	1868	C00097	HMDB00574	5862	3.82	0.62	0.0000	0.0000	0.0278	0.0199
LC/MS pos early	1586	C06809	HMDB01890	12035	1.15	0.60	0.6242	0.1468	0.0246	0.0182
LC/MS polar	56	C00491	HMDB00192	67678	2.95	0.47	0.0392	0.0131	0.0514	0.0319
LC/MS pos early	590	C00519	HMDB00965	107812	2.92	0.66	0.0000	0.0000	0.0014	0.0020
LC/MS pos early	2125	C00245	HMDB00251	1123	2.97	0.65	0.0000	0.0000	0.0072	0.0072
LC/MS neg	48187			159864	1.01	0.71	0.9366	0.2071	0.0043	0.0048
LC/MS polar	47089	C00506	HMDB02757	72886	1.88	0.42	0.0201	0.0073	0.0004	0.0007
LC/MS pos early	1638	C00062	HMDB00517	232	0.95	1.04	0.5795	0.1376	0.9230	0.3061
LC/MS pos early	15497	C03406	HMDB00052	828	2.37	0.81	0.0055	0.0024	0.1261	0.0663
LC/MS pos early	1493	C00077	HMDB03374	6262	1.34	0.82	0.0178	0.0066	0.1095	0.0585
LC/MS pos early	2132	C00327	HMDB00904	9750	4.18	0.62	0.0003	0.0003	0.1459	0.0752
LC/MS pos early	22138	C02427	HMDB00679	65072	7.61	0.58	0.0001	0.0001	0.0041	0.0048
LC/MS pos early	1898	C00148	HMDB00162	145742	0.58	0.58	0.0010	0.0006	0.0001	0.0002
LC/MS pos early	36808	C03626	HMDB01539	123831	1.47	0.48	0.0099	0.0040	0.0002	0.0005
LC/MS pos early	33953	C02562	HMDB04620	67427	0.75	1.03	0.1442	0.0397	0.8386	0.2869
LC/MS pos early	43249			9920500	3.66	0.59	0.0000	0.0000	0.0026	0.0034
LC/MS pos early	32306	C01157	HMDB00725	5810	1.62	0.89	0.0076	0.0032	0.1859	0.0909
LC/MS pos early	35127		HMDB06695	11673055	0.97	0.78	0.7488	0.1720	0.9996	0.3241
LC/MS pos early	37431			557	1.28	1.31	0.0645	0.0201	0.0199	0.0155
LC/MS pos early	43586	C03884	HMDB29416	132862	1.28	0.79	0.0262	0.0092	0.1882	0.0915
LC/MS pos early	43802	C00581	HMDB00128	763	3.53	1.55	0.0001	0.0001	0.0383	0.0253
LC/MS pos early	27718	C00300	HMDB00064	586	1.21	1.03	0.1639	0.0444	0.8053	0.2779
LC/MS pos early	513	C00791	HMDB00562	588	1.94	0.72	0.0004	0.0003	0.0031	0.0038
LC/MS pos early	1408	C00134	HMDB01414	1045	10.54	0.81	0.0000	0.0000	0.1353	0.0705
LC/MS pos early	485	C00315	HMDB01257	1102	3.26	0.60	0.0000	0.0000	0.0276	0.0198
LC/MS pos early	52987	C03413	HMDB02172	132680	1.00	1.00				
LC/MS pos early	1419	C00170	HMDB01173	439176	1.59	0.51	0.0071	0.0030	0.0005	0.0009
LC/MS pos early	37496	C02714	HMDB02064	122356	40.70	0.19	0.0000	0.0000	0.0002	0.0005
LC/MS pos early	57814				6.71	0.54	0.0000	0.0000	0.0063	0.0065
LC/MS pos early	15681	C01035	HMDB03464	500	1.68	1.32	0.0018	0.0009	0.0794	0.0454
LC/MS pos early	2127	C00051	HMDB00125	124886	2.01	0.47	0.0001	0.0001	0.0004	0.0008
LC/MS pos early	27727	C00127	HMDB03337	65359	1.73	0.55	0.0142	0.0055	0.0118	0.0102

LC/MS pos early	35159		HMDB00656	4247235	3.83	1.37	0.0000	0.0000	0.2239	0.1028
LC/MS neg	33944	C11347		3605667	2.83	0.23	0.0000	0.0000	0.0000	0.0001
LC/MS pos early	35637	C01419	HMDB00078	439498	2.95	0.41	0.0000	0.0000	0.0001	0.0003
LC/MS neg	1494	C01879	HMDB00267	7405	1.77	0.86	0.0041	0.0019	0.0788	0.0452
LC/MS polar	52281				0.74	0.97	0.0677	0.0209	0.8930	0.3005
LC/MS neg	48504				1.50	0.62	0.1289	0.0359	0.0724	0.0422
LC/MS pos early	1778	C00669	HMDB01049	842	3.16	0.48	0.0001	0.0001	0.0030	0.0037
LC/MS pos early	36738	C05282	HMDB11737	92865	1.27	0.78	0.2093	0.0557	0.2272	0.1038
LC/MS pos early	2730	C05283	HMDB11738	150914	51.70	0.14	0.0000	0.0000	0.0000	0.0002
LC/MS pos early	33949		HMDB11667	165527	5.64	0.29	0.0001	0.0001	0.0001	0.0003
LC/MS neg	34457		HMDB11170	14253342	4.98	0.33	0.0000	0.0001	0.0000	0.0000
LC/MS neg	18369		HMDB11171	151023	4.20	0.47	0.0000	0.0000	0.0000	0.0001
LC/MS pos early	33934		HMDB03869	7015685	0.58	1.33	0.0137	0.0054	0.0227	0.0170
LC/MS pos early	44872		HMDB29155	7009567	4.27	0.81	0.0018	0.0009	0.1918	0.0918
LC/MS neg	33422		HMDB00594	111299	5.02	0.35	0.0000	0.0000	0.0002	0.0005
LC/MS pos early	33364		HMDB29159	76078708	3.02	0.88	0.0004	0.0003	0.3622	0.1529
LC/MS neg	2734		HMDB11741	94340	6.01	0.36	0.0000	0.0000	0.0725	0.0422
LC/MS pos early	43829		HMDB11172	7015683	4.73	0.37	0.0002	0.0002	0.0009	0.0014
LC/MS pos early	37092				0.27	1.92	0.0052	0.0023	0.0001	0.0004
LC/MS neg	36659		HMDB28844	88079	0.71	1.66	0.4094	0.1011	0.5795	0.2218
LC/MS neg	34398	C02155	HMDB00759	92843	0.92	1.91	0.9612	0.2110	0.5153	0.2022
LC/MS neg	18357		HMDB28854	97417	0.98	1.20	0.9331	0.2066	0.9947	0.3230
LC/MS neg	40008		HMDB28907	342532	0.50	1.11	0.0000	0.0000	0.6415	0.2355
LC/MS neg	40045		HMDB28929	79070	0.18	2.98	0.0006	0.0004	0.1675	0.0847
LC/MS pos early	41370		HMDB28995	98207	0.77	1.70	0.2287	0.0602	0.4408	0.1781
LC/MS pos early	40703		HMDB11178	6426709	4.93	0.71	0.0000	0.0000	0.0936	0.0516
LC/MS neg	31530		HMDB29068	4099799	0.18	3.92	0.0000	0.0000	0.0878	0.0492
LC/MS neg	41375		HMDB29105	259323	1.35	1.10	0.0974	0.0286	0.8302	0.2848
LC/MS neg	40475		HMDB29127	136487	0.30	2.27	0.0000	0.0000	0.0069	0.0069
LC/MS pos early	39994		HMDB29131	352039	0.19	3.87	0.0010	0.0006	0.1821	0.0899
LC/MS pos early	48189		HMDB28927	4305457	0.33	3.32	0.0732	0.0223	0.2846	0.1252
LC/MS neg	33945	C05598	HMDB00821	68144	0.61	0.89	0.0013	0.0007	0.1035	0.0557
LC/MS polar	20488	C00031	HMDB00122	79025	0.30	1.31	0.0247	0.0088	0.3547	0.1506

LC/MS polar	31260	C00668	HMDB01401	5958	0.38	0.72	0.0043	0.0020	0.1812	0.0899
LC/MS polar	15561	C00103	HMDB01586	65533	0.63	1.86	0.0136	0.0053	0.0268	0.0195
LC/MS neg	46896	C00354			0.33	1.01	0.0170	0.0064	0.6286	0.2335
LC/MS pos early	15522	C00111	HMDB01473	668	0.37	0.50	0.0517	0.0165	0.3811	0.1582
LC/MS polar	35629	C00631	HMDB03391	59	0.11	0.85	0.0000	0.0001	0.3709	0.1562
LC/MS neg	1414	C00597	HMDB00807	724	0.17	1.06	0.0003	0.0002	0.7169	0.2543
LC/MS neg	597	C00074	HMDB00263	1005	0.14	0.92	0.0005	0.0003	0.6019	0.2267
LC/MS polar	22250	C00022	HMDB00243	1060	0.46	0.75	0.0020	0.0010	0.0111	0.0099
LC/MS neg	527	C00186	HMDB00190	612	1.09	1.07	0.4535	0.1105	0.4796	0.1909
LC/MS polar	1572	C00258	HMDB00139	752	0.23	1.16	0.0045	0.0020	0.5552	0.2147
LC/MS neg	15442	C00345	HMDB01316	91493	0.34	1.75	0.0006	0.0004	0.2289	0.1043
LC/MS polar	1763	C00620	HMDB01489	439236	1.39	1.43	0.0147	0.0057	0.1923	0.0918
LC/MS neg	36840	C00119	HMDB00280	7339	0.20	1.00	0.0171	0.0064		
LC/MS neg	35649	C05382	HMDB01068	616	2.95	0.82	0.0007	0.0004	0.7875	0.2727
LC/MS polar	37288	C00199			0.57	0.69	0.1249	0.0352	0.1815	0.0899
LC/MS polar	1471	C00121	HMDB00283	5779	1.43	0.92	0.1146	0.0328	0.7600	0.2665
LC/MS polar	15772	C00474	HMDB00508	6912	2.23	1.09	0.0001	0.0001	0.3447	0.1468
LC/MS polar	27731	C01685	HMDB00867	5460677	1.41	0.58	0.0276	0.0096	0.0003	0.0006
LC/MS polar	48885	C01904		6912	1.26	1.02	0.0729	0.0223	0.8141	0.2803
LC/MS polar	48255				1.75	0.40	0.0191	0.0070	0.0002	0.0005
LC/MS polar	53237		HMDB03219	5459879	5.63	0.53	0.0001	0.0001	0.0275	0.0198
LC/MS polar	61858				0.69	0.95	0.0552	0.0176	0.6748	0.2430
LC/MS polar	567	C00243	HMDB00186	84571	0.39	1.77	0.0020	0.0010	0.0093	0.0086
LC/MS polar	577	C00095	HMDB00660	5984	3.98	1.74	0.0001	0.0001	0.0112	0.0099
LC/MS polar	46142	C00794	HMDB00247	5780	3.17	1.58	0.0001	0.0001	0.0037	0.0044
LC/MS polar	584	C00159	HMDB00169	18950	0.98	0.85	0.9889	0.2149	0.9654	0.3162
LC/MS polar	1469	C00275	HMDB01078	439198	0.54	0.66	0.0188	0.0069	0.1526	0.0781
LC/MS polar	1117	C01697	HMDB00107	11850	1.22	1.07	0.9419	0.2075	0.8270	0.2842
LC/MS polar	15706	C00446	HMDB00645	123912	0.36	1.82	0.0102	0.0041	0.4610	0.1851
LC/MS polar	32344	C00029	HMDB00286	8629	0.93	1.13	0.5640	0.1346	0.2633	0.1177
LC/MS polar	15860	C00052	HMDB00302	18068	1.05	0.92	0.6591	0.1539	0.4884	0.1932
LC/MS neg	2763	C00167	HMDB00935	17473	0.83	0.66	0.2577	0.0670	0.0051	0.0055
LC/MS neg	15903				1.00	0.84	0.8757	0.1956	0.2754	0.1226

LC/MS polar	46148				0.89	1.02	0.4232	0.1041	0.7764	0.2703
LC/MS polar	36831	C00128	HMDB01176	448209	1.28	0.87	0.1159	0.0330	0.3374	0.1440
LC/MS polar	15443	C00191	HMDB00127	444791	2.01	0.73	0.1075	0.0309	0.3962	0.1632
LC/MS polar	15107	C00357	HMDB02817	439219	0.75	0.82	0.0580	0.0184	0.9706	0.3174
LC/MS polar	15741	C04256	HMDB01367	440364	2.50	0.77	0.0000	0.0000	0.0759	0.0438
LC/MS polar	32377	C00270	HMDB00230	439197	0.53	1.17	0.0020	0.0010	0.0460	0.0293
LC/MS pos early	48149	C04540	HMDB00489	123826	0.81	0.99	0.2161	0.0573	0.9116	0.3044
LC/MS polar	42420		HMDB00613	2781043	0.83	0.76	0.1399	0.0387	0.0114	0.0099
LC/MS pos early	46539		HMDB00215	24139	0.55	0.93	0.0050	0.0022	0.7273	0.2565
LC/MS neg	1564	C00158	HMDB00094	311	52.00	0.72	0.0000	0.0000	0.0348	0.0236
LC/MS neg	46173				34.29	0.85	0.0000	0.0000	0.1813	0.0899
LC/MS polar	12110	C00311	HMDB00193	1198	51.49	0.54	0.0001	0.0001	0.0366	0.0245
LC/MS polar	54724			98259	5.84	0.46	0.0001	0.0001	0.0000	0.0001
LC/MS polar	528	C00026	HMDB00208	51	2.85	0.33	0.0008	0.0005	0.0122	0.0104
LC/MS pos early	37058		HMDB61717	71464481	0.46	1.34	0.0041	0.0019	0.0211	0.0161
LC/MS polar	1437	C00042	HMDB00254	1110	7.45	0.42	0.0000	0.0000	0.0002	0.0006
LC/MS polar	1643	C00122	HMDB00134	444972	3.35	0.57	0.0000	0.0000	0.0002	0.0005
LC/MS neg	1303	C00149	HMDB00156	525	2.83	0.63	0.0000	0.0000	0.0003	0.0007
LC/MS neg	52282				0.45	0.83	0.0016	0.0009	0.0470	0.0298
LC/MS polar	15488	C00227	HMDB01494	186	0.40	0.88	0.0180	0.0067	0.7736	0.2698
LC/MS pos early	42109	C00009	HMDB01429	1061	1.26	0.85	0.1079	0.0309	0.2222	0.1025
LC/MS neg	1645	C02679	HMDB00638	3893	0.70	1.18	0.0234	0.0083	0.2245	0.1028
LC/MS neg	33968		HMDB00529	5312378	0.72	0.63	0.7377	0.1698	0.1844	0.0906
LC/MS neg	1365	C06424	HMDB00806	11005	0.50	1.46	0.0022	0.0011	0.3833	0.1586
LC/MS neg	32418	C08322	HMDB02000	5281119	0.55	0.73	0.0008	0.0005	0.0254	0.0187
LC/MS neg	1361	C16537	HMDB00826	13849	0.89	1.36	0.5063	0.1220	0.6379	0.2351
LC/MS neg	1336	C00249	HMDB00220	985	0.99	1.37	0.9482	0.2085	0.2412	0.1094
LC/MS neg	33447	C08362	HMDB03229	445638	0.81	1.12	0.1834	0.0494	0.9109	0.3044
LC/MS neg	1121		HMDB02259	10465	1.59	1.83	0.0128	0.0051	0.2445	0.1107
LC/MS neg	33971		HMDB60038	5312435	2.02	1.47	0.0014	0.0008	0.6210	0.2320
LC/MS neg	1358	C01530	HMDB00827	5281	1.19	1.43	0.2848	0.0736	0.2785	0.1230
LC/MS neg	52285				1.23	1.99	0.1966	0.0525	0.0408	0.0265
LC/MS neg	1356	C16535	HMDB00772	12591	1.58	2.06	0.0132	0.0052	0.2147	0.0995

LC/MS neg	33972		HMDB13622	5312513	2.58	2.74	0.0013	0.0007	0.0632	0.0375
LC/MS neg	1118	C06425	HMDB02212	10467	1.59	1.84	0.0370	0.0124	0.1775	0.0888
LC/MS neg	33587	C16526	HMDB02231	5282768	1.41	4.08	0.0361	0.0122	0.0111	0.0099
LC/MS neg	12125	C08281	HMDB00944	8215	1.95	0.80	0.1077	0.0309	0.3033	0.1319
LC/MS neg	1552	C08316	HMDB02068	5281116	1.34	7.79	0.1557	0.0426	0.0142	0.0118
LC/MS neg	57658			11998573	8.07	1.89	0.0001	0.0001	0.4447	0.1793
LC/MS neg	33969	C16300	HMDB06547	5312508	8.76	1.11	0.0000	0.0000	0.8788	0.2972
LC/MS neg	18467	C06428	HMDB01999	446284	10.34	0.75	0.0000	0.0000	0.1917	0.0918
LC/MS neg	32504	C16513	HMDB06528	6441454	8.43	1.94	0.0000	0.0000	0.3051	0.1323
LC/MS neg	44675	C06429	HMDB02183	445580	5.95	1.20	0.0000	0.0000	0.8627	0.2928
LC/MS neg	57810		HMDB02007	11792612	20.40	2.74	0.0000	0.0000	0.0094	0.0087
LC/MS neg	1105	C01595	HMDB00673	5280450	3.24	1.42	0.0001	0.0001	0.5949	0.2254
LC/MS neg	34035	C06426	HMDB03073	5280934	4.60	1.01	0.0000	0.0000	0.5948	0.2254
LC/MS neg	35718	C03242	HMDB02925	5280581	4.13	1.61	0.0000	0.0001	0.2395	0.1089
LC/MS neg	1110	C00219	HMDB01043	444899	4.61	1.04	0.0000	0.0000	0.6191	0.2318
LC/MS neg	32980	C16527	HMDB02226	5497181	12.20	4.24	0.0000	0.0000	0.0110	0.0099
LC/MS neg	37478	C16513	HMDB01976	6441454	4.94	1.32	0.0000	0.0001	0.4883	0.1932
LC/MS neg	32415	C16533	HMDB61714	5282807	2.37	7.75	0.0020	0.0010	0.0046	0.0051
LC/MS neg	17805	C16525	HMDB05060	6439848	5.85	4.56	0.0001	0.0001	0.0084	0.0082
LC/MS neg	32420	C01595	HMDB06270	5282457	1.00	1.00				
LC/MS neg	35174		HMDB10378	5312531	5.31	1.26	0.0000	0.0000	0.6442	0.2360
LC/MS neg	57467				9.84	8.41	0.0000	0.0000	0.0000	0.0001
LC/MS neg	38293			151014	0.54	1.83	0.0043	0.0020	0.1357	0.0705
LC/MS neg	38768			17903417	0.67	1.74	0.0479	0.0155	0.2244	0.1028
LC/MS neg	38296		HMDB37397	3083779	0.78	2.20	0.1052	0.0304	0.1320	0.0690
LC/MS polar	396	C00489	HMDB00661	743	0.57	0.74	0.0052	0.0023	0.0028	0.0035
LC/MS pos early	52294	C02630	HMDB00606	43	0.23	0.63	0.0000	0.0000	0.0018	0.0025
LC/MS polar	20676	C01384	HMDB00176	444266	4.46	0.41	0.0000	0.0000	0.0000	0.0001
LC/MS pos early	32412	C02862	HMDB02013	439829	1.73	0.60	0.0158	0.0060	0.0001	0.0003
LC/MS pos early	32452	C03017	HMDB00824	107738	1.36	1.06	0.0449	0.0146	0.5199	0.2035
LC/MS polar	1496	C02170	HMDB00202	487	1.54	0.41	0.0181	0.0067	0.0000	0.0001
LC/MS pos early	32198	C02571	HMDB00201	1	2.48	1.12	0.0001	0.0001	0.1680	0.0847
LC/MS pos early	43264		HMDB13127	53481617	1.74	1.30	0.0027	0.0013	0.0065	0.0066

LC/MS pos early	52984		HMDB13127		1.49	1.70	0.0124	0.0049	0.0006	0.0011
LC/MS pos early	34406		HMDB13128	6426903	1.09	2.59	0.4093	0.1011	0.0000	0.0001
LC/MS pos early	32328		HMDB00705	6426853	1.20	1.41	0.1271	0.0356	0.0373	0.0248
LC/MS pos late	33936	C02838	HMDB00791	123701	2.12	1.29	0.0141	0.0055	0.1020	0.0550
LC/MS pos late	33941		HMDB00651	10245190	4.05	0.56	0.0006	0.0004	0.0150	0.0123
LC/MS pos late	61769				2.86	0.32	0.0003	0.0002	0.0000	0.0001
LC/MS pos late	34534		HMDB02250	10427569	3.82	0.88	0.0005	0.0004	0.4135	0.1696
LC/MS pos late	33952		HMDB05066	6426854	1.07	1.50	0.4846	0.1177	0.0592	0.0357
LC/MS pos late	44681	C02990	HMDB00222	461	0.82	1.47	0.1529	0.0420	0.0399	0.0261
LC/MS pos late	53223			71464547	0.89	0.36	0.9651	0.2115	0.0092	0.0086
LC/MS pos late	34409		HMDB00848	6426855	2.03	2.27	0.0023	0.0011	0.0001	0.0002
LC/MS pos late	46223		HMDB06469	6450015	2.99	0.53	0.0044	0.0020	0.1274	0.0668
LC/MS pos late	57511				5.16	0.37	0.0040	0.0019	0.2002	0.0949
LC/MS pos late	35160		HMDB05065	6441392	1.36	0.90	0.1282	0.0359	0.9425	0.3111
LC/MS pos late	48182			90659872	2.13	0.32	0.0023	0.0011	0.0054	0.0057
LC/MS pos late	57513		HMDB06460		3.62	1.69	0.0004	0.0003	0.0042	0.0048
LC/MS pos late	57518				4.97	0.38	0.0009	0.0005	0.0055	0.0058
LC/MS pos late	57514				1.01	1.00	0.3739	0.0929		
LC/MS pos late	57520				4.97	1.29	0.0040	0.0019	0.2559	0.1150
LC/MS pos late	57519				1.94	2.16	0.0270	0.0095	0.0006	0.0010
LC/MS pos late	57527				1.12	1.00	0.3739	0.0929		
LC/MS pos late	57529				15.97	0.74	0.0002	0.0001	0.8619	0.2928
LC/MS pos late	57515				1.00	1.00				
LC/MS pos late	57512		HMDB06210		0.98	1.43	0.9677	0.2115	0.0159	0.0129
LC/MS pos late	57531				2.14	1.07	0.0174	0.0065	0.2073	0.0971
LC/MS pos early	36747	C01181	HMDB01161	134	1.45	1.22	0.0083	0.0034	0.0733	0.0426
LC/MS pos early	15500	C00318	HMDB00062	10917	0.62	2.32	0.0055	0.0024	0.0004	0.0008
LC/MS polar	542	C01089	HMDB00357	441	2.05	1.54	0.1035	0.0301	0.3739	0.1563
LC/MS pos late	53260				2.36	0.87	0.0010	0.0006	0.3091	0.1338
LC/MS neg	61698			5312783	0.94	9.61	0.8477	0.1910	0.0045	0.0050
LC/MS neg	35675		HMDB31057	92836	0.78	0.98	0.2177	0.0577	0.5402	0.2102
LC/MS neg	22053		HMDB02203	26612	0.97	0.89	0.6063	0.1432	0.0864	0.0485
LC/MS neg	32457		HMDB00387	94216	0.76	0.93	0.1004	0.0293	0.4643	0.1859

LC/MS neg	21158			16064	1.00	1.00				
LC/MS neg	27503		HMDB10734	301590	0.33	0.97	0.0000	0.0000	0.6299	0.2335
LC/MS neg	52938			5282907	0.40	0.52	0.0015	0.0009	0.0173	0.0137
LC/MS pos late	38102		HMDB02088	5283454	0.84	1.24	0.0053	0.0023	0.0128	0.0108
LC/MS pos late	38165	C16512	HMDB02100	4671	1.00	0.56	0.9681	0.2115	0.0000	0.0001
LC/MS pos late	32463	C11695	HMDB04080	5281969	2.53	0.73	0.0000	0.0000	0.0087	0.0083
LC/MS neg	39732			6437033	5.32	1.02	0.0001	0.0001	0.5435	0.2110
LC/MS neg	39730			168274	4.90	1.46	0.0002	0.0002	0.6510	0.2367
LC/MS neg	39835				6.00	0.60	0.0000	0.0000	0.0620	0.0369
LC/MS pos late	57541		HMDB13648	9835868	0.53	0.77	0.0000	0.0001	0.0267	0.0195
LC/MS polar	1124	C00137	HMDB00211	892	1.30	2.74	0.2311	0.0606	0.0000	0.0001
LC/MS polar	37112	C19891	HMDB34220		1.00	1.00				
LC/MS polar	43849	C01177	HMDB00213	440194	0.39	1.63	0.0018	0.0010	0.1571	0.0801
LC/MS pos early	15506	C00114	HMDB00097	305	3.25	0.38	0.0001	0.0001	0.0004	0.0007
LC/MS pos early	34396	C00588	HMDB01565	1014	81.55	0.15	0.0000	0.0000	0.0006	0.0010
LC/MS polar	34418	C00307	HMDB01413	13804	2.14	0.62	0.0001	0.0001	0.0001	0.0004
LC/MS pos early	15990	C00670	HMDB00086	71920	1.98	0.59	0.0002	0.0002	0.0002	0.0006
LC/MS neg	1600	C00346	HMDB00224	1015	6.87	0.35	0.0016	0.0009	0.1482	0.0762
LC/MS polar	34410	C00570	HMDB01564	123727	0.88	0.47	0.3457	0.0877	0.0001	0.0003
LC/MS polar	37455	C01233	HMDB00114	123874	1.34	0.53	0.0310	0.0107	0.0001	0.0004
LC/MS pos early	57404			3081457	0.90	0.64	0.5656	0.1348	0.0282	0.0200
LC/MS polar	47155			167572	0.96	1.24	0.8187	0.1855	0.1913	0.0918
LC/MS pos late	19258		HMDB07869	129657	0.73	1.18	0.0408	0.0135	0.1183	0.0629
LC/MS pos late	53195		HMDB07883		2.22	0.63	0.0003	0.0002	0.0006	0.0010
LC/MS pos late	19130	D03585	HMDB00564	452110	1.46	0.79	0.0212	0.0077	0.1124	0.0599
LC/MS pos late	52470		HMDB07969		0.77	0.82	0.0847	0.0252	0.0979	0.0533
LC/MS pos late	52616		HMDB07970		2.53	0.79	0.0016	0.0009	0.3223	0.1388
LC/MS pos late	52461		HMDB07972	6436017	1.11	1.13	0.4036	0.1001	0.2791	0.1230
LC/MS pos late	42446		HMDB07973	5287971	1.75	0.76	0.0058	0.0025	0.0595	0.0358
LC/MS pos late	52458				0.24	1.18	0.0000	0.0000	0.2063	0.0969
LC/MS pos late	53180		HMDB08008		3.15	0.28	0.0000	0.0000	0.0000	0.0000
LC/MS pos late	52454				1.54	1.00	0.0764	0.0231	0.9191	0.3053
LC/MS pos late	52462		HMDB07982	10747814	1.98	0.89	0.0017	0.0009	0.4035	0.1659

LC/MS pos late	52610		HMDB07991	6441886	2.04	1.00	0.0007	0.0004	0.9579	0.3149
LC/MS pos late	52438		HMDB08038		1.16	1.47	0.2837	0.0736	0.0118	0.0102
LC/MS pos late	52452		HMDB08039		1.89	1.08	0.0220	0.0079	0.9288	0.3075
LC/MS pos late	52457			10350317	0.70	1.53	0.0192	0.0070	0.0028	0.0035
LC/MS pos late	52453				1.98	1.00	0.0007	0.0004	0.9874	0.3221
LC/MS pos late	52603		HMDB08138	5288075	1.88	0.94	0.0080	0.0033	0.6225	0.2320
LC/MS pos late	42450		HMDB08048	16219824	4.80	0.78	0.0000	0.0000	0.1700	0.0853
LC/MS pos late	52710		HMDB08147		8.17	0.58	0.0000	0.0000	0.0005	0.0009
LC/MS pos late	52611		HMDB08057		6.26	0.71	0.0000	0.0000	0.0343	0.0234
LC/MS pos late	52697		HMDB08123		2.06	1.31	0.0007	0.0005	0.0719	0.0421
LC/MS pos late	57341		HMDB08923	445468	1.50	0.46	0.0988	0.0290	0.0044	0.0049
LC/MS pos late	57388		HMDB08925	5326793	2.10	0.36	0.0499	0.0160	0.0174	0.0137
LC/MS pos late	19263		HMDB05320	5283496	0.72	0.94	0.0476	0.0154	0.6453	0.2360
LC/MS pos late	42449		HMDB05322	9546747	2.01	0.62	0.0041	0.0019	0.0297	0.0208
LC/MS pos late	52469				0.12	1.18	0.0000	0.0000	0.2098	0.0978
LC/MS pos late	52464		HMDB05323	9546800	1.33	0.77	0.0588	0.0186	0.0798	0.0454
LC/MS pos late	52465		HMDB05324	9546799	1.69	0.89	0.0037	0.0018	0.2874	0.1258
LC/MS pos late	42448		HMDB08993		1.20	1.15	0.2561	0.0667	0.4247	0.1734
LC/MS pos late	52609			9546757	0.71	1.49	0.0359	0.0122	0.0174	0.0137
LC/MS pos late	52687		HMDB05349	9546753	0.93	1.05	0.6490	0.1521	0.6964	0.2484
LC/MS pos late	52447		HMDB09003	5289133	2.59	0.76	0.0003	0.0002	0.0952	0.0521
LC/MS pos late	55041		HMDB09069		1.62	1.07	0.0053	0.0023	0.5785	0.2218
LC/MS pos late	52466		HMDB05334	9546798	1.46	0.92	0.0160	0.0061	0.6064	0.2279
LC/MS pos late	53209				1.06	1.37	0.6747	0.1570	0.0168	0.0135
LC/MS pos late	19261	C13880	HMDB12357	5283499	0.74	0.81	0.0600	0.0189	0.2036	0.0963
LC/MS pos late	19265		HMDB10163	9547087	1.16	1.43	0.3571	0.0898	0.0973	0.0531
LC/MS pos late	52235		HMDB12383		2.26	0.54	0.0006	0.0004	0.0048	0.0052
LC/MS pos late	52625		HMDB10570	11846227	1.57	0.37	0.0119	0.0047	0.0001	0.0005
LC/MS pos late	52448			5283509	1.20	1.08	0.1253	0.0352	0.4404	0.1781
LC/MS pos late	52623				1.76	1.07	0.0007	0.0004	0.3553	0.1506
LC/MS pos late	19142			11846228	1.53	1.58	0.0081	0.0034	0.0206	0.0159
LC/MS pos late	57375		HMDB09778		0.16	0.77	0.0000	0.0000	0.1520	0.0779
LC/MS pos late	52669		HMDB09783		0.38	1.00	0.0001	0.0001	0.9886	0.3221

LC/MS pos late	52467		HMDB09789		0.97	0.56	0.7943	0.1806	0.0016	0.0022
LC/MS pos late	52726				0.48	1.32	0.0002	0.0001	0.0349	0.0236
LC/MS pos late	52468		HMDB09809		2.10	0.95	0.0004	0.0003	0.6087	0.2283
LC/MS pos late	52619		HMDB09837		0.32	1.59	0.0000	0.0001	0.0053	0.0056
LC/MS pos late	52449		HMDB09815		1.62	0.90	0.0043	0.0020	0.3952	0.1632
LC/MS pos late	54994		HMDB09844		1.11	0.95	0.4355	0.1066	0.6499	0.2367
LC/MS pos late	33955		HMDB10382	86554	0.62	0.80	0.0031	0.0015	0.2766	0.1227
LC/MS pos late	35253		HMDB61702	15061532	1.19	0.34	0.2513	0.0656	0.0012	0.0019
LC/MS pos late	33230		HMDB10383	24779461	0.76	0.42	0.0895	0.0265	0.0114	0.0099
LC/MS pos late	35819		HMDB10383		0.39	0.34	0.0003	0.0002	0.0027	0.0035
LC/MS pos late	33961		HMDB10384	497299	1.30	0.71	0.0429	0.0141	0.0285	0.0201
LC/MS pos late	48258		HMDB02815	16081932	0.83	1.06	0.1290	0.0359	0.5924	0.2254
LC/MS pos late	34419	C04100	HMDB10386	11988421	2.53	0.45	0.0020	0.0010	0.0147	0.0121
LC/MS pos late	49617		HMDB10405		1.00	1.06			0.2944	0.1283
LC/MS pos late	35631		HMDB11503	9547069	0.46	0.74	0.0000	0.0000	0.0091	0.0086
LC/MS pos late	42398		HMDB11130	9547068	0.93	0.72	0.5126	0.1233	0.0042	0.0048
LC/MS neg	41220		HMDB11129		0.93	0.97	0.7772	0.1775	0.6544	0.2370
LC/MS pos late	35628		HMDB11506	9547071	0.52	1.11	0.0004	0.0003	0.3257	0.1397
LC/MS neg	32635		HMDB11507	52925130	1.12	1.55	0.4964	0.1201	0.5884	0.2247
LC/MS neg	35186		HMDB11517	42607465	1.99	1.48	0.0484	0.0156	0.5642	0.2168
LC/MS neg	46130			9547100	0.60	0.67	0.1892	0.0508	0.1192	0.0632
LC/MS pos late	45966			9547101	0.70	0.66	0.0370	0.0124	0.0049	0.0053
LC/MS neg	19260		HMDB61694	9547099	0.99	1.50	0.7280	0.1679	0.6537	0.2370
LC/MS neg	45970			3300276	0.66	0.94	0.0788	0.0236	0.5019	0.1973
LC/MS neg	34437				1.27	0.97	0.3214	0.0817	0.4876	0.1932
LC/MS neg	45968				1.04	1.24	0.8594	0.1932	0.8055	0.2779
LC/MS neg	54885				2.22	1.80	0.0041	0.0019	0.2627	0.1177
LC/MS neg	35305		HMDB61695		0.44	1.94	0.0514	0.0165	0.2932	0.1280
LC/MS pos late	19324		HMDB61696		0.73	1.16	0.0899	0.0265	0.4499	0.1810
LC/MS neg	36602				0.49	2.94	0.1535	0.0420	0.0606	0.0363
LC/MS neg	36594				1.89	1.65	0.3009	0.0771	0.6766	0.2430
LC/MS neg	34214		HMDB61690		2.23	1.53	0.0137	0.0054	0.4651	0.1859
LC/MS polar	57345	C05401	HMDB06790	16048618	0.57	1.68	0.0010	0.0006	0.0001	0.0004

LC/MS pos late	52477		HMDB11342		0.33	1.34	0.0000	0.0000	0.0643	0.0380
LC/MS pos late	52677		HMDB11343		0.47	0.71	0.0005	0.0003	0.0608	0.0363
LC/MS pos late	52716		HMDB11206	11146967	1.09	0.65	0.5506	0.1319	0.0077	0.0075
LC/MS pos late	52713		HMDB11207		0.62	0.59	0.0289	0.0100	0.0032	0.0038
LC/MS pos late	52673		HMDB11352		1.08	0.83	0.5670	0.1349	0.1883	0.0915
LC/MS pos late	52478				0.63	0.89	0.0188	0.0069	0.3745	0.1563
LC/MS pos late	52614		HMDB11375		0.42	1.54	0.0006	0.0004	0.0407	0.0265
LC/MS pos late	52689		HMDB11220		4.45	0.73	0.0000	0.0000	0.0519	0.0320
LC/MS pos late	52682		HMDB11211		0.96	0.64	0.9418	0.2075	0.0100	0.0091
LC/MS pos late	52475		HMDB05779	9547058	2.99	1.13	0.0001	0.0001	0.5017	0.1973
LC/MS pos late	52474		HMDB10407	10917802	1.24	0.77	0.0412	0.0136	0.0507	0.0317
LC/MS pos late	39270				0.45	0.76	0.0000	0.0000	0.0087	0.0083
LC/MS pos late	44621				0.50	1.30	0.0000	0.0000	0.0191	0.0149
LC/MS pos late	39271				1.01	1.22	0.8605	0.1932	0.0237	0.0177
LC/MS pos late	54691		HMDB11441		0.35	2.09	0.0001	0.0001	0.0006	0.0010
LC/MS neg	15122	C00116	HMDB00131	753	2.01	1.11	0.0043	0.0020	0.1946	0.0925
LC/MS pos early	43847	C00093	HMDB00126	754	3.75	0.61	0.0026	0.0013	0.1412	0.0730
LC/MS polar	48857	C03274		439964	1.69	0.96	0.0017	0.0009	0.4781	0.1907
LC/MS neg	35625	C01885	HMDB11561	79050	0.30	1.86	0.0001	0.0001	0.1361	0.0705
LC/MS neg	47898			190750	0.33	2.08	0.0002	0.0001	0.1912	0.0918
LC/MS neg	21127		HMDB31074	14900	0.82	2.21	0.3500	0.0883	0.0738	0.0427
LC/MS neg	52431		HMDB11565		0.24	1.24	0.0001	0.0001	0.9439	0.3111
LC/MS neg	34391			107036	0.38	2.16	0.0003	0.0002	0.0883	0.0493
LC/MS neg	21184		HMDB11567	5283468	0.49	3.10	0.0031	0.0015	0.0323	0.0224
LC/MS neg	27447			5283469	0.96	1.79	0.8963	0.1992	0.5626	0.2166
LC/MS neg	48341				0.69	2.16	0.2269	0.0598	0.4268	0.1739
LC/MS neg	34397	C13857	HMDB11549	5282281	1.47	1.45	0.0530	0.0169	0.9144	0.3048
LC/MS neg	35153		HMDB11587		1.72	1.29	0.0088	0.0036	0.9175	0.3053
LC/MS neg	34383		HMDB11530	137938	0.23	2.11	0.0001	0.0001	0.0771	0.0443
LC/MS neg	33419		HMDB11533	123409	0.72	2.58	0.1639	0.0444	0.1195	0.0632
LC/MS neg	52432		HMDB11565		0.14	1.39	0.0000	0.0000	0.6990	0.2488
LC/MS neg	21232		HMDB11537	5319879	0.31	3.32	0.0007	0.0004	0.0427	0.0275
LC/MS neg	32506		HMDB11538	5365676	0.75	1.53	0.1011	0.0294	0.6235	0.2320

LC/MS neg	19266	C13856	HMDB04666	5282280	0.92	1.54	0.7782	0.1775	0.6383	0.2351
LC/MS neg	48675		HMDB11557		1.09	1.23	0.7260	0.1677	0.9107	0.3044
LC/MS pos late	55002				0.50	0.41	0.0029	0.0014	0.0003	0.0007
LC/MS pos late	55001				0.31	0.64	0.0000	0.0000	0.0000	0.0000
LC/MS pos late	54953				0.98	0.59	0.9281	0.2059	0.0027	0.0035
LC/MS pos late	54954				0.75	0.76	0.0418	0.0138	0.0032	0.0039
LC/MS pos late	54966				2.14	0.47	0.0006	0.0004	0.0000	0.0000
LC/MS pos late	61709				0.68	0.88	0.0753	0.0228	0.4218	0.1726
LC/MS pos late	57364		HMDB07095		0.54	1.08	0.0087	0.0036	0.5453	0.2113
LC/MS pos late	54991		HMDB07098		1.20	0.75	0.3492	0.0883	0.1078	0.0578
LC/MS pos late	54990		HMDB07098		0.77	0.82	0.3071	0.0786	0.1941	0.0925
LC/MS pos late	57409				0.46	0.40	0.0005	0.0003	0.0000	0.0001
LC/MS pos late	54943	C13861	HMDB07102		1.93	1.13	0.0019	0.0010	0.2204	0.1019
LC/MS pos late	54942	C13861	HMDB07102		1.21	1.23	0.1431	0.0395	0.0114	0.0099
LC/MS pos late	52634		HMDB07103		3.67	0.53	0.0000	0.0000	0.0002	0.0005
LC/MS pos late	54965		HMDB07105		2.39	0.36	0.0016	0.0009	0.0011	0.0016
LC/MS pos late	52632		HMDB07131	9543694	0.17	0.66	0.0094	0.0039	0.0017	0.0023
LC/MS pos late	52631				0.78	0.80	0.0731	0.0223	0.0150	0.0123
LC/MS pos late	54941				3.31	0.76	0.0000	0.0000	0.0362	0.0243
LC/MS pos late	54957		HMDB07112		6.93	0.48	0.0001	0.0001	0.0031	0.0038
LC/MS pos late	54958		HMDB07112		5.59	0.56	0.0000	0.0000	0.0000	0.0001
LC/MS pos late	54945		HMDB07218		2.01	1.54	0.0017	0.0009	0.0030	0.0038
LC/MS pos late	54946		HMDB07218		1.40	1.71	0.0230	0.0082	0.0002	0.0006
LC/MS pos late	46798		HMDB07219		6.30	0.53	0.0001	0.0001	0.0472	0.0298
LC/MS pos late	46799		HMDB07219		3.48	0.95	0.0000	0.0000	0.3105	0.1341
LC/MS pos late	57450				3.81	0.60	0.0007	0.0004	0.0545	0.0333
LC/MS pos late	57449				3.72	0.75	0.0001	0.0001	0.0125	0.0106
LC/MS pos late	54961		HMDB07228		6.01	0.79	0.0000	0.0000	0.0004	0.0008
LC/MS pos late	57368				6.67	0.68	0.0000	0.0000	0.0010	0.0016
LC/MS pos late	17769	C00836	HMDB00269	3126	1.74	0.35	0.0007	0.0005	0.0000	0.0001
LC/MS pos late	34381	C02934	HMDB01480	631	0.79	0.34	0.1205	0.0341	0.0009	0.0015
LC/MS pos late	52604		HMDB11760	5283572	3.68	0.55	0.0000	0.0000	0.0000	0.0001
LC/MS pos late	57416				0.82	0.52	0.5291	0.1270	0.0374	0.0248

LC/MS pos late	57372				1.87	0.65	0.0007	0.0004	0.0015	0.0022
LC/MS pos late	57365		HMDB12085		2.83	0.53	0.0001	0.0001	0.0022	0.0029
LC/MS pos late	52434			9939965	4.30	0.50	0.0000	0.0000	0.0014	0.0020
LC/MS pos late	57331		HMDB12091		21.89	0.32	0.0001	0.0001	0.0003	0.0006
LC/MS pos late	37506			9939941	1.02	0.84	0.8816	0.1966	0.1855	0.0909
LC/MS pos late	19503	C00550	HMDB01348	6453725	1.22	0.48	0.1631	0.0444	0.0008	0.0014
LC/MS pos late	48492		HMDB12103		1.92	0.55	0.0013	0.0007	0.0007	0.0012
LC/MS pos late	52436		HMDB12105		1.82	0.83	0.0005	0.0003	0.0811	0.0459
LC/MS pos late	57330				2.21	1.77	0.0000	0.0001	0.0000	0.0001
LC/MS pos late	42463		HMDB12097	11433862	0.79	0.61	0.0890	0.0265	0.0015	0.0022
LC/MS pos late	47154				0.50	0.47	0.0008	0.0005	0.0004	0.0007
LC/MS pos late	52433				0.69	1.05	0.0275	0.0096	0.6918	0.2472
LC/MS pos late	42459				0.87	1.03	0.3524	0.0888	0.7586	0.2665
LC/MS pos late	52615				1.65	0.57	0.0161	0.0061	0.0040	0.0047
LC/MS pos late	37529		HMDB12101	6443882	1.05	0.83	0.6512	0.1523	0.1887	0.0915
LC/MS pos late	48490		HMDB12102		2.02	0.28	0.0007	0.0005	0.0000	0.0001
LC/MS pos late	52495				1.98	0.41	0.0002	0.0001	0.0002	0.0006
LC/MS pos late	48493		HMDB12104		1.04	0.57	0.7816	0.1780	0.0012	0.0019
LC/MS pos late	52435				1.40	1.64	0.0405	0.0135	0.0043	0.0048
LC/MS pos late	47153		HMDB12107		1.02	1.70	0.8320	0.1878	0.0004	0.0007
LC/MS pos late	52437				1.10	1.39	0.4316	0.1059	0.0223	0.0168
LC/MS pos late	17747	C00319	HMDB00252	5353955	1.41	0.70	0.0063	0.0027	0.0046	0.0051
LC/MS pos late	1510	C12144	HMDB04610	122121	0.84	0.73	0.2311	0.0606	0.0223	0.0168
LC/MS pos late	57482				0.99	1.18	0.9739	0.2124	0.4324	0.1758
LC/MS pos late	57479				1.92	1.35	0.0047	0.0021	0.0987	0.0535
LC/MS pos late	57478				1.60	1.61	0.0104	0.0042	0.0073	0.0072
LC/MS pos late	57477				0.99	0.61	0.9857	0.2146	0.0111	0.0099
LC/MS pos late	57476				25.40	0.10	0.0001	0.0001	0.0005	0.0009
LC/MS pos late	57473		HMDB12087		25.38	1.00	0.0000	0.0000		
LC/MS pos late	57483				1.12	0.44	0.2944	0.0756	0.0000	0.0002
LC/MS pos late	57475				4.56	0.14	0.0009	0.0005	0.0000	0.0000
LC/MS pos late	57427			5283557	1.48	0.46	0.0075	0.0032	0.0009	0.0015
LC/MS pos late	57428				1.31	0.36	0.0341	0.0116	0.0001	0.0002

LC/MS pos late	57430				1.28	0.37	0.0432	0.0142	0.0000	0.0001
LC/MS pos late	1759			5283573	19.76	0.14	0.0000	0.0000	0.0000	0.0001
LC/MS pos late	57426			6449795	0.77	0.85	0.0893	0.0265	0.0708	0.0417
LC/MS pos late	57451				0.92	2.05	0.3187	0.0812	0.0000	0.0001
LC/MS pos late	44877		HMDB04949	5283564	0.97	0.52	0.7999	0.1815	0.0021	0.0027
LC/MS pos late	54979		HMDB04950	5283565	1.70	0.46	0.0035	0.0017	0.0000	0.0001
LC/MS pos late	57417				0.63	0.76	0.0111	0.0045	0.0426	0.0275
LC/MS pos late	57437				1.40	0.77	0.0155	0.0059	0.0118	0.0102
LC/MS pos late	57432				1.02	0.28	0.7706	0.1767	0.0064	0.0066
LC/MS pos late	57434				2.31	0.47	0.0000	0.0000	0.0003	0.0006
LC/MS pos late	57443				1.31	1.78	0.0270	0.0095	0.0003	0.0006
LC/MS pos late	53013				0.68	0.36	0.0700	0.0216	0.0006	0.0010
LC/MS pos late	52234				0.84	0.26	0.4321	0.1059	0.0002	0.0005
LC/MS pos late	57423			6321358	1.21	0.16	0.1446	0.0398	0.0000	0.0000
LC/MS pos late	57421				1.25	0.55	0.0330	0.0113	0.0003	0.0007
LC/MS pos late	57418			6321364	2.39	0.81	0.0077	0.0032	0.0854	0.0481
LC/MS pos late	53010				0.51	0.42	0.0042	0.0019	0.0001	0.0003
LC/MS pos late	57457				0.53	0.47	0.0001	0.0001	0.0002	0.0005
LC/MS pos late	57448				0.73	0.84	0.0395	0.0132	0.0549	0.0333
LC/MS polar	531	C03761	HMDB00355	1662	4.84	0.32	0.0001	0.0001	0.0004	0.0007
LC/MS pos late	63	C00187	HMDB00067	11025495	1.37	0.68	0.0057	0.0025	0.0011	0.0017
LC/MS pos late	47890		HMDB06119	107722	0.90	0.97	0.5910	0.1401	0.8935	0.3005
LC/MS polar	2133	C00130	HMDB00175	8582	0.43	0.22	0.0027	0.0013	0.0113	0.0099
LC/MS pos early	1123	C00294	HMDB00195	6021	0.93	1.35	0.6055	0.1432	0.0512	0.0319
LC/MS neg	3127	C00262	HMDB00157	790	1.51	0.75	0.0200	0.0073	0.0177	0.0139
LC/MS neg	3147	C00385	HMDB00292	1188	1.54	0.86	0.0290	0.0100	0.1612	0.0818
LC/MS neg	15136	C01762	HMDB00299	64959	2.84	0.34	0.0016	0.0009	0.0382	0.0253
LC/MS neg	15076	C05512	HMDB00071	65058	1.58	0.81	0.0173	0.0065	0.1579	0.0803
LC/MS neg	1604	C00366	HMDB00289	1175	1.14	0.73	0.5561	0.1330	0.0486	0.0305
LC/MS polar	1107	C02350	HMDB00462	204	2.06	0.66	0.0003	0.0002	0.0001	0.0003
LC/MS neg	3108	C00008	HMDB01341	6022	0.56	0.93	0.0151	0.0058	0.5915	0.2254
LC/MS neg	32342	C00020	HMDB00045	6083	1.31	1.06	0.1189	0.0337	0.6001	0.2264
LC/MS neg	36815	C00946	HMDB11617	94136	1.18	1.00	0.2848	0.0736		

LC/MS neg	2831	C00575	HMDB00058	6076	1.08	1.00	0.2922	0.0752	0.9043	0.3036
LC/MS neg	57838	C03794	HMDB00536	195	6.26	0.55	0.0000	0.0000	0.4399	0.1781
LC/MS pos early	555	C00212	HMDB00050	60961	1.72	0.99	0.0024	0.0012	0.9903	0.3222
LC/MS pos early	554	C00147	HMDB00034	190	2.96	0.87	0.0002	0.0002	0.7694	0.2693
LC/MS pos early	1527	C02216	HMDB11599	78821	1.33	0.24	0.1038	0.0301	0.0016	0.0022
LC/MS neg	35157		HMDB41623	161466	0.93	0.98	0.4472	0.1092	0.8394	0.2869
LC/MS neg	15116	C00206	HMDB01508	188966	1.10	1.00	0.3739	0.0929		
LC/MS neg	46333	C00360	HMDB00905	12599	2.23	1.00	0.0026	0.0013		
LC/MS neg	47397	C06197	HMDB01155		0.23	1.41	0.0180	0.0067	0.1839	0.0906
LC/MS neg	48130		HMDB00912	165243	4.69	0.44	0.0000	0.0000	0.0000	0.0001
LC/MS neg	2848	C00035	HMDB01201	8977	0.27	1.00	0.0013	0.0007		
LC/MS pos early	2849	C00144	HMDB01397	6804	0.68	1.61	0.0291	0.0101	0.1226	0.0646
LC/MS neg	1573	C00387	HMDB00133	6802	1.47	1.46	0.0256	0.0091	0.0140	0.0116
LC/MS pos early	32352	C00242	HMDB00132	764	1.44	0.84	0.0483	0.0156	0.2552	0.1149
LC/MS pos early	35114	C02242	HMDB00897	11361	0.95	0.52	0.6801	0.1580	0.0075	0.0074
LC/MS neg	1411	C00330	HMDB00085	187790	2.32	0.86	0.0029	0.0014	0.3286	0.1406
LC/MS polar	1505	C00295	HMDB00226	967	5.43	0.07	0.0001	0.0001	0.0011	0.0017
LC/MS polar	35172		HMDB00788	92751	1.58	0.89	0.0048	0.0022	0.2145	0.0995
LC/MS neg	33448	C00075	HMDB00285	6133	0.03	1.00	0.0005	0.0003		
LC/MS neg	5345	C00015	HMDB00295	6031	0.51	0.61	0.0058	0.0025	0.0003	0.0007
LC/MS polar	2856	C00105	HMDB00288	6030	1.78	1.06	0.0145	0.0056	0.7003	0.2489
LC/MS neg	606	C00299	HMDB00296	6029	2.39	0.86	0.0005	0.0004	0.0515	0.0319
LC/MS polar	605	C00106	HMDB00300	1174	8.25	0.16	0.0000	0.0000	0.0000	0.0002
LC/MS neg	33442	C02067	HMDB00767	15047	1.08	0.68	0.3704	0.0928	0.0102	0.0092
LC/MS neg	61833			94312	5.27	0.18	0.0008	0.0005	0.0014	0.0020
LC/MS neg	35136		HMDB00884	445408	6.33	0.41	0.0000	0.0000	0.0002	0.0005
LC/MS polar	1412	C00526	HMDB00012	13712	4.72	0.44	0.0006	0.0004	0.0064	0.0066
LC/MS pos early	3155	C02642	HMDB00026	111	0.22	0.47	0.0001	0.0001	0.0005	0.0009
LC/MS pos early	55	C00099	HMDB00056	239	1.03	1.14	0.8722	0.1952	0.1813	0.0899
LC/MS neg	2841	C00112	HMDB01546	6132	0.32	0.92	0.0036	0.0017	0.3739	0.1563
LC/MS pos early	2372	C00055	HMDB00095	6131	1.27	0.97	0.1367	0.0379	0.6775	0.2430
LC/MS neg	514	C00475	HMDB00089	6175	3.46	0.38	0.0779	0.0234	0.0038	0.0045
LC/MS pos early	533	C00239	HMDB01202	13945	1.65	1.00	0.3126	0.0798		

LC/MS pos early	57554			150971	1.10	0.36	0.2260	0.0597	0.0011	0.0016
LC/MS neg	12023	C00364	HMDB01227	9700	2.36	0.79	0.0000	0.0000	0.7240	0.2562
LC/MS neg	2183	C00214	HMDB00273	5789	6.30	0.80	0.0258	0.0091	0.6504	0.2367
LC/MS neg	604	C00178	HMDB00262	1135	5.84	0.37	0.0016	0.0009	0.0119	0.0102
LC/MS pos early	37070		HMDB61711	13130	1.46	0.77	0.0227	0.0081	0.0458	0.0293
LC/MS pos early	594	C00153	HMDB01406	936	0.83	1.17	0.2901	0.0748	0.2058	0.0969
LC/MS pos early	22152	C00455	HMDB00229	14180	1.84	0.30	0.0115	0.0046	0.0092	0.0086
LC/MS neg	5278	C00003	HMDB00902	5893	2.04	0.59	0.0004	0.0003	0.0002	0.0006
LC/MS neg	31475	C00004	HMDB01487	439153	5.04	0.53	0.0000	0.0000	0.0936	0.0516
LC/MS pos early	27665	C02918	HMDB00699	10129985	0.73	0.63	0.0635	0.0199	0.0171	0.0136
LC/MS pos early	32401	C01004	HMDB00875	5570	0.63	1.69	0.0055	0.0024	0.0028	0.0036
LC/MS neg	558	C00301	HMDB01178	192	0.19	1.74	0.0002	0.0002	0.0010	0.0016
LC/MS neg	2134	C00016	HMDB01248	643975	0.90	0.88	0.6182	0.1457	0.2857	0.1254
LC/MS neg	15797	C00061	HMDB01520	710	5.04	0.27	0.0001	0.0001	0.0017	0.0023
LC/MS pos early	1508	C00864	HMDB00210	6613	0.71	0.61	0.0610	0.0192	0.0058	0.0061
LC/MS neg	15504	C01134	HMDB01416	987	1.65	0.52	0.3739	0.0929	0.7250	0.2562
LC/MS neg	18289	C00882	HMDB01373	444485	3.57	0.91	0.0000	0.0000	0.6392	0.2351
LC/MS neg	57837	C00010	HMDB01423	317	0.71	0.41	0.0437	0.0143	0.0168	0.0135
LC/MS neg	57555	C00831		439322	1.41	0.52	0.0371	0.0124	0.1015	0.0549
LC/MS polar	27738	C01620	HMDB00943	151152	1.08	0.41	0.8258	0.1867	0.0907	0.0505
LC/MS polar	46957	C00257	HMDB03290	9794176	1.62	0.48	0.0020	0.0010	0.0039	0.0046
LC/MS pos late	1561	C02477	HMDB01893	14985	1.17	0.87	0.7716	0.1767	0.5285	0.2065
LC/MS pos early	568	C00120	HMDB00030	171548	1.00	1.00				
LC/MS neg	18330	C00440	HMDB01396	146	0.32	2.07	0.0001	0.0001	0.0003	0.0006
LC/MS pos early	43023	C00715	HMDB00802	73000	1.90	0.98	0.0021	0.0011	0.7585	0.2665
LC/MS pos late	43807	C00486	HMDB00054	5280352	0.69	0.58	0.0767	0.0231	0.0210	0.0161
LC/MS pos early	5341	C00378	HMDB00235	1130	1.64	0.75	0.0009	0.0005	0.0402	0.0262
LC/MS pos late	1806	C00473	HMDB00305	445354	3.18	0.41	0.0000	0.0000	0.0000	0.0001
LC/MS pos early	608	C00314	HMDB02075	1054	3.43	0.67	0.0006	0.0004	0.0088	0.0084
LC/MS pos early	2150	C00534	HMDB01431	1052	1.26	1.05	0.0101	0.0041	0.6349	0.2349
LC/MS pos early	3138	C00647	HMDB01555	1053	0.85	1.58	0.7227	0.1673	0.0390	0.0256
LC/MS neg	5331	C00018	HMDB01491	1051	0.43	0.85	0.0626	0.0196	0.3739	0.1563
LC/MS pos early	1651	C00250	HMDB01545	1050	1.45	1.09	0.0038	0.0018	0.5009	0.1973

LC/MS neg	15753	C01586	HMDB00714	464	1.12	0.87	0.0611	0.0192	0.2099	0.0978
LC/MS neg	46111		HMDB60013	22473	0.38	1.55	0.0000	0.0001	0.0032	0.0039
LC/MS neg	36103		HMDB11635	4615423	0.63	1.01	0.0000	0.0000	0.8541	0.2909
LC/MS polar	587	C00257	HMDB00625	10690	1.29	0.95	0.0803	0.0240	0.7720	0.2698
LC/MS pos early	35101	C03065	HMDB13222	67701	3.61	0.61	0.0005	0.0003	0.0019	0.0025
LC/MS pos early	37459	C05570	HMDB03045	3032311	1.50	1.30	0.0085	0.0035	0.0301	0.0209
LC/MS polar	20699	C00503	HMDB02994	222285	2.49	1.15	0.0005	0.0004	0.2065	0.0969
LC/MS pos early	33009	C08283	HMDB33433	441447	0.75	1.60	0.0444	0.0145	0.0003	0.0007
LC/MS pos early	37123	C03410	HMDB00833	123802	0.54	0.96	0.0105	0.0042	0.5976	0.2260
LC/MS pos early	34384	C10172	HMDB04827	115244	0.91	1.45	0.5055	0.1220	0.0038	0.0045
LC/MS neg	37468	C05551	HMDB15186	5904	1.10	0.61	0.1736	0.0469	0.0002	0.0005
LC/MS pos early	47897	C03727	HMDB29415	1080	0.61	1.19	0.1976	0.0526	0.2712	0.1210
LC/MS neg	46960	C00059	HMDB01448	1118	0.86	1.13	0.4856	0.1177	0.3767	0.1569
LC/MS neg	45413			514186	1.18	0.91	0.2491	0.0652	0.2474	0.1117
LC/MS neg	43266		HMDB61116	181670	0.43	2.25	0.0000	0.0000	0.0000	0.0001
LC/MS pos early	42002			98504	1.94	1.63	0.0140	0.0054	0.0483	0.0304
LC/MS neg	36817	C12600		4766	0.88	0.96	0.1603	0.0437	0.5596	0.2159
LC/MS polar	41888	C07273		11439	1.60	0.98	0.0434	0.0142	0.7825	0.2719
LC/MS pos early	53231			93176	2.15	0.70	0.0003	0.0002	0.0248	0.0183

Mean Values				% Filled Values				Super Pathway
CTRL KO	IDH3A KO	OE 6	OE CTRL	CTRL KO	IDH3A KO	OE 6	OE CTRL	
0.9682	2.2519	0.9067	2.2740	100	100	100	100	Amino Acid
1.2455	0.9879	1.7459	1.6381	100	100	100	100	Amino Acid
0.8296	1.3162	1.0748	0.8901	100	100	100	100	Amino Acid
0.7134	1.3411	0.6035	0.8751	100	100	100	100	Amino Acid
1.5298	1.1294	2.1141	2.1353	100	100	100	100	Amino Acid
0.5200	1.5678	0.6486	1.0801	100	100	100	100	Amino Acid
1.3081	1.0581	1.7552	2.3359	100	100	100	100	Amino Acid
0.6470	0.7048	0.7285	0.9453	100	100	100	100	Amino Acid
1.1234	0.9466	1.4102	1.9632	100	100	100	100	Amino Acid
0.8867	3.3901	0.6088	1.3881	100	100	100	100	Amino Acid
0.7960	1.2911	0.9917	1.4745	100	100	100	100	Amino Acid
0.6969	1.0818	0.6894	0.9297	100	100	100	100	Amino Acid
1.4986	1.1116	2.3461	1.6367	100	100	100	100	Amino Acid
0.4985	1.0041	0.4178	1.0958	100	100	100	100	Amino Acid
0.2021	1.6989	0.2503	0.9290	100	100	100	100	Amino Acid
1.2702	0.8980	1.0655	2.2976	100	100	100	100	Amino Acid
0.9561	1.2185	0.8793	1.1998	100	100	100	100	Amino Acid
0.4341	1.2554	0.1742	0.3328	100	100	100	100	Amino Acid

0.5212	0.2631	1.0201	0.4770	100	100	100	100	Amino Acid
1.0584	0.3746	1.1567	1.0882	100	100	100	100	Amino Acid
1.0054	1.2799	0.9822	1.0029	100	100	100	100	Amino Acid
0.6801	3.0668	0.6188	0.9565	100	100	100	100	Amino Acid
0.8205	7.8390	1.1409	0.6240	100	100	100	100	Amino Acid
0.5139	0.8213	0.7442	2.3679	80	100	100	100	Amino Acid
0.8134	2.0230	0.8316	1.1782	100	100	100	100	Amino Acid
0.7899	3.9530	1.0291	1.7355	100	100	100	100	Amino Acid
0.4401	2.1483	0.6425	1.2013	60	100	100	100	Amino Acid
0.7635	0.7267	0.9474	0.9295	100	100	100	100	Amino Acid
0.9795	1.8646	2.2374	4.4367	100	100	100	100	Amino Acid
1.0423	0.2069	6.1104	0.9646	100	100	100	100	Amino Acid
0.9292	1.1932	0.9543	1.1046	100	100	100	100	Amino Acid
0.3010	0.4439	0.7042	0.9329	100	100	100	100	Amino Acid
1.0116	1.1046	0.8314	0.8828	100	100	100	100	Amino Acid
1.6165	0.6042	1.4993	1.1152	100	100	100	100	Amino Acid
1.5982	0.5217	2.4597	0.9014	100	80	100	100	Amino Acid
1.2355	0.6751	1.2700	0.9502	100	100	100	100	Amino Acid
1.1057	2.4777	0.7998	1.0622	100	100	100	100	Amino Acid
1.0709	1.4388	1.0514	0.9023	100	100	100	100	Amino Acid
0.7826	0.9855	1.9933	1.4969	100	100	100	100	Amino Acid
0.7559	6.2915	1.1269	2.2369	100	100	100	100	Amino Acid
0.8930	1.2687	1.0674	0.9084	100	100	100	100	Amino Acid
0.9656	1.9762	0.9431	1.2965	100	100	100	100	Amino Acid
0.8234	1.0259	0.9983	1.2607	100	100	100	100	Amino Acid
0.4668	0.4830	1.5998	0.6372	60	60	100	100	Amino Acid
0.9071	2.0481	0.9088	1.1745	100	100	100	100	Amino Acid
1.0423	0.8686	1.1536	1.1323	100	80	100	100	Amino Acid
1.1935	0.2948	6.0437	0.9925	100	100	100	100	Amino Acid
1.8277	0.7595	1.9836	1.3198	100	100	100	100	Amino Acid
0.7218	1.4759	0.6091	0.6725	100	100	80	80	Amino Acid
0.6194	1.2621	0.3508	0.6296	100	100	100	100	Amino Acid
1.2911	1.2050	0.7607	0.9201	100	100	60	100	Amino Acid

1.0910	2.2343	1.1171	1.4439	100	100	100	100	Amino Acid
0.9458	1.2317	0.8632	1.0750	100	100	100	100	Amino Acid
0.9715	6.7148	0.8853	2.2875	100	100	100	100	Amino Acid
0.1384	1.8175	0.2350	1.2208	60	100	100	100	Amino Acid
1.7849	0.2483	13.5665	1.1142	100	0	100	100	Amino Acid
0.8965	2.1676	0.8661	1.2091	100	100	100	100	Amino Acid
1.1380	1.5091	0.9645	1.5201	100	100	100	100	Amino Acid
0.1600	1.1816	1.2812	2.5912	60	100	100	100	Amino Acid
1.1868	1.4377	1.1053	1.3692	100	100	100	100	Amino Acid
0.6400	1.4928	0.6552	1.4841	100	100	100	100	Amino Acid
1.5164	1.0412	1.7583	3.2555	100	100	100	100	Amino Acid
0.9466	2.4665	0.9163	1.4317	100	100	100	100	Amino Acid
1.1980	1.7837	1.0773	1.5521	100	100	100	100	Amino Acid
0.1546	1.6171	1.4626	3.1570	60	100	100	100	Amino Acid
0.8601	0.6944	1.9858	1.2643	100	100	100	100	Amino Acid
1.3283	1.1345	1.6174	1.0041	100	100	100	100	Amino Acid
1.1821	0.9172	1.0998	0.8967	100	100	100	100	Amino Acid
0.7070	0.5676	0.9925	2.3963	100	100	100	100	Amino Acid
0.9281	0.3895	1.1369	1.2302	100	100	100	100	Amino Acid
0.7824	2.3787	0.8155	1.3175	100	100	100	100	Amino Acid
1.2704	1.0721	1.4031	1.5340	100	100	100	100	Amino Acid
0.2084	2.0645	1.8395	4.1341	80	100	100	100	Amino Acid
1.0815	6.6749	1.6131	1.1780	100	100	100	100	Amino Acid
0.7042	1.0921	0.7518	1.6472	80	100	80	100	Amino Acid
0.6910	1.8201	0.6969	1.0647	100	100	100	100	Amino Acid
1.2171	1.1553	1.3579	1.3723	100	100	100	100	Amino Acid
0.9793	0.4506	1.1869	1.8440	100	100	100	100	Amino Acid
0.8837	2.4364	0.8954	1.1923	100	100	100	100	Amino Acid
0.8613	1.1511	0.8085	0.8771	100	100	100	100	Amino Acid
1.9647	0.8123	1.5551	1.0620	100	100	100	100	Amino Acid
0.9546	1.2781	0.7461	1.2836	100	100	100	100	Amino Acid
1.7367	1.0622	1.4549	1.2387	100	100	100	100	Amino Acid
1.3812	0.3845	1.3775	1.3741	100	100	100	100	Amino Acid

0.4452	1.0198	1.2383	0.9333	100	100	100	100	Amino Acid
0.3946	1.5065	0.5513	0.8824	100	100	100	100	Amino Acid
0.7394	0.8534	0.6956	1.1615	100	100	100	100	Amino Acid
0.1872	0.5528	0.7271	1.5577	0	80	60	100	Amino Acid
1.1610	3.3949	1.2263	1.8515	100	100	100	100	Amino Acid
1.0784	3.2082	1.2117	1.8603	100	100	100	100	Amino Acid
0.9625	0.9699	0.9216	1.2903	100	100	100	100	Amino Acid
0.3173	0.5962	0.4041	0.9624	100	100	100	100	Amino Acid
0.9410	0.8927	0.7696	0.7389	100	100	100	100	Amino Acid
0.4410	1.0473	0.7922	0.9731	100	100	100	100	Amino Acid
0.6386	0.8573	1.0399	1.2644	100	100	100	100	Amino Acid
0.2653	1.1095	0.4847	0.7771	100	100	100	100	Amino Acid
0.2562	1.9503	0.7088	1.2135	80	100	100	100	Amino Acid
1.0795	0.6282	0.7947	1.3703	100	100	100	100	Amino Acid
0.8059	1.1863	0.8582	1.7960	100	100	100	100	Amino Acid
0.3021	0.2270	0.3234	0.3141	60	40	60	60	Amino Acid
0.7874	2.8790	1.0789	1.8297	100	100	100	100	Amino Acid
1.0994	1.7811	1.2370	1.3922	100	100	100	100	Amino Acid
1.6638	1.6078	0.9075	1.1698	80	100	100	80	Amino Acid
0.7998	1.0233	1.2842	0.9784	100	100	100	100	Amino Acid
0.9578	1.2233	0.9161	1.1562	100	100	100	100	Amino Acid
0.5686	2.0048	1.1509	0.7409	60	100	100	100	Amino Acid
1.2588	1.5208	1.3510	1.3083	100	100	100	100	Amino Acid
1.1038	2.1464	1.4198	1.9650	100	100	100	100	Amino Acid
0.0797	0.8403	0.6250	0.7754	100	100	100	100	Amino Acid
0.4371	1.4234	0.7248	1.2052	100	100	100	100	Amino Acid
0.1439	0.1439	0.1439	0.1439	0	0	0	0	Amino Acid
0.9224	1.4680	0.6438	1.2721	100	100	100	100	Amino Acid
0.0408	1.6604	0.2911	1.5170	100	100	100	100	Amino Acid
0.1809	1.2145	0.3861	0.7212	100	100	100	100	Amino Acid
0.3624	0.6096	1.0676	0.8067	100	100	100	100	Amino Acid
0.6579	1.3244	0.5673	1.2059	100	100	100	100	Amino Acid
0.8703	1.5095	0.6933	1.2715	100	100	100	100	Amino Acid

0.2932	1.1244	0.3865	0.2830	40	100	40	20	Amino Acid
0.3917	1.1083	0.3520	1.5295	100	100	100	100	Amino Acid
0.4968	1.4659	0.4689	1.1378	100	100	100	100	Amino Acid
0.5112	0.9061	0.7675	0.8916	100	100	100	100	Amino Acid
1.1306	0.8332	2.3689	2.4455	100	100	100	100	Amino Acid
1.5772	2.3682	0.8303	1.3313	100	100	100	100	Amino Acid
0.5787	1.8306	0.6853	1.4168	100	100	100	100	Peptide
0.7616	0.9699	0.8896	1.1449	100	100	100	100	Peptide
0.0822	4.2496	0.0579	0.4159	100	100	100	100	Peptide
0.1918	1.0821	0.3001	1.0247	20	100	80	100	Peptide
0.3330	1.6594	0.3805	1.1630	100	100	100	100	Peptide
0.3571	1.4984	0.3662	0.7734	100	100	100	100	Peptide
1.5928	0.9161	0.9168	0.6915	100	100	100	100	Peptide
0.2111	0.9019	0.2111	0.2622	0	100	20	40	Peptide
0.2520	1.2658	0.2814	0.8055	40	100	80	100	Peptide
0.2706	0.8159	0.2852	0.3243	0	100	40	40	Peptide
0.1923	1.1559	0.1923	0.5406	20	100	0	60	Peptide
0.3432	1.6221	0.3534	0.9428	60	100	60	100	Peptide
1.4413	0.3825	1.6490	0.8600	100	60	100	100	Peptide
0.4851	0.3455	0.5355	0.3219	60	40	40	40	Peptide
0.8223	0.7556	0.9304	0.4873	80	100	80	80	Peptide
0.9645	0.9484	0.8642	0.7230	100	100	100	100	Peptide
1.4714	0.7347	1.1163	1.0037	100	100	100	100	Peptide
3.8476	0.6881	2.4238	0.8133	100	100	100	100	Peptide
0.7596	0.5882	0.6012	0.3539	100	100	80	100	Peptide
0.2126	1.0488	0.3416	0.4844	100	100	100	100	Peptide
4.5445	0.8395	2.0817	0.5310	100	100	100	80	Peptide
0.5381	0.7239	0.4545	0.4143	100	100	80	80	Peptide
2.1071	0.6232	1.6114	0.7101	100	100	100	100	Peptide
1.4649	0.2714	0.9706	0.2506	100	40	80	40	Peptide
1.0505	0.3499	1.1869	0.3576	80	40	60	40	Peptide
0.7927	0.4862	1.0878	1.2182	100	100	100	100	Peptide
3.9862	1.1833	15.3353	11.7379	100	100	100	100	Carbohydrate

4.9900	1.8913	1.3060	1.8166	100	100	100	100	Carbohydrate
2.0230	1.2842	1.3092	0.7053	100	100	100	100	Carbohydrate
4.1557	1.3625	0.1560	0.1550	100	100	100	100	Carbohydrate
2.0854	0.7815	0.0761	0.1510	100	100	40	20	Carbohydrate
7.1027	0.7937	0.6068	0.7108	100	100	100	100	Carbohydrate
8.6415	1.4786	0.8414	0.7947	100	100	100	100	Carbohydrate
8.2338	1.1507	1.1494	1.2451	100	100	100	100	Carbohydrate
0.8342	0.3796	1.0030	1.3391	100	100	100	100	Carbohydrate
1.0243	1.1195	0.9810	0.9145	100	100	100	100	Carbohydrate
5.3156	1.2002	8.8928	7.6884	100	100	100	100	Carbohydrate
28.7774	9.6585	1.3592	0.7755	100	100	100	100	Carbohydrate
1.1345	1.5739	0.4214	0.2955	100	100	100	100	Carbohydrate
1.1448	0.2296	0.2296	0.2296	100	0	0	0	Carbohydrate
1.6131	4.7528	0.3123	0.3821	100	100	100	100	Carbohydrate
1.5220	0.8615	0.0833	0.1209	100	100	20	40	Carbohydrate
0.8814	1.2623	5.3761	5.8223	100	100	100	100	Carbohydrate
0.5701	1.2708	1.0063	0.9263	100	100	100	100	Carbohydrate
1.0584	1.4956	1.0866	1.8741	100	100	100	100	Carbohydrate
0.9732	1.2297	1.0952	1.0697	100	100	100	100	Carbohydrate
1.0714	1.8791	0.8230	2.0577	100	100	100	100	Carbohydrate
0.4995	2.8122	1.5209	2.8586	100	100	100	100	Carbohydrate
0.8073	0.5595	1.1755	1.2361	100	100	100	100	Carbohydrate
1.5758	0.6078	1.3556	0.7647	100	100	100	100	Carbohydrate
1.0634	4.2318	1.6242	0.9349	100	100	100	100	Carbohydrate
1.0441	3.3087	0.9783	0.6199	100	100	100	100	Carbohydrate
0.6347	0.6214	1.9298	2.2700	100	100	100	100	Carbohydrate
3.6472	1.9734	0.7012	1.0608	100	100	100	100	Carbohydrate
0.7433	0.9065	0.8730	0.8138	100	20	100	100	Carbohydrate
0.7029	0.2513	0.1192	0.0655	100	100	40	40	Carbohydrate
1.1242	1.0450	1.7069	1.5165	100	100	100	100	Carbohydrate
0.8895	0.9334	0.8358	0.9047	100	100	100	100	Carbohydrate
1.4100	1.1722	2.1913	3.3394	100	100	100	100	Carbohydrate
0.9573	0.9597	0.7308	0.8714	100	100	100	100	Carbohydrate

1.4891	1.3183	1.2844	1.2532	100	100	100	100	Carbohydrate
1.2816	1.6422	1.2349	1.4236	100	100	100	100	Carbohydrate
0.8247	1.6592	0.6679	0.9120	80	100	80	100	Carbohydrate
1.2550	0.9424	0.1742	0.2124	100	100	100	100	Carbohydrate
0.5481	1.3706	0.2317	0.3022	100	100	100	100	Carbohydrate
1.8918	0.9989	2.0452	1.7453	100	100	100	100	Carbohydrate
1.1233	0.9078	0.9880	0.9993	100	100	100	100	Carbohydrate
1.1710	0.9751	1.2731	1.6707	100	100	100	100	Carbohydrate
1.8599	1.0165	1.8854	2.0218	100	100	100	100	Carbohydrate
0.3158	16.4228	0.1729	0.2410	100	100	100	100	Energy
0.5451	18.6935	0.3168	0.3737	100	100	100	100	Energy
0.8317	42.8207	0.1814	0.3346	100	100	80	100	Energy
0.1493	0.8713	0.5676	1.2308	20	100	100	100	Energy
0.4520	1.2897	1.2357	3.7205	100	100	100	100	Energy
1.0883	0.4955	0.8671	0.6448	100	100	100	100	Energy
0.2851	2.1242	0.3983	0.9502	100	100	100	100	Energy
0.4531	1.5165	0.6966	1.2259	100	100	100	100	Energy
0.4632	1.3123	0.6058	0.9653	100	100	100	100	Energy
1.5917	0.7190	2.2729	2.7252	100	100	100	100	Energy
1.9211	0.7746	0.2476	0.2815	100	100	100	100	Energy
0.9824	1.2399	0.9487	1.1115	100	100	100	100	Energy
1.3698	0.9637	1.2960	1.0979	100	100	100	100	Lipid
0.9967	0.7192	0.9004	1.4345	80	100	80	100	Lipid
1.9648	0.9833	2.3192	1.5833	100	100	100	100	Lipid
1.4644	0.8069	1.2381	1.7005	100	100	100	100	Lipid
1.3947	1.2402	1.6162	1.1902	100	100	100	100	Lipid
1.3634	1.3435	1.4320	1.0468	100	100	100	100	Lipid
1.4703	1.1847	1.5765	1.4109	100	100	100	100	Lipid
1.6280	2.5900	1.9275	1.0542	100	100	100	100	Lipid
1.4359	2.8965	1.8610	1.2665	100	100	100	100	Lipid
1.1782	1.3994	1.2058	0.8436	100	100	100	100	Lipid
1.6090	1.9748	1.8785	0.9433	100	100	100	100	Lipid
1.6064	2.5448	2.1243	1.0328	100	100	100	100	Lipid

1.7335	4.4667	2.7658	1.0108	100	100	100	100	Lipid
1.2368	1.9709	1.3818	0.7513	100	100	100	100	Lipid
1.1615	1.6396	1.6812	0.4121	100	100	100	100	Lipid
0.8037	1.5651	1.1015	1.3710	100	100	100	100	Lipid
1.4008	1.8708	2.6018	0.3339	100	100	100	100	Lipid
1.0226	8.2504	1.5514	0.8195	100	100	100	100	Lipid
0.4060	3.5560	0.5685	0.5124	60	100	60	60	Lipid
1.4982	15.4946	1.4659	1.9428	100	100	100	100	Lipid
1.4513	12.2364	2.1906	1.1279	100	100	100	100	Lipid
1.3784	8.1968	2.0468	1.7050	100	100	100	100	Lipid
0.3268	6.6667	0.6794	0.2480	80	100	100	0	Lipid
1.2634	4.0904	1.8240	1.2866	100	100	100	100	Lipid
1.2465	5.7322	1.5804	1.5659	100	100	100	100	Lipid
1.2721	5.2529	1.7391	1.0790	100	100	100	100	Lipid
1.5642	7.2096	1.9077	1.8376	100	100	100	100	Lipid
1.5994	19.5048	3.1838	0.7503	100	100	100	100	Lipid
1.0897	5.3812	1.3055	0.9919	100	100	100	100	Lipid
0.6937	1.6433	1.2434	0.1604	100	100	100	100	Lipid
0.9054	5.2952	1.6651	0.3649	100	100	100	100	Lipid
0.5421	0.5421	0.5421	0.5421	0	0	0	0	Lipid
0.2009	1.0674	0.2344	0.1859	100	100	100	100	Lipid
0.0984	0.9682	0.1547	0.0184	100	100	100	80	Lipid
1.7208	0.9325	2.3800	1.2977	100	100	100	100	Lipid
1.6338	1.0875	2.1179	1.2163	100	100	100	100	Lipid
1.5726	1.2256	2.2877	1.0389	100	100	100	100	Lipid
1.0330	0.5870	1.1310	1.5367	100	100	100	100	Lipid
1.2541	0.2886	1.8088	2.8752	100	100	100	100	Lipid
0.3568	1.5915	0.5007	1.2126	100	100	100	100	Lipid
0.8103	1.4039	0.9988	1.6775	100	100	100	100	Lipid
1.0396	1.4106	1.3516	1.2699	100	100	100	100	Lipid
0.9753	1.5050	1.1983	2.9372	100	100	100	100	Lipid
0.5683	1.4094	0.7874	0.7022	100	100	100	100	Lipid
0.7109	1.2397	0.9043	0.6950	100	100	100	100	Lipid

0.5262	0.7827	0.8984	0.5284	100	100	100	100	Lipid
0.8822	0.9591	2.6095	1.0090	80	100	100	100	Lipid
0.6993	0.8377	1.0928	0.7751	100	100	100	100	Lipid
0.5181	1.0966	0.8220	0.6383	100	100	100	100	Lipid
0.2385	0.9655	0.4608	0.8168	40	100	100	100	Lipid
0.3188	0.9123	0.3577	1.1327	40	100	100	100	Lipid
0.2830	1.0824	0.6831	0.7772	100	100	100	100	Lipid
0.8629	0.9212	1.2588	0.8388	100	100	100	100	Lipid
1.1183	0.9216	1.2093	0.8232	100	100	100	100	Lipid
0.5924	0.5294	0.4639	1.2946	100	100	100	100	Lipid
0.4739	0.9616	0.5299	0.2331	100	100	100	100	Lipid
0.4158	1.2414	0.3785	0.7189	100	100	100	100	Lipid
0.2277	1.1757	0.1785	0.4764	60	100	60	100	Lipid
0.5601	0.7596	0.6284	0.6963	100	100	100	100	Lipid
0.1958	0.4174	0.1672	0.5213	20	100	40	100	Lipid
0.2462	0.8913	0.3036	0.1800	80	100	100	80	Lipid
0.7429	3.6896	0.9703	2.5552	100	100	100	100	Lipid
0.1610	0.1632	0.1610	0.1610	0	40	0	0	Lipid
0.1838	0.9130	0.2736	0.2119	80	100	100	80	Lipid
0.4828	0.9382	0.6324	0.2924	80	100	100	100	Lipid
0.0703	0.0785	0.0703	0.0703	0	40	0	0	Lipid
0.3860	6.1643	0.7923	1.0644	60	100	100	80	Lipid
0.2167	0.2167	0.2167	0.2167	0	20	0	0	Lipid
1.0855	1.0689	1.0183	0.7139	100	100	100	100	Lipid
0.0566	0.1214	0.0605	0.0566	0	80	60	0	Lipid
1.1507	1.6718	1.3260	1.0832	100	100	100	100	Lipid
1.3272	0.8275	1.0454	0.4502	100	100	100	100	Lipid
0.2552	0.5225	0.3303	0.2150	20	100	20	0	Lipid
0.2806	0.6633	0.2806	0.3229	0	100	0	60	Lipid
0.8358	0.7885	2.8215	0.2937	100	80	100	20	Lipid
1.7496	1.3673	1.7812	1.8265	100	100	100	100	Lipid
0.1892	0.1834	0.1843	0.2081	40	40	60	80	Lipid
0.8763	0.6675	0.6642	0.7105	100	100	100	100	Lipid

0.4988	0.4988	0.4988	0.4988	0	0	0	0	Lipid
2.4480	0.8060	2.1759	2.2430	100	100	100	100	Lipid
2.8156	1.1210	1.8619	3.6116	100	100	100	100	Lipid
1.3022	1.0918	1.2431	1.0026	100	100	100	100	Lipid
1.2286	1.2285	1.0707	1.9210	100	100	100	100	Lipid
0.6984	1.7667	0.7914	1.0896	100	100	100	100	Lipid
0.6516	3.4675	1.1642	1.1368	100	100	100	100	Lipid
0.7727	3.7866	1.5435	1.0541	100	100	100	100	Lipid
0.4122	2.4751	0.6560	1.0993	100	100	100	100	Lipid
1.6759	0.8842	1.3765	1.7913	100	100	100	100	Lipid
0.7041	0.9178	0.9133	0.3336	100	100	100	100	Lipid
0.4141	0.4141	0.4141	0.4141	0	0	0	0	Lipid
1.3686	0.5395	0.0732	0.0448	100	100	100	20	Lipid
0.5527	1.7949	0.5409	1.4349	100	100	100	100	Lipid
0.0582	4.7465	0.0562	0.3780	100	100	100	100	Lipid
0.5357	1.1441	0.6448	1.0470	100	100	100	100	Lipid
1.3601	2.6994	1.0583	1.7883	100	100	100	100	Lipid
0.2236	1.5354	0.0265	0.0756	100	100	0	100	Lipid
0.9810	0.8646	0.1974	0.4203	100	100	100	100	Lipid
0.9212	1.2299	0.7755	1.4718	100	100	100	100	Lipid
0.7770	0.6978	0.7264	1.1398	100	100	100	100	Lipid
0.9192	0.8841	0.9144	0.7400	100	100	100	100	Lipid
1.3266	0.9745	1.0519	0.8877	100	100	100	100	Lipid
0.9811	2.1800	1.0007	1.5878	100	100	100	100	Lipid
1.3321	1.9450	0.9551	1.2110	100	100	100	100	Lipid
1.2113	0.9359	0.9556	1.1711	100	100	100	100	Lipid
1.0577	2.6800	0.7507	0.9552	100	100	100	100	Lipid
1.0675	1.1879	0.9138	0.8063	100	100	100	100	Lipid
0.7204	1.2583	0.5771	0.7567	100	100	100	100	Lipid
1.4076	0.3443	1.0661	0.9043	100	100	100	100	Lipid
0.5481	1.7262	0.4176	1.4695	100	100	100	100	Lipid
0.7130	1.0967	0.4805	0.4827	100	100	100	100	Lipid
1.3156	2.5995	1.0009	1.1290	100	100	100	100	Lipid

1.4213	2.8989	1.1187	1.1221	100	100	100	100	Lipid
0.8149	0.9462	0.6338	0.4308	100	100	100	100	Lipid
0.8076	1.5280	0.6974	0.6487	100	100	100	100	Lipid
0.9400	0.6543	0.8824	0.5762	100	100	100	100	Lipid
1.0592	2.0932	1.0074	1.0085	100	100	100	100	Lipid
1.0660	2.0031	0.9597	1.0238	100	100	100	100	Lipid
0.6713	3.2219	0.5088	0.6499	100	100	100	100	Lipid
1.0846	8.8572	1.0762	1.8581	100	100	100	100	Lipid
0.9345	5.8539	0.6297	0.8822	100	100	100	100	Lipid
1.1186	2.3050	1.0069	0.7714	100	100	100	100	Lipid
0.9773	1.4700	0.5404	1.1765	100	100	100	100	Lipid
0.7450	1.5653	0.2784	0.7784	100	100	100	100	Lipid
1.4880	1.0721	1.2585	1.3392	100	100	100	100	Lipid
0.7482	1.5028	0.6881	1.1152	100	100	100	100	Lipid
4.6533	0.5775	3.4333	2.9139	100	100	100	100	Lipid
1.4301	1.9066	1.1527	1.4918	100	100	100	100	Lipid
1.4285	2.4162	1.1475	1.2878	100	100	100	100	Lipid
0.9551	1.1493	0.7897	0.6861	100	100	100	100	Lipid
1.1597	0.8192	0.9139	0.6129	100	100	100	100	Lipid
1.5177	1.4146	1.2033	1.1463	100	100	100	100	Lipid
1.1546	2.9935	0.8650	1.1384	100	100	100	100	Lipid
1.2458	2.0229	1.0471	0.9793	100	100	100	100	Lipid
1.5599	2.2797	1.0528	1.1444	100	100	100	100	Lipid
1.6990	1.7982	1.3383	0.9769	100	100	100	100	Lipid
1.6689	1.2378	1.5686	1.9249	100	100	100	100	Lipid
1.0816	1.2528	0.8362	0.5861	100	100	100	100	Lipid
1.2257	2.7698	0.9319	1.7387	100	100	100	100	Lipid
0.7791	1.2214	0.3828	1.0212	100	100	100	100	Lipid
1.0046	1.2036	0.8497	0.7886	100	100	100	100	Lipid
1.1098	1.9484	0.7420	0.6927	100	100	100	100	Lipid
0.8403	1.2897	0.6859	0.4338	100	100	100	100	Lipid
1.0919	0.1745	1.2507	1.6296	100	100	100	100	Lipid
2.4829	0.9322	2.6856	2.6747	100	100	100	100	Lipid

1.4671	1.4158	1.0248	1.8395	100	100	100	100	Lipid
1.4791	0.7167	1.5310	1.1607	100	100	100	100	Lipid
1.0641	2.2312	1.0326	1.0901	100	100	100	100	Lipid
1.2759	0.4104	1.2560	0.7906	100	100	100	100	Lipid
1.4205	2.3045	1.0238	1.1402	100	100	100	100	Lipid
1.4352	1.5872	1.2386	1.2994	100	100	100	100	Lipid
1.7446	1.0730	2.5399	3.1560	100	100	100	100	Lipid
1.0031	1.1949	1.1048	3.2574	100	100	100	100	Lipid
1.3965	1.0553	1.9277	4.6235	100	100	100	100	Lipid
2.3244	0.9151	2.4841	7.3857	100	100	100	100	Lipid
0.8735	1.1337	1.0299	1.4561	100	100	100	100	Lipid
1.2600	1.0432	2.1887	2.0714	100	100	100	100	Lipid
0.9731	2.4607	1.3092	2.9041	100	100	100	100	Lipid
0.0695	0.0695	0.0740	0.0695	0	0	60	0	Lipid
2.3211	1.0712	2.4098	3.2522	100	100	100	100	Lipid
1.2275	1.1417	1.1018	1.5408	100	100	100	100	Lipid
2.0019	1.8670	1.4345	1.4843	100	100	100	100	Lipid
2.1075	1.0875	2.0527	1.8528	100	100	100	100	Lipid
1.1518	1.2912	1.6775	1.0851	100	100	100	100	Lipid
1.5976	3.1800	2.3935	1.6175	100	100	100	100	Lipid
1.0200	0.6069	1.7954	2.6668	100	80	100	100	Lipid
1.3324	0.9358	1.1258	1.6997	100	100	100	100	Lipid
1.4825	1.4649	2.2697	1.5084	100	100	100	100	Lipid
1.5695	1.0414	1.8478	1.9668	100	100	100	100	Lipid
1.2099	1.5409	1.2911	1.3377	100	100	100	100	Lipid
1.6634	1.7301	1.8662	1.5071	100	100	100	100	Lipid
1.2937	2.8735	1.8205	1.0090	100	100	100	80	Lipid
1.5869	0.6991	2.2630	1.1641	100	100	100	100	Lipid
1.9218	1.4083	1.4809	1.2729	100	100	100	100	Lipid
2.5341	1.2335	3.5861	1.2193	100	100	100	100	Lipid
1.3234	2.4996	1.6867	1.0226	100	80	100	100	Lipid
1.3235	2.9559	1.4734	0.9616	100	100	100	100	Lipid
1.1437	0.6518	2.7970	1.6626	100	100	100	100	Lipid

2.1793	0.7295	1.5201	1.1339	100	100	100	100	Lipid
2.1007	0.9859	1.1155	1.5789	100	100	100	100	Lipid
1.5947	1.7445	0.9393	1.4512	100	100	100	100	Lipid
1.5781	0.9797	1.0890	1.8557	100	100	100	100	Lipid
1.5089	1.6306	1.1567	1.3907	100	100	100	100	Lipid
1.5560	0.9841	1.2403	1.3881	100	100	100	100	Lipid
0.9268	0.3893	0.7137	0.4636	100	100	100	100	Lipid
1.1946	5.3123	1.0231	1.3971	100	100	100	100	Lipid
1.3963	1.3404	0.7424	1.1643	100	100	100	100	Lipid
0.8035	2.4042	0.7122	0.6307	100	100	100	100	Lipid
0.7317	0.9047	1.0723	1.3999	100	100	100	100	Lipid
2.3086	1.0391	2.2434	2.9707	100	100	100	100	Lipid
2.0852	1.0379	2.1172	1.6334	100	100	100	100	Lipid
0.9613	0.9734	1.1484	0.9386	100	100	100	100	Lipid
1.5202	0.5389	1.1222	0.5361	100	100	100	100	Lipid
1.0287	2.0643	1.1750	1.0616	100	100	100	100	Lipid
0.8452	3.1701	0.4760	0.7837	100	100	100	100	Lipid
1.3221	2.2296	1.0556	1.1006	100	100	100	100	Lipid
2.3724	0.7068	2.7483	1.4783	100	100	100	100	Lipid
2.8242	0.9283	3.7768	1.8177	100	100	100	100	Lipid
1.6123	1.3249	2.0426	0.9225	100	100	100	100	Lipid
3.7182	0.8771	3.3715	2.7219	100	100	100	100	Lipid
2.9027	1.1114	3.2401	1.4982	100	100	100	100	Lipid
1.9331	0.9447	2.2713	0.7318	100	100	100	100	Lipid
1.7115	1.6440	2.1675	1.2090	100	100	100	100	Lipid
0.8965	0.6174	1.0577	0.4898	100	100	100	100	Lipid
1.5399	2.2624	1.8143	1.2480	100	100	100	100	Lipid
1.3856	2.3766	1.6955	1.3147	100	100	100	100	Lipid
2.2897	0.5211	2.7408	1.2990	100	100	100	100	Lipid
1.4563	1.0445	2.2600	0.8758	100	100	100	100	Lipid
4.4436	0.6280	4.0629	2.9333	100	100	100	100	Lipid
1.6726	0.5247	2.1995	0.6623	100	100	100	100	Lipid
1.8044	1.3533	2.1158	1.3837	100	100	100	100	Lipid

1.5362	1.4147	1.7499	1.1367	100	100	100	100	Lipid
1.2580	1.3747	1.4640	1.1876	100	100	100	100	Lipid
1.5790	0.7885	0.9478	2.2984	100	100	100	100	Lipid
3.2456	1.0099	2.4619	3.8523	100	100	100	100	Lipid
1.2425	1.2217	1.1142	1.8942	100	100	100	100	Lipid
1.4830	1.1112	1.2860	1.6812	100	100	100	100	Lipid
1.5236	3.2531	1.0299	2.2090	100	100	100	100	Lipid
1.5925	1.0869	1.5732	1.7884	100	100	100	100	Lipid
1.9577	1.0600	1.8351	1.7066	100	100	100	100	Lipid
1.3769	1.6515	1.2825	1.7211	100	100	100	100	Lipid
1.5597	1.1937	1.3114	1.6060	100	100	100	100	Lipid
2.2165	1.0197	1.3605	3.4069	100	100	100	100	Lipid
1.1375	2.1931	1.2459	1.0979	100	100	100	100	Lipid
1.2931	1.5682	1.2414	1.0070	100	100	100	100	Lipid
1.2917	4.7406	1.0107	1.9001	100	100	100	100	Lipid
1.1488	2.7485	0.6570	1.8005	100	100	100	100	Lipid
1.2129	0.2073	1.0537	1.5904	100	20	100	100	Lipid
1.4286	1.1097	1.0243	1.2836	100	100	100	100	Lipid
1.0148	3.3558	0.9135	1.1990	100	100	100	100	Lipid
0.7693	5.3292	0.7327	1.5151	100	100	100	100	Lipid
1.0849	6.0659	1.0987	1.9631	100	100	100	100	Lipid
1.0293	2.0683	1.0047	0.6510	100	100	100	100	Lipid
1.1506	1.6080	1.0562	0.6188	100	100	100	100	Lipid
1.2460	7.8465	0.8376	1.5844	100	100	100	100	Lipid
1.1644	4.0467	1.0516	1.1057	100	100	100	100	Lipid
0.3539	1.3498	0.2315	0.3851	100	100	100	100	Lipid
1.3365	4.9756	1.0667	1.4310	100	100	100	100	Lipid
1.1723	7.0401	1.0443	1.3286	100	100	100	100	Lipid
0.9899	6.6022	1.0632	1.5590	100	100	100	100	Lipid
0.6441	1.1208	0.5665	1.6159	100	100	100	100	Lipid
0.6779	0.5346	0.8242	2.4025	100	20	100	100	Lipid
0.3051	1.1231	0.3174	0.5740	100	100	100	100	Lipid
1.6153	1.3240	1.8458	3.5402	100	100	100	100	Lipid

1.0014	1.8772	1.1525	1.7666	100	100	100	100	Lipid
0.4492	1.2691	0.3432	0.6421	100	100	100	100	Lipid
0.3613	1.5526	0.2859	0.5733	100	100	100	100	Lipid
0.0923	2.0209	0.1058	0.3257	80	100	100	100	Lipid
0.9903	1.0097	0.7953	0.9421	100	100	100	100	Lipid
0.9810	1.1964	0.5686	1.1861	100	100	100	100	Lipid
1.1379	2.1875	0.8441	1.5251	100	100	100	100	Lipid
1.0187	1.8493	1.0328	1.2515	100	100	100	100	Lipid
1.0280	2.2725	0.9896	0.5589	100	100	100	100	Lipid
1.0085	0.8007	0.7141	1.1802	100	100	100	100	Lipid
1.7740	0.8848	1.2640	2.6742	100	100	100	100	Lipid
1.8523	1.2702	1.4522	1.3826	100	100	100	100	Lipid
1.3621	1.1892	1.0457	1.0118	100	100	100	100	Lipid
0.8042	1.3285	0.4926	0.8689	100	100	100	100	Lipid
1.5186	1.5889	0.9407	1.1349	100	100	100	100	Lipid
1.2896	2.6059	0.9069	3.2102	100	100	100	100	Lipid
1.0015	1.9844	0.9465	2.2968	100	100	100	100	Lipid
1.3743	1.4267	0.9576	1.6874	100	100	100	100	Lipid
1.3289	1.8663	1.2850	0.7858	100	100	100	100	Lipid
1.0365	1.0609	0.8970	0.5261	100	100	100	100	Lipid
1.6139	1.7826	1.4147	1.0160	100	100	100	100	Lipid
0.9847	1.3890	1.1028	1.5695	100	100	100	100	Lipid
1.0547	0.8909	1.0915	1.4968	100	100	100	100	Lipid
1.2134	1.2008	0.8708	0.7398	100	100	100	100	Lipid
0.9789	1.8813	0.9737	0.7222	100	100	100	100	Lipid
0.7825	1.2494	0.9476	0.5875	100	100	100	100	Lipid
1.0955	1.0866	0.6709	1.1013	100	100	100	100	Lipid
0.1270	3.2258	0.0693	0.7142	80	100	40	100	Lipid
0.0551	1.3982	0.0551	0.0551	0	100	0	20	Lipid
0.8988	1.0054	0.7812	1.7952	100	100	100	100	Lipid
0.2299	1.0489	0.1902	1.3508	20	100	60	100	Lipid
0.7384	1.0910	0.9770	2.1144	100	100	100	100	Lipid
0.8511	1.1174	1.1177	3.0812	100	100	100	100	Lipid

0.8863	1.1387	0.7607	2.0427	100	100	100	100	Lipid
0.0344	0.6796	0.0324	0.2304	40	100	20	100	Lipid
1.4019	1.0807	1.9723	2.3101	100	100	100	100	Lipid
1.5843	1.4506	1.9825	0.9653	100	100	100	100	Lipid
1.0282	0.9965	0.8785	1.6773	100	100	100	100	Lipid
0.7878	1.3365	0.6582	1.4230	100	100	100	100	Lipid
1.3439	0.8468	0.9989	1.3208	100	100	100	100	Lipid
0.8803	1.2312	0.9653	1.2486	100	100	100	100	Lipid
0.8716	0.8892	0.8589	3.0838	100	100	100	100	Lipid
1.0551	2.4347	0.9358	1.9979	100	100	100	100	Lipid
1.2034	1.5740	1.6877	0.9498	100	100	100	100	Lipid
1.7418	1.1818	1.2546	3.5220	100	100	100	100	Lipid
1.2537	1.0554	0.6243	2.4089	100	100	100	100	Lipid
0.8371	1.0127	0.4236	2.5782	100	100	100	100	Lipid
1.0437	1.3077	0.8562	1.5532	100	100	100	100	Lipid
0.3587	0.8570	0.3587	0.4438	0	100	0	100	Lipid
1.6432	0.8319	1.4136	3.4043	100	100	100	100	Lipid
1.5993	0.8420	0.9816	2.0996	100	100	100	100	Lipid
1.3489	0.9886	0.9619	1.1474	100	100	100	100	Lipid
0.1136	0.5497	0.5190	1.6392	100	100	100	100	Lipid
1.0463	1.4338	1.0753	1.5825	100	100	100	100	Lipid
1.4918	1.3407	0.9083	0.9326	100	100	100	100	Lipid
0.8021	0.3436	0.0099	0.0455	100	100	40	100	Nucleotide
1.3439	1.2438	1.0814	0.7983	100	100	100	100	Nucleotide
0.9605	1.4529	1.5218	2.0334	100	100	100	100	Nucleotide
1.1110	1.7077	1.8447	2.1410	100	100	100	100	Nucleotide
0.7922	2.2475	2.3121	6.7036	100	100	100	100	Nucleotide
0.9982	1.5780	1.5691	1.9376	100	100	100	100	Nucleotide
0.6595	0.7489	0.8540	1.1674	100	100	100	100	Nucleotide
0.8927	1.8418	1.0148	1.5265	100	100	100	100	Nucleotide
1.3577	0.7571	0.2047	0.2191	100	100	100	100	Nucleotide
0.7417	0.9752	0.0974	0.0922	100	100	100	100	Nucleotide
0.7064	0.8312	0.4657	0.4657	80	100	0	0	Nucleotide

0.9211	0.9918	0.9346	0.9376	100	100	100	100	Nucleotide
0.1788	1.1190	0.0412	0.0743	100	100	100	100	Nucleotide
0.8328	1.4344	0.5406	0.5445	100	100	100	100	Nucleotide
0.2801	0.8304	0.7787	0.8968	100	100	100	100	Nucleotide
0.7446	0.9940	0.5141	2.1548	100	100	100	100	Nucleotide
0.9790	0.9138	1.7789	1.8128	100	100	100	100	Nucleotide
0.1347	0.1482	0.1347	0.1347	0	40	0	0	Nucleotide
0.5453	1.2171	0.2037	0.2037	100	100	0	20	Nucleotide
0.7604	0.1742	0.2460	0.1742	80	20	40	0	Nucleotide
0.3593	1.6843	1.3659	3.1237	100	100	100	100	Nucleotide
0.7266	0.1967	0.1967	0.1967	100	20	0	0	Nucleotide
0.9970	0.6794	0.1329	0.0823	100	100	100	100	Nucleotide
0.8868	1.3038	0.9896	0.6767	100	100	100	100	Nucleotide
0.6354	0.9156	0.5346	0.6345	100	100	100	100	Nucleotide
0.6976	0.6596	1.0213	1.9481	100	100	100	100	Nucleotide
0.6387	1.4839	1.0192	1.1890	100	100	100	100	Nucleotide
0.1993	1.0813	0.3395	4.6592	100	100	100	100	Nucleotide
1.1262	1.7772	1.0107	1.1403	100	100	100	100	Nucleotide
1.2995	0.0408	0.0408	0.0408	100	0	0	20	Nucleotide
1.3080	0.6724	0.6416	1.0557	100	100	100	100	Nucleotide
0.6991	1.2412	0.1330	0.1250	100	100	100	100	Nucleotide
1.0513	2.5117	2.2566	2.6294	100	100	100	100	Nucleotide
0.3334	2.7503	0.5696	3.5344	100	100	100	100	Nucleotide
0.8713	0.9450	0.9724	1.4242	100	100	100	100	Nucleotide
0.6571	3.4605	0.6434	3.5523	80	100	60	100	Nucleotide
0.6573	4.1625	1.1159	2.7052	100	100	100	100	Nucleotide
0.3414	1.6105	1.3985	3.1955	100	100	100	100	Nucleotide
2.1851	0.4898	0.4786	1.0172	100	100	100	100	Nucleotide
1.1327	1.1692	1.1668	1.0202	100	100	100	100	Nucleotide
1.0046	0.3228	0.1948	0.2123	100	100	0	20	Nucleotide
0.8671	1.1036	0.5704	0.5899	100	100	100	100	Nucleotide
0.7126	2.4688	0.5303	1.3880	100	100	100	100	Nucleotide
0.8802	1.4551	0.3839	0.3839	100	80	0	0	Nucleotide

0.3052	0.3348	0.3742	1.0391	0	60	40	100	Nucleotide
0.8297	1.9608	0.2113	0.2676	100	100	80	100	Nucleotide
0.4534	2.8553	5.8167	7.2615	100	100	100	100	Nucleotide
0.2825	1.6490	1.5451	4.1365	80	100	100	100	Nucleotide
1.0882	1.5900	3.0325	3.9542	100	100	100	100	Nucleotide
1.1317	0.9426	1.0604	0.9097	100	100	100	100	Cofactors and Vitamins
0.5471	1.0078	0.7415	2.4632	100	100	100	100	Cofactors and Vitamins
0.6618	1.3522	0.5821	0.9835	100	100	100	100	Cofactors and Vitamins
0.1982	0.9995	0.2170	0.4118	40	100	40	80	Cofactors and Vitamins
1.2110	0.8898	0.9198	1.4494	100	100	100	100	Cofactors and Vitamins
1.3070	0.8206	1.9793	1.1744	100	100	100	100	Cofactors and Vitamins
2.9325	0.5562	1.0870	0.6250	100	100	100	100	Cofactors and Vitamins
1.0761	0.9689	0.8618	0.9784	100	100	100	100	Cofactors and Vitamins
0.1743	0.8784	0.1667	0.6103	20	100	20	100	Cofactors and Vitamins
1.2228	0.8652	0.9977	1.6470	100	100	100	100	Cofactors and Vitamins
0.0930	0.1536	0.9671	1.8702	0	40	100	80	Cofactors and Vitamins
0.3521	1.2582	2.6356	2.9032	100	100	100	100	Cofactors and Vitamins
1.3181	0.9320	0.2103	0.5084	100	100	100	100	Cofactors and Vitamins
0.4834	0.6829	0.8837	1.7099	100	100	100	100	Cofactors and Vitamins
1.1892	1.2892	1.1414	2.7684	100	100	100	100	Cofactors and Vitamins
0.7507	1.2125	0.9877	2.0447	100	100	100	100	Cofactors and Vitamins
0.6014	0.7035	0.4908	0.5628	100	100	100	100	Cofactors and Vitamins
0.2994	0.2994	0.2994	0.2994	0	0	0	0	Cofactors and Vitamins
1.3604	0.4406	1.6352	0.7904	100	100	100	100	Cofactors and Vitamins
0.9436	1.7887	0.9308	0.9476	100	100	100	100	Cofactors and Vitamins
1.1073	0.7607	1.2433	2.1605	100	100	100	100	Cofactors and Vitamins
0.6487	1.0655	1.0352	1.3821	100	100	100	100	Cofactors and Vitamins
0.2995	0.9521	0.3222	0.7950	100	100	100	100	Cofactors and Vitamins
0.4162	1.4285	0.7397	1.0999	100	100	100	100	Cofactors and Vitamins
1.0642	1.3413	1.4615	1.3968	100	100	100	100	Cofactors and Vitamins
0.9547	0.8084	1.1456	0.7237	80	100	100	100	Cofactors and Vitamins
0.2432	0.1051	0.0708	0.0830	80	40	0	40	Cofactors and Vitamins
0.9234	1.3402	1.3974	1.2855	100	100	100	100	Cofactors and Vitamins

0.8236	0.9231	1.0940	1.2578	100	100	100	100	Xenobiotics
1.4303	0.5445	1.3926	0.8989	100	80	100	100	Xenobiotics
1.0883	0.6807	1.0590	1.0494	100	100	100	100	Xenobiotics
2.7388	3.5351	1.2527	1.3186	100	100	100	100	Xenobiotics
0.6228	2.2480	0.7937	1.3005	100	100	100	100	Xenobiotics
1.0408	1.5567	1.0808	0.8326	100	100	100	100	Xenobiotics
0.8481	2.1149	1.0692	0.9328	100	100	100	100	Xenobiotics
1.1549	0.8674	1.4603	0.9100	100	100	100	100	Xenobiotics
0.9993	0.5355	1.1437	1.1908	100	100	100	100	Xenobiotics
0.9701	0.8832	1.4758	1.0213	100	100	100	100	Xenobiotics
0.5701	0.6284	0.6915	1.1391	100	100	100	100	Xenobiotics
0.8643	0.5311	1.0502	0.8791	80	100	100	100	Xenobiotics
0.5787	0.4952	0.9498	0.8405	100	100	100	100	Xenobiotics
1.0449	1.2355	1.5079	1.6559	100	100	100	100	Xenobiotics
1.8607	0.7917	1.1917	0.5297	100	100	100	100	Xenobiotics
0.5675	1.1036	1.6110	0.9897	100	100	100	100	Xenobiotics
1.1928	1.0521	1.2614	1.3159	100	100	100	100	Xenobiotics
1.2527	2.0072	2.0474	2.0901	100	100	100	100	Xenobiotics
0.8107	1.7467	0.8047	1.1564	100	100	100	100	Xenobiotics

Sub Pathway	Chemical ID	CAS	RI	Mass
Glycine, Serine and Threonine Metabolism	340	56-40-6	1375	76.03931
Glycine, Serine and Threonine Metabolism	100001006	543-24-8	826	118.04987
Glycine, Serine and Threonine Metabolism	799	107-43-7	1064	118.08626
Glycine, Serine and Threonine Metabolism	503	56-45-1	1239	106.04987
Glycine, Serine and Threonine Metabolism	100001851	97-14-3	811	148.06044
Glycine, Serine and Threonine Metabolism	564	72-19-5	1514	120.06552
Glycine, Serine and Threonine Metabolism	100001274	17093-74-2	821.6	160.06153
Alanine and Aspartate Metabolism	811	56-41-7	1700	90.05496
Alanine and Aspartate Metabolism	1110	97-69-8	861.2	130.05096
Alanine and Aspartate Metabolism	234	56-84-8	1165	134.04479
Alanine and Aspartate Metabolism	100000787	997-55-7;997-55-7	3143	174.04079
Alanine and Aspartate Metabolism	917	70-47-3	1225	133.06077
Alanine and Aspartate Metabolism	100001257	4033-40-3	785	175.07134
Glutamate Metabolism	561	56-86-0	1500	148.06044
Glutamate Metabolism	563	56-85-9	1291	147.07642
Glutamate Metabolism	100000282	8/3/17	1050	190.071
Glutamate Metabolism	100001253	2490-97-3	845	189.08699
Glutamate Metabolism	100001103	1499-55-4;1499-55-4	2170	162.07609

Glutamate Metabolism	100001540	2353-44-8	1900	129.06586
Glutamate Metabolism	100001612	3106-85-2	1035	305.09795
Glutamate Metabolism	100003271	73590-26-8	530	320.06232
Glutamate Metabolism	141	56-12-2	2048	104.07061
Glutamate Metabolism	100003152	1119-48-8	2109	118.08626
Glutamate Metabolism	35	2906-39-0	1528	114.05496
Histidine Metabolism	355	5934-29-2	755.9	154.0622
Histidine Metabolism	100001051	332-80-9	2755	170.09241
Histidine Metabolism	100000042	368-16-1	906.3	168.07785
Histidine Metabolism	100001293	39145-52-3	2065	198.08732
Histidine Metabolism	100003434	1074-59-5	2263	141.06586
Histidine Metabolism	100000263	14403-45-3	2040	157.06077
Histidine Metabolism	249	305-84-0	2942	227.11387
Histidine Metabolism	100001207	645-65-8	2055	127.05021
Lysine Metabolism	407	56-87-1	2850	147.11281
Lysine Metabolism	100001721	1946-82-3	3372.6	187.10881
Lysine Metabolism	100001734	692-04-6	2612.6	187.10881
Lysine Metabolism	189	23284-33-5	2825	189.15976
Lysine Metabolism	100002462	32448-36-5	2755	325.16055
Lysine Metabolism	381	542-32-5;1118-90-7	3500	160.06153
Lysine Metabolism	1025	4043-87-2	2200	130.08626
Lysine Metabolism	100000454	660-88-8	2220	118.08626
Lysine Metabolism	100015962		2186	160.13321
Phenylalanine Metabolism	460	63-91-2	2878	166.08626
Phenylalanine Metabolism	100001256	2018-61-3	2597	206.08226
Phenylalanine Metabolism	100000774	828-01-3	2208	165.05571
Tyrosine Metabolism	815	60-18-4	2430	182.08117
Tyrosine Metabolism	1141	156-39-8	1690	179.03498
Tyrosine Metabolism	240	6482-98-0	1379	181.05063
Tyrosine Metabolism	100001510	937-34-8	2156	172.9914
Tyrosine Metabolism	100004290	2370-61-8	2772	182.08117
Tyrosine Metabolism	100002078	1080-06-4	2790	196.09682
Tyrosine Metabolism	100006056	13200-85-6	2360	192.06661

Tryptophan Metabolism	565	73-22-3	2986	205.09716
Tryptophan Metabolism	100006379	180509-18-6	1777	365.13542
Tryptophan Metabolism	100000265	2922-83-0	2739	209.09207
Tryptophan Metabolism	504	153-98-0	2550	177.10224
Tryptophan Metabolism	100000463	832-97-3	2286	204.06661
Leucine, Isoleucine and Valine Metabolism	397	61-90-5	2864	132.10191
Leucine, Isoleucine and Valine Metabolism	1082	1188-21-2	2400	172.09791
Leucine, Isoleucine and Valine Metabolism	100000551	816-66-0	2170	129.05571
Leucine, Isoleucine and Valine Metabolism	100001393	31023-24-2	3085	246.16999
Leucine, Isoleucine and Valine Metabolism	1442	625-08-1	1149.8	117.05572
Leucine, Isoleucine and Valine Metabolism	100002458	5746-90-7	2700	99.04518
Leucine, Isoleucine and Valine Metabolism	376	73-32-5	2800	132.10191
Leucine, Isoleucine and Valine Metabolism	100001276	3077-46-1	2325	172.09791
Leucine, Isoleucine and Valine Metabolism	100000036	1460-34-0;51829-07-3	2064.2	129.05572
Leucine, Isoleucine and Valine Metabolism	100001300	600-37-3	1052	117.05571
Leucine, Isoleucine and Valine Metabolism	100001509	31023-25-3	3035	246.16999
Leucine, Isoleucine and Valine Metabolism	100001597	64191-86-2	2962	244.15434
Leucine, Isoleucine and Valine Metabolism	2054	601-75-2	2785	131.03498
Leucine, Isoleucine and Valine Metabolism	2051	498-21-5	2800	131.03498
Leucine, Isoleucine and Valine Metabolism	566	72-18-4	2479	118.08626
Leucine, Isoleucine and Valine Metabolism	1084	96-81-1	1704	158.08226
Leucine, Isoleucine and Valine Metabolism	100000936	3715-29-5	911	115.04006
Leucine, Isoleucine and Valine Metabolism	100001055	25518-49-4	2810	232.15434
Leucine, Isoleucine and Valine Metabolism	111	2068-83-9	1619	103.04007
Methionine, Cysteine, SAM and Taurine Metabolism	415	63-68-3	2526	150.05833
Methionine, Cysteine, SAM and Taurine Metabolism	1083	65-82-7	1787	190.05434
Methionine, Cysteine, SAM and Taurine Metabolism	194	4289-98-9	1543.8	176.03869
Methionine, Cysteine, SAM and Taurine Metabolism	100004635	820-10-0	1250	182.04816
Methionine, Cysteine, SAM and Taurine Metabolism	100000039	3226-65-1	1272	166.05325
Methionine, Cysteine, SAM and Taurine Metabolism	100005463	108646-71-5	880	208.06381
Methionine, Cysteine, SAM and Taurine Metabolism	1263	24346-00-7;86867-01-8;86867-0108	3002	399.14452
Methionine, Cysteine, SAM and Taurine Metabolism	197	979-92-0	1832.4	383.11431
Methionine, Cysteine, SAM and Taurine Metabolism	311	454-29-5	2155	136.04268

Methionine, Cysteine, SAM and Taurine Metabolism	310	535-34-2	2270	223.07471
Methionine, Cysteine, SAM and Taurine Metabolism	800	52-90-4;56-89-3	1488	122.02703
Methionine, Cysteine, SAM and Taurine Metabolism	1107	616-91-1	1416	164.0376
Methionine, Cysteine, SAM and Taurine Metabolism	279	56-89-3	3424	239.01657
Methionine, Cysteine, SAM and Taurine Metabolism	358	300-84-5	724	110.02703
Methionine, Cysteine, SAM and Taurine Metabolism	512	107-35-7	660	126.02195
Methionine, Cysteine, SAM and Taurine Metabolism	100005466		800	166.01795
Methionine, Cysteine, SAM and Taurine Metabolism	382	498-40-8	2890	167.99722
Urea cycle; Arginine and Proline Metabolism	231	1119-34-2	2825	175.11896
Urea cycle; Arginine and Proline Metabolism	232	156637-58-0	2745	291.12992
Urea cycle; Arginine and Proline Metabolism	444	3184-13-2	2800	133.09716
Urea cycle; Arginine and Proline Metabolism	391	372-75-8	1520	176.10297
Urea cycle; Arginine and Proline Metabolism	100000963	1190-49-4	1908	190.11862
Urea cycle; Arginine and Proline Metabolism	480	147-85-3	1603	116.07061
Urea cycle; Arginine and Proline Metabolism	100001810	102783-24-4	2850	203.15026
Urea cycle; Arginine and Proline Metabolism	100001266	155-84-0	2245	217.12952
Urea cycle; Arginine and Proline Metabolism	100004523		1877	175.10772
Urea cycle; Arginine and Proline Metabolism	1001	51-35-4	1064	132.06552
Urea cycle; Arginine and Proline Metabolism	100001167	18684-24-7	2128	229.11829
Urea cycle; Arginine and Proline Metabolism	100001956	475-11-6	1335	130.08626
Urea cycle; Arginine and Proline Metabolism	100004488	53308-83-1	2845	189.13461
Creatine Metabolism	344	352-97-6	1937	118.06111
Creatine Metabolism	1221	57-00-1	1947	132.07676
Creatine Metabolism	275	60-27-5	2055	114.06619
Polyamine Metabolism	49	110-60-1	3027	89.10733
Polyamine Metabolism	50	124-20-9	3355	146.16518
Polyamine Metabolism	100002132	61345-83-3	3105	287.24416
Polyamine Metabolism	212	2457-80-9	2752	298.09684
Polyamine Metabolism	192	18233-70-0	2230	131.11789
Polyamine Metabolism	100016038		3080	188.17574
Guanidino and Acetamido Metabolism	100000096	463-003;463-00-3	2320	146.09241
Glutathione Metabolism	496	70-18-8	2000	308.09109
Glutathione Metabolism	448	103239-24-3	2667	613.15925

Glutathione Metabolism	100001437	13081-14-6	2465	427.09519
Glutathione Metabolism	100001259	2922-56-7	1075	320.09218
Glutathione Metabolism	278	19246-18-5	2132	179.0485
Glutathione Metabolism	1021	98-79-3	738.5	128.03531
Glutathione Metabolism	100008928		1258	103.04006
Glutathione Metabolism	100006240	99927-70-5	3387.5	462.19156
Gamma-glutamyl Amino Acid	1036	636-58-8	2118	251.06963
Gamma-glutamyl Amino Acid	331	1116-22-9	1775	277.10303
Gamma-glutamyl Amino Acid	1140	10148-81-9	1430	276.11902
Gamma-glutamyl Amino Acid	100001294	1948-29-4	1535	205.0819
Gamma-glutamyl Amino Acid	100001485		1600	259.12994
Gamma-glutamyl Amino Acid	1268	2566-39-4	1685	259.12994
Gamma-glutamyl Amino Acid	100001262	17105-15-6	2717	276.1554
Gamma-glutamyl Amino Acid	100001313	17663-87-5	2640	279.10092
Gamma-glutamyl Amino Acid	100000491	7432-24-8	1825	293.11429
Gamma-glutamyl Amino Acid	100001314	5652-48-2	1750	249.10812
Gamma-glutamyl Amino Acid	1102	7432-23-7	1240	309.10921
Gamma-glutamyl Amino Acid	100001126	2746-34-1	2700	247.12885
Gamma-glutamyl Amino Acid	100001502	16869-42-4	2380	233.1132
Dipeptide	100001790	19461-38-2	1820	187.10881
Dipeptide	100001258	869-19-2	1891	187.10881
Dipeptide	100000487	1963-21-9	1320	173.09316
Dipeptide	100003169	868-28-0	1992	187.10881
Dipeptide	100003185	686-50-0	2050	187.10881
Dipeptide	100003588	721-90-4	2898	223.10772
Dipeptide	100003674	2578-57-6	2136	173.09207
Dipeptide	100001125	16875-27-7	2322	265.11938
Dipeptide	100003598	673-05-5	1635	237.08808
Dipeptide	100003641	686-43-1	1506	173.09316
Dipeptide	100003210	22906-55-4	3138	231.17032
Dipeptide	100003183		2620	260.1605
Acetylated Peptides	100001275	500-98-1	2375	192.06661
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	572	50-99-7	2342	179.05611

Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	291	103192-55-8	4537	259.02244
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	1233	56401-20-8	4277	259.02244
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	100002180		551	338.98897
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	309	102783-56-2	539	171.00531
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	100000093	70195-25-4	4346	184.98566
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	132	80731-10-8	583	184.98566
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	463	10526-80-4	587.3	166.9751
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	823	127-17-3	2650	175.02481
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	482	79-33-4	681.6	89.02442
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	1052	600-19-1	2070.4	105.01933
Pentose Phosphate Pathway	100000341	921-62-0;53411-70-4	583.9	275.01735
Pentose Phosphate Pathway	219	50-99-7;58459-37-3	4025	229.01188
Pentose Phosphate Pathway	166	108321-05-7	570	308.97822
Pentose Phosphate Pathway	100001628	2646-35-7	599.6	289.033
Pentose Phosphate Pathway	100002179		3888	229.01187
Pentose Metabolism	914	50-69-1	1508.2	195.05103
Pentose Metabolism	100000406	488-81-3	1789.6	151.06119
Pentose Metabolism	100001007	8/3/36	2425	165.04046
Pentose Metabolism	100006430		1932.4	151.0612
Pentose Metabolism	100006115		2700	165.04046
Pentose Metabolism	100002619	3019-74-7	2255	209.06667
Pentose Metabolism	100019968		2350	165.04046
Disaccharides and Oligosaccharides	393	5965-66-2	3500	387.11442
Fructose, Mannose and Galactose Metabolism	878	57-48-7	2065	179.05611
Fructose, Mannose and Galactose Metabolism	100001740		2320	181.07176
Fructose, Mannose and Galactose Metabolism	803	3458-28-4	2200	179.05611
Fructose, Mannose and Galactose Metabolism	294	70442-25-0;104872-94-8	4510	259.02244
Fructose, Mannose and Galactose Metabolism	1003	608-66-2	2360	181.07176
Fructose, Mannose and Galactose Metabolism	100000300	19046-60-7	4552	259.02244
Nucleotide Sugar	1096	117756-22-6	3950	565.04775
Nucleotide Sugar	100000298	2956-16-3;91183-98-1;137868-52-1	4000	565.04774
Nucleotide Sugar	1097	28053-08-9;63700-19-6	588	579.02701
Nucleotide Sugar	335	15839-70-0	755	588.07497

Nucleotide Sugar	100002957		3665	606.07429
Nucleotide Sugar	1223	3063-71-6	3900	613.13999
Aminosugar Metabolism	100000257	207300-70-7	3233.3	193.03537
Aminosugar Metabolism	1213	102029-88-9	4114	300.04899
Aminosugar Metabolism	1212	31281-59-1	4052	300.04899
Aminosugar Metabolism	1162	131-48-6	3072.6	308.0987
Aminosugar Metabolism	1215	2776-93-4	1212	336.14015
Aminosugar Metabolism	100001320	88759-55-1	2186	135.02989
Aminosugar Metabolism	100006435		715	222.0972
TCA Cycle	1124	77-92-9	582	191.01973
TCA Cycle	100001359		580	173.00916
TCA Cycle	1206	20226-99-7	4400	191.01973
TCA Cycle	100009239	4702-32-3	2970	173.00916
TCA Cycle	93	305-72-6;328-50-7;22202-68-2	2700	145.01425
TCA Cycle	100001948	256928-74-2	2291	262.12852
TCA Cycle	252	110-15-6	3149	117.01933
TCA Cycle	330	100-17-8	3084	115.00368
TCA Cycle	409	6915-15-7	615.6	133.01425
TCA Cycle	100008929		575	205.03538
Oxidative Phosphorylation	1211	94249-01-1	4013.9	138.98018
Oxidative Phosphorylation	461	7664-38-2	576	98.98418
Medium Chain Fatty Acid	181	143-07-7	5300	199.17035
Medium Chain Fatty Acid	100001232	2430-94-6	5224	197.1547
Long Chain Fatty Acid	519	544-63-8	5440	227.20165
Long Chain Fatty Acid	100001198	544-64-9	5346.9	225.186
Long Chain Fatty Acid	980	1002-84-2;10002-84-2	5521	241.2173
Long Chain Fatty Acid	424	57-10-3	5618	255.23295
Long Chain Fatty Acid	452	373-49-9	5475	253.2173
Long Chain Fatty Acid	891	506-12-7	5731	269.2486
Long Chain Fatty Acid	100001278	29743-97-3	5555	267.23295
Long Chain Fatty Acid	439	57-11-4	5872	283.26425
Long Chain Fatty Acid	100008930		5655	281.2486
Long Chain Fatty Acid	892	646-30-0	6068	297.2799

Long Chain Fatty Acid	100001277	73033-09-7	5780	295.26425
Long Chain Fatty Acid	893	506-30-9	6240	311.29555
Long Chain Fatty Acid	100001335		5950	309.2799
Long Chain Fatty Acid	314	112-85-6	6745	339.32685
Long Chain Fatty Acid	1087	112-86-7	6355.6	337.3112
Polyunsaturated Fatty Acid (n3 and n6)	100015797	24257-10-1	5514	315.23295
Polyunsaturated Fatty Acid (n3 and n6)	100001229	111174-40-4	5395	275.20165
Polyunsaturated Fatty Acid (n3 and n6)	2050	10-2005-9;10417-94-4	5450	301.2173
Polyunsaturated Fatty Acid (n3 and n6)	100001181	2234-74-4	5571	329.2486
Polyunsaturated Fatty Acid (n3 and n6)	100000665	6217-54-5	5525	327.23295
Polyunsaturated Fatty Acid (n3 and n6)	100015785	68378-49-4	5657	355.26425
Polyunsaturated Fatty Acid (n3 and n6)	180	60-33-3	5535	279.23295
Polyunsaturated Fatty Acid (n3 and n6)	100001337		5450	277.2173
Polyunsaturated Fatty Acid (n3 and n6)	100001739	17046-59-2	5596	305.2486
Polyunsaturated Fatty Acid (n3 and n6)	229	506-32-1	5535	303.23295
Polyunsaturated Fatty Acid (n3 and n6)	100001193	2091-25-0	5678	331.26425
Polyunsaturated Fatty Acid (n3 and n6)	100001580	25182-74-5	5624.5	329.2486
Polyunsaturated Fatty Acid (n3 and n6)	100001182	7370-49-2	6034	335.29555
Polyunsaturated Fatty Acid (n3 and n6)	1231	2091-39-6	5730	307.26425
Polyunsaturated Fatty Acid (n3 and n6)	100001200	506-21-8	5575	279.23295
Polyunsaturated Fatty Acid (n3 and n6)	100001472	20590-32-3	5650	305.2486
Polyunsaturated Fatty Acid (n3 and n6)	100015762		5850	333.27989
Fatty Acid, Branched	100002344	2485-71-4	5499	241.2173
Fatty Acid, Branched	100002945		5695	269.24868
Fatty Acid, Branched	100002356	2724-59-6	5993	297.2799
Fatty Acid, Dicarboxylate	339	110-94-1	2900	131.03498
Fatty Acid, Dicarboxylate	100002070	40951-21-1	958	166.071
Fatty Acid, Dicarboxylate	100000707	110-16-7	2510	115.00368
Fatty Acid Metabolism (also BCAA Metabolism)	100001054	25576-40-3	2860	232.15434
Fatty Acid Metabolism (also BCAA Metabolism)	100001162	17298-37-2	2590	218.13869
Fatty Acid Metabolism (also BCAA Metabolism)	418	516-05-2	3078.4	117.01933
Fatty Acid Metabolism(Acyl Carnitine)	100000802	5080-50-2	2282	204.12304
Fatty Acid Metabolism(Acyl Carnitine)	100003926		2400	248.14925

Fatty Acid Metabolism(Acyl Carnitine)	100009271		2340	248.14925
Fatty Acid Metabolism(Acyl Carnitine)	100001394	40225-14-7	3112	246.16999
Fatty Acid Metabolism(Acyl Carnitine)	100000781	6920-35-0	3308	260.18564
Fatty Acid Metabolism(Acyl Carnitine)	100001247	3671-77-0	950	288.21694
Fatty Acid Metabolism(Acyl Carnitine)	100001251	1492-27-9	1130	316.24824
Fatty Acid Metabolism(Acyl Carnitine)	100016069		1135	342.26389
Fatty Acid Metabolism(Acyl Carnitine)	100001392	25518-54-1	1235	344.27954
Fatty Acid Metabolism(Acyl Carnitine)	100001270	18822-89-4	1350	372.31084
Fatty Acid Metabolism(Acyl Carnitine)	100000776	6865-14-1	1425	400.34214
Fatty Acid Metabolism(Acyl Carnitine)	100009406		1357	398.32649
Fatty Acid Metabolism(Acyl Carnitine)	100001391	18822-91-8	1485	428.37344
Fatty Acid Metabolism(Acyl Carnitine)	100003151	36816-10-1	1430	424.34214
Fatty Acid Metabolism(Acyl Carnitine)	100015831		1310	422.32649
Fatty Acid Metabolism(Acyl Carnitine)	100001501	38677-66-6	1423	426.35779
Fatty Acid Metabolism(Acyl Carnitine)	100006051	889848-55-9	1316	370.29471
Fatty Acid Metabolism(Acyl Carnitine)	100015833		1512	456.40474
Fatty Acid Metabolism(Acyl Carnitine)	100015837		1353	448.34215
Fatty Acid Metabolism(Acyl Carnitine)	100015832		1561	484.43604
Fatty Acid Metabolism(Acyl Carnitine)	100015839		1436	452.37343
Fatty Acid Metabolism(Acyl Carnitine)	100015838		1484	454.38909
Fatty Acid Metabolism(Acyl Carnitine)	100015849		1460	478.38909
Fatty Acid Metabolism(Acyl Carnitine)	100015851		1387	474.35777
Fatty Acid Metabolism(Acyl Carnitine)	100015834		1603	512.46733
Fatty Acid Metabolism(Acyl Carnitine)	100004054	106182-29-0	1424	414.35779
Fatty Acid Metabolism(Acyl Carnitine)	100015846		1602	510.45168
Carnitine Metabolism	100001662	6249-56-5	2052	146.11756
Carnitine Metabolism	100000007	461-05-2	1978	162.11247
Ketone Bodies	254	625-72-9	1444	103.04007
Fatty Acid Metabolism (Acyl Choline)	100009331		1449	368.35231
Fatty Acid, Monohydroxy	100015638		6345	381.33742
Fatty Acid, Monohydroxy	100001579	764-67-0	5511.2	271.22786
Fatty Acid, Monohydroxy	100000997	5561-87-5	4634.7	187.13396
Fatty Acid, Monohydroxy	100001112	53941-38-1	5175	215.16526

Fatty Acid, Monohydroxy	100000882	3422-31-9	5335	243.19656
Fatty Acid, Monohydroxy	100000983	928-17-6	5476	271.22786
Fatty Acid, Monohydroxy	100008933	45261-96-9	5674	299.25917
Endocannabinoid	1137	11-58-0;111-58-0	1661	326.30536
Endocannabinoid	1489	544-31-0	1643	300.28971
Endocannabinoid	1488	94421-68-8	1535	348.28971
Endocannabinoid	100003119	52514-04-2	5610	388.2527
Endocannabinoid	100003240	63155-80-6	5782	390.26835
Endocannabinoid	100003239	83982-06-3	5560	362.23705
Endocannabinoid	100015862		1546	298.27406
Inositol Metabolism	363	87-89-8	3506.3	225.06159
Inositol Metabolism	100001859	643-12-9	3191.2	225.06159
Inositol Metabolism	370	573-35-3;106032-59-1	4785	259.02244
Phospholipid Metabolism	1256	67-48-1	1961	104.10699
Phospholipid Metabolism	267	72556-74-2	700	184.07332
Phospholipid Metabolism	1220	33818-15-4	4200	533.10553
Phospholipid Metabolism	100000269	28319-77-9	672	258.1101
Phospholipid Metabolism	1026	1071-23-4	638	140.01182
Phospholipid Metabolism	100001407	72842-05-8	4210	445.0531
Phospholipid Metabolism	100001620	33049-08-0	3075	214.04859
Phospholipid Metabolism	100015666		577	260.05298
Phospholipid Metabolism	100001621	16824-65-0	3850	333.05922
Phosphatidylcholine (PC)	100000672	69525-80-0	2147	706.53813
Phosphatidylcholine (PC)	100009139		1914	754.53813
Phosphatidylcholine (PC)	100000657	63-89-8	2365	734.56944
Phosphatidylcholine (PC)	100008984		2160	732.55378
Phosphatidylcholine (PC)	100008921	59403-51-9	2653	762.60074
Phosphatidylcholine (PC)	1539	26853-31-6;26853-31-6	2358	760.58509
Phosphatidylcholine (PC)	1537	40811-94-7	2160	758.56944
Phosphatidylcholine (PC)	100008983		2155	758.56944
Phosphatidylcholine (PC)	100009345		1850	754.53813
Phosphatidylcholine (PC)	100008985		2199	784.58509
Phosphatidylcholine (PC)	100008914	35418-58-7	2091	782.56944

Phosphatidylcholine (PC)	100008915	59403-54-2	2023	806.56944
Phosphatidylcholine (PC)	100008904	56421-10-4	2644	788.61639
Phosphatidylcholine (PC)	100008980		2380	786.60074
Phosphatidylcholine (PC)	100008905	4235-95-4	2346	786.60074
Phosphatidylcholine (PC)	100008981		2165	784.58509
Phosphatidylcholine (PC)	100008903	998-06-1	2006	782.56944
Phosphatidylcholine (PC)	100001869	35418-59-8	2300	810.60074
Phosphatidylcholine (PC)	100009131		1969	806.56944
Phosphatidylcholine (PC)	100008916	59403-52-0	2197	834.60128
Phosphatidylcholine (PC)	100009130		2011	832.58509
Phosphatidylethanolamine (PE)	100009204		2498	692.52248
Phosphatidylethanolamine (PE)	100009205		2850	720.55378
Phosphatidylethanolamine (PE)	1526	26662-94-2	2509	718.53813
Phosphatidylethanolamine (PE)	100001870		2275	716.52248
Phosphatidylethanolamine (PE)	100008995		2250	716.52248
Phosphatidylethanolamine (PE)	100008990		2198	740.52248
Phosphatidylethanolamine (PE)	100008991		2119	764.52248
Phosphatidylethanolamine (PE)	100001856		2858	746.56944
Phosphatidylethanolamine (PE)	100008906	5/1/04	2485	744.55378
Phosphatidylethanolamine (PE)	100009078		2270	742.53813
Phosphatidylethanolamine (PE)	100008977		2424	768.55378
Phosphatidylethanolamine (PE)	100009219		2200	766.53813
Phosphatidylethanolamine (PE)	100008992		2317	792.55378
Phosphatidylethanolamine (PE)	100009220		2119	790.53813
Phosphatidylserine (PS)	1531	40290-44-6	2660	762.52797
Phosphatidylserine (PS)	100000639		3000	790.55926
Phosphatidylserine (PS)	100001872		2565	812.54361
Phosphatidylglycerol (PG)	100000652	200880-41-7	3157	740.54362
Phosphatidylglycerol (PG)	100000641		3206	766.55927
Phosphatidylglycerol (PG)	100001866	322647-48-3	3714	794.59057
Phosphatidylglycerol (PG)	1541	67254-28-8	3149	792.57492
Phosphatidylinositol (PI)	100009169		3122	828.55966
Phosphatidylinositol (PI)	100009066		3140	854.57531

Phosphatidylinositol (PI)	100008993		2567	876.55966
Phosphatidylinositol (PI)	100009181		3711	882.60661
Phosphatidylinositol (PI)	100008994		3185	880.59096
Phosphatidylinositol (PI)	100008908		3121	880.59096
Phosphatidylinositol (PI)	100000616	383907-33-3	3000	904.59096
Phosphatidylinositol (PI)	100010951		2568	902.57531
Lysophospholipid	100001263	17364-16-8	1525	496.33977
Lysophospholipid	100001562		1505	496.33977
Lysophospholipid	100001511		1450	494.32412
Lysophospholipid	100001561		1425	494.32412
Lysophospholipid	100001271	19420-57-6	1606	524.37107
Lysophospholipid	100001272	19420-56-5	1540	522.35542
Lysophospholipid	100001395		1465	520.33977
Lysophospholipid	100002873	325171-59-3	1907	608.46497
Lysophospholipid	100001567	53862-35-4	1544	454.29282
Lysophospholipid	100001461	69747-55-3	1626	482.32412
Lysophospholipid	100003901		6350	480.30956
Lysophospholipid	100001569	89576-29-4	1554	480.30847
Lysophospholipid	100001570		5900	476.27826
Lysophospholipid	100001571		5874	500.27826
Lysophospholipid	100005805		5572	496.26809
Lysophospholipid	100004327		1634	526.31395
Lysophospholipid	100000630	326589-90-6	5607	522.28374
Lysophospholipid	100005717		5570	483.27284
Lysophospholipid	100001462		5816	511.30414
Lysophospholipid	100005716		5610	509.28849
Lysophospholipid	100009227		5516	507.27284
Lysophospholipid	100001655		5564	571.28888
Lysophospholipid	100000656	796963-93-4	1700	601.33474
Lysophospholipid	100001777		5599	597.30453
Lysophospholipid	100001778		5494	595.28888
Lysophospholipid	100001654		5482	619.28888
Glycolipid Metabolism	100003064	16232-91-0	2518	299.09837

Plasmalogen	100009005		2600	702.54322
Plasmalogen	100009069		2351	700.52757
Plasmalogen	100009162		2454	718.57452
Plasmalogen	100009160		2218	716.55887
Plasmalogen	100009002		2270	724.52757
Plasmalogen	100009007		2443	744.59017
Plasmalogen	100008919	144371-68-6	2950	730.57452
Plasmalogen	100009014		2154	766.57452
Plasmalogen	100009009		2226	742.57452
Plasmalogen	100008999		2511	752.55887
Lysoplasmalogen	100002875		1547	480.34485
Lysoplasmalogen	100003000		1558	438.2979
Lysoplasmalogen	100005372		1566	464.3136
Lysoplasmalogen	100003001		1649	466.3292
Lysoplasmalogen	100010839		2534	728.55887
Glycerolipid Metabolism	1254	56-81-5	758	91.04007
Glycerolipid Metabolism	100000258	29849-82-9	580	173.02095
Glycerolipid Metabolism	100001619		2430	245.04317
Monoacylglycerol	100001618	75685-84-6	6353.3	227.20163
Monoacylglycerol	100001431	104140-07-0	6200	241.21728
Monoacylglycerol	100000827	542-44-9	6550	255.23293
Monoacylglycerol	100008952		6094	253.21727
Monoacylglycerol	100001429	68002-72-2	6571	269.24858
Monoacylglycerol	100000924	111-03-5	6650	281.24858
Monoacylglycerol	100001040	2277-28-3	6477	279.23293
Monoacylglycerol	100006121		6400	305.24858
Monoacylglycerol	100001433	35474-99-8	6250	303.23293
Monoacylglycerol	100001481		6150	309.22236
Monoacylglycerol	100001408	27214-38-6	6230	227.20163
Monoacylglycerol	100001048	23470-00-0	6400	255.23293
Monoacylglycerol	100008953		6016	253.21727
Monoacylglycerol	100000943	3443-84-3	6500	281.24858
Monoacylglycerol	100000987	3443-82-1	6250	279.23293

Monoacylglycerol	10000584	53847-30-6	6170	303.23293
Monoacylglycerol	100006352		6050	309.22236
Diacylglycerol	100010958		2636	556.49356
Diacylglycerol	100010959		2716	556.49356
Diacylglycerol	100010934		3057	584.52486
Diacylglycerol	100010935		3183	584.52486
Diacylglycerol	100010940		2733	608.52486
Diacylglycerol	100015682		3054	558.50921
Diacylglycerol	100015610		3180	558.50921
Diacylglycerol	100010947		3568	586.54051
Diacylglycerol	100010948		3734	586.54051
Diacylglycerol	100015686		2708	582.50921
Diacylglycerol	100010916		3562	612.55616
Diacylglycerol	100010917		3695	612.55616
Diacylglycerol	100009055		3197	610.54051
Diacylglycerol	100010939		2834	608.52486
Diacylglycerol	100009053		3035	610.54051
Diacylglycerol	100009054		3154	610.54051
Diacylglycerol	100010915		3265	636.55616
Diacylglycerol	100010924		2916	634.54051
Diacylglycerol	100010925		3015	634.54051
Diacylglycerol	100010918		3571	638.57181
Diacylglycerol	100010919		3695	638.57181
Diacylglycerol	100002989	106292-55-1	3115	636.55616
Diacylglycerol	100002990	104346-53-4	3223	636.55616
Diacylglycerol	100010949		3404	662.57181
Diacylglycerol	100010950		3522	662.57181
Diacylglycerol	100010937		2990	660.55616
Diacylglycerol	100015617		3256	686.57181
Sphingolipid Metabolism	313	3102-56-5	1413	302.30536
Sphingolipid Metabolism	100001436	18944-28-0	1400	300.28971
Sphingolipid Metabolism	100009028	5966-29-0	3090	540.53503
Sphingolipid Metabolism	100015609		2490	536.50372

Sphingolipid Metabolism	100015624		3911	620.59763
Sphingolipid Metabolism	100009038		2060	677.5592
Sphingolipid Metabolism	100008954		2290	705.5905
Sphingolipid Metabolism	100009026		3150	789.68441
Sphingolipid Metabolism	100002107	6254-89-3	2168	703.57485
Sphingolipid Metabolism	1538	85187-10-6;85187-10-6	2400	731.60615
Sphingolipid Metabolism	100006294		3083	787.66876
Sphingolipid Metabolism	100008955		3200	801.68441
Sphingolipid Metabolism	100006298	60037-60-7	3437	815.70006
Sphingolipid Metabolism	100004328		1998	675.54355
Sphingolipid Metabolism	100005985		1860	673.5279
Sphingolipid Metabolism	100006314	121999-58-4	2082	689.5592
Sphingolipid Metabolism	100004329		2002	701.5592
Sphingolipid Metabolism	100008920	121999-64-2	2312	717.5905
Sphingolipid Metabolism	100002106	108392-10-5	2167	729.5905
Sphingolipid Metabolism	100006290		2685	759.6375
Sphingolipid Metabolism	100009025		2793	773.65311
Sphingolipid Metabolism	100006295		2666	785.65311
Sphingolipid Metabolism	100008956		2845	799.66868
Sphingolipid Metabolism	100005986	94359-13-4	3033	813.68441
Sphingolipid Metabolism	100008957		2635	811.66868
Sphingolipid Metabolism	297	123-78-4	1393	300.28971
Sphingolipid Metabolism	469	554-62-1	1367	318.30027
Sphingolipid Metabolism	100015791		2315	797.65308
Sphingolipid Metabolism	100015789		2215	809.65308
Sphingolipid Metabolism	100015792		3220	829.71571
Sphingolipid Metabolism	100006296		2209	783.63746
Sphingolipid Metabolism	100015786		2600	761.65311
Sphingolipid Metabolism	100009027		2362	733.6218
Sphingolipid Metabolism	100015793		1837	687.54355
Sphingolipid Metabolism	100015787		2330	745.62178
Sphingolipid Metabolism	100015724	6918-48-5	1377	286.27406
Sphingolipid Metabolism	100015723		1289	272.25841

Sphingolipid Metabolism	100015731		2645	524.50374
Sphingolipid Metabolism	922	2304-80-5	3526	568.56632
Sphingolipid Metabolism	100015643	25696-03-1	1350	298.27406
Sphingolipid Metabolism	100015700		3380	808.66608
Ceramides	1518	24696-26-2	2893	538.51937
Ceramides	1547	104404-17-3	3392	566.55067
Ceramides	100015632		2846	564.53503
Ceramides	100015727		3850	620.59763
Ceramides	100015735		2477	510.48808
Ceramides	100015737		3055	552.53505
Ceramides	100015744		3858	646.6133
Ceramides	100009272		2623	700.5722
Ceramides	100001882		3053	728.6035
Ceramides	100015714		3432	756.6348
Ceramides	100015625		3420	782.65045
Ceramides	100015694		3134	730.61915
Ceramides	100009030	4201-62-1	2527	862.62502
Ceramides	100015730		3373	782.65045
Ceramides	100015751		3667	796.66609
Mevalonate Metabolism	112	503-49-1	2850	161.04555
Sterol	266	57-88-5	2707	369.35159
Sterol	100005999		1930	367.33594
Purine Metabolism, (Hypo)Xanthine/Inosine containing	362	4691-65-0	4267.7	347.03982
Purine Metabolism, (Hypo)Xanthine/Inosine containing	361	58-63-9	1269	269.08805
Purine Metabolism, (Hypo)Xanthine/Inosine containing	171	68-94-0	1291.2	135.03123
Purine Metabolism, (Hypo)Xanthine/Inosine containing	1004	69-89-6	910	151.02615
Purine Metabolism, (Hypo)Xanthine/Inosine containing	100000299	146-80-5	1075	283.0684
Purine Metabolism, (Hypo)Xanthine/Inosine containing	100000135	890-38-0	1688	251.07857
Purine Metabolism, (Hypo)Xanthine/Inosine containing	1134	69-93-2;120K5305	757.1	167.02106
Purine Metabolism, (Hypo)Xanthine/Inosine containing	1002	97-59-6	1672	157.03671
Purine Metabolism, Adenine containing	208	20398-34-9	680	426.02214
Purine Metabolism, Adenine containing	209	149022-20-8	822	346.05581
Purine Metabolism, Adenine containing	100001694	130-49-4	1497.7	346.0558

Purine Metabolism, Adenine containing	207	60-92-4	1952.2	328.04524
Purine Metabolism, Adenine containing	1303	19046-78-7	560	462.0668
Purine Metabolism, Adenine containing	798	58-61-7	2169	268.10404
Purine Metabolism, Adenine containing	880	73-24-5	2221	136.06178
Purine Metabolism, Adenine containing	54	5142-22-3	2133	150.07743
Purine Metabolism, Adenine containing	100001415	24719-82-2	2164	411.12698
Purine Metabolism, Adenine containing	1228	72003-83-9	1050	410.02723
Purine Metabolism, Adenine containing	100000485	653-63-4	1315	330.06089
Purine Metabolism, Adenine containing	100002712	56432-02-1	1213.7	755.07465
Purine Metabolism, Adenine containing	100001664	4542-23-8	940	382.10043
Purine Metabolism, Guanine containing	346	43139-22-6	639	442.01706
Purine Metabolism, Guanine containing	347	12/9/50	800	364.06528
Purine Metabolism, Guanine containing	1099	118-00-3	1662	282.08439
Purine Metabolism, Guanine containing	172	73-40-5	2032	152.05669
Purine Metabolism, Guanine containing	100001456	578-76-7	2175	166.07234
Purine Metabolism, Guanine containing	348	961-07-9	1751	266.08948
Pyrimidine Metabolism, Orotate containing	445	50887-69-9	1638.1	155.00983
Pyrimidine Metabolism, Orotate containing	100001416	314-50-1	2250	287.05209
Pyrimidine Metabolism, Uracil containing	871	19817-92-6	572	482.96126
Pyrimidine Metabolism, Uracil containing	870	21931-53-3	599.5	402.99492
Pyrimidine Metabolism, Uracil containing	869	3387-36-8	4150	323.02859
Pyrimidine Metabolism, Uracil containing	535	58-96-8	1457.6	243.06226
Pyrimidine Metabolism, Uracil containing	825	66-22-8	1089.7	111.02
Pyrimidine Metabolism, Uracil containing	821	1445-07-4	1100	243.06226
Pyrimidine Metabolism, Uracil containing	100001425	5/4/27	1119	245.07791
Pyrimidine Metabolism, Uracil containing	100001446	1463-10-1	1778.1	257.07791
Pyrimidine Metabolism, Uracil containing	536	951-78-0	1100	273.07281
Pyrimidine Metabolism, Uracil containing	1053	462-88-4	875	133.06077
Pyrimidine Metabolism, Uracil containing	244	56-41-7;107-95-9	1905	90.05496
Pyrimidine Metabolism, Cytidine containing	280	34393-59-4	580	402.01091
Pyrimidine Metabolism, Cytidine containing	282	63-37-6	835	324.05914
Pyrimidine Metabolism, Cytidine containing	827	65-46-3	1325	242.07824
Pyrimidine Metabolism, Cytidine containing	298	1032-65-1	975	308.06422

Pyrimidine Metabolism, Cytidine containing	100010895	2140-72-9	2411	258.10845
Pyrimidine Metabolism, Thymine containing	1248	33430-62-5	883	321.04933
Pyrimidine Metabolism, Thymine containing	872	50-89-5	1963.7	241.08299
Pyrimidine Metabolism, Thymine containing	882	65-71-4	1654	125.03565
Purine and Pyrimidine Metabolism	100001805	7023-27-0	544	112.99983
Nicotinate and Nicotinamide Metabolism	432	98-92-0	1942	123.05529
Nicotinate and Nicotinamide Metabolism	1312	1094-61-7	766	335.06388
Nicotinate and Nicotinamide Metabolism	1310	53-84-9	1434	662.10184
Nicotinate and Nicotinamide Metabolism	428	58-68-4;606-68-8	1540	664.1175
Nicotinate and Nicotinamide Metabolism	55	1005-24-9	1940	137.07094
Nicotinate and Nicotinamide Metabolism	100001092	535-83-1	1388	138.05496
Nicotinate and Nicotinamide Metabolism	215	68414-18-6	920	558.06439
Riboflavin Metabolism	327	146-14-5;84366-81-4	2425	784.14985
Riboflavin Metabolism	100000251	130-40-5	2390	455.09733
Pantothenate and CoA Metabolism	1024	137-08-6	1667	220.11795
Pantothenate and CoA Metabolism	100000328	NA	1597	357.08908
Pantothenate and CoA Metabolism	100000138	3633-59-8	2013	686.1416
Pantothenate and CoA Metabolism	270	85-61-0;18439-24-2	1448	766.1079
Pantothenate and CoA Metabolism	100001495	496-65-1	2765	277.12275
Ascorbate and Aldarate Metabolism	100001022	70753-61-6	2384	135.02989
Ascorbate and Aldarate Metabolism	100001586	20246-53-1	2750	195.05102
Tocopherol Metabolism	1105	59-02-9;10191-41-0	2522	430.37818
Biotin Metabolism	251	58-85-5	2253	245.09545
Folate Metabolism	1244	68703-91-3;68792-52-9	1820	458.17935
Pterin Metabolism	100004216	22363-60-4	1805	164.05669
Hemoglobin and Porphyrin Metabolism	1090	635-65-4	1840	585.27076
Thiamine Metabolism	873	59-43-8	3050	265.11176
Vitamin A Metabolism	498	68-26-8	1636	269.22639
Vitamin B6 Metabolism	936	58-56-0	2442	170.08117
Vitamin B6 Metabolism	568	58052-48-5	2975	169.09716
Vitamin B6 Metabolism	493	529-96-4	1932	249.06349
Vitamin B6 Metabolism	492	41468-25-1	943	246.0173
Vitamin B6 Metabolism	491	65-22-5	2343	168.06552

Benzoate Metabolism	100000014	495-69-2	2106.9	178.05096
Benzoate Metabolism	100004208		2344	203.00196
Benzoate Metabolism	100001315	3233-57-7	2890	187.00705
Food Component/Plant	338	527-07-1	2922	195.05102
Food Component/Plant	100001411	353-09-3	2145	132.07676
Food Component/Plant	100002154	58511-63-0	850	230.09578
Food Component/Plant	100000846	149-32-6	1491	167.05611
Food Component/Plant	100001550	1195-94-4	1750	158.11756
Food Component/Plant	100001491	1113-83-3	636	326.10818
Food Component/Plant	100001296	4136-37-2	1440	144.10191
Drug - Antibiotic	100002155	69-57-8	3855	333.09145
Drug - Other	100002324	638-23-3	1490	180.03251
Chemical	100002528	14808-79-8	616	96.9601
Chemical	100005384		990	260.02343
Chemical	100004322		1677	188.0023
Chemical	100003892	8/2/83	1730	209.05906
Chemical	100001724	143-74-8	3665.9	353.04891
Chemical	100003696	123-56-8	2155	116.03532
Chemical	100009232	34592-47-4	1250	134.02703