

Table S2: Metabolomics comparisons in p53-activated cells (+Nutlin, 20 hr)

KEY:

0.55 **Green:** significant difference ($p \leq 0.05$) between groups shown, metabolite ratio of < 1.00

0.76 **Light Green:** statistical significance $0.05 < p < 0.10$, metabolite ratio of < 1.00

1.71 **Red:** significant difference ($p \leq 0.05$) between groups shown; metabolite ratio of ≥ 1.00

1.32 **Light Red:** statistical significance $0.05 < p < 0.10$, metabolite ratio of ≥ 1.00

1.20 **Non-colored text and cell:** mean values not significantly different for that comparison

Super Pathway	Sub Pathway	Biochemical Name	Nutlin WTp53:WTp53	Nutlin $\Delta 40p53$:WTp53
Amino Acid	Glycine, Serine and Threonine Metabolism	glycine	1.17	1.03
		betaine	0.80	11.69
		serine	1.20	1.01
		N-acetylserine	1.00	1.13
		threonine	1.13	1.03
		N-acetylthreonine	1.58	1.47
	Alanine and Aspartate Metabolism	alanine	1.08	0.95
		N-acetylalanine	0.78	0.83
		aspartate	0.86	0.88
		N-acetylaspartate (NAA)	1.81	2.31
		asparagine	1.07	0.88
	Glutamate Metabolism	glutamate	1.25	1.01
		glutamine	0.90	0.75
		N-acetylglutamate	1.01	0.85
		N-acetylglutamine	0.85	0.78
		glutamate, gamma-methyl ester	0.82	0.70
		pyroglutamine*	0.87	0.75
		beta-citrylglutamate	1.33	1.56
	Histidine Metabolism	S-1-pyrroline-5-carboxylate	1.71	1.10
		histidine	0.96	0.88
		formiminoglutamate	1.52	1.23
		imidazole lactate	0.59	0.89
	Lysine Metabolism	4-imidazoleacetate	0.75	0.68
		lysine	1.05	0.84
		N6-acetyllysine	1.14	1.10
		N6-methyllysine	1.14	1.02
		N6,N6-dimethyllysine	1.18	0.94
N6,N6,N6-trimethyllysine		1.12	0.98	
5-(galactosylhydroxy)-L-lysine		0.99	0.51	
Amin Acid	Phenylalanine Metabolism	phenylalanine	1.12	0.96
	Tyrosine Metabolism	tyrosine	1.13	0.97

	3-(4-hydroxyphenyl)lactate	0.95	1.02
	phenol sulfate	3.71	2.78
	O-methyltyrosine	0.90	0.81
	N-formylphenylalanine	1.32	1.44
Tryptophan Metabolism	tryptophan	0.95	0.91
	kynurenine	1.07	1.04
Leucine, Isoleucine and Valine Metabolism	leucine	1.09	0.93
	isovalerylcarnitine (C5)	1.72	1.10
	beta-hydroxyisovalerate	1.21	1.03
	isoleucine	1.09	0.91
	2-methylbutyrylcarnitine (C5)	1.50	0.81
	tiglylcarnitine (C5:1-DC)	1.01	1.16
	methylsuccinate	1.25	0.80
	valine	1.05	0.98
	alpha-hydroxyisovalerate	0.99	0.87
	isobutyrylcarnitine (C4)	2.02	1.42
Methionine, Cysteine, SAM and Taurine Metabolism	methionine	1.03	0.89
	N-acetylmethionine	0.92	1.02
	N-formylmethionine	1.03	1.00
	methionine sulfoxide	1.22	0.90
	N-acetylmethionine sulfoxide	1.14	0.87
	S-adenosylhomocysteine (SAH)	0.98	0.96
	cystathionine	0.68	1.68
	cysteine	1.05	0.83
	N-acetylcysteine	1.15	1.15
	S-methylcysteine	1.19	0.99
	cystine	1.04	0.60
	cysteine sulfinic acid	1.24	0.89
	hypotaurine	0.41	1.07
	taurine	0.89	1.04
Urea cycle; Arginine and Proline Metabolism	arginine	1.06	0.82
	argininosuccinate	1.11	1.04
	urea	2.31	1.36
	ornithine	3.05	1.27
	2-oxoarginine*	0.74	0.82
	citrulline	1.52	2.55
	proline	0.96	0.92
	dimethylarginine (SDMA + ADMA)	1.13	0.92
	trans-4-hydroxyproline	1.14	1.07
	N-monomethylarginine	1.18	0.94
Creatine Metabolism	guanidinoacetate	0.10	0.08
	creatine	0.77	0.99
	creatinine	0.88	0.87

Amino Acid	Polyamine Metabolism	putrescine	1.63	1.01
		N-acetylputrescine	3.07	1.48
		spermidine	0.49	0.85
		(N(1) + N(8))-acetylspermidine	1.62	0.23
		spermine	0.60	0.90
		N(1)-acetylspermine	0.63	0.21
		5-methylthioadenosine (MTA)	0.95	0.82
	Guanidino and Acetamido Metabolism	4-guanidinobutanoate	1.13	1.00
	Glutathione Metabolism	glutathione, reduced (GSH)	0.44	0.98
		glutathione, oxidized (GSSG)	0.62	1.03
		cysteine-glutathione disulfide	0.94	0.83
		5-oxoproline	0.95	0.95
	Peptide	Gamma-glutamyl Amino Acid	gamma-glutamylcysteine	0.48
gamma-glutamylglutamine			1.05	0.50
gamma-glutamylleucine			1.36	1.01
Dipeptide		alanylleucine	0.97	0.48
		glutaminylleucine	1.01	0.89
		glycylleucine	1.49	1.03
		glycylvaline	0.99	0.79
		histidylalanine	1.13	0.91
		isoleucylglycine	1.17	0.84
		leucylalanine	1.44	0.87
		leucylglycine	1.55	0.94
		phenylalanylalanine	1.14	0.74
		phenylalanylglycine	1.24	0.97
		prolylglycine	0.95	0.86
		threonylphenylalanine	1.27	0.76
		tryptophylglycine	1.16	0.83
		tyrosylglycine	1.51	1.08
		valylglutamine	1.46	0.84
		valylglycine	1.32	0.90
		valylleucine	1.66	0.77
leucylglutamine*	1.20	0.70		
Acetylated Peptides	phenylacetylglycine	0.99	1.05	
Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	glucose	0.90	0.70
		fructose 1,6-diphosphate/glucose 1,6-diphosphate/myo-inositol diphosphates	1.12	1.13
		dihydroxyacetone phosphate (DHAP)	1.12	1.40
		3-phosphoglycerate	0.98	1.02
		phosphoenolpyruvate (PEP)	0.84	1.08
		pyruvate	0.81	1.23
		lactate	1.08	1.14
		glycerate	0.78	0.99

Carbohydrate	Pentose Phosphate Pathway	sedoheptulose-7-phosphate	0.90	1.00
	Pentose Metabolism	ribose	1.12	1.14
	Fructose, Mannose and Galactose Metabolism	mannitol/sorbitol	0.89	2.38
		mannose	1.11	0.96
		galactitol (dulcitol)	0.87	1.01
	Nucleotide Sugar	UDP-glucose/UDP-galactose	2.07	1.17
		UDP-glucuronate	0.89	1.37
		UDP-N-acetylglucosamine/galactosamine	0.82	1.24
	Aminosugar Metabolism	N-acetylglucosamine 6-phosphate	0.63	1.24
		N-acetyl-glucosamine 1-phosphate	1.19	1.04
		N-acetylneuraminate	0.95	1.14
		N-acetylglucosaminylasparagine	0.91	1.06
		erythronate*	1.02	1.05
N-acetylglucosamine/N-acetylgalactosamine		0.87	1.12	
N-glycolylneuraminate		1.14	1.13	
Energy	TCA Cycle	citrate	1.26	1.01
		aconitate [cis or trans]	1.39	1.22
		isocitrate	1.52	1.14
		alpha-ketoglutarate	1.14	1.03
		fumarate	0.84	1.20
		malate	0.99	1.29
	Oxidative Phosphorylation	acetylphosphate	1.08	0.77
		phosphate	1.04	0.99
Lipid	Long Chain Saturated Fatty Acid	myristate (14:0)	0.89	0.84
		pentadecanoate (15:0)	1.03	0.79
		palmitate (16:0)	0.97	0.77
		margarate (17:0)	1.21	0.85
		stearate (18:0)	1.05	0.81
		nonadecanoate (19:0)	1.08	0.85
		arachidate (20:0)	0.95	0.99
	Long Chain Monounsaturated Fatty Acid	palmitoleate (16:1n7)	0.92	0.85
		10-heptadecenoate (17:1n7)	1.08	0.91
		oleate/vaccenate (18:1)	0.94	0.94
		10-nonadecenoate (19:1n9)	1.07	0.98
		eicosenoate (20:1)	0.89	1.15
		erucate (22:1n9)	0.86	1.21
	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	tetradecadienoate (14:2)*	1.77	0.96
		stearidonate (18:4n3)	0.95	0.74
		eicosapentaenoate (EPA; 20:5n3)	0.90	0.64
		docosapentaenoate (n3 DPA; 22:5n3)	1.18	0.98
		docosahexaenoate (DHA; 22:6n3)	1.59	1.03
docosatrienoate (22:3n3)		1.37	1.41	

Lipid

Long Chain Polyunsaturated Fatty Acid (n3 and n6)	nisinate (24:6n3)	1.70	1.19
	hexadecadienoate (16:2n6)	0.86	0.99
	linoleate (18:2n6)	1.00	0.99
	linolenate [alpha or gamma; (18:3n3 or 6)]	1.07	0.91
	dihomo-linoleate (20:2n6)	1.07	1.11
	dihomo-linolenate (20:3n3 or n6)	1.11	1.01
	arachidonate (20:4n6)	1.21	1.05
	docosatrienoate (22:3n6)*	1.08	1.19
	adrenate (22:4n6)	1.07	1.06
	docosadienoate (22:2n6)	1.07	1.11
	mead acid (20:3n9)	0.82	0.87
Fatty Acid, Branched	(14 or 15)-methylpalmitate (a17:0 or i17:0)	1.10	0.86
	(16 or 17)-methylstearate (a19:0 or i19:0)	1.11	0.77
Fatty Acid, Dicarboxylate	glutarate (C5-DC)	1.41	0.59
	azelate (C9-DC)	0.99	0.91
	dodecadienoate (12:2)*	1.00	1.00
Fatty Acid Metabolism (also BCAA Metabolism)	butyrylcarnitine (C4)	1.14	0.93
	propionylcarnitine (C3)	1.90	1.21
	methylmalonate (MMA)	0.94	1.14
Fatty Acid Metabolism (Acyl Carnitine, Short Chain)	acetylcarnitine (C2)	1.13	1.48
Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	palmitoylcarnitine (C16)	1.86	1.19
	stearoylcarnitine (C18)	2.85	1.45
	lignoceroylcarnitine (C24)*	2.67	2.01
	cerotoylcarnitine (C26)*	1.44	1.38
Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	oleoylcarnitine (C18:1)	3.00	1.92
	nervonoylcarnitine (C24:1)*	2.26	2.52
	ximenoylcarnitine (C26:1)*	1.55	1.67
Carnitine Metabolism	deoxycarnitine	1.48	1.32
	carnitine	0.96	0.99
Fatty Acid, Monohydroxy	2-hydroxypalmitate	1.31	1.04
	2-hydroxyoleate	1.22	1.15
	2-hydroxystearate	1.60	1.28
	3-hydroxylaurate	1.31	0.96
	13-HODE + 9-HODE	1.13	1.01
Endocannabinoid	oleoyl ethanolamide	1.10	0.94
	palmitoyl ethanolamide	1.12	1.03
	stearoyl ethanolamide	1.45	1.20
	linoleoyl ethanolamide	1.04	0.95
Inositol Metabolism	myo-inositol	0.78	1.37
Phospholipid Metabolism	choline	1.11	1.38
	choline phosphate	0.62	1.10

Lipid

	glycerophosphorylcholine (GPC)	1.19	0.78
	phosphoethanolamine	1.93	1.24
	glycerophosphoethanolamine	1.36	0.76
	glycerophosphoserine*	1.09	0.73
	glycerophosphoinositol*	1.07	0.97
Phosphatidylcholine (PC)	1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	1.22	0.99
	1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)*	1.45	0.97
	1,2-dipalmitoyl-GPC (16:0/16:0)	1.36	1.01
	1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*	1.07	0.80
	1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	1.91	1.16
	1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	1.17	0.86
	1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	1.08	0.76
	1-palmitoyl-2-gamma-linolenoyl-GPC (16:0/18:3n6)*	1.16	0.93
Phosphatidylcholine (PC)	1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	1.18	0.78
	1,2-distearoyl-GPC (18:0/18:0)	1.81	2.09
	1-stearoyl-2-oleoyl-GPC (18:0/18:1)	1.22	0.98
	1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	1.35	0.81
	1-oleoyl-2-linoleoyl-GPC (18:1/18:2)*	1.09	0.81
	1-oleoyl-2-docosaheptaenoyl-GPC (18:1/22:6)*	1.61	0.95
	1,2-dilinoleoyl-GPC (18:2/18:2)	1.10	0.78
	1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)*	1.10	0.76
Phosphatidylethanolamine (PE)	1,2-dipalmitoyl-GPE (16:0/16:0)*	1.16	0.93
	1-palmitoyl-2-oleoyl-GPE (16:0/18:1)	0.88	0.73
	1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	0.89	0.75
	1-palmitoleoyl-2-oleoyl-GPE (16:1/18:1)*	0.67	0.61
	1-stearoyl-2-oleoyl-GPE (18:0/18:1)	1.11	0.94
	1-stearoyl-2-linoleoyl-GPE (18:0/18:2)*	0.96	0.70
	1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	1.17	0.83
	1,2-dioleoyl-GPE (18:1/18:1)	0.92	0.93
	1-oleoyl-2-linoleoyl-GPE (18:1/18:2)*	0.89	0.78
	1-oleoyl-2-arachidonoyl-GPE (18:1/20:4)*	1.26	0.90
Phosphatidylserine (PS)	1-palmitoyl-2-oleoyl-GPS (16:0/18:1)	1.00	0.81
	1-stearoyl-2-oleoyl-GPS (18:0/18:1)	1.28	1.24
	1-stearoyl-2-linoleoyl-GPS (18:0/18:2)	0.99	0.76
Phosphatidylglycerol (PG)	1-palmitoyl-2-oleoyl-GPG (16:0/18:1)	0.97	0.93
	1,2-distearoyl-GPG (18:0/18:0)	1.60	1.27
	1-stearoyl-2-oleoyl-GPG (18:0/18:1)	1.34	1.07
Phosphatidylinositol (PI)	1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*	1.11	0.67
	1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*	1.23	0.79
	1-stearoyl-2-oleoyl-GPI (18:0/18:1)*	1.09	0.80
	1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	1.03	0.74
	1,2-dioleoyl-GPI (18:1/18:1)	0.81	0.85
	1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	1.31	1.10

	1-oleoyl-2-arachidonoyl-GPI (18:1/20:4)*	1.15	0.92	
Lysophospholipid	1-palmitoyl-GPC (16:0)	0.70	0.66	
	2-palmitoyl-GPC (16:0)*	0.86	0.79	
	1-palmitoleoyl-GPC (16:1)*	0.49	0.43	
	2-palmitoleoyl-GPC (16:1)*	1.10	1.05	
	1-stearoyl-GPC (18:0)	0.82	0.71	
	1-oleoyl-GPC (18:1)	0.72	0.50	
	1-linoleoyl-GPC (18:2)	0.60	0.59	
	1-lignoceroyl-GPC (24:0)	0.84	0.72	
	1-palmitoyl-GPE (16:0)	0.61	0.61	
	1-stearoyl-GPE (18:0)	0.75	0.66	
	2-stearoyl-GPE (18:0)*	0.85	0.49	
	1-oleoyl-GPE (18:1)	0.60	0.72	
	1-linoleoyl-GPE (18:2)*	0.74	0.67	
	1-arachidonoyl-GPE (20:4n6)*	1.11	0.70	
	1-stearoyl-GPS (18:0)*	0.77	0.66	
Lysophospholipid	1-oleoyl-GPS (18:1)	0.56	0.60	
	1-palmitoyl-GPG (16:0)*	0.82	0.75	
	1-stearoyl-GPG (18:0)	0.94	0.85	
	1-oleoyl-GPG (18:1)*	1.05	0.84	
	1-linoleoyl-GPG (18:2)*	1.37	0.84	
	1-palmitoyl-GPI (16:0)	0.58	0.62	
	1-stearoyl-GPI (18:0)	0.63	0.67	
	1-oleoyl-GPI (18:1)	0.66	0.66	
	1-linoleoyl-GPI (18:2)*	0.82	0.65	
	1-arachidonoyl-GPI (20:4)*	1.15	0.88	
Lipid	Plasmalogen	1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)*	1.20	0.99
		1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*	1.16	0.69
		1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*	1.25	1.01
		1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*	1.16	0.95
		1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	1.23	0.98
		1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	1.20	0.93
		1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	1.41	1.31
		1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)*	1.32	0.84
		1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*	1.19	1.01
		1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	1.29	0.85
		1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	1.56	1.17
		Lysoplasmalogen	1-(1-enyl-palmitoyl)-GPC (P-16:0)*	0.82
1-(1-enyl-palmitoyl)-GPE (P-16:0)*	0.76		0.73	
1-(1-enyl-oleoyl)-GPE (P-18:1)*	0.73		0.76	
1-(1-enyl-stearoyl)-GPE (P-18:0)*	0.96		0.88	
1-(1-enyl-oleoyl)-2-oleoyl-GPE (P-18:1/18:1)*	1.01		1.00	
Glycerolipid Metabolism	glycerol	1.08	1.23	

Lipid

	glycerol 3-phosphate	1.03	0.95
	glycerophosphoglycerol	1.13	0.87
Monoacylglycerol	1-pentadecanoylglycerol (15:0)	0.70	1.05
	1-palmitoylglycerol (16:0)	1.50	0.76
	1-margaroylglycerol (17:0)	1.56	1.06
	1-oleoylglycerol (18:1)	1.16	0.86
	1-linoleoylglycerol (18:2)	0.76	1.09
	2-dihomo-linoleoylglycerol (20:2)*	0.77	0.75
	1-dihomo-linolenylglycerol (20:3)	0.84	0.51
	1-arachidonoylglycerol (20:4)	0.82	0.97
	2-palmitoylglycerol (16:0)	1.01	0.77
	2-palmitoleoylglycerol (16:1)*	0.57	0.58
	2-oleoylglycerol (18:1)	1.05	0.66
	2-linoleoylglycerol (18:2)	0.77	0.95
	2-arachidonoylglycerol (20:4)	0.76	0.80
	Monoacylglycerol	1-heptadecenoylglycerol (17:1)*	0.66
2-heptadecenoylglycerol (17:1)*		0.70	0.88
1-meadoylglycerol (20:3n9)*		1.70	0.46
1-dihomo-linoleoylglycerol (20:2)		0.48	0.91
Diacylglycerol	diacylglycerol (14:0/18:1, 16:0/16:1) [2]*	0.51	0.72
	diacylglycerol (16:1/18:2 [2], 16:0/18:3 [1])*	0.91	0.72
	palmitoyl-oleoyl-glycerol (16:0/18:1) [2]*	0.80	0.83
	palmitoyl-linoleoyl-glycerol (16:0/18:2) [2]*	1.11	0.66
	palmitoleoyl-oleoyl-glycerol (16:1/18:1) [2]*	0.57	0.59
	palmitoyl-arachidonoyl-glycerol (16:0/20:4) [2]*	1.01	0.73
	oleoyl-oleoyl-glycerol (18:1/18:1) [2]*	0.94	1.09
	oleoyl-linoleoyl-glycerol (18:1/18:2) [1]	0.93	0.94
	oleoyl-linoleoyl-glycerol (18:1/18:2) [2]	0.96	0.83
	linoleoyl-linolenoyl-glycerol (18:2/18:3) [2]*	1.33	0.59
	stearoyl-arachidonoyl-glycerol (18:0/20:4) [1]*	0.92	0.93
	stearoyl-arachidonoyl-glycerol (18:0/20:4) [2]*	1.41	1.02
	oleoyl-arachidonoyl-glycerol (18:1/20:4) [2]*	1.30	0.87
Sphingolipid Synthesis	sphinganine	0.73	0.71
	sphingadienine	0.53	0.34
	phytosphingosine	0.53	0.51
Dihydroceramides	N-palmitoyl-sphinganine (d18:0/16:0)	0.97	1.52
Ceramides	N-palmitoyl-sphingosine (d18:1/16:0)	0.78	0.73
	N-stearoyl-sphingosine (d18:1/18:0)*	1.03	1.21
	N-palmitoyl-sphingadienine (d18:2/16:0)*	0.89	0.40
	N-palmitoyl-heptadecasphingosine (d17:1/16:0)*	0.82	0.67
	ceramide (d18:1/14:0, d16:1/16:0)*	0.78	0.68
	ceramide (d18:1/17:0, d17:1/18:0)*	1.19	1.01
	glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	0.97	0.54

Lipid	Hexosylceramides (HCER)	glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	0.88	0.66
		glycosyl ceramide (d18:1/20:0, d16:1/22:0)*	1.04	1.00
		glycosyl ceramide (d18:2/24:1, d18:1/24:2)*	1.06	0.38
	Lactosylceramides (LCER)	lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)	0.86	0.63
		lactosyl-N-nervonoyl-sphingosine (d18:1/24:1)*	0.89	0.86
	Dihydrosphingomyelins	myristoyl dihydrosphingomyelin (d18:0/14:0)*	0.94	1.67
		palmitoyl dihydrosphingomyelin (d18:0/16:0)*	1.05	1.66
		behenoyl dihydrosphingomyelin (d18:0/22:0)*	1.20	2.49
		sphingomyelin (d18:0/18:0, d19:0/17:0)*	1.08	3.52
		sphingomyelin (d18:0/20:0, d16:0/22:0)*	1.20	3.66
	Sphingomyelins	palmitoyl sphingomyelin (d18:1/16:0)	1.11	1.00
		hydroxypalmitoyl sphingomyelin (d18:1/16:0(OH))**	1.66	1.55
		stearoyl sphingomyelin (d18:1/18:0)	1.38	1.38
		behenoyl sphingomyelin (d18:1/22:0)*	1.19	1.45
		lignoceroyl sphingomyelin (d18:1/24:0)	1.23	1.34
		sphingomyelin (d18:2/24:2)*	1.45	0.96
		sphingomyelin (d17:1/14:0, d16:1/15:0)*	0.99	1.15
		sphingomyelin (d18:1/14:0, d16:1/16:0)*	1.04	1.00
		sphingomyelin (d18:2/14:0, d18:1/14:1)*	1.16	0.90
		sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*	1.06	0.98
	Sphingomyelins	sphingomyelin (d18:2/16:0, d18:1/16:1)*	1.15	0.70
		sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)	1.38	1.19
		sphingomyelin (d18:1/18:1, d18:2/18:0)	1.54	1.38
		sphingomyelin (d18:1/20:0, d16:1/22:0)*	1.20	1.34
		sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*	1.23	0.99
		sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*	1.03	1.08
		sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*	1.09	1.15
		sphingomyelin (d18:1/24:1, d18:2/24:0)*	1.19	0.99
		sphingomyelin (d18:2/24:1, d18:1/24:2)*	1.10	1.11
		sphingomyelin (d18:1/25:0, d19:0/24:1, d20:1/23:0, d19:1/24:0)*	1.44	1.05
Ceramide PEs	palmitoyl-sphingosine-phosphoethanolamine (d18:1/16:0)	1.41	1.13	
Sphingosines	sphingosine	0.51	0.45	
	hexadecasphingosine (d16:1)*	0.59	0.40	
	heptadecasphingosine (d17:1)	0.64	0.50	
	eicosanoylsphingosine (d20:1)*	0.76	0.63	
Mevalonate Metabolism	3-hydroxy-3-methylglutarate	1.34	1.09	
Sterol	cholesterol	1.03	1.09	
	4-cholesten-3-one	0.72	0.77	
	7-hydroxycholesterol (alpha or beta)	0.99	0.81	
Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	AICA ribonucleotide	1.00	2.03
		inosine	1.11	1.09
		hypoxanthine	1.00	1.36
		xanthine	0.79	0.58

Nucleotide		2'-deoxyinosine	0.04	0.04	
		urate	0.57	0.30	
	Purine Metabolism, Adenine containing		adenosine 5'-triphosphate (ATP)	0.83	0.72
			adenosine 5'-monophosphate (AMP)	0.84	0.69
			adenosine 3'-monophosphate (3'-AMP)	0.78	0.57
			adenosine 2'-monophosphate (2'-AMP)	0.82	0.45
			adenosine	1.10	1.08
			adenine	0.27	0.08
			N6-methyladenosine	0.80	1.31
			N6,N6-dimethyladenosine	1.01	1.48
		2'-deoxyadenosine	0.01	0.00	
	Purine Metabolism, Guanine containing		guanosine 5'- diphosphate (GDP)	0.98	1.37
			guanosine 5'- monophosphate (5'-GMP)	0.88	0.65
			guanosine 3'-monophosphate (3'-GMP)	0.75	0.56
			guanosine	1.04	1.70
			guanine	1.85	7.93
	Purine Metabolism, Guanine containing		7-methylguanine	0.89	0.89
			2'-deoxyguanosine	0.04	0.07
	Pyrimidine Metabolism, Orotate containing		orotate	1.94	1.52
	Pyrimidine Metabolism, Uracil containing		uridine 3'-monophosphate (3'-UMP)	0.90	0.66
			uridine	1.10	1.14
			uracil	0.76	1.38
			pseudouridine	0.79	1.45
			3-ureidopropionate	0.52	0.81
	Pyrimidine Metabolism, Cytidine containing		cytidine 5'-monophosphate (5'-CMP)	1.33	1.11
			cytidine 2' or 3'-monophosphate (2' or 3'-CMP)	0.63	0.51
			cytidine	0.74	1.09
			cytosine	0.52	0.39
		2'-deoxycytidine 5'-monophosphate	0.05	0.05	
		2'-deoxycytidine	0.16	0.08	
		2'-O-methylcytidine	0.57	1.22	
Pyrimidine Metabolism, Thymine containing		thymidine 5'-monophosphate	0.80	0.80	
		thymidine	1.00	1.00	
Purine and Pyrimidine Metabolism		methylphosphate	0.76	0.89	
Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	nicotinamide	0.64	0.97	
		nicotinamide ribonucleotide (NMN)	0.83	1.00	
		nicotinamide riboside	1.30	0.81	
		nicotinamide adenine dinucleotide (NAD+)	0.87	0.81	
		1-methylnicotinamide	0.80	0.60	
		adenosine 5'-diphosphoribose (ADP-ribose)	0.51	0.73	
	Riboflavin Metabolism	riboflavin (Vitamin B2)	0.68	0.76	

		flavin adenine dinucleotide (FAD)	1.00	0.97
Pantothenate and CoA Metabolism		pantothenate	0.86	0.86
		pantetheine	0.99	1.17
		phosphopantetheine	1.03	1.27
Tocopherol Metabolism		alpha-tocopherol	1.08	0.89
		gamma-tocopherol/beta-tocopherol	0.58	0.66
Hemoglobin and Porphyrin Metabolism		heme	0.45	0.97
Thiamine Metabolism		thiamin (Vitamin B1)	0.61	1.17
Vitamin A Metabolism		retinol (Vitamin A)	0.86	0.96
Vitamin B6 Metabolism		pyridoxine (Vitamin B6)	0.97	0.83
		pyridoxamine	1.24	0.98
		pyridoxamine phosphate	0.95	0.89
		pyridoxal phosphate	0.74	1.02
		pyridoxal	0.97	1.20
Xenobiotics	Benzoate Metabolism	hippurate	1.02	0.99
		p-cresol sulfate	0.79	0.90
Xenobiotics	Food Component/Plant	3-formylindole	0.97	0.78
		ergothioneine	0.43	1.21
		stachydrine	1.02	1.02
		methyl glucopyranoside (alpha + beta)	1.26	0.94
		Drug - Antibiotic	penicillin G	1.02
Xenobiotics	Drug - Antineoplastic	tamoxifen	0.81	0.73
	Chemical	HEPES	1.13	0.91
		2,4-di-tert-butylphenol	0.91	0.93
		phenol red	1.02	0.89
		thioprolone	1.19	0.91
4-chlorobenzoic acid		1.10	0.80	