Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profiling Assay

Supplemental Table 1. Biochemicals Detected in Plasma, Urine, and CSF

Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
alanine	811	Amino Acid	Alanine and Aspartate Metabolism	+	+	+
asparagine	917	Amino Acid	Alanine and Aspartate Metabolism	+	+	+
aspartate	234	Amino Acid	Alanine and Aspartate Metabolism	+	+	+
N-acetylalanine	1110	Amino Acid	Alanine and Aspartate Metabolism	+	+	+
N-acetylaspartate (NAA)	100000787	Amino Acid	Alanine and Aspartate Metabolism	+	+	+
N-acetylasparagine	100001257	Amino Acid	Alanine and Aspartate Metabolism	+	-	+
creatine	1221	Amino Acid	Creatine Metabolism	+	+	+
creatinine	275	Amino Acid	Creatine Metabolism	+	+	+
guanidinoacetate	344	Amino Acid	Creatine Metabolism	+	+	+
creatine phosphate	100000112	Amino Acid	Creatine Metabolism	+	-	-
gamma-glutamyl-alpha-lysine		Amino Acid	Gamma-glutamyl Amino Acid	+	+	+
beta-citryl-glutamate		Amino Acid	Glutamate Metabolism	+	+	+
glutamate	561	Amino Acid	Glutamate Metabolism	+	+	+
glutamine	563	Amino Acid	Glutamate Metabolism	+	+	+
N-acetyl-aspartyl-glutamate (NAAG)	100001612	Amino Acid	Glutamate Metabolism	+	+	+
N-acetylglutamate	100000282	Amino Acid	Glutamate Metabolism	+	+	+
N-acetylglutamine	100001253	Amino Acid	Glutamate Metabolism	+	+	+
pyroglutamine		Amino Acid	Glutamate Metabolism	+	+	+
citramalate	100000998	Amino Acid	Glutamate Metabolism	+	+	-
carboxyethyl-GABA	100003260	Amino Acid	Glutamate Metabolism	+	-	+
gamma-aminobutyrate (GABA)	141	Amino Acid	Glutamate Metabolism	+	-	+
glutamate, gamma-methyl ester	100001103	Amino Acid	Glutamate Metabolism	+	-	-
S-1-pyrroline-5-carboxylate	35	Amino Acid	Glutamate Metabolism	+	-	-
5-oxoproline	1021	Amino Acid	Glutathione Metabolism	+	+	+
cysteinylglycine	278	Amino Acid	Glutathione Metabolism	+	+	+
cys-gly, oxidized	1224	Amino Acid	Glutathione Metabolism	+	+	-
glutathione, oxidized (GSSG)	448	Amino Acid	Glutathione Metabolism	+	-	-
betaine	799	Amino Acid	Glycine, Serine and Threonine Metabolism	+	+	+
dimethylglycine	806	Amino Acid	Glycine, Serine and Threonine Metabolism	+	+	+
glycine	340	Amino Acid	Glycine, Serine and Threonine Metabolism	+	+	+
N-acetylglycine	100001006	Amino Acid	Glycine, Serine and Threonine Metabolism	+	+	+
N-acetylserine	100001851	Amino Acid	Glycine, Serine and Threonine Metabolism	+	+	+
N-acetylthreonine	100001274	Amino Acid	Glycine, Serine and Threonine Metabolism	+	+	+
serine	503	Amino Acid	Glycine, Serine and Threonine Metabolism	+	+	+
threonine	564	Amino Acid	Glycine, Serine and Threonine Metabolism	+	+	+
2-methylserine		Amino Acid	Glycine, Serine, and Threonine Metabolism	+	-	+
4-guanidinobutanoate	100000096	Amino Acid	Guanidino and Acetamido Metabolism	+	+	+
1-methylguanidine	100000715	Amino Acid	Guanidino and Acetamido Metabolism	+	-	+
1-methylhistidine	100001051	Amino Acid	Histidine Metabolism	+	+	+
1-methylimidazoleacetate	100001208	Amino Acid	Histidine Metabolism	+	+	+
3-methylhistidine	100000042	Amino Acid	Histidine Metabolism	+	+	+
4-imidazoleacetate	100001207	Amino Acid	Histidine Metabolism	+	+	+
histidine	355	Amino Acid	Histidine Metabolism	+	+	+
imidazole lactate	100000263	Amino Acid	Histidine Metabolism	+	+	+
imidazole propionate	100003434	Amino Acid	Histidine Metabolism	+	+	+
N-acetylhistidine	100001293	Amino Acid	Histidine Metabolism	+	+	+
1-methylhistamine	100001204	Amino Acid	Histidine Metabolism	+	-	+
N-acetyl-3-methylhistidine		Amino Acid	Histidine Metabolism	+	-	+
2-hydroxy-3-methylvalerate	100001541	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
2-methylbutyroylcarnitine (C5)		Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
3-hydroxy-2-ethylpropionate	100001170	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
3-hydroxyisobutyrate	111	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
3-methyl-2-oxobutyrate	100000936	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
3-methyl-2-oxovalerate	100000036	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
3-methylglutaconate	100002458	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
4-methyl-2-oxopentanoate	100000551	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
alpha-hydroxyisocaproate	100000706	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
alpha-hydroxyisovalerate	100001300	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
beta-hydroxyisovalerate	1442	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
beta-hydroxyisovaleroylcarnitine	100001594	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
ethylmalonate	2054	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
isobutyrylcarnitine (C4)	100001055	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
isoleucine	376	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
isovalerylcarnitine (C5)	100001393	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
leucine	397	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
methylsuccinate	2051	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
N-acetylisoleucine	100001276	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
N-acetylleucine	1082	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
N-acetylvaline	1084	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
tiglyl carnitine (C5)		Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
valine	566	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	+
isovalerate (C5)		Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	+	-
methylsuccinoylcarnitine (1)	100009275	Amino Acid	Leucine, Isoleucine and Valine Metabolism	+	-	-
3-methylglutarylcarnitine (2)	100005850	Amino Acid	Lysine Metabolism	+	+	+
5-hydroxylysine	100000054	Amino Acid	Lysine Metabolism	+	+	+
glutarate (pentanedioate)	339	Amino Acid	Lysine Metabolism	+	+	+
glutaroylcarnitine (C5)		Amino Acid	Lysine Metabolism	+	+	+
lysine	407	Amino Acid	Lysine Metabolism	+	+	+
N6,N6,N6-trimethyllysine	189	Amino Acid	Lysine Metabolism	+	+	+
pipecolate	1025	Amino Acid	Lysine Metabolism	+	+	-
2-oxoadipate	92	Amino Acid	Lysine Metabolism	+	-	+
N2-acetyllysine/N6-acetyllysine	100008925	Amino Acid	Lysine Metabolism	+	-	-
2-aminobutyrate	1128	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
2-hydroxybutyrate/2-hydroxyisobutyrate	100008928	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
cystathionine	310	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
cysteine	800	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
methionine	415	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
methionine sulfone	100004635	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
methionine sulfoxide	100000039	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+

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Supplemental Table 1. Biochemicals Detected in Plasma, Urine, and CSF

Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
N-acetylmethionine	1083	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
N-acetyltaurine	100005466	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
N-formylmethionine	194	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
S-adenosylhomocysteine (SAH)	197	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
S-methylcysteine	100002749	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
taurine	512	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	+	+
N-acetylmethionine sulfoxide	100005463	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	+	-	+
3-(4-hydroxyphenyl)lactate (HPLA)		Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
3-methoxytyramine sulfate	100004634	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
3-methoxytyrosine	1342	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
dopamine 3-O-sulfate		Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
N-acetylphenylalanine	100001256	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
N-acetyltyrosine	100001104	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
p-cresol sulfate	100001315	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
phenol sulfate	100001510	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
phenylacetylglutamine	100001417	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
phenylalanine	460	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
phenyllactate (PLA)	100000774	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
tyrosine	815	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	+	+
homovanillate (HVA)	117	Amino Acid	Phenylalanine and Tyrosine Metabolism	+	-	+
4-acetamidobutanoate	1113	Amino Acid	Polyamine Metabolism	+	+	+
5-methylthioadenosine (MTA)	212	Amino Acid	Polyamine Metabolism	+	+	+
acisoga	100004541	Amino Acid	Polyamine Metabolism	+	+	+
N-acetylputrescine	192	Amino Acid	Polyamine Metabolism	+	+	+
spermidine	50	Amino Acid	Polyamine Metabolism	+	+	+
3-indoxyl sulfate	100000467	Amino Acid	Tryptophan Metabolism	+	+	+
5-hydroxyindoleacetate	71	Amino Acid	Tryptophan Metabolism	+	+	+
anthranilate	1258	Amino Acid	Tryptophan Metabolism	+	+	+
C-glycosyltryptophan	100006379	Amino Acid	Tryptophan Metabolism	+	+	+
indole-3-carboxylic acid	100002185	Amino Acid	Tryptophan Metabolism	+	+	+
indoleacetate	100001034	Amino Acid	Tryptophan Metabolism	+	+	+
indolelactate	100000463	Amino Acid	Tryptophan Metabolism	+	+	+
indolepropionate	100001083	Amino Acid	Tryptophan Metabolism	+	+	+
kynurenate	98	Amino Acid	Tryptophan Metabolism	+	+	+
kynurenine	100000265	Amino Acid	Tryptophan Metabolism	+	+	+
picolinate	1022	Amino Acid	Tryptophan Metabolism	+	+	+
thioproline		Amino Acid	Tryptophan Metabolism	+	+	+
tryptophan	565	Amino Acid	Tryptophan Metabolism	+	+	+
tryptophan betaine	100001743	Amino Acid	Tryptophan Metabolism	+	+	+
arginate		Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
arginine	231	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
argininosuccinate	232	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
citrulline	391	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
dimethylarginine (ADMA + SDMA)		Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
homoarginine	100000961	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
homocitrulline	100000963	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
hydroxyproline		Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
N-acetylarginine	100001266	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
N-delta-acetylornithine	100004523	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
N-methylproline	100001956	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
ornithine	444	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
proline	480	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
prolylhydroxyproline		Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
urea	533	Amino Acid	Urea cycle; Arginine and Proline Metabolism	+	+	+
erythronate		Carbohydrate	Aminosugar Metabolism	+	+	+
glucuronate	100000257	Carbohydrate	Aminosugar Metabolism	+	+	+
N-acetylneuraminate	1162	Carbohydrate	Aminosugar Metabolism	+	+	+
N-acetylglucosaminylasparagine		Carbohydrate	Aminosugar Metabolism	+	-	+
sucrose	935	Carbohydrate	Disaccharides and Oligosaccharides	+	+	+
fructose	878	Carbohydrate	Fructose, Mannose and Galactose Metabolism	+	+	+
galactitol (dulcitol)	1003	Carbohydrate	Fructose, Mannose and Galactose Metabolism	+	+	+
galactonate	100001026	Carbohydrate	Fructose, Mannose and Galactose Metabolism	+	+	+
mannitol/sorbitol	100001740	Carbohydrate	Fructose, Mannose and Galactose Metabolism	+	+	+
mannose	803	Carbohydrate	Fructose, Mannose and Galactose Metabolism	+	+	+
1,5-anhydroglucitol (1,5-AG)	100000580	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	+	+	+
glucose	572	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	+	+	+
glycerate	1052	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	+	+	+
lactate	482	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	+	+	+
pyruvate	823	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	+	+	-
arabitol/xylitol	100006430	Carbohydrate	Pentose Metabolism	+	+	+
ribitol	100000406	Carbohydrate	Pentose Metabolism	+	+	+
ribonate (ribonolactone)		Carbohydrate	Pentose Metabolism	+	+	+
ribose	914	Carbohydrate	Pentose Metabolism	+	-	+
arabonate/xylonate	100006115	Carbohydrate	Pentose Phosphate Pathway	+	+	+
gulonic acid		Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	+	+	+
oxalate (ethanedioate)	100000841	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	+	+	+
threonate	100001022	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	+	+	+
5-methyltetrahydrofolate (5MeTHF)	1244	Cofactors and Vitamins	Folate Metabolism	+	-	+
bilirubin		Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	+	+	-
bilirubin (E,E)		Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	+	+	-
heme	100001386	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	+	+	-
1-methylnicotinamide	55	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	+	+	+
N1-Methyl-2-pyridone-5-carboxamide	100001468	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	+	+	+
nicotinamide	432	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	+	+	+
quinolinate	182	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	+	+	+
trigonelline (N'-methylnicotinate)	100001092	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	+	+	+
nicotinamide riboside	100001310	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	+	-	+
pantothenate (Vitamin B5)		Cofactors and Vitamins	Pantothenate and CoA Metabolism	+	+	+
gamma-CEHC	100002094	Cofactors and Vitamins	Tocopherol Metabolism	+	+	+

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Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
gamma-tocopherol/beta-tocopherol	100008998	Cofactors and Vitamins	Tocopherol Metabolism	+	-	-
retinol (Vitamin A)	498	Cofactors and Vitamins	Vitamin A Metabolism	+	+	-
pyridoxal	491	Cofactors and Vitamins	Vitamin B6 Metabolism	+	+	+
pyridoxate	100001121	Cofactors and Vitamins	Vitamin B6 Metabolism	+	+	+
pyridoxine (Vitamin B6)	936	Cofactors and Vitamins	Vitamin B6 Metabolism	+	-	+
phosphate	461	Energy	Oxidative Phosphorylation	+	+	+
2-methylcitrate	90	Energy	TCA Cycle	+	+	+
alpha-ketoglutarate	93	Energy	TCA Cycle	+	+	+
citrate	1124	Energy	TCA Cycle	+	+	+
fumarate	330	Energy	TCA Cycle	+	+	+
malate	409	Energy	TCA Cycle	+	+	+
succinate	252	Energy	TCA Cycle	+	+	+
succinylcarnitine (C4)		Energy	TCA Cycle	+	+	+
aconitate [cis or trans]	100001359	Energy	TCA Cycle	+	+	-
isocitrate	1206	Energy	TCA Cycle	+	-	+
carnitine	100000007	Lipid	Carnitine Metabolism	+	+	+
deoxycarnitine	100001662	Lipid	Carnitine Metabolism	+	+	+
methylmalonate (MMA)	418	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	+	+	+
propionylcarnitine (C3)	100001162	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	+	+	+
butyrylcarnitine (C4)	100001054	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	+	+	-
acetylcarnitine (C2)	100000802	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	+	+	+
decanoylcarnitine (C10)	100001251	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	+	+	+
hexanoylcarnitine (C6)	100000781	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	+	+	+
octanoylcarnitine (C8)	100001247	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	+	+	+
cis-4-decenoyl carnitine		Lipid	Fatty Acid Metabolism(Acyl Carnitine)	+	+	-
laurylcarnitine (C12)	100001392	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	+	+	-
3-hydroxybutyrylcarnitine (1)	100003926	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	+	-	-
malonate	818	Lipid	Fatty Acid Synthesis	+	+	+
malonylcarnitine	100001526	Lipid	Fatty Acid Synthesis	+	-	+
oleamide	1504	Lipid	Fatty Acid, Amide	+	+	-
palmitic amide	100003915	Lipid	Fatty Acid, Amide	+	+	-
2-aminoheptanoate	100004542	Lipid	Fatty Acid, Amino	+	+	+
2-aminooctanoate	100004227	Lipid	Fatty Acid, Amino	+	+	+
2-hydroxyadipate	100001153	Lipid	Fatty Acid, Dicarboxylate	+	+	+
3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)	100001178	Lipid	Fatty Acid, Dicarboxylate	+	+	+
maleate	100000707	Lipid	Fatty Acid, Dicarboxylate	+	+	+
dimethylmalonic acid	100004251	Lipid	Fatty Acid, Dicarboxylate	+	-	+
3-hydroxyhexanoic acid		Lipid	Fatty Acid, Monohydroxy	+	+	+
3-hydroxyoctanoate	100000773	Lipid	Fatty Acid, Monohydroxy	+	+	+
3-hydroxysebacate	100001145	Lipid	Fatty Acid, Monohydroxy	+	+	+
5-hydroxyhexanoate	100001148	Lipid	Fatty Acid, Monohydroxy	+	+	+
2-hydroxydecanoate	100004089	Lipid	Fatty Acid, Monohydroxy	+	+	-
glycerol 3-phosphate	100000258	Lipid	Glycerolipid Metabolism	+	+	+
glycerol	1254	Lipid	Glycerolipid Metabolism	+	+	-
galactosylglycerol		Lipid	Glycerolipid Metabolism	+	-	+
myo-inositol	363	Lipid	Inositol Metabolism	+	+	+
3-hydroxybutyrate (BHBA)	254	Lipid	Ketone Bodies	+	+	+
acetoacetate	1218	Lipid	Ketone Bodies	+	-	-
1-(1-enyl-stearoyl)-GPE (P-18:0)		Lipid	Lysolipid	+	+	-
1-adrenoyl-GPC (22:4)		Lipid	Lysolipid	+	+	-
1-arachidonoyl-GPC (20:4)		Lipid	Lysolipid	+	+	-
1-arachidonoyl-GPE (20:4)		Lipid	Lysolipid	+	+	-
1-docosahexaenoyl-GPC (22:6)		Lipid	Lysolipid	+	+	-
1-docosahexaenoyl-GPE (22:6)		Lipid	Lysolipid	+	+	-
1-docosapentaenoyl-GPC (22:5n3)		Lipid	Lysolipid	+	+	-
1-docosapentaenoyl-GPC (22:5n6)		Lipid	Lysolipid	+	+	-
1-eicosadienoyl-GPC (20:2)		Lipid	Lysolipid	+	+	-
1-eicosatrienoyl-GPC (20:3)		Lipid	Lysolipid	+	+	-
1-linoleoyl-GPC (18:2)	100001395	Lipid	Lysolipid	+	+	-
1-myristoyl-GPC (14:0)	100001383	Lipid	Lysolipid	+	+	-
1-O-hexadecyl-GPC (C16)		Lipid	Lysolipid	+	+	-
1-oleoyl-GPC (18:1)	100001272	Lipid	Lysolipid	+	+	-
1-palmitoleoyl-GPC (16:1)		Lipid	Lysolipid	+	+	-
1-palmitoyl-GPA (16:0)	100001445	Lipid	Lysolipid	+	+	-
1-palmitoyl-GPC (16:0)	100001263	Lipid	Lysolipid	+	+	-
1-pentadecanoyl-GPC (15:0)		Lipid	Lysolipid	+	+	-
1-stearoyl-GPC (18:0)	100001271	Lipid	Lysolipid	+	+	-
1-stearoyl-GPE (18:0)	100001461	Lipid	Lysolipid	+	+	-
1-oleoylglycerophosphate (18:1)		Lipid	Lysolipid	+	-	-
1-(1-enyl-palmitoyl)-GPC (P-16:0)		Lipid	Lysoplasmalogen	+	+	-
3-hydroxy-3-methylglutarate	112	Lipid	Mevalonate Metabolism	+	+	+
1-arachidonylglycerol (20:4)	100001433	Lipid	Monoacylglycerol	+	+	-
1-dihomo-linolenylglycerol (20:3)	100006121	Lipid	Monoacylglycerol	+	+	-
1-oleoylglycerol (18:1)	100000924	Lipid	Monoacylglycerol	+	+	-
1-palmitoylglycerol (16:0)	100000827	Lipid	Monoacylglycerol	+	+	-
choline	1256	Lipid	Phospholipid Metabolism	+	+	+
glycerophosphoethanolamine	100001620	Lipid	Phospholipid Metabolism	+	+	+
glycerophosphoinositol*	100001621	Lipid	Phospholipid Metabolism	+	+	+
glycerophosphorylcholine (GPC)	100000269	Lipid	Phospholipid Metabolism	+	+	+
phosphocholine		Lipid	Phospholipid Metabolism	+	+	+
phosphoethanolamine (PE)		Lipid	Phospholipid Metabolism	+	+	+
trimethylamine N-oxide	100003397	Lipid	Phospholipid Metabolism	+	+	+
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)		Lipid	Phospholipid Metabolism	+	+	-
1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)		Lipid	Phospholipid Metabolism	+	+	-
1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)		Lipid	Phospholipid Metabolism	+	+	-
1-(1-enyl-stearoyl)-2-arachidonoyl-GPC (P-18:0/20:4)	100008918	Lipid	Phospholipid Metabolism	+	+	-
1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)		Lipid	Phospholipid Metabolism	+	+	-
1-(1-enyl-stearoyl)-2-docosahexaenoyl-GPE (P-18:0/22:6)		Lipid	Phospholipid Metabolism	+	+	-
1,2-dilinoleoyl-GPC (18:2/18:2)	100008903	Lipid	Phospholipid Metabolism	+	+	-

Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profiling Assay

Supplemental Table 1. Biochemicals Detected in Plasma, Urine, and CSF

Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
1,2-dimyristoyl-GPC (14:0/14:0)	100000647	Lipid	Phospholipid Metabolism	+	+	-
1,2-dioleoyl-GPC (18:1/18:1)	100008905	Lipid	Phospholipid Metabolism	+	+	-
1,2-dipalmitoyl-GPC (16:0/16:0)	100000657	Lipid	Phospholipid Metabolism	+	+	-
1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4)		Lipid	Phospholipid Metabolism	+	+	-
1-margaroyl-2-linoleoyl-GPC (17:0/18:2)		Lipid	Phospholipid Metabolism	+	+	-
1-margaroyl-2-oleoyl-GPC (17:0/18:1)		Lipid	Phospholipid Metabolism	+	+	-
1-myristoyl-2-linoleoyl-GPC (14:0/18:2)		Lipid	Phospholipid Metabolism	+	+	-
1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	100000672	Lipid	Phospholipid Metabolism	+	+	-
1-oleoyl-2-dihomo-linolenoyl-GPC (18:1/20:3)		Lipid	Phospholipid Metabolism	+	+	-
1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)		Lipid	Phospholipid Metabolism	+	+	-
1-oleoyl-2-linoleoyl-GPC (18:1/18:2)		Lipid	Phospholipid Metabolism	+	+	-
1-palmitoleoyl-2-linoleoyl-GPC (16:1/18:2)		Lipid	Phospholipid Metabolism	+	+	-
1-palmitoyl-2-adrenoyl-GPC (16:0/22:4)		Lipid	Phospholipid Metabolism	+	+	-
1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4)		Lipid	Phospholipid Metabolism	+	+	-
1-palmitoyl-2-dihomo-linolenoyl-GPC (16:0/20:3n3 or 6)		Lipid	Phospholipid Metabolism	+	+	-
1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)	100008915	Lipid	Phospholipid Metabolism	+	+	-
1-palmitoyl-2-eicosapentaenoyl-GPC (16:0/20:5)		Lipid	Phospholipid Metabolism	+	+	-
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	1537	Lipid	Phospholipid Metabolism	+	+	-
1-palmitoyl-2-meadoyl-GPC (16:0/20:3n9)		Lipid	Phospholipid Metabolism	+	+	-
1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	1539	Lipid	Phospholipid Metabolism	+	+	-
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)		Lipid	Phospholipid Metabolism	+	+	-
1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	100008921	Lipid	Phospholipid Metabolism	+	+	-
1-palmityl-2-oleoyl-GPC (O-16:0/18:1)		Lipid	Phospholipid Metabolism	+	+	-
1-pentadecanoyl-2-oleoyl-GPC (15:0/18:1)		Lipid	Phospholipid Metabolism	+	+	-
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	100001869	Lipid	Phospholipid Metabolism	+	+	-
1-stearoyl-2-dihomo-linolenoyl-GPC (18:0/20:3n3 or 6)		Lipid	Phospholipid Metabolism	+	+	-
1-stearoyl-2-docosahexaenoyl-GPC (18:0/22:6)	100008916	Lipid	Phospholipid Metabolism	+	+	-
1-stearoyl-2-docosahexaenoyl-GPE (18:0/22:6)		Lipid	Phospholipid Metabolism	+	+	-
1-stearoyl-2-docosapentaenoyl-GPC (18:0/22:5n3)		Lipid	Phospholipid Metabolism	+	+	-
1-stearoyl-2-docosapentaenoyl-GPC (18:0/22:5n6)		Lipid	Phospholipid Metabolism	+	+	-
1-stearoyl-2-linoleoyl-GPC (18:0/18:2)		Lipid	Phospholipid Metabolism	+	+	-
1-stearoyl-2-meadoyl-GPC (18:0/20:3n9)		Lipid	Phospholipid Metabolism	+	+	-
1-stearoyl-2-oleoyl-GPC (18:0/18:1)	100008904	Lipid	Phospholipid Metabolism	+	+	-
1-palmityl-2-arachidonoyl-GPC (O-16:0/20:4)		Lipid	Phospholipid Metabolism	+	-	-
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)		Lipid	Plasmalogen	+	+	-
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPC (P-16:0/22:6)		Lipid	Plasmalogen	+	+	-
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPE (P-16:0/22:6)		Lipid	Plasmalogen	+	+	-
1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)		Lipid	Plasmalogen	+	+	-
1-(1-enyl-palmitoyl)-2-dihomo-linolenoyl-GPC (P-18:0/20:3)		Lipid	Plasmalogen	+	-	-
dihomolinoleate (20:2n6)		Lipid	Polyunsaturated Fatty Acid (n3 and n6)	+	+	-
dihomolinolenate (20:3n3 or 3n6)		Lipid	Polyunsaturated Fatty Acid (n3 and n6)	+	+	-
glycochenodeoxycholate	1628	Lipid	Primary Bile Acid Metabolism	+	+	+
glycocholate	342	Lipid	Primary Bile Acid Metabolism	+	+	+
glycocholenate sulfate		Lipid	Secondary Bile Acid Metabolism	+	+	+
glycohyocholate	100004083	Lipid	Secondary Bile Acid Metabolism	+	+	+
hyocholate	100001279	Lipid	Secondary Bile Acid Metabolism	+	+	-
behenoyl sphingomyelin (d18:1/22:0)		Lipid	Sphingolipid Metabolism	+	+	-
palmitoyl sphingomyelin (d18:1/16:0)	100002107	Lipid	Sphingolipid Metabolism	+	+	-
sphingomyelin		Lipid	Sphingolipid Metabolism	+	+	-
sphingomyelin (d18:1/14:0, d16:1/16:0)		Lipid	Sphingolipid Metabolism	+	+	-
sphingomyelin (d18:1/18:1, d18:2/18:0)	100002106	Lipid	Sphingolipid Metabolism	+	+	-
sphingomyelin (d18:1/20:0, d16:1/22:0)		Lipid	Sphingolipid Metabolism	+	+	-
sphingomyelin (d18:1/24:1, d18:2/24:0)		Lipid	Sphingolipid Metabolism	+	+	-
sphingomyelin (d18:2/16:0, d18:1/16:1)		Lipid	Sphingolipid Metabolism	+	+	-
sphingosine	297	Lipid	Sphingolipid Metabolism	+	+	-
16a-hydroxy DHEA 3-sulfate	100002126	Lipid	Steroid	+	+	+
4-androsten-3beta,17beta-diol disulfate (1)	100001992	Lipid	Steroid	+	+	+
4-androsten-3beta,17beta-diol disulfate (2)	100001994	Lipid	Steroid	+	+	+
5alpha-pregnan-3beta,20alpha-diol disulfate	100001988	Lipid	Steroid	+	+	+
andro steroid monosulfate (1)		Lipid	Steroid	+	+	+
cortisol	356	Lipid	Steroid	+	+	+
cortisone	273	Lipid	Steroid	+	+	+
dehydroisoandrosterone sulfate (DHEA-S)	100000792	Lipid	Steroid	+	+	+
7-HOCA		Lipid	Sterol	+	+	-
cholesterol	266	Lipid	Sterol	+	+	-
allantoin	1002	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	+	+	+
hypoxanthine	171	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	+	+	+
inosine	361	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	+	+	+
N1-methylinosine		Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	+	+	+
urate	1134	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	+	+	+
xanthine	1004	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	+	+	+
xanthosine	100000299	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	+	-	+
2'-deoxyinosine	100000135	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	+	-	-
1-methyladenosine		Nucleotide	Purine Metabolism, Adenine containing	+	+	+
adenine	880	Nucleotide	Purine Metabolism, Adenine containing	+	+	+
adenosine 3',5'-cyclic monophosphate (cAMP)	207	Nucleotide	Purine Metabolism, Adenine containing	+	+	+
AMP		Nucleotide	Purine Metabolism, Adenine containing	+	+	+
N6-carbamoylthreonyladenosine	100001415	Nucleotide	Purine Metabolism, Adenine containing	+	+	+
N6-succinyladenosine	100001664	Nucleotide	Purine Metabolism, Adenine containing	+	+	+
adenosine	798	Nucleotide	Purine Metabolism, Adenine containing	+	-	+
N6-methyladenosine	213	Nucleotide	Purine Metabolism, Adenine containing	+	-	+
7-methylguanine	100001456	Nucleotide	Purine Metabolism, Guanine containing	+	+	+
N2,N2-dimethylguanosine	100001412	Nucleotide	Purine Metabolism, Guanine containing	+	+	+
guanosine	1099	Nucleotide	Purine Metabolism, Guanine containing	+	-	+
N2-methylguanosine	100001467	Nucleotide	Purine Metabolism, Guanine containing	+	-	+
cytidine	827	Nucleotide	Pyrimidine Metabolism, Cytidine containing	+	+	+
2'-deoxycytidine	100000125	Nucleotide	Pyrimidine Metabolism, Cytidine containing	+	-	-
orotate	445	Nucleotide	Pyrimidine Metabolism, Orotate containing	+	+	+
orotidine	100001416	Nucleotide	Pyrimidine Metabolism, Orotate containing	+	+	+

Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profiling Assay

Supplemental Table 1. Biochemicals Detected in Plasma, Urine, and CSF

Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
3-aminoisobutyrate	1114	Nucleotide	Pyrimidine Metabolism, Thymine containing	+	+	+
5,6-dihydrothymine	158	Nucleotide	Pyrimidine Metabolism, Thymine containing	+	+	+
3-ureidopropionate	1053	Nucleotide	Pyrimidine Metabolism, Uracil containing	+	+	+
5-methyluridine (ribothymidine)	100001446	Nucleotide	Pyrimidine Metabolism, Uracil containing	+	+	+
N-acetyl-beta-alanine	100002102	Nucleotide	Pyrimidine Metabolism, Uracil containing	+	+	+
pseudouridine	821	Nucleotide	Pyrimidine Metabolism, Uracil containing	+	+	+
uracil	825	Nucleotide	Pyrimidine Metabolism, Uracil containing	+	+	+
uridine	535	Nucleotide	Pyrimidine Metabolism, Uracil containing	+	+	+
2'-deoxyuridine	536	Nucleotide	Pyrimidine Metabolism, Uracil containing	+	+	-
pyroglutamylglutamine	100000966	Peptide	Dipeptide	+	+	+
glycylproline	100000976	Peptide	Dipeptide	+	-	+
leucylproline	100001574	Peptide	Dipeptide	+	-	+
cyclo(ala-pro)	100004646	Peptide	Dipeptide	+	-	-
cyclo(pro-val)	100006065	Peptide	Dipeptide	+	-	-
homocarnosine	41	Peptide	Dipeptide Derivative	+	-	+
gamma-glutamyl-epsilon-lysine	100001262	Peptide	Gamma-glutamyl Amino Acid	+	+	+
gamma-glutamylglutamine	1140	Peptide	Gamma-glutamyl Amino Acid	+	+	+
gamma-glutamylhistidine	1235	Peptide	Gamma-glutamyl Amino Acid	+	+	+
gamma-glutamylisoleucine		Peptide	Gamma-glutamyl Amino Acid	+	+	+
gamma-glutamylleucine	1268	Peptide	Gamma-glutamyl Amino Acid	+	+	+
gamma-glutamylphenylalanine	100000491	Peptide	Gamma-glutamyl Amino Acid	+	+	+
gamma-glutamyltyrosine	1102	Peptide	Gamma-glutamyl Amino Acid	+	+	+
gamma-glutamylvaline	100001126	Peptide	Gamma-glutamyl Amino Acid	+	+	+
gamma-glutamylalanine	100001843	Peptide	Gamma-glutamyl Amino Acid	+	+	-
gamma-glutamylmethionine	100001313	Peptide	Gamma-glutamyl Amino Acid	+	+	-
gamma-glutamylthreonine	100001314	Peptide	Gamma-glutamyl Amino Acid	+	+	-
tartronate (hydroxymalonate)	100000840	Xenobiotics	Bacterial/Fungal	+	+	+
4-methylcatechol sulfate	100004111	Xenobiotics	Benzoate Metabolism	+	+	+
catechol sulfate	100001605	Xenobiotics	Benzoate Metabolism	+	+	+
hippurate	100000014	Xenobiotics	Benzoate Metabolism	+	+	+
methyl-4-hydroxybenzoate sulfate	100006116	Xenobiotics	Benzoate Metabolism	+	+	+
2-aminophenol sulfate	100004322	Xenobiotics	Chemical	+	+	+
3-hydroxypyridine sulfate	100006098	Xenobiotics	Chemical	+	+	+
O-sulfo-L-tyrosine	100005384	Xenobiotics	Chemical	+	+	+
succinimide	100003696	Xenobiotics	Chemical	+	+	+
sulfate		Xenobiotics	Chemical	+	+	+
dimethyl sulfone	100004284	Xenobiotics	Chemical	+	-	+
trizma acetate	100000856	Xenobiotics	Chemical	+	-	+
1,2-propanediol	100001176	Xenobiotics	Chemical	+	-	-
1,3-propanediol	100001175	Xenobiotics	Chemical	+	-	-
2-hydroxyacetaminophen sulfate		Xenobiotics	Drug	+	+	+
2-methoxyacetaminophen glucuronide		Xenobiotics	Drug	+	+	+
2-methoxyacetaminophen sulfate		Xenobiotics	Drug	+	+	+
3-(cystein-S-yl)acetaminophen		Xenobiotics	Drug	+	+	+
4-acetamidophenol	1383	Xenobiotics	Drug	+	+	+
4-acetamidophenylglucuronide	100000043	Xenobiotics	Drug	+	+	+
4-acetaminophen sulfate	2049	Xenobiotics	Drug	+	+	+
6-oxopiperidine-2-carboxylic acid		Xenobiotics	Drug	+	+	+
Cetirizine		Xenobiotics	Drug	+	+	+
salicylate	501	Xenobiotics	Drug	+	+	+
topiramate	1388	Xenobiotics	Drug	+	+	-
carbamazepine 10,11-epoxide		Xenobiotics	Drug	+	-	+
lidocaine	100001538	Xenobiotics	Drug	+	-	+
N-ethylglycinexylidide	100001539	Xenobiotics	Drug	+	-	+
5-sulfosalicylate	100000815	Xenobiotics	Drug	+	-	-
fluoxetine	1382	Xenobiotics	Drug	+	-	-
pregabalin	100008943	Xenobiotics	Drug	+	-	-
sulfamethoxazole		Xenobiotics	Drug	+	-	-
2,3-dihydroxyisovalerate	100002417	Xenobiotics	Food Component/Plant	+	+	+
2-piperidinone	100004295	Xenobiotics	Food Component/Plant	+	+	+
acesulfame		Xenobiotics	Food Component/Plant	+	+	+
betonicine	100002153	Xenobiotics	Food Component/Plant	+	+	+
ergothioneine	100002154	Xenobiotics	Food Component/Plant	+	+	+
erythritol	100000846	Xenobiotics	Food Component/Plant	+	+	+
gluconate	338	Xenobiotics	Food Component/Plant	+	+	+
piperine	100001267	Xenobiotics	Food Component/Plant	+	+	+
quinate	100000442	Xenobiotics	Food Component/Plant	+	+	+
stachydrine	100001296	Xenobiotics	Food Component/Plant	+	+	+
tartarate	100000295	Xenobiotics	Food Component/Plant	+	+	+
S-allylcysteine	100004509	Xenobiotics	Food Component/Plant	+	+	-
indolin-2-one	100004318	Xenobiotics	Food Component/Plant	+	-	+
levulinate (4-oxovalerate)	100000765	Xenobiotics	Food Component/Plant	+	-	+
3-methylxanthine	100001108	Xenobiotics	Xanthine Metabolism	+	+	+
5-acetylamino-6-amino-3-methyluracil	100001403	Xenobiotics	Xanthine Metabolism	+	+	+
7-methylxanthine	100001396	Xenobiotics	Xanthine Metabolism	+	+	+
caffeine	849	Xenobiotics	Xanthine Metabolism	+	+	+
paraxanthine	100000453	Xenobiotics	Xanthine Metabolism	+	+	+
theobromine	100000445	Xenobiotics	Xanthine Metabolism	+	+	+
theophylline	100000437	Xenobiotics	Xanthine Metabolism	+	+	+
N-carbamoylalanine	100006369	Amino Acid	Alanine and Aspartate Metabolism	-	+	+
N-methylalanine	100001823	Amino Acid	Alanine and Aspartate Metabolism	-	+	+
N-carbamoylsarcosine	100002606	Amino Acid	Creatine Metabolism	-	-	+
N-methylhydantoin	100002557	Amino Acid	Creatine Metabolism	-	-	+
4-hydroxyglutamate	100002544	Amino Acid	Glutamate Metabolism	-	-	+
gamma-carboxyglutamate	100002679	Amino Acid	Glutamate Metabolism	-	-	+
N-methyl-4-aminobutyric acid		Amino Acid	Glutamate Metabolism	-	-	+
N-methylglutamate	100001131	Amino Acid	Glutamate Metabolism	-	-	+
cysteine-glutathione disulfide	100001437	Amino Acid	Glutathione Metabolism	-	+	+
sarcosine (N-Methylglycine)		Amino Acid	Glycine, Serine and Threonine Metabolism	-	+	+

Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profiling Assay

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Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
allo-threonine	100000272	Amino Acid	Glycine, Serine and Threonine Metabolism	-	-	+
beta-hydroxypyruvate	100000055	Amino Acid	Glycine, Serine and Threonine Metabolism	-	-	+
guanidinosuccinate	100001212	Amino Acid	Guanidino and Acetamido Metabolism	-	+	+
cis-urocanate	100003425	Amino Acid	Histidine Metabolism	-	+	+
hydantoin-5-propionic acid	100002514	Amino Acid	Histidine Metabolism	-	+	+
N-acetyl-l-methylhistidine		Amino Acid	Histidine Metabolism	-	+	+
trans-urocanate	537	Amino Acid	Histidine Metabolism	-	+	+
histamine	354	Amino Acid	Histidine Metabolism	-	-	+
N-acetylhistamine	100006123	Amino Acid	Histidine Metabolism	-	-	+
2-methylbutyrylglycine (C5)		Amino Acid	Leucine, Isoleucine and Valine Metabolism	-	+	+
isobutyrylglycine (C4)		Amino Acid	Leucine, Isoleucine and Valine Metabolism	-	+	+
isovalerylglycine	100001452	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-	+	+
tigloylglycine	1161	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-	+	+
allo-isoleucine	100005840	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-	+	-
3-methylcrotonylglycine	100001149	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-	-	+
3-methylglutarate	1122	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-	-	+
beta-hydroxyisovaleryl glycine		Amino Acid	Leucine, Isoleucine, and Valine Metabolism	-	-	+
methylsuccinoylcarnitine (1)		Amino Acid	Leucine, Isoleucine, and Valine Metabolism	-	-	+
2-aminoadipate	381	Amino Acid	Lysine Metabolism	-	+	+
3-methylglutarylcarnitine (1)	100005849	Amino Acid	Lysine Metabolism	-	+	+
N6-acetyllysine	100001734	Amino Acid	Lysine Metabolism	-	+	+
N-acetyl-cadaverine	100002249	Amino Acid	Lysine Metabolism	-	+	+
3-hydroxyglutarate	100001146	Amino Acid	Lysine Metabolism	-	-	+
5-(galactosylhydroxy)-L-lysine	100002462	Amino Acid	Lysine Metabolism	-	-	+
5-aminovalerate	100000454	Amino Acid	Lysine Metabolism	-	-	+
cadaverine	100000110	Amino Acid	Lysine Metabolism	-	-	+
N2,N6-diacetyllysine	100006124	Amino Acid	Lysine Metabolism	-	-	+
N2-acetyllysine	100001721	Amino Acid	Lysine Metabolism	-	-	+
saccharopine	392	Amino Acid	Lysine Metabolism	-	-	+
cysteine s-sulfate	100000808	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-	+	+
cystine	279	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-	+	+
hypotaurine	358	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-	+	+
alpha-ketobutyrate	796	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-	+	-
cysteine sulfinic acid	100002113	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-	+	-
N-acetylcysteine	1107	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-	-	+
N-methyltaurine	100004056	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-	-	+
S-adenosylmethionine (SAM)	1263	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-	-	+
taurocyamine	100001418	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-	-	+
2-hydroxyphenylacetate	235	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
3-(3-hydroxyphenyl)propionate	100001624	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
3-(3-hydroxyphenyl)propionate sulfate	100005391	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
3-(4-hydroxyphenyl)propionate	100002914	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
4-hydroxyphenylacetate	144	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
4-hydroxyphenylpyruvate	1141	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
5-bromotryptophan		Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
dopamine 4-sulfate		Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
gentisate	100000447	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
o-cresol sulfate	100001806	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
p-cresol-glucuronide		Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
phenylacetylcarnitine	100006108	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
phenylacetylglycine	100001275	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
tyramine O-sulfate	100006092	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
vanillic alcohol sulfate	100006125	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
vanillylmandelate (VMA)	1111	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	+
3-phenylpropionate (hydrocinnamate)	100000010	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	-
N-formylphenylalanine	100006056	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	-
phenylacetate	100000011	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	-
phenylpyruvate	241	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	-
thyroxine	1094	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	+	-
3,4-dihydroxyphenylacetate	100000449	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
3,4-dihydroxyphenylacetate sulfate	100006254	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
3-hydroxyphenylacetate	114	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
3-hydroxyphenylacetyl carnitine		Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
3-hydroxyphenylacetyl sulfate		Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
3-methoxytyramine	118	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
4-hydroxycinnamate sulfate	100006095	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
4-hydroxyphenylacetyl glycine	100004418	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
4-hydroxyphenylacetylcarnitine		Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
5-hydroxymethyl-2-furoic acid	100003954	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
catechol glucuronide		Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
dopamine	1748	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
homovanillate sulfate	100002250	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
m-tyramine	100002797	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
phenethylamine	1207	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
phenylpropionylglycine	100001591	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
tyramine	1133	Amino Acid	Phenylalanine and Tyrosine Metabolism	-	-	+
putrescine	49	Amino Acid	Polyamine Metabolism	-	-	+
3-hydroxykynurenine	100000986	Amino Acid	Tryptophan Metabolism	-	+	+
indoleacetylglutamine	100001731	Amino Acid	Tryptophan Metabolism	-	+	+
N-acetylkynurenine (2)	100006378	Amino Acid	Tryptophan Metabolism	-	+	+
N-acetyltryptophan	100001254	Amino Acid	Tryptophan Metabolism	-	+	+
serotonin	504	Amino Acid	Tryptophan Metabolism	-	+	+
xanthurenate	100000015	Amino Acid	Tryptophan Metabolism	-	+	+
3-hydroxyanthranilate	243	Amino Acid	Tryptophan Metabolism	-	-	+
indolepropionylglycine		Amino Acid	Tryptophan Metabolism	-	-	+
tryptamine	1095	Amino Acid	Tryptophan Metabolism	-	-	+
2-oxoarginine		Amino Acid	Urea cycle; Arginine and Proline Metabolism	-	+	+
N-acetylcitrulline	100001577	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-	+	+
3-hydroxyproline	100002089	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-	-	+

Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profiling Assay

Supplemental Table 1. Biochemicals Detected in Plasma, Urine, and CSF

Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
N2,N5-diacetylornithine	100004575	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-	-	+
N-acetylproline	100001334	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-	-	+
N-alpha-acetylornithine	100000285	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-	-	+
N6-carboxymethyllysine	100001768	Carbohydrate	Advanced Glycation End-product	-	+	+
N-acetylglucosamine/N-acetylgalactosamine	100006435	Carbohydrate	Aminosugar Metabolism	-	+	-
3'-a-sialyl-N-acetyllactosamine	100003257	Carbohydrate	Aminosugar Metabolism	-	-	+
6-sialyl-N-acetyllactosamine	100003259	Carbohydrate	Aminosugar Metabolism	-	-	+
lactose	393	Carbohydrate	Disaccharides and Oligosaccharides	-	+	+
2-fucosyllactose	100002930	Carbohydrate	Disaccharides and Oligosaccharides	-	-	+
3-fucosyllactose	100002931	Carbohydrate	Disaccharides and Oligosaccharides	-	-	+
3-sialyllactose	100003408	Carbohydrate	Disaccharides and Oligosaccharides	-	-	+
6'-sialyllactose	100003132	Carbohydrate	Disaccharides and Oligosaccharides	-	-	+
lacto-N-fucopentaose I	100002938	Carbohydrate	Disaccharides and Oligosaccharides	-	-	+
lacto-N-fucopentaose II	100002936	Carbohydrate	Disaccharides and Oligosaccharides	-	-	+
lacto-N-tetraose	100004063	Carbohydrate	Disaccharides and Oligosaccharides	-	-	+
raffinose	879	Carbohydrate	Disaccharides and Oligosaccharides	-	-	+
maltose	913	Carbohydrate	Glycogen Metabolism	-	+	-
maltotriose	100000276	Carbohydrate	Glycogen Metabolism	-	+	-
3-phosphoglycerate	132	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-	+	+
2,3-diphosphoglycerate	1227	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-	+	-
arabinose	828	Carbohydrate	Pentose Metabolism	-	-	+
ribulose/xylulose	100006122	Carbohydrate	Pentose Metabolism	-	-	+
sedoheptulose		Carbohydrate	Pentose Metabolism	-	-	+
xylose	826	Carbohydrate	Pentose Metabolism	-	-	+
6-phosphogluconate	100000341	Carbohydrate	Pentose Phosphate Pathway	-	-	+
ascorbate (Vitamin C)	233	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-	-	+
dehydroascorbate	301	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-	-	+
glucarate (saccharate)	1020	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-	-	+
biotin	251	Cofactors and Vitamins	Biotin Metabolism	-	-	+
folate	328	Cofactors and Vitamins	Folate Metabolism	-	-	+
bilirubin (E,Z or Z,E)		Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-	+	-
biliverdin	250	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-	+	-
5-aminolevulinate	1306	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-	-	+
L-urobilin	100002568	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-	-	+
adenosine 5'-diphosphoribose (ADP-ribose)	215	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-	+	-
nicotinate ribonucleoside	100001316	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-	-	+
7,8-dihydroneopterin	100000142	Cofactors and Vitamins	Pterin Metabolism	-	-	+
isoxanthopterin	100000749	Cofactors and Vitamins	Pterin Metabolism	-	-	+
neopterin	100001474	Cofactors and Vitamins	Pterin Metabolism	-	-	+
pterin	100004216	Cofactors and Vitamins	Pterin Metabolism	-	-	+
sepiapterin	100005969	Cofactors and Vitamins	Pterin Metabolism	-	-	+
riboflavin (Vitamin B2)	500	Cofactors and Vitamins	Riboflavin Metabolism	-	+	+
FAD		Cofactors and Vitamins	Riboflavin Metabolism	-	+	-
biopterin	1548	Cofactors and Vitamins	Tetrahydrobiopterin Metabolism	-	-	+
dihydrobiopterin	100001506	Cofactors and Vitamins	Tetrahydrobiopterin Metabolism	-	-	+
thiamin (Vitamin B1)	873	Cofactors and Vitamins	Thiamine Metabolism	-	+	+
alpha-CEHC sulfate	100005972	Cofactors and Vitamins	Tocopherol Metabolism	-	+	+
gamma-CEHC glucuronide		Cofactors and Vitamins	Tocopherol Metabolism	-	+	+
alpha-tocopherol	1105	Cofactors and Vitamins	Tocopherol Metabolism	-	+	-
delta-tocopherol	100001216	Cofactors and Vitamins	Tocopherol Metabolism	-	+	-
alpha-CEHC	100002206	Cofactors and Vitamins	Tocopherol Metabolism	-	-	+
alpha-CEHC glucuronide		Cofactors and Vitamins	Tocopherol Metabolism	-	-	+
pyridoxamine	568	Cofactors and Vitamins	Vitamin B6 Metabolism	-	-	+
citraconate/glutaconate	100006438	Energy	TCA Cycle	-	-	+
trans-aconitate	100001043	Energy	TCA Cycle	-	-	+
tricarballylate	2053	Energy	TCA Cycle	-	-	+
1-oleoyl-2-linoleoyl-glycerol (18:1/18:2)		Lipid	Diacylglycerol	-	+	-
1-oleoyl-3-linoleoyl-glycerol (18:1/18:2)		Lipid	Diacylglycerol	-	+	-
diacylglycerol (14:0/18:1, 16:0/16:1) (1)		Lipid	Diacylglycerol	-	+	-
diacylglycerol (14:0/18:1, 16:0/16:1) (2)		Lipid	Diacylglycerol	-	+	-
linoleoyl-arachidonoyl-glycerol (18:2/20:4) (1)		Lipid	Diacylglycerol	-	+	-
linoleoyl-arachidonoyl-glycerol (18:2/20:4) (2)		Lipid	Diacylglycerol	-	+	-
N-oleoyltaurine	100003119	Lipid	Endocannabinoid	-	+	-
N-palmitoyltaurine	100003239	Lipid	Endocannabinoid	-	+	-
N-stearoyltaurine	100003240	Lipid	Endocannabinoid	-	+	-
oleic ethanolamide		Lipid	Endocannabinoid	-	+	-
palmitoyl ethanolamide	1489	Lipid	Endocannabinoid	-	+	-
stearoyl ethanolamide	100002254	Lipid	Endocannabinoid	-	+	-
3-hydroxybutyrylcarnitine (2)		Lipid	Fatty Acid Metabolism (Acyl Carnitine)	-	+	+
suberoylcarnitine		Lipid	Fatty Acid Metabolism (Acyl Carnitine)	-	+	+
arachidonoylcholine		Lipid	Fatty Acid Metabolism (Acyl Choline)	-	+	-
linoleoylcholine		Lipid	Fatty Acid Metabolism (Acyl Choline)	-	+	-
oleoylcholine		Lipid	Fatty Acid Metabolism (Acyl Choline)	-	+	-
palmitoylcholine		Lipid	Fatty Acid Metabolism (Acyl Choline)	-	+	-
stearoylcholine		Lipid	Fatty Acid Metabolism (Acyl Choline)	-	+	-
hexanoylglutamine		Lipid	Fatty Acid Metabolism (Acyl Glutamine)	-	+	+
3,4-methylene-heptanoylglycine		Lipid	Fatty Acid Metabolism (Acyl Glycine)	-	-	+
propionylglycine (C3)		Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	-	+	+
hydroxybutyrylcarnitine		Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-	+	+
myristoleoylcarnitine		Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-	+	+
myristoylcarnitine		Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-	+	+
linoleoylcarnitine		Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-	+	-
oleoylcarnitine (C18)		Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-	+	-
palmitoylcarnitine (C16)	100000776	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-	+	-
stearoylcarnitine (C18)	100001391	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-	+	-
hexanoylglycine (C6)		Lipid	Fatty Acid Metabolism(Acyl Glycine)	-	+	+
N-octanoylglycine	100003940	Lipid	Fatty Acid Metabolism(Acyl Glycine)	-	+	+
N-linoleoylglycine	1506	Lipid	Fatty Acid Metabolism(Acyl Glycine)	-	+	-
N-palmitoyl glycine		Lipid	Fatty Acid Metabolism(Acyl Glycine)	-	+	-

Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profiling Assay

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Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
heptanoyl glycine	100004195	Lipid	Fatty Acid Metabolism(Acyl Glycine)	-	-	+
2-methylmalonyl carnitine		Lipid	Fatty Acid Synthesis	-	+	+
linoleamide (18:2n6)	1492	Lipid	Fatty Acid, Amide	-	+	-
17-methylstearate	100002356	Lipid	Fatty Acid, Branched	-	+	-
methylpalmitate (15 or 2)		Lipid	Fatty Acid, Branched	-	+	-
2-hydroxyglutarate	100002070	Lipid	Fatty Acid, Dicarboxylate	-	+	+
3-methyladipate	100001765	Lipid	Fatty Acid, Dicarboxylate	-	+	+
adipate	100000863	Lipid	Fatty Acid, Dicarboxylate	-	+	+
azelate (nonanedioate; C9)		Lipid	Fatty Acid, Dicarboxylate	-	+	+
pimelate (heptanedioate)	100000101	Lipid	Fatty Acid, Dicarboxylate	-	+	+
sebacate (decanedioate)	100001211	Lipid	Fatty Acid, Dicarboxylate	-	+	+
suberate (octanedioate)	100000016	Lipid	Fatty Acid, Dicarboxylate	-	+	+
docosadioate	100002952	Lipid	Fatty Acid, Dicarboxylate	-	+	-
dodecanedioate (C12)		Lipid	Fatty Acid, Dicarboxylate	-	+	-
eicosanodioate	100002951	Lipid	Fatty Acid, Dicarboxylate	-	+	-
hexadecanedioate (C16)		Lipid	Fatty Acid, Dicarboxylate	-	+	-
octadecanedioate (C18)		Lipid	Fatty Acid, Dicarboxylate	-	+	-
tetradecanedioate (C14)		Lipid	Fatty Acid, Dicarboxylate	-	+	-
4-octenedioate	100001152	Lipid	Fatty Acid, Dicarboxylate	-	-	+
9,10-DiHOME	179	Lipid	Fatty Acid, Dihydroxy	-	+	-
2-hydroxyoctanoate	100000743	Lipid	Fatty Acid, Monohydroxy	-	+	+
7-hydroxyoctanoate	100001223	Lipid	Fatty Acid, Monohydroxy	-	+	+
13-HODE + 9-HODE	100002196	Lipid	Fatty Acid, Monohydroxy	-	+	-
16-hydroxypalmitate	100002953	Lipid	Fatty Acid, Monohydroxy	-	+	-
2-hydroxypalmitate	100001579	Lipid	Fatty Acid, Monohydroxy	-	+	-
2-hydroxystearate	1239	Lipid	Fatty Acid, Monohydroxy	-	+	-
3-hydroxydecanoate	100000997	Lipid	Fatty Acid, Monohydroxy	-	+	-
3-hydroxylaurate	100001112	Lipid	Fatty Acid, Monohydroxy	-	+	-
8-hydroxyoctanoate	100000956	Lipid	Fatty Acid, Monohydroxy	-	+	-
9-hydroxystearate	100005834	Lipid	Fatty Acid, Monohydroxy	-	+	-
alpha-hydroxycaproate	100001723	Lipid	Fatty Acid, Monohydroxy	-	+	-
3-hydroxypropanoate	115	Lipid	Fatty Acid, Monohydroxy	-	-	+
3-hydroxysuberate	100001143	Lipid	Fatty Acid, Monohydroxy	-	-	+
3-hydroxytetradecanedioate	100001147	Lipid	Fatty Acid, Monohydroxy	-	-	+
epiandrosterone glucuronide	100005400	Lipid	Fatty Acid, Monohydroxy	-	-	+
glycerophosphoglycerol	100001619	Lipid	Glycerolipid Metabolism	-	+	+
chiro-inositol	100001859	Lipid	Inositol Metabolism	-	+	+
scyllo-inositol	100001215	Lipid	Inositol Metabolism	-	-	+
10-heptadecenoate (17:1n7)	100001278	Lipid	Long Chain Fatty Acid	-	+	-
10-nonadecenoate (19:1n9)	100001277	Lipid	Long Chain Fatty Acid	-	+	-
arachidate (20:0)	893	Lipid	Long Chain Fatty Acid	-	+	-
eicosenoate (20:1n9 or 1n11)		Lipid	Long Chain Fatty Acid	-	+	-
erucate (22:1n9)	1087	Lipid	Long Chain Fatty Acid	-	+	-
margarate (17:0)	891	Lipid	Long Chain Fatty Acid	-	+	-
myristate (14:0)	519	Lipid	Long Chain Fatty Acid	-	+	-
myristoleate (14:1n5)	100001198	Lipid	Long Chain Fatty Acid	-	+	-
nonadecanoate (19:0)	892	Lipid	Long Chain Fatty Acid	-	+	-
oleate/vaccenate (18:1)	100008930	Lipid	Long Chain Fatty Acid	-	+	-
palmitate (16:0)	424	Lipid	Long Chain Fatty Acid	-	+	-
palmitoleate (16:1n7)	452	Lipid	Long Chain Fatty Acid	-	+	-
stearate (18:0)	439	Lipid	Long Chain Fatty Acid	-	+	-
1-(1-enyl-oleoyl)-GPC (P-18:1)		Lipid	Lysolipid	-	+	-
1-(1-enyl-oleoyl)-GPE (P-18:1)		Lipid	Lysolipid	-	+	-
1-arachidonoyl-GPA (20:4)	100004442	Lipid	Lysolipid	-	+	-
1-arachidonoyl-GPI (20:4)		Lipid	Lysolipid	-	+	-
1-arachidoyl-GPC (20:0)	100001384	Lipid	Lysolipid	-	+	-
1-dihomo-linolenoyl-GPE (20:3n3 or 6)		Lipid	Lysolipid	-	+	-
1-eicosapentaenoyl-GPC (20:5)		Lipid	Lysolipid	-	+	-
1-eicosapentaenoyl-GPE (20:5)		Lipid	Lysolipid	-	+	-
1-eicosenoyl-GPC (20:1)		Lipid	Lysolipid	-	+	-
1-heptadecanoyl-GPC (17:0)		Lipid	Lysolipid	-	+	-
1-lignoceroyl-GPC (24:0)	100002873	Lipid	Lysolipid	-	+	-
1-linolenoyl-GPC (18:3)		Lipid	Lysolipid	-	+	-
1-linoleoyl-GPA (18:2)		Lipid	Lysolipid	-	+	-
1-linoleoyl-GPE (18:2)		Lipid	Lysolipid	-	+	-
1-linoleoyl-GPI (18:2)		Lipid	Lysolipid	-	+	-
1-margaroyl-GPE (17:0)		Lipid	Lysolipid	-	+	-
1-nonadecanoyl-GPC (19:0)	100005353	Lipid	Lysolipid	-	+	-
1-oleoyl-GPE (18:1)	100001569	Lipid	Lysolipid	-	+	-
1-oleoyl-GPG (18:1)		Lipid	Lysolipid	-	+	-
1-oleoyl-GPI (18:1)		Lipid	Lysolipid	-	+	-
1-oleoyl-GPS (18:1)	100000630	Lipid	Lysolipid	-	+	-
1-palmitoyl-GPE (16:0)	100001567	Lipid	Lysolipid	-	+	-
1-palmitoyl-GPI (16:0)	100001655	Lipid	Lysolipid	-	+	-
1-stearoyl-GPI (18:0)	100000656	Lipid	Lysolipid	-	+	-
1-stearoyl-GPS (18:0)		Lipid	Lysolipid	-	+	-
2-arachidonoyl-GPC (20:4)		Lipid	Lysolipid	-	+	-
2-arachidonoyl-GPE (20:4)		Lipid	Lysolipid	-	+	-
2-docosahexaenoyl-GPC (22:6)		Lipid	Lysolipid	-	+	-
2-docosahexaenoyl-GPE (22:6)		Lipid	Lysolipid	-	+	-
2-linoleoyl-GPC (18:2)		Lipid	Lysolipid	-	+	-
2-linoleoyl-GPE (18:2)		Lipid	Lysolipid	-	+	-
2-oleoyl-GPC (18:1)		Lipid	Lysolipid	-	+	-
2-oleoyl-GPE (18:1)		Lipid	Lysolipid	-	+	-
2-palmitoleoyl-GPC (16:1)		Lipid	Lysolipid	-	+	-
2-palmitoyl-GPC (16:0)		Lipid	Lysolipid	-	+	-
2-palmitoyl-GPE (16:0)		Lipid	Lysolipid	-	+	-
2-stearoyl-GPE (18:0)		Lipid	Lysolipid	-	+	-
2-stearoyl-GPI (18:0)		Lipid	Lysolipid	-	+	-

Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profiling Assay

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Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
1-(1-enyl-palmitoyl)-GPE (P-16:0)		Lipid	Lysoplasmalogen	-	+	-
caprylate (8:0)	932	Lipid	Medium Chain Fatty Acid	-	+	+
heptanoate (7:0)	925	Lipid	Medium Chain Fatty Acid	-	+	+
10-undecenoate (11:1n1)	100001197	Lipid	Medium Chain Fatty Acid	-	+	-
5-dodecenoate (12:1n7)	100001232	Lipid	Medium Chain Fatty Acid	-	+	-
caprate (10:0)	888	Lipid	Medium Chain Fatty Acid	-	+	-
caproate (6:0)	926	Lipid	Medium Chain Fatty Acid	-	+	-
laurate (12:0)	181	Lipid	Medium Chain Fatty Acid	-	+	-
1-docosahexaenoylglycerol (22:6)	100001481	Lipid	Monoacylglycerol	-	+	-
1-linolenoylglycerol (18:3)	100001435	Lipid	Monoacylglycerol	-	+	-
1-linoleoylglycerol (18:2)	100001040	Lipid	Monoacylglycerol	-	+	-
1-margaroylglycerol (17:0)	100001429	Lipid	Monoacylglycerol	-	+	-
1-pentadecanoylglycerol (15:0)	100001431	Lipid	Monoacylglycerol	-	+	-
2-arachidonoylglycerol (20:4)	100000584	Lipid	Monoacylglycerol	-	+	-
2-linoleoylglycerol (18:2)	100000987	Lipid	Monoacylglycerol	-	+	-
2-oleoylglycerol (18:1)	100000943	Lipid	Monoacylglycerol	-	+	-
2-palmitoylglycerol (16:0)	100001048	Lipid	Monoacylglycerol	-	+	-
1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)		Lipid	Phospholipid Metabolism	-	+	-
1-(1-enyl-stearoyl)-2-docosahexaenoyl-GPC (P-18:0/22:6)		Lipid	Phospholipid Metabolism	-	+	-
1-(1-enyl-stearoyl)-2-linoleoyl-GPC (P-18:0/18:2)		Lipid	Phospholipid Metabolism	-	+	-
1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)		Lipid	Phospholipid Metabolism	-	+	-
1-(1-enyl-stearoyl)-2-oleoyl-GPC (P-18:0/18:1)	100008917	Lipid	Phospholipid Metabolism	-	+	-
1-(1-enyl-stearoyl)-GPC (P-18:0)		Lipid	Phospholipid Metabolism	-	+	-
1,2-dioleoyl-GPE (18:1/18:1)	100008906	Lipid	Phospholipid Metabolism	-	+	-
1,2-distearoyl-GPC (18:0/18:0)	100000660	Lipid	Phospholipid Metabolism	-	+	-
1-oleoyl-2-eicosapentaenoyl-GPC (18:1/20:5)		Lipid	Phospholipid Metabolism	-	+	-
1-oleoyl-2-linoleoyl-GPE (18:1/18:2)		Lipid	Phospholipid Metabolism	-	+	-
1-palmitoleoyl-2-oleoyl-glycerol (16:1/18:1)		Lipid	Phospholipid Metabolism	-	+	-
1-palmitoleoyl-3-oleoyl-glycerol (16:1/18:1)		Lipid	Phospholipid Metabolism	-	+	-
1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)		Lipid	Phospholipid Metabolism	-	+	-
1-palmitoyl-2-dihomo-linolenoyl-GPE (16:0/20:3)		Lipid	Phospholipid Metabolism	-	+	-
1-palmitoyl-2-docosahexaenoyl-GPE (16:0/22:6)		Lipid	Phospholipid Metabolism	-	+	-
1-palmitoyl-2-linolenoyl-GPC (16:0/18:3)		Lipid	Phospholipid Metabolism	-	+	-
1-palmitoyl-2-linoleoyl-glycerol (16:0/18:2)		Lipid	Phospholipid Metabolism	-	+	-
1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	100001870	Lipid	Phospholipid Metabolism	-	+	-
1-palmitoyl-2-oleoyl-GPE (16:0/18:1)	1526	Lipid	Phospholipid Metabolism	-	+	-
1-palmitoyl-3-linoleoyl-glycerol (16:0/18:2)		Lipid	Phospholipid Metabolism	-	+	-
1-pentadecanoyl-2-linoleoyl-GPC (15:0/18:2)		Lipid	Phospholipid Metabolism	-	+	-
1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	100008977	Lipid	Phospholipid Metabolism	-	+	-
1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	100000616	Lipid	Phospholipid Metabolism	-	+	-
1-stearoyl-2-linoleoyl-GPC (18:0/18:2(OH))		Lipid	Phospholipid Metabolism	-	+	-
1-stearoyl-2-linoleoyl-GPE (18:0/18:2)		Lipid	Phospholipid Metabolism	-	+	-
1-stearoyl-2-oleoyl-GPE (18:0/18:1)	100001856	Lipid	Phospholipid Metabolism	-	+	-
1-stearyl-GPC (O-18:0)		Lipid	Phospholipid Metabolism	-	+	-
dihomo-linolenoyl-choline		Lipid	Phospholipid Metabolism	-	+	-
docosahexaenoylcholine		Lipid	Phospholipid Metabolism	-	+	-
PC (14:0/16:1)		Lipid	Phospholipid Metabolism	-	+	-
PC (O-16:0/16:0)		Lipid	Phospholipid Metabolism	-	+	-
PC (P-18:1/18:2)		Lipid	Phospholipid Metabolism	-	+	-
phosphocholine (16:0/22:5n3, 18:1/20:4)		Lipid	Phospholipid Metabolism	-	+	-
phosphocholine (18:0/20:5, 16:0/22:5n6)		Lipid	Phospholipid Metabolism	-	+	-
ethanolamine	420	Lipid	Phospholipid Metabolism	-	-	+
1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)		Lipid	Plasmalogen	-	+	-
1-(1-enyl-palmitoyl)-2-myristoyl-GPC (P-16:0/14:0)		Lipid	Plasmalogen	-	+	-
1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)		Lipid	Plasmalogen	-	+	-
1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	100008919	Lipid	Plasmalogen	-	+	-
adrenate (22:4n6)	100001193	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
arachidonate (20:4n6)	229	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
docosadienoate (22:2n6)	100001182	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
docosahexaenoate (DHA; 22:6n3)	100000665	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
docosapentaenoate (DPA; 22:5n3)		Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
docosapentaenoate (n6 DPA; 22:5n6)	100001580	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
docosatrienoate (22:3n3)	100001195	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
eicosapentaenoate (EPA; 20:5n3)	2050	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
linoleate (18:2n6)	180	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
linolenate (18:3n3 or 3n6)		Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
mead acid (20:3n9)	100001472	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
stearidonate (18:4n3)	100001229	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-	+	-
cholate	136	Lipid	Primary Bile Acid Metabolism	-	+	+
glycochenodeoxycholate glucuronide		Lipid	Primary Bile Acid Metabolism	-	+	+
glycochenodeoxycholate sulfate		Lipid	Primary Bile Acid Metabolism	-	+	+
tauro-beta-muricholate	100001250	Lipid	Primary Bile Acid Metabolism	-	+	+
taurochenodeoxycholate	1629	Lipid	Primary Bile Acid Metabolism	-	+	+
taurocholate	1648	Lipid	Primary Bile Acid Metabolism	-	+	+
chenodeoxycholate	1123	Lipid	Primary Bile Acid Metabolism	-	+	-
glycodeoxycholate	100000436	Lipid	Secondary Bile Acid Metabolism	-	+	+
glycolithocholate sulfate		Lipid	Secondary Bile Acid Metabolism	-	+	+
glycoursodeoxycholate	100002911	Lipid	Secondary Bile Acid Metabolism	-	+	+
taurocholenate sulfate	100001990	Lipid	Secondary Bile Acid Metabolism	-	+	+
taurolithocholate 3-sulfate	100001658	Lipid	Secondary Bile Acid Metabolism	-	+	+
deoxycholate	302	Lipid	Secondary Bile Acid Metabolism	-	+	-
taurodeoxycholate	1668	Lipid	Secondary Bile Acid Metabolism	-	+	-
tauroursodeoxycholate	100002912	Lipid	Secondary Bile Acid Metabolism	-	+	-
ursodeoxycholate	1135	Lipid	Secondary Bile Acid Metabolism	-	+	-
12-dehydrocholate	100001072	Lipid	Secondary Bile Acid Metabolism	-	-	+
7-ketodeoxycholate	100001063	Lipid	Secondary Bile Acid Metabolism	-	-	+
glycodeoxycholate sulfate		Lipid	Secondary Bile Acid Metabolism	-	-	+
lactosyl-N-palmitoyl-spingosine (C16 lactosyl ceramide)		Lipid	Sphingolipid Metabolism	-	+	-
N-palmitoyl-sphingosine (d18:1/16:0)	1518	Lipid	Sphingolipid Metabolism	-	+	-

Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profiling Assay

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Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
palmitoyl dihydrosphingomyelin (d18:0/16:0)		Lipid	Sphingolipid Metabolism	-	+	-
sphinganine	313	Lipid	Sphingolipid Metabolism	-	+	-
sphinganine-1-phosphate	100001876	Lipid	Sphingolipid Metabolism	-	+	-
sphingomyelin (d18:1/15:0, d16:1/17:0)		Lipid	Sphingolipid Metabolism	-	+	-
sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)	100008920	Lipid	Sphingolipid Metabolism	-	+	-
sphingomyelin (d18:1/20:1, d18:2/20:0)		Lipid	Sphingolipid Metabolism	-	+	-
sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)		Lipid	Sphingolipid Metabolism	-	+	-
sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)		Lipid	Sphingolipid Metabolism	-	+	-
sphingomyelin (d18:2/14:0, d18:1/14:1)		Lipid	Sphingolipid Metabolism	-	+	-
sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)		Lipid	Sphingolipid Metabolism	-	+	-
sphingomyelin (d18:2/24:1, d18:1/24:2)		Lipid	Sphingolipid Metabolism	-	+	-
sphingosine 1-phosphate	100000626	Lipid	Sphingolipid Metabolism	-	+	-
tricosanoyl sphingomyelin (d18:1/23:0)		Lipid	Sphingolipid Metabolism	-	+	-
21-hydroxypregnenolone disulfate	100001999	Lipid	Steroid	-	+	+
4-androsten-3beta,17beta-diol monosulfate (1)	100002028	Lipid	Steroid	-	+	+
5alpha-androstan-3beta,17beta-diol disulfate	100001987	Lipid	Steroid	-	+	+
5alpha-pregnan-3(alpha or beta),20beta-diol disulfate	100002015	Lipid	Steroid	-	+	+
androsterone sulfate	100001073	Lipid	Steroid	-	+	+
etiocholanolone glucuronide	100005403	Lipid	Steroid	-	+	+
pregnanediol-3-glucuronide	100003470	Lipid	Steroid	-	+	+
pregnen-diol disulfate		Lipid	Steroid	-	+	+
21-hydroxypregnenolone monosulfate (1)	100002003	Lipid	Steroid	-	+	-
4-androsten-3alpha,17alpha-diol monosulfate (2)	100002026	Lipid	Steroid	-	+	-
4-androsten-3alpha,17alpha-diol monosulfate (3)	100002027	Lipid	Steroid	-	+	-
4-androsten-3beta,17beta-diol monosulfate (2)	100002029	Lipid	Steroid	-	+	-
5alpha-androstan-3alpha,17beta-diol disulfate	100002017	Lipid	Steroid	-	+	-
5alpha-androstan-3alpha,17beta-diol monosulfate (1)	100002018	Lipid	Steroid	-	+	-
5alpha-androstan-3alpha,17beta-diol monosulfate (2)	100006005	Lipid	Steroid	-	+	-
5alpha-androstan-3beta,17alpha-diol disulfate	100002021	Lipid	Steroid	-	+	-
5alpha-androstan-3beta,17beta-diol monosulfate (1)	100002023	Lipid	Steroid	-	+	-
5alpha-pregnan-3beta,20alpha-diol monosulfate (2)	100002014	Lipid	Steroid	-	+	-
5alpha-pregnan-3beta,20beta-diol monosulfate (1)	100002009	Lipid	Steroid	-	+	-
5-pregnen-3b, 17-diol-20-one 3-sulfate		Lipid	Steroid	-	+	-
epiandrosterone sulfate	100001287	Lipid	Steroid	-	+	-
pregn steroid monosulfate*	100002067	Lipid	Steroid	-	+	-
pregnenolone sulfate	100002129	Lipid	Steroid	-	+	-
11-ketoetiocholanolone glucuronide	100005402	Lipid	Steroid	-	-	+
17alpha-hydroxypregnanolone glucuronide	100005418	Lipid	Steroid	-	-	+
5beta-pregnan-3alpha,21-diol-11,20-dione 21-glucosiduronate	100005417	Lipid	Steroid	-	-	+
cortisol glucuronide	100005434	Lipid	Steroid	-	-	+
cortisone monosulfate	100001995	Lipid	Steroid	-	-	+
etiocholanolone sulfate	100001282	Lipid	Steroid	-	-	+
tetrahydrocortisone	100002403	Lipid	Steroid	-	-	+
7-hydroxycholesterol (alpha or beta)	100005999	Lipid	Sterol	-	+	-
campesterol	100001269	Lipid	Sterol	-	+	-
inosine 5'-monophosphate (IMP)	362	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-	+	-
allantoic acid	218	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-	-	+
ADP		Nucleotide	Purine Metabolism, Adenine containing	-	+	-
1-methyladenine	54	Nucleotide	Purine Metabolism, Adenine containing	-	-	+
2'-deoxyadenosine	211	Nucleotide	Purine Metabolism, Adenine containing	-	-	+
1-methylguanosine		Nucleotide	Purine Metabolism, Guanine containing	-	-	+
2'-deoxyguanosine	348	Nucleotide	Purine Metabolism, Guanine containing	-	-	+
7-methylguanosine	100001118	Nucleotide	Purine Metabolism, Guanine containing	-	-	+
guanine	172	Nucleotide	Purine Metabolism, Guanine containing	-	-	+
guanosine-3',5'-cyclic monophosphate (cGMP)	104	Nucleotide	Purine Metabolism, Guanine containing	-	-	+
N2,N2-dimethylguanine	100001853	Nucleotide	Purine Metabolism, Guanine containing	-	-	+
N4-acetylcytidine	100001413	Nucleotide	Pyrimidine Metabolism, Cytidine containing	-	+	+
CDP-choline		Nucleotide	Pyrimidine Metabolism, Cytidine containing	-	+	-
CMP		Nucleotide	Pyrimidine Metabolism, Cytidine containing	-	+	-
3-methylcytidine	100001466	Nucleotide	Pyrimidine Metabolism, Cytidine containing	-	-	+
cytosine	881	Nucleotide	Pyrimidine Metabolism, Cytidine containing	-	-	+
N-carbamoylaspartate	1108	Nucleotide	Pyrimidine Metabolism, Orotate containing	-	+	+
dihydroorotate	923	Nucleotide	Pyrimidine Metabolism, Orotate containing	-	-	+
thymine	882	Nucleotide	Pyrimidine Metabolism, Thymine containing	-	+	+
5,6-dihydrouracil	1125	Nucleotide	Pyrimidine Metabolism, Uracil containing	-	+	+
beta-alanine	244	Nucleotide	Pyrimidine Metabolism, Uracil containing	-	+	+
4-ureidobutyrate	100000718	Nucleotide	Pyrimidine Metabolism, Uracil containing	-	-	+
N3-methyluridine	100001424	Nucleotide	Pyrimidine Metabolism, Uracil containing	-	-	+
4-hydroxyphenylacetylglutamine		Peptide	Acetylate Peptide	-	+	+
phenylacetylglutamate		Peptide	Acetylated Peptides	-	-	+
phenylacetylhistidine		Peptide	Acetylated Peptides	-	-	+
phenylacetylmethionine		Peptide	Acetylated Peptides	-	-	+
phenylacetylthreonine		Peptide	Acetylated Peptides	-	-	+
prolylglycine	100003674	Peptide	Dipeptide	-	+	+
prolylvaline	100003682	Peptide	Dipeptide	-	+	+
pyroglutamylvaline	100001132	Peptide	Dipeptide	-	+	+
valylglycine	100003641	Peptide	Dipeptide	-	+	+
glycylleucine	100001258	Peptide	Dipeptide	-	+	-
glycylphenylalanine	100001268	Peptide	Dipeptide	-	+	-
histidinylglutamate		Peptide	Dipeptide	-	+	-
isoleucylglycine	100003169	Peptide	Dipeptide	-	+	-
isoleucylleucine/leucylisoleucine	100008939	Peptide	Dipeptide	-	+	-
leucylglycine	100003185	Peptide	Dipeptide	-	+	-
leucylleucine	100001710	Peptide	Dipeptide	-	+	-
phenylalanylalanine	100003589	Peptide	Dipeptide	-	+	-
phenylalanylaspartate	100003595	Peptide	Dipeptide	-	+	-
phenylalanylphenylalanine	100002293	Peptide	Dipeptide	-	+	-
phenylalanyltryptophan	100003594	Peptide	Dipeptide	-	+	-
prolylserine	100003679	Peptide	Dipeptide	-	+	-

Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profiling Assay

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Biochemical	Chem ID	Super Family	Sub Family	CSF	EDTA Plasma	Urine
tryptophylleucine	100003206	Peptide	Dipeptide	-	+	-
alanylalanine	100000113	Peptide	Dipeptide	-	-	+
alanylproline	100001888	Peptide	Dipeptide	-	-	+
cyclo(his-pro)	100002745	Peptide	Dipeptide	-	-	+
glutaminyllysine		Peptide	Dipeptide	-	-	+
glutaminylmethionine		Peptide	Dipeptide	-	-	+
glycylglycine	100000898	Peptide	Dipeptide	-	-	+
histidylproline	100003546	Peptide	Dipeptide	-	-	+
phenylacetylphenylalanine	100003760	Peptide	Dipeptide	-	-	+
phenylalanylglycine	100003588	Peptide	Dipeptide	-	-	+
phenylalanylproline	100003592	Peptide	Dipeptide	-	-	+
prolylalanine	100003668	Peptide	Dipeptide	-	-	+
prolylglutamate	100003673	Peptide	Dipeptide	-	-	+
prolylglutamine	100003672	Peptide	Dipeptide	-	-	+
prolylproline	100003678	Peptide	Dipeptide	-	-	+
tryptophylproline	100003614	Peptide	Dipeptide	-	-	+
valylleucine	100003210	Peptide	Dipeptide	-	-	+
anserine	100000044	Peptide	Dipeptide Derivative	-	+	+
carnosine	249	Peptide	Dipeptide Derivative	-	+	+
N-acetylcarnosine	100004046	Peptide	Dipeptide Derivative	-	+	+
DSGEGDFXAEGGGVR		Peptide	Fibrinogen Cleavage Peptide	-	+	-
gamma-glutamylglycine	100001294	Peptide	Gamma-glutamyl Amino Acid	-	+	+
gamma-glutamylglutamate	331	Peptide	Gamma-glutamyl Amino Acid	-	+	-
pro-pro-pro	100003708	Peptide	Polypeptide	-	-	+
epsilon-caprolactam		Xenobiotics	Bacterial/Fungal	-	+	-
2-hydroxyhippurate (salicylurate)	1869	Xenobiotics	Benzoate Metabolism	-	+	+
3-hydroxyhippurate	100002122	Xenobiotics	Benzoate Metabolism	-	+	+
3-methoxycatechol sulfate (1)	100006375	Xenobiotics	Benzoate Metabolism	-	+	+
3-methyl catechol sulfate (1)	100004112	Xenobiotics	Benzoate Metabolism	-	+	+
3-methyl catechol sulfate (2)	100004110	Xenobiotics	Benzoate Metabolism	-	+	+
4-ethylphenyl sulfate		Xenobiotics	Benzoate Metabolism	-	+	+
4-hydroxyhippurate	100001423	Xenobiotics	Benzoate Metabolism	-	+	+
4-vinylphenol sulfate	100001755	Xenobiotics	Benzoate Metabolism	-	+	+
4-methylcatechol sulfate	100004208	Xenobiotics	Benzoate Metabolism	-	+	+
propyl 4-hydroxybenzoate sulfate	100006264	Xenobiotics	Benzoate Metabolism	-	+	+
2,4,6-trihydroxybenzoate	100001718	Xenobiotics	Benzoate Metabolism	-	-	+
2-methylhippurate	100000052	Xenobiotics	Benzoate Metabolism	-	-	+
3-methoxycatechol sulfate (2)	100006376	Xenobiotics	Benzoate Metabolism	-	-	+
4-hydroxybenzoate	100000862	Xenobiotics	Benzoate Metabolism	-	-	+
4-hydroxymandelate	1115	Xenobiotics	Benzoate Metabolism	-	-	+
benzene-1,2,3-triol	100002323	Xenobiotics	Benzoate Metabolism	-	-	+
benzoate	100000008	Xenobiotics	Benzoate Metabolism	-	-	+
mandelate	100000710	Xenobiotics	Benzoate Metabolism	-	-	+
1,2,3-benzenetriol sulfate (2)	100006374	Xenobiotics	Chemical	-	+	+
2-pyrrolidinone	100001081	Xenobiotics	Chemical	-	+	+
6-hydroxyindole sulfate		Xenobiotics	Chemical	-	+	+
N-methylpipecolate	100005383	Xenobiotics	Chemical	-	+	+
S-(3-hydroxypropyl)mercapturic acid (HPMA)	100004568	Xenobiotics	Chemical	-	+	+
4-hydroxychlorothalonil	100006082	Xenobiotics	Chemical	-	+	-
EDTA	100001002	Xenobiotics	Chemical	-	+	-
ethyl paraben sulfate	100006271	Xenobiotics	Chemical	-	+	-
iminodiacetate (IDA)	100000900	Xenobiotics	Chemical	-	+	-
1-(3-aminopropyl)-2-pyrrolidone	100003263	Xenobiotics	Chemical	-	-	+
1,2,3-benzenetriol sulfate (1)	100006373	Xenobiotics	Chemical	-	-	+
2-methoxyresorcinol sulfate	100006184	Xenobiotics	Chemical	-	-	+
2-oxo-1-pyrrolidinepropionate	100003265	Xenobiotics	Chemical	-	-	+
3-acetylphenol sulfate		Xenobiotics	Chemical	-	-	+
3-hydroxyindolin-2-one sulfate	100006103	Xenobiotics	Chemical	-	-	+
4'-hydroxypropiophenone sulfate	100006269	Xenobiotics	Chemical	-	-	+
4-methylbenzenesulfonate	100002390	Xenobiotics	Chemical	-	-	+
dexpanthenol	100002376	Xenobiotics	Chemical	-	-	+
diethylamine	100004379	Xenobiotics	Chemical	-	-	+
diglycerol	100003700	Xenobiotics	Chemical	-	-	+
ectoine	100001635	Xenobiotics	Chemical	-	-	+
gentisic acid-5-glucoside	100006372	Xenobiotics	Chemical	-	-	+
heptaethylene glycol	100002318	Xenobiotics	Chemical	-	-	+
hexaethylene glycol	100002317	Xenobiotics	Chemical	-	-	+
octaethylene glycol	100002319	Xenobiotics	Chemical	-	-	+
pentaethylene glycol	100002316	Xenobiotics	Chemical	-	-	+
phenylcarnitine		Xenobiotics	Chemical	-	-	+
2-acetamidophenol sulfate	100006190	Xenobiotics	Drug	-	+	+
3-(N-acetyl-L-cystein-S-yl) acetaminophen	2048	Xenobiotics	Drug	-	+	+
4-acetylphenyl sulfate		Xenobiotics	Drug	-	+	+
atenolol	100002726	Xenobiotics	Drug	-	+	+
hydroquinone sulfate	100001604	Xenobiotics	Drug	-	+	+
salicyluric glucuronide		Xenobiotics	Drug	-	+	+
2-hydroxyibuprofen	100004169	Xenobiotics	Drug	-	+	-
carboxyibuprofen	100004171	Xenobiotics	Drug	-	+	-
ibuprofen	1487	Xenobiotics	Drug	-	+	-
ibuprofen acyl glucuronide	100002406	Xenobiotics	Drug	-	+	-
naproxen	1384	Xenobiotics	Drug	-	+	-
ranitidine	100002735	Xenobiotics	Drug	-	+	-
4-hydroxycoumarin	100002049	Xenobiotics	Drug	-	-	+
4-phenylbutyrate	100004197	Xenobiotics	Drug	-	-	+
6-aminopenicillanate	100002627	Xenobiotics	Drug	-	-	+
carbamazepine	100001933	Xenobiotics	Drug	-	-	+
metformin	100002405	Xenobiotics	Drug	-	-	+
metoprolol acid metabolite		Xenobiotics	Drug	-	-	+
ofloxacin	100000673	Xenobiotics	Drug	-	-	+

Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profiling Assay

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penicillin G	100002155	Xenobiotics	Drug	-	-	+
pivaloylcarnitine (C5)	100001589	Xenobiotics	Drug	-	-	+
S-carboxymethyl-L-cysteine	100002324	Xenobiotics	Drug	-	-	+
2-isopropylmalate	100000409	Xenobiotics	Food Component/Plant	-	+	+
2-oxindole-3-acetate	100003109	Xenobiotics	Food Component/Plant	-	+	+
4-allylphenol sulfate	100001868	Xenobiotics	Food Component/Plant	-	+	+
4-vinylguaiacol sulfate	100006126	Xenobiotics	Food Component/Plant	-	+	+
cinnamoylglycine	100002253	Xenobiotics	Food Component/Plant	-	+	+
daidzein sulfate (2)	100006363	Xenobiotics	Food Component/Plant	-	+	+
dihydroferulic acid	100003432	Xenobiotics	Food Component/Plant	-	+	+
eugenol sulfate	100006171	Xenobiotics	Food Component/Plant	-	+	+
ferulic acid 4-sulfate	100005389	Xenobiotics	Food Component/Plant	-	+	+
homostachydrine		Xenobiotics	Food Component/Plant	-	+	+
methyl indole-3-acetate	1104	Xenobiotics	Food Component/Plant	-	+	+
N-(2-furoyl)glycine	100001086	Xenobiotics	Food Component/Plant	-	+	+
N-acetylalliin	100005367	Xenobiotics	Food Component/Plant	-	+	+
pyrraline	100001767	Xenobiotics	Food Component/Plant	-	+	+
saccharin	100000870	Xenobiotics	Food Component/Plant	-	+	+
sucralose	100001789	Xenobiotics	Food Component/Plant	-	+	+
thymol sulfate	100001757	Xenobiotics	Food Component/Plant	-	+	+
umbelliferone sulfate	100006282	Xenobiotics	Food Component/Plant	-	+	+
methyl glucopyranoside (alpha + beta)	100005864	Xenobiotics	Food Component/Plant	-	+	-
1,1-kestotetraose	100003047	Xenobiotics	Food Component/Plant	-	-	+
1,6-anhydroglucose	100000939	Xenobiotics	Food Component/Plant	-	-	+
1-kestose	100000980	Xenobiotics	Food Component/Plant	-	-	+
2,8-quinolinediol sulfate		Xenobiotics	Food Component/Plant	-	-	+
2-keto-3-deoxy-gluconate	100005946	Xenobiotics	Food Component/Plant	-	-	+
3,5-dihydroxybenzoic acid	100002054	Xenobiotics	Food Component/Plant	-	-	+
3-hydroxycinnamate (m-coumarate)	100000842	Xenobiotics	Food Component/Plant	-	-	+
3-hydroxycinnamate sulfate	100006094	Xenobiotics	Food Component/Plant	-	-	+
3-hydroxyindolin-2-one	100003823	Xenobiotics	Food Component/Plant	-	-	+
4-ethylphenol glucuronide		Xenobiotics	Food Component/Plant	-	-	+
abscisate	100000879	Xenobiotics	Food Component/Plant	-	-	+
acetolactate	100002418	Xenobiotics	Food Component/Plant	-	-	+
daidzein	100001219	Xenobiotics	Food Component/Plant	-	-	+
ethyl pyruvate	100001573	Xenobiotics	Food Component/Plant	-	-	+
ferulate	100001542	Xenobiotics	Food Component/Plant	-	-	+
ferulylglycine (1)		Xenobiotics	Food Component/Plant	-	-	+
fucitol	100002455	Xenobiotics	Food Component/Plant	-	-	+
furaneol sulfate		Xenobiotics	Food Component/Plant	-	-	+
genistein	100001221	Xenobiotics	Food Component/Plant	-	-	+
hesperetin	100001039	Xenobiotics	Food Component/Plant	-	-	+
homocitrate	100002554	Xenobiotics	Food Component/Plant	-	-	+
isoeugenol sulfate	100006089	Xenobiotics	Food Component/Plant	-	-	+
N-acetylpyrraline	100006120	Xenobiotics	Food Component/Plant	-	-	+
N-acetyl-S-allyl-L-cysteine	100005818	Xenobiotics	Food Component/Plant	-	-	+
naringenin 7-glucuronide		Xenobiotics	Food Component/Plant	-	-	+
piperidine	100002398	Xenobiotics	Food Component/Plant	-	-	+
syringic acid	100001919	Xenobiotics	Food Component/Plant	-	-	+
syringol sulfate	100006256	Xenobiotics	Food Component/Plant	-	-	+
vanillate	100001634	Xenobiotics	Food Component/Plant	-	-	+
cotinine	848	Xenobiotics	Tobacco Metabolite	-	-	+
hydroxycotinine	100002717	Xenobiotics	Tobacco Metabolite	-	-	+
1,3,7-trimethylurate	100001397	Xenobiotics	Xanthine Metabolism	-	+	+
1,3-dimethylurate	100001106	Xenobiotics	Xanthine Metabolism	-	+	+
1,7-dimethylurate	100001399	Xenobiotics	Xanthine Metabolism	-	+	+
1-methylurate	100001400	Xenobiotics	Xanthine Metabolism	-	+	+
1-methylxanthine	100001405	Xenobiotics	Xanthine Metabolism	-	+	+
3,7-dimethylurate	100001398	Xenobiotics	Xanthine Metabolism	-	+	+
5-acetylamino-6-formylamino-3-methyluracil	100001402	Xenobiotics	Xanthine Metabolism	-	+	+
7-methylurate	100002241	Xenobiotics	Xanthine Metabolism	-	+	+
3-methylurate		Xenobiotics	Xanthine Metabolism	-	-	+
caffeic acid sulfate		Xenobiotics	Xanthine Metabolism	-	-	+

Supplemental Table 2. Z-scores for Population Baseline

No heme detec

Biochemical	Super Pathway	Sub Pathway	CSF301	CSF302	CSF303	CSF304	CSF306	CSF307	CSF308	CSF309	CSF313	CSF317
alanine	Amino Acid	Alanine and Aspartate Metabolism	-1.1506	0.5372	0.5999	0.2402	-2.4839	-0.5127	0.0932	0.3744	-1.5477	0.0530
asparagine	Amino Acid	Alanine and Aspartate Metabolism	-0.5922	-1.3469	1.1883	-0.6660	-0.7640	-0.5734	0.6208	-0.3885	-0.5478	0.0849
aspartate	Amino Acid	Alanine and Aspartate Metabolism	0.2139	-0.7887	-0.2555	1.1478	0.1770	-1.4338	-0.7123	1.2770	1.5686	-1.1327
N-acetylalanine	Amino Acid	Alanine and Aspartate Metabolism	-0.7016	-2.7704	-0.8811	-1.1749	-0.6009	0.1402	1.4465	-1.1142	1.4912	-0.3323
N-acetylasparagine	Amino Acid	Alanine and Aspartate Metabolism	-0.1198	-2.1012	0.4854	-0.0609	-0.0156	0.0069	0.3258	-0.0308	1.5161	-1.2082
N-acetylaspartate (NAA)	Amino Acid	Alanine and Aspartate Metabolism	-0.6059	-1.5155	-1.5298	-0.9372	0.5720	-0.1616	0.6546	-0.5412	-0.6967	1.0288
creatine	Amino Acid	Creatine Metabolism	0.5903	0.8231	0.8905	0.9018	-0.1915	1.9967	0.1337	0.5595	-1.1920	0.5445
creatine phosphate	Amino Acid	Creatine Metabolism	-0.0724	0.7592	1.7502	-0.6676	-0.0003	3.0062	-0.6642	-0.6705	-0.6771	-0.6768
creatinine	Amino Acid	Creatine Metabolism	0.5349	-1.1310	0.5618	0.8414	-0.8067	0.9558	1.4858	1.6393	1.3077	-0.8435
guanidinoacetate	Amino Acid	Creatine Metabolism	-0.2848	0.3042	0.2687	0.1009	0.0205	-0.9201	1.0703	-0.2664	-2.7725	-0.2500
carboxyethyl-GABA	Amino Acid	Glutamate Metabolism	0.5325	-1.3670	0.2786	-0.5075	-0.9719	0.1587	1.0431	0.9767	0.0483	-3.6766
citramalate	Amino Acid	Glutamate Metabolism	-0.6722	0.9115	0.2186	-1.4011	-0.5528	-1.8829	0.0773	-0.0945	-1.8865	-0.0017
gamma-aminobutyrate (GABA)	Amino Acid	Glutamate Metabolism	0.4649	-0.5684	0.5935	0.7368	0.5117	-0.5717	-0.4959	1.1537	0.1990	0.8181
glutamate	Amino Acid	Glutamate Metabolism	-1.2826	-0.8998	-0.2835	-0.6768	-0.7595	-1.4063	-0.3118	-0.1096	0.8255	-0.6958
glutamate, gamma-methyl ester	Amino Acid	Glutamate Metabolism	0.2459	-3.2305	-0.5703	0.4340	-1.1608	1.2576	-0.6338	0.0329	0.6132	-0.3908
glutamine	Amino Acid	Glutamate Metabolism	-0.8186	-1.4260	-0.0441	0.1526	-1.2575	1.7208	-0.4138	-0.2078	1.3309	0.4779
N-acetyl-aspartyl-glutamate (NAAG)	Amino Acid	Glutamate Metabolism	0.1864	-2.1705	-0.0690	0.1207	0.4303	-0.3994	1.2660	-1.1982	0.3048	-0.8203
N-acetylglutamate	Amino Acid	Glutamate Metabolism	-0.2501	-1.8406	-1.0009	-1.3364	0.3012	-1.0367	0.6840	-1.1133	-0.5676	0.7069
N-acetylglutamine	Amino Acid	Glutamate Metabolism	-0.6768	-2.7384	-0.0070	-0.5435	-0.7598	-0.6769	0.6715	0.2644	1.7803	-0.8484
pyroglutamine*	Amino Acid	Glutamate Metabolism	-0.2449	-0.5950	0.4375	-0.4862	-0.4326	-0.2874	0.6317	1.2886	0.5235	0.5358
S-1-pyrroline-5-carboxylate	Amino Acid	Glutamate Metabolism	0.8411	-0.2950	0.8799	-0.4641	0.8049	0.7375	-1.0744	0.3865	-1.5840	1.7094
beta-citrylglutamate	Amino Acid	Glutamate Metabolism	-0.6332	-0.9662	-0.4999	-0.6896	-1.5894	0.21224	0.6854	-0.2251	-0.0159	-1.8282
5-oxoproline	Amino Acid	Glutathione Metabolism	-0.9711	-0.2543	0.0298	0.0209	-0.2226	-0.1542	-0.3009	-0.1509	1.0897	-0.1628
cys-gly, oxidized	Amino Acid	Glutathione Metabolism	0.2211	1.6352	0.5637	0.3408	-0.7906	1.1155	1.9201	-0.4110	-1.8039	0.8386
cysteinylglycine	Amino Acid	Glutathione Metabolism	-0.5809	-0.5820	1.4380	-0.5899	-0.5795	-0.5778	2.5313	-0.5810	-0.5787	1.1409
glutathione, oxidized (GSSG)	Amino Acid	Glutathione Metabolism	-0.3699	-0.3617	-0.3663	-0.3689	-0.3621	-0.3596	2.3675	-0.3625	-0.3598	-0.3786
betaine	Amino Acid	Glycine, Serine and Threonine Metabolism	-1.0854	-1.2120	-0.6481	-0.7078	-1.5756	-0.0674	1.6572	-0.2581	-0.7082	-0.1413
dimethylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.8631	-1.3719	0.2184	-0.7393	-1.3789	-0.5801	1.7071	-0.8158	0.2469	0.2764
glycine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.4835	-0.4149	0.1277	0.4815	0.4197	-2.0274	2.7544	-0.0804	-1.6893	1.2979
N-acetylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.8102	-1.1025	-0.3249	0.2298	-0.8425	0.0536	1.3115	-0.6028	2.0634	0.9277
N-acetylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.3023	-2.4151	-0.4168	-1.1872	-0.7792	-0.0991	1.2110	-0.0475	1.2872	-0.4077
N-acetylthreonine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.5286	-2.4289	-0.5706	-0.6554	-0.4589	-0.2402	1.0930	-0.4898	1.7381	-0.7968
serine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.7213	-2.2909	-1.2661	-0.1242	0.1888	-0.9779	1.3059	-1.0115	-0.5279	1.0213
threonine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.2530	-1.7446	0.2716	0.9099	0.2332	-0.1998	0.0263	0.7675	-1.0937	0.1086
2-methylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.1118	0.16822	-0.4918	-0.3504	1.06319	-1.2868	0.53537	-1.1379	-0.7742	-0.6027
1-methylguanidine	Amino Acid	Guanidino and Acetamido Metabolism	-0.5781	-0.6219	-0.4126	-0.6156	0.2988	0.4780	0.0365	-0.6260	3.6353	-0.6176
4-guanidinobutanoate	Amino Acid	Guanidino and Acetamido Metabolism	0.0116	0.6870	-0.0054	0.2597	-1.1191	0.2805	-1.1757	0.5402	-0.0789	1.3574
1-methylhistamine	Amino Acid	Histidine Metabolism	-0.3638	-0.3488	-0.3616	-0.3583	-0.3467	-0.3643	-0.3437	-0.3587	-0.3611	1.5279
1-methylhistidine	Amino Acid	Histidine Metabolism	1.4806	-0.9765	1.3374	1.5754	-0.5618	0.6326	-0.0216	-0.3141	2.1185	-0.9479
1-methylimidazoleacetate	Amino Acid	Histidine Metabolism	-0.0451	-2.2767	-1.1664	-0.2863	0.7974	-0.6872	-0.1840	-0.0709	-0.0303	-0.0772
3-methylhistidine	Amino Acid	Histidine Metabolism	1.4326	-0.3071	1.5871	1.5278	-0.0891	-1.0737	0.5391	-0.2566	2.0453	-0.4416
4-imidazoleacetate	Amino Acid	Histidine Metabolism	-1.0211	0.8832	1.0828	-1.0245	-0.0982	-1.0217	-1.0262	0.7949	0.8877	-1.0243
histidine	Amino Acid	Histidine Metabolism	-1.4373	-1.1840	0.4077	0.6838	1.1004	-2.3118	0.8530	-0.6451	0.4038	0.0540
imidazole lactate	Amino Acid	Histidine Metabolism	1.0639	-1.7111	0.8829	-0.2828	-0.6681	-0.9325	1.2912	0.5512	0.0788	-1.3548
imidazole propionate	Amino Acid	Histidine Metabolism	-0.5779	-0.5892	-0.5822	0.2262	-0.5815	-0.5829	-0.5814	-0.5802	-0.5827	-0.5876
N-acetyl-3-methylhistidine*	Amino Acid	Histidine Metabolism	0.6609	-0.3772	1.2036	1.3779	0.4608	-1.6421	0.8144	-0.1913	1.4265	-0.5588
N-acetylhistidine	Amino Acid	Histidine Metabolism	-1.8548	-1.9696	0.8320	-0.3289	-0.6333	-1.6171	0.1295	-0.7726	0.0679	-1.1921
2-hydroxy-3-methylvalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.2531	-0.9779	0.6852	-0.2100	-1.1430	3.0459	-0.7203	0.6244	2.3639	0.0429
2-methylbutyrylcarnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.4888	-1.9037	0.4972	-0.1650	-1.9161	1.1828	0.8011	0.4997	0.8847	-0.3202
3-hydroxy-2-ethylpropionate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.2644	-0.6980	-0.2290	0.1498	-1.3478	1.1344	-0.5736	0.5373	0.7063	0.2102
3-hydroxyisobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.4987	-1.2695	-1.3852	-0.4668	-1.3526	0.3904	1.4103	0.4838	2.2931	0.5282
3-methyl-2-oxobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.5018	-0.6943	-1.2987	-0.5700	0.7882	-0.5176	1.2132	-1.2907	-1.2944	1.4954
3-methyl-2-oxovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.1472	-1.7601	-0.9834	-0.4633	0.3000	0.5544	1.2582	-0.6267	-0.3853	1.3102
3-methylglutaconate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.4230	-1.9009	-0.4371	-0.4035	-0.9635	1.6684	1.1795	0.5161	3.1338	0.1550
4-methyl-2-oxopentanoate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.5281	-1.2315	-1.2318	-1.2234	0.8785	-0.1903	1.4734	-1.2306	-0.1844	1.4029
alpha-hydroxyisocaproate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.3687	-1.8510	0.4632	0.4142	-1.8614	0.8518	0.5843	1.1848	1.2748	0.3479

Supplemental Table 2. Z-scores for Population Baseline

No heme detec

Biochemical	Super Pathway	Sub Pathway	CSF301	CSF302	CSF303	CSF304	CSF306	CSF307	CSF308	CSF309	CSF313	CSF317
alpha-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.1583	-0.8991	0.3122	-0.5585	-0.1704	3.4954	-0.6906	0.5641	2.8362	-0.1366
beta-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.1944	-1.4801	0.3408	0.1777	-1.0012	1.7660	-0.7434	0.6600	3.2242	0.8347
beta-hydroxyisovaleroylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.0284	-2.3343	-0.6358	-0.7748	0.2692	0.5441	1.3691	0.1379	0.9117	-0.0040
ethylmalonate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.1571	-1.2686	-0.9397	-1.2726	-1.9088	-0.0808	2.4175	0.2007	1.1585	-0.2186
isobutyrylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.1430	0.8006	0.0278	0.3654	-1.7427	1.4730	1.7514	1.2762	1.9965	-0.6102
isoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.7578	-1.3540	-0.2840	-0.6653	-1.0298	2.2378	-0.1643	-0.7797	1.4510	0.6179
isovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.7191	-0.0802	-0.1000	0.1674	-1.1566	1.5834	-0.2205	0.4028	2.1978	-1.1629
isovalerylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.0833	-0.3329	0.9589	-1.1718	-0.7211	1.5419	2.4537	1.5673	1.0888	-0.9603
leucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.8374	-0.7505	-0.7787	-0.7858	-0.7111	1.9879	0.6800	-0.6773	1.8199	0.9794
methylsuccinate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.6928	-0.7413	-0.9211	-0.2928	-0.5686	-1.0681	2.2945	0.0572	0.1101	0.7155
methylsuccinoylcarnitine (1)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.4006	-0.9053	0.0410	0.0951	-1.0274	0.5644	2.6130	0.4535	0.7136	0.5728
N-acetylisoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.6638	-2.5000	-0.1639	-1.1276	-0.6200	-0.1323	1.5908	-0.9971	1.6871	0.3470
N-acetylleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.0278	-1.3618	-1.3528	0.2698	0.3610	-0.6414	2.1009	-1.2640	1.0684	0.6268
N-acetylvaline	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.6446	-2.3940	-0.7456	-0.8206	-0.6562	-0.4082	1.3490	-0.4727	1.4570	-0.5020
tiglylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.0811	-1.6508	-0.5085	0.1253	-2.0315	1.3173	-0.1192	0.7033	1.6935	-0.2379
valine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.9581	-1.3458	-0.8210	-0.7189	-1.0038	2.0060	0.4087	-0.1232	1.8363	1.6291
2,3-dihydroxy-2-methylbutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.1432	-0.8989	0.4068	-0.2598	-0.4103	0.58556	0.47	0.37542	1.00809	-1.6594
2-oxoadipate	Amino Acid	Lysine Metabolism	-0.5371	-0.5391	-0.5453	-0.5478	1.0778	-0.5408	2.1349	-0.5451	-0.5442	3.0173
3-methylglutarylcarnitine (2)	Amino Acid	Lysine Metabolism	-0.4639	-1.2009	0.0864	0.1877	-2.4899	1.4601	1.8738	0.1327	0.7821	0.5380
5-hydroxylysine	Amino Acid	Lysine Metabolism	-0.3672	-0.9503	-1.5470	-0.4887	-0.2882	-0.1981	0.6999	-0.5527	-1.2615	0.4876
6-oxopiperidine-2-carboxylic acid	Amino Acid	Lysine Metabolism	0.0653	-0.9826	1.4441	-0.2700	0.9712	0.9937	-0.2943	0.8684	2.0288	1.3871
glutarate (pentanedioate)	Amino Acid	Lysine Metabolism	-1.0010	-1.8884	0.1037	-1.0188	0.6786	-0.2945	0.9797	-0.1715	-0.6653	0.2041
glutarylcarnitine (C5)	Amino Acid	Lysine Metabolism	-0.4449	-0.6230	0.0822	-0.5970	-1.6205	0.1260	0.5186	0.0591	1.0014	-0.3644
lysine	Amino Acid	Lysine Metabolism	0.0059	-0.1469	0.5236	0.0166	-0.9823	2.4015	0.6921	1.0590	1.9969	0.1763
N2-acetyllysine/N6-acetyllysine	Amino Acid	Lysine Metabolism	-2.4835	-0.4173	-0.3154	-0.8532	-0.4569	1.0013	-0.9915	-1.2689	2.1282	0.0821
N6,N6,N6-trimethyllysine	Amino Acid	Lysine Metabolism	-0.3889	-1.9027	-0.4492	-0.6314	-0.6823	1.0237	0.8159	-0.5559	1.7293	-0.7444
pipecolate	Amino Acid	Lysine Metabolism	-1.1740	-0.3966	0.4869	-0.5742	-0.4400	-1.2898	2.2106	0.0937	0.9585	1.2779
2-aminobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.1156	-1.6531	-0.9969	-1.4262	-1.3497	0.8313	0.0796	0.1366	2.1405	1.9317
2-hydroxybutyrate/2-hydroxyisobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.1288	-1.1049	-1.3924	-1.0341	-1.3767	1.3132	0.2153	0.3684	2.4776	0.7984
cystathionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-1.9761	-2.0135	-0.3230	0.7811	0.5018	-0.0929	0.6841	-1.1611	0.2488	0.1465
cysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.5912	-2.3415	0.0469	-0.9253	-2.3435	0.0711	1.3933	-0.1949	0.6065	-1.1587
methionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.2271	-1.7114	0.7797	-0.0348	0.3403	0.5329	0.5008	-0.1280	0.2144	-0.2050
methionine sulfone	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.1448	-0.0725	-0.2536	-0.4006	-0.9156	1.5420	0.7786	-1.9713	0.1959	0.5969
methionine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.7226	0.4447	1.2542	0.7792	-1.0734	0.6366	-1.2106	0.5637	1.2220	-1.6646
N-acetylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.5643	-2.8699	-1.4927	-0.3993	-0.5230	-0.3228	2.1976	-0.8249	0.7581	1.0763
N-acetylmethionine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-1.0641	-1.0647	-0.4315	0.4532	-1.0660	0.0626	0.2973	0.0165	1.4221	-1.0593
N-acetyltaurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.6188	-2.3732	-0.3049	-0.7475	0.2089	-0.9659	1.7770	-0.9769	0.6511	0.8768
N-formylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.2574	-3.0900	-1.4478	-0.5972	-0.5143	-0.2213	2.0550	-0.5712	0.8600	1.3729
S-adenosylhomocysteine (SAH)	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.4885	-0.4870	-0.4801	-0.4998	-0.4796	-0.4733	-0.4951	-0.4893	3.5855	-0.4852
S-methylcysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.7216	-1.3477	-0.2843	-0.7687	-0.5575	-0.9242	0.2045	-0.3216	1.8646	1.2655
taurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-1.3157	-0.8059	-1.1249	-0.2479	-1.3078	0.0932	1.1888	0.4726	-0.9957	0.9945
3-(4-hydroxyphenyl)lactate	Amino Acid	Phenylalanine and Tyrosine Metabolism	-1.7918	-2.9070	-1.0971	-0.8165	0.3170	0.0312	1.7426	0.0865	1.2040	-0.1320
3-methoxytyramine sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.8313	-0.5795	-1.7566	0.2005	0.5680	-0.4430	1.3913	0.2608	1.0175	-0.3185
3-methoxytyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.6524	-1.5969	-1.2361	-0.5644	0.4086	-0.9667	0.4314	-1.3350	-1.5435	-1.6031
dopamine 3-O-sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	1.3796	2.7020	-0.4788	-0.4794	-0.4808	0.1452	-0.1390	2.2509	-0.4736	-0.4722
homovanillate (HVA)	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.5687	-3.2458	-1.5389	-0.4607	0.2597	0.1580	1.2299	-0.4646	0.1452	0.6059
N-acetylphenylalanine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-1.1289	-1.1267	-1.1134	0.2275	0.0413	-1.1224	1.9129	-0.0690	0.7463	0.9441
N-acetyltyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.2802	-0.2767	-0.2734	-0.2729	-0.2755	-0.2763	-0.2714	-0.2790	-0.2813	-0.2690
p-cresol sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.1681	0.1650	1.1106	0.2586	0.1590	-0.1824	1.7357	0.0978	0.8796	-1.8585
phenol sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.5264	-1.1427	-0.2327	-0.4834	-0.1217	0.0539	0.5702	0.4262	1.6134	-0.5833
phenylacetylglutamine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.3885	-0.4890	0.3690	-0.1846	-0.3226	-0.8241	2.5119	-0.6848	0.7292	-1.5838
phenylalanine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.8376	-0.2903	-0.1137	0.1700	0.8154	-0.1872	-0.4437	0.4601	1.4998	-1.0509
phenyllactate (PLA)	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.5374	-1.8749	-0.0614	0.0534	1.2626	-0.8124	0.9135	0.6286	1.0383	-0.9686
tyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-2.3096	-0.5113	-0.8501	-0.3910	-0.0699	0.9008	-0.4400	-0.1904	1.2358	0.0273
4-acetamidobutanoate	Amino Acid	Polyamine Metabolism	-0.3603	-1.6761	-1.0496	-0.2286	-1.0238	0.2358	1.4982	0.3244	-1.6865	0.8399
5-methylthioadenosine (MTA)	Amino Acid	Polyamine Metabolism	-0.6938	-1.7126	-0.9242	-0.4651	-0.3827	0.0985	-2.1258	0.2429	0.5573	-0.8663

Supplemental Table 2. Z-scores for Population Baseline

No heme detec

Biochemical	Super Pathway	Sub Pathway	CSF301	CSF302	CSF303	CSF304	CSF306	CSF307	CSF308	CSF309	CSF313	CSF317
acisoga	Amino Acid	Polyamine Metabolism	-0.0977	-0.6214	-1.1454	-1.0687	0.1308	-1.3611	0.3892	-0.4584	2.2444	-0.9093
N-acetylputrescine	Amino Acid	Polyamine Metabolism	-0.5921	-0.8363	-0.9587	-0.4669	-0.4263	-1.0906	1.0223	-0.8872	-0.4287	0.4398
spermidine	Amino Acid	Polyamine Metabolism	0.3914	1.3756	0.4326	0.2609	0.3289	0.6059	-0.4809	1.0640	0.0625	0.8174
3-indoxyl sulfate	Amino Acid	Tryptophan Metabolism	-0.7029	-0.7129	0.5188	-0.7094	-0.7072	-0.7126	0.5442	-0.1103	0.2896	-0.7115
5-hydroxyindoleacetate	Amino Acid	Tryptophan Metabolism	-0.6935	-2.7733	-1.2213	-0.7057	-0.4477	-0.2074	1.2756	-0.6750	-0.4021	0.5177
anthranilate	Amino Acid	Tryptophan Metabolism	0.3580	1.1948	1.3306	0.7046	-0.2807	-0.1571	0.1568	0.4913	0.8661	-1.4500
C-glycosyltryptophan	Amino Acid	Tryptophan Metabolism	-0.5373	-1.7774	-0.2699	-1.0399	-0.6377	-0.1597	0.5264	-0.1042	0.9908	-1.4003
indole-3-carboxylic acid	Amino Acid	Tryptophan Metabolism	-0.3182	0.3829	0.0511	-2.1175	0.3302	-0.7829	0.2438	-1.1151	1.7553	-1.1098
indoleacetate	Amino Acid	Tryptophan Metabolism	-1.0966	-0.9971	-0.9244	-0.1600	-1.5770	0.4433	1.0803	-0.8533	0.8235	0.5608
indolelactate	Amino Acid	Tryptophan Metabolism	-0.3025	-0.3028	-0.3013	-0.3205	-0.3190	-0.3063	2.0890	-0.3196	-0.3085	-0.3034
indolepropionate	Amino Acid	Tryptophan Metabolism	-0.3703	-0.3612	-0.3656	-0.3597	-0.3641	-0.3654	-0.3737	0.3368	-0.3799	-0.3761
kynurenate	Amino Acid	Tryptophan Metabolism	-0.5199	-1.3113	-1.3139	-1.3150	0.2746	0.0963	2.0667	-0.7511	0.3435	-0.1109
kynurenine	Amino Acid	Tryptophan Metabolism	-0.5399	-1.9713	-2.5479	-0.7946	-0.4757	-0.1163	1.2454	-0.1773	0.3944	0.2801
picolinate	Amino Acid	Tryptophan Metabolism	0.4751	-1.2589	-0.2909	-0.8562	-1.7991	-0.0375	1.9055	-0.7687	2.0310	1.3269
tryptophan	Amino Acid	Tryptophan Metabolism	-1.0022	-1.3906	-0.7630	-0.1172	-0.2875	-0.2495	-0.2534	-0.2306	1.7105	0.3197
tryptophan betaine	Amino Acid	Tryptophan Metabolism	0.3798	1.0051	0.6452	-1.1215	1.0289	-1.1198	-0.7701	0.7142	2.0842	0.6569
arginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.4705	0.3302	0.4638	-0.1814	0.0248	-0.1273	0.5386	-0.0960	-2.3347	-0.5001
argininosuccinate	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.3014	-0.0383	-0.2858	-1.0764	-0.7515	-1.8187	1.0634	-0.4261	-1.3925	-1.1112
citrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-1.4560	-0.4425	0.5063	0.2933	-0.3194	-0.4934	-0.4083	-0.6556	-1.4401	-0.2159
dimethylarginine (SDMA + ADMA)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.5971	-0.8076	-1.3539	-0.6762	0.0050	-0.2547	0.9238	-0.7121	-1.6080	0.2146
homoarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.0446	0.0744	0.5193	1.5608	0.9905	-1.4685	0.2846	1.1009	1.3340	0.1484
homocitrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.3495	-0.6684	-0.2754	-0.1236	-0.4942	0.8750	0.4080	-0.8124	1.0079	-0.5938
N-acetylarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.4297	-1.8050	0.1166	-0.2589	-0.5257	0.1115	0.9092	0.1234	1.1705	-1.0310
N-delta-acetylornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.4184	0.2228	0.2709	0.6818	-1.0830	-0.3519	-0.3470	-1.4578	0.6374	0.4482
N-methylproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.9183	-0.9163	2.3127	-0.5436	0.5607	-0.9211	-0.9129	1.6988	-0.9162	-0.9161
ornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.2425	-0.4548	0.2790	-0.4838	0.2049	-0.7506	0.2082	0.1004	-1.9963	2.3207
pro-hydroxy-pro	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.0629	-1.1409	-0.2167	-1.6126	-1.2536	0.0129	0.6871	-1.4049	-0.2483	0.1093
proline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-1.2475	-0.9284	-0.6158	-1.1486	-0.2445	0.1459	0.4801	0.8392	-1.3012	0.7223
trans-4-hydroxyproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.2599	-1.7186	0.5151	-0.4233	-0.5321	-1.5804	1.0782	-0.0256	-1.5773	0.7785
urea	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.7762	0.1365	0.0314	0.0190	-0.3282	1.5140	-0.1486	0.2499	2.4697	0.2557
argininate*	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.91982	0.111	-1.1483	-0.6502	-0.8191	-0.7689	0.54717	1.40817	-0.3439	-0.7758
erythronate*	Carbohydrate	Aminosugar Metabolism	-0.3141	-1.3330	-0.0540	-0.4544	-0.8154	0.9284	1.0485	0.7352	1.7994	-1.7761
glucuronate	Carbohydrate	Aminosugar Metabolism	-0.4744	-1.9834	-0.5242	-0.8109	-0.3316	1.7467	0.7051	0.0243	0.0413	-0.5638
N-acetylglucosaminylasparagine	Carbohydrate	Aminosugar Metabolism	-0.6326	-1.5512	-1.1705	-1.2345	-0.5173	0.2387	1.3317	-1.7212	1.1688	-0.5561
N-acetylneuraminate	Carbohydrate	Aminosugar Metabolism	0.0175	-2.0271	-0.5715	-1.2171	-0.4581	0.0599	0.8157	0.5298	0.7601	-1.2490
sucrose	Carbohydrate	Disaccharides and Oligosaccharides	0.0420	0.2389	-1.5654	0.9095	1.4794	1.2476	0.5764	0.1941	-0.5910	-1.5644
fructose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.2532	1.4131	0.7906	1.3424	1.2292	1.5777	-0.4334	0.1868	-2.6312	0.0059
galactitol (dulcitol)	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.8111	-1.1518	0.0555	-1.6396	-0.7234	0.2091	-0.1886	0.2204	0.2386	-0.2019
galactonate	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.5241	0.2520	-0.5237	-0.5248	-0.5237	-0.5265	-0.5250	1.1191	-0.5252	0.9804
mannitol/sorbitol	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.4098	-0.0937	0.1479	-0.3467	-0.4749	1.0175	-0.2876	0.1164	-0.1730	-1.4723
mannose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.2484	1.4102	0.2822	1.2690	0.5494	1.8209	-0.3829	0.7410	-2.1527	0.2542
1,5-anhydroglucitol (1,5-AG)	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.8513	0.0934	0.7002	0.5589	0.7511	-1.0809	-0.5177	0.4724	0.4606	-0.3634
glucose	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.6264	0.0751	-0.3344	0.0736	0.9109	0.4354	0.2728	0.3834	-2.9049	0.1993
glycerate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.7345	0.2050	-0.1856	-0.1254	-0.8029	0.1126	-0.1003	0.4636	0.1990	-2.3826
lactate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.4830	0.2356	-0.1824	-0.3554	-0.2446	-0.4008	0.5906	0.0621	-1.6950	-0.8437
pyruvate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.1611	-0.7951	-0.7986	-0.7975	0.5743	-0.7955	1.1488	-0.7953	-0.7946	2.0793
arabitol/xylitol	Carbohydrate	Pentose Metabolism	-0.5605	-1.3628	0.2849	-0.8233	-1.1676	1.1261	0.9289	0.8649	1.2686	-1.2960
arabonate/xylonate	Carbohydrate	Pentose Metabolism	-0.0951	-1.1068	0.0086	0.7880	-1.1157	1.4556	0.5022	0.0374	1.5886	-0.8422
ribitol	Carbohydrate	Pentose Metabolism	0.2611	0.2197	0.7495	-0.2803	-0.7359	0.8565	0.3136	0.4048	1.1873	-1.9109
ribonate	Carbohydrate	Pentose Metabolism	0.0272	-1.2559	0.6109	-0.1401	-0.6282	1.4885	1.0644	0.2606	1.7235	-1.8259
ribose	Carbohydrate	Pentose Metabolism	-1.3699	-1.3718	0.6626	0.9307	0.5190	0.3015	0.4732	0.7074	-1.3609	-1.3643
gulonic acid*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.2367	-2.0003	0.4570	-0.6159	-0.2922	0.2445	0.1111	-0.4304	0.5219	-1.6838
oxalate (ethanedioate)	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.1977	0.0461	0.0769	-0.1233	0.0815	1.3177	-0.1152	0.2820	-0.2480	-1.8377
threonate	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.0200	-0.2904	-0.2047	-0.0385	-0.5480	1.3952	-0.4314	0.4597	-0.6115	-2.2696
5-methyltetrahydrofolate (5MeTHF)	Cofactors and Vitamins	Folate Metabolism	-0.1778	0.5909	-0.2576	-1.5491	0.6556	-1.5611	0.9028	-0.7925	-1.2239	0.3013
bilirubin (E,E)*	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.4034	-0.4073	1.7568	-0.3991	-0.4021	-0.4110	-0.0434	-0.4120	-0.4068	-0.4074

Supplemental Table 2. Z-scores for Population Baseline

No heme detec

Biochemical	Super Pathway	Sub Pathway	CSF301	CSF302	CSF303	CSF304	CSF306	CSF307	CSF308	CSF309	CSF313	CSF317
bilirubin (Z,Z)	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.2306	-0.2406	1.1613	-0.2491	-0.2400	-0.2467	-0.2502	-0.2403	-0.2498	-0.2502
heme	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.5197	-0.5232	-0.5189	-0.5234	-0.5197	-0.5184	-0.5173	-0.5229	-0.5189	-0.5219
1-methylnicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.1801	-1.3633	-1.8079	-0.2017	-0.1838	0.0866	1.5162	-0.8697	0.7652	0.1998
N1-Methyl-2-pyridone-5-carboxamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.6025	0.7410	-0.9352	0.0277	-0.7240	0.7811	0.1988	-0.8518	0.8313	-0.1724
nicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-1.1762	-0.0301	-0.9316	0.6378	-1.1780	0.4790	0.6961	-0.6445	0.6479	0.5309
nicotinamide riboside	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.6961	-1.8646	-0.5523	0.2435	0.0028	0.2953	1.5425	0.8678	0.8792	-0.6550
quinolinate	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.4953	-0.5027	-0.4988	-0.4959	-0.5016	-0.4987	0.2999	-0.0309	-0.0179	-0.4999
trigonelline (N'-methylnicotinate)	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	1.0700	1.3618	0.6964	1.2930	0.0197	-1.3350	0.7492	1.1252	-0.1360	0.7615
pantothenate	Cofactors and Vitamins	Pantothenate and CoA Metabolism	-0.7488	0.5870	-1.7131	-1.1517	-1.2453	0.7256	1.4839	-0.4180	0.4183	-0.0875
gamma-CEHC	Cofactors and Vitamins	Tocopherol Metabolism	1.0359	0.6403	-0.9146	0.7710	-1.5552	1.3139	1.9429	-0.2107	1.1984	-1.0868
gamma-tocopherol/beta-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	-0.3581	-0.3592	1.2312	-0.3652	-0.3598	-0.3576	-0.3673	0.3874	-0.3629	-0.3621
retinol (Vitamin A)	Cofactors and Vitamins	Vitamin A Metabolism	-0.7984	0.1603	-0.6499	-0.8045	-0.8034	0.1118	1.6701	-0.8039	0.3149	-0.8091
pyridoxal	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.1815	-0.0293	-0.9941	-0.7294	-0.2250	0.2404	0.2767	-0.7832	1.2650	-0.4697
pyridoxate	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.5811	-0.2719	-1.2405	-0.9057	-0.6892	-0.0199	0.1369	-0.6269	1.7143	-0.6492
pyridoxine (Vitamin B6)	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.1861	-0.1899	-0.1777	-0.1798	-0.1890	-0.1723	-0.1735	-0.1852	-0.1908	-0.1886
phosphate	Energy	Oxidative Phosphorylation	-1.8957	0.1009	0.4174	0.7144	2.5486	-0.6054	-0.1576	-0.3922	0.8547	0.6066
2-methylcitrate	Energy	TCA Cycle	-0.6565	-2.0303	-0.2427	-0.9393	-0.5754	0.2840	1.2094	-0.6221	2.3422	-0.6128
aconitate [cis or trans]	Energy	TCA Cycle	-0.2275	-0.3304	0.3395	-0.6158	-0.6354	-0.3423	-0.6724	-0.0200	0.0914	-0.1047
alpha-ketoglutarate	Energy	TCA Cycle	-0.6525	-1.3360	-0.9251	-0.9726	-0.4250	-0.7273	1.1213	-0.1123	-0.5034	2.7763
citrate	Energy	TCA Cycle	0.2444	1.6706	1.6097	0.0941	-1.4009	-0.2872	-0.6614	0.7662	-1.7935	-0.9418
fumarate	Energy	TCA Cycle	-0.9701	-0.9750	-0.9701	-0.9779	-0.0139	-0.9764	0.7629	-0.9751	-0.9668	0.7040
isocitrate	Energy	TCA Cycle	0.5144	0.8526	1.2665	0.3789	-0.1551	-0.6864	-1.3675	-0.2754	-1.1948	-1.3620
malate	Energy	TCA Cycle	-0.5090	-0.9274	-1.3299	-0.7993	-0.4757	-0.5484	0.2014	-0.6525	-0.7231	0.8481
succinate	Energy	TCA Cycle	-0.7767	-0.8471	-1.0740	-0.6853	0.4472	-0.4130	0.7417	-0.9124	-0.8222	0.0471
succinylcarnitine	Energy	TCA Cycle	0.1458	-1.6586	0.5509	-0.3847	-0.5097	0.1960	1.3580	1.1554	0.9293	-0.3114
carnitine	Lipid	Carnitine Metabolism	-0.4170	-0.1828	1.0477	-0.0224	-1.5595	0.7451	1.6204	1.2630	-0.8689	-1.1330
deoxycarnitine	Lipid	Carnitine Metabolism	-0.1063	-0.7294	1.9074	0.9551	-1.3187	0.6179	-0.1694	0.9952	0.0590	-1.1792
butyrylcarnitine	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	-0.7222	0.1065	-0.1086	-1.4012	-0.0929	0.2086	2.2514	0.6506	-0.0124	0.0950
methylmalonate (MMA)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.1209	-0.7034	-0.1580	-0.9651	-1.5641	0.1994	-0.8359	0.4557	1.1468	0.1021
propionylcarnitine	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.0207	-1.7042	0.1768	-0.5102	-0.2866	0.7453	1.1990	0.8247	0.5779	-0.7280
3-hydroxybutyrylcarnitine (1)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.5931	-0.5832	-0.5929	-0.5893	-0.5885	-0.5865	1.4647	-0.5926	1.3285	-0.5802
acetylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.7774	-1.4599	0.5336	-0.1517	-0.9805	0.1304	1.9271	0.0409	0.2449	-0.6313
cis-4-decenoyl carnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.4858	-0.7097	-1.2850	-1.0043	-0.4904	0.6748	2.0733	0.4177	-0.2115	-1.1935
decanoylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.6271	-1.3852	-0.0386	-1.3916	-1.3862	-0.2322	1.5029	0.6675	0.3488	-0.7799
hexanoylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.9376	-0.9339	-0.9238	-0.9277	-0.9367	-0.9242	2.0466	0.7557	0.9454	-0.9256
laurylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.4621	-0.4645	-0.4548	-0.4563	-0.4682	-0.4829	-0.4608	0.6262	-0.4803	-0.4760
octanoylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.8593	-1.3075	-0.2064	-1.7144	-0.0748	-0.0692	1.4688	0.7899	0.4876	-0.4759
malonate	Lipid	Fatty Acid Synthesis	0.6151	1.3680	0.6832	0.0819	-1.6311	-0.0135	-0.2505	0.8661	-0.8776	-0.8005
malonylcarnitine	Lipid	Fatty Acid Synthesis	-0.0326	-1.3404	0.4908	-0.4289	-1.0143	-1.3407	1.2087	-0.6348	0.5830	-1.3289
oleamide	Lipid	Fatty Acid, Amide	0.7040	0.7032	1.0284	0.6124	0.3596	0.9762	1.1802	-0.9814	-1.0815	0.4149
palmitic amide	Lipid	Fatty Acid, Amide	0.5585	0.6335	1.0683	0.5099	0.1682	1.1139	1.4081	-1.1229	-1.1567	0.1675
2-aminoheptanoate	Lipid	Fatty Acid, Amino	-0.7743	-1.0754	0.6179	-0.0441	-0.3377	-0.0074	-1.3780	-1.4476	1.0283	1.1064
2-aminooctanoate	Lipid	Fatty Acid, Amino	0.7915	1.1741	1.9826	-0.3636	-0.2915	-1.1313	-1.0659	-1.0747	-1.1252	0.6474
2-hydroxyadipate	Lipid	Fatty Acid, Dicarboxylate	-0.2554	-1.9637	1.5429	-0.4354	1.2970	0.5119	0.5728	1.0746	-1.2694	0.9590
3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)	Lipid	Fatty Acid, Dicarboxylate	-0.1916	-0.1908	-0.1567	-0.1686	-0.2083	-0.1947	-0.1532	-0.1857	-0.2107	-0.1569
dimethylmalonic acid	Lipid	Fatty Acid, Dicarboxylate	-0.5279	-1.8660	-0.5396	-0.5226	-1.0555	1.1202	1.5454	-0.4781	2.1239	-0.3894
maleate	Lipid	Fatty Acid, Dicarboxylate	-0.4615	-1.0360	-1.5585	-1.3820	-1.1063	-0.5433	0.6992	0.0367	0.4673	-0.9368
2-hydroxydecanoate	Lipid	Fatty Acid, Monohydroxy	-0.4458	-0.4401	0.7530	-0.4388	-0.4339	-0.4292	-0.4308	-0.4308	-0.4330	-0.4561
3-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	-0.2134	-1.524	-0.4334	-1.4358	-1.5293	-0.4732	0.85669	0.15646	0.20742	0.66691
3-hydroxyoctanoate	Lipid	Fatty Acid, Monohydroxy	-1.1075	-1.1020	-0.8641	-1.0995	-1.1095	-1.0971	0.5238	0.1246	-0.2181	0.2313
3-hydroxysebacate	Lipid	Fatty Acid, Monohydroxy	-0.1159	0.0193	-0.0676	-0.3121	-0.2475	0.0388	-0.0619	-0.4179	-0.3894	-0.4815
5-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	-0.4592	-0.7528	-0.1064	-0.7386	-0.7447	1.4494	-0.7575	0.2383	-0.7463	0.6659
glycerol	Lipid	Glycerolipid Metabolism	-0.3268	-0.2106	-0.1353	-0.5609	-0.1593	0.3771	0.0994	0.0769	-0.2743	-0.5276
glycerol 3-phosphate	Lipid	Glycerolipid Metabolism	0.2847	1.0955	1.9109	0.7675	0.4260	-0.3726	-0.5503	-1.3731	-2.0217	-0.3606
galactosylglycerol*	Lipid	Glycerolipid Metabolism	-0.2475	-0.8006	-0.1815	-1.0469	0.01169	-0.5685	0.6028	-0.0503	0.36003	-1.6021
myo-inositol	Lipid	Inositol Metabolism	-0.3125	-0.4539	-0.8231	-1.0522	-0.4156	-0.7897	-0.4635	0.2491	0.3001	-0.4257

Supplemental Table 2. Z-scores for Population Baseline

No heme detec

Biochemical	Super Pathway	Sub Pathway	CSF301	CSF302	CSF303	CSF304	CSF306	CSF307	CSF308	CSF309	CSF313	CSF317
3-hydroxybutyrate (BHBA)	Lipid	Ketone Bodies	-0.4766	-1.2418	-1.2800	-1.2667	-1.3317	-1.0323	1.1503	-0.3908	1.6800	-0.1982
acetoacetate	Lipid	Ketone Bodies	-0.1942	-1.1146	-1.0610	-1.2422	-0.9117	-0.4534	1.1391	-0.4617	1.8221	-0.2494
1-adrenoyl-GPC (22:4)*	Lipid	Lysolipid	1.6648	-0.3873	-0.6531	-1.2498	0.9453	-0.5361	-0.1352	-1.1247	0.3535	-0.8215
1-arachidonoyl-GPC (20:4)*	Lipid	Lysolipid	0.2224	-1.4971	0.1487	-0.5569	-1.5018	0.1895	0.2987	-0.0041	1.0061	-1.4915
1-arachidonoyl-GPE (20:4)*	Lipid	Lysolipid	0.5245	-1.1730	-0.2209	-1.1595	-1.1638	-0.0930	1.3870	-0.1771	0.6210	-1.1658
1-dihomo-linolenoyl-GPC (20:3n3 or 6)*	Lipid	Lysolipid	-0.2381	-0.2228	-0.2362	-0.2355	-0.2402	-0.2250	0.4432	-0.2394	-0.2260	-0.2291
1-dihomo-linoleoyl-GPC (20:2)*	Lipid	Lysolipid	-1.2204	-0.4961	-0.4929	-0.1402	0.4874	-1.4665	-1.5910	-0.7551	-1.3929	0.3700
1-docosahexaenoyl-GPC (22:6)*	Lipid	Lysolipid	-0.2957	-0.2908	-0.2989	-0.2919	-0.2784	-0.2863	-0.2954	-0.2787	1.5822	-0.2923
1-docosahexaenoyl-GPE (22:6)*	Lipid	Lysolipid	0.9169	-1.1978	-1.1936	-1.1918	-0.0463	1.1024	1.1300	0.4966	1.9545	-1.1862
1-docosapentaenoyl-GPC (22:5n3)*	Lipid	Lysolipid	1.2482	-1.3079	0.5269	-0.0221	-1.1655	0.6348	0.2175	-1.3963	-1.0853	-0.9570
1-docosapentaenoyl-GPC (22:5n6)*	Lipid	Lysolipid	1.1191	0.4165	0.0887	-0.0036	1.3731	1.3512	-1.3542	-0.4436	-0.5708	0.6254
1-linoleoyl-GPC (18:2)	Lipid	Lysolipid	-0.1547	-1.4845	-0.2244	-0.5814	-1.4911	-0.3365	0.9326	-0.1151	0.5799	-0.8878
1-myristoyl-GPC (14:0)	Lipid	Lysolipid	-0.2253	-0.2454	-0.2361	-0.2266	-0.2426	-0.2380	-0.2348	-0.2436	-0.2350	-0.2294
1-oleoyl-GPA (18:1)	Lipid	Lysolipid	-0.3264	1.5666	-0.4377	-0.9570	1.8857	-1.3682	0.9579	1.0153	0.9528	-0.6764
1-oleoyl-GPC (18:1)	Lipid	Lysolipid	0.1287	-2.0347	0.2733	-0.7927	-0.9357	0.4849	0.9411	-0.2257	1.5086	-1.7718
1-palmitoleoyl-GPC (16:1)*	Lipid	Lysolipid	-0.2088	-0.2240	-0.2225	-0.2247	-0.2203	-0.2149	-0.2118	-0.2246	0.8115	-0.2074
1-palmitoyl-GPA (16:0)	Lipid	Lysolipid	-0.4785	-0.4878	-0.4812	-0.4912	-0.4891	0.4018	-0.4800	-0.1793	2.0137	-0.4796
1-palmitoyl-GPC (16:0)	Lipid	Lysolipid	-0.0711	-1.6836	0.1841	-0.7718	-0.8251	0.2399	0.8409	-0.1976	1.2468	-1.7714
1-pentadecanoyl-GPC (15:0)*	Lipid	Lysolipid	-0.8472	-0.4025	-1.2137	-0.2001	1.1570	-0.5174	0.1439	-1.0342	0.0748	1.5255
1-stearoyl-GPC (18:0)	Lipid	Lysolipid	-0.1498	-1.1698	-0.0698	-0.7871	-1.4748	-0.3060	0.5922	-0.2781	0.9136	-1.4720
1-stearoyl-GPE (18:0)	Lipid	Lysolipid	-0.6360	-0.6505	-0.6461	-0.6474	-0.6305	-0.6297	-0.6240	-0.6380	1.8713	-0.6419
1-palmityl-GPC (O-16:0)	Lipid	Lyso-phospho-ether	-0.7451	0.1426	-1.1485	-1.1252	0.5797	0.8001	1.0386	-0.2919	-1.2927	-0.3526
1-(1-enyl-palmitoyl)-GPC (P-16:0)*	Lipid	Lysoplasmalogen	-1.2239	0.2755	1.2938	0.7094	1.4297	-1.6291	1.0376	0.6121	-1.4671	-0.8357
1-(1-enyl-stearoyl)-GPE (P-18:0)*	Lipid	Lysoplasmalogen	0.1910	0.8085	0.9314	-0.0962	0.1747	0.8750	0.9357	-0.7341	-1.0914	0.8004
3-hydroxy-3-methylglutarate	Lipid	Mevalonate Metabolism	-0.2930	-1.2588	-1.2250	-1.6908	0.2806	-0.8120	0.7991	-0.3985	-0.5707	0.6856
1-arachidonylglycerol (20:4)	Lipid	Monoacylglycerol	0.6652	-0.8825	-0.8428	-1.3092	0.2944	1.0792	0.8047	-0.9692	0.4577	0.6293
1-dihomo-linolenylglycerol (20:3)	Lipid	Monoacylglycerol	-1.6815	-0.3581	0.4960	-1.1988	0.3509	1.1041	-0.2629	-0.9976	0.1041	-0.3890
1-oleoylglycerol (18:1)	Lipid	Monoacylglycerol	1.4302	-0.4332	-0.0738	-0.5846	-1.7070	-0.0154	0.1822	0.5396	1.0666	-1.7088
1-palmitoylglycerol (16:0)	Lipid	Monoacylglycerol	1.1820	-0.1475	1.0348	0.7651	-0.5976	0.5209	0.4507	0.7656	2.9040	-1.3778
1,2-dilinoleoyl-GPC (18:2/18:2)	Lipid	Phospholipid Metabolism	-0.1849	-0.1771	-0.1836	-0.1958	-0.1719	-0.1893	-0.1742	-0.1869	-0.1864	-0.1884
1,2-dimyristoyl-GPC (14:0/14:0)	Lipid	Phospholipid Metabolism	0.6596	-0.4987	0.9238	0.4193	-0.5470	-1.5883	-0.5454	-1.3304	-0.3572	0.1679
1,2-dioleoyl-GPC (18:1/18:1)*	Lipid	Phospholipid Metabolism	0.0439	-1.2930	0.8999	-0.5971	-1.0467	0.2163	1.1003	0.2850	1.3345	-2.2366
1,2-dipalmitoyl-GPC (16:0/16:0)	Lipid	Phospholipid Metabolism	0.1382	-1.2613	0.6313	-0.9429	-0.5407	0.1254	0.9290	0.1562	1.3973	-1.7009
1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4)*	Lipid	Phospholipid Metabolism	-0.9822	-1.4846	0.8326	-1.1227	-0.3388	0.8484	-0.6516	-1.4665	0.4452	1.3757
1-margaroyl-2-linoleoyl-GPC (17:0/18:2)*	Lipid	Phospholipid Metabolism	-0.4955	0.4037	-1.5346	-1.4312	0.0310	1.2756	-0.3012	1.4891	0.4688	1.1477
1-margaroyl-2-oleoyl-GPC (17:0/18:1)*	Lipid	Phospholipid Metabolism	-0.2865	-0.2956	-0.2968	-0.2970	-0.3037	-0.2840	-0.2930	-0.2953	3.0725	-0.3071
1-myristoyl-2-linoleoyl-GPC (14:0/18:2)*	Lipid	Phospholipid Metabolism	-1.5324	-0.1946	-1.5693	-0.1445	-0.2520	1.0664	0.3748	0.3207	-0.6289	-0.7901
1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	Lipid	Phospholipid Metabolism	-0.4204	-1.0678	0.1643	-1.4764	-1.1295	0.2866	0.8584	0.1270	0.6847	-1.3520
1-oleoyl-2-dihomo-linolenoyl-GPC (18:1/20:3)*	Lipid	Phospholipid Metabolism	-0.2076	-0.1994	-0.2016	-0.2102	-0.1985	-0.2102	0.3144	-0.1968	-0.1878	-0.2103
1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)*	Lipid	Phospholipid Metabolism	0.4825	1.3921	1.0508	-1.4787	1.1398	-1.1526	-0.5009	-0.4352	0.8506	-1.0283
1-oleoyl-2-linoleoyl-GPC (18:1/18:2)*	Lipid	Phospholipid Metabolism	-0.9080	-0.9181	0.3676	-0.9134	-0.9098	-0.5931	1.2091	-0.0512	0.4785	-0.9079
1-palmitoleoyl-2-linoleoyl-GPC (16:1/18:2)*	Lipid	Phospholipid Metabolism	-1.7170	0.1762	0.9984	0.1235	-0.1184	-1.4250	0.3166	-0.9321	0.5082	0.1293
1-palmitoyl-2-adrenoyl-GPC (16:0/22:4)*	Lipid	Phospholipid Metabolism	-0.5519	-0.5465	0.4979	-0.5575	-0.5451	-0.5534	1.0385	-0.5534	0.8864	-0.5542
1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4)	Lipid	Phospholipid Metabolism	0.0293	-1.4053	0.3254	-1.0508	-0.6772	0.2196	0.7488	-0.0721	0.9312	-1.7397
1-palmitoyl-2-dihomo-linolenoyl-GPC (16:0/20:3n3 or 6)*	Lipid	Phospholipid Metabolism	-1.1865	-0.8894	0.1478	-0.8865	-1.1844	-0.0320	1.3636	0.1381	0.7689	-0.8290
1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)	Lipid	Phospholipid Metabolism	-0.0696	-1.0380	0.4890	-1.0274	-0.2104	0.2940	0.9300	-0.2584	1.4701	-1.6496
1-palmitoyl-2-eicosapentaenoyl-GPC (16:0/20:5)*	Lipid	Phospholipid Metabolism	-1.0310	-1.4898	-0.0472	-0.0983	1.5825	0.6301	0.7316	0.1414	0.4520	-0.5632
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	Lipid	Phospholipid Metabolism	-0.7069	-0.8089	0.0932	-1.2588	-1.0227	-0.4428	1.2800	-0.0310	0.5456	-1.2269
1-palmitoyl-2-meadoyl-GPC (16:0/20:3n9)*	Lipid	Phospholipid Metabolism	0.9895	0.5280	-2.0441	-0.0287	-1.4638	1.5705	-0.6290	-1.1357	-0.1252	0.3030
1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	Lipid	Phospholipid Metabolism	0.3012	-1.1329	0.8053	-0.8558	-0.7591	0.4944	1.3184	0.1846	1.4646	-1.7858
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*	Lipid	Phospholipid Metabolism	0.0412	-1.0241	0.2022	-1.1294	-0.5941	0.1447	0.9974	0.0355	1.0150	-0.9709
1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	Lipid	Phospholipid Metabolism	-0.2447	-0.2499	-0.2486	-0.2581	-0.2714	-0.2647	-0.2670	-0.2629	-0.2516	-0.2659
1-palmityl-2-arachidonoyl-GPC (O-16:0/20:4)*	Lipid	Phospholipid Metabolism	-0.4000	-0.3886	-0.4009	-0.3951	-0.3887	-0.4017	0.8647	-0.3949	-0.1864	-0.3945
1-palmityl-2-oleoyl-GPC (O-16:0/18:1)*	Lipid	Phospholipid Metabolism	-0.6855	-0.9272	1.0499	-0.9269	-1.1192	0.6971	1.2757	0.0744	0.9913	-1.1143
1-pentadecanoyl-2-oleoyl-GPC (15:0/18:1)*	Lipid	Phospholipid Metabolism	-0.2266	-0.2118	-0.2307	-0.2360	-0.2217	-0.2198	-0.2095	-0.2201	1.1530	-0.2231
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	Lipid	Phospholipid Metabolism	0.0420	-1.2150	0.3411	-1.2572	-0.6636	-0.0216	0.6745	-0.0043	1.0140	-1.8347

Supplemental Table 2. Z-scores for Population Baseline

No heme detec

Biochemical	Super Pathway	Sub Pathway	CSF301	CSF302	CSF303	CSF304	CSF306	CSF307	CSF308	CSF309	CSF313	CSF317
1-stearoyl-2-dihomo-linolenoyl-GPC (18:0/20:3n3 or 6)*	Lipid	Phospholipid Metabolism	-0.7390	-0.2679	-0.2661	-0.7421	-0.7458	-0.7467	1.3357	-0.4330	0.7264	-0.7454
1-stearoyl-2-docosahexaenoyl-GPC (18:0/22:6)	Lipid	Phospholipid Metabolism	0.1433	-1.5071	0.4125	-1.0796	-0.7970	0.0843	0.7519	0.4409	1.4808	-1.5110
1-stearoyl-2-docosahexaenoyl-GPE (18:0/22:6)*	Lipid	Phospholipid Metabolism	0.8327	-0.9090	1.0148	-0.9045	-0.0732	0.3461	0.5406	1.3986	2.3210	-0.9074
1-stearoyl-2-docosapentaenoyl-GPC (18:0/22:5n3)*	Lipid	Phospholipid Metabolism	-1.1306	-0.9824	1.4357	-0.0002	-0.0023	-0.0161	-1.1838	0.1721	-0.5459	1.2085
1-stearoyl-2-docosapentaenoyl-GPC (18:0/22:5n6)*	Lipid	Phospholipid Metabolism	0.7911	-0.8268	1.0853	1.3672	-0.2815	-0.9822	0.5491	-1.2004	-0.6334	0.2494
1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*	Lipid	Phospholipid Metabolism	-0.5400	-0.9403	0.2597	-1.1907	-0.8755	-0.7002	1.1470	0.0811	0.5118	-1.2673
1-stearoyl-2-meadoyl-GPC (18:0/20:3n9)*	Lipid	Phospholipid Metabolism	-1.0424	0.5872	0.5946	-0.8159	1.0679	-1.7783	-0.5000	0.4882	-0.9593	-0.1002
1-stearoyl-2-oleoyl-GPC (18:0/18:1)	Lipid	Phospholipid Metabolism	0.2028	-1.4000	0.5910	-0.4361	-0.5474	0.3548	0.7771	0.6863	1.2779	-1.7315
choline	Lipid	Phospholipid Metabolism	-0.4527	-1.0318	-1.2595	0.5221	0.3499	1.5732	0.4493	0.3705	1.2344	0.5578
choline phosphate	Lipid	Phospholipid Metabolism	-0.5031	-1.5500	0.9744	0.2924	0.2571	0.2649	-0.0075	-0.8345	0.0219	-0.4925
glycerophosphoethanolamine	Lipid	Phospholipid Metabolism	-0.6392	-0.6322	-0.6404	-0.6411	0.8265	-0.6350	0.1919	-0.6357	-0.6396	0.0071
glycerophosphoinositol*	Lipid	Phospholipid Metabolism	0.7546	-1.8941	0.6795	-1.9035	-0.2507	0.5949	1.1699	0.1874	1.7406	0.1276
glycerophosphorylcholine (GPC)	Lipid	Phospholipid Metabolism	-0.0383	-0.2382	-0.8831	-1.9406	-1.9442	-0.3046	0.4908	0.2604	-0.2396	-0.6269
phosphoethanolamine	Lipid	Phospholipid Metabolism	-0.4523	1.0510	2.9208	0.5622	0.3984	0.8024	-1.0572	-1.0244	-0.5314	-1.0304
trimethylamine N-oxide	Lipid	Phospholipid Metabolism	-0.2216	-0.4971	0.6015	-0.3984	-0.5993	0.8752	0.4868	0.0152	0.6456	-0.8162
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*	Lipid	Plasmalogen	-0.4399	-0.4411	-0.2999	-0.4371	-0.4367	-0.4307	0.7160	-0.4448	-0.0210	-0.4321
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	Lipid	Plasmalogen	-0.4008	-0.4163	-0.4112	-0.4095	-0.4048	-0.3939	-0.3935	-0.3916	-0.4181	-0.3917
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPC (P-16:0/22:6	Lipid	Plasmalogen	-0.5225	0.1046	1.0395	1.2636	0.1832	-0.2599	0.0367	-1.1415	0.5839	-1.4882
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPE (P-16:0/22:6	Lipid	Plasmalogen	0.5096	-0.8200	0.7525	-0.8203	-0.8143	0.7316	1.0998	-0.8202	1.9684	-0.8213
1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	Lipid	Plasmalogen	-0.2923	-1.2607	-0.3178	-1.2521	0.1676	-0.0156	-0.6829	-0.4897	0.7959	-1.9608
1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	Lipid	Plasmalogen	-0.8545	-0.3375	1.3211	-0.8487	-0.8527	0.6535	1.3552	-0.0222	0.3893	-0.8493
1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*	Lipid	Plasmalogen	-0.3258	0.2619	0.6995	0.9616	0.2203	-1.0262	-0.7260	0.6605	-0.0977	-1.1459
1-(1-enyl-stearoyl)-2-arachidonoyl-GPC (P-18:0/20:4)	Lipid	Plasmalogen	0.0546	-0.8025	-1.8278	1.1229	0.9614	-0.0076	-0.8493	-0.1691	-0.4988	1.3884
1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	Lipid	Plasmalogen	0.2752	-0.8542	0.7863	-0.8488	-0.6022	-0.7115	1.4442	-0.4298	1.4187	-0.8506
1-(1-enyl-stearoyl)-2-docosahexaenoyl-GPE (P-18:0/22:6)	Lipid	Plasmalogen	0.8171	-1.5877	0.6060	-0.6567	-0.1201	0.5392	0.9703	0.1177	1.9087	-2.0699
1-(1-enyl-palmitoyl)-2-dihomo-linolenoyl-GPC (P-18:0/20	Lipid	Plasmalogen	-0.1411	0.1164	1.7250	-0.7746	0.3290	-0.6001	-0.5332	0.0263	-0.6788	0.7386
dihomo-linoleate (20:2n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-0.3414	-0.9279	1.0913	-0.9355	-0.9228	-0.3853	0.8712	-0.9320	1.0763	-0.9364
dihomo-linolenate (20:3n3 or n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-0.8453	-0.8267	-0.0110	-0.8322	-0.2213	-0.7183	0.7213	0.0742	0.0917	-0.8274
glycochenodeoxycholate	Lipid	Primary Bile Acid Metabolism	-0.2460	-0.1803	-0.1634	-0.0786	-0.0605	-0.0663	-0.3442	-0.2210	-0.0756	-0.2074
glycocholate	Lipid	Primary Bile Acid Metabolism	-0.1830	-0.1843	-0.1789	-0.1840	-0.1935	-0.1791	-0.1726	-0.1937	-0.1959	-0.1803
glycocholenate sulfate*	Lipid	Secondary Bile Acid Metabolism	-0.1794	-0.1744	-0.1873	-0.1861	-0.1755	-0.1895	-0.1831	-0.1886	-0.1889	-0.1796
glycohyocholate	Lipid	Secondary Bile Acid Metabolism	-0.1631	-0.1940	-0.1756	-0.1904	-0.2044	-0.1879	-0.1518	-0.2050	-0.1496	-0.2050
hyocholate	Lipid	Secondary Bile Acid Metabolism	-0.5348	-0.6149	0.1055	0.5118	1.0428	-0.9942	-1.4342	-0.9968	0.2379	1.0603
behenoyl sphingomyelin (d18:1/22:0)*	Lipid	Sphingolipid Metabolism	-0.3849	-0.3984	0.9632	-0.3866	-0.3912	-0.3834	0.5374	-0.3913	-0.3992	-0.3869
palmitoyl sphingomyelin (d18:1/16:0)	Lipid	Sphingolipid Metabolism	-0.3662	-0.8963	0.4757	-1.1216	-0.8563	0.1533	0.8458	-0.1150	1.0319	-1.6641
sphingomyelin (d18:1/14:0, d16:1/16:0)*	Lipid	Sphingolipid Metabolism	-0.6166	-0.9403	0.2268	-0.9362	-0.9374	-0.0251	0.3956	0.0142	1.0170	-0.9409
sphingomyelin (d18:1/18:1, d18:2/18:0)	Lipid	Sphingolipid Metabolism	0.4565	-1.0441	0.8651	-0.6000	-0.9003	0.4815	0.8879	0.3762	1.4827	-1.8098
sphingomyelin (d18:1/20:0, d16:1/22:0)*	Lipid	Sphingolipid Metabolism	0.5258	-1.0324	0.6037	-1.0249	-1.0253	0.5208	0.6283	0.3382	0.9800	-1.0268
sphingomyelin (d18:1/24:1, d18:2/24:0)*	Lipid	Sphingolipid Metabolism	-1.0666	-0.7788	0.7632	-1.0607	-1.0664	0.1539	1.0386	0.1061	0.4167	-1.0627
sphingomyelin (d18:2/16:0, d18:1/16:1)*	Lipid	Sphingolipid Metabolism	0.1125	-0.9845	0.7889	-0.9870	-0.9874	-0.0295	0.9019	-0.1250	1.1420	-0.9887
sphingosine	Lipid	Sphingolipid Metabolism	-1.0048	1.2370	-1.0120	0.6663	-1.0042	0.0168	-1.0112	-0.2020	-1.0127	0.5063
stearoyl sphingomyelin (d18:1/18:0)	Lipid	Sphingolipid Metabolism	0.4416	-1.4706	0.9977	-0.6355	-0.4401	0.6270	1.3019	0.0645	1.4249	-1.7825
16a-hydroxy DHEA 3-sulfate	Lipid	Steroid	-0.2242	-0.2315	-0.2335	-0.2339	-0.2344	-0.2229	-0.2253	-0.2307	-0.2340	-0.2219
4-androsten-3beta,17beta-diol disulfate (1)	Lipid	Steroid	-0.4090	-0.4054	1.2053	-0.4083	-0.4130	0.4656	-0.4133	0.6251	-0.4067	-0.4133
4-androsten-3beta,17beta-diol disulfate (2)	Lipid	Steroid	-0.1821	-0.1813	-0.1804	-0.1859	-0.1887	-0.1827	-0.1855	-0.1845	-0.1887	-0.1788
5alpha-pregnan-3beta,20alpha-diol disulfate	Lipid	Steroid	-1.1326	1.4716	0.0232	-1.1482	1.0924	-1.3071	-0.7722	0.7217	-0.3145	-1.1371
andro steroid monosulfate (1)*	Lipid	Steroid	-0.9390	1.2149	-0.5790	-0.3626	1.0720	-0.7604	1.1535	0.3231	0.3112	-1.1528
cortisol	Lipid	Steroid	0.1502	0.2454	-0.2435	-0.6465	0.2689	-0.6450	-0.4961	0.4365	0.9137	-0.6481
cortisone	Lipid	Steroid	0.2117	-1.5398	-0.0910	-0.4028	0.0653	-1.5392	0.0260	0.3853	0.4827	0.1159
dehydroisoandrosterone sulfate (DHEA-S)	Lipid	Steroid	-0.1138	-0.1100	-0.1057	-0.1444	-0.1897	-0.2161	-0.1070	-0.1493	-0.1731	-0.1123
7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)	Lipid	Sterol	-0.0637	-0.1489	0.5319	-0.4597	-0.0933	0.5234	0.5693	0.1110	-0.4567	-1.3882
cholesterol	Lipid	Sterol	-0.0481	-1.3976	0.4157	-0.7062	-0.1983	0.0700	0.7025	0.1047	0.9554	-2.2498
2'-deoxyinosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.0759	0.1481	-1.1783	-0.2529	-1.4874	-1.4301	-1.4039	-0.1373	-0.8505	0.9594
allantoin	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.3787	-0.6469	0.0656	-0.1556	-1.1469	0.9100	-0.6284	0.1905	-0.2072	-0.6739
hypoxanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.1849	-1.5549	-1.6582	-0.9308	0.0863	-0.3239	0.8301	1.1775	0.9349	0.8236
inosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.0892	0.8140	1.0406	1.7207	0.6824	-1.2471	-1.2463	0.4759	-0.6893	-0.3817

Supplemental Table 2. Z-scores for Population Baseline

No heme detec

Biochemical	Super Pathway	Sub Pathway	CSF301	CSF302	CSF303	CSF304	CSF306	CSF307	CSF308	CSF309	CSF313	CSF317
urate	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.2560	-0.2138	0.6434	-0.0832	-0.2163	1.1814	0.4044	0.2775	-0.0805	-0.6241
xanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-1.0346	-2.5373	-1.3548	-1.3401	-0.6077	-0.1024	1.3651	0.3066	0.9498	1.0408
xanthosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.0777	-1.4413	-1.4302	-1.4400	-1.4472	-0.2111	0.6517	1.4300	-1.4421	1.3787
N1-methylinosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.1358	-3.4977	-1.2615	-0.322	-0.4496	-0.7268	1.13917	-0.021	1.01125	0.86328
adenine	Nucleotide	Purine Metabolism, Adenine containing	-0.1786	-0.2438	-0.9107	-0.5842	-0.6485	-0.1343	-2.1732	1.1515	0.2909	-1.2496
adenosine	Nucleotide	Purine Metabolism, Adenine containing	-0.5593	-0.9145	-0.7220	-0.2894	-2.0692	-0.4123	0.2795	-0.3284	-0.8098	-0.5956
adenosine 3',5'-cyclic monophosphate (cAMP)	Nucleotide	Purine Metabolism, Adenine containing	0.3311	0.4151	0.8665	-0.1206	0.0701	0.0281	1.4792	0.6436	-0.3475	1.6776
adenosine 5'-monophosphate (AMP)	Nucleotide	Purine Metabolism, Adenine containing	0.5442	0.8766	-0.9753	1.0095	-0.1638	-0.1923	0.4322	1.0119	-0.1284	-0.4999
N1-methyladenosine	Nucleotide	Purine Metabolism, Adenine containing	-0.2918	-1.7969	-1.8425	-0.3198	-0.8491	-0.4411	1.3488	0.1194	0.3095	1.4824
N6-carbamoylthreonyladenosine	Nucleotide	Purine Metabolism, Adenine containing	-0.1698	-2.6770	-0.8542	-0.4408	-1.1837	0.0202	1.8217	0.0050	2.2219	0.0391
N6-methyladenosine	Nucleotide	Purine Metabolism, Adenine containing	0.2494	0.0555	-0.8383	0.4783	0.8562	-0.7014	0.6669	0.0890	0.1705	1.4420
N6-succinyladenosine	Nucleotide	Purine Metabolism, Adenine containing	0.4718	-1.0285	0.5612	0.2857	-0.4480	0.0953	0.6877	1.3090	1.3256	-1.5011
7-methylguanine	Nucleotide	Purine Metabolism, Guanine containing	-0.3613	-2.0062	-1.1889	-0.2831	-0.7820	-0.6464	0.5161	-0.2825	0.6009	0.7914
guanosine	Nucleotide	Purine Metabolism, Guanine containing	-1.4733	-0.2000	-0.7378	0.4238	1.0043	-2.5873	0.3665	0.3393	1.1799	0.9416
N2,N2-dimethylguanosine	Nucleotide	Purine Metabolism, Guanine containing	-0.0391	-2.2710	-1.6670	-0.4337	-0.9378	-0.7348	1.3859	0.0449	0.7850	1.2254
N2-methylguanosine	Nucleotide	Purine Metabolism, Guanine containing	-0.0162	-1.4252	-0.1734	-0.4591	-0.0980	-1.5365	1.2519	-0.3926	0.9415	1.0007
2'-deoxycytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	-1.3258	-1.6353	-0.0377	-0.3657	-0.4814	0.3147	1.2788	0.0763	0.4076	-0.1645
cytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	0.7082	-1.0293	-0.1127	-0.9387	-0.4359	-0.1861	1.1905	0.0846	1.3428	-1.7427
orotate	Nucleotide	Pyrimidine Metabolism, Orotate containing	-1.2087	-2.4310	-0.7483	-0.6842	-1.6746	0.5942	1.0182	0.2907	0.9310	0.5673
orotidine	Nucleotide	Pyrimidine Metabolism, Orotate containing	-0.6074	-1.3536	-1.4132	-1.2832	-1.7345	0.4974	0.0953	0.2892	0.8424	-1.7490
3-aminoisobutyrate	Nucleotide	Pyrimidine Metabolism, Thymine containing	-1.0358	-0.4074	0.7558	-1.0472	-1.0352	-1.0397	0.5003	1.3222	-1.0370	-1.0402
5,6-dihydrothymine	Nucleotide	Pyrimidine Metabolism, Thymine containing	-1.3820	-0.2937	-0.8297	-0.7447	-0.5837	-0.0171	-0.5631	-0.3571	-0.0243	1.0800
2'-deoxyuridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	-1.1077	-0.8700	0.5885	0.3395	-1.1122	-1.1064	0.5736	-0.4246	0.4353	-0.7534
3-ureidopropionate	Nucleotide	Pyrimidine Metabolism, Uracil containing	-1.5677	-1.3959	-0.2138	-0.0064	2.2961	0.0294	-0.0015	1.2361	0.9099	1.1976
5-methyluridine (ribothymidine)	Nucleotide	Pyrimidine Metabolism, Uracil containing	1.1002	-0.9642	0.0983	0.2075	-0.7514	-1.2496	0.0113	-0.4901	0.2503	-1.3154
N-acetyl-beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.5485	-2.4722	-0.0520	-1.0704	-0.6725	-0.5903	2.6492	0.1255	-0.4323	1.5029
pseudouridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.3379	-0.5513	-0.7623	-0.7255	-0.9664	1.2591	1.0032	-0.3168	0.6883	-1.6516
uracil	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.3635	-0.9368	-0.9355	-0.9337	-0.4137	-0.4166	1.0949	-0.9631	1.6744	0.8511
uridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	1.5659	-0.2285	-1.0477	-0.4249	0.0338	-1.7918	1.0371	-0.7641	1.6610	-0.4173
cyclo(ala-pro)	Peptide	Dipeptide	-0.1408	0.1405	-0.1225	-0.0663	-2.0413	-1.4370	0.4619	-0.3061	0.3572	-1.0439
cyclo(pro-val)	Peptide	Dipeptide	0.5618	0.6812	-0.5400	0.0189	-0.5414	-0.5410	-0.5356	0.6433	-0.5354	-0.5390
glycylproline	Peptide	Dipeptide	-0.6119	-1.3128	-0.8182	-0.9834	-1.1768	-0.4689	0.3482	-1.6340	-0.6857	0.6151
leucylproline	Peptide	Dipeptide	2.2358	0.4831	1.8941	1.0932	-0.6210	-0.6500	-0.0557	-0.6178	-0.5245	-0.6184
pyroglutamylglutamine	Peptide	Dipeptide	-0.3169	-1.4529	0.3362	0.0856	0.1774	-0.2735	0.5467	0.2355	3.0530	0.4309
homocarnosine	Peptide	Dipeptide Derivative	-1.2023	-0.9391	-1.5526	0.0703	0.8930	-1.7177	-0.5834	-1.2540	-0.2127	1.7071
gamma-glutamyl-epsilon-lysine	Peptide	Gamma-glutamyl Amino Acid	0.2091	-1.1931	0.3749	-0.5635	-1.7807	0.0407	0.5584	0.2880	1.9226	-1.2037
gamma-glutamylalanine	Peptide	Gamma-glutamyl Amino Acid	-0.3408	-0.0932	0.0743	-1.0845	-0.2491	-0.8361	1.2058	-0.2911	-0.7022	-0.3875
gamma-glutamylglutamine	Peptide	Gamma-glutamyl Amino Acid	-0.6239	-0.7790	-0.3897	-0.7011	-0.3283	0.6928	0.9041	-0.7606	-0.9991	0.4456
gamma-glutamylhistidine	Peptide	Gamma-glutamyl Amino Acid	-1.5635	-1.9744	0.4985	-0.8133	-0.2173	-0.9848	1.0469	-0.8644	0.5387	-1.3120
gamma-glutamylisoleucine*	Peptide	Gamma-glutamyl Amino Acid	0.5362	-1.0187	0.8750	-0.3322	-1.0346	1.3542	-1.0185	0.7437	1.2869	-0.3139
gamma-glutamylleucine	Peptide	Gamma-glutamyl Amino Acid	0.7592	-1.2936	0.6875	-0.9848	-1.2803	1.3320	-0.1663	-0.0775	1.5276	0.1785
gamma-glutamylmethionine	Peptide	Gamma-glutamyl Amino Acid	-0.8703	-1.0739	0.6279	-1.0633	-0.4817	-0.3195	1.6378	0.2926	0.1459	0.2470
gamma-glutamylphenylalanine	Peptide	Gamma-glutamyl Amino Acid	-0.6373	1.0276	1.1950	-0.6383	-0.6377	-0.6474	-0.6474	0.4208	-0.6366	-0.6281
gamma-glutamylthreonine*	Peptide	Gamma-glutamyl Amino Acid	0.1217	-1.3163	0.4039	0.4702	-0.9231	-0.5742	0.4074	0.4385	-0.4626	-0.7501
gamma-glutamyltyrosine	Peptide	Gamma-glutamyl Amino Acid	-0.3799	-0.3961	-0.4016	-0.3802	-0.4079	-0.3786	-0.3974	-0.3908	2.7262	-0.3976
gamma-glutamylvaline	Peptide	Gamma-glutamyl Amino Acid	0.1956	-0.4801	0.5123	-0.2735	-2.0997	1.6454	0.6469	0.1955	0.5833	-0.1968
gamma-glutamyl-alpha-lysine	Peptide	Gamma-glutamyl Amino Acid	-0.365	-1.2612	0.19583	-0.5333	-1.2856	1.43816	0.77587	-0.2466	1.86862	-0.1801
tartronate (hydroxymalonate)	Xenobiotics	Bacterial/Fungal	-0.4547	0.5533	0.4725	0.0759	-0.0928	0.5054	-0.3865	0.6722	0.3443	-3.5188
4-methylcatechol sulfate	Xenobiotics	Benzoate Metabolism	-0.2015	5.2939	-0.1974	-0.1564	-0.1787	-0.1716	-0.2020	-0.1542	-0.1935	-0.1674
catechol sulfate	Xenobiotics	Benzoate Metabolism	1.4920	1.8574	1.5085	1.2768	-0.6937	-0.7070	0.1631	1.1532	-0.7064	-0.7087
hippurate	Xenobiotics	Benzoate Metabolism	-0.9284	-0.0530	0.2758	-0.8133	-0.0783	-1.3184	-0.4830	0.1720	1.2005	-0.4823
methyl-4-hydroxybenzoate sulfate	Xenobiotics	Benzoate Metabolism	-0.7190	-0.7157	-0.7208	-0.7178	-0.7180	-0.2216	1.0485	0.0163	-0.7178	1.5230
1,2-propanediol	Xenobiotics	Chemical	-0.4476	-0.4517	-0.4511	-0.4492	-0.4461	0.4050	-0.4509	-0.4520	-0.4477	-0.4495
1,3-propanediol	Xenobiotics	Chemical	-0.7790	-0.3769	-0.8237	0.1892	-0.2746	-0.8406	-0.8346	-0.3414	0.3070	0.1477
2-aminophenol sulfate	Xenobiotics	Chemical	-0.3712	0.1511	-0.3682	-0.3703	-0.3752	-0.3720	-0.3771	-0.3647	-0.3718	-0.3756
3-hydroxypyridine sulfate	Xenobiotics	Chemical	0.3901	1.0909	-0.5228	-0.9566	0.9248	-0.9405	0.1410	-1.0496	-0.3649	1.2667

Supplemental Table 2. Z-scores for Population Baseline

Biochemical	Super Pathway	Sub Pathway	CSF301	CSF302	CSF303	CSF304	CSF306	CSF307	CSF308	CSF309	CSF313	CSF317
dimethyl sulfone	Xenobiotics	Chemical	1.2250	1.3983	-0.5645	1.1958	-0.2417	-1.2388	0.0367	0.7872	1.0567	1.2458
O-sulfo-L-tyrosine	Xenobiotics	Chemical	-0.5734	-1.5147	-0.0755	-1.0172	-1.2077	0.5700	0.8838	-0.3838	1.1303	-1.2458
succinimide	Xenobiotics	Chemical	-0.1651	0.0370	-0.0352	0.0433	-0.3467	0.3557	-0.9636	-0.3018	0.8461	2.4233
sulfate*	Xenobiotics	Chemical	0.2341	-1.7802	-0.9727	-0.1346	0.2895	1.1655	0.1604	0.2850	2.2626	-1.3456
trizma acetate	Xenobiotics	Chemical	-0.4461	-0.5320	-0.6186	-0.5039	-0.3829	1.8641	2.8813	-0.4311	-0.1215	-0.4766
2-hydroxyacetaminophen sulfate*	Xenobiotics	Drug	2.7076	-0.3256	-0.3390	-0.3398	-0.3220	0.1078	-0.3278	-0.3252	-0.3301	-0.3315
2-methoxyacetaminophen glucuronide*	Xenobiotics	Drug	4.5264	-0.2961	-0.2848	-0.2977	-0.2851	-0.2844	-0.3069	-0.2998	-0.3026	-0.3068
2-methoxyacetaminophen sulfate*	Xenobiotics	Drug	-0.2568	-0.2652	-0.2532	-0.2695	-0.2541	-0.2529	-0.2604	-0.2631	-0.2555	-0.2648
3-(cystein-S-yl)acetaminophen*	Xenobiotics	Drug	4.9016	-0.2443	-0.2566	-0.2340	-0.2324	-0.2533	-0.2294	-0.2509	-0.2271	-0.2543
4-acetamidophenol	Xenobiotics	Drug	1.9007	-0.4774	-0.4744	-0.4757	-0.4768	0.9272	-0.4756	-0.4773	-0.4755	-0.4779
4-acetamidophenylglucuronide	Xenobiotics	Drug	3.1398	-0.4244	-0.4248	-0.4217	-0.4283	1.6826	-0.4250	-0.4274	-0.4270	-0.4222
4-acetaminophen sulfate	Xenobiotics	Drug	1.8294	-0.4751	-0.4790	-0.4767	-0.4781	1.3170	-0.4782	-0.4798	-0.4738	-0.4781
5-sulfosalicylate	Xenobiotics	Drug	-0.6054	-0.6050	-0.6040	-0.6028	-0.6058	-0.6028	-0.6063	1.7102	-0.6002	-0.6050
carbamazepine 10,11-epoxide*	Xenobiotics	Drug	-0.1768	-0.1755	-0.1757	-0.1771	-0.1845	-0.1878	-0.1832	-0.1822	-0.1792	-0.1888
fluoxetine	Xenobiotics	Drug	-0.1881	5.2946	-0.1802	-0.1777	-0.1820	-0.1887	-0.1879	-0.1774	-0.1854	-0.1789
lidocaine	Xenobiotics	Drug	1.2521	0.2235	1.5710	0.5646	-0.5704	0.3531	-1.2245	0.2567	-1.3383	-0.8542
N-ethylglycinexylidide	Xenobiotics	Drug	-0.5129	-0.5173	0.1128	-0.5179	-0.5168	-0.5156	-0.5165	0.8847	-0.5139	-0.5167
salicylate	Xenobiotics	Drug	-0.2167	-0.9303	-0.9303	0.5504	-0.9273	-0.0418	-0.5665	0.5711	-0.9258	0.8980
topiramate	Xenobiotics	Drug	-0.2631	-0.2655	-0.2610	-0.2616	-0.2632	-0.2631	-0.2647	-0.2607	-0.2653	-0.2623
pregabalin	Xenobiotics	Drug	-0.1835	5.2946	-0.1783	-0.1866	-0.1827	-0.1871	-0.1834	-0.1805	-0.1823	-0.1809
sulfamethoxazole	Xenobiotics	Drug	-0.1848	-0.1814	-0.1813	-0.1837	-0.1806	-0.1795	5.29464	-0.1847	-0.1838	-0.1795
cetirizine	Xenobiotics	Drug	-0.3252	2.92369	-0.3286	2.44734	-0.3225	-0.3273	-0.325	-0.3246	-0.3287	-0.3278
2-piperidinone	Xenobiotics	Food Component/Plant	-1.5792	0.0367	0.7759	-0.3120	-0.5343	-1.6879	-2.1094	-0.5164	1.3419	0.9205
betonicine	Xenobiotics	Food Component/Plant	0.7763	0.1900	1.4564	0.5093	0.3638	1.3831	-1.0811	1.4193	0.4602	-1.0828
ergothioneine	Xenobiotics	Food Component/Plant	0.3815	-1.5929	-0.4355	-0.2005	-1.0634	0.2557	-0.3035	0.0911	0.6653	0.8448
erythritol	Xenobiotics	Food Component/Plant	-0.6118	0.6905	0.8285	-0.3944	0.0276	1.7217	0.4503	0.6833	1.3293	-1.9179
gluconate	Xenobiotics	Food Component/Plant	-0.2780	-0.6007	-0.3500	-0.5048	0.0867	0.8620	-0.2053	0.3214	-0.9679	-0.0462
indolin-2-one	Xenobiotics	Food Component/Plant	-1.1490	-0.8251	-0.0246	1.9461	-1.1494	-1.1466	0.8387	-0.4308	0.8257	-1.1379
levulinate (4-oxovalerate)	Xenobiotics	Food Component/Plant	-1.2387	0.0046	0.7320	1.4203	-0.4831	0.1398	0.2722	-0.0357	-1.0352	-0.1201
piperine	Xenobiotics	Food Component/Plant	1.5655	0.8956	2.6487	1.4263	-0.6602	-0.6598	-0.6643	1.0671	1.0318	0.0660
quinate	Xenobiotics	Food Component/Plant	1.7441	0.5220	0.0285	1.2844	0.3004	-0.7262	-0.7187	1.8996	-0.7254	-0.7239
S-allylcysteine	Xenobiotics	Food Component/Plant	0.7311	1.7758	2.2833	-0.5511	-0.5578	-0.5534	-0.5617	2.7328	-0.5604	-0.5605
stachydrine	Xenobiotics	Food Component/Plant	0.8317	-0.0401	1.4710	0.4603	0.8401	0.5148	-1.4424	1.4449	0.0920	-0.5420
tartarate	Xenobiotics	Food Component/Plant	0.1352	-0.2605	-0.5308	-1.3992	0.7028	-1.2232	0.3754	-0.4887	-1.3981	-0.3303
acesulfame	Xenobiotics	Food Component/Plant	-0.5028	-0.5081	-0.5109	-0.5051	-0.5102	-0.503	-0.1488	-0.5124	-0.5095	-0.5118
3-methylxanthine	Xenobiotics	Xanthine Metabolism	-0.4899	1.7480	-0.5054	1.1765	-0.5051	-0.4999	-0.5059	0.2519	-0.5009	-0.4872
5-acetylamino-6-amino-3-methyluracil	Xenobiotics	Xanthine Metabolism	2.1683	-0.2741	4.7140	-0.2538	-0.2785	-0.2761	-0.2652	-0.2722	-0.2723	-0.2722
7-methylxanthine	Xenobiotics	Xanthine Metabolism	0.7012	0.7130	-0.5062	1.5223	0.8768	-0.6318	-0.6153	1.5937	-0.6185	-0.6324
caffeine	Xenobiotics	Xanthine Metabolism	0.5800	0.2851	2.5494	0.9645	-0.6163	-0.6148	-0.6153	0.7118	-0.6123	-0.6146
paraxanthine	Xenobiotics	Xanthine Metabolism	0.9874	0.6147	2.9245	1.7417	-0.6494	-0.6511	-0.6570	0.9871	-0.6532	-0.6490
theobromine	Xenobiotics	Xanthine Metabolism	0.7628	1.4621	0.7791	1.1444	0.8392	-0.9362	-0.9355	1.1342	-0.9386	-0.5923
theophylline	Xenobiotics	Xanthine Metabolism	1.0032	-0.4926	3.4202	2.0935	-0.4900	-0.4964	-0.4962	0.2505	-0.4962	-0.4976
thioproline	Xenobiotics	Chemical	-0.7971	0.96069	-0.0657	-1.1546	-1.2425	-1.2388	0.4556	-0.2488	-0.161	0.06954

Supplemental Table 2. Z-scores for Population Baseline

Biochemical	Super Pathway	Sub Pathway	CSF318	CSF319	CSF320	CSF322	CSF323	CSF325	CSF327	CSF328	CSF329	CSF305
alanine	Amino Acid	Alanine and Aspartate Metabolism	1.5508	0.1355	0.0119	1.4837	1.3003	-2.1704	-0.1434	0.6453	0.1438	-0.3532
asparagine	Amino Acid	Alanine and Aspartate Metabolism	0.9225	0.5168	-0.7872	2.2283	1.3377	-0.7118	-1.0137	0.0050	0.7856	0.5501
aspartate	Amino Acid	Alanine and Aspartate Metabolism	-0.4126	-1.2060	-0.1126	0.0407	-0.0646	0.4270	0.8776	0.6743	0.2534	0.7091
N-acetylalanine	Amino Acid	Alanine and Aspartate Metabolism	0.8002	-0.6247	-0.1801	1.5262	0.6844	0.4915	0.5285	1.7090	0.5920	-0.3390
N-acetylasparagine	Amino Acid	Alanine and Aspartate Metabolism	-0.5728	-0.3142	-0.3125	0.6289	-1.4170	1.6947	0.5877	0.9818	-0.2307	1.1504
N-acetylaspartate (NAA)	Amino Acid	Alanine and Aspartate Metabolism	2.1077	0.4256	-0.1219	-0.1883	1.3091	0.0743	0.4581	1.5858	1.0377	0.5501
creatine	Amino Acid	Creatine Metabolism	0.2933	1.4429	-0.0301	-0.3144	-2.6221	-1.4614	-1.1648	-0.1589	-1.0897	0.9486
creatine phosphate	Amino Acid	Creatine Metabolism	0.7721	-0.6009	1.2175	-0.6186	-0.6746	-0.6589	0.7726	1.7392	0.8110	-0.3004
creatinine	Amino Acid	Creatine Metabolism	-0.5651	-0.4119	-0.4201	-1.1110	-1.4695	0.7100	0.7252	0.1937	-0.6874	1.3515
guanidinoacetate	Amino Acid	Creatine Metabolism	0.6636	2.0040	0.4616	-1.4283	0.5875	-0.3357	0.8416	0.4172	0.0546	-0.7219
carboxyethyl-GABA	Amino Acid	Glutamate Metabolism	0.3722	-0.3681	-0.1924	-0.4173	0.4189	1.2627	-0.3594	0.6520	-1.3974	1.1836
citramalate	Amino Acid	Glutamate Metabolism	1.3749	0.5660	1.0648	0.0345	-0.7961	-1.8820	0.7604	-1.1240	0.5392	0.3715
gamma-aminobutyrate (GABA)	Amino Acid	Glutamate Metabolism	-2.3521	0.6186	0.4976	-2.2787	-1.0527	1.7009	0.6286	-0.5141	-0.1025	1.7146
glutamate	Amino Acid	Glutamate Metabolism	-0.0941	-0.9547	-0.0972	1.9647	0.1957	0.5872	1.0939	1.0637	0.8228	-0.0869
glutamate, gamma-methyl ester	Amino Acid	Glutamate Metabolism	-0.5371	0.6411	-0.6475	0.4442	0.7799	0.4209	0.3635	0.1395	1.1288	1.0109
glutamine	Amino Acid	Glutamate Metabolism	-0.5063	0.0572	-1.0820	1.6452	-0.3003	0.3976	0.1282	-0.8063	-0.0264	0.8838
N-acetyl-aspartyl-glutamate (NAAG)	Amino Acid	Glutamate Metabolism	0.5775	0.3436	1.1005	1.0002	0.5246	-0.2919	0.7951	1.5536	-0.0818	0.2215
N-acetylglutamate	Amino Acid	Glutamate Metabolism	1.6685	0.0115	-0.2959	0.5062	1.1580	0.8069	0.6141	1.4838	1.3001	0.5511
N-acetylglutamine	Amino Acid	Glutamate Metabolism	0.3131	-0.6359	-0.3281	1.6697	-1.0129	1.4129	0.2976	1.2933	0.3635	0.4827
pyroglutamine*	Amino Acid	Glutamate Metabolism	0.8358	-0.1225	-1.0916	-2.2871	0.7992	0.6681	0.2406	-0.0762	0.0507	-0.2995
S-1-pyrroline-5-carboxylate	Amino Acid	Glutamate Metabolism	-1.5726	0.9615	0.1942	1.9627	-0.1471	-0.0533	0.0172	-1.5735	-0.0990	1.0077
beta-citrylglutamate	Amino Acid	Glutamate Metabolism	0.90543	-0.8612	0.03105	3.08573	0.20752	0.3883	-0.1879	1.59831	0.60745	0.61886
5-oxoproline	Amino Acid	Glutathione Metabolism	-0.2131	-0.8779	-0.2911	-0.4679	-0.6783	1.6970	1.2330	0.1952	0.6241	-0.4548
cys-gly, oxidized	Amino Acid	Glutathione Metabolism	-1.4030	0.2914	0.9561	0.7470	0.0971	-0.4733	0.6595	-0.7498	-0.3764	-0.5470
cysteinylglycine	Amino Acid	Glutathione Metabolism	0.5598	2.0051	-0.1536	1.6961	-0.5895	-0.5895	-0.5887	-0.5911	-0.5902	-0.5873
glutathione, oxidized (GSSG)	Amino Acid	Glutathione Metabolism	1.8634	-0.3749	-0.3685	4.0059	0.3606	-0.3720	-0.3671	-0.3674	-0.3600	-0.3660
betaine	Amino Acid	Glycine, Serine and Threonine Metabolism	1.6635	0.6606	-1.8860	1.6391	1.1371	0.0415	-0.5560	1.2690	0.7196	0.5403
dimethylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.0614	0.6147	-1.7076	1.5243	1.1063	-0.7889	-0.6609	1.2424	0.1966	-0.2361
glycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.2461	-0.0361	-0.5611	1.2958	0.9832	-1.3540	-0.0493	-0.5102	-0.4022	1.1047
N-acetylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.5187	-0.9694	-0.5606	0.1387	-1.1322	0.2239	0.0968	-0.4006	2.6178	-0.1868
N-acetylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.4139	-0.7046	-0.4862	1.7274	0.4618	0.3280	0.3978	2.0353	0.3449	0.4779
N-acetylthreonine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.1906	-0.3991	-0.7868	2.0198	0.2098	0.6740	0.3515	1.7430	0.3559	0.2902
serine	Amino Acid	Glycine, Serine and Threonine Metabolism	1.6553	0.3401	-0.2817	1.0078	1.1517	-0.7905	-0.0709	0.7989	0.6913	0.5304
threonine	Amino Acid	Glycine, Serine and Threonine Metabolism	1.5466	0.5465	-0.9626	1.6947	0.6380	-1.2960	-0.0085	-1.2393	-0.2134	0.2813
2-methylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	1.92439	0.06982	1.4038	0.22908	2.72027	-0.8261	-0.4371	-0.731	0.38643	-0.9354
1-methylguanidine	Amino Acid	Guanidino and Acetamido Metabolism	-0.2930	0.0328	-0.6239	1.6671	-0.0134	-0.6169	0.2183	2.3724	-0.6229	0.0042
4-guanidinobutanoate	Amino Acid	Guanidino and Acetamido Metabolism	1.2643	-0.7088	0.0426	0.3725	0.6972	-0.3614	0.2334	0.1094	2.6449	-0.8447
1-methylhistamine	Amino Acid	Histidine Metabolism	1.6823	-0.3534	-0.3625	-0.3487	-0.3641	-0.3557	4.0722	-0.3575	1.9866	-0.3582
1-methylhistidine	Amino Acid	Histidine Metabolism	-1.4467	-0.0004	0.0206	0.1597	-0.4427	-0.9128	0.7278	-1.8933	-0.5535	-0.0614
1-methylimidazoleacetate	Amino Acid	Histidine Metabolism	2.1283	1.0386	0.4789	0.2988	0.9147	-0.5598	-0.5107	1.0580	0.0946	0.9157
3-methylhistidine	Amino Acid	Histidine Metabolism	-1.0724	0.8440	1.0996	-1.0736	-0.8300	-1.0751	1.4994	-0.9820	-1.0696	0.4211
4-imidazoleacetate	Amino Acid	Histidine Metabolism	0.9412	-0.5334	1.4732	-1.0249	1.6163	-1.0213	0.3634	1.3204	1.6413	-1.0267
histidine	Amino Acid	Histidine Metabolism	-0.4463	1.5211	-0.1740	0.8971	0.1674	0.7278	-0.3295	-2.0775	0.0087	0.6113
imidazole lactate	Amino Acid	Histidine Metabolism	-0.0038	0.3438	-2.1049	0.3809	0.8932	0.1475	-0.3956	-0.3072	-1.4418	1.2598
imidazole propionate	Amino Acid	Histidine Metabolism	-0.5826	-0.5845	-0.5894	2.9695	1.3790	-0.5781	-0.5823	-0.5850	1.3580	0.3711
N-acetyl-3-methylhistidine*	Amino Acid	Histidine Metabolism	-1.2619	0.7746	0.7588	-0.9129	-1.1764	0.1051	1.4082	-1.0903	-1.6564	0.9480
N-acetylhistidine	Amino Acid	Histidine Metabolism	0.8421	-0.0498	-0.3607	2.0122	0.8717	1.1105	0.0269	1.2147	0.2040	0.0320
2-hydroxy-3-methylvalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.0250	-1.6981	-0.1147	0.4724	-1.7014	0.2555	0.5220	0.1899	-0.6194	0.6493
2-methylbutyrylcarnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.3266	0.3199	-1.4689	1.5937	-0.6278	-0.0468	0.6534	0.3498	-0.2809	0.9934
3-hydroxy-2-ethylpropionate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.1134	-0.7580	0.3311	1.7820	-1.9944	-1.0985	0.5262	-1.9837	-0.1780	0.3607
3-hydroxyisobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.4667	0.3864	0.3853	0.9790	-0.5832	-1.8809	0.2994	0.7233	0.4676	-0.4164
3-methyl-2-oxobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.2944	0.9175	-0.7489	0.7185	-1.2947	0.6736	-1.2971	0.4060	-1.2958	1.0793
3-methyl-2-oxovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.0465	0.1388	-1.7575	0.8910	-1.7582	0.8189	-0.4673	0.8079	-1.7645	0.8688
3-methylglutaconate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.1862	-0.4979	-0.6640	-0.4244	-1.2547	0.0544	0.6690	0.9406	0.0587	0.7502
4-methyl-2-oxopentanoate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.7467	0.4800	-1.2240	1.2243	-1.2320	0.8258	-1.2251	0.3701	-1.2308	0.9759
alpha-hydroxyisocaproate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.8593	-1.8606	-0.0444	-0.0472	-1.8659	0.4590	0.5009	-0.5203	0.3085	1.2004

Supplemental Table 2. Z-scores for Population Baseline

Biochemical	Super Pathway	Sub Pathway	CSF318	CSF319	CSF320	CSF322	CSF323	CSF325	CSF327	CSF328	CSF329	CSF305
alpha-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.2217	-0.0292	0.6253	-0.5683	-0.8467	-0.0762	0.4799	-1.1317	-0.6034	0.4348
beta-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.2683	0.1287	0.2244	-0.7252	-2.1206	0.2761	0.8115	-0.2030	-1.3511	0.2626
beta-hydroxyisovaleroylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.0514	-0.0559	-0.5941	1.5374	-1.3888	0.2268	0.7183	1.1305	0.0909	1.4292
ethylmalonate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.0882	-0.6958	-0.0415	1.1815	0.1180	0.3887	-0.5066	1.9934	0.8256	1.1768
isobutyrylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.2597	0.3867	-0.3799	1.5062	-0.8317	-0.9617	-0.5646	-0.5665	-1.0137	0.3540
isoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.7662	-0.1479	-0.8524	1.9544	0.3312	-0.6232	-0.5898	1.1495	-0.3312	0.1244
isovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.4965	-1.1536	0.1749	-0.3507	0.9510	0.3353	0.6299	0.1044	1.1467	-1.1511
isovalerylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.3437	-0.2703	-0.1605	0.5300	-0.1319	-0.5601	-1.7875	-0.3241	-0.4633	0.8812
leucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.0267	0.1598	-0.5942	1.8999	-0.1387	-0.4361	-0.6156	0.1614	-0.2435	0.6784
methylsuccinate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.4936	-0.1247	0.0330	-1.1687	0.9485	-0.5824	0.3239	3.1696	0.7132	0.7543
methylsuccinoylcarnitine (1)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.5762	0.3868	0.3014	-1.6250	-0.2167	0.6448	-0.0123	0.7902	0.3941	1.2210
N-acetylisoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.8579	-0.3698	-0.3099	1.1158	-0.5488	0.0490	0.2947	1.6754	0.7533	-0.1657
N-acetylleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.9546	0.1010	-1.3721	0.7358	-0.4478	0.4218	0.7475	1.5580	0.3225	-0.4349
N-acetylvaline	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.9633	-0.5464	-0.3346	2.1467	0.5513	0.3637	0.3976	1.6344	0.6031	-0.4443
tiglylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.0048	0.0397	1.2036	1.5084	-0.5255	-0.2380	-0.1052	1.3765	-0.3206	0.1250
valine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.0170	0.8763	-0.5858	1.0712	0.0463	-1.7506	0.2181	-0.2984	0.1782	1.0517
2,3-dihydroxy-2-methylbutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.3571	0.04332	1.34623	-0.0554	-1.2133	-0.4932	0.18305	0.62299	-2.3509	0.42211
2-oxoadipate	Amino Acid	Lysine Metabolism	-0.5402	0.9284	-0.5453	-0.5367	-0.5384	-0.5397	-0.5398	-0.5418	-0.5469	1.5575
3-methylglutarylcarnitine (2)	Amino Acid	Lysine Metabolism	-0.4935	-0.0615	-0.1399	-0.3101	-0.9202	0.3809	0.0958	0.7505	-0.5207	0.7749
5-hydroxylysine	Amino Acid	Lysine Metabolism	1.1985	-0.1133	-0.7492	2.0665	1.1975	-1.5562	-0.1051	0.6617	1.2803	0.7327
6-oxopiperidine-2-carboxylic acid	Amino Acid	Lysine Metabolism	-0.0848	-0.9434	-0.6603	-1.6503	-1.8051	-0.5803	0.5303	-0.6389	1.3128	-0.1495
glutarate (pentanedioate)	Amino Acid	Lysine Metabolism	2.0498	0.4040	-0.2009	-0.4022	0.8840	-0.4217	0.6409	1.6929	0.3450	0.3472
glutarylcarnitine (C5)	Amino Acid	Lysine Metabolism	-0.0439	1.3937	-0.9481	3.1157	-0.5728	-0.4677	-1.2142	0.3554	-0.3346	0.7150
lysine	Amino Acid	Lysine Metabolism	-0.0464	-0.1460	-0.0830	1.4583	0.2336	-1.5794	-0.6865	-0.9429	-1.2290	0.5610
N2-acetyllysine/N6-acetyllysine	Amino Acid	Lysine Metabolism	-0.3819	0.6772	-1.2985	2.1213	0.0472	-0.6991	-1.0222	0.7528	-0.4744	0.2909
N6,N6,N6-trimethyllysine	Amino Acid	Lysine Metabolism	-0.0215	-0.8086	-0.2072	2.6133	0.5843	-0.2183	0.1131	0.7943	0.6172	0.2931
pipecolate	Amino Acid	Lysine Metabolism	-0.6305	0.1910	-0.2753	0.5789	-0.0415	-1.0759	1.1219	0.6480	1.9168	0.3420
2-aminobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.7157	0.0538	-0.3841	-0.0034	-0.7777	-2.0500	0.0768	0.4923	0.7031	1.0997
2-hydroxybutyrate/2-hydroxyisobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.4755	0.1562	0.2087	0.4252	-1.2202	-1.2975	0.1028	0.6410	-0.5881	0.3750
cystathionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.8745	0.3569	-0.1017	1.6867	0.3997	-0.1306	0.3956	0.8615	0.1126	0.4708
cysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.3423	-0.6206	-0.3247	0.9570	-0.3150	0.8867	-0.3706	1.1472	0.3518	1.3131
methionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.6895	0.4932	-1.6530	0.8912	-0.5764	0.3563	-0.7075	0.1815	-1.7336	1.2923
methionine sulfone	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.6504	-0.9108	-0.8644	2.7563	-0.7283	-0.6946	0.6794	-0.9011	1.1878	-0.3323
methionine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.0309	-1.4263	0.9000	0.4112	1.4919	-0.6344	0.4661	0.3180	1.4407	-1.2272
N-acetylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.2574	-0.1072	-0.3985	0.0210	0.0438	0.8128	0.3523	1.4127	0.2377	0.4582
N-acetylmethionine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.5466	-1.0611	1.1786	-0.6898	1.5658	0.3184	0.6727	1.1776	2.0505	-1.0649
N-acetyltaurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.4640	-0.1142	-0.0647	0.2419	1.0087	0.2791	0.4230	1.9758	0.4688	-0.2037
N-formylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.1121	-0.0141	-0.2821	-0.5432	-0.1485	0.7896	0.6032	1.1581	0.0169	0.5299
S-adenosylhomocysteine (SAH)	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.4863	-0.4900	-0.4829	1.4639	-0.4785	1.3910	-0.4989	1.3533	-0.4669	-0.3903
S-methylcysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.3197	0.4201	0.3422	-0.0598	-0.2892	-0.3497	3.0257	-0.3441	-1.2930	0.2598
taurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.4165	1.2151	0.5788	2.1043	0.1179	-0.1471	0.8618	0.2463	0.3147	0.3036
3-(4-hydroxyphenyl)lactate	Amino Acid	Phenylalanine and Tyrosine Metabolism	1.1934	0.0414	0.6823	-0.1919	0.2230	0.5209	1.0580	0.2233	-0.7283	0.3622
3-methoxytyramine sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.1517	0.8783	-1.9954	0.9159	0.2887	-0.8289	1.0144	0.8794	-0.3747	1.8486
3-methoxytyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	1.0135	0.0037	-0.3620	1.4101	1.5953	0.5065	-0.3288	0.5733	1.3557	0.0399
dopamine 3-O-sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.4847	-0.4698	-0.4834	2.7711	-0.0650	-0.4723	-0.4804	-0.4703	-0.4806	-0.4732
homovanillate (HVA)	Amino Acid	Phenylalanine and Tyrosine Metabolism	1.9129	0.6794	-0.4865	-0.6047	0.8861	0.2130	0.1492	0.5440	0.7038	0.6006
N-acetylphenylalanine	Amino Acid	Phenylalanine and Tyrosine Metabolism	1.1848	-0.1238	-1.1216	0.9123	-1.1305	-1.1275	0.5435	0.9197	0.9398	0.8009
N-acetyltyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.1457	-0.2768	-0.2834	3.3467	-0.2703	-0.2741	-0.2673	3.9646	-0.2743	-0.2705
p-cresol sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.1029	-1.1260	-0.0836	-0.6143	0.5177	-1.5608	-0.4374	-0.4663	0.3827	0.3785
phenol sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	-1.0670	0.7745	-0.2134	-1.0387	-1.3196	-0.1005	-0.8819	1.7689	-0.2381	0.6348
phenylacetylglutamine	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.1200	1.1575	-1.0050	0.7783	1.0050	-0.5268	-0.5551	-1.4612	-0.0491	-0.3016
phenylalanine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.8606	0.5143	-0.5251	0.2797	0.8350	-2.0757	0.4662	-0.3026	-0.2732	0.1861
phenyllactate (PLA)	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.5887	-0.1135	-0.5660	0.1426	-1.4240	-0.7072	0.5260	1.0511	-1.5782	0.6862
tyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	1.1379	0.7151	-0.2135	1.2508	1.2674	-0.3970	0.4293	-1.9741	0.4469	-0.2375
4-acetamidobutanoate	Amino Acid	Polyamine Metabolism	0.8841	-1.6929	-1.6876	1.7420	0.7101	0.8907	0.3397	0.8541	1.0104	0.4707
5-methylthioadenosine (MTA)	Amino Acid	Polyamine Metabolism	1.7903	0.7034	-0.6168	1.5247	1.0725	0.0050	0.0341	0.4497	1.3329	0.1667

Supplemental Table 2. Z-scores for Population Baseline

Biochemical	Super Pathway	Sub Pathway	CSF318	CSF319	CSF320	CSF322	CSF323	CSF325	CSF327	CSF328	CSF329	CSF305
acisoga	Amino Acid	Polyamine Metabolism	-0.6550	-1.1448	0.2187	-0.4367	0.3123	-0.8562	1.2281	0.0993	-0.1230	0.6031
N-acetylputrescine	Amino Acid	Polyamine Metabolism	0.9655	-0.4417	-0.9059	2.7412	1.2726	-0.3381	0.8679	0.3009	1.2978	-0.2624
spermidine	Amino Acid	Polyamine Metabolism	1.4125	-0.7148	-0.4219	-0.5792	-0.0125	-2.2955	-0.8101	-0.4734	0.7613	0.7834
3-indoxyl sulfate	Amino Acid	Tryptophan Metabolism	-0.7096	0.7399	-0.5372	3.4337	1.0507	-0.7052	-0.3421	-0.7025	-0.7123	-0.0307
5-hydroxyindoleacetate	Amino Acid	Tryptophan Metabolism	2.0390	0.4608	-0.7773	0.4360	0.9038	-0.0734	-0.0394	0.5276	0.8688	-0.1126
anthranilate	Amino Acid	Tryptophan Metabolism	-1.5222	0.1253	1.4887	1.2196	-0.0225	-0.6113	-1.6880	-1.0029	-1.6931	-0.6045
C-glycosyltryptophan	Amino Acid	Tryptophan Metabolism	0.1007	-0.7297	-0.8183	3.2001	0.3309	0.2700	-0.0071	1.4700	0.7089	0.2383
indole-3-carboxylic acid	Amino Acid	Tryptophan Metabolism	-0.5025	1.1091	-0.2856	1.1957	1.1782	1.1571	1.4145	-0.8573	1.2419	-0.7996
indoleacetate	Amino Acid	Tryptophan Metabolism	0.3389	0.7701	-0.1057	1.3057	0.8956	-1.1292	-0.0958	-0.3353	0.8210	-1.0868
indolelactate	Amino Acid	Tryptophan Metabolism	-0.3022	-0.3164	-0.3005	4.3000	-0.3051	-0.2998	-0.3210	-0.3131	-0.3065	-0.3143
indolepropionate	Amino Acid	Tryptophan Metabolism	-0.3590	-0.3739	-0.3701	-0.3538	2.9298	0.1364	2.6875	-0.3525	-0.3603	3.1103
kynurenate	Amino Acid	Tryptophan Metabolism	0.9924	0.2929	-1.3104	1.5108	1.1010	0.2774	0.5907	1.1801	-1.3065	0.5015
kynurenine	Amino Acid	Tryptophan Metabolism	0.0320	0.5453	-0.7501	2.2186	1.2021	0.3557	0.0757	0.8561	0.4065	0.1671
picolinate	Amino Acid	Tryptophan Metabolism	0.0305	-0.3639	-0.8387	0.2046	-0.8982	-0.9221	0.0012	0.7423	-0.3633	0.5483
tryptophan	Amino Acid	Tryptophan Metabolism	1.0984	1.2165	0.5397	0.5892	1.4096	-0.8032	-0.0282	-0.5586	1.6876	-0.2716
tryptophan betaine	Amino Acid	Tryptophan Metabolism	-1.1168	0.8603	-0.2690	0.1710	-1.1165	0.9971	0.9384	-1.1148	-1.1196	1.2388
arginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1.2738	0.5776	-0.1493	0.3311	1.2902	-0.4772	0.0784	-0.3551	1.3171	0.4032
argininosuccinate	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.3192	-0.9639	-0.3121	2.2508	0.3646	-0.3951	-0.2749	1.3543	0.9241	-0.2600
citrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.6933	1.1486	-0.8045	1.5316	1.2781	-0.6508	-0.4355	-1.5024	1.0847	1.1804
dimethylarginine (SDMA + ADMA)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.6717	-0.4177	-0.3759	1.0287	1.9004	-0.7483	-0.3822	0.2772	1.3262	-0.2704
homoarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.1503	0.1886	-0.0802	-2.1318	-0.1450	-1.4262	0.0365	-1.1802	-1.3912	0.1705
homocitrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.2535	-0.8593	-0.3032	2.7759	-0.4344	-1.4703	0.9356	-1.4646	0.0796	-0.5290
N-acetylarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.3148	0.2950	-0.7967	2.6629	-0.4489	0.4813	-0.4076	1.1964	-0.1289	0.5341
N-delta-acetylornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.4725	-0.4995	-0.5085	2.2065	0.6212	-1.1815	1.9082	-0.8336	0.2343	-0.3628
N-methylproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.9128	1.7131	0.7591	-0.6843	-0.9214	-0.9147	-0.3698	-0.9117	0.1903	0.0552
ornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.8353	-0.5175	-0.4454	2.2942	1.5818	-0.6959	-0.5648	0.6015	1.6930	0.1002
pro-hydroxy-pro	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.0184	0.5450	-0.6727	2.3401	1.0972	-0.7638	-0.2295	0.0049	0.8004	0.7924
proline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.5787	0.9347	-0.3133	2.6315	1.5153	-1.2222	-1.4076	0.6126	0.5318	-0.6926
trans-4-hydroxyproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1.0194	1.0792	-0.8729	2.6226	1.0477	-0.6438	-0.7917	-0.1821	1.0474	-0.1168
urea	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-1.5671	0.4985	-0.1530	-0.0331	-1.3969	-1.9617	0.4636	-0.9030	-0.7283	-0.1265
argininate*	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.75657	1.85084	-1.0339	0.82545	-0.849	0.24342	-0.2784	-0.6082	0.69936	1.30115
erythronate*	Carbohydrate	Aminosugar Metabolism	-0.4469	-0.9215	0.4044	1.5669	-0.6516	0.3478	0.6077	1.5407	-1.0547	1.7099
glucuronate	Carbohydrate	Aminosugar Metabolism	0.2164	-0.9274	-0.8930	2.8797	-0.0440	0.2430	0.4250	1.0404	0.1694	0.0627
N-acetylglucosaminylasparagine	Carbohydrate	Aminosugar Metabolism	-0.1415	-0.6317	-0.0078	1.5028	0.9196	-0.1670	-0.3934	0.9965	0.1041	-0.0822
N-acetylneuraminate	Carbohydrate	Aminosugar Metabolism	-0.0878	-0.7964	-0.6488	2.6735	-0.3199	0.4285	0.6589	2.0477	-0.1209	0.7915
sucrose	Carbohydrate	Disaccharides and Oligosaccharides	-1.5590	-0.5708	-1.2041	3.2751	0.5065	-0.3100	0.1072	-0.1025	-1.0198	0.0746
fructose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.0198	-1.7247	-0.2232	-0.5928	-0.6545	-0.8914	-0.9433	0.5524	-0.2647	0.6346
galactitol (dulcitol)	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.2619	-1.0892	-1.1366	2.3092	-0.4035	-0.2453	-1.4347	2.0516	1.4535	0.0644
galactonate	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.5235	-0.5310	-0.5228	3.1637	-0.5271	-0.5313	-0.5243	-0.5251	1.9906	-0.5245
mannitol/sorbitol	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.7455	-1.6125	-0.1764	1.6031	-0.9517	0.1907	-1.5531	1.3655	-0.6881	0.0176
mannose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.1138	-1.2411	-0.7680	-0.7057	-0.6767	-0.4453	-0.0934	0.1275	-0.6543	-0.1349
1,5-anhydroglucitol (1,5-AG)	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.5980	0.3781	-0.5721	-3.9045	0.2814	0.3289	0.2402	1.3415	-1.4462	1.1913
glucose	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.9757	-0.8422	-0.1344	-0.8889	-0.5697	0.0439	0.6518	0.4338	-0.5865	0.2114
glycerate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	1.2372	-1.1069	0.5329	0.4063	0.7457	-2.1145	0.4398	1.0092	1.5249	-0.6253
lactate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.5185	0.2162	0.7128	0.1086	-0.5318	-1.1412	-0.0399	-0.4308	-1.1835	0.4590
pyruvate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.7947	1.0372	-0.7963	0.6342	-0.7955	-0.7946	-0.7965	-0.5930	-0.7978	1.1604
arabitol/xylitol	Carbohydrate	Pentose Metabolism	-0.5268	-1.3421	-0.8278	1.9272	-0.8934	0.4122	-0.5646	1.7091	-0.7798	0.7329
arabonate/xylonate	Carbohydrate	Pentose Metabolism	-1.4509	-0.5697	-0.7909	2.0153	-2.0058	0.3231	0.1728	1.2238	-1.0020	0.6721
ribitol	Carbohydrate	Pentose Metabolism	-0.7276	-0.9320	0.3670	2.3742	-0.5808	0.7406	-2.4278	1.4306	-1.5555	0.5447
ribonate	Carbohydrate	Pentose Metabolism	-1.4333	-1.1173	-0.5633	1.3147	-1.4815	0.6881	0.6522	1.5333	-1.1425	1.1844
ribose	Carbohydrate	Pentose Metabolism	0.8441	-1.3693	-1.3651	1.1144	-0.1916	0.1843	0.7699	1.1293	0.4405	-0.0819
gulonic acid*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-0.6889	-0.3416	0.1774	2.6379	-0.0791	1.1251	0.6856	1.9299	-0.4227	0.5844
oxalate (ethanedioate)	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.5845	0.9341	-0.3549	1.8763	0.0633	-2.1116	-0.9464	-1.1340	0.5202	-0.0461
threonate	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.9139	0.7217	-0.6823	1.8059	1.0382	-0.9768	-1.3459	0.8091	1.1571	-0.5110
5-methyltetrahydrofolate (5MeTHF)	Cofactors and Vitamins	Folate Metabolism	1.5038	1.3603	-0.2726	1.4221	1.2503	-1.5558	-1.2161	-1.5537	0.6968	0.5174
bilirubin (E,E)*	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.3991	1.0775	-0.4015	3.7248	-0.4032	-0.4070	-0.4070	-0.4043	-0.4039	2.5679

Supplemental Table 2. Z-scores for Population Baseline

Biochemical	Super Pathway	Sub Pathway	CSF318	CSF319	CSF320	CSF322	CSF323	CSF325	CSF327	CSF328	CSF329	CSF305
bilirubin (Z,Z)	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.2339	-0.2450	-0.2307	5.0992	-0.2500	-0.2326	-0.2446	-0.2313	-0.2374	0.2660
heme	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.5188	-0.5203	-0.5194	-0.5220	-0.5185	-0.5197	-0.5197	-0.5217	-0.5197	-0.0034
1-methylnicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	1.5108	-0.0962	-0.7405	0.5213	0.3743	-0.4224	-0.4184	1.0621	0.8202	0.5699
N1-Methyl-2-pyridone-5-carboxamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.0818	0.2681	-0.7699	0.8938	0.3992	-1.2011	-0.5963	-0.2439	0.0446	-0.1947
nicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.4602	0.0085	-0.2481	-0.4451	-1.1801	0.8329	-1.1813	1.4085	-1.1836	-0.5088
nicotinamide riboside	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-1.2104	-0.7226	-0.4119	0.9300	-0.9449	0.9814	0.7585	0.9977	-1.1794	1.4636
quinolinate	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.4987	0.8312	-0.5049	2.4684	-0.4979	-0.5082	-0.5048	-0.4958	-0.4979	-0.2907
trigonelline (N'-methylnicotinate)	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.5011	0.3404	0.4138	-1.8612	-1.3216	-0.3395	2.2139	-1.8543	-0.3593	-0.2027
pantothenate	Cofactors and Vitamins	Pantothenate and CoA Metabolism	0.7739	-0.4989	-0.8659	2.1465	0.9958	-0.8953	-0.3099	0.1065	1.0375	-0.5109
gamma-CEHC	Cofactors and Vitamins	Tocopherol Metabolism	0.0316	1.5346	-1.0983	0.2976	-1.3080	-1.2717	0.6319	-0.5958	-0.5621	0.2561
gamma-tocopherol/beta-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	-0.3656	0.6649	-0.3690	4.6880	-0.3644	-0.3585	-0.3650	0.1808	-0.1653	1.3530
retinol (Vitamin A)	Cofactors and Vitamins	Vitamin A Metabolism	0.3613	-0.3865	-0.7999	3.6678	-0.4520	-0.8122	0.6289	0.2669	0.3429	0.8974
pyridoxal	Cofactors and Vitamins	Vitamin B6 Metabolism	3.8195	-0.0231	-0.3522	1.9243	0.4161	-0.2288	-1.1337	-2.0086	0.1646	-0.0361
pyridoxate	Cofactors and Vitamins	Vitamin B6 Metabolism	3.5474	-0.1507	-0.8120	2.5146	0.1903	-0.2620	-0.1332	0.4415	0.0417	0.0439
pyridoxine (Vitamin B6)	Cofactors and Vitamins	Vitamin B6 Metabolism	5.2945	-0.1800	-0.1704	-0.1799	-0.1909	-0.1887	-0.1725	-0.1779	-0.1914	-0.1748
phosphate	Energy	Oxidative Phosphorylation	-1.1128	-0.0005	-0.5932	0.3892	0.1045	2.3025	-0.3974	-0.8101	0.7252	0.1475
2-methylcitrate	Energy	TCA Cycle	0.2324	-0.7937	-1.1941	2.3405	-0.2644	-0.5051	0.0382	1.3697	0.4788	0.2405
aconitate [cis or trans]	Energy	TCA Cycle	2.1422	-0.4779	0.5977	-2.0522	-0.3799	-1.3516	0.8624	1.7009	1.1382	-0.4871
alpha-ketoglutarate	Energy	TCA Cycle	-0.1992	1.0711	-0.7336	-0.1147	-1.1014	-0.8409	0.8441	0.6771	-0.1218	0.7827
citrate	Energy	TCA Cycle	-0.1528	-0.3018	0.1564	-0.0304	-0.2793	-1.4950	-0.1172	0.1781	-0.0225	0.5008
fumarate	Energy	TCA Cycle	2.7527	0.3592	-0.3310	-0.9678	0.9911	-0.9780	0.5373	1.1363	1.1913	0.7215
isocitrate	Energy	TCA Cycle	0.3154	1.3468	0.2942	-0.2667	-1.2016	-0.1510	-0.3186	-0.2647	-0.3487	0.2200
malate	Energy	TCA Cycle	2.8245	0.5873	-0.2986	0.0394	1.3159	-0.6635	0.0070	1.5088	1.3501	0.4966
succinate	Energy	TCA Cycle	2.8106	-0.2279	-0.3814	-0.1887	1.2415	-0.5330	0.7440	1.4476	1.4892	0.1847
succinylcarnitine	Energy	TCA Cycle	-0.9714	-0.1242	-2.4478	0.7146	-0.6964	1.0424	-1.0618	1.0793	0.1694	1.4066
carnitine	Lipid	Carnitine Metabolism	0.5036	0.7109	-0.6824	0.9107	0.4696	-0.8094	-1.7278	0.2696	0.2286	0.6443
deoxycarnitine	Lipid	Carnitine Metabolism	0.3427	0.2513	-0.3936	1.8274	0.2065	-1.3009	-1.0682	0.7158	0.4467	0.8903
butyrylcarnitine	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.2159	0.1435	0.0170	1.5549	0.5958	-0.3406	-0.4979	1.1670	0.3090	0.2311
methylmalonate (MMA)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.4162	0.3865	-0.7541	3.0164	-1.0209	0.0301	-0.4173	-0.3729	0.7044	0.3205
propionylcarnitine	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.7005	0.6316	-0.8862	2.4434	0.2599	-1.1762	-0.9500	0.3999	0.0922	0.4099
3-hydroxybutyrylcarnitine (1)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.5805	0.0952	-0.5938	-0.5812	-0.5941	-0.5920	-0.5887	2.1915	-0.5852	-0.5827
acetylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.1747	0.5941	-0.9313	1.3411	0.5586	-0.7920	-1.5429	0.5054	0.4591	0.3630
cis-4-decenoyl carnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.3470	1.0148	-1.1009	0.8083	0.9104	-2.3649	0.0527	1.0701	0.2862	-0.6123
decanoylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.8578	0.4013	-0.8404	1.3811	0.6431	-1.3883	-0.7052	1.2638	0.1541	0.9020
hexanoylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.9154	1.1677	-0.9235	1.4241	1.1692	-0.9268	-0.9274	0.6046	-0.0109	0.7635
laurylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.0216	-0.4685	-0.4605	1.4209	0.9492	-0.4807	-0.4602	-0.4628	-0.4594	-0.4727
octanoylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.9004	0.7857	-0.9421	1.2648	0.8177	-0.3094	-1.7205	1.2054	0.4203	0.5167
malonate	Lipid	Fatty Acid Synthesis	0.3664	0.5129	-0.0973	-0.1866	0.4755	-0.6796	0.0900	-3.7366	0.8815	0.7622
malonylcarnitine	Lipid	Fatty Acid Synthesis	-0.0233	0.2042	-1.3375	2.4091	-0.2767	0.3611	-0.6076	1.8742	0.8955	0.2965
oleamide	Lipid	Fatty Acid, Amide	-1.1382	0.7910	0.4721	-1.2370	-0.9080	0.9460	-1.1338	-1.1592	-1.6696	1.0505
palmitic amide	Lipid	Fatty Acid, Amide	-1.1693	0.9302	0.5264	-1.0779	-1.1644	1.0866	-1.1164	-1.0959	-1.2261	1.1626
2-aminoheptanoate	Lipid	Fatty Acid, Amino	-0.2505	0.8698	0.0485	0.2277	-0.6343	0.5234	-0.6374	2.6023	0.0125	0.5413
2-aminooctanoate	Lipid	Fatty Acid, Amino	-1.1234	0.3763	0.2857	0.8882	-1.0590	-1.1266	0.0715	2.4076	0.7610	0.4189
2-hydroxyadipate	Lipid	Fatty Acid, Dicarboxylate	0.6476	1.2659	0.1199	-1.8645	0.1432	-0.0319	0.0681	0.5123	-0.5697	0.1250
3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)	Lipid	Fatty Acid, Dicarboxylate	-0.1574	-0.2071	-0.1677	5.2936	-0.1593	-0.1954	-0.1827	-0.2032	-0.1605	-0.2108
dimethylmalonic acid	Lipid	Fatty Acid, Dicarboxylate	-0.1681	-0.3940	-0.7036	-0.4795	0.0784	-0.8288	0.5132	1.5133	1.0013	0.1962
maleate	Lipid	Fatty Acid, Dicarboxylate	-0.4706	0.4725	1.1050	0.7137	0.0921	-1.1894	0.1741	2.5999	0.1821	0.1381
2-hydroxydecanoate	Lipid	Fatty Acid, Monohydroxy	-0.4557	-0.4376	-0.4522	4.0852	-0.4573	0.2950	-0.4516	1.7682	-0.4562	-0.4507
3-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	-0.188	-0.125	-0.5356	0.31167	-0.7296	-0.2886	-0.5971	3.51815	0.64825	-0.252
3-hydroxyoctanoate	Lipid	Fatty Acid, Monohydroxy	0.9058	0.3089	0.8186	0.8796	-0.2884	-0.2458	-0.8658	3.6283	0.4631	-0.1439
3-hydroxysebacate	Lipid	Fatty Acid, Monohydroxy	-0.5179	-0.5166	0.0436	0.0746	-0.4841	0.0787	-0.4483	5.1507	-0.0874	-0.4618
5-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	-0.7454	-0.7443	-0.7466	1.5953	-0.7520	0.0450	-0.7408	2.1802	-0.0062	0.3911
glycerol	Lipid	Glycerolipid Metabolism	-0.5772	-0.3194	-0.3878	1.0320	-0.4714	-0.4702	-0.0037	-0.0196	-0.7087	0.1367
glycerol 3-phosphate	Lipid	Glycerolipid Metabolism	1.2639	0.3852	1.3561	-2.4085	0.4390	0.8900	0.5030	-0.0616	-0.7691	-0.2122
galactosylglycerol*	Lipid	Glycerolipid Metabolism	0.12641	-0.822	-1.5038	2.77	0.4073	-0.3654	-0.4309	1.3924	0.29758	0.76638
myo-inositol	Lipid	Inositol Metabolism	1.0188	-0.3142	-0.3577	3.7450	0.5206	-0.6426	-0.0183	1.2021	0.8700	-0.5712

Supplemental Table 2. Z-scores for Population Baseline

Biochemical	Super Pathway	Sub Pathway	CSF318	CSF319	CSF320	CSF322	CSF323	CSF325	CSF327	CSF328	CSF329	CSF305
3-hydroxybutyrate (BHBA)	Lipid	Ketone Bodies	-0.5448	0.1016	0.1526	-0.5652	-0.3799	-0.1455	-0.5631	2.1508	1.0951	0.1920
acetoacetate	Lipid	Ketone Bodies	-0.2170	0.1150	-0.2992	-0.3683	-0.5669	-0.5365	-0.7407	2.3063	0.9364	-0.1480
1-adrenoyl-GPC (22:4)*	Lipid	Lysolipid	0.6621	-0.2944	0.6715	1.9146	-1.2241	-0.0374	-1.4727	-0.8150	0.7541	-0.6255
1-arachidonoyl-GPC (20:4)*	Lipid	Lysolipid	-0.2859	0.2545	-0.6415	2.9294	0.3941	-0.0258	0.5119	1.3384	0.1770	-1.4979
1-arachidonoyl-GPE (20:4)*	Lipid	Lysolipid	-1.1735	-0.3204	-1.1717	1.6256	0.1269	0.0547	-1.1716	1.7934	-0.0568	1.2792
1-dihomo-linolenoyl-GPC (20:3n3 or 6)*	Lipid	Lysolipid	-0.2267	-0.2246	-0.2246	5.2291	0.0785	-0.2262	-0.2336	0.2559	-0.2254	-0.2270
1-dihomo-linoleoyl-GPC (20:2)*	Lipid	Lysolipid	0.5695	0.5446	-0.3933	1.8328	1.5801	0.5187	-1.0285	-0.0685	-1.2186	0.8123
1-docosahexaenoyl-GPC (22:6)*	Lipid	Lysolipid	-0.2920	-0.2788	-0.2831	4.6904	-0.2964	-0.2924	-0.3015	1.5022	-0.2978	-0.2876
1-docosahexaenoyl-GPE (22:6)*	Lipid	Lysolipid	-1.1926	-0.4259	0.4562	0.3873	-1.1846	0.9306	1.2945	1.2306	-1.0202	1.1723
1-docosapentaenoyl-GPC (22:5n3)*	Lipid	Lysolipid	-0.2632	0.7596	1.1128	1.5604	0.7268	0.8451	1.1208	0.3262	-1.4455	0.6913
1-docosapentaenoyl-GPC (22:5n6)*	Lipid	Lysolipid	-1.6287	-1.3562	0.1005	1.5978	0.0762	1.1500	-1.2135	1.2141	-1.6836	1.0026
1-linoleoyl-GPC (18:2)	Lipid	Lysolipid	-0.8188	-0.0175	-1.4968	3.3715	0.6454	-0.4090	0.1925	1.3447	0.5456	0.3752
1-myristoyl-GPC (14:0)	Lipid	Lysolipid	-0.2281	-0.2429	-0.2441	5.1397	-0.2208	-0.2225	-0.2223	1.0593	-0.2225	-0.2410
1-oleoyl-GPA (18:1)	Lipid	Lysolipid	0.1655	0.3362	1.1335	2.0370	-0.5288	1.2159	-0.8768	-0.9427	-0.3234	-0.4079
1-oleoyl-GPC (18:1)	Lipid	Lysolipid	-0.5236	-0.3306	-0.7177	3.0708	-0.0060	0.0646	0.7386	1.3321	-0.5503	0.9643
1-palmitoleoyl-GPC (16:1)*	Lipid	Lysolipid	-0.2110	-0.2131	-0.2232	5.2009	-0.2087	-0.2168	-0.2113	-0.2212	-0.2036	-0.2263
1-palmitoyl-GPA (16:0)	Lipid	Lysolipid	-0.4927	-0.4863	-0.4923	3.9570	-0.4716	-0.4691	1.4190	0.9873	-0.4894	0.2575
1-palmitoyl-GPC (16:0)	Lipid	Lysolipid	-0.4000	-0.3340	-0.9727	3.4891	-0.0170	0.1006	0.3414	1.3087	-0.3285	0.8243
1-pentadecanoyl-GPC (15:0)*	Lipid	Lysolipid	0.6859	0.7297	0.8673	1.5333	-1.3429	-1.3937	-0.5426	-0.8873	-0.3344	1.0320
1-stearoyl-GPC (18:0)	Lipid	Lysolipid	-0.6621	-0.2416	-0.7794	3.8047	0.4047	-0.1369	0.3383	1.2472	-0.0350	0.8038
1-stearoyl-GPE (18:0)	Lipid	Lysolipid	-0.6370	-0.6153	-0.6403	2.3901	-0.6233	1.1815	1.0396	2.1315	-0.6284	1.5350
1-palmityl-GPC (O-16:0)	Lipid	Lyso-phospho-ether	0.8852	0.3227	0.3634	1.5152	0.6046	-1.2944	-0.2260	-0.7656	0.5732	1.4432
1-(1-enyl-palmitoyl)-GPC (P-16:0)*	Lipid	Lysoplasmalogen	-0.8503	-0.9395	-1.5978	1.5927	-0.3861	-0.1365	0.5523	-0.2860	0.9948	0.2863
1-(1-enyl-stearoyl)-GPE (P-18:0)*	Lipid	Lysoplasmalogen	-0.6823	-0.0003	-0.8769	1.5899	-0.9868	-0.3552	1.7035	-0.7360	-1.8009	-1.5314
3-hydroxy-3-methylglutarate	Lipid	Mevalonate Metabolism	1.7890	0.3353	-0.8665	1.1685	1.1980	-0.2650	0.1179	2.0010	0.6798	0.4169
1-arachidonylglycerol (20:4)	Lipid	Monoacylglycerol	-1.5093	-0.4099	-0.5356	1.6692	-0.2475	-1.7024	1.3477	0.1448	-0.6023	-0.0700
1-dihomo-linolenylglycerol (20:3)	Lipid	Monoacylglycerol	-1.2345	-0.2388	1.0113	1.7322	0.8026	-1.1373	1.6556	0.9045	-0.5684	1.5684
1-oleoylglycerol (18:1)	Lipid	Monoacylglycerol	-0.3883	0.5104	0.4778	1.7148	-0.8322	-0.3468	0.0714	0.6403	-1.0600	0.3708
1-palmitoylglycerol (16:0)	Lipid	Monoacylglycerol	-0.8075	-0.8873	-0.3496	0.7849	-0.3494	-1.3140	0.2730	-0.1476	-1.8947	0.5680
1,2-dilinoleoyl-GPC (18:2/18:2)	Lipid	Phospholipid Metabolism	-0.1721	-0.1754	-0.1733	5.2945	-0.1835	-0.1911	-0.1955	-0.1874	-0.1872	-0.1869
1,2-dimyristoyl-GPC (14:0/14:0)	Lipid	Phospholipid Metabolism	-0.5321	1.2490	-0.6857	1.7536	1.5167	-1.7738	0.6285	-1.4320	0.8039	-0.3933
1,2-dioleoyl-GPC (18:1/18:1)*	Lipid	Phospholipid Metabolism	-1.0065	-0.3909	-0.4949	2.8819	-0.3510	-0.2914	0.6608	0.6319	-0.6247	1.0284
1,2-dipalmitoyl-GPC (16:0/16:0)	Lipid	Phospholipid Metabolism	-0.7502	-0.6499	-0.8892	2.8598	-0.2205	-0.0232	0.4126	1.5756	-0.8094	1.0615
1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4)*	Lipid	Phospholipid Metabolism	0.1815	1.0442	-1.1751	1.5865	-0.7124	0.6785	1.3432	0.6778	0.8493	1.1637
1-margaroyl-2-linoleoyl-GPC (17:0/18:2)*	Lipid	Phospholipid Metabolism	-0.6859	-1.1030	0.7413	1.7167	1.4828	-0.7471	-0.4966	-0.2595	0.5863	-1.7498
1-margaroyl-2-oleoyl-GPC (17:0/18:1)*	Lipid	Phospholipid Metabolism	-0.2958	-0.2803	-0.2977	4.0878	-0.2930	-0.3022	-0.2866	-0.2959	-0.2748	-0.2722
1-myristoyl-2-linoleoyl-GPC (14:0/18:2)*	Lipid	Phospholipid Metabolism	1.6833	1.3574	1.2820	1.7037	-0.7493	0.9823	-1.1813	-0.7532	0.4522	0.5447
1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	Lipid	Phospholipid Metabolism	-0.0321	-0.7030	-0.9702	3.3335	0.5391	-0.2838	0.1839	1.3579	0.3209	0.6441
1-oleoyl-2-dihomo-linolenoyl-GPC (18:1/20:3)*	Lipid	Phospholipid Metabolism	-0.2026	-0.2046	-0.2113	5.2711	-0.1952	-0.1908	-0.1924	-0.1853	-0.2034	-0.1969
1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)*	Lipid	Phospholipid Metabolism	-0.5368	-0.5252	1.4615	1.6319	-0.5689	-1.5422	1.3398	-1.0354	-1.2695	1.3680
1-oleoyl-2-linoleoyl-GPC (18:1/18:2)*	Lipid	Phospholipid Metabolism	-0.9117	0.0437	-0.9155	3.6762	0.7222	-0.9065	-0.0150	1.0747	0.6093	0.3152
1-palmitoleoyl-2-linoleoyl-GPC (16:1/18:2)*	Lipid	Phospholipid Metabolism	1.5764	0.2855	-1.7200	1.6090	-0.0953	0.1299	0.6895	-1.8239	0.2881	-0.6233
1-palmitoyl-2-adrenoyl-GPC (16:0/22:4)*	Lipid	Phospholipid Metabolism	-0.5593	-0.5568	-0.5592	3.9017	-0.5446	-0.5501	0.8162	0.9434	-0.5498	1.6971
1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4)	Lipid	Phospholipid Metabolism	-0.7113	-0.4617	-1.0574	3.4278	-0.1158	-0.2707	0.5130	0.9725	-0.2971	1.0391
1-palmitoyl-2-dihomo-linolenoyl-GPC (16:0/20:3n3 or 6)*	Lipid	Phospholipid Metabolism	-0.3393	0.0904	-1.1839	3.4283	0.4416	-1.1878	0.2517	1.0190	0.0871	0.8789
1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)	Lipid	Phospholipid Metabolism	-0.8365	-0.6582	-1.3741	2.9769	-0.0593	-0.3267	0.4992	0.5373	-0.5701	0.8833
1-palmitoyl-2-eicosapentaenoyl-GPC (16:0/20:5)*	Lipid	Phospholipid Metabolism	-1.5852	0.8914	0.0358	1.6883	-0.3637	-0.5516	-0.4772	0.3432	-0.2186	-0.6102
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	Lipid	Phospholipid Metabolism	-0.6953	-0.1617	-1.2136	3.5460	0.2099	-0.9542	0.0776	1.1903	0.1436	0.6240
1-palmitoyl-2-meadoyl-GPC (16:0/20:3n9)*	Lipid	Phospholipid Metabolism	0.9871	1.5561	-0.8800	1.5837	-1.0557	-1.1997	-0.6919	0.4968	1.5822	-0.1612
1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	Lipid	Phospholipid Metabolism	-0.9440	-0.5312	-0.7366	2.6087	-0.4580	0.0300	0.6290	1.1365	-0.9772	1.2668
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*	Lipid	Phospholipid Metabolism	-0.4709	-0.4326	-0.9631	3.8168	0.3240	-0.7768	0.2724	1.2529	-0.1284	0.5178
1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	Lipid	Phospholipid Metabolism	-0.2724	-0.2710	-0.2505	4.1875	-0.2537	-0.2618	-0.2555	3.0936	-0.2520	-0.2632
1-palmityl-2-arachidonoyl-GPC (O-16:0/20:4)*	Lipid	Phospholipid Metabolism	-0.3895	-0.3962	-0.3965	4.4911	-0.3886	-0.3973	-0.3906	1.2531	-0.3893	-0.4025
1-palmityl-2-oleoyl-GPC (O-16:0/18:1)*	Lipid	Phospholipid Metabolism	-1.1111	-0.9188	-1.1236	2.8913	0.2243	-1.1246	0.2940	0.9854	-0.4290	1.1469
1-pentadecanoyl-2-oleoyl-GPC (15:0/18:1)*	Lipid	Phospholipid Metabolism	-0.2233	-0.2238	-0.2251	5.1246	-0.2177	-0.2242	-0.2128	-0.2213	-0.2272	-0.2118
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	Lipid	Phospholipid Metabolism	-0.5786	-0.2850	-0.9292	3.1652	-0.0105	-0.3142	0.4402	1.1937	-0.4565	1.0630

Supplemental Table 2. Z-scores for Population Baseline

Biochemical	Super Pathway	Sub Pathway	CSF318	CSF319	CSF320	CSF322	CSF323	CSF325	CSF327	CSF328	CSF329	CSF305
1-stearoyl-2-dihomo-linolenoyl-GPC (18:0/20:3n3 or 6)*	Lipid	Phospholipid Metabolism	-0.6695	-0.7402	-0.7424	3.8335	0.9183	-0.7416	0.2085	1.1381	0.1025	0.6324
1-stearoyl-2-docosahexaenoyl-GPC (18:0/22:6)	Lipid	Phospholipid Metabolism	-1.5148	-0.4969	-0.8509	2.7010	0.3203	-0.2601	0.6224	1.0014	-0.4658	0.9401
1-stearoyl-2-docosahexaenoyl-GPE (18:0/22:6)*	Lipid	Phospholipid Metabolism	-0.9114	-0.6462	-0.9047	-0.2956	-0.8955	-0.5389	1.1499	1.8354	-0.9028	1.1711
1-stearoyl-2-docosapentaenoyl-GPC (18:0/22:5n3)*	Lipid	Phospholipid Metabolism	-0.2668	0.7306	0.3984	2.1157	0.1875	-1.6123	1.0457	-0.8339	-0.1797	-1.0759
1-stearoyl-2-docosapentaenoyl-GPC (18:0/22:5n6)*	Lipid	Phospholipid Metabolism	-0.7935	-1.5153	-0.0848	1.4969	0.7130	1.2514	1.4878	-1.1488	-0.6651	0.1152
1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*	Lipid	Phospholipid Metabolism	-0.6270	-0.3043	-1.1573	3.4748	0.6418	-0.8207	0.0383	1.0849	0.2468	0.6551
1-stearoyl-2-meadoyl-GPC (18:0/20:3n9)*	Lipid	Phospholipid Metabolism	-0.4931	-1.4454	-0.6110	1.6411	1.0925	1.1050	-1.4072	0.0170	-0.0666	0.8937
1-stearoyl-2-oleoyl-GPC (18:0/18:1)	Lipid	Phospholipid Metabolism	-0.4510	-0.6193	-0.6972	2.4447	-0.0244	-0.2939	0.5630	1.1523	-2.1604	1.1121
choline	Lipid	Phospholipid Metabolism	0.9494	-0.0356	-0.7583	1.3370	-0.0381	0.4991	-0.2715	0.6081	-0.5574	1.0990
choline phosphate	Lipid	Phospholipid Metabolism	1.4498	0.0669	1.7193	-0.9916	0.9374	0.9009	0.6294	0.4839	1.1297	0.0881
glycerophosphoethanolamine	Lipid	Phospholipid Metabolism	1.3255	3.2066	-0.4229	2.0372	1.2600	-0.6337	0.7541	1.1584	1.0973	-0.0577
glycerophosphoinositol*	Lipid	Phospholipid Metabolism	-1.8882	-1.2400	0.2448	1.3344	0.2395	0.3728	1.0127	1.3400	-1.3199	-0.1004
glycerophosphorylcholine (GPC)	Lipid	Phospholipid Metabolism	1.1545	0.0464	-0.0510	2.0344	0.3658	0.4248	0.7782	0.6827	-0.1635	0.7836
phosphoethanolamine	Lipid	Phospholipid Metabolism	0.8679	-0.3740	1.4952	-1.4475	0.3325	0.3175	0.7816	0.6789	0.1045	-0.3602
trimethylamine N-oxide	Lipid	Phospholipid Metabolism	-0.4752	0.4186	-1.5320	1.7980	-0.3011	-1.1434	-0.1408	0.4444	-0.3515	1.7454
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*	Lipid	Plasmalogen	-0.4337	-0.4338	-0.4391	4.5438	-0.0818	-0.4377	-0.3706	1.4648	-0.4379	0.0248
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	Lipid	Plasmalogen	-0.4066	-0.3944	-0.4075	4.0581	-0.4043	-0.4187	-0.4187	1.9270	-0.4070	1.0117
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPC (P-16:0/22:6	Lipid	Plasmalogen	-1.6396	1.0352	-1.3075	1.5994	-0.3355	-0.5726	-1.8042	1.3753	0.9744	0.9723
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPE (P-16:0/22:6	Lipid	Plasmalogen	-0.8211	-0.8248	-0.8100	2.0374	-0.8201	-0.8190	1.1668	1.6385	-0.8204	1.4494
1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	Lipid	Plasmalogen	0.7485	0.5777	-1.4921	1.5873	0.9477	0.8235	1.3287	-1.2771	0.8504	0.1986
1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	Lipid	Plasmalogen	-0.8520	-0.8481	-0.8559	3.2107	-0.8335	-0.8572	-0.0048	0.8101	-0.8589	1.1856
1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*	Lipid	Plasmalogen	-1.5707	-0.9803	-1.0426	1.6042	0.5961	-0.4766	-1.6245	1.4907	-0.6680	-0.0331
1-(1-enyl-stearoyl)-2-arachidonoyl-GPC (P-18:0/20:4)	Lipid	Plasmalogen	0.3794	0.5475	0.7414	1.7363	-1.7696	1.1710	-1.7657	-1.5070	1.0208	1.5413
1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	Lipid	Plasmalogen	-0.8585	-0.8390	-0.8595	1.8203	-0.8525	-0.8389	0.8615	1.3276	-0.8558	1.6269
1-(1-enyl-stearoyl)-2-docosahexaenoyl-GPE (P-18:0/22:6)	Lipid	Plasmalogen	-1.4215	-0.0932	-0.7051	0.3495	-0.8152	0.3472	0.9703	1.0486	-1.1635	1.3970
1-(1-enyl-palmitoyl)-2-dihomo-linolenoyl-GPC (P-18:0/20	Lipid	Plasmalogen	0.0638	1.7715	-1.0973	1.8576	-1.0953	0.1996	0.8063	-1.2161	1.6761	1.2883
dihomo-linoleate (20:2n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-0.9223	0.3615	-0.9366	2.4671	-0.9286	0.2111	-0.9313	-0.9228	0.1926	0.7196
dihomo-linolenate (20:3n3 or n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	1.0442	0.4438	-0.8476	3.9478	-0.8480	-0.7498	0.8830	0.3595	-0.8369	0.1296
glycochenodeoxycholate	Lipid	Primary Bile Acid Metabolism	-0.0709	-0.2120	-0.0466	5.2700	-0.0893	-0.0782	-0.1377	-0.2377	-0.3559	-0.1808
glycocholate	Lipid	Primary Bile Acid Metabolism	-0.1911	-0.1898	-0.1934	5.2945	-0.1760	-0.1724	-0.1692	-0.1833	-0.1741	-0.1874
glycocholenate sulfate*	Lipid	Secondary Bile Acid Metabolism	-0.1874	-0.1854	-0.1787	5.2946	-0.1763	-0.1743	-0.1882	-0.1878	-0.1812	-0.1830
glycohyocholate	Lipid	Secondary Bile Acid Metabolism	-0.1669	-0.1490	-0.2168	5.2934	-0.1879	-0.1852	-0.1719	-0.1654	-0.2064	-0.1589
hyocholate	Lipid	Secondary Bile Acid Metabolism	-0.0711	-1.5882	-0.0715	2.3844	-0.1116	-0.8294	-0.1755	-0.4463	0.6963	-0.2660
behenoyl sphingomyelin (d18:1/22:0)*	Lipid	Sphingolipid Metabolism	-0.3938	-0.3963	-0.3855	4.5855	-0.3986	-0.3957	-0.3917	0.8424	-0.3941	-0.3979
palmitoyl sphingomyelin (d18:1/16:0)	Lipid	Sphingolipid Metabolism	-0.7423	-0.7543	-1.2357	3.3903	-0.0828	-0.4574	0.1411	1.1856	-0.5462	0.7530
sphingomyelin (d18:1/14:0, d16:1/16:0)*	Lipid	Sphingolipid Metabolism	-0.9424	-0.9436	-0.9369	3.0599	0.4327	-0.9306	-0.0707	1.0159	0.5875	0.7756
sphingomyelin (d18:1/18:1, d18:2/18:0)	Lipid	Sphingolipid Metabolism	-0.5928	-0.6564	-1.1245	2.6859	-0.0285	-0.1455	0.5219	0.9311	-1.2311	0.9843
sphingomyelin (d18:1/20:0, d16:1/22:0)*	Lipid	Sphingolipid Metabolism	-1.0327	-1.0247	-1.0292	3.0731	0.1616	0.0813	0.2833	0.3286	-1.0231	1.3539
sphingomyelin (d18:1/24:1, d18:2/24:0)*	Lipid	Sphingolipid Metabolism	0.1313	-1.0651	-1.0676	2.9490	0.1988	-1.0630	-0.5497	0.9334	-0.4881	0.7713
sphingomyelin (d18:2/16:0, d18:1/16:1)*	Lipid	Sphingolipid Metabolism	-0.9775	-0.9803	-0.9854	3.4418	-0.1821	-0.7974	0.0228	1.0965	-0.5170	0.6858
sphingosine	Lipid	Sphingolipid Metabolism	-1.0123	-1.0121	1.7119	-0.9997	0.5174	-0.9971	0.3215	-0.0517	-1.0044	1.0237
stearoyl sphingomyelin (d18:1/18:0)	Lipid	Sphingolipid Metabolism	-1.0443	-0.6098	-0.4311	1.7347	-0.5832	0.4705	0.8610	0.9552	-1.0273	1.2863
16a-hydroxy DHEA 3-sulfate	Lipid	Steroid	-0.2290	-0.2305	-0.2335	5.0793	-0.2319	-0.2282	-0.2251	1.3184	-0.2290	-0.2236
4-androsten-3beta,17beta-diol disulfate (1)	Lipid	Steroid	-0.4100	-0.4095	-0.4081	4.3922	-0.4078	-0.4139	-0.4065	-0.4102	-0.4090	-0.4102
4-androsten-3beta,17beta-diol disulfate (2)	Lipid	Steroid	-0.1830	-0.1795	-0.1788	5.2946	-0.1818	-0.1789	-0.1806	-0.1840	-0.1798	-0.1805
5alpha-pregnan-3beta,20alpha-diol disulfate	Lipid	Steroid	1.3677	-0.7485	-0.2561	1.7621	0.1669	0.4991	0.2195	-1.0131	1.0910	-0.4344
andro steroid monosulfate (1)*	Lipid	Steroid	-1.3605	0.3153	1.2529	1.3853	-0.1526	1.0430	1.3677	-0.6437	-1.0865	0.5090
cortisol	Lipid	Steroid	0.4532	-0.6494	-0.6450	-0.6546	-0.6526	-0.6447	-0.6420	0.7985	-0.4939	-0.6529
cortisone	Lipid	Steroid	1.4536	-0.0713	-0.2854	1.1714	1.0490	-0.5256	-0.5291	0.8316	0.9325	-0.2078
dehydroisoandrosterone sulfate (DHEA-S)	Lipid	Steroid	-0.2736	-0.2894	-0.1827	5.2855	-0.2083	-0.1853	-0.1608	-0.2126	-0.2889	-0.2460
7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)	Lipid	Sterol	-1.5169	0.9333	-0.2640	3.0785	0.4095	-0.7701	0.0094	-0.4668	-1.9026	1.5134
cholesterol	Lipid	Sterol	-0.7945	-0.5585	-0.6499	2.9480	-0.5310	-0.1849	0.1753	1.2048	-0.9679	0.7343
2'-deoxyinosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.1149	1.7658	0.5176	1.8482	-1.0424	0.9993	-1.0433	0.1271	-0.7690	-0.3032
allantoin	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-1.7623	0.8969	-0.8366	1.0735	-0.6659	-1.0912	0.3292	0.7002	-0.0365	0.0752
hypoxanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.0208	0.0377	0.5747	-0.8512	0.5779	1.0296	1.0597	0.8961	-0.0685	1.8294
inosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.7476	-0.3388	0.0974	0.3836	-0.4886	0.4034	-0.3868	-0.3051	-0.4199	0.5938

Supplemental Table 2. Z-scores for Population Baseline

Biochemical	Super Pathway	Sub Pathway	CSF318	CSF319	CSF320	CSF322	CSF323	CSF325	CSF327	CSF328	CSF329	CSF305
urate	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-1.3960	0.1895	-1.5925	0.0772	0.0430	-1.4526	-0.9279	-0.8846	-0.2566	0.5376
xanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.7827	0.7321	-0.0208	-0.0184	0.2178	0.7088	0.1503	1.4211	0.5415	1.1381
xanthosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	1.7130	-0.1935	0.1711	0.4281	0.4476	-1.4401	0.6055	1.0261	0.6326	1.3306
N1-methylinosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.76889	0.16751	-0.4687	0.8909	0.62722	0.0589	-0.0625	0.82743	0.23632	0.84696
adenine	Nucleotide	Purine Metabolism, Adenine containing	2.3986	0.4579	0.4549	-0.2680	0.4843	0.8421	0.5257	-0.2584	0.2930	0.2540
adenosine	Nucleotide	Purine Metabolism, Adenine containing	0.1649	0.2451	-0.1036	0.2839	0.4167	-0.3648	0.3061	0.5246	0.5184	-0.2705
adenosine 3',5'-cyclic monophosphate (cAMP)	Nucleotide	Purine Metabolism, Adenine containing	0.3198	1.6904	-1.5077	0.1670	-0.2832	-0.3494	0.3595	-2.2616	-0.3115	0.5002
adenosine 5'-monophosphate (AMP)	Nucleotide	Purine Metabolism, Adenine containing	-0.1716	1.3140	-1.5151	1.8097	-0.6792	-1.6434	1.1701	-1.4976	-0.5569	-0.2264
N1-methyladenosine	Nucleotide	Purine Metabolism, Adenine containing	1.3547	-0.0571	-0.1952	1.6234	0.7402	-0.5027	-0.1551	0.8634	1.5291	0.4115
N6-carbamoylthreonyladenosine	Nucleotide	Purine Metabolism, Adenine containing	0.0291	-0.4513	-0.5997	0.9622	-0.3064	0.4143	0.4482	0.8851	0.0487	0.8245
N6-methyladenosine	Nucleotide	Purine Metabolism, Adenine containing	1.5538	-0.4719	-0.2198	0.3260	0.5748	0.1140	-0.1748	0.1853	-0.1185	-0.1312
N6-succinyladenosine	Nucleotide	Purine Metabolism, Adenine containing	-1.0234	-0.4191	0.5940	-0.7827	-1.2119	0.8109	0.0052	1.6873	-1.9138	1.3683
7-methylguanine	Nucleotide	Purine Metabolism, Guanine containing	1.0233	0.1264	-0.4962	2.3343	1.0022	-0.4241	-1.0978	0.9097	0.7542	0.3045
guanosine	Nucleotide	Purine Metabolism, Guanine containing	0.2083	0.3526	-1.0872	1.4891	0.5616	-0.0836	-0.4003	1.5036	-0.9688	0.7261
N2,N2-dimethylguanosine	Nucleotide	Purine Metabolism, Guanine containing	0.3530	0.1944	-0.5627	1.5254	0.5461	-0.0197	-0.3780	0.6906	0.4187	1.1826
N2-methylguanosine	Nucleotide	Purine Metabolism, Guanine containing	0.7133	0.5464	-1.9481	1.0715	0.2707	0.1829	-0.1837	0.6658	0.3679	0.9091
2'-deoxycytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	1.1618	0.6562	-0.3066	2.6588	0.8849	-0.9862	-0.7573	0.4067	0.8847	0.2501
cytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	2.2932	-0.3987	-0.1669	0.7184	0.2897	-1.2869	0.2268	1.6340	0.3827	0.1944
orotate	Nucleotide	Pyrimidine Metabolism, Orotate containing	2.7844	0.2732	0.1242	0.1029	-0.2192	0.2814	-0.0301	1.2927	0.5783	-0.0763
orotidine	Nucleotide	Pyrimidine Metabolism, Orotate containing	1.6787	-0.9163	-1.1154	1.9606	0.5453	0.3883	0.1769	1.1264	0.7118	0.3720
3-aminoisobutyrate	Nucleotide	Pyrimidine Metabolism, Thymine containing	1.7224	-0.3847	-1.0407	-1.0400	0.2757	-0.4844	-1.0360	1.9589	0.6688	0.5037
5,6-dihydrothymine	Nucleotide	Pyrimidine Metabolism, Thymine containing	0.0529	0.2558	-1.2310	-0.7295	1.5317	-0.2114	0.0938	-0.1628	-0.4589	0.1680
2'-deoxyuridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	1.0780	-1.1170	0.8825	2.1388	1.1437	0.0174	-0.7055	-1.1174	1.2255	1.1936
3-ureidopropionate	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.4777	0.8097	-0.9433	0.1562	-0.9755	0.1007	0.1488	-0.5061	-0.7078	1.3574
5-methyluridine (ribothymidine)	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.4350	-0.5000	0.0545	2.0747	1.3807	0.9410	-1.1935	0.8360	1.6188	-0.2354
N-acetyl-beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	1.4383	-0.0531	-0.9276	0.7583	0.4146	-0.6410	-0.5043	1.3959	0.6199	-0.3019
pseudouridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.7299	-1.1270	-0.6229	2.2803	0.4363	-0.2673	-0.0955	0.9343	0.1455	0.2479
uracil	Nucleotide	Pyrimidine Metabolism, Uracil containing	1.8968	-0.4014	-0.3532	0.8305	0.7071	-0.7667	0.5923	1.2413	0.6351	-0.3416
uridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	1.5969	-0.3715	-0.8441	0.7534	0.5141	-1.1616	-0.1558	0.8874	0.2121	0.2559
cyclo(ala-pro)	Peptide	Dipeptide	-0.2923	-0.4926	0.1305	0.9210	-0.2064	0.4741	0.0658	0.1697	0.3967	-0.5373
cyclo(pro-val)	Peptide	Dipeptide	-0.5370	-0.5383	1.4296	-0.5378	-0.5418	-0.5371	-0.0173	1.0371	-0.5360	0.0092
glycylproline	Peptide	Dipeptide	0.0459	0.4682	-0.2437	2.3708	1.3762	-0.4577	-0.4310	0.8497	0.5240	0.7159
leucylproline	Peptide	Dipeptide	-0.6123	-0.6413	2.0176	-0.6181	1.3450	-0.6080	-0.6276	2.0948	-0.6442	-0.6239
pyroglutamylglutamine	Peptide	Dipeptide	-1.1169	-0.4032	-1.4061	0.3392	-0.8563	1.2686	0.8476	-1.0939	0.3989	0.1370
homocarnosine	Peptide	Dipeptide Derivative	0.4223	0.2550	-0.0555	-0.8549	0.8531	1.6078	0.0731	1.0862	1.8892	-0.9281
gamma-glutamyl-epsilon-lysine	Peptide	Gamma-glutamyl Amino Acid	-0.2605	0.0883	-1.2534	3.3072	-0.0138	-0.7357	0.2510	0.1218	0.4387	0.3441
gamma-glutamylalanine	Peptide	Gamma-glutamyl Amino Acid	2.8163	-0.3915	0.2071	1.3335	1.9854	-1.6440	0.4261	-0.3007	0.4932	0.3425
gamma-glutamylglutamine	Peptide	Gamma-glutamyl Amino Acid	1.5894	-0.3248	-0.3172	2.6269	1.0550	-0.3311	0.2419	-0.5404	1.3542	-0.5023
gamma-glutamylhistidine	Peptide	Gamma-glutamyl Amino Acid	-0.0493	0.2080	-0.6766	3.0067	0.0523	-0.1388	0.1959	-0.2772	0.4231	0.4085
gamma-glutamylisoleucine*	Peptide	Gamma-glutamyl Amino Acid	-0.2223	0.4855	-1.0351	2.4250	-0.2794	-1.0304	0.7758	0.4114	-1.0261	0.1522
gamma-glutamylleucine	Peptide	Gamma-glutamyl Amino Acid	0.9800	0.5634	-1.1092	2.2911	-0.1478	-0.6698	0.7422	-0.0196	0.5093	0.2308
gamma-glutamylmethionine	Peptide	Gamma-glutamyl Amino Acid	1.5991	0.7022	-1.0683	2.0914	0.4911	0.7280	0.3468	-1.0647	-1.0740	1.3651
gamma-glutamylphenylalanine	Peptide	Gamma-glutamyl Amino Acid	0.8370	-0.6245	-0.6289	3.0108	0.1384	-0.6325	1.7549	-0.6271	-0.2446	-0.6262
gamma-glutamylthreonine*	Peptide	Gamma-glutamyl Amino Acid	0.8440	-0.3138	0.2146	2.6090	0.5976	-0.8463	0.2097	-0.7618	-0.5003	-0.0247
gamma-glutamyltyrosine	Peptide	Gamma-glutamyl Amino Acid	1.3277	-0.4202	-0.4146	3.4347	-0.4160	-0.4094	-0.4104	-0.4155	-0.4069	-0.3798
gamma-glutamylvaline	Peptide	Gamma-glutamyl Amino Acid	-0.8904	-0.0709	-0.9559	3.1837	-0.2600	-1.3820	0.3194	-1.1690	-0.2773	0.6556
gamma-glutamyl-alpha-lysine	Peptide	Gamma-glutamyl Amino Acid	0.61318	-0.5307	-0.5034	3.14074	0.68851	-1.5127	-0.0168	-0.4856	-0.0007	0.48826
tartronate (hydroxymalonate)	Xenobiotics	Bacterial/Fungal	0.7984	-0.5966	0.5708	0.3826	0.4196	-1.8860	-0.5410	0.0157	0.3459	-0.6457
4-methylcatechol sulfate	Xenobiotics	Benzoate Metabolism	-0.1941	-0.1677	-0.1932	-0.2106	-0.1787	-0.1766	-0.2005	-0.1907	-0.1811	-0.1667
catechol sulfate	Xenobiotics	Benzoate Metabolism	-0.7004	0.2184	-0.6973	-0.6980	-0.7079	-0.6959	1.4517	-0.7118	-0.6954	-0.0804
hippurate	Xenobiotics	Benzoate Metabolism	-0.8061	0.2304	-1.3058	1.7137	1.6365	-1.3130	-0.2104	0.0713	-1.3169	-0.4845
methyl-4-hydroxybenzoate sulfate	Xenobiotics	Benzoate Metabolism	-0.7251	0.0008	-0.7197	2.5405	1.8184	-0.7178	0.8307	1.8787	0.4738	-0.7154
1,2-propanediol	Xenobiotics	Chemical	-0.4460	-0.4422	-0.4506	3.0410	-0.4505	-0.0993	-0.4496	0.2409	-0.4438	-0.4450
1,3-propanediol	Xenobiotics	Chemical	-0.4617	-0.4644	-0.4582	3.7381	2.2123	-0.8417	-0.1325	0.9320	0.7269	-0.3845
2-aminophenol sulfate	Xenobiotics	Chemical	-0.3747	1.8290	-0.3763	-0.3661	-0.3701	-0.3739	-0.3754	-0.3649	-0.3700	0.1300
3-hydroxypyridine sulfate	Xenobiotics	Chemical	-1.3889	0.8144	1.3549	0.3477	1.1982	-0.2289	1.4689	-0.9885	0.0728	1.3117

Supplemental Table 2. Z-scores for Population Baseline

Biochemical	Super Pathway	Sub Pathway	CSF318	CSF319	CSF320	CSF322	CSF323	CSF325	CSF327	CSF328	CSF329	CSF305
dimethyl sulfone	Xenobiotics	Chemical	-0.3219	0.2710	-0.0305	-1.8444	-1.5261	-0.4936	0.5355	-1.6102	0.6967	-0.8741
O-sulfo-L-tyrosine	Xenobiotics	Chemical	-0.6466	-0.0936	-0.0086	2.9473	0.1495	-0.7636	-0.1241	0.7856	-0.2251	0.3330
succinimide	Xenobiotics	Chemical	-0.7923	0.0641	0.1795	-0.5418	-0.2563	-0.2218	-0.2186	0.1780	3.8657	-0.7093
sulfate*	Xenobiotics	Chemical	0.5117	-0.3458	-0.9596	-0.2244	-0.8250	-0.7003	0.5648	-0.1785	0.6548	-0.0676
trizma acetate	Xenobiotics	Chemical	-0.3753	-0.8141	-0.5757	1.6684	-0.2046	-0.2142	-0.3568	0.0499	-0.4205	-0.1818
2-hydroxyacetaminophen sulfate*	Xenobiotics	Drug	-0.3344	-0.3354	-0.3401	-0.3208	-0.3209	-0.3296	-0.3215	-0.3278	-0.3364	-0.3323
2-methoxyacetaminophen glucuronide*	Xenobiotics	Drug	-0.3044	-0.2948	-0.3035	-0.2937	-0.2862	-0.2900	-0.2930	-0.2903	-0.3046	-0.2972
2-methoxyacetaminophen sulfate*	Xenobiotics	Drug	-0.2673	-0.2675	-0.2575	-0.2609	-0.2543	-0.2579	-0.2647	-0.2581	-0.2630	-0.2674
3-(cystein-S-yl)acetaminophen*	Xenobiotics	Drug	-0.2560	-0.2417	-0.2470	-0.2391	-0.2483	-0.2326	-0.2372	-0.2324	-0.2324	-0.2266
4-acetamidophenol	Xenobiotics	Drug	-0.4777	-0.4759	-0.4762	-0.4752	-0.4739	-0.4773	-0.4753	-0.4745	-0.4740	-0.4756
4-acetamidophenylglucuronide	Xenobiotics	Drug	-0.4260	-0.4280	-0.4269	-0.4219	-0.4250	-0.4225	-0.4225	-0.4245	-0.4244	-0.4283
4-acetaminophen sulfate	Xenobiotics	Drug	-0.4778	-0.4795	-0.4768	-0.4782	-0.4782	-0.4777	-0.4781	-0.4795	-0.4742	-0.4768
5-sulfosalicylate	Xenobiotics	Drug	-0.3806	0.7585	-0.6015	0.3756	1.0633	-0.6066	1.6088	1.1189	-0.6014	-0.6019
carbamazepine 10,11-epoxide*	Xenobiotics	Drug	-0.1823	-0.1817	-0.1822	-0.1767	-0.1802	-0.1829	-0.1807	-0.1920	-0.1850	-0.1861
fluoxetine	Xenobiotics	Drug	-0.1806	-0.1839	-0.1880	-0.1775	-0.1811	-0.1843	-0.1867	-0.1864	-0.1790	-0.1789
lidocaine	Xenobiotics	Drug	1.3651	-1.3063	-0.3564	-1.0964	0.2944	-0.5306	-0.5217	0.5298	-1.3383	0.4515
N-ethylglycinexylidide	Xenobiotics	Drug	1.3304	-0.5188	-0.5176	-0.5181	0.9220	-0.5180	-0.5165	2.8194	-0.5158	3.0335
salicylate	Xenobiotics	Drug	-0.9318	2.4320	-0.9202	-0.9228	0.6549	0.7315	1.3133	-0.9268	-0.9306	-0.1864
topiramate	Xenobiotics	Drug	-0.2597	-0.2604	-0.2629	-0.2620	-0.2622	-0.2634	-0.2606	-0.2644	-0.2638	-0.2638
pregabalin	Xenobiotics	Drug	-0.1810	-0.1865	-0.1786	-0.1786	-0.1836	-0.1833	-0.1799	-0.1857	-0.1864	-0.1801
sulfamethoxazole	Xenobiotics	Drug	-0.1833	-0.1798	-0.1841	-0.1856	-0.1842	-0.1824	-0.1795	-0.1827	-0.1834	-0.1809
cetirizine	Xenobiotics	Drug	-0.323	-0.3231	-0.3216	-0.3255	-0.3282	-0.3223	-0.3223	-0.3226	-0.3241	-0.3276
2-piperidinone	Xenobiotics	Food Component/Plant	0.5179	1.3779	0.1474	-1.1651	1.2705	-0.7342	-0.8447	-0.5246	0.5809	0.5072
betonicine	Xenobiotics	Food Component/Plant	-1.0818	0.7454	1.4904	-1.0793	-0.3833	0.3871	-0.5891	-1.0828	-1.0831	0.6039
ergothioneine	Xenobiotics	Food Component/Plant	-1.8592	-0.0267	1.1402	1.0529	0.9669	0.8705	-1.6712	0.2456	0.1795	0.8350
erythritol	Xenobiotics	Food Component/Plant	-0.6499	-1.7191	-0.1745	1.4963	-1.3265	-0.2717	-0.8345	0.1379	-1.3012	0.7023
gluconate	Xenobiotics	Food Component/Plant	-0.4971	-0.4083	-1.1524	3.0011	-1.5339	-1.1180	0.3092	2.9033	-0.5885	0.8121
indolin-2-one	Xenobiotics	Food Component/Plant	-1.1378	0.4306	-1.1383	-0.2538	0.5010	1.4626	-0.2068	-1.1383	-1.1440	0.9786
levulinate (4-oxovalerate)	Xenobiotics	Food Component/Plant	1.2841	0.9092	-0.1962	1.3455	-1.3926	0.3260	-1.2056	1.4165	0.5063	-1.1641
piperine	Xenobiotics	Food Component/Plant	-0.6609	-0.6649	-0.6640	-0.6625	-0.6590	-0.6654	-0.6650	-0.6631	-0.6637	-0.6589
quinate	Xenobiotics	Food Component/Plant	-0.1766	-0.7195	2.1729	-0.7248	-0.7184	-0.7250	-0.7176	-0.7198	-0.7187	-0.7233
S-allylcysteine	Xenobiotics	Food Component/Plant	-0.5617	-0.5539	0.9482	-0.5600	-0.5565	-0.5512	-0.5572	-0.5601	-0.5543	1.3908
stachydrine	Xenobiotics	Food Component/Plant	-1.3161	1.2867	1.2840	-1.3755	-0.8439	0.6643	0.0000	-0.6460	-0.5709	0.5130
tartarate	Xenobiotics	Food Component/Plant	-0.4897	1.1664	-0.9086	1.5902	-0.6197	-0.3305	-1.2860	-0.0340	-1.3879	0.7329
acesulfame	Xenobiotics	Food Component/Plant	-0.5124	-0.5123	-0.5027	2.12045	1.50576	-0.5024	1.2569	-0.5036	0.04918	-0.5073
3-methylxanthine	Xenobiotics	Xanthine Metabolism	-0.4904	-0.5090	3.6419	-0.5028	-0.5099	-0.4940	1.0605	-0.5042	-0.4895	1.0718
5-acetylamino-6-amino-3-methyluracil	Xenobiotics	Xanthine Metabolism	-0.2546	-0.2680	-0.2702	-0.2667	-0.2662	-0.2788	-0.2643	-0.2715	-0.2739	-0.2603
7-methylxanthine	Xenobiotics	Xanthine Metabolism	-0.6298	-0.6309	2.3702	-0.6281	-0.6340	-0.6210	2.0426	-0.6193	-0.6162	1.5231
caffeine	Xenobiotics	Xanthine Metabolism	-0.6120	-0.6165	1.8860	0.1135	-0.6114	-0.6160	-0.6106	-0.6103	-0.6158	-0.6146
paraxanthine	Xenobiotics	Xanthine Metabolism	-0.6572	-0.6544	1.7587	-0.6549	0.6867	-0.6564	-0.6484	-0.6564	-0.6499	-0.6581
theobromine	Xenobiotics	Xanthine Metabolism	-0.9382	0.4153	1.9423	-0.9353	-0.9353	-0.2986	0.9005	-0.9350	-0.9384	1.0140
theophylline	Xenobiotics	Xanthine Metabolism	-0.4910	-0.4963	1.4488	-0.4992	-0.4990	-0.2178	-0.4980	-0.4978	-0.5013	-0.4898
thioproline	Xenobiotics	Chemical	0.66449	0.20873	-1.141	0.62398	-0.6845	0.58106	-1.024	-0.961	-1.2358	0.09949

Supplemental Table 2. Z-scores for Population Baseline

			Heme present in samples								
Biochemical	Super Pathway	Sub Pathway	CSF310	CSF311	CSF312	CSF314	CSF315	CSF316	CSF321	CSF324	CSF326	CSF330
alanine	Amino Acid	Alanine and Aspartate Metabolism	-0.1479	1.6847	-0.4696	0.2811	0.4043	0.7352	0.4628	-0.7833	-1.2668	0.2922
asparagine	Amino Acid	Alanine and Aspartate Metabolism	-0.7162	0.4687	-1.5356	0.5904	-0.3766	1.6635	0.0442	-0.2614	-2.0353	1.3097
aspartate	Amino Acid	Alanine and Aspartate Metabolism	0.4271	2.1165	-1.3504	-0.6020	-1.0936	1.7021	-1.1891	-1.6051	-0.2580	0.6048
N-acetylalanine	Amino Acid	Alanine and Aspartate Metabolism	-0.8266	-0.2604	-0.3982	-0.3364	0.6980	0.8568	-1.4535	0.2564	0.1246	0.6487
N-acetylasparagine	Amino Acid	Alanine and Aspartate Metabolism	-0.0083	0.5059	0.4350	0.9499	0.3318	0.2978	-3.1453	0.2656	-0.6831	0.0567
N-acetylaspartate (NAA)	Amino Acid	Alanine and Aspartate Metabolism	-1.3631	-0.9508	-0.0515	-0.7161	-1.1159	0.9012	-1.8207	1.1021	0.1928	0.3163
creatine	Amino Acid	Creatine Metabolism	-0.5647	1.3942	0.3534	-0.7452	0.3416	-0.1338	0.4741	-0.2099	-1.4358	-0.3741
creatine phosphate	Amino Acid	Creatine Metabolism	-0.6690	-0.6616	-0.6650	-0.6590	1.4229	-0.6336	-0.6705	-0.6718	-0.6730	-0.6650
creatinine	Amino Acid	Creatine Metabolism	-0.2501	1.6835	-0.3446	0.7451	-0.9870	-0.5801	-1.8285	-1.0768	0.4786	-0.7010
guanidinoacetate	Amino Acid	Creatine Metabolism	-0.0705	0.8797	1.1376	0.4589	-0.8648	-1.5037	-1.9054	0.8137	0.5722	0.6670
carboxyethyl-GABA	Amino Acid	Glutamate Metabolism	-0.4223	0.4947	0.8809	0.6448	0.0875	0.4910	-1.0787	0.0680	0.8150	0.3495
citramalate	Amino Acid	Glutamate Metabolism	0.6598	1.1661	-0.8137	-0.1877	0.9599	-1.0370	1.6269	0.7340	0.7126	0.5543
gamma-aminobutyrate (GABA)	Amino Acid	Glutamate Metabolism	-0.0333	1.3091	0.7041	-0.0741	-1.1676	0.1691	-1.1669	-0.3469	-0.4139	-0.6814
glutamate	Amino Acid	Glutamate Metabolism	0.5002	0.5748	-1.3422	-0.2001	-0.9870	2.0257	-0.4253	-1.5099	0.5329	1.9360
glutamate, gamma-methyl ester	Amino Acid	Glutamate Metabolism	-0.2408	-0.0739	-1.6497	2.1061	0.0962	-1.2934	-0.4206	0.5169	0.4543	0.1631
glutamine	Amino Acid	Glutamate Metabolism	-0.3316	0.5224	-0.6378	2.7945	-1.8618	0.7881	0.3316	-0.7831	-0.3055	-0.4221
N-acetyl-aspartyl-glutamate (NAAG)	Amino Acid	Glutamate Metabolism	-0.0316	0.4542	0.4961	-1.0639	-0.3679	1.1207	-3.2850	-0.2710	-0.3247	-0.1208
N-acetylglutamate	Amino Acid	Glutamate Metabolism	-1.0789	-1.2583	-0.2586	-0.7126	-0.7121	1.4227	-1.4777	0.9915	0.1596	0.5737
N-acetylglutamine	Amino Acid	Glutamate Metabolism	-0.7281	0.8633	0.2512	1.2920	-1.2867	0.0182	-1.2115	0.7480	-0.2542	-0.0136
pyroglutamine*	Amino Acid	Glutamate Metabolism	-1.1604	2.8107	0.0791	1.0564	-2.3961	0.4325	-0.7295	-0.0472	0.0913	-0.2253
S-1-pyrroline-5-carboxylate	Amino Acid	Glutamate Metabolism	-0.1128	-0.1268	0.5147	1.2934	0.3872	-1.5812	0.2997	-1.1813	-1.2897	-0.8428
beta-citrylglutamate	Amino Acid	Glutamate Metabolism	-0.8943	-1.0055	-0.662	-0.3674	1.08245	1.29488	-0.7349	0.16614	-0.0155	0.29234
5-oxoproline	Amino Acid	Glutathione Metabolism	0.5781	-0.6708	-1.5763	0.5869	-2.1444	2.9357	0.2234	-1.1799	0.2830	1.2743
cys-gly, oxidized	Amino Acid	Glutathione Metabolism	0.4957	0.3433	0.7824	1.2574	-1.2213	-1.4475	-1.6410	0.4127	-0.5104	-1.3024
cysteinylglycine	Amino Acid	Glutathione Metabolism	-0.5927	1.3362	-0.5888	-0.5890	1.7353	-0.5819	-0.5795	-0.5786	-0.5849	-0.5875
glutathione, oxidized (GSSG)	Amino Acid	Glutathione Metabolism	-0.3787	-0.3744	-0.3713	-0.3760	-0.3721	-0.3751	-0.3629	0.6004	-0.3612	-0.3607
betaine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.0542	-0.2975	-0.1688	-0.6083	-0.5797	1.4323	-1.2036	1.3129	-0.2170	-0.2064
dimethylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.0829	-0.5329	-0.1702	-0.8305	0.8576	1.8641	-1.6687	0.9009	0.4398	1.1281
glycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.0959	0.1158	-1.7354	-0.4938	-0.2860	0.2270	1.0429	0.7456	-0.5492	-0.2654
N-acetylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.8610	-0.9544	-0.4717	-0.3122	-0.7836	-0.1223	-0.5160	0.3542	2.4084	-0.5738
N-acetylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	-1.0214	0.0540	-0.1853	-0.3152	0.5564	0.5610	-2.5174	0.5592	-0.0505	0.5198
N-acetylthreonine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.5751	-0.1000	-0.0644	-0.3259	0.8453	0.9074	-2.3786	0.2470	0.0318	0.4834
serine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.9243	-0.4141	0.1359	0.4553	-0.0052	2.0176	-1.4705	0.3260	-1.2097	0.4604
threonine	Amino Acid	Glycine, Serine and Threonine Metabolism	1.3852	0.7722	-1.1492	1.7485	0.0479	0.8597	-0.7511	-1.1918	-1.7260	-0.5145
2-methylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	-1.5727	0.46551	-1.0785	-0.2647	1.47952	0.22378	-0.9748	-0.1336	0.39877	0.64137
1-methylguanidine	Amino Acid	Guanidino and Acetamido Metabolism	-0.6201	-0.6220	-0.6177	0.4735	0.8913	-0.6159	-0.6240	-0.6157	-0.1303	-0.6206
4-guanidinobutanoate	Amino Acid	Guanidino and Acetamido Metabolism	-0.0424	-2.1160	-0.3762	0.3763	-0.7267	0.9151	-2.1432	-0.4974	1.1824	-0.7785
1-methylhistamine	Amino Acid	Histidine Metabolism	-0.3612	-0.3542	-0.3563	-0.3571	-0.3565	-0.3433	-0.3621	-0.3634	-0.3594	-0.3486
1-methylhistidine	Amino Acid	Histidine Metabolism	0.4762	0.6888	-0.3641	0.2352	1.8402	0.6075	-0.8103	-1.1661	-0.9688	-0.4584
1-methylimidazoleacetate	Amino Acid	Histidine Metabolism	-2.2919	-0.9683	0.7006	-1.3366	0.3092	1.1988	-1.0074	0.6834	0.2952	0.5866
3-methylhistidine	Amino Acid	Histidine Metabolism	1.2116	0.0989	0.2030	-0.8974	-0.0384	-0.1318	-1.0245	-1.0733	-0.9733	-0.0999
4-imidazoleacetate	Amino Acid	Histidine Metabolism	0.5166	-1.0298	-0.5592	-0.2034	-1.0250	0.2633	-1.0231	0.2566	1.4516	-0.8299
histidine	Amino Acid	Histidine Metabolism	0.4499	1.2412	0.7819	0.9237	-1.3143	1.1638	-0.9382	-0.3995	-0.9724	0.2334
imidazole lactate	Amino Acid	Histidine Metabolism	1.5518	1.1699	-0.4645	1.3510	0.9373	-0.9539	-0.4568	0.4546	-0.0562	-1.2236
imidazole propionate	Amino Acid	Histidine Metabolism	-0.5845	1.3455	-0.5816	-0.5782	-0.5827	1.8256	-0.5877	1.6316	-0.5845	1.1401
N-acetyl-3-methylhistidine*	Amino Acid	Histidine Metabolism	0.4364	1.0083	1.1205	-0.8794	-0.8813	-0.2437	0.4674	-1.5575	0.2000	-0.7422
N-acetylhistidine	Amino Acid	Histidine Metabolism	-0.8767	0.6367	0.5419	1.1737	-0.6597	1.6026	-0.9288	0.3435	0.3075	-0.7055
2-hydroxy-3-methylvalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.2270	-0.6365	-0.1467	0.7948	-0.6675	-0.2688	0.4069	-0.4789	-0.0115	0.3405
2-methylbutyrylcarnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.3205	-1.0327	-0.7474	-2.0318	0.1338	1.2950	-0.6662	-0.7302	0.3460	0.8925
3-hydroxy-2-ethylpropionate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.9761	0.6560	0.0402	-0.5701	1.8754	0.0945	0.8429	0.5717	1.2033	0.0071
3-hydroxyisobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.5942	-0.4679	-0.9726	-0.7307	0.7401	0.5191	0.9238	-0.8864	0.0228	1.4856
3-methyl-2-oxobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.1878	0.9764	0.8377	0.3063	0.6283	0.0057	1.0531	1.0320	-0.9637	1.1149
3-methyl-2-oxovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.4653	0.0814	0.7044	0.2750	0.0376	0.9154	1.0941	0.8957	-1.7646	1.1437
3-methylglutaconate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.8697	-0.0791	0.1071	-0.0621	-0.6063	0.0044	-1.5079	-1.0380	0.6340	0.6013
4-methyl-2-oxopentanoate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.2312	0.2610	0.8641	0.1783	0.3039	0.4536	1.1043	0.9277	-1.2315	1.1612
alpha-hydroxyisocaproate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.5328	-0.4859	0.1182	0.5139	-0.9410	-0.1025	1.2543	-0.3929	1.0566	0.3982

Supplemental Table 2. Z-scores for Population Baseline

			Heme present in samples								
Biochemical	Super Pathway	Sub Pathway	CSF310	CSF311	CSF312	CSF314	CSF315	CSF316	CSF321	CSF324	CSF326	CSF330
alpha-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.2876	-0.3965	0.0793	0.5571	-0.3191	-0.5477	0.1318	-0.3438	-0.1030	-0.7443
beta-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.2300	-0.0568	-0.1635	-0.7103	0.5111	-0.6863	0.8463	-0.6901	-0.2793	-0.0094
beta-hydroxyisovaleroylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.1691	-0.0177	-2.1291	-0.0623	-0.0400	-0.0323	-1.1349	-1.1728	0.3825	1.8781
ethylmalonate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.0278	-0.8566	-0.1393	-0.5140	0.3309	1.3173	-0.5161	0.0458	-0.1654	0.2426
isobutyrylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.3212	-0.3824	-1.4007	-0.8200	0.2138	0.3244	-1.9937	-0.2351	-0.2823	0.8715
isoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.4340	-0.7405	0.1384	-1.0438	-0.3466	2.3045	-0.5938	-0.8592	-0.4202	0.9423
isovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.0770	-1.1552	-0.6554	-0.7114	-1.1650	1.2139	-0.1696	-1.1567	1.7384	-0.9573
isovalerylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.7365	-1.0990	-1.3763	-1.4121	0.3289	0.4441	-1.0119	-0.0542	0.0381	1.0075
leucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.4982	-1.0594	0.5950	-1.7556	-0.7724	2.2115	-0.5030	-0.7283	-0.0710	0.8104
methylsuccinate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.1793	-0.6580	-0.8194	-0.6657	0.0501	0.6967	-1.2456	-0.4830	0.1886	0.6628
methylsuccinoylcarnitine (1)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.5031	-0.3031	0.5346	0.4403	-0.2586	-0.3618	-2.7706	-1.8191	0.1211	0.8920
N-acetylisoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.7153	-0.1376	-0.1303	-0.4480	0.5378	0.8611	-2.2938	0.7829	0.1020	0.6692
N-acetylleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-1.3629	-1.1562	-0.1516	-1.1544	0.1287	0.9433	-1.1765	1.0600	0.7617	0.7427
N-acetylvaline	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.6203	-0.1522	-0.3827	-0.8824	0.6550	0.8155	-1.9489	0.3096	-0.0075	0.7169
tiglylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.6246	-0.4200	-1.9029	-0.6260	1.3126	0.4991	-1.6501	-0.4579	0.0896	0.3389
valine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.7671	0.2350	0.0374	-1.5143	-0.4017	1.4656	0.3794	-1.0989	-0.5833	0.5487
2,3-dihydroxy-2-methylbutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.5887	0.18473	0.20068	-0.2978	2.00096	-0.0177	2.63087	0.08097	-0.3083	-0.5078
2-oxoadipate	Amino Acid	Lysine Metabolism	-0.5475	-0.5361	-0.5413	-0.5387	-0.2368	-0.5422	0.3918	2.0839	-0.5402	0.4195
3-methylglutarylcarnitine (2)	Amino Acid	Lysine Metabolism	-0.9463	0.2916	0.8293	0.7194	0.2852	0.1192	-2.8563	-0.2799	0.3167	1.0591
5-hydroxylysine	Amino Acid	Lysine Metabolism	-1.5523	-1.5550	0.0316	-0.7353	0.7652	1.4381	-0.4751	0.4124	0.4131	1.1102
6-oxopiperidine-2-carboxylic acid	Amino Acid	Lysine Metabolism	0.4344	1.1978	-1.3268	-0.5747	-0.6292	0.1735	1.1941	-0.8151	-0.7154	-0.4808
glutarate (pentanedioate)	Amino Acid	Lysine Metabolism	-1.5158	-1.8995	-0.4977	-0.9029	-0.6498	1.7689	-0.4611	1.0963	0.5844	0.2117
glutarylcarnitine (C5)	Amino Acid	Lysine Metabolism	0.2095	0.1727	-1.2424	0.1152	0.3696	0.1386	-1.6688	-0.1769	-0.0715	2.0178
lysine	Amino Acid	Lysine Metabolism	0.5698	1.5543	-0.2271	-0.4111	-1.5797	-0.3523	-0.8409	0.0289	-1.2615	-0.7626
N2-acetyllysine/N6-acetyllysine	Amino Acid	Lysine Metabolism	-0.3105	0.9615	0.1046	0.0568	1.5103	-0.4614	0.3224	0.5376	0.3405	0.4996
N6,N6,N6-trimethyllysine	Amino Acid	Lysine Metabolism	-0.7009	0.1942	-0.3200	0.0660	0.3495	0.9927	-2.6687	0.6864	-0.4717	-0.1013
pipecolate	Amino Acid	Lysine Metabolism	-0.9273	0.2416	-1.9025	-1.6963	0.6694	-0.6994	-0.1853	0.3825	-0.7911	0.9801
2-aminobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.7108	0.2900	-0.5813	-0.6387	0.1252	0.9067	0.5628	-1.1418	0.4978	0.9545
2-hydroxybutyrate/2-hydroxyisobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-1.0554	-1.2398	-0.8111	-0.2888	0.4686	0.5458	1.7922	-0.3215	1.0912	1.0980
cystathionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.6004	0.1408	-0.3805	0.8016	-2.0155	1.2708	-2.0205	1.4234	-0.3918	0.0504
cysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-1.2178	0.2046	-0.4260	-0.7461	0.5246	0.4424	1.9998	0.2467	0.7149	0.3271
methionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.1804	1.2102	-0.3873	0.3931	-0.5187	1.7912	0.6051	-0.3214	-2.7098	-0.5380
methionine sulfone	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.5366	0.5373	-0.7074	1.2442	1.1161	0.2402	-1.3937	0.1277	1.0256	-0.5498
methionine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.9339	-1.1539	-1.0239	-0.0376	-1.1917	0.7050	-0.0699	-1.4282	0.6991	-0.4326
N-acetylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-1.2146	-0.6794	-0.2285	-0.4625	-0.0099	0.8532	-0.9875	1.2237	-0.0930	0.4732
N-acetylmethionine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.4997	-1.0639	-0.8804	-0.5541	-1.0668	0.7119	-0.9238	-0.4317	1.2978	0.1501
N-acetyltaurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.8948	-0.4233	0.0098	-1.4200	-0.1274	0.8861	-2.0899	1.3090	0.0850	0.6599
N-formylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-1.2360	-0.7392	-0.1885	-0.2758	0.4701	0.5394	-1.0401	0.9417	-0.0139	0.7317
S-adenosylhomocysteine (SAH)	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.4886	-0.2479	-0.4995	-0.4747	-0.4745	2.1413	-0.4658	-0.4744	0.1588	0.7033
S-methylcysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.8079	2.0340	-0.2250	-0.2909	-0.4454	1.1492	0.1316	0.0855	-1.2112	-0.2212
taurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-1.6075	-0.6401	0.0212	-1.9841	-0.4600	0.6694	1.1644	-0.2404	-1.2664	1.3803
3-(4-hydroxyphenyl)lactate	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.3284	-0.2226	-0.1795	-0.5926	-0.5698	0.3509	2.3193	-0.5850	0.0400	-0.2538
3-methoxytyramine sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	-1.9693	1.2169	0.1955	-0.4460	-0.0920	-1.1082	0.7444	-1.3611	0.4402	0.0926
3-methoxytyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.5946	-0.0513	-0.0655	-0.2804	1.3726	1.8924	-0.1888	0.8475	-0.8373	0.7564
dopamine 3-O-sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.4827	-0.4760	-0.4815	-0.4648	1.4228	-0.4687	-0.4744	-0.4843	-0.4677	-0.4684
homovanillate (HVA)	Amino Acid	Phenylalanine and Tyrosine Metabolism	-1.2709	-0.5863	0.8722	-0.6968	-0.8336	1.0812	-0.7422	0.0579	0.7979	0.6027
N-acetylphenylalanine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-1.1261	-0.3203	-1.1308	-1.1237	-1.1283	0.8151	-0.0769	1.8842	0.7196	0.3780
N-acetyltyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.2839	-0.2856	-0.2686	-0.2768	-0.2720	-0.2850	-0.2676	-0.2717	-0.2872	-0.2865
p-cresol sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.4501	0.5373	0.0841	-2.0770	1.6569	1.1416	0.7824	-2.0700	1.0499	-0.6405
phenol sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.9773	-0.6637	-0.1877	-1.8430	2.2589	-0.7642	0.2963	2.0189	-0.0330	0.0477
phenylacetylglutamine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.0321	-0.1671	-0.3537	-2.0930	1.1525	0.7827	0.5427	1.5282	1.1417	-0.7968
phenylalanine	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.7735	1.2410	-1.3455	0.6326	0.0930	1.5316	2.0106	-1.2966	-2.1112	0.2051
phenyllactate (PLA)	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.8250	-0.3333	-0.6797	0.5423	0.8629	0.1649	3.0370	-0.6952	-0.2944	0.0757
tyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	1.2829	0.9161	0.1033	-0.1469	-1.0588	1.4155	0.8672	-1.0260	-1.6440	-0.5362
4-acetamidobutanoate	Amino Acid	Polyamine Metabolism	-1.6804	-0.4591	-0.0204	-0.0412	0.7547	1.0209	-0.0638	-0.1644	-0.2413	0.5006
5-methylthioadenosine (MTA)	Amino Acid	Polyamine Metabolism	-0.5803	-0.9054	-1.6007	0.1026	0.1682	2.1971	-0.4315	0.2214	0.0610	0.5770

Supplemental Table 2. Z-scores for Population Baseline

			Heme present in samples									
Biochemical	Super Pathway	Sub Pathway	CSF310	CSF311	CSF312	CSF314	CSF315	CSF316	CSF321	CSF324	CSF326	CSF330
acisoga	Amino Acid	Polyamine Metabolism	-1.3471	-0.8433	0.7543	-0.7129	2.4488	0.6633	-0.2304	1.2648	1.2068	0.4472
N-acetylputrescine	Amino Acid	Polyamine Metabolism	-1.3045	-0.2084	-1.1139	-1.0371	0.0176	1.5598	0.5260	0.6827	-1.2282	0.8329
spermidine	Amino Acid	Polyamine Metabolism	-2.2980	0.7566	-1.1470	-0.3786	-2.0114	0.0292	0.7802	0.8387	-0.1431	1.0652
3-indoxyl sulfate	Amino Acid	Tryptophan Metabolism	-0.7125	0.2717	-0.7128	-0.7111	1.8915	1.4043	-0.7055	1.0471	0.4701	-0.7136
5-hydroxyindoleacetate	Amino Acid	Tryptophan Metabolism	-0.9242	-1.5630	0.1094	-0.5164	-0.2208	1.9097	0.9420	0.6758	0.0293	0.6576
anthranilate	Amino Acid	Tryptophan Metabolism	1.1111	0.4494	1.6736	-1.3890	0.7046	-0.2282	0.1106	0.2654	-0.3655	-1.2354
C-glycosyltryptophan	Amino Acid	Tryptophan Metabolism	-0.7084	-0.4126	-0.0938	-0.2466	1.0542	1.0314	-1.7976	0.2735	0.2079	0.3373
indole-3-carboxylic acid	Amino Acid	Tryptophan Metabolism	-1.1586	-0.8943	-0.8034	-0.1479	-1.1975	0.1773	0.3362	-0.6022	0.6766	1.4425
indoleacetate	Amino Acid	Tryptophan Metabolism	-1.1575	-0.1407	-0.0991	-1.5889	1.8492	1.4331	-1.3188	1.2771	1.0659	0.0017
indolelactate	Amino Acid	Tryptophan Metabolism	-0.3079	-0.2974	-0.3108	-0.2988	-0.2955	-0.3063	1.8977	-0.3158	-0.3011	-0.2904
indolepropionate	Amino Acid	Tryptophan Metabolism	-0.3651	-0.3727	-0.3802	-0.3664	-0.3733	-0.3548	-0.3787	-0.3740	-0.3717	-0.3781
kynurenate	Amino Acid	Tryptophan Metabolism	-1.3079	-1.3120	0.2330	-0.9043	0.3686	0.6581	-1.3054	1.0300	0.5149	0.7360
kynurenine	Amino Acid	Tryptophan Metabolism	-1.1388	-1.1569	0.0753	-0.7151	0.9517	0.6608	-0.6073	0.9901	-0.5603	1.0945
picolinate	Amino Acid	Tryptophan Metabolism	-0.5994	0.0526	-0.1982	-0.8274	1.0001	1.6156	-1.8075	0.4494	0.3392	1.1078
tryptophan	Amino Acid	Tryptophan Metabolism	-0.3279	-1.4722	-0.0077	-0.6015	-1.0705	1.7525	0.7813	-0.6335	-2.0316	0.9955
tryptophan betaine	Amino Acid	Tryptophan Metabolism	-1.1169	0.9113	0.9501	-1.1155	-1.1158	0.1577	-1.1213	-0.2321	0.8278	-1.1171
arginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.1663	1.2473	0.0035	0.3015	-0.7510	0.5950	-3.6157	0.6888	-0.4564	0.2159
argininosuccinate	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.4367	0.4732	0.2872	1.0420	1.1893	1.4519	-1.9414	-0.6668	0.4295	0.7002
citrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.2762	-0.4748	0.4487	1.2520	-1.0578	1.1054	-1.8645	1.1152	-0.5476	1.4076
dimethylarginine (SDMA + ADMA)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-1.9345	0.1523	-0.6248	-1.0306	1.9054	1.8001	-0.0059	0.2404	0.1628	1.1913
homoarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1.1442	2.1397	0.3392	-0.3196	-1.5598	-0.6545	-0.3811	0.4703	-0.3350	0.7663
homocitrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.7830	-0.0866	-0.0780	-0.1172	2.4265	1.4583	-0.3683	-1.3848	-0.1174	0.3945
N-acetylarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.9176	0.6287	0.2639	0.1618	1.3972	0.0687	-2.7736	0.1435	-0.7494	0.3230
N-delta-acetylornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.1209	0.7859	-0.5256	-0.1963	1.5119	1.2949	-2.6069	-0.3110	-0.6174	-0.0082
N-methylproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	2.2119	0.2105	-0.3014	-0.9204	0.6567	0.9616	0.4881	-0.2042	0.3036	0.0629
ornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.2653	0.5844	-0.6589	-0.2195	-1.6221	0.2879	-0.7076	-0.0678	-1.1059	-0.2928
pro-hydroxy-pro	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-1.4469	-0.4377	-0.0301	-0.5454	1.6361	1.6044	-1.4095	0.4474	0.1210	1.2590
proline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.3702	0.4959	-1.1802	-1.1633	0.9664	0.9985	0.1459	-0.2075	-0.5807	1.0249
trans-4-hydroxyproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-1.1867	0.1432	-0.1855	-1.0166	0.2616	1.2845	0.2887	-0.6015	-0.2545	0.8032
urea	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.0546	-0.8005	-0.0016	0.1311	2.4852	-0.0508	-1.0498	-0.9423	0.8542	0.2521
argininate*	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-1.1482	-0.9848	-0.4581	1.89535	0.06672	-0.1765	-2.2902	-0.0149	1.10844	0.61485
erythronate*	Carbohydrate	Aminosugar Metabolism	-0.8690	-0.1735	-0.0868	0.2622	1.1008	-0.5914	-1.1037	-1.4970	0.5341	-0.4431
glucuronate	Carbohydrate	Aminosugar Metabolism	-2.4965	0.1143	-0.1258	0.4312	1.2187	0.4728	-0.6052	0.1854	-0.1164	-0.0799
N-acetylglucosaminylasparagine	Carbohydrate	Aminosugar Metabolism	-0.3860	-0.4470	0.2472	-0.5886	1.8563	1.4216	-1.7303	1.5216	0.5525	0.0973
N-acetylneuraminate	Carbohydrate	Aminosugar Metabolism	-1.2763	0.4980	0.2823	0.3037	0.1360	0.6599	-1.3514	0.4716	-1.1975	0.1869
sucrose	Carbohydrate	Disaccharides and Oligosaccharides	-0.4289	0.4015	-0.0172	-0.5700	1.0622	-0.3844	-0.5208	0.0179	0.4053	-0.1300
fructose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.3428	0.7110	-0.7888	-0.8021	-0.0512	-0.5537	1.1343	1.5022	-1.1650	0.0241
galactitol (dulcitol)	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.5363	0.1289	-0.2518	-0.0957	0.5388	2.0396	-0.8271	0.9569	-0.4617	0.6700
galactonate	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.5242	-0.5245	0.5961	-0.5222	-0.5227	2.1352	-0.5275	-0.5294	-0.5302	1.3263
mannitol/sorbitol	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.2012	1.2901	-0.4054	0.7474	-0.4840	-0.0258	2.0468	2.5167	-0.3514	-0.6066
mannose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.0226	0.7623	-1.0864	-0.0841	-0.6535	-0.6414	2.4964	1.6277	-0.9318	-0.3491
1,5-anhydroglucitol (1,5-AG)	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.0449	0.2572	0.8115	-0.2637	-0.4574	0.9748	-0.8898	0.6946	-0.0664	-0.1825
glucose	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.5965	0.9688	-0.3067	0.0749	-1.1229	-0.5813	2.9099	1.6660	-0.8534	0.0614
glycerate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.6164	-1.0553	-1.2622	-0.0430	-0.3163	0.1620	1.0258	-0.6902	0.8144	2.0501
lactate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.5158	0.5785	-0.5110	0.3913	1.3589	0.5419	3.9800	-1.0567	0.0934	-0.2317
pyruvate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	-0.7942	1.7540	0.0617	-0.7949	1.5471	-0.7965	1.3836	1.2579	-0.7960	0.8488
arabitol/xylitol	Carbohydrate	Pentose Metabolism	-0.5601	0.7764	-0.1821	0.5869	1.7082	-0.3074	-1.5193	0.2746	-0.0168	0.1295
arabonate/xylonate	Carbohydrate	Pentose Metabolism	-0.6030	0.9168	1.4933	-0.0502	0.1606	-0.1107	-1.5397	0.0773	-0.3957	0.2429
ribitol	Carbohydrate	Pentose Metabolism	0.2438	0.9754	-0.4130	-0.0865	0.7307	0.0840	-0.0871	-0.9154	-0.4951	-0.3354
ribonate	Carbohydrate	Pentose Metabolism	-0.4483	0.4546	0.7142	-0.1618	0.4542	0.1098	-1.2257	-0.7701	0.2311	-0.3181
ribose	Carbohydrate	Pentose Metabolism	0.0056	-1.3743	0.0973	-1.3746	1.6453	-1.3648	-0.0849	1.0961	0.5566	1.1959
gulonic acid*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-0.4342	0.0607	0.4007	-0.7312	0.6396	1.1217	-2.0532	-0.2654	-0.2304	-0.6652
oxalate (ethanedioate)	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.0670	0.8074	0.3791	1.5291	1.5320	-1.8968	-0.4095	0.8614	-0.8549	-1.0779
threonate	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	-1.0474	0.6335	0.0382	1.2475	1.0342	0.0950	-1.4822	0.8606	-0.2440	-1.5459
5-methyltetrahydrofolate (5MeTHF)	Cofactors and Vitamins	Folate Metabolism	0.2732	0.2355	0.4984	-0.1677	1.5582	0.3298	-0.0230	-0.1740	-0.0090	-1.5628
bilirubin (E,E)*	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.4086	0.6072	-0.3996	-0.4031	-0.3981	-0.3967	-0.4037	-0.3973	-0.4039	-0.4050

Supplemental Table 2. Z-scores for Population Baseline

			Heme present in samples									
Biochemical	Super Pathway	Sub Pathway	CSF310	CSF311	CSF312	CSF314	CSF315	CSF316	CSF321	CSF324	CSF326	CSF330
bilirubin (Z,Z)	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	-0.2381	-0.2355	-0.2477	-0.2525	-0.2475	-0.2313	-0.2322	-0.2346	-0.2524	-0.2515
heme	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	1.8012	2.8751	0.4537	-0.5173	1.2003	-0.2599	0.1465	0.9466	0.1724	3.0690
1-methylnicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-1.8053	-0.5581	0.4413	-1.8011	-0.0098	1.6377	-1.4711	1.3433	0.3141	0.7667
N1-Methyl-2-pyridone-5-carboxamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.5568	0.0215	-0.1239	0.3104	3.0706	-0.1431	-3.1515	0.7088	-0.0244	0.8714
nicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-1.1823	0.7604	1.5465	-1.1837	1.3509	2.1382	-1.1806	-0.0942	1.3262	0.4446
nicotinamide riboside	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-2.3732	1.2466	-0.1476	0.4026	-0.9673	1.0481	-0.3334	0.1209	-0.3111	-0.8030
quinolinate	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.5049	-0.5042	-0.5047	-0.2186	3.8402	0.6754	-0.4995	0.7798	-0.5089	1.1865
trigonelline (N'-methylnicotinate)	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.4731	0.5364	-0.1222	-0.5365	0.4414	-0.3664	-1.8611	0.2855	-0.7029	-0.2814
pantothenate	Cofactors and Vitamins	Pantothenate and CoA Metabolism	-0.4658	-0.6118	-0.7149	0.0647	1.3896	1.0722	-2.0424	0.3659	-0.0103	1.1231
gamma-CEHC	Cofactors and Vitamins	Tocopherol Metabolism	-0.9943	-0.1925	0.1957	1.6803	-1.1217	-0.8882	-0.5530	0.0910	-0.2948	1.0266
gamma-tocopherol/beta-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	-0.3656	-0.3590	-0.3622	-0.3657	-0.3636	-0.3604	-0.3665	-0.3588	-0.3599	-0.3639
retinol (Vitamin A)	Cofactors and Vitamins	Vitamin A Metabolism	-0.8084	0.7508	-0.8114	0.5777	1.2433	0.2816	-0.8052	-0.8096	-0.1207	-0.8007
pyridoxal	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.3736	-0.0235	-0.3256	-0.2092	0.2000	0.3758	-0.4597	0.1161	-0.3497	0.1375
pyridoxate	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.7315	-0.2878	-0.0758	-0.4387	0.4631	0.3760	-0.7989	-0.3376	-0.3744	-0.0827
pyridoxine (Vitamin B6)	Cofactors and Vitamins	Vitamin B6 Metabolism	-0.1904	-0.1878	-0.1897	-0.1839	-0.1782	-0.1712	-0.1859	-0.1806	-0.1875	-0.1800
phosphate	Energy	Oxidative Phosphorylation	0.0527	-0.8399	-0.0169	-1.3817	-0.0305	-2.1527	0.0016	0.0963	0.7562	0.5684
2-methylcitrate	Energy	TCA Cycle	-0.7445	0.1466	-0.3458	-0.6078	0.4891	0.4697	-1.3641	1.2654	0.0290	0.5632
aconitate [cis or trans]	Energy	TCA Cycle	0.1617	-1.1117	-1.6932	0.3640	-0.9917	0.9321	1.8871	0.5827	0.8808	-0.1869
alpha-ketoglutarate	Energy	TCA Cycle	-1.5622	-0.1483	-0.3573	-0.8403	0.3391	0.0395	1.8992	1.4642	0.6532	0.0061
citrate	Energy	TCA Cycle	0.7065	0.7058	-1.5806	0.7359	-1.2659	1.1265	2.3453	-0.1564	0.5750	-0.9287
fumarate	Energy	TCA Cycle	-0.9774	-0.9784	0.4584	-0.9691	-0.9710	1.0804	0.6237	1.1415	0.0758	0.4619
isocitrate	Energy	TCA Cycle	0.3017	0.4491	-0.8128	1.5456	0.4418	-0.5531	1.2649	2.5866	-0.8870	-1.9332
malate	Energy	TCA Cycle	-1.5165	-0.7990	-0.2259	-0.5348	-0.9572	0.8889	-1.1817	1.2062	0.2142	0.6538
succinate	Energy	TCA Cycle	-1.2330	-1.4569	-0.2529	-1.1022	-0.6798	1.1507	-0.7824	0.6740	0.8054	0.5853
succinylcarnitine	Energy	TCA Cycle	-0.1902	0.7416	0.0131	0.4882	0.4816	0.0780	-2.4808	0.0292	-0.4854	0.7432
carnitine	Lipid	Carnitine Metabolism	0.5186	0.6616	-0.8145	-1.6451	1.4335	0.7050	-1.5949	-0.4876	-1.0249	1.2378
deoxycarnitine	Lipid	Carnitine Metabolism	1.5133	1.0755	-0.5470	-1.8885	-0.2596	0.0864	-1.2835	-0.4873	-1.4081	0.2494
butyrylcarnitine	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	-0.2222	-2.6180	-0.9251	-1.5525	0.9452	1.0650	-1.4382	0.1610	-0.8699	1.0843
methylmalonate (MMA)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	-0.5596	-0.3838	-0.2567	-0.2121	-1.6224	-0.1902	0.5998	2.6435	0.3086	-0.4345
propionylcarnitine	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.1383	0.0763	-2.6204	-0.8776	0.8125	0.9727	-1.2283	0.4366	-0.6391	0.6886
3-hydroxybutyrylcarnitine (1)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.5844	-0.5822	-0.5859	-0.5948	2.1785	1.8647	-0.5866	1.1720	0.2019	1.8414
acetylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.2231	0.8296	-2.2895	-1.0714	1.3924	1.4988	-0.9359	0.0498	-0.2180	1.2644
cis-4-decenoyl carnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.0991	-0.1863	-1.2034	-1.1116	0.3802	1.1153	0.0890	0.2757	0.4761	1.8689
decanoylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.1170	-0.8042	-0.1986	-1.3888	0.5248	0.5803	-1.3858	1.6232	-0.0755	1.6599
hexanoylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.1806	-0.9315	-0.9333	-0.9327	0.8912	0.5044	-0.3698	0.1791	-0.9364	1.8548
laurylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.4845	-0.4638	-0.4646	-0.4811	3.0227	-0.4770	-0.4666	2.1967	-0.4692	2.5833
octanoylcarnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	-0.1387	-0.1400	-1.3110	-1.7220	0.7057	0.6960	-1.4156	1.1467	-0.1181	1.3190
malonate	Lipid	Fatty Acid Synthesis	-0.0614	0.4876	-0.8601	0.5670	-1.1383	0.7919	0.3279	1.0522	0.6559	-0.2524
malonylcarnitine	Lipid	Fatty Acid Synthesis	-0.9474	0.8665	-1.3258	0.3852	0.5986	1.2267	-1.3280	0.2535	-0.0348	0.3480
oleamide	Lipid	Fatty Acid, Amide	0.6624	0.8623	0.7167	0.9166	-1.2741	-1.2743	-0.9318	0.5981	-1.2971	1.0912
palmitic amide	Lipid	Fatty Acid, Amide	0.4275	0.8440	0.6631	0.8596	-1.3525	-1.0337	-1.1352	0.5342	-1.2203	1.2091
2-aminoheptanoate	Lipid	Fatty Acid, Amino	-0.0862	1.0734	0.6047	0.2315	-0.9335	0.3972	-1.3830	1.8086	-1.3662	-1.3381
2-aminooctanoate	Lipid	Fatty Acid, Amino	0.4522	-1.1320	0.8259	-1.1370	-0.4909	0.8997	-1.1228	0.5857	-0.4804	0.1560
2-hydroxyadipate	Lipid	Fatty Acid, Dicarboxylate	-0.9655	-0.5671	-0.5135	-1.0660	-1.9722	1.5891	0.9512	0.3852	-0.4954	0.2040
3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)	Lipid	Fatty Acid, Dicarboxylate	-0.2060	-0.1502	-0.1832	-0.1852	-0.2054	-0.2022	-0.1579	-0.1638	-0.2003	-0.1780
dimethylmalonic acid	Lipid	Fatty Acid, Dicarboxylate	-0.5474	0.4707	0.2569	-0.4166	-0.5491	-0.3212	-2.2100	0.5358	1.2751	1.3671
maleate	Lipid	Fatty Acid, Dicarboxylate	-1.3479	-0.5886	-0.3827	-0.3769	0.5851	-0.0958	2.2860	0.3417	0.3276	1.2554
2-hydroxydecanoate	Lipid	Fatty Acid, Monohydroxy	-0.4313	-0.4281	-0.4321	-0.4478	-0.4376	1.6510	0.8530	0.7617	-0.4506	-0.4400
3-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	-0.5196	-0.4791	-0.3511	-0.5571	1.54697	0.74771	0.23225	0.84023	-0.6266	1.12578
3-hydroxyoctanoate	Lipid	Fatty Acid, Monohydroxy	-0.4251	-0.7951	-0.7065	-1.1069	1.3025	0.4514	0.3722	0.5007	0.1352	0.5296
3-hydroxysebacate	Lipid	Fatty Acid, Monohydroxy	0.0562	0.1506	-0.0746	-0.4463	0.1474	-0.1359	-0.0332	-0.1578	0.1507	-0.4530
5-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	-0.7546	-0.7547	-0.7468	-0.7434	1.9605	1.6510	-0.7441	-0.7414	0.6932	1.6558
glycerol	Lipid	Glycerolipid Metabolism	-0.3625	-0.2160	-0.3908	-0.0573	4.8478	0.1122	0.9025	-0.6378	-0.3723	-0.3953
glycerol 3-phosphate	Lipid	Glycerolipid Metabolism	0.4754	-1.2416	0.4087	-0.5395	-1.5942	0.6847	0.4973	0.0413	0.0228	0.0531
galactosylglycerol*	Lipid	Glycerolipid Metabolism	-0.1676	-0.4244	-0.7599	-0.5353	0.86607	1.57468	-1.9829	0.9312	0.70586	0.67715
myo-inositol	Lipid	Inositol Metabolism	-1.3489	-0.1348	-0.4942	0.5424	0.7589	0.7913	-0.3804	0.2574	-1.7433	0.4860

Supplemental Table 2. Z-scores for Population Baseline

			Heme present in samples								
Biochemical	Super Pathway	Sub Pathway	CSF310	CSF311	CSF312	CSF314	CSF315	CSF316	CSF321	CSF324	CSF326	CSF330
3-hydroxybutyrate (BHBA)	Lipid	Ketone Bodies	-0.8908	-0.8925	0.0061	-1.1841	0.6840	0.9262	0.2675	1.5284	1.0107	1.4385
acetoacetate	Lipid	Ketone Bodies	-0.7511	-1.3812	-0.3394	-0.9819	0.4776	0.8362	-0.1479	1.7697	1.4458	1.3183
1-adrenoyl-GPC (22:4)*	Lipid	Lysolipid	0.8632	-0.4595	-0.5371	1.8092	-0.6379	0.6257	-0.4400	-1.2416	0.5473	1.8815
1-arachidonoyl-GPC (20:4)*	Lipid	Lysolipid	0.0721	0.1872	0.4218	-1.4947	0.8905	0.8146	-1.4934	-0.5461	0.5556	0.6241
1-arachidonoyl-GPE (20:4)*	Lipid	Lysolipid	0.0746	1.1761	0.4370	-1.1656	0.3726	0.8452	-1.1733	-1.1646	0.8576	1.3748
1-dihomo-linolenoyl-GPC (20:3n3 or 6)*	Lipid	Lysolipid	-0.2321	-0.2351	-0.2295	-0.2351	-0.2296	-0.2392	-0.2251	-0.2394	-0.2223	-0.2390
1-dihomo-linoleoyl-GPC (20:2)*	Lipid	Lysolipid	1.5071	-0.3996	-0.6536	-0.7418	1.1431	0.3831	0.9143	0.6604	1.5767	-0.8412
1-docosahexaenoyl-GPC (22:6)*	Lipid	Lysolipid	-0.2760	-0.2769	-0.2836	-0.2924	-0.2810	-0.2956	-0.2763	-0.2828	-0.2895	-0.2826
1-docosahexaenoyl-GPE (22:6)*	Lipid	Lysolipid	-0.0209	0.4772	0.9347	-1.1903	-0.3635	0.2083	-1.1930	-1.1935	0.4685	-0.5603
1-docosapentaenoyl-GPC (22:5n3)*	Lipid	Lysolipid	0.7165	-0.2608	-1.2358	-0.2143	-0.7046	1.2963	-1.9652	1.0192	-0.9251	0.1461
1-docosapentaenoyl-GPC (22:5n6)*	Lipid	Lysolipid	0.8947	0.9315	-0.4725	-1.4842	-0.9220	-0.1026	0.1716	-0.6734	-0.5917	0.3874
1-linoleoyl-GPC (18:2)	Lipid	Lysolipid	-0.0451	0.4341	-0.3983	-1.4937	0.7857	0.1458	-0.4256	-0.0244	-0.1601	1.2116
1-myristoyl-GPC (14:0)	Lipid	Lysolipid	-0.2351	-0.2216	-0.2405	-0.2258	-0.2341	0.0682	-0.2292	-0.2329	-0.2228	-0.2245
1-oleoyl-GPA (18:1)	Lipid	Lysolipid	0.8062	0.4291	-1.4000	-0.5910	-0.1205	-0.5826	-0.9382	-1.5446	-0.7150	0.2354
1-oleoyl-GPC (18:1)	Lipid	Lysolipid	-0.1331	0.1104	0.3113	-0.3497	0.0724	0.2410	-1.3262	-0.7437	0.3723	-0.1728
1-palmitoleoyl-GPC (16:1)*	Lipid	Lysolipid	-0.2156	-0.2076	-0.2035	-0.2229	-0.2032	-0.2128	-0.2237	-0.2035	-0.2169	-0.2085
1-palmitoyl-GPA (16:0)	Lipid	Lysolipid	-0.4857	-0.4763	-0.4825	-0.4925	0.2138	1.0537	-0.4844	-0.4702	-0.4741	-0.4700
1-palmitoyl-GPC (16:0)	Lipid	Lysolipid	-0.2873	0.1124	0.2030	-0.4609	0.2875	0.3101	-1.4076	-0.7289	0.3837	0.3851
1-pentadecanoyl-GPC (15:0)*	Lipid	Lysolipid	0.4121	-0.8065	-1.4867	1.4848	-1.5080	1.5218	-0.0899	-0.0013	0.1736	1.2666
1-stearoyl-GPC (18:0)	Lipid	Lysolipid	-0.2135	0.1190	0.1058	-0.8148	0.4290	0.4330	-0.9717	-0.5844	0.0546	0.9009
1-stearoyl-GPE (18:0)	Lipid	Lysolipid	0.7522	-0.0271	-0.6225	-0.6176	-0.6308	-0.6300	-0.6220	-0.6470	1.2368	0.5474
1-palmityl-GPC (O-16:0)	Lipid	Lyso-phospho-ether	0.3102	-1.5924	-0.3276	0.7379	1.2729	-1.5197	1.0345	1.4379	-1.5868	-0.7934
1-(1-enyl-palmitoyl)-GPC (P-16:0)*	Lipid	Lysoplasmalogen	0.4235	0.1274	-1.5134	-1.4576	1.1027	0.8225	0.3571	1.0945	-0.0864	-0.3026
1-(1-enyl-stearoyl)-GPE (P-18:0)*	Lipid	Lysoplasmalogen	-1.0159	1.0478	0.9242	0.2194	-1.3038	0.4414	-0.8340	-0.9874	1.0463	1.3432
3-hydroxy-3-methylglutarate	Lipid	Mevalonate Metabolism	-1.4125	-0.9239	-0.0943	-1.3785	-0.3858	1.1809	-1.0412	1.0203	0.1727	0.7709
1-arachidonylglycerol (20:4)	Lipid	Monoacylglycerol	-0.5134	1.0865	0.8952	0.7415	1.6577	-1.3794	-0.8133	-1.2976	1.0686	0.5427
1-dihomo-linolenylglycerol (20:3)	Lipid	Monoacylglycerol	1.5790	-0.4434	-0.4507	0.5179	-1.1249	0.4798	-1.4615	0.0458	-1.0308	0.2260
1-oleoylglycerol (18:1)	Lipid	Monoacylglycerol	-0.4962	1.2203	1.3414	0.5513	0.2992	0.9095	-1.7214	-1.7092	-1.2162	0.9674
1-palmitoylglycerol (16:0)	Lipid	Monoacylglycerol	0.1394	-0.2873	0.2059	-0.3335	-0.8123	-0.1449	-0.4158	-1.1572	-0.4407	1.8703
1,2-dilinoleoyl-GPC (18:2/18:2)	Lipid	Phospholipid Metabolism	-0.1744	-0.1802	-0.1763	-0.1820	-0.1738	-0.1791	-0.1817	-0.1815	-0.1885	-0.1862
1,2-dimyristoyl-GPC (14:0/14:0)	Lipid	Phospholipid Metabolism	-0.1561	-0.6006	0.9908	0.0180	0.0350	-1.3412	1.6725	1.4368	-0.1801	-0.3137
1,2-dioleoyl-GPC (18:1/18:1)*	Lipid	Phospholipid Metabolism	-0.5152	0.6409	0.3924	0.4183	0.3084	0.3005	-0.8320	-1.6541	0.3157	-0.1251
1,2-dipalmitoyl-GPC (16:0/16:0)	Lipid	Phospholipid Metabolism	-0.6603	0.6523	0.2979	-0.1683	0.2510	0.6587	-1.7664	-0.9157	0.3746	-0.2225
1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4)*	Lipid	Phospholipid Metabolism	0.6516	0.0540	1.4462	-1.0564	-0.5509	-1.4213	-1.2002	0.1072	-0.6242	-0.4988
1-margaroyl-2-linoleoyl-GPC (17:0/18:2)*	Lipid	Phospholipid Metabolism	0.9669	0.5514	0.1316	-1.3070	-1.0265	0.8355	-0.4167	-0.1716	0.9811	-1.0831
1-margaroyl-2-oleoyl-GPC (17:0/18:1)*	Lipid	Phospholipid Metabolism	-0.2973	0.7340	-0.2893	-0.2825	-0.2793	-0.3042	-0.2741	-0.3039	-0.2950	-0.3111
1-myristoyl-2-linoleoyl-GPC (14:0/18:2)*	Lipid	Phospholipid Metabolism	-0.0460	-0.8632	-1.1830	0.1030	0.3925	0.6773	-1.1940	0.5404	-1.5934	1.1946
1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	Lipid	Phospholipid Metabolism	-0.8111	0.3830	-0.2505	-0.4780	0.9412	0.8124	-1.5078	-0.7946	0.2892	0.3510
1-oleoyl-2-dihomo-linolenoyl-GPC (18:1/20:3)*	Lipid	Phospholipid Metabolism	-0.1881	-0.1907	-0.1960	-0.1889	-0.2056	-0.2057	-0.2109	-0.1965	-0.2104	-0.1881
1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)*	Lipid	Phospholipid Metabolism	0.5453	-0.1782	-0.0971	-0.7285	0.4014	0.4602	-0.2851	0.7135	0.0856	-1.5604
1-oleoyl-2-linoleoyl-GPC (18:1/18:2)*	Lipid	Phospholipid Metabolism	-0.2785	0.3519	-0.5282	-0.9064	1.0638	0.5354	-0.5955	-0.9136	-0.0494	0.7742
1-palmitoleoyl-2-linoleoyl-GPC (16:1/18:2)*	Lipid	Phospholipid Metabolism	-1.1701	-1.1436	0.3672	-1.1160	-0.2344	0.7106	1.4508	1.0923	0.8091	0.8584
1-palmitoyl-2-adrenoyl-GPC (16:0/22:4)*	Lipid	Phospholipid Metabolism	-0.5567	-0.5490	-0.5478	-0.5553	0.5854	0.8641	-0.5581	-0.5567	-0.5452	-0.1800
1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4)	Lipid	Phospholipid Metabolism	-0.4226	0.7509	0.3436	-0.5891	0.6631	0.2993	-0.8678	-1.3791	0.2839	0.5701
1-palmitoyl-2-dihomo-linolenoyl-GPC (16:0/20:3n3 or 6)*	Lipid	Phospholipid Metabolism	-1.1124	0.7100	-0.2819	-0.3664	0.7052	0.4434	-0.5673	-1.1851	0.4266	0.3313
1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)	Lipid	Phospholipid Metabolism	-0.4868	0.8939	0.0309	-0.3756	0.7380	0.2243	-0.8863	-1.6396	0.1712	1.3287
1-palmitoyl-2-eicosapentaenoyl-GPC (16:0/20:5)*	Lipid	Phospholipid Metabolism	-0.0300	-1.4740	1.1944	-1.6342	0.6854	-1.7463	0.2047	0.3815	1.5595	1.3989
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	Lipid	Phospholipid Metabolism	-0.3444	0.8777	-0.3279	-0.9493	0.8704	0.2536	-0.2000	-0.6477	0.3042	0.9761
1-palmitoyl-2-meadoyl-GPC (16:0/20:3n9)*	Lipid	Phospholipid Metabolism	0.3248	-0.8450	-0.6442	0.0131	-0.4310	0.9000	-0.9628	1.1614	-0.0963	0.3977
1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	Lipid	Phospholipid Metabolism	-0.6307	0.6539	0.3187	-0.0259	0.1682	0.1998	-1.5421	-1.2840	0.4370	-0.3539
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*	Lipid	Phospholipid Metabolism	-1.3070	0.0747	0.0316	-0.2862	0.6788	0.3358	-0.7253	-1.2841	0.4427	-0.0904
1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	Lipid	Phospholipid Metabolism	-0.2584	-0.2611	-0.2653	-0.2658	-0.2570	-0.2623	-0.2568	-0.2579	-0.2676	-0.2638
1-palmityl-2-arachidonoyl-GPC (O-16:0/20:4)*	Lipid	Phospholipid Metabolism	-0.3942	-0.4002	-0.3969	-0.3942	0.9326	1.3689	-0.4032	-0.3967	-0.3941	0.3701
1-palmityl-2-oleoyl-GPC (O-16:0/18:1)*	Lipid	Phospholipid Metabolism	-0.4435	1.1140	-0.1080	0.2526	0.4529	0.5511	-0.9774	-1.1180	0.4537	-0.3276
1-pentadecanoyl-2-oleoyl-GPC (15:0/18:1)*	Lipid	Phospholipid Metabolism	-0.2386	-0.2228	-0.2238	-0.2267	-0.2230	-0.2163	-0.2263	-0.2360	-0.2380	-0.2395
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	Lipid	Phospholipid Metabolism	-0.3658	0.7043	0.4030	-0.7331	0.8835	0.6072	-1.2564	-1.3230	0.1170	0.6000

Supplemental Table 2. Z-scores for Population Baseline

			Heme present in samples									
Biochemical	Super Pathway	Sub Pathway	CSF310	CSF311	CSF312	CSF314	CSF315	CSF316	CSF321	CSF324	CSF326	CSF330
1-stearoyl-2-dihomo-linolenoyl-GPC (18:0/20:3n3 or 6)*	Lipid	Phospholipid Metabolism	-0.7489	0.9124	-0.5203	-0.7469	0.7680	0.4746	-0.7479	-0.7473	-0.1392	0.1799
1-stearoyl-2-docosahexaenoyl-GPC (18:0/22:6)	Lipid	Phospholipid Metabolism	-0.3911	0.7663	0.5098	0.0495	0.5765	0.3659	-1.5046	-1.5046	0.2606	0.4561
1-stearoyl-2-docosahexaenoyl-GPE (18:0/22:6)*	Lipid	Phospholipid Metabolism	-0.8894	1.0308	0.8017	0.4154	-0.9023	-0.8882	-0.9115	-0.9102	0.4311	-0.8984
1-stearoyl-2-docosapentaenoyl-GPC (18:0/22:5n3)*	Lipid	Phospholipid Metabolism	1.9963	0.5806	-0.1075	-1.1505	-0.6086	-0.5361	0.8445	0.8033	0.3940	-1.6803
1-stearoyl-2-docosapentaenoyl-GPC (18:0/22:5n6)*	Lipid	Phospholipid Metabolism	-0.2282	0.3251	0.2967	0.6534	1.2820	0.8876	-1.5693	-1.3356	-1.6377	0.3515
1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*	Lipid	Phospholipid Metabolism	-0.2740	0.9248	-0.3700	-1.3291	0.9971	0.4210	-0.2015	-0.6877	-0.0458	0.8474
1-stearoyl-2-meadoyl-GPC (18:0/20:3n9)*	Lipid	Phospholipid Metabolism	1.0170	-1.5247	1.2400	1.2106	-0.4620	0.7712	-1.5731	0.6526	0.0002	0.4003
1-stearoyl-2-oleoyl-GPC (18:0/18:1)	Lipid	Phospholipid Metabolism	-0.4987	0.8885	0.4194	-0.0197	0.5108	0.4095	-0.7992	-1.8088	0.2543	-0.1569
choline	Lipid	Phospholipid Metabolism	-0.9804	0.8102	0.3290	-1.2278	-1.2121	1.0867	-3.0353	-0.5142	-0.5012	0.1001
choline phosphate	Lipid	Phospholipid Metabolism	-1.4703	0.7682	0.5854	0.8473	-1.1630	-0.7249	-2.5853	0.7331	-0.8843	-0.9431
glycerophosphoethanolamine	Lipid	Phospholipid Metabolism	-0.6463	-0.6406	-0.6286	-0.6344	-0.6348	-0.6425	-0.6257	-0.5598	-0.6340	-0.6405
glycerophosphoinositol*	Lipid	Phospholipid Metabolism	0.0432	0.1359	0.9455	0.4214	0.0324	-0.4155	-1.1280	0.3456	-0.4241	-1.1580
glycerophosphorylcholine (GPC)	Lipid	Phospholipid Metabolism	-1.9074	-0.7615	1.9283	-0.1026	0.9249	-1.2839	-0.7602	0.6736	-0.1686	0.8661
phosphoethanolamine	Lipid	Phospholipid Metabolism	0.0690	-1.3164	0.3158	0.1821	-0.4573	-0.2601	-2.1905	0.6371	-0.4200	-0.5952
trimethylamine N-oxide	Lipid	Phospholipid Metabolism	0.8184	0.1611	-0.0316	-1.8345	2.8088	0.1955	-1.3552	-1.0506	-0.0751	-0.1907
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*	Lipid	Plasmalogen	-0.4312	0.3461	-0.4357	-0.4311	-0.1322	1.3306	-0.4410	-0.4421	-0.4377	0.3428
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	Lipid	Plasmalogen	-0.3906	1.6937	-0.4126	-0.4023	-0.4067	0.9953	-0.4075	-0.4078	-0.3995	0.0297
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPC (P-16:0/22:6	Lipid	Plasmalogen	-0.3903	-0.2855	0.4248	0.7930	0.1154	0.7755	-1.8212	-0.9244	0.6068	0.6092
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPE (P-16:0/22:6	Lipid	Plasmalogen	-0.8156	0.8477	0.7173	-0.8101	-0.3619	0.1235	-0.8127	-0.8182	0.4097	-0.8222
1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	Lipid	Plasmalogen	-0.6421	0.1297	-0.2677	-0.4572	1.2571	1.2157	-1.9352	0.6988	-0.0168	1.0327
1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	Lipid	Plasmalogen	0.1886	1.7855	-0.5465	0.0703	0.0310	-0.1013	0.4683	-0.8616	-0.4357	-0.6489
1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*	Lipid	Plasmalogen	1.3702	-1.3901	0.9965	0.8230	1.0224	-0.6199	1.5577	-0.7783	-0.6120	0.8529
1-(1-enyl-stearoyl)-2-arachidonoyl-GPC (P-18:0/20:4)	Lipid	Plasmalogen	-0.4912	-0.4411	-0.7629	0.2159	-0.3754	-0.7016	0.7937	-0.1650	-0.0174	0.4771
1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	Lipid	Plasmalogen	-0.8529	1.7521	0.5983	-0.8450	0.3197	-0.8422	-0.8491	-0.8449	0.5141	0.8905
1-(1-enyl-stearoyl)-2-docosahexaenoyl-GPE (P-18:0/22:6)	Lipid	Plasmalogen	-0.1649	0.7546	0.8197	0.3767	-0.1495	0.1904	-2.0738	-0.8982	0.6840	0.0225
1-(1-enyl-palmitoyl)-2-dihomo-linolenoyl-GPC (P-18:0/20	Lipid	Plasmalogen	-1.2937	-1.0857	-0.5627	-1.1716	-0.3175	1.5966	-0.4078	-0.6407	-0.4638	-0.1152
dihomo-linoleate (20:2n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	0.6276	0.1065	-0.9256	-0.9244	1.7445	0.3161	0.2920	-0.9260	0.9989	1.7226
dihomo-linolenate (20:3n3 or n6)	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	-0.8533	0.1970	-0.4940	-0.8266	0.5387	0.3288	1.1680	-0.0357	-0.8375	0.6840
glycochenodeoxycholate	Lipid	Primary Bile Acid Metabolism	-0.2643	-0.3186	-0.2203	-0.2271	-0.0872	-0.2059	-0.2011	-0.3554	-0.2921	-0.0458
glycocholate	Lipid	Primary Bile Acid Metabolism	-0.1694	-0.1709	-0.1947	-0.1845	-0.1740	-0.1766	-0.1888	-0.1691	-0.1903	-0.1940
glycocholenate sulfate*	Lipid	Secondary Bile Acid Metabolism	-0.1753	-0.1873	-0.1777	-0.1811	-0.1886	-0.1854	-0.1874	-0.1747	-0.1739	-0.1887
glycohyocholate	Lipid	Secondary Bile Acid Metabolism	-0.1659	-0.1724	-0.1712	-0.2173	-0.1497	-0.1788	-0.2137	-0.1746	-0.2011	-0.2132
hyocholate	Lipid	Secondary Bile Acid Metabolism	-0.7837	-0.0063	-0.5085	0.0727	-1.2753	1.5584	0.1538	1.4969	-0.7013	2.0888
behenoyl sphingomyelin (d18:1/22:0)*	Lipid	Sphingolipid Metabolism	-0.3877	1.0959	-0.3940	-0.3985	-0.3852	-0.1574	-0.3884	-0.3909	-0.3846	1.1378
palmitoyl sphingomyelin (d18:1/16:0)	Lipid	Sphingolipid Metabolism	-0.5652	0.8807	-0.2000	-0.1893	0.9296	0.8645	-0.7494	-0.9285	0.2229	0.5962
sphingomyelin (d18:1/14:0, d16:1/16:0)*	Lipid	Sphingolipid Metabolism	-0.5584	0.3052	-0.4331	-0.9356	1.0514	1.0087	-0.9420	-0.9393	0.3116	1.8270
sphingomyelin (d18:1/18:1, d18:2/18:0)	Lipid	Sphingolipid Metabolism	-0.4239	0.8223	-0.0858	0.2405	0.1338	0.6290	-1.2571	-1.7790	0.3588	-0.1785
sphingomyelin (d18:1/20:0, d16:1/22:0)*	Lipid	Sphingolipid Metabolism	-1.0344	1.0768	-1.0350	0.4410	0.3995	0.7347	-1.0348	-1.0330	0.3754	0.4504
sphingomyelin (d18:1/24:1, d18:2/24:0)*	Lipid	Sphingolipid Metabolism	-0.1898	1.3145	-1.0597	0.4102	1.0788	0.5652	0.5335	-1.0638	-0.8534	1.0711
sphingomyelin (d18:2/16:0, d18:1/16:1)*	Lipid	Sphingolipid Metabolism	-0.3644	1.2044	-0.9888	0.1516	0.6092	0.4531	-0.6425	-0.9840	0.3224	0.5888
sphingosine	Lipid	Sphingolipid Metabolism	1.7142	1.4240	0.1750	0.7983	1.0784	0.7925	-1.0049	1.3433	-1.0001	-0.9973
stearoyl sphingomyelin (d18:1/18:0)	Lipid	Sphingolipid Metabolism	-0.3740	0.7518	0.5243	0.2791	-0.0670	0.1658	-2.2133	-1.3977	0.4169	-0.2267
16a-hydroxy DHEA 3-sulfate	Lipid	Steroid	-0.2185	-0.2242	-0.2258	-0.2352	-0.2274	-0.2292	-0.2228	-0.2340	-0.2355	-0.2219
4-androsten-3beta,17beta-diol disulfate (1)	Lipid	Steroid	-0.4059	0.5188	-0.4094	1.8430	0.3617	-0.4071	-0.4061	-0.4105	-0.4112	-0.4071
4-androsten-3beta,17beta-diol disulfate (2)	Lipid	Steroid	-0.1833	-0.1800	-0.1834	-0.1893	-0.1808	-0.1845	-0.1799	-0.1810	-0.1876	-0.1792
5alpha-pregnan-3beta,20alpha-diol disulfate	Lipid	Steroid	-1.0239	0.1261	1.5290	1.4641	1.2373	-1.2914	-0.7302	-0.5763	-0.9366	0.0504
andro steroid monosulfate (1)*	Lipid	Steroid	-1.0952	0.9074	-1.1480	-0.7975	-0.3405	1.3318	-1.1271	-0.5572	-1.4318	1.3473
cortisol	Lipid	Steroid	0.9884	0.0942	-0.6427	-0.6517	0.6206	-0.6521	2.3721	3.6218	-0.6550	-0.6479
cortisone	Lipid	Steroid	-0.7039	-1.0039	-1.5332	-0.5401	0.7645	1.1068	1.3937	2.0513	-1.5326	-1.5355
dehydroisoandrosterone sulfate (DHEA-S)	Lipid	Steroid	-0.2895	-0.1257	-0.1304	-0.2091	-0.1304	-0.1082	-0.2058	-0.2583	-0.1633	-0.1961
7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)	Lipid	Sterol	-0.1521	0.2911	-1.0531	0.7874	1.2987	0.5722	-1.1510	-0.7355	-0.4504	0.4443
cholesterol	Lipid	Sterol	-0.8605	0.7624	0.1060	-0.4145	-0.0570	0.2571	1.9237	-1.0880	0.1570	0.1899
2'-deoxyinosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.9621	1.4887	-1.2200	1.2562	-0.7785	0.4087	0.0853	0.2538	1.3402	-0.3027
allantoin	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.3225	0.5058	-1.8467	-1.0058	2.2374	1.2491	0.0635	-0.2341	1.2574	2.0852
hypoxanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-1.8629	-0.7447	0.0150	-0.2470	-0.7099	-0.4723	-2.2696	0.9197	0.6960	0.4114
inosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.4937	2.4052	-0.0629	0.9115	-2.0903	-1.7940	-0.2924	0.3425	-1.2477	1.2844

Supplemental Table 2. Z-scores for Population Baseline

			Heme present in samples									
Biochemical	Super Pathway	Sub Pathway	CSF310	CSF311	CSF312	CSF314	CSF315	CSF316	CSF321	CSF324	CSF326	CSF330
urate	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.1208	1.9305	-1.1791	1.1335	2.3161	1.0401	-1.9486	1.0161	-0.0401	0.2406
xanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-2.1499	-1.0099	-0.0507	-0.2857	0.6529	0.7550	-1.0318	0.6180	0.1946	-0.0312
xanthosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-1.4367	-0.5864	-0.7418	0.8110	0.3721	0.2142	0.1345	1.0477	-0.0129	-0.4937
N1-methylinosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-1.1993	-0.8754	0.03	-0.7711	0.53145	1.46694	-1.2298	0.75824	0.14803	0.6488
adenine	Nucleotide	Purine Metabolism, Adenine containing	-1.7135	-1.7578	1.1227	-0.0991	0.4445	1.9321	-0.4441	-0.0462	-0.4698	0.5276
adenosine	Nucleotide	Purine Metabolism, Adenine containing	-0.0403	-0.4684	-0.5476	-0.6198	1.1612	0.2783	0.6690	-0.2711	0.3657	4.1732
adenosine 3',5'-cyclic monophosphate (cAMP)	Nucleotide	Purine Metabolism, Adenine containing	-0.5503	-1.0036	-0.1514	0.6957	-0.5099	0.0317	-1.5154	0.9774	0.9305	-2.2715
adenosine 5'-monophosphate (AMP)	Nucleotide	Purine Metabolism, Adenine containing	1.0534	0.1244	-0.8939	1.0002	-0.9582	-0.9714	-1.2512	0.3366	-0.2159	1.8576
N1-methyladenosine	Nucleotide	Purine Metabolism, Adenine containing	-1.8330	-0.0170	-0.7550	-1.6511	-0.0056	0.7152	-0.8385	0.7056	-0.0784	0.4269
N6-carbamoylthreonyladenosine	Nucleotide	Purine Metabolism, Adenine containing	-0.7679	0.7002	-0.0461	-0.2013	0.2138	0.6855	-2.4221	0.2034	0.1044	0.4930
N6-methyladenosine	Nucleotide	Purine Metabolism, Adenine containing	-1.1333	0.2062	-0.1713	-2.4382	-1.0885	2.8687	-0.5409	0.5889	-1.8139	-0.5835
N6-succinyladenosine	Nucleotide	Purine Metabolism, Adenine containing	0.4222	1.5417	0.3012	0.8465	-1.0910	-0.9546	-1.5339	-0.6057	0.0098	0.1904
7-methylguanine	Nucleotide	Purine Metabolism, Guanine containing	-1.4785	-0.4756	-0.4778	-0.6630	0.7231	1.9987	-1.2235	1.0911	-0.2555	-0.0334
guanosine	Nucleotide	Purine Metabolism, Guanine containing	-0.6785	-0.2359	-1.1136	0.1216	0.3844	0.6946	-0.9699	1.3992	0.4410	-1.6012
N2,N2-dimethylguanosine	Nucleotide	Purine Metabolism, Guanine containing	-1.2249	-0.7945	-0.3554	-1.4217	0.9009	1.7043	-0.7969	0.6706	-0.7151	0.7243
N2-methylguanosine	Nucleotide	Purine Metabolism, Guanine containing	-0.6844	-2.6433	-0.7416	-1.5444	0.9710	0.8868	0.3381	0.6980	0.8309	0.2000
2'-deoxycytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	-0.2925	-0.6886	0.1800	-1.7927	1.2464	1.0158	-1.8095	-0.5229	-0.2056	-0.0507
cytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	-1.3292	0.1148	-0.7990	-0.0315	1.5279	0.1450	-2.1519	0.0042	-0.0444	-0.2031
orotate	Nucleotide	Pyrimidine Metabolism, Orotate containing	-1.3950	0.6879	-1.1037	0.0029	-0.2614	-0.6467	0.6651	0.6347	0.0600	-0.4098
orotidine	Nucleotide	Pyrimidine Metabolism, Orotate containing	-0.5570	0.6885	-0.2973	0.1129	1.5899	0.8050	-0.8802	-0.0164	-0.1549	0.1979
3-aminoisobutyrate	Nucleotide	Pyrimidine Metabolism, Thymine containing	-1.0462	0.7468	-0.4321	-1.0415	1.4664	0.1356	-0.1130	1.1251	0.8810	1.1983
5,6-dihydrothymine	Nucleotide	Pyrimidine Metabolism, Thymine containing	-0.9378	-1.6754	0.1372	1.4149	-0.1986	2.6985	-0.7841	1.7675	0.6110	1.3736
2'-deoxyuridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	-1.1192	-0.5038	0.2160	-0.7077	-1.1113	1.5336	-1.1243	-0.3846	1.2861	0.6128
3-ureidopropionate	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.2793	-0.8365	1.0055	0.8644	-0.7912	-0.7325	-2.3789	0.4905	0.6142	-0.3580
5-methyluridine (ribothymidine)	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.3159	-0.7099	-1.5540	-1.0884	-1.4252	1.4564	0.4823	0.3914	1.2501	0.0745
N-acetyl-beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.2640	-0.0910	-1.0054	-1.1922	-0.0325	0.9471	0.3744	0.2762	-0.4191	0.7681
pseudouridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	-1.0227	-0.1558	-0.9498	0.3269	2.8245	0.6588	-1.2166	-0.1799	0.1567	0.0416
uracil	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.8615	-1.2940	-0.5639	-1.0591	1.0416	0.5602	-2.4518	0.2259	0.0555	0.9223
uridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	-0.9355	-0.6615	-0.7666	-0.4939	0.2598	0.7223	-2.2539	0.4617	0.9514	1.4062
cyclo(ala-pro)	Peptide	Dipeptide	-0.1941	-0.1727	0.0833	1.1539	1.1950	-0.2260	-2.0441	2.9575	1.6534	-0.8371
cyclo(pro-val)	Peptide	Dipeptide	-0.5388	0.3231	0.7116	-0.0399	-0.5411	-0.5414	-0.5406	4.3413	-0.5375	-0.5404
glycylproline	Peptide	Dipeptide	-1.1606	-0.2627	0.1621	-0.9459	1.6327	0.0564	-0.9018	1.2532	-0.0350	1.7118
leucylproline	Peptide	Dipeptide	-0.6371	-0.6407	0.5438	-0.6483	-0.6331	-0.6165	-0.6399	0.8046	-0.6125	-0.6211
pyroglutamylglutamine	Peptide	Dipeptide	-0.3822	1.0640	-1.4390	1.6662	-1.4578	0.4924	-0.4163	-0.2236	-0.0244	-0.2161
homocarnosine	Peptide	Dipeptide Derivative	-1.2398	-0.3474	0.3446	-0.7602	0.5643	1.0285	-0.9417	0.4509	0.7324	0.6115
gamma-glutamyl-epsilon-lysine	Peptide	Gamma-glutamyl Amino Acid	-0.3437	0.5843	-0.5716	0.6972	-0.3589	1.0597	-1.3543	-0.1951	-0.6451	0.1870
gamma-glutamylalanine	Peptide	Gamma-glutamyl Amino Acid	-0.3106	0.5495	0.2607	1.5481	0.0330	-1.0342	-1.1026	-0.4493	-1.2514	-0.8065
gamma-glutamylglutamine	Peptide	Gamma-glutamyl Amino Acid	-0.5177	-1.1266	-0.1370	1.8395	-2.3001	0.0618	-0.2447	0.6341	-0.0945	-0.4273
gamma-glutamylhistidine	Peptide	Gamma-glutamyl Amino Acid	0.0022	0.8217	0.2052	1.5658	0.0688	1.4741	-0.9809	-0.4930	-0.4612	0.2904
gamma-glutamylisoleucine*	Peptide	Gamma-glutamyl Amino Acid	-0.2991	-1.0216	-0.8760	1.4180	0.9560	1.5215	-1.0203	-0.9411	-1.0319	-0.4403
gamma-glutamylleucine	Peptide	Gamma-glutamyl Amino Acid	-0.9164	-1.4844	0.1937	0.3331	0.0519	1.2957	-0.9978	-1.4737	-1.4779	0.4229
gamma-glutamylmethionine	Peptide	Gamma-glutamyl Amino Acid	1.1761	0.9411	-1.0585	-1.0664	-1.0755	0.7158	-0.3186	-0.4349	-1.0663	-1.0721
gamma-glutamylphenylalanine	Peptide	Gamma-glutamyl Amino Acid	-0.5604	-0.6480	-0.6283	2.0264	0.7929	-0.6483	1.0443	-0.6378	-0.6308	-0.6378
gamma-glutamylthreonine*	Peptide	Gamma-glutamyl Amino Acid	0.9841	0.3413	-1.0253	2.0429	0.8741	1.1709	-2.1786	-0.5994	-1.1350	-0.3183
gamma-glutamyltyrosine	Peptide	Gamma-glutamyl Amino Acid	-0.3815	-0.4180	-0.3988	0.5487	-0.3916	1.9308	-0.3923	-0.3932	-0.4081	-0.3819
gamma-glutamylvaline	Peptide	Gamma-glutamyl Amino Acid	-0.1289	0.5672	-0.2930	0.9413	0.6730	0.7740	-1.0365	-1.0695	-0.2363	-0.0734
gamma-glutamyl-alpha-lysine	Peptide	Gamma-glutamyl Amino Acid	0.02231	0.77519	-0.5857	0.50681	-0.5513	0.49835	-1.5078	-0.0855	-0.8728	-0.4872
tartronate (hydroxymalonate)	Xenobiotics	Bacterial/Fungal	1.3398	-0.5341	-0.7297	0.1297	-0.2139	-0.3291	1.2338	-0.5951	0.7597	1.9045
4-methylcatechol sulfate	Xenobiotics	Benzoate Metabolism	-0.1637	-0.1987	-0.1723	-0.1982	-0.2045	-0.1567	-0.2040	-0.1806	-0.1578	-0.1749
catechol sulfate	Xenobiotics	Benzoate Metabolism	2.1887	1.5078	-0.6417	-0.7061	-0.7098	-0.7119	-0.6968	-0.1432	-0.6981	-0.7071
hippurate	Xenobiotics	Benzoate Metabolism	0.0893	-1.1304	0.0059	-0.7647	0.6866	0.7814	2.4330	-0.1250	1.5942	0.7229
methyl-4-hydroxybenzoate sulfate	Xenobiotics	Benzoate Metabolism	-0.7243	-0.7233	-0.7235	-0.6712	0.6101	-0.7250	-0.7172	0.1961	1.4742	-0.7180
1,2-propanediol	Xenobiotics	Chemical	-0.4492	0.2094	-0.4422	0.9081	-0.4523	1.6483	3.4054	-0.4490	-0.4431	-0.3495
1,3-propanediol	Xenobiotics	Chemical	0.2353	0.1712	-0.8401	-0.8369	0.4580	0.5685	-0.7061	0.8538	-0.8397	-0.3036
2-aminophenol sulfate	Xenobiotics	Chemical	-0.3709	-0.3657	-0.3736	-0.3770	3.1487	-0.3715	-0.3749	3.5151	0.1532	-0.3761
3-hydroxypyridine sulfate	Xenobiotics	Chemical	-1.0426	1.5589	-1.4563	-0.7896	-1.2784	0.4519	-0.5527	-1.3238	0.8347	-0.3436

Supplemental Table 2. Z-scores for Population Baseline

			Heme present in samples								
Biochemical	Super Pathway	Sub Pathway	CSF310	CSF311	CSF312	CSF314	CSF315	CSF316	CSF321	CSF324	CSF326	CSF330
dimethyl sulfone	Xenobiotics	Chemical	-0.7754	0.1848	-0.1271	-0.9910	-0.5377	-0.3038	-0.4267	0.2181	2.4548	0.6008
O-sulfo-L-tyrosine	Xenobiotics	Chemical	-0.9185	0.3005	-0.6874	0.0293	2.2114	1.2014	-0.8195	-0.0989	-0.7211	0.5829
succinimide	Xenobiotics	Chemical	-0.2797	-0.9432	-0.5943	-0.6203	0.1358	-0.0118	-1.6143	0.1105	0.4136	-0.0366
sulfate*	Xenobiotics	Chemical	-0.5069	0.4666	-0.4076	-0.0933	1.7610	1.7323	-2.4360	0.1340	0.2443	0.5115
trizma acetate	Xenobiotics	Chemical	-0.6013	-0.2677	-0.3064	0.0208	-0.1346	-0.2117	3.1244	-0.6428	-0.6265	-0.1624
2-hydroxyacetaminophen sulfate*	Xenobiotics	Drug	-0.3347	-0.3308	-0.3326	3.9115	-0.3284	-0.3369	1.8738	-0.3411	-0.3219	-0.3341
2-methoxyacetaminophen glucuronide*	Xenobiotics	Drug	-0.2877	-0.2868	-0.3012	2.0971	-0.2957	-0.2857	1.3303	-0.2870	-0.2864	-0.3014
2-methoxyacetaminophen sulfate*	Xenobiotics	Drug	-0.2671	-0.2661	-0.2677	1.0815	-0.2685	-0.2565	5.0023	0.9793	-0.2698	-0.2532
3-(cystein-S-yl)acetaminophen*	Xenobiotics	Drug	-0.2419	-0.2372	-0.2518	-0.2264	-0.2564	-0.2310	1.8310	-0.2336	-0.2490	-0.2297
4-acetamidophenol	Xenobiotics	Drug	-0.4782	-0.4756	-0.4758	2.3011	0.7566	-0.1223	2.6082	2.5753	-0.4748	-0.4765
4-acetamidophenylglucuronide	Xenobiotics	Drug	-0.4253	-0.4281	-0.4243	2.5407	1.4563	-0.4209	1.7963	-0.4208	-0.4213	-0.4240
4-acetaminophen sulfate	Xenobiotics	Drug	-0.4788	-0.4790	-0.4773	2.1998	1.2132	-0.4746	2.6945	2.2077	-0.4780	-0.4785
5-sulfosalicylate	Xenobiotics	Drug	-0.6024	-0.6011	-0.6017	-0.6002	2.1973	-0.6023	2.7047	-0.6011	0.9072	-0.6063
carbamazepine 10,11-epoxide*	Xenobiotics	Drug	-0.1823	-0.1767	-0.1845	-0.1748	-0.1917	-0.1913	-0.1828	-0.1855	5.2946	-0.1844
fluoxetine	Xenobiotics	Drug	-0.1863	-0.1813	-0.1847	-0.1844	-0.1762	-0.1886	-0.1772	-0.1772	-0.1863	-0.1799
lidocaine	Xenobiotics	Drug	2.0325	1.6113	1.2600	-0.0488	0.3758	0.2524	-0.2126	-1.3356	-0.3219	-1.3377
N-ethylglycinexylidide	Xenobiotics	Drug	1.2385	1.0176	-0.5154	-0.5166	-0.5142	-0.5183	-0.5156	-0.5146	-0.5132	-0.5187
salicylate	Xenobiotics	Drug	0.3279	1.2508	-0.9283	-0.9200	0.8470	-0.9241	1.0080	1.9219	0.5481	-0.9250
topiramate	Xenobiotics	Drug	-0.2631	3.6784	-0.2596	3.6792	-0.2657	-0.2623	-0.2645	-0.2652	-0.2596	-0.2639
pregabalin	Xenobiotics	Drug	-0.1788	-0.1825	-0.1851	-0.1862	-0.1844	-0.1869	-0.1783	-0.1818	-0.1833	-0.1782
sulfamethoxazole	Xenobiotics	Drug	-0.1809	-0.1836	-0.1801	-0.1832	-0.1818	-0.185	-0.1828	-0.1855	-0.1826	-0.1838
cetirizine	Xenobiotics	Drug	-0.3241	3.40713	-0.3253	-0.3235	-0.3237	-0.3277	-0.3254	-0.3276	-0.3291	-0.3217
2-piperidinone	Xenobiotics	Food Component/Plant	0.2708	-1.1324	-0.1380	-0.4801	1.2785	1.5564	0.6733	0.1558	-0.7819	1.1284
betonicine	Xenobiotics	Food Component/Plant	2.0970	0.9123	-0.2515	-1.0830	-1.0820	-1.0798	0.3740	-1.0854	-0.8355	-0.2879
ergothioneine	Xenobiotics	Food Component/Plant	-0.6292	1.2757	1.0571	1.1859	-1.1667	-1.4321	-1.4370	1.1209	-0.9339	0.5831
erythritol	Xenobiotics	Food Component/Plant	0.2587	1.5158	-0.3607	0.9176	1.5532	-0.6063	0.0965	-0.8391	-0.5736	-0.8281
gluconate	Xenobiotics	Food Component/Plant	-0.8240	0.2824	-0.1660	-0.5429	0.7893	-0.5425	0.1177	0.6610	0.0596	0.1205
indolin-2-one	Xenobiotics	Food Component/Plant	0.6663	-0.0191	1.1238	-1.1370	0.9046	1.3437	0.6494	1.2043	0.2986	-1.1356
levulinate (4-oxovalerate)	Xenobiotics	Food Component/Plant	-1.1373	0.4718	-0.1614	1.3292	0.9544	-0.8401	-1.2807	1.5642	-0.8761	-1.5090
piperine	Xenobiotics	Food Component/Plant	2.1153	1.0338	-0.6613	-0.6632	-0.0473	-0.6632	0.7809	-0.6600	-0.6633	-0.6609
quinate	Xenobiotics	Food Component/Plant	-0.3313	1.4059	0.4874	-0.7232	1.3024	-0.7251	-0.7225	-0.7239	-0.7245	1.6409
S-allylcysteine	Xenobiotics	Food Component/Plant	1.4363	0.9540	-0.5536	-0.5610	-0.5554	-0.5608	-0.5550	-0.5534	-0.5565	-0.5570
stachydrine	Xenobiotics	Food Component/Plant	1.8312	0.8421	0.3325	-1.6429	-0.7936	-1.5702	0.0761	-1.0287	-0.6044	-0.0682
tartarate	Xenobiotics	Food Component/Plant	-0.0160	1.2306	0.4535	0.8982	1.3337	0.0099	0.0704	1.1152	-1.3896	2.2778
acesulfame	Xenobiotics	Food Component/Plant	-0.5105	-0.5078	-0.5039	1.51598	3.07635	-0.5111	-0.5094	-0.5026	1.78966	-0.5057
3-methylxanthine	Xenobiotics	Xanthine Metabolism	-0.4980	0.1689	1.8581	-0.5086	-0.4914	-0.5082	-0.5005	-0.5099	-0.4821	-0.4847
5-acetylamino-6-amino-3-methyluracil	Xenobiotics	Xanthine Metabolism	-0.2591	-0.2634	0.3623	-0.2617	-0.2655	-0.2744	-0.2772	-0.2741	-0.2741	-0.2560
7-methylxanthine	Xenobiotics	Xanthine Metabolism	-0.6328	-0.5207	1.5322	-0.6195	-0.6209	-0.6163	-0.6173	-0.6253	-0.6191	-0.6197
caffeine	Xenobiotics	Xanthine Metabolism	0.3283	2.9961	0.8229	-0.6112	-0.6131	0.4129	-0.6104	-0.6140	-0.6103	-0.6111
paraxanthine	Xenobiotics	Xanthine Metabolism	0.4836	1.4830	0.9641	-0.6485	-0.6564	-0.2159	-0.6542	-0.6557	-0.6558	-0.6495
theobromine	Xenobiotics	Xanthine Metabolism	0.8079	1.4439	1.1750	-0.9352	-0.9362	0.0373	-0.9379	-0.9351	-0.7941	-0.9362
theophylline	Xenobiotics	Xanthine Metabolism	-0.4954	1.4326	1.4926	-0.4936	-0.4978	-0.4892	-0.5024	-0.5010	-0.4994	-0.5033
thioproline	Xenobiotics	Chemical	0.1844	1.26525	0.68037	-0.7707	2.44639	1.30658	0.72709	-0.5159	-1.0305	1.99833

Supplemental Table 3. Key Z-scored molecules in 30 CSF samples and samples with heme.

Sample ID	Key Z-scored compounds (Z-scores in parentheses)	Comments
CSF301	6/8 top z-scored compounds acetaminophen metabolites	Observable intervention markers
CSF302	pregabalin (5.29), fluoxetine (5.29), cetirizine (2.92), dopamine 3-O-sulfate (2.70), homovanillate (-3.25)	Observable intervention markers; possible dopamine/catecholamine pathway disorder
CSF304	cetirizine (2.45)	Observable intervention marker
CSF305	heme detected in sample	
CSF308	sulfamethoxazole (5.29)	Observable intervention marker
CSF310	heme detected in sample	
CSF311	topiramate (3.68), cetirizine (3.41), heme detected in sample	Observable intervention markers
CSF312	heme detected in sample	
CSF313	glucose (-2.90), fructose (-2.63), mannose (-2.02)	No *GLUT1* variants detected. Succinyladenosine testing revealed level of 0.3 µM
CSF314	6/8 top z-scored compounds acetaminophen metabolites and topiramate, heme detected in sample.	Observable intervention markers
CSF315	glycerol (4.85), glycerol-3-phosphate (-1.59), heme detected in sample	Glycerol quantitative trait loci identified rs117066088, rs140943510, rs76608797 [MIM:614411; GLYCQTL]
CSF316	heme detected in sample	
CSF318	pyridoxine (5.29), pyridoxal (3.82), pyridoxate (3.55)	Observable intervention markers
CSF321	acetaminophen and aspirin metabolites among top z-scored compounds, heme detected in sample.	Observable intervention markers
CSF322	136 compounds (including several steroid hormones) had z-scores greater than 2	
CSF324	heme detected in sample	
CSF326	carbamazerine-10,11- epoxide* (5.29), heme detected in sample	Observable intervention marker
CSF329	succinimide (3.87)	
CSF330	heme detected in sample	

Kennedy et al. Elucidation of the Complex Metabolic Profile of Cerebrospinal Fluid Using an Untargeted Biochemical Profi

Supplemental Table 3. Correlation of Molecules Between CSF and EDTA Plasma

BIOCHEMICAL	Super Family	Subfamily	R Value
stachydrine	Xenobiotics	Food Component/Plant	0.971044
pyridoxate	Cofactors and Vitamins	Vitamin B6 Metabolism	0.969893
1,5-anhydroglucitol (1,5-AG)	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.933673
p-cresol sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.915477
pantothenate (vitamin B5)	Cofactors and Vitamins	Pantothenate and CoA Metabolism	0.88484
urea	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.879918
methionine sulfone	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.877218
3-methoxytyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.872818
3-hydroxybutyrate (BHBA)	Lipid	Ketone Bodies	0.868016
N6-succinyladenosine	Nucleotide	Purine Metabolism, Adenine containing	0.855326
3-hydroxy-3-methylglutarate	Lipid	Mevalonate Metabolism	0.818865
myo-inositol	Lipid	Inositol Metabolism	0.805937
N-delta-acetylornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.797318
phenol sulfate	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.794274
beta-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.787116
alpha-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.771023
trimethylamine N-oxide	Lipid	Phospholipid Metabolism	0.770927
phenylacetylglutamine	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.768393
picolinate	Amino Acid	Tryptophan Metabolism	0.743864
N1-Methyl-2-pyridone-5-carboxamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.734004
1-methylnicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.72052
N-acetylaspartate (NAA)	Amino Acid	Alanine and Aspartate Metabolism	0.720091
dimethylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.716961
kynurenine	Amino Acid	Tryptophan Metabolism	0.711586
arginate	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.704855
homoarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.703587
2-hydroxybutyrate/2-hydroxyisobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.680585
7-methylguanine	Nucleotide	Purine Metabolism, Guanine containing	0.678521
1-methyladenosine	Nucleotide	Purine Metabolism, Adenine containing	0.670817
N-acetylputrescine	Amino Acid	Polyamine Metabolism	0.667395
urate	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.662498
N2,N2-dimethylguanosine	Nucleotide	Purine Metabolism, Guanine containing	0.650957
prolylhydroxyproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.640048
lactate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.637187
pipecolate	Amino Acid	Lysine Metabolism	0.623308
serine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.622439
N-acetylhistidine	Amino Acid	Histidine Metabolism	0.619984
mannose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.619432
4-guanidinobutanoate	Amino Acid	Guanidino and Acetamido Metabolism	0.615404
carnitine	Lipid	Carnitine Metabolism	0.610975
N-acetylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.602264
beta-citryl-glutamate	Amino Acid	Glutamate Metabolism	0.58386
hydroxyproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.580528
2-aminobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.578511
4-acetamidobutanoate	Amino Acid	Polyamine Metabolism	0.577443
C-glycosyltryptophan*	Amino Acid	Tryptophan Metabolism	0.567648
glutamate	Amino Acid	Glutamate Metabolism	0.566928
creatinine	Amino Acid	Creatine Metabolism	0.563536
N-acetylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.552807
1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	Lipid	Phospholipid Metabolism	0.535208
acetylcarnitine (C2)	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.53111
1-methylhistidine	Amino Acid	Histidine Metabolism	0.52394
sulfate*	Xenobiotics	Chemical	0.517726
N-acetylneuraminate	Carbohydrate	Aminosugar Metabolism	0.499693
choline	Lipid	Phospholipid Metabolism	0.493838
N-acetylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.488254
propionylcarnitine (C3)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.483763
N-acetylthreonine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.481687
5-methyluridine (ribothymidine)	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.472621
N-acetylalanine	Amino Acid	Alanine and Aspartate Metabolism	0.46724
tartronate (hydroxymalonate)	Xenobiotics	Bacterial/Fungal	0.460685
1-methylimidazoleacetate	Amino Acid	Histidine Metabolism	0.446182
isobutyrylcarnitine (C4)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.443013
creatine	Amino Acid	Creatine Metabolism	0.440123
gamma-glutamylvaline	Peptide	Gamma-glutamyl Amino Acid	0.436698
xanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.434722
ethylmalonate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.430952
N-formylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.405444
glycerate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.403274
asparagine	Amino Acid	Alanine and Aspartate Metabolism	0.395706
6-oxopiperidine-2-carboxylic acid	Xenobiotics	Drug	0.391818
1,2-dipalmitoyl-GPC (16:0/16:0)	Lipid	Phospholipid Metabolism	0.39163
threonine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.390394
N-acetylvaline	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.371849
indoleacetate	Amino Acid	Tryptophan Metabolism	0.366371

Supplemental Table 3. Correlation of Molecules Between CSF and EDTA Plasma

BIOCHEMICAL	Super Family	Subfamily	R Value
pseudouridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.362021
gamma-glutamylglutamine	Peptide	Gamma-glutamyl Amino Acid	0.35823
methionine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.351347
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	Lipid	Phospholipid Metabolism	0.335564
glycerol	Lipid	Glycerolipid Metabolism	0.321109
betaine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.317125
phosphocholine	Lipid	Phospholipid Metabolism	0.310433
succinylcarnitine (C4)	Energy	TCA Cycle	0.306347
5,6-dihydrothymine	Nucleotide	Pyrimidine Metabolism, Thymine containing	0.296726
1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*	Lipid	Phospholipid Metabolism	0.279967
2-hydroxy-3-methylvalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.275055
N-acetylglutamate	Amino Acid	Glutamate Metabolism	0.267855
O-sulfo-L-tyrosine	Xenobiotics	Chemical	0.265452
N-acetyl-beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.247168
cis-4-decenoyl carnitine	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	0.241869
adenine	Nucleotide	Purine Metabolism, Adenine containing	0.238977
cysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.234002
gamma-glutamylthreonine*	Peptide	Gamma-glutamyl Amino Acid	0.223436
1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	Lipid	Phospholipid Metabolism	0.219881
3-hydroxy-2-ethylpropionate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.2056
2-aminoheptanoate	Lipid	Fatty Acid, Amino	0.204523
ornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.202843
methylmalonate (MMA)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.200623
1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4)	Lipid	Phospholipid Metabolism	0.194201
guanidinoacetate	Amino Acid	Creatine Metabolism	0.193038
inosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.183467
ribitol	Carbohydrate	Pentose Metabolism	0.175958
dimethylarginine (SDMA + ADMA)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.170091
aspartate	Amino Acid	Alanine and Aspartate Metabolism	0.156139
gulonic acid*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.152583
N6,N6,N6-trimethyllysine	Amino Acid	Lysine Metabolism	0.151
glutamine	Amino Acid	Glutamate Metabolism	0.147714
glucose	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.14399
palmitoyl sphingomyelin (d18:1/16:0)	Lipid	Sphingolipid Metabolism	0.131589
hypoxanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.125361
phosphate	Energy	Oxidative Phosphorylation	0.119409
uridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.118148
glycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.116811
fructose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.106116
5-oxoproline	Amino Acid	Glutathione Metabolism	0.104451
glucuronate	Carbohydrate	Aminosugar Metabolism	0.101878
1-stearoyl-GPC (18:0)	Lipid	Lysolipid	0.101615
alanine	Amino Acid	Alanine and Aspartate Metabolism	0.095938
arabonate/xylonate	Carbohydrate	Pentose Phosphate Pathway	0.092224
arabitol/xylitol	Carbohydrate	Pentose Metabolism	0.086287
tyrosine	Amino Acid	Phenylalanine and Tyrosine Metabolism	0.078154
2-methylbutyroylcarnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.071792
threonate	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.070256
3-methylglutaconate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.060601
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	Lipid	Phospholipid Metabolism	0.0604
proline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.059144
3-methyl-2-oxovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.058473
arginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.057716
oxalate (ethanedioate)	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.053909
N-acetylarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.040555
1-palmitoyl-GPC (16:0)	Lipid	Lysolipid	0.034549
lysine	Amino Acid	Lysine Metabolism	0.030192
maleate	Lipid	Fatty Acid, Dicarboxylate	0.021532
cholesterol	Lipid	Sterol	0.006758
taurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.00539
leucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.00807
alpha-ketoglutarate	Energy	TCA Cycle	-0.01831
orotate	Nucleotide	Pyrimidine Metabolism, Orotate containing	-0.02063
malate	Energy	TCA Cycle	-0.0366
erythritol	Xenobiotics	Food Component/Plant	-0.03691
valine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.0471
citrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	-0.05305
mannitol/sorbitol	Carbohydrate	Fructose, Mannose and Galactose Metabolism	-0.05889
erythronate*	Carbohydrate	Aminosugar Metabolism	-0.07068
isoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.07734
3-hydroxyisobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.07925
succinate	Energy	TCA Cycle	-0.08315
1,2-dioleoyl-GPC (18:1/18:1)*	Lipid	Phospholipid Metabolism	-0.08885
gluconate	Xenobiotics	Food Component/Plant	-0.12787
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*	Lipid	Phospholipid Metabolism	-0.13108

Supplemental Table 3. Correlation of Molecules Between CSF and EDTA Plasma

BIOCHEMICAL	Super Family	Subfamily	R Value
deoxycarnitine	Lipid	Carnitine Metabolism	-0.14361
sphingomyelin	Lipid	Sphingolipid Metabolism	-0.14794
histidine	Amino Acid	Histidine Metabolism	-0.14893
methionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.14901
1-stearoyl-2-oleoyl-GPC (18:0/18:1)	Lipid	Phospholipid Metabolism	-0.16262
oleoyl sphingomyelin	Lipid	Sphingolipid Metabolism	-0.16609
3-(4-hydroxyphenyl)lactate (HPLA)	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.16784
tryptophan	Amino Acid	Tryptophan Metabolism	-0.17372
1-palmitoyl-2-dihomo-linolenoyl-GPC (16:0/20:3n3 or 6)*	Lipid	Phospholipid Metabolism	-0.1809
ribonate	Carbohydrate	Pentose Metabolism	-0.19397
1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)	Lipid	Phospholipid Metabolism	-0.20872
malonate	Lipid	Fatty Acid Synthesis	-0.22534
citrate	Energy	TCA Cycle	-0.23207
phenylalanine	Amino Acid	Phenylalanine and Tyrosine Metabolism	-0.26911
allantoin	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	-0.34467
tiglyl carnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	-0.35128
1-oleoyl-GPC (18:1)	Lipid	Lysolipid	-0.36701
glutaroylcarnitine (C5)	Amino Acid	Lysine Metabolism	-0.42072