

Supplementary Table 1.

Metabolic Pathway	Metabolite Names
Glycosphingolipid metabolism	Choline phosphate; Phosphorylcholine; Phosphocholine; D-Glucose; Grape sugar; Sphinganine; Dihydrosphingosine; Psychosine; Galactosylsphingosine; N-Acetylneuraminate; N-Acetylneuraminic acid; 5-Acetamido-3,5-dideoxy-D-glycero-D-galacto-2-nonulosonic acid; CMP; Cytidine-5'-monophosphate; Sphingosine; Sphingenine; Sphingoid; 3-Dehydrosphinganine; beta-D-Galactose
Glycerophospholipid metabolism	Choline phosphate; Phosphorylcholine; Phosphocholine; Glycerol; Glycerin; 1,2,3-Trihydroxypropane; Acetylcholine; Sphinganine; Dihydrosphingosine; myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; CTP; Cytidine 5'-triphosphate; Linoleate; Linoleic acid; (9Z,12Z)-Octadecadienoic acid; 9-cis,12-cis-Octadecadienoate; CMP; Cytidine-5'-monophosphate; (5Z,8Z,11Z,14Z)-Icosatetraenoic acid; Arachidonate; Arachidonic acid; Sphingosine; Sphingenine; Sphingoid; Inositol 1-phosphate; myo-Inositol 1-phosphate; 1D-myo-Inositol 1-phosphate; D-myo-Inositol 1-phosphate; 1D-myo-Inositol 1-monophosphate
Biopterin metabolism	L-Phenylalanine; L-Tyrosine; (S)-3-(p-Hydroxyphenyl)alanine; (S)-2-Amino-3-(p-hydroxyphenyl)propionic acid; Tetrahydrobiopterin; 5,6,7,8-Tetrahydrobiopterin; 6-Pyruvoyltetrahydropterin; 6-(1,2-Dioxopropyl)-5,6,7,8-tetrahydropterin; quinonoid dihydrobiopterin
Tyrosine metabolism	Phenethylamine; Tetrahydrobiopterin; 5,6,7,8-Tetrahydrobiopterin; L-Phenylalanine; Ascorbate; Ascorbic acid; L-Ascorbate; L-Ascorbic acid; L-Tyrosine; (S)-3-(p-Hydroxyphenyl)alanine; (S)-2-Amino-3-(p-hydroxyphenyl)propionic acid; Dopamine; 4-(2-Aminoethyl)-1,2-benzenediol; 4-(2-Aminoethyl)benzene-1,2-diol; 3,4-Dihydroxyphenylacetaldehyde; 3-O-methyl dopa
N-Glycan biosynthesis	D-Mannose; Mannose; Seminose; CMP; Cytidine-5'-monophosphate; CTP; Cytidine 5'-triphosphate; Dolichyl phosphate D-mannose; D-Glucose; Grape sugar; Dextrose
Linoleate metabolism	Ascorbate; Ascorbic acid; L-Ascorbate; L-Ascorbic acid; Linoleate; Linoleic acid; (9Z,12Z)-Octadecadienoic acid; 9-cis,12-cis-Octadecadienoate; 9(S)-HPODE; 9(S)-HPOD; (9Z,11E)-(13S)-13-Hydroperoxyoctadeca-9,11-dienoic acid; (9Z,11E)-(13S)-13-Hydroperoxyoctadeca-9,11-dienoate; 13(S)-HPODE; 13S-Hydroperoxy-9Z,11E-octadecadienoic acid
N-Glycan Degradation	D-Mannose; Mannose; Seminose; N-Acetylneuraminate; N-Acetylneuraminic acid; 5-Acetamido-3,5-dideoxy-D-glycero-D-galacto-2-nonulosonic acid; D-Galactose
Pentose phosphate pathway	D-Sedoheptulose 1,7-bisphosphate; Deoxyribose; 2-Deoxy-D-erythro-pentose; Thyminose; D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Sedoheptulose 1-phosphate; Sedoheptulose 7-phosphate; D-Glucose 6-phosphate; Glucose 6-phosphate; D-Sedoheptulose 7-phosphate; beta-D-Fructose 6-phosphate
Caffeine metabolism	1,7-Dimethylxanthine; 1-Methylxanthine
Alkaloid biosynthesis II	Benzoate; Benzoic acid; Benzenecarboxylic acid; Phenylformic acid; N-Methylputrescine
Glycosphingolipid biosynthesis - ganglioseries	CMP; Cytidine-5'-monophosphate; Chondroitin; D-Galactose\$Galactose
Pyrimidine metabolism	Deoxyribose; 2-Deoxy-D-erythro-pentose; Thyminose; \$dTMP; Thymidine 5'-phosphate; Deoxythymidine 5'-phosphate; Thymidylic acid; 5'-Thymidylic acid; Thymidine monophosphate; Deoxythymidylic acid; dUMP; Deoxyuridylic acid; Deoxyuridine monophosphate; Deoxyuridine 5'-phosphate; 2'-Deoxyuridine 5'-phosphate\$D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; 5,6-Dihydrouracil; 2,4(1H,3H)-Pyrimidinedione, dihydro-; Dihydrouracile; Dihydrouracil; 5,6-Dihydro-2,4-dihydroxypyrimidine; Dihydrofolate; Dihydrofolic acid; 7,8-Dihydrofolate; 7,8-Dihydrofolic acid; CTP; Cytidine 5'-triphosphate; CMP; Cytidine-5'-monophosphate; 2-Deoxy-D-ribose 1-phosphate; dGTP; 2'-Deoxyguanosine 5'-triphosphate; Deoxyguanosine 5'-triphosphate; dUDP; 2'-Deoxyuridine 5'-diphosphate
Tryptophan metabolism	L-Tryptophan; Tryptophan; Indole-3-acetaldehyde; 2-(Indol-3-yl)acetaldehyde; 3-Hydroxyanthranilate; Indolepyruvate; Indolepyruvic acid; (Indol-3-yl)pyruvate; Indole-3-pyruvate; Tetrahydrobiopterin; 5,6,7,8-Tetrahydrobiopterin; 4,6-Dihydroxyquinoline; Quinoline-4,6-diol

