

**Supplemental table S1: List of Metabolites: MxP® Quant 500 Kit
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Alkaloids (1)	
Trigonelline	
Amine Oxides (1)	
Trimethylamine N-oxide	
Amino Acids (20)	
Alanine	Leucine
Arginine	Lysine
Asparagine	Methionine
Aspartate	Phenylalanine
Cysteine	Proline
Glutamate	Serine
Glutamine	Threonine
Glycine	Tryptophan
Histidine	Tyrosine
Isoleucine	Valine
Amino Acid Related (30)	
α -Aminoadipic acid	cis-4-Hydroxyproline
α -Aminobutyric acid	trans-4-Hydroxyproline
Acetylmethionine	Kynurenine
Asymmetric dimethylarginine	Methionine sulfoxide
Anserine	1-Methylhistidine
5-Aminovaleric acid	3-Methylhistidine
β -Aminobutyric acid	Nitrotyrosine
Betaine	Ornithine
Carnosine	Phenylacetyl glycine
Citrulline	Phenylalanine betaine
Creatinine	Proline betaine
Cystine	Sarcosine
Dihydroxyphenylalanine	Symmetric dimethylarginine
Homoarginine	Taurine
Homocysteine	Tryptophan betaine
Bile Acids (14)	
Cholic acid	Glycolithocholic acid sulfate
Chenodeoxycholic acid	Glycoursodeoxycholic acid
Deoxycholic acid	Taurocholic acid
Glycocholic acid	Taurochenodeoxycholic acid
Glycodeoxycholic acid	Taurodeoxycholic acid
Glycochenodeoxycholic acid	Taurolithocholic acid
Glycolithocholic acid	Tauromurocholic acid
Biogenic Amines (9)	
β -Alanine	Putrescine
γ -Aminobutyric acid	Serotonine
Dopamine	Spermidine
Histamine	Spermine

Phenylethylamine	
Carbohydrates and Related (1)	
Hexoses (including glucose)	
Carboxylic Acids (7)	
Aconitic acid	3-Hydroxyglutaric acid
Dodecanedioic acid	Lactic acid
Tetradecanedioic acid	Succinic acid
Hippuric acid	
Cresols (1)	
p-Cresol sulfate	
Fatty Acids (12)	
Lauric acid	Eicosenoic acid
Myristic acid	Eicosadienoic acid
Palmitic acid	Eicosatrienoic acid
Stearic acid	Arachidonic acid
Octadecenoic acid	Eicosapentaenoic acid
Octadecadienoic acid	Docosahexaenoic acid
Hormones and Related (4)	
Abscissic acid	Cortisone
Cortisol	Dehydroepiandrosterone sulfate
Indoles and Derivatives (4)	
Indole	3-Indolepropionic acid
3-Indoleacetic acid	Indoxyl sulfate
Nucleobases and Related (2)	
Hypoxanthine	Xanthine
Vitamins and Cofactors (1)	
Choline	
Acylcarnitines (40)	
Carnitine	Decenoylcarnitine
Acetylcarnitine	Decadienoylcarnitine
Propionylcarnitine	Dodecanoylcarnitine
Malonylcarnitine	Dodecanediocylcarnitine
Hydroxypropionylcarnitine	Dodecenoylcarnitine
Propenoylcarnitine	Tetradecanoylcarnitine
Butyrylcarnitine	Tetradecenoylcarnitine
Butenylcarnitine	Hydroxytetradecadienoylcarnitine
Valeryl carnitine	Tetradecadienoylcarnitine
Glutaryl carnitine	Hydrocytetradecadienoylcarnitine
Methylglutaryl carnitine	Hexadecanoylcarnitine
Hydroxyvaleryl carnitine	Hydroxyhexadecanoylcarnitine
Tiglylcarnitine	Hexadecenoylcarnitine
Glutaconyl carnitine	Hydroxyhexadecenoylcarnitine
Hexanoylcarnitine	Hexadecadienoylcarnitine
Hexenoylcarnitine	Hydroxyhexadecadienoylcarnitine
Pimeloylcarnitine	Octadecanoylcarnitine
Octanoylcarnitine	Octadecenoylcarnitine
Nonanoylcarnitine	Hydroxyoctadecenoylcarnitine

Decanoylcarnitine	Octadecadienylcarnitine
Lysophosphatidylcholines (14)	
lysoPC a C14:0	lysoPC a C20:3
lysoPC a C16:0	lysoPC a C20:4
lysoPC a C16:1	lysoPC a C24:0
lysoPC a C17:0	lysoPC a C26:0
lysoPC a C18:0	lysoPC a C26:1
lysoPC a C18:1	lysoPC a C28:0
lysoPC a C18:2	lysoPC a C28:1
Phosphatidylcholines (76)	
PC aa C24:0	PC ae C30:0
PC aa C26:0	PC ae C30:1
PC aa C28:1	PC ae C30:2
PC aa C30:0	PC ae C32:1
PC aa C30:2	PC ae C32:2
PC aa C32:0	PC ae C34:0
PC aa C32:1	PC ae C34:1
PC aa C32:2	PC ae C34:2
PC aa C32:3	PC ae C34:3
PC aa C34:1	PC ae C36:0
PC aa C34:2	PC ae C36:1
PC aa C34:3	PC ae C36:2
PC aa C34:4	PC ae C36:3
PC aa C36:0	PC ae C36:4
PC aa C36:1	PC ae C36:5
PC aa C36:2	PC ae C38:0
PC aa C36:3	PC ae C38:1
PC aa C36:4	PC ae C38:2
PC aa C36:5	PC ae C38:3
PC aa C36:6	PC ae C38:4
PC aa C38:0	PC ae C38:5
PC aa C38:1	PC ae C38:6
PC aa C38:3	PC ae C40:1
PC aa C38:4	PC ae C40:2
PC aa C38:5	PC ae C40:3
PC aa C38:6	PC ae C40:4
PC aa C40:1	PC ae C40:5
PC aa C40:2	PC ae C40:6
PC aa C40:3	PC ae C42:0
PC aa C40:4	PC ae C42:1
PC aa C40:5	PC ae C42:2
PC aa C40:6	PC ae C42:3
PC aa C42:0	PC ae C42:4
PC aa C42:1	PC ae C42:5
PC aa C42:2	PC ae C44:3
PC aa C42:4	PC ae C44:4
PC aa C42:5	PC ae C44:5

PC aa C42:6	PC ae C44:6
Sphingomyelins (15)	
SM (OH) C14:1	SM (OH) C22:2
SM C16:0	SM C22:3
SM C16:1	SM C24:0
SM (OH) C16:1	SM C24:1
SM C18:0	SM (OH) C24:1
SM C18:1	SM C26:0
SM C20:2	SM C26:1
SM (OH) C22:1	
Ceramides (28)	
Cer(d16:1/18:0)	Cer(d18:1/24:0)
Cer(d16:1/20:0)	Cer(d18:1/24:1)
Cer(d16:1/22:0)	Cer(d18:1/25:0)
Cer(d16:1/23:0)	Cer(d18:1/26:0)
Cer(d16:1/24:0)	Cer(d18:1/26:1)
Cer(d18:1/14:0)	Cer(d18:2/14:0)
Cer(d18:1/16:0)	Cer(d18:2/16:0)
Cer(d18:1/18:0(OH))	Cer(d18:2/18:0)
Cer(d18:1/18:0)	Cer(d18:2/18:1)
Cer(d18:1/18:1)	Cer(d18:2/20:0)
Cer(d18:1/20:0(OH))	Cer(d18:2/22:0)
Cer(d18:1/20:0)	Cer(d18:2/23:0)
Cer(d18:1/22:0)	Cer(d18:2/24:0)
Cer(d18:1/23:0)	Cer(d18:2/24:1)
Dihydroceramides (8)	
Cer(d18:0/18:0(OH))	Cer(d18:0/24:0)
Cer(d18:0/18:0)	Cer(d18:0/24:1)
Cer(d18:0/20:0)	Cer(d18:0/26:1(OH))
Cer(d18:0/22:0)	Cer(d18:0/26:1)
Hexosylceramides (19)	
HexCer(d16:1/22:0)	HexCer(d18:1/24:1)
HexCer(d16:1/24:0)	HexCer(d18:1/26:0)
HexCer(d18:1/14:0)	HexCer(d18:1/26:1)
HexCer(d18:1/16:0)	HexCer(d18:2/16:0)
HexCer(d18:1/18:0)	HexCer(d18:2/18:0)
HexCer(d18:1/18:1)	HexCer(d18:2/20:0)
HexCer(d18:1/20:0)	HexCer(d18:2/22:0)
HexCer(d18:1/22:0)	HexCer(d18:2/23:0)
HexCer(d18:1/23:0)	HexCer(d18:2/24:0)
HexCer(d18:1/24:0)	
Dihexosylceramides (9)	
Hex2Cer(d18:1/14:0)	Hex2Cer(d18:1/24:0)
Hex2Cer(d18:1/16:0)	Hex2Cer(d18:1/24:1)
Hex2Cer(d18:1/18:0)	Hex2Cer(d18:1/26:0)
Hex2Cer(d18:1/20:0)	Hex2Cer(d18:1/26:1)
Hex2Cer(d18:1/22:0)	

Trihexosylceramides (6)	
Hex3Cer(d18:1/16:0)	Hex3Cer(d18:1/26:1)
Hex3Cer(d18:1/18:0)	Hex3Cer(d18:1/20:0)
Hex3Cer(d18:1/24:1)	Hex3Cer(d18:1/22:0)
Cholesteryl Esters (22)	
CE(14:0)	CE(18:3)
CE(14:1)	CE(20:0)
CE(15:0)	CE(20:1)
CE(15:1)	CE(20:3)
CE(16:0)	CE(20:4)
CE(16:1)	CE(20:5)
CE(17:0)	CE(22:0)
CE(17:1)	CE(22:1)
CE(18:0)	CE(22:2)
CE(18:1)	CE(22:5)
CE(18:2)	CE(22:6)
Diglycerides (44)	
DG(14:0_14:0)	DG(18:1_18:2)
DG(14:0_18:1)	DG(18:1_18:3)
DG(14:0_18:2)	DG(18:1_18:4)
DG(14:0_20:0)	DG(18:1_20:0)
DG(14:1_18:1)	DG(18:1_20:1)
DG(14:1_20:2)	DG(18:1_20:2)
DG(16:0_16:0)	DG(18:1_20:3)
DG(16:0_16:1)	DG(18:1_20:4)
DG(16:0_18:1)	DG(18:1_22:5)
DG(16:0_18:2)	DG(18:1_22:6)
DG(16:0_20:0)	DG(18:2_18:2)
DG(16:0_20:3)	DG(18:2_18:3)
DG(16:0_20:4)	DG(18:2_18:4)
DG(16:1_18:0)	DG(18:2_20:0)
DG(16:1_18:1)	DG(18:2_20:4)
DG(16:1_18:2)	DG(18:3_18:3)
DG(16:1_20:0)	DG(18:3_20:2)
DG(17:0_17:1)	DG(21:0_22:6)
DG(17:0_18:1)	DG(22:1_22:2)
DG(18:0_20:0)	DG-O(14:0_18:2)
DG(18:0_20:4)	DG-O(16:0_18:1)
DG(18:1_18:1)	DG-O(16:0_20:4)
Triglycerides (242)	
TG(14:0_32:2)	TG(18:1_35:2)
TG(14:0_34:0)	TG(18:1_35:3)
TG(14:0_34:1)	TG(18:1_36:0)
TG(14:0_34:2)	TG(18:1_36:1)
TG(14:0_34:3)	TG(18:1_36:2)
TG(14:0_35:1)	TG(18:1_36:3)
TG(14:0_35:2)	TG(18:1_36:4)

TG(14:0_36:1)	TG(18:1_36:5)
TG(14:0_36:2)	TG(18:1_36:6)
TG(14:0_36:3)	TG(18:1_38:5)
TG(14:0_36:4)	TG(18:1_38:6)
TG(14:0_38:4)	TG(18:1_38:7)
TG(14:0_38:5)	TG(18:2_28:0)
TG(14:0_39:3)	TG(18:2_30:0)
TG(16:0_28:1)	TG(18:2_30:1)
TG(16:0_28:2)	TG(18:2_31:0)
TG(16:0_30:2)	TG(18:2_32:0)
TG(16:0_32:0)	TG(18:2_32:1)
TG(16:0_32:1)	TG(18:2_32:2)
TG(16:0_32:2)	TG(18:2_33:0)
TG(16:0_32:3)	TG(18:2_33:1)
TG(16:0_33:1)	TG(18:2_33:2)
TG(16:0_33:2)	TG(18:2_34:0)
TG(16:0_34:0)	TG(18:2_34:1)
TG(16:0_34:1)	TG(18:2_34:2)
TG(16:0_34:2)	TG(18:2_34:3)
TG(16:0_34:3)	TG(18:2_34:4)
TG(16:0_34:4)	TG(18:2_35:1)
TG(16:0_35:1)	TG(18:2_35:2)
TG(16:0_35:2)	TG(18:2_35:3)
TG(16:0_35:3)	TG(18:2_36:0)
TG(16:0_36:2)	TG(18:2_36:1)
TG(16:0_36:3)	TG(18:2_36:2)
TG(16:0_36:4)	TG(18:2_36:3)
TG(16:0_36:5)	TG(18:2_36:4)
TG(16:0_36:6)	TG(18:2_36:5)
TG(16:0_37:3)	TG(18:2_38:4)
TG(16:0_38:1)	TG(18:2_38:5)
TG(16:0_36:2)	TG(18:2_38:6)
TG(16:0_38:3)	TG(18:3_30:0)
TG(16:0_38:4)	TG(18:3_32:0)
TG(16:0_38:5)	TG(18:3_32:1)
TG(16:0_38:6)	TG(18:3_33:2)
TG(16:0_38:7)	TG(18:3_34:0)
TG(16:0_40:6)	TG(18:3_34:1)
TG(16:0_40:7)	TG(18:3_34:2)
TG(16:0_40:8)	TG(18:3_34:3)
TG(16:1_28:0)	TG(18:3_35:2)
TG(16:1_30:1)	TG(18:3_36:1)
TG(16:1_32:0)	TG(18:3_36:2)
TG(16:1_32:1)	TG(18:3_36:3)
TG(16:1_32:2)	TG(18:3_36:4)
TG(16:1_33:1)	TG(18:3_38:5)
TG(16:1_34:0)	TG(18:3_38:6)

TG(16:1_34:1)	TG(20:0_32:3)
TG(16:1_34:2)	TG(20:0_32:4)
TG(16:1_34:3)	TG(20:1_34:1)
TG(16:1_36:1)	TG(20:1_24:3)
TG(16:1_36:2)	TG(20:1_26:1)
TG(16:1_36:3)	TG(20:1_30:1)
TG(16:1_36:4)	TG(20:1_31:0)
TG(16:1_36:5)	TG(20:1_32:1)
TG(16:1_38:3)	TG(20:1_32:2)
TG(16:1_38:4)	TG(20:1_32:3)
TG(16:1_38:5)	TG(20:1_34:0)
TG(17:0_32:1)	TG(20:1_34:1)
TG(17:0_34:1)	TG(20:1_34:2)
TG(17:0_34:2)	TG(20:1_34:3)
TG(17:0_34:3)	TG(20:2_32:0)
TG(17:0_36:3)	TG(20:2_32:1)
TG(17:0_36:4)	TG(20:2_34:1)
TG(17:1_32:1)	TG(20:2_34:2)
TG(17:1_34:1)	TG(20:2_34:3)
TG(17:1_34:2)	TG(20:2_34:4)
TG(17:1_34:3)	TG(20:2_36:5)
TG(17:1_36:3)	TG(20:3_32:0)
TG(17:1_36:4)	TG(20:3_32:1)
TG(17:1_36:5)	TG(20:3_32:2)
TG(17:1_38:5)	TG(20:3_34:0)
TG(17:1_38:6)	TG(20:3_34:1)
TG(17:1_38:7)	TG(20:3_34:2)
TG(17:2_34:2)	TG(20:3_34:3)
TG(17:2_34:3)	TG(20:3_36:3)
TG(17:2_36:2)	TG(20:3_36:4)
TG(17:2_36:3)	TG(20:3_36:5)
TG(17:2_36:4)	TG(20:4_30:0)
TG(17:2_38:5)	TG(20:4_32:0)
TG(17:2_38:6)	TG(20:4_32:1)
TG(17:2_38:7)	TG(20:4_32:2)
TG(18:0_30:0)	TG(20:4_33:2)
TG(18:0_30:1)	TG(20:4_34:0)
TG(18:0_32:0)	TG(20:4_34:1)
TG(18:0_32:1)	TG(20:4_34:2)
TG(18:0_32:2)	TG(20:4_34:3)
TG(18:0_34:2)	TG(20:4_35:3)
TG(18:0_34:3)	TG(20:4_36:2)
TG(18:0_36:1)	TG(20:4_36:3)
TG(18:0_36:2)	TG(20:4_36:4)
TG(18:0_36:3)	TG(20:4_36:5)
TG(18:0_36:4)	TG(20:5_34:0)
TG(18:0_36:5)	TG(20:5_34:1)

TG(18:0_38:6)	TG(20:5_34:2)
TG(18:0_38:7)	TG(20:5_36:2)
TG(18:1_26:0)	TG(20:5_36:3)
TG(18:1_28:1)	TG(22:0_32:4)
TG(18:1_30:0)	TG(22:1_32:5)
TG(18:1_30:1)	TG(22:2_32:4)
TG(18:1_30:2)	TG(22:3_30:2)
TG(18:1_31:0)	TG(22:4_32:0)
TG(18:1_32:0)	TG(22:4_32:2)
TG(18:1_32:1)	TG(22:4_34:2)
TG(18:1_32:2)	TG(22:5_32:0)
TG(18:1_32:3)	TG(22:5_32:1)
TG(18:1_33:0)	TG(22:5_34:1)
TG(18:1_33:1)	TG(22:5_34:2)
TG(18:1_33:2)	TG(22:5_34:3)
TG(18:1_33:3)	TG(22:6_32:0)
TG(18:1_34:1)	TG(22:6_32:1)
TG(18:1_34:2)	TG(22:6_34:1)
TG(18:1_34:3)	TG(22:6_34:2)
TG(18:1_34:4)	TG(22:6_34:3)