

Supplemental table 1. List of metabolites by type, subtype and method used for compound identification

Metabolite	Type	Subtype	Analysis method
Glutamic acid	Amino acids	Acid	GC/QTOF
Alanine	Amino acids	Aliphatic	GC/QTOF
Glycine			
Valine			
Leucine			
Isoleucine			
Phenylalanine	Amino acids	Aromatic	GC/QTOF
Tyrosine			
Tryptophan			
Lysine	Amino acids	Basic	GC/QTOF
Proline	Amino acids	Cyclic	GC/QTOF
Serine	Amino acids	Hydroxyl-containing	GC/QTOF
Threonine			
Ornithine	Amino acids	Non-proteinogenic	GC/QTOF
Methionine	Amino acids	Sulfur-containing	GC/QTOF
Sucrose	Carbohydrates	Disaccharides	GC/QTOF
Glyceric acid	Carbohydrates	Glyceric acids	GC/QTOF
Fructose, Glucose	Carbohydrates	Monosaccharides	GC/QTOF
Glycerol	Carbohydrates	Sugar alcohols	GC/QTOF
Citric acid	Carboxylic acids	Citrates	GC/QTOF
2-Hydroxybutanoic acid	Carboxylic acids	Hydroxybutirates	GC/QTOF
3-Hydroxybutanoic acid			
Lactic acid	Carboxylic acids	Lactates	GC/QTOF
PC 30:0, PC 31:0, PC 32:0, PC 32:1, PC 32:1 e, PC 32:2, PC 33:0, PC 33:1, PC 34:0, PC 34:1, PC 34:1, PC 34:2, PC 34:2 e, PC 34:3, PC 34:3 e, PC 34:4, PC 35:1, PC 35:2, PC 35:4, PC 36:0, PC 36:1, PC 36:2, PC 36:2 e, PC 36:3, PC 36:3 e, PC 36:4, PC 36:4 e, PC 36:5, PC 36:5 e, PC 37:4, PC 37:6, PC 38:2, PC 38:3, PC 38:3 e, PC 38:4, PC 38:4 e, PC 38:5, PC 38:5 e, PC 38:6, PC 38:6 e, PC 40:4, PC 40:4 e, PC 40:5, PC 40:5 e, PC 40:6, PC 42:4 e, PC 42:5 e, PE 36:4, PE 36:5 e, PE 38:5 e, PE 38:6 e	Glycerophospholipids	LC/QTOF	

Arachidonic Acid (ARA+EPA)			
Docosahexaenoic acid (DHA)			
Polyunsaturated fatty acids (PUFA)			
Monounsaturated fatty acids (MUFA)			
Palmitic acid			
Linoleic acid	Lipids	Fatty acids	NMR
Oleic acid			
Stearic acid			
Fatty acyl chains			
Omega-3			
Phosphatidyl Choline			
Lysophosphatidyl Choline	Lipids	Phospholipids	NMR
Sphingomyelin			
Cholesterol	Lipids	Sterols	GC/QTOF
alpha-Tocopherol	Lipids	Vitamin E	GC/QTOF
LPC 14:0, LPC 15:0, LPC 16:0m, LPC 16:0 em, LPC 16:1, LPC 16:1 e, LPC 17:0, LPC 18:0, LPC 18:0 e, LPC 18:1, LPC 18:2, LPC 18:3, LPC 18:4, LPC 20:0, LPC 20:1, LPC 20:2, LPC 20:3, LPC 20:4, LPC 20:5, LPC 22:5,LPC 22:6	Lysophosphatidylcholines		LC/QTOF
SM 32:0, SM 32:1, SM 32:2, SM 33:1, SM 34:1, SM 34:2, SM 35:0, SM 35:1, SM 36:0, SM 36:1, SM 36:2, SM 38:1, SM 38:2, SM 39:1, SM 40:0, SM 40:1, SM 40:2, SM 41:1, SM 41:2, SM 42:1, SM 42:2, SM 42:3, SM 43:1, SM 43:2	Sphingomyelins		LC/QTOF
TG 46:0, TG 46:1, TG 46:2, TG 48:0, TG 48:1, TG 48:2, TG 48:3, TG 50:0, TG 50:1, TG 50:2, TG 50:3, TG 50:4, TG 51:2, TG 52:1, TG 52:2, TG 52:3, TG 52:4, TG 52:5, TG 52:6, TG 54:2, TG 54:3, TG 54:4, TG 54:5, TG 54:6, TG 54:7	Triglycerides		LC/QTOF
Triglycerides	Triglycerides		NMR

LC/QTOF, liquid chromatography in combination with hybrid quadrupole time-of-flight mass spectrometry; NMR, nuclear magnetic resonance; GC/QTOF, gas chromatography in combination with hybrid quadrupole time-of-flight mass spectrometry