

Table S1. Classification of metabolome-related metabolites. Metabolite categories identified following targeted ultra-high-performance liquid chromatography coupled to high resolution Orbitrap mass spectrometry (UHPLC-LC-MLS/MS).

Metabolite categories	
Small molecule category	Lipid category
Alkaloids	Acylcarnitines
Amino acids	Phosphatidylcholines
Amino acid related	Lysophosphatidylcholines
Bile acids	Sphingomyelins
Biogenic amines	Cholesteryl esters
Carboxylic acids	Ceramides
Cresols	Dihydroceramides
Hormones	Glucosylceramides
Indoles and derivatives	Lactosylceramides
Nucleobases and related	Trihexosylceramides
Vitamins and cofactors	Diacylglycerols
Sugars	Triacylglycerols