

**Table S2.** Subclass analysis of differentially accumulated metabolites in GC-MS/MS

Category	Number of metabolites	Proportion (%)
Amino acids, peptides, and analogues	26	23.42%
Others	26	23.42%
Carbohydrates and carbohydrate conjugates	13	11.71%
Fatty acids and conjugates	4	3.60%
Alcohols and polyols	3	2.70%
Benzoic acids and derivatives	2	1.80%
Indolyl carboxylic acids and derivatives	2	1.80%
Monoradylglycerols	2	1.80%
Purines and purine derivatives	2	1.80%
Pyrimidines and pyrimidine derivatives	2	1.80%
Quinone and hydroquinone lipids	2	1.80%
5'-deoxy-5'-thionucleosides	1	0.90%
Alpha-keto acids and derivatives	1	0.90%
Amines	1	0.90%
Benzaldehydes	1	0.90%
Benzenediols	1	0.90%
Bile acids, alcohols and derivatives	1	0.90%
Bipyridines and oligopyridines	1	0.90%
Cresols	1	0.90%
Fatty acyl glycosides	1	0.90%
Fatty alcohols	1	0.90%
Flavans	1	0.90%
Furoic acid and derivatives	1	0.90%
Gamma butyrolactones	1	0.90%
Glycerophosphates	1	0.90%
Glycosyl compounds	1	0.90%
Guanidines	1	0.90%
Hydroxycinnamic acids and derivatives	1	0.90%
Hydroxycoumarins	1	0.90%
Hydroxyindoles	1	0.90%
Imidazoles	1	0.90%
Medium-chain hydroxy acids and derivatives	1	0.90%
Methoxyphenols	1	0.90%
Organic phosphonic acids	1	0.90%
Pterins and derivatives	1	0.90%
Pyrrolidinylpyridines	1	0.90%
Steroids and steroid derivatives	1	0.90%
Tricarboxylic acids and derivatives	1	0.90%