

Table S1. Subclass analysis of differentially accumulated metabolites in LC-MS/MS

Category	Number of metabolites	Proportion (%)
Others	177	27.23%
Carbohydrates and carbohydrate conjugates	66	10.15%
Amino acids, peptides, and analogues	55	8.46%
Flavonoid glycosides	26	4.00%
Flavonoids	22	3.38%
Fatty acids and conjugates	20	3.08%
Fatty acyl glycosides	17	2.62%
Hydroxycinnamic acids and derivatives	16	2.46%
Terpene glycosides	10	1.54%
Alcohols and polyols	9	1.38%
Glycerophosphates	7	1.08%
Glycerophosphoinositols	7	1.08%
Carbonyl compounds	6	0.92%
Purine ribonucleotides	6	0.92%
Glycerophosphoglycerols	5	0.77%
Octadecanoids	5	0.77%
Sesquiterpenoids	5	0.77%
Amines	4	0.62%
Benzoic acids and derivatives	4	0.62%
Diterpenoids	4	0.62%
Fatty amides	4	0.62%
Isoflavonoid O-glycosides	4	0.62%
Oxidized glycerophospholipids	4	0.62%
Triradylglycerols	4	0.62%
Benzoquinolines	3	0.46%
Bile acids, alcohols and derivatives	3	0.46%
Eicosanoids	3	0.46%
Ethers	3	0.46%
Fatty acyl thioesters	3	0.46%
Fatty alcohols	3	0.46%
Flavones	3	0.46%
Gamma butyrolactones	3	0.46%
Glycerophosphocholines	3	0.46%
Linoleic acids and derivatives	3	0.46%
Medium-chain keto acids and derivatives	3	0.46%
Monoradylglycerols	3	0.46%
Other Sphingolipids	3	0.46%
Porphyrins	3	0.46%
Steroidal glycosides	3	0.46%
Terpene lactones	3	0.46%
Tetraterpenoids	3	0.46%
1-benzopyrans	2	0.31%

Arylsulfates	2	0.31%
Beta hydroxy acids and derivatives	2	0.31%
Chalcones and dihydrochalcones	2	0.31%
Cinnamylphenols	2	0.31%
Coumarin glycosides	2	0.31%
Cyclic purine nucleotides	2	0.31%
Fatty acid esters	2	0.31%
Furanoquinolines	2	0.31%
Glycerophosphoserines	2	0.31%
Glycosylglycerols	2	0.31%
Hydrocarbons	2	0.31%
Hydrolyzable tannins	2	0.31%
Isosorbides	2	0.31%
Linear diarylheptanoids	2	0.31%
Methoxyphenols	2	0.31%
Other Fatty Acyls	2	0.31%
Phosphosphingolipids	2	0.31%
Purines and purine derivatives	2	0.31%
Pyrimidines and pyrimidine derivatives	2	0.31%
Steroid esters	2	0.31%
Steroid lactones	2	0.31%
Steroids	2	0.31%
Sterols	2	0.31%
Tricarboxylic acids and derivatives	2	0.31%
Triterpenoids	2	0.31%
1-hydroxy-2-unsubstituted benzenoids	1	0.15%
2-benzopyrans	1	0.15%
Alkylthiols	1	0.15%
Alloxazines and isoalloxazines	1	0.15%
Anisoles	1	0.15%
Benzenediols	1	0.15%
Bisphosphonates	1	0.15%
Chlorins	1	0.15%
Cinnamic acid esters	1	0.15%
Cinnamic acids	1	0.15%
Dialkyldisulfides	1	0.15%
Dialkylthioethers	1	0.15%
Dicarboxylic acids and derivatives	1	0.15%
Furanocoumarins	1	0.15%
Furanoisoflavonoids	1	0.15%
Furanones	1	0.15%
Glycerophosphoinositolglycans	1	0.15%
Glycosphingolipids	1	0.15%
Glycosyldiradylglycerols	1	0.15%

Halobenzenes	1	0.15%
Hopanoids	1	0.15%
HyBcid peptides	1	0.15%
Hydropyridines	1	0.15%
Hydroxycoumarins	1	0.15%
Hydroxyflavonoids	1	0.15%
Hydroxyindoles	1	0.15%
Hydroxyisoflavonoids	1	0.15%
Indoles	1	0.15%
Indolines	1	0.15%
Indolyl carboxylic acids and derivatives	1	0.15%
Isoprenoids	1	0.15%
Macrolides and lactone polyketides	1	0.15%
Medium-chain hydroxy acids and derivatives	1	0.15%
Methoxybenzenes	1	0.15%
Monosaccharides	1	0.15%
Monoterpenoids	1	0.15%
N-acylpiperidines	1	0.15%
Naphthalene sulfonic acids and derivatives	1	0.15%
Nicotinamide nucleotides	1	0.15%
O-methylated flavonoids	1	0.15%
Organic pyrophosphates	1	0.15%
Other Polyketides	1	0.15%
Oxazolidines	1	0.15%
Oxygenated hydrocarbons	1	0.15%
Piperazines	1	0.15%
Polyprenols	1	0.15%
Polyprenylphenols	1	0.15%
Pregnane steroids	1	0.15%
Purine deoxyribonucleotides	1	0.15%
Pyridinecarboxylic acids and derivatives	1	0.15%
Quaternary ammonium salts	1	0.15%
Quinone and hydroquinone lipids	1	0.15%
Secosteroids	1	0.15%
Sphingoid bases	1	0.15%
Steroid conjugates	1	0.15%
Stilbene glycosides	1	0.15%
Sulfuric acid esters	1	0.15%
Triradylglycerols	1	0.15%
Tryptamines and derivatives	1	0.15%
Unsaturated aliphatic hydrocarbons	1	0.15%