Supplement Table 1 Top metabolites identified by different ML algorithms

Least Absolute Shrinkage and Selection Operator	Support Vector Machine-Recursive Feature Elimination	Random forest
(10E,12Z)-9-HODE	N-Acetylcarnosine	CerP(d18:1/12:0)
2-Hydroxy-3-methylbutyricacid	2-Stearylcitrate	2-Stearylcitrate
N-Acetylcarnosine	CerP(d18:1/12:0)	N-Acetylcarnosine
Acetovanillone	3-Methyl-alpha-ionylacetate	PC(20:1(11Z)/15:0)
2-Methylbutyroylcarnitine	Atrolacticacid	3-Methyl-alpha-ionylacetate
PC(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	Acetovanillone	2-Methylbutyroylcarnitine
2-Stearylcitrate	2-Hydroxy-2-methylbutyricacid	Atrolacticacid
3-Methyl-alpha-ionylacetate	SanguisorbinB	Creatinine
CerP(d18:1/12:0)	(10E,12Z)-9-HODE	DG(18:3(9Z,12Z,15Z)/15:0/0:0)
DG(15:0/18:4(6Z,9Z,12Z,15Z)/0:0)	DG(15:0/18:4(6Z,9Z,12Z,15Z)/0:0)	PC(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
PC(P-16:0/18:2(9Z,12Z))		
PC(20:1(11Z)/15:0)		
PC(P-18:0/22:5(4Z,7Z,10Z,13Z,16Z))		
Diethylenetriaminecrosslinkedwithepichlorohydrin		
Simulansine		