Systems and parameters	Non-polar metabolite profiling	Polar metabolite profiling
LC system	Accela™ system	Accela™ system
MS system	Exactive(R)	Exactive(R)
Column type	Agilent SB C8 column (1.8 µm, 2.1 x 100 mm)	C18(2) column (2.5 µm, 3 x 100 mm)
Column Temperature (°C)	40	40
Mobile phase A	0.1% w/v Ammonium acetate in water	0.1 % v/v formic acid in water
Mobile phase B	0.1% Ammonium acetate in mixture of acetonitrile/isopropanol (60:40 v/v)	0.1 % v/v formic acid in acetonitrile
Gradient step	Time (min) %A %B 0 75 25 5 10 90 10 0 100 12 0 100 15 75 25	Time (min) %A %B 0 80 20 5 40 60 10 20 80 12 20 80 15 80 20
Flow rate (µl/min)	500	500
Sample injection volume (µl)	10	10