

**Supplementary Table 1 Chromatographic conditions of metabolomics**

<b>Time</b>	<b>A%</b>	<b>B%</b>
0	95	5
2	95	5
4	70	30
8	50	50
10	20	80
14	0	100
15	0	100
15.1	95	5
16	95	5

**Supplementary Table 2 Mass spectrum conditions of metabolomics**

<b>Argument</b>	<b>Positive ion</b>	<b>Negative ion</b>
Spray Voltage (V)	3800	-3000
Capillary Temperature (°C)	320	320
Aux gas heater temperature (°C)	350	350
Sheath Gas Flow Rate (Arb)	35	35
Aux gas flow rate (Arb)	8	8
S-lens RF level	50	50
Mass range (m/z)	100-1200	100-1200
Full ms resolution	70000	70000
MS/MS resolution	17500	17500
NCE/stepped NCE	10, 20, 40	10, 20, 40