

### Supplementary Table 1

#### UPLC-QTOF-MS instrument conditions

<b>UPLC condition</b>	Mobile phase	A: water containing 0.1% (v/v) formic acid B: Acetonitrile containing 0.1% (v/v) formic acid					
	Gradient time (min)	0	2	10	12	13	15
	A (%)	95	95	5	5	95	95
	B (%)	5	5	95	95	5	5
	Total flow	0.4 mL/min					
	Temperature of column oven	35 °C					
	Column	Waters ACQUITY HSS T3 column (2.1 × 100 mm, i.d., 1.8 µm)					
<b>MS condition</b>	Ionisation mode	ESI positive			ESI negative		
	Collision energy	20-40 eV					
	Capillary voltage	2.5 kV					
	Cone voltage	40V					
	Desolvation gas	800 L/h					
	Cone gas	50 L/h					
	Source temperature	100° C					
	Desolvation gas temperature	450° C					
	Scan time	0.5 s					
	Inter-scan time	0.1 s					
	Mass range	50 to 1500 Da					