

**Table SI.** Mobile phase gradients.

Time (min)	A%	B%
0-5	0-20	100-80
5-25	20-40	80-60
25-35	40-45	60-55
35-45	45-60	55-40
45-60	60-90	40-10
60-63	90	10
63-63.1	90-0	10-100
63.1-66	0	100

Column: Waters CORTECS C8 UPLC<sup>®</sup> T3 (2.1x100pin; 1.6 ufm), mobile phase (A) acetonitrile (B) 0.1% formic acid aqueous solution; injection volume of 2  $\mu$ l, flow rate of 0.3 ml/min, column temperature 30°C, gradient elution.

**Table SII.** Mass spectrometry parameters.

MS parameters	Parameter value	MS/MS Parameters	Parameter value
TOF mass range	50-1700	MS/MS mass range	50-1250
Ion source gas 1 (psi)	50	Declustering potential (V)	100
Ion source gas 2 (psi)	50	Collision energy (eV)	±40
Curtain gas (psi)	35	Collision energy spread (eV)	20
Ion spray voltage floating(V)	-4500/5000	Ion release delay (msec)	30
Ion source temperature(°C)	500	Ion release width (msec)	15
Declustering potential (V)	100		
Collision energy (eV)	10		

Mass spectrometry conditions: Mass spectrometry detection mode is electrospray ionization source (-positive/negative ion mode, mass spectrometry parameters. MS, mass spectrometry; TOF, time-of-flight.