

Table S3. MS Parameters for Q Exactive		
Polarity	Top 5	
	Positive	Negative
Full Scan		Full Scan
Resolution	70000	70000
AGC	1.00E+06	1.00E+06
Maximum IT(ms)	50	50
Scan range (m/z)	300-1800	300-1800
TopN (ddMS2)		TopN (ddMS2)
	5	5
Resolution	17500	17500
AGC	1.00E+05	1.00E+05
Maximum IT(ms)	117	117
Isolation window (m/z)	1	1
NCE	25,30	25,30
Dynamic exclusion (s)	20	20
Minimum AGC	2.00E+02	2.00E+02

AGC

Automatic gain control

IT

Injection time

NCE

Normalized collision energy