

Table S1. Instrumental and LC-MS data processing methods.

Thermo Scientific Vanquish UHPLC system parameters		
Time (min)	Flow (mL/min)	%A (Water + 0.1% Formic Acid)
0.00	0.500	98
1.00	0.500	98
2.50	0.500	2
4.50	0.500	2
5.50	0.500	98
7.50	0.500	98
7.50	Stop Run	
Divert valve parameters		
Switch at	0.2 min	
Q Exactive Plus (Thermo Scientific) mass spectrometer parameters		
Source		
Sheath Gas Flow Rate	35	
Aux Gas Flow Rate	10	
Sweep Gas Flow Rate	0	
Spray Voltage	3.80 (+)	
Capillary Temperature	320°C	
S-lens RF Level	50.0	
Aux Gas Heater Temperature	350.0°C	
Full MS		
Resolution	70,000	
AGC Target	3.0E6	
Maximum IT	246 milliseconds	
Scan Range	100 to 1500 <i>m/z</i>	
dd-MS ²		
Resolution	17,500	
AGC Target	1.0E5	
Maximum IT	54 milliseconds	
Top N	5	
Isolation Window	1.0 <i>m/z</i>	
Fixed First Mass	---	
(N)CE/ Stepped	NCE: 20, 40, 60	
dd Settings		
Min. AGC Target	8.00E3	
Intensity Threshold	1.50E5	
Apex Trigger	---	
Charge Exclusion	---	

Peptide Match	preferred	
Exclude Isotope	On	
Dynamic Exclusion	10.0 seconds	
MZmine version 2.5.3 parameters		
		Polarity: Positive
MS ¹	Noise Level	9.0E5
MS ²	Noise Level	1.0E3
Chromatogram Builder	Mass List	masses
	Minimum Time Span (min)	0.01
	Minimum Height	9.0E5
	<i>m/z</i> Tolerance (ppm)	10.0
Chromatogram Deconvolution	Algorithm	Local minimum search
	<i>m/z</i> Range for MS ² Scan Pairing (Da)	0.01
	RT Range for MS ² Scan Pairing (min)	0.2
	Chromatographic Threshold	20%
	Search Minimum in RT range	0.03
	Minimum Relative Height	26%
	Minimum Absolute Height	1.0E4
	Minimum ratio of peak top/edge	1
	Peak Duration range (min)	0.01-1.00
Deisotoping	<i>m/z</i> Tolerance (ppm)	10.0
	Retention Time Tolerance (min)	0.5
	Monotonic Shape	Checked
	Maximum Charge	3
	Representative Isotope	Lowest <i>m/z</i>
Alignment	<i>m/z</i> Tolerance (ppm)	10.0
	Weight for <i>m/z</i>	1
	Weight for Retention Time	1
	Retention Time Tolerance (min)	0.5
Row Filtering	Minimum Peaks in a Row	3
	Retention Time (min)	0.3-7
	Keeps Only Peaks with MS ² Scans	Checked
	Reset Peak No. ID	Checked