

Mode Source Tune MS/MS Chromatogram

Source Change... ESI

End Plate Offset 500 V
 Capillary 4500 V
 Nebulizer 2.0 Bar
 Dry Gas 8.0 l/min
 Dry Temp 250 °C

Divert Valve
 Valve Head 6 Port
 Position Source 1-2
 Waste 1-6

Ion Polarity TIMS
 positive Enable

Scan Mode
 Auto MS/MS

Mass Range
 From 50 to 2800 m/z

Rolling Average Spectra Rate
 On 2 x 1.00 Hz

Apply

Both Polarities All Segments

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General

Transfer
 Funnel 1 RF 350.0 Vpp Funnel 2 RF 600.0 Vpp
 isCID Energy 0.0 eV Multipole RF 400.0 Vpp
 Deflection Delta 70.0 V

Quadrupole
 Ion Energy 5.0 eV Low Mass 300.0 m/z

Collision Cell
 Collision Energy 7.0 eV
 Pre Pulse Storage 12.0 μs

Stepping
 Mode Basic

Always	From	To
Collision RF	1500.0	2100.0 Vpp
Transfer Time	121.0	181.0 μs
Timing	50	50 %
MS/MS only		
Collision Energy	80	100 %
Timing	50	50 %

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Auto MS/MS

Preference
 SILE
 CID
 AcqCtrl
 Multi CE
 MRM
 isCID
 bbCID

Precursor Ion List
 Exclude
 Width ± 0.5
 Mass Range
 50.00-300.00
 1221.90-1225.00
 Import...
 Add
 Delete
 Delete All

Precursor Ions
 No. of Precursors 2
 Cycle Time 3.0 sec

Threshold
 Absolute (per 1000 sum.)
 Absolute 300 cts Exclude after 1 Spectra
 Absolute 1628 cts Release after 2.00 min

Active Exclusion
 Reconsider Precursor, if Current Intens. / Previous Intens. 2.5

Smart Exclusion 5 x

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MS/MS Acquisition Control

Spectra Rate
 MS 1.00 Hz

Fixed MS/MS Acquisition 0.68 Hz
 Dynamic MS/MS Spectra Acquisition

Target Intensity (MS/MS TIC) 20000 cts
 Max. MS/MS Spectra Acquisition 2.00 Hz
 Min. MS/MS Spectra Acquisition 0.50 Hz

Total Cycle Time Range 3 sec
 Absolute Threshold 1628 cts

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Supplementary Figure 2. Mass spectrometric parameters applied in the study.