Supplementary Table 1. LC-MS instrument parameters

Acquisition Experiment Report

File: c:\masslynx\project2017.pro\data\18ejanesms135.raw

Header

Acquired File Name: 18EJANESMS135

Acquired Date: 22-Jan-2019

Acquired Time: 10:29:20

Job Code: JAN\_EXT2019

Task Code:

User Name:

Laboratory Name:

Instrument: ACQ-TQD#QBB1152

Conditions:

Submitter:

SampleID: 14-H [SAIF566]

Bottle Number: 1:A,2

Description: ACCUCORE C18, 150 X 2.1, 2.6um

Instrument Calibration:

Calibration File: C:\MassLynx\IntelliStart\Results\Unit Mass Resolution\_180517\Calibration\_20181031\_1.cal

Parameters

MS1 Static:

Mass: 20 Da to 1974 Da.

Resolution: 8.9/15.1

Ion Energy: 0.3

Reference File: Naics2

Acquisition File: STATMS1

MS1 Scanning:

Mass: 2 Da to 2048 Da.

Resolution: 8.9/15.1

Ion Energy: 0.3

Reference File: Naics2

Acquisition File: SCNMS1

MS1 Scan Speed Compensation:

Scan: 100 to 2000 amu/sec.

Resolution: 8.9/15.1

Ion Energy: 0.3

Reference File: Naics2

Acquisition File: FASTMS1

MS2 Static: None

MS2 Scanning: None

MS2 Scan Speed Compensation: None

Calibration Time: 11:28

Calibration Date: 10/31/18

Coefficients

MS1 Static: -0.000000000000\*x^4 + 0.000000000496\*x^3 + -0.000000912943\*x^2 + 1.000775223259\*x +-0.120910276204

MS2 Static: -0.000000000000\*x^4 + 0.000000000858\*x^3 + -0.000001694529\*x^2 + 1.001395382120\*x +-0.206712798330

Function 1: 0.000000000000\*x^4 + -0.000000000145\*x^3 + 0.000000401562\*x^2 + 0.999589858766\*x +-0.192535990770

Function 2: 0.000000000000\*x^4 + -0.000000000145\*x^3 + 0.000000401562\*x^2 + 0.999589858766\*x +-0.192535990770

Parameters for C:\MassLynx\PROJECT2017.PRO\ACQUDB\FULLSCANESPN150-1000ACN.EXP

Data Processing:

SIR / MRM Chromatogram Spike Removal ON

SIR / MRM Smoothing OFF

Smoothing window size (scans) 3

Number of smooths 2

Prescan Statistics:

Initial Average Intensity 21.5123

Initial Average Std Dev 1.9238

Bunch Zero Level 0.0123

Bunch Std Dev 0.0182

Bunch Threshold 0.1459

Spike Removal Std Dev 1.9158

Method Events:

Initial Stop Flow: No Change

Initial Switch 2: No Change

Initial Switch 3: No Change

Initial Switch 4: No Change

Initial Infusion: No Change

Initial Flow State: LC

Initial Flow Rate: 5

Initial Reservoir: No Action

API Probe Delay Temp: 20

Initial Refill: No Action

Timed Events Enabled

Event Time Name Action

1 0 Flow State LC

Instrument Parameters - Function 1:

Parameter File - C:\MassLynx\PROJECT2017.PRO\ACQUDB\PROJECT2017.IPR

Polarity ES+

Calibration Dynamic 1

Capillary (kV) 3.50 3.49

Cone (V) 30.00 -16.85

Extractor (V) 3.00 -1.71

RF (V) 0.00

Source Temperature (°C) 120 119

Desolvation Temperature (°C) 350 350

Cone Gas Flow (L/Hr) 30 30

Desolvation Gas Flow (L/Hr) 650 650

Collision Gas Flow (mL/Min) 0.23 0.00

LM 1 Resolution 15.00

HM 1 Resolution 15.00

Ion Energy 1 0.50

MS Mode Entrance 50.00

MS Mode Collision Energy 2.00

MS Mode Exit 50.00

MSMS Mode Entrance 2.00

MSMS Mode Collision Energy 2.00

MSMS Mode Exit 2.00

LM 2 Resolution 15.00

HM 2 Resolution 15.00

Ion Energy 2 3.00

Gain 1.00

Multiplier -503.97

Active Reservoir B

Instrument Parameters - Function 2:

Parameter File - C:\MassLynx\PROJECT2017.PRO\ACQUDB\PROJECT2017.IPR

Polarity ES-

Calibration Dynamic 1

Capillary (kV) 3.50 3.49

Cone (V) 30.00 -16.85

Extractor (V) 3.00 -1.71

RF (V) 0.00

Source Temperature (°C) 120 119

Desolvation Temperature (°C) 350 350

Cone Gas Flow (L/Hr) 30 30

Desolvation Gas Flow (L/Hr) 650 650

Collision Gas Flow (mL/Min) 0.10 0.00

LM 1 Resolution 15.00

HM 1 Resolution 15.00

Ion Energy 1 0.50

MS Mode Entrance 50.00

MS Mode Collision Energy 2.00

MS Mode Exit 50.00

MSMS Mode Entrance 2.00

MSMS Mode Collision Energy 20.00

MSMS Mode Exit 2.00

LM 2 Resolution 15.00

HM 2 Resolution 15.00

Ion Energy 2 3.00

Gain 1.00

Multiplier -503.97

Active Reservoir B

Engineers Settings:

MS1 Low Mass Position 519

MS1 High Mass Position 377

MS1 Low Mass Resolution 518

MS1 High Mass Resolution 301

MS1 Resolution Linearity 822

MS1 High Mass DC Balance -0

MS1 DC Polarity Negative

MS2 Low Mass Position 520

MS2 High Mass Position 420

MS2 Low Mass Resolution 518

MS2 High Mass Resolution 181

MS2 Resolution Linearity 767

MS2 High Mass DC Balance 0

MS2 DC Polarity Positive

HM RF Lens Correction + 0

HM RF Lens Correction - 0

Inter-scan delays:

Automatic Mode

MS 1 Delay Table:

 R delay

<= 0.500 0.005

<= 2.000 0.008

<= 4.000 0.010

<= 11.000 0.012

> 11.000 0.014

MS 2 Delay Table:

 R delay

<= 8.000 0.005

<= 25.000 0.006

> 25.000 0.007

ACE Experimental Record

Inlet Method File: c:\masslynx\project2017.pro\acqudb\gap0188

--------------------- Run method parameters ----------------

-- PUMP --

Waters ACQUITY QSM

 Solvent A Name: 95%H2O IN ACN

 Solvent B Name: Acetonitrile

 Solvent C Name: Methanol

 Solvent D Name: 5 mM NH4Ac IN 95:5 H2O:ACN

 Low Pressure Limit: 0 psi

 High Pressure Limit: 15000 psi

 Seal Wash Period: 5.00 min

 [Gradient Table]

 Time(min) Flow Rate(mL/min) %A %B %C %D Curve

 1. Initial 0.250 0.0 5.0 0.0 95.0 Initial

 2. 1.00 0.250 0.0 5.0 0.0 95.0 6

 3. 10.00 0.250 0.0 30.0 0.0 70.0 6

 4. 14.00 0.250 0.0 60.0 0.0 40.0 6

 5. 16.00 0.250 0.0 60.0 0.0 40.0 6

 6. 24.00 0.250 0.0 80.0 0.0 20.0 6

 7. 32.00 0.250 0.0 80.0 0.0 20.0 6

 8. 35.00 0.250 0.0 5.0 0.0 95.0 6

 9. 40.00 0.250 0.0 5.0 0.0 95.0 6

 Comment: gradiant gap0188

 Flow Ramp Rate: 0.45 min

 D Solvent Selection (if supported): No Change

 System Pressure Data Channel: No

 Flow Rate Data Channel: No

 %A Data Channel: No

 %B Data Channel: No

 %C Data Channel: No

 %D Data Channel: No

 Primary Data Channel: No

 Accumulator Data Channel: No

 Degasser Data Channel: No

 Gradient Start: At Injection

 Gradient Start Volume: 0 uL

 Gradient Start Time: 0.00 min

 Participate in pre-analysis: No

-- END PUMP --

-- AUTOSAMPLER --

Waters ACQUITY FTN AutoSampler

 Run Time: 40.00 min

 Comment:

 Load Ahead: Disabled

 Loop Offline: Automatic min

 Wash Solvent Name: Water

 Pre-Inject Wash Time: 2.0 sec

 Post-Inject Wash Time: 6.0 sec

 Purge Solvent Name: ACN:MEOH:H2O

 Dilution: Disabled

 Dilution Volume: 0 uL

 Delay Time: 0 min

 Dilution Needle Placement: Automatic mm

 Target Column Temperature: 30.0 C

 Column Temperature Alarm Band: 5.0 C

 Target Sample Temperature: 20.0 C

 Sample Temperature Alarm Band: Disabled

 Syringe Draw Rate: Automatic

 Needle Placement: Automatic

 Pre-Aspirate Air Gap: Automatic

 Post-Aspirate Air Gap: Automatic

 Column Temperature Data Channel: No

 Room Temperature Data Channel: No

 Sample Temperature Data Channel: No

 Sample Organizer Temperature Data Channel: No

 Sample Pressure Data Channel: No

 Preheater Temperature Data Channel: No

 Seal Force Data Channel: No

 No Injection Mode Enabled: No

 Run Events: No

Sample Run Injection Parameter

Injection Volume (ul) - 1.00

-- END AUTOSAMPLER --

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End of experimental record.

------------------- Waters ACQUITY QSM Postrun Report ---------------

 Firmware Version: 1.50.237 (May 18 2011) Software Version: 1.50.1621 Checksum: 0xae400516 Serial Number: L10QSM943A Minimum System Pressure: 0.0 psi Maximum System Pressure: 0.0 psi Average System Pressure: 0.0 psi

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------------------- Waters ACQUITY FTN Postrun Report ---------------

Software Version: 1.50.1481 Firmware Version: 1.50.317 (Jul 11 2011) Checksum: 0x3e83519d Serial Number: M10SDI443M Sample Syringe Size: 100.0 Extension Loop Size: 0.0 Needle Size: 15.0 Minimum Sample Temperature: 0.0 Maximum Sample Temperature: 0.0 Average Sample Temperature: 0.0 Minimum Column Temperature: 26.0 Maximum Column Temperature: 31.6 Average Column Temperature: 0.0

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Function 1

Scans in function: 1930

Cycle time (secs): Automatic

Scan duration (secs): 0.600

Inter Scan Delay (secs): Automatic

Start and End Time(mins): 0.000 to 40.000

Ionization mode: ES+

Data type: Enhanced Mass

Function type: Scan

Mass range: 100 to 1000

Function 2

Scans in function: 1929

Cycle time (secs): Automatic

Scan duration (secs): 0.600

Inter Scan Delay (secs): Automatic

Start and End Time (mins): 0.000 to 40.000

Ionization mode: ES-

Data type: Enhanced Mass

Function type: Scan

Mass range: 100 to 1000