File Information for Sample 1 (Test) of AQNEG01.wiff

File Name: AQNEG01.wiff

File Path: D:\Analyst Data\Projects\Mengmeng\2013\_06\_17\Data\

Original Name: AQNEG01.wiff

Software Version: Analyst TF 1.5.1

Log Information from Devices at Start of acquisition:

Integrated System Shimadzu Controller CBM20A

 Serial# L20234953303

 ROM Version 2.30

 Pressure Units psi

Time from start =0.0000 min Pump Shimadzu LC20ADXR

 Serial# L20434950766

 ROM Version 1.22

Time from start =0.0000 min Pump Shimadzu LC20ADXR

 Serial# L20434950767

 ROM Version 1.22

Time from start =0.0000 min AutoSampler Shimadzu SIL20ACXR

 Serial# L20454950207

 ROM Version 1.25

Time from start =0.0000 min Column Oven Shimadzu CTO20A

 Serial# L20204951547

 ROM Version 1.07

Time from start =0.0000 min

Time from start =0.0000 min Injection Volume used 5.00 µl

Time from start =0.0000 min Mass Spectrometer TripleTOF 5600 0

 Config Table Version 01

 Firmware Version M402001 B4T0301 M3L2002 B3T0300

 Component Name Hybrid Quadrupole-TOF LC/MS/MS Mass Spectrometer

 Component ID Triple TOF 5600

 Manufacturer AB Sciex Instruments

 Model 1032150/N

 Serial Number AY21451105

 Source Housing DuoSpray Ion Source

Time from start =0.0167 min Mass Spectrometer TripleTOF 5600 0

Start of Run - Detailed Status

Vacuum Status At Pressure

Vacuum Gauge (10e-5 Torr) 3.6

Backing Pump Ok

Q1 Turbo Pump Normal

Q2/TOF Turbo Pump Normal

Sample Introduction Status Ready

Source/Ion Path Electronics On

Source Type DuoSpray Ion Source

Source Temperature (at setpoint) 500.0 C

Source Exhaust Pump Ok

Injection Manifold Bypass

Time from start =0.0333 min Mass Spectrometer TripleTOF 5600 0

End of Run - Detailed Status

Vacuum Status At Pressure

Vacuum Gauge (10e-5 Torr) 3.6

Backing Pump Ok

Q1 Turbo Pump Normal

Q2/TOF Turbo Pump Normal

Sample Introduction Status Ready

Source/Ion Path Electronics On

Source Type DuoSpray Ion Source

Source Temperature (at setpoint) 500.0 C

Source Exhaust Pump Ok

Injection Manifold Bypass

Time from start =21.7500 min

Acquisition Info

Pulser frequency has been adjusted to the value of 16.644 kHz for this method.

Pulse 1 Duration was 3 µs for this method.

File has been acquired with TDCx8.

Acquisition Method: \Waters20Neg5IDA.dam

Acquisition Path: D:\Analyst Data\Projects\Mengmeng\2013\_06\_17\Acquisition Methods\

First Sample Started: Monday, June 17, 2013 12:46:47 PM

Last Sample Finished: Monday, June 17, 2013 12:46:47 PM

Sample Acq Time: Monday, June 17, 2013 12:46:47 PM

Sample Acq Duration: 20min1sec

Number of Scans: 0

Periods in File: 1

Batch Name: \New Batch.dab

Batch Path: D:\Analyst Data\Projects\Mengmeng\2013\_06\_17\Batch\

Submitted by: 9WGC8P1\Administrator()

Logged-on User: 9WGC8P1\Administrator

Synchronization Mode: LC Sync

Auto-Equilibration: Off

Comment:

Software Version: Analyst TF 1.5.1

Set Name: SET1

Sample Name: Test

Sample ID:

Sample Comments:

Autosampler Vial: 3

Rack Code: 1.5mL Standard

Rack Position: 1

Plate Code: 1.5mL Standard

Plate Position: 1

Shimadzu LC Method Properties (Not Used)

Shimadzu LC system Equlibration time = 1.00 min

Shimadzu LC system Injection Volume = 5.00 ul

Shimadzu LC Method Parameters

 Pumps

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Pump A Model: LC-20ADXR

Pump B Model: LC-20ADXR

Pumping Mode: Binary Flow

Total Flow: 0.2500 mL/min.

Pump B Conc: 3.0 %

B Curve: 0

Pressure Range (Pump A/B): 0 - 9000 psi

 Autosampler

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Model: SIL-20ACXR

Rinsing Volume: 500 uL

Needle Stroke: 52 mm.

Rinsing Speed: 35 uL/sec.

Sampling Speed: 5.0 uL/sec.

Purge Time: 25.0 min.

Rinse Dip Time: 10 sec.

Rinse Mode: Before and after aspiration

Cooler Enabled: Yes

Cooler Temperature: 15 deg. C

Control Vial Needle Stroke: 52 mm

 Oven

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Model: CTO-20A

Temperature Control: Enabled

Temperature: 55 deg. C

Max. Temperature: 90 deg. C

 System Controller

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Model: CBM-20A

Power: On

Event 1: Off

Event 2: Off

Event 3: Off

Event 4: Off

 Time Program

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 Time Module Events Parameter

 0.01 Pumps Pump B Conc. 3

10.00 Pumps Pump B Conc. 45

12.00 Pumps Pump B Conc. 75

17.50 Pumps Pump B Conc. 75

18.00 Pumps Pump B Conc. 3

20.00 System Controller Stop

Information Dependent Acquisition

 Switch Criteria

 For ions greater than: 100.000 m/z

 For ions smaller than: 1200.000 m/z

 With charge state: 1 to 2

 Which exceeds: 200 cps

 Exclude former target ions: For: 15 seconds

 Exclude former ions after: 2 Repeats

 Maximum number of candidate ions to monitor per cycle: 5 spectra

 Mass Defect Filter: No

 Ions Tolerance: 50.000 mDa

 Include / Exclude

 IDA Advanced

 Match Isotopes: No

 Dynamic Background Subtract: Yes

 Rolling Collision Energy: No

 Adjust CE when using iTRAQ Reagent: No

Quantitation Information:

Sample Type: Unknown

Dilution Factor: 1.000000

Custom Data:

Quantitation Table:

Period: 1

Duration: 20.010 mins

Cycle Time: 0.7999 secs

# Cycles: 1501

Period Delay: 0.00 secs

Period: 1 Experiment: 1

Scan Mode: None

Scan Type: Negative TOF MS

Intensity Thres.: 1 cps

Settling Time: 0.000 ms

MR Pause: 1.021 ms

MCA: No

GS1: 50.00

GS2: 50.00

CUR: 25.00

TEM: 500.00

ISVF: 4000.00

TOF Masses (Da): Min = 50.0000 Max = 1250.0000

Accumulation Time (sec): 0.2500

Time Bins to Sum: 4 Channels: 1 2 3 4

Q1 Mass (Da) % Time Param Start Stop

40.00 33.0 DP -50.00 -50.00

 CE -10.00 -10.00

 XA1 140.15 140.15

Q1 Mass (Da) % Time Param Start Stop

130.00 33.0 DP -50.00 -50.00

 CE -10.00 -10.00

 XA1 140.15 140.15

Q1 Mass (Da) % Time Param Start Stop

400.00 34.0 DP -50.00 -50.00

 CE -10.00 -10.00

 XA1 140.15 140.15

Period: 1 Experiment: 2

Scan Mode: None

Scan Type: Negative Product Ion

Product of Peak: IDA

Resolution Q1: UNIT

Intensity Thres.: 0 cps

Settling Time: 0.000 ms

MR Pause: 1.021 ms

MCA: No

GS1: 50.00

GS2: 50.00

CUR: 25.00

TEM: 500.00

ISVF: 4000.00

TOF Masses (Da): Min = 50.0000 Max = 1250.0000

Accumulation Time (sec): 0.1000

Time Bins to Sum: 4 Channels: 1 2 3 4 High Sensitivity

Q2 Mass (Da) % Time Param Start Stop

40.00 50.0 DP -80.00 -80.00

 CE -45.00 -45.00

 CES 30.00 30.00

 IRD 30.00 30.00

 IRW 15.00 15.00

 XA1 70.16 70.16

Q2 Mass (Da) % Time Param Start Stop

130.00 50.0 DP -80.00 -80.00

 CE -45.00 -45.00

 CES 30.00 30.00

 IRD 30.00 30.00

 IRW 15.00 15.00

 XA1 70.16 70.16

Resolution tables

Quad 1 Negative Unit TOF Resolution Mode: High Resolution

Last Modification Date Time: January 17, 2013 11:21:25

IE1 -2.200

VS1 0.329

HST 0.000

VS2 0.000

Mass (Da) Offset Value

 44.998 62.295

 411.260 62.551

 585.385 62.556

 933.637 62.556

 1165.804 62.552

Calibration tables

Quad 1 Negative Unit Resolution

Last Modification Date Time: January 17, 2013 11:21:03

Mass (Da) Dac Value

 44.998 1855

 411.260 17192

 585.385 24486

 933.637 39076

 1165.804 48804

Instrument Parameters:

TOF Mass Calibration Parameters:

Polarity Scan Slope Delay (nsec)

Negative: TOFMS 7.025933212407666800e-004 7.543183221457944200e-001

Negative: MS/MS High Resolution 7.026334136747718800e-004 9.016819020151080100e-001

Negative: MS/MS High Sensitivity 7.025890961131382700e-004 8.997354693740290400e-001

Show TOF Resolution Parameters in Manual Tune: No

Keyed Text:

File was created with the software version: Analyst TF 1.5.1