File Information for Sample 1 (Test) of AQPOS01.wiff

File Name: AQPOS01.wiff

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

Original Name: AQPOS01.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 =0.0000 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 =21.7667 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: \waters20minHEIDA.dam

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

First Sample Started: Monday, June 17, 2013 12:18:23 PM

Last Sample Finished: Monday, June 17, 2013 12:18:23 PM

Sample Acq Time: Monday, June 17, 2013 12:18:23 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: 10 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: 20.016 mins

Cycle Time: 1.2998 secs

# Cycles: 924

Period Delay: 0.00 secs

Period: 1 Experiment: 1

Scan Mode: None

Scan Type: Positive 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: 5500.00

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 80.00 80.00

CE 10.00 10.00

XA1 140.15 140.15

Q1 Mass (Da) % Time Param Start Stop

130.00 33.0 DP 80.00 80.00

CE 10.00 10.00

XA1 140.15 140.15

Q1 Mass (Da) % Time Param Start Stop

400.00 34.0 DP 80.00 80.00

CE 10.00 10.00

XA1 140.15 140.15

Period: 1 Experiment: 2

Scan Mode: None

Scan Type: Positive 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: 5500.00

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 Positive Unit TOF Resolution Mode: High Resolution

Last Modification Date Time: January 17, 2013 12:08:28

IE1 2.100

VS1 -0.220

HST 0.000

VS2 0.000

Mass (Da) Offset Value

59.049 62.305

175.133 62.500

442.337 62.551

674.505 62.556

906.672 62.558

1196.882 62.558

Calibration tables

Quad 1 Positive Unit Resolution

Last Modification Date Time: January 17, 2013 11:12:14

Mass (Da) Dac Value

59.049 2444

175.133 7304

442.337 18495

674.505 28221

906.672 37946

1196.882 50105

Instrument Parameters:

TOF Mass Calibration Parameters:

Polarity Scan Slope Delay (nsec)

Positive: TOFMS 7.025558672032314200e-004 1.092937681426426700e+000

Positive: MS/MS High Resolution 7.025673679348962800e-004 1.034688928602508700e+000

Positive: MS/MS High Sensitivity 7.025582560165323500e-004 1.088663895926203200e+000

Show TOF Resolution Parameters in Manual Tune: No

Keyed Text:

File was created with the software version: Analyst TF 1.5.1