**Analytical Method Negative Mode**

**Sample Info**

Sample: 20221004-NEG-AN-4.wiff (sample 1)

Sample Name: 20221004-NEG-AN-4

Sample ID: N/A

Comment: N/A

**Acquisition Info**

Method Path: D:\Analyst Data\Projects\C501\Acquisition Methods\20220930-NEG-AN.dam

Batch Path: D:\Analyst Data\Projects\C501\Batch\New Batch.dab

Acquisition Date: Monday, April 5, 2022

Acquisition Time: 5:01:31 AM

User Name: TRIPLETOF5600\Administrator

Acquisition Method: 20220930-NEG-AN.dam

Rack: 1

Plate: 1

Vial: 79

Injection Volume: 2.00

**Quantitation Info**

Sample Type: Unknown

Dilution Factor: 1.0000

**Log Info**

Integrated System: Shimadzu Controller, CBM20Alite

Serial#: L20225219100

ROM Version: 2.72

Pressure Units: psi

Pump: Shimadzu LC30AD

Serial#: L20555204364

ROM Version: 3.10

Pump: Shimadzu LC30AD

Serial#: L20555104258

ROM Version: 3.10

AutoSampler: Shimadzu SIL30AC

Serial#: L20565202103

ROM Version: 3.10

Column Oven: Shimadzu CTO30A

Serial#: L20575100652

ROM Version: 3.00

Injection Volume used: 2.00 µl

Mass Spectrometer: TripleTOF 5600-1

Config Table Version: 01

Firmware Version: MIA3000 ------- MIL3000 MIB3000

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

Component ID: TripleTOF 5600+

Manufacturer: AB Sciex Instruments

Model: 5016230/L

Serial Number: BN22351402

Source Housing: DuoSpray Ion Source

Time (from start of run): 00:00:01

Mass Spectrometer: TripleTOF 5600-1

Start of Run - Detailed Status: N/A

Vacuum Status: At Pressure

Vacuum Gauge (10e-5 Torr): 2.5

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 of run): 00:40:28

Mass Spectrometer: TripleTOF 5600-1

End of Run - Detailed Status: N/A

Vacuum Status: At Pressure

Vacuum Gauge (10e-5 Torr): 2.5

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

**IDA**

With intensity greater than: 10

Switch after: 6 spectra

Use advanced settings: True

Always exclude: True

Exclude for: 0 sec

Mass tolerance units: mDa

Mass tolerance: 50

Use inclusion list: False

Use exclusion list: False

Ignore peaks within: 6 Da

Real time: None

Spectrum file: N/A

Dynamic background subtraction: True

Fragment intensity multiplier: 2

Maximum accumulation: 2 sec

Allow standard filters for Smart IDA: True

Exclude former target ions: True

Exclude isotopes window: 4 Da

**Period 1, Experiment 4**

Experiment Type: TOF MS^2

Num. Cycles: 2432

Polarity: Negative

Product : IDA

Period Cycle Time: 900 ms

Pulser Frequency: 15.392 kHz

Accumulation Time: 100.0 ms

**Experiment Parameters**

*Parameter Value*

CUR 40.000

GS1 50.000

GS2 50.000

ISVF 4500.000

TEM 500.000

**Mass Range Parameters**

*Parameter Value*

CE -35.000

CES 15.000

DP -100.000

IDIx 0.000

IDUx 5.000

IRD 66.633

IRDx 28287.602

IRW 24.917

IRWx 24917.307

IWIx 0.000

IWUx 5.000

XA1 70.480

Start Mass: 50.0

End Mass: 1250.0

**RF Transmission**

*Mass Time (%)*

40.0 50.0

120.0 50.0

**Instrument Tables and Parameters**

**Resolution Table, Quad 1, Negative, Unit, TOF Resolution Mode: High Resolution**

Last Modification Date Time: April 16, 2022 14:40:58

IE1: -2.000

VS1: -0.536

HST: -0.195

VS2: 0.000

*Mass (Da) Offset Value*

44.998 61.550

411.260 61.915

585.385 61.927

933.637 61.934

1165.804 61.934

**Resolution Table, Quad 1, Negative, Unit, TOF Resolution Mode: High Sensitivity**

Last Modification Date Time: April 08, 2022 12:29:18

IE1: -1.200

VS1: 0.120

HST: -0.234

VS2: 0.000

*Mass (Da) Offset Value*

44.998 61.550

411.260 61.915

585.385 61.927

933.637 61.934

1165.804 61.934

**Mass Calibration Table, Quad 1, Negative, Unit Resolution**

Last Modification Date Time: April 08, 2022 12:36:39

*Mass (Da) Dac Value*

44.998 1874

411.260 17370

585.385 24738

933.637 39478

1165.804 49306

**TOF Mass Calibration Parameters**

*Polarity Scan Slope Delay (nsec)*

Positive TOFMS 7.018887027320172300e-004 1.026524375283072200e+000

Positive MS/MS High Resolution 7.019077858213306300e-004 7.494127005391801900e-001

Positive MS/MS High Sensitivity 7.018733228168398800e-004 1.059622710398323800e+000

Negative TOFMS 7.018759022350879900e-004 7.043493037955130800e-001

Negative MS/MS High Resolution 7.018893845378848500e-004 1.850125599822521900e+000

Negative MS/MS High Sensitivity 7.018645513363496900e-004 7.159541879773057000e-001

Show TOF Resolution Parameters in Manual Tune: No

**Keyed Text**

File was created with the software version: Analyst TF 1.6

**Shimadzu Integrated System**

500 mL/min

Pump B Conc: 5.0 %

B Curve: 0

Pressure Range (Pump A/B): 0 - 12000 psi

**Autosampler**

Model: SIL-30AC

Use Autosampler: Yes

Rinsing Volume: 500 uL

Needle Stroke: 52 mm.

Rinsing Speed: 35 uL/sec

Sampling Speed: 5.0 uL/sec

Rinse Dip Time: 0 sec

Rinse Mode: Before and after aspiration

Cooler Enabled: No

Control Vial Needle Stroke: 52 mm

Rinse Method: Rinse Port Only

Rinse Time: 2 sec

Measuring Line Purge Volume: 100 uL

Discharge Speed: 1.0 uL/sec

Air Gap: Off

Rinse Port Liquid Selection: R1

Rinsing Type: External

Purge Time of Rinse Port R0: 10.0 min

Purge Time of Measuring Line R0: 10.0 min

Rinsing Start Time Mode: After Acquisition

Rinsing Sequence 1: none

Rinsing Sequence 2: none

Rinsing Sequence 3: none

Rinsing Sequence 4: none

Rinsing Volume (R0 R1 R2): 300 uL

Injection Port Rinsing With R0: On

Injection Port Rinsing With R1: On

Injection Port Rinsing With R2: On

Sample Loop Equilibration: Off

**Oven**

Model: CTO-30A

Temperature Control: Enabled

Temperature: 40 deg. C

Max. Temperature: 160 deg. C

Heat Compensation: Auto

Heat Compensation Flow: 0.2500 mL\min

**System Controller**

Model: CBM-20A Lite

Event 1: Off

Event 2: Off

**Time Program**

*Time Module Events Parameter*

0.01 Pumps Pump B Conc. 5

18.00 Pumps Pump B Conc. 40

35.00 Pumps Pump B Conc. 95

37.00 Pumps Pump B Conc. 95

37.10 Pumps Pump B Conc. 5

40.00 System Controller Stop

**Pretreatment**

Mode: Standard.

**Analytical Method Positive Mode**

**Sample Info**

Sample: 20220404-POS-AN-4.wiff (sample 1)

Sample Name: 20220404-POS-AN-4

Sample ID: N/A

Comment: N/A

**Acquisition Info**

Method Path: D:\Analyst Data\Projects\C501\Acquisition Methods\20220930-POS-AN.dam

Batch Path: D:\Analyst Data\Projects\C501\Batch\New Batch.dab

Acquisition Date: Sunday, April 24, 2022

Acquisition Time: 11:30:24 PM

User Name: TRIPLETOF5600\Administrator

Acquisition Method: 20220930-POS-AN.dam

Rack: 1

Plate: 1

Vial: 79

Injection Volume: 2.00

**Quantitation Info**

Sample Type: Unknown

Dilution Factor: 1.0000

**Log Info**

Mass Spectrometer: TripleTOF 5600-1

Config Table Version: 01

Firmware Version: MIA3000 ------- MIL3000 MIB3000

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

Component ID: TripleTOF 5600+

Manufacturer: AB Sciex Instruments

Model: 5016230/L

Serial Number: BN22351402

Source Housing: DuoSpray Ion Source

Mass Spectrometer: TripleTOF 5600-1

Start of Run - Detailed Status: N/A

Vacuum Status: At Pressure

Vacuum Gauge (10e-5 Torr): 2.4

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 of run): 00:00:02

Integrated System: Shimadzu Controller, CBM20Alite

Serial#: L20225219100

ROM Version: 2.72

Pressure Units: psi

Pump: Shimadzu LC30AD

Serial#: L20555204364

ROM Version: 3.10

Pump: Shimadzu LC30AD

Serial#: L20555104258

ROM Version: 3.10

AutoSampler: Shimadzu SIL30AC

Serial#: L20565202103

ROM Version: 3.10

Column Oven: Shimadzu CTO30A

Serial#: L20575100652

ROM Version: 3.00

Injection Volume used: 2.00 µl

Time (from start of run): 00:40:33

Mass Spectrometer: TripleTOF 5600-1

End of Run - Detailed Status: N/A

Vacuum Status: At Pressure

Vacuum Gauge (10e-5 Torr): 2.4

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

**IDA**

With intensity greater than: 10

Switch after: 6 spectra

Use advanced settings: True

Always exclude: True

Exclude for: 0 sec

Mass tolerance units: mDa

Mass tolerance: 50

Use inclusion list: False

Use exclusion list: False

Ignore peaks within: 6 Da

Real time: None

Spectrum file: N/A

Dynamic background subtraction: True

Fragment intensity multiplier: 2

Maximum accumulation: 2 sec

Allow standard filters for Smart IDA: True

Exclude former target ions: True

Exclude isotopes window: 4 Da

**Period 1, Experiment 4**

Experiment Type: TOF MS^2

Num. Cycles: 2409

Polarity: Positive

Product : IDA

Period Cycle Time: 900 ms

Pulser Frequency: 15.392 kHz

Accumulation Time: 100.0 ms

**Experiment Parameters**

*Parameter Value*

CUR 40.000

GS1 50.000

GS2 50.000

ISVF 5500.000

TEM 500.000

**Mass Range Parameters**

*Parameter Value*

CE 35.000

CES 15.000

DP 100.000

IDIx 0.000

IDUx 5.000

IRD 66.633

IRDx 28287.602

IRW 24.917

IRWx 24917.307

IWIx 0.000

IWUx 5.000

XA1 70.480

Start Mass: 50.0

End Mass: 1250.0

**RF Transmission**

*Mass Time (%)*

40.0 50.0

120.0 50.0

**Instrument Tables and Parameters**

**Resolution Table, Quad 1, Positive, Unit, TOF Resolution Mode: High Resolution**

Last Modification Date Time: April 04, 2022 12:17:10

IE1: 2.000

VS1: 0.540

HST: 0.000

VS2: 0.000

*Mass (Da) Offset Value*

59.049 61.720

175.133 61.895

442.337 61.938

674.505 61.940

906.672 61.935

1196.882 61.935

**Resolution Table, Quad 1, Positive, Unit, TOF Resolution Mode: High Sensitivity**

Last Modification Date Time: April 04, 2022 12:15:27

IE1: 2.000

VS1: -0.203

HST: -1.113

VS2: 0.000

*Mass (Da) Offset Value*

59.049 61.720

175.133 61.895

442.337 61.938

674.505 61.940

906.672 61.935

1196.882 61.935

**Mass Calibration Table, Quad 1, Positive, Unit Resolution**

Last Modification Date Time: April 04, 2022 12:19:21

*Mass (Da) Dac Value*

59.049 2468

175.133 7380

442.337 18687

674.505 28513

906.672 38339

1196.882 50622

**TOF Mass Calibration Parameters**

*Polarity Scan Slope Delay (nsec)*

Positive TOFMS 7.018880027725008800e-004 1.017994863329238400e+000

Positive MS/MS High Resolution 7.019077858213306300e-004 7.494127005391801900e-001

Positive MS/MS High Sensitivity 7.018726228726613000e-004 1.051093198444490200e+000

Negative TOFMS 7.018761535024436500e-004 6.063937870770647100e-001

Negative MS/MS High Resolution 7.018893845378848500e-004 1.850125599822521900e+000

Negative MS/MS High Sensitivity 7.018658116844302600e-004 6.440652657408516600e-001

Show TOF Resolution Parameters in Manual Tune: No

**Keyed Text**

File was created with the software version: Analyst TF 1.6

**Shimadzu Integrated System**

500 mL/min

Pump B Conc: 5.0 %

B Curve: 0

Pressure Range (Pump A/B): 0 - 12000 psi

**Autosampler**

Model: SIL-30AC

Use Autosampler: Yes

Rinsing Volume: 500 uL

Needle Stroke: 52 mm.

Rinsing Speed: 35 uL/sec

Sampling Speed: 5.0 uL/sec

Rinse Dip Time: 0 sec

Rinse Mode: Before and after aspiration

Cooler Enabled: No

Control Vial Needle Stroke: 52 mm

Rinse Method: Rinse Port Only

Rinse Time: 2 sec

Measuring Line Purge Volume: 100 uL

Discharge Speed: 1.0 uL/sec

Air Gap: Off

Rinse Port Liquid Selection: R1

Rinsing Type: External

Purge Time of Rinse Port R0: 10.0 min

Purge Time of Measuring Line R0: 10.0 min

Rinsing Start Time Mode: After Acquisition

Rinsing Sequence 1: none

Rinsing Sequence 2: none

Rinsing Sequence 3: none

Rinsing Sequence 4: none

Rinsing Volume (R0 R1 R2): 300 uL

Injection Port Rinsing With R0: On

Injection Port Rinsing With R1: On

Injection Port Rinsing With R2: On

Sample Loop Equilibration: Off

**Oven**

Model: CTO-30A

Temperature Control: Enabled

Temperature: 40 deg. C

Max. Temperature: 160 deg. C

Heat Compensation: Auto

Heat Compensation Flow: 0.2500 mL\min

**System Controller**

Model: CBM-20A Lite

Event 1: Off

Event 2: Off

**Time Program**

*Time Module Events Parameter*

0.01 Pumps Pump B Conc. 5

18.00 Pumps Pump B Conc. 40

35.00 Pumps Pump B Conc. 95

37.00 Pumps Pump B Conc. 95

37.10 Pumps Pump B Conc. 5

40.00 System Controller Stop

**Pretreatment**

Mode: Standard