**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