TBI-FORENSIC SERVICES DIVISION
PERFORMANCE VERIFICATION FORM

Instrument/Method to Verify:

Heisenberg CN16483010 / US1648M021

Check the appropriate box: New Validation ☐ Modification ☐ Performance Check ☑

Laboratory: NCL ☑ KCL ☐ MCL ☐ Unit: Forensic Chemistry

Based on training and competency, the following analyst(s) are authorized by the Technical Leader to participate in this study:

Name Ben Hubert Title SA/FS Initials BH

Completed: Signature/Date Ben Hubert

Name _____ Title _____ Initials _____

Completed: Signature/Date _____

Name _____ Title _____ Initials _____

Completed: Signature/Date _____

Verification of final review:

Unit Supervisor/Date Rebecca Hernandez

Unit Supervisor/Date Brett Trotter

Unit Manger/Date Glenn Everett

Crime Laboratory Regional Supervisor/Date Jenifer Hall (Mar 13, 2023 10:45 CDT)

Crime Laboratory Regional Supervisor/Date _____

Forensic IT Manager/Date Matthew Buck

Quality Assurance Manager/Date Chad Johnson (Mar 14, 2023 09:27 CDT)

By signing below, I have verified this study meets all requirements and I deem this procedure/instrument fit for the intended use:

Technical Leader/Date Brett Trotter

All information must be submitted to the Quality Assurance Manager prior to the implementation of the procedure/instrument. If applicable, include training plan and competency testing schedule.

Validation Study for updating Heisenberg to Windows 10

Tennessee Bureau of Investigation Nashville Crime Lab

3-12-23

1. **Purpose of validation**
   The purpose of this validation study is to verify the performance of Heisenberg. This study will verify the methods, performance, and accuracy of identifications by comparative analysis. This is required as Heisenberg received firmware updates, and a new computer, requiring a limited revalidation to demonstrate that it still produces acceptable data for casework.

2. **Objectives**
   a. Demonstrate the accurate operation of the gas chromatograph mass spectrometer and gas chromatograph flame ionization detector after receiving firmware updates to the instrument and the computer being updated.
   b. Demonstrate the ability of the Masshunter and Chemstation software to function as intended software to continue to function with the updated system software.

3. **Setup and Procedures**
   Forensic chemistry MS and GC identification methods were created with the same parameters as a previously validated methods on this instrument before being updated. The hand injection methods were developed from the autosample methods.

   Appropriate standards were run on each autosample method to demonstrate performance and consistency. Two different standards/standard mixes were run on each autosample method. Instrument repeatability was confirmed by running the same standard mix three times on the ASMSDRUGS100 and ASGC100.

   For the hand injection methods, appropriate standards were run on the only on MSDRUGS100 and GC100 methods to demonstrate performance for the hand injection methods. Because these methods are based off the autosample methods, additional testing was not required.

   Two separate standard mixes were used depending on the method; one containing tramadol, -anilino-N-phenethylpiperidine, heroin, acetyl fentanyl, para-fluorofentanyl and fentanyl and the other containing cocaine, hydrocodone, and pethidine. A buprenorphine standard was also run on the appropriate methods.

   The spectra obtained from these standards were compared to spectra to library spectra and the chromatographs were compared to chromatographic data obtained before the update.

4. **Results and Conclusion**
   Analysis of the standards run on Heisenberg have consistently shown compliance with standard operating procedures in chapter 21. All methods have been utilized in the analysis of known drug standards. The data obtained from these standards is consistent with previously verified standards in the Nashville forensic chemistry standard library. The instrument response was compared to older data taken from before the period of maintenance. The chromatography, peak shape, and separation all appear to be consistent to the data that the instrument was generating prior to the update.

5. **Training and Competency**

The instrument used for the question methods is configured the same as the other existing instruments in the laboratory. There are no significant changes in instrumentation that would warrant an initial demonstration of proficiency for these methods.

6. **Conclusions**

After monitoring parameters specified in Forensic Chemistry Standard Operating Procedure found in chapter 21 and verifying the functionality of the methods with known drug standards, it has been demonstrated that Heisenberg produced comparable results to previous instrument response and GCMS libraries. This confirms the correct operation of the updated firmware and software.

Materials

Computer:

Device:	Heisenberg
Processor	11th Gen Intel(R) Core(TM) i5-11600 @ 2.80GHz 2.81 GHz
Installed RAM	16.0 GB (15.7 GB usable)
Device ID	B937707C-6C34-41B6-A16F-7145A01E5A2F
Product ID	00355-63022-12005-AAOEM
System type	64-bit operating system, x64-based processor
Pen and touch	No pen or touch input is available for this display

Windows Edition: Windows 10 Pro

Version	22H2
Installed on	12/7/2022
OS build	19045.2604
Experience	Windows Feature Experience Pack 120.2212.4190.0

Productivity tools:
Enhanced Chemstation
F.01.03.2357

Agilent MassHunter Workstation:
Version 10.0.368

GC:
Aiglent 7890B GC system
Serial: CN16483010

MS:
Aiglent 5977B
Serial: US1648M021

Columns:
GC: Agilent J&W GC HP-1MS 15 meter, 0.32 mm ID, 0.25 µm film thickness
MS: Agilent J&W GC HP-1MS 12.5 meter, 0.20 mm ID, 0.33 µm film thickness

GCMS Standard Mix
MEOH (Fisher lot# 214330)
Pethidine (S.B. Penick 413 NMN-027)
Cocaine Base (Merck lot # U7472)
Hydrocodone (Merck lot # V1526)
Made: BTT 5-2-22 Exp. 5-2-23

THFF4A Retention Time Mix
MEOH lot #215157 Bottle #5
Tramdol (Sigma Alrdrich# BCBB9210)
4-ANPP (Cayman# 0540831-6)
Heroin (Cayman# 0559235-2)
Acetyl fentanyl (Cayman# 04197037)
Para-fluorofentanyl (Cayman#0541563-27)
Fentanyl (USPC# 1275-F)
Made by RH 10-20-22 exp, 10-20-23

Buprenorphine
Cerilliant lot# FE0.191903 Exp. 6-2024

GC and GC/MS methods

Gas Chromatography /Mass Spectrometry methods

Manual Injection	
MSDRUGS100	100-280^{o}C for 10 minutes
MSDRUGS200	200-280^{o}C for 10 minutes
MSDRUGS60	60-280^{o}C for 10 minutes
MSDRUGSTI	100-280^{o}C for 30 minutes

Auto-sample Injection	
ASMSDRUGS100	100-280^{o}C for 10 minutes
ASMSDRUGS200	200-280^{o}C for 10 minutes
ASMSDRUGS60	60-280^{o}C for 10 minutes
ASMSDRUGSTI	100-280^{o}C for 30 minutes
THC-MS (Quant)	230-280^{o}C for 5 minutes (Select instruments only)

Gas Chromatography Methods

Manual Injection	
GC100	100-280^{o}C for 10 minutes
GC200	200-280^{o}C for 10 minutes
GC280ISOTI	280^{o}C isothermal for 30 minutes

Auto-sample Injection	
ASGC100	100-280^{o}C for 10 minutes
ASGC200	200-280^{o}C for 10 minutes
ASGC280ISOTI	280^{o}C isothermal for 30 minutes

BH
3-11-23

C:\MassHunter\GCMS\1\methods\ASGC100.M
Fri Mar 10 14:50:21 2023

Control Information

Sample Inlet : GC
Injection Source : GC ALS
Injection Location: Rear
Mass Spectrometer : Disabled

No Sample Prep method has been assigned to this method.

GC
GC Summary

Run Time	10.001 min
Post Run Time	0 min

Oven
Temperature

Setpoint	On
(Initial)	100 °C
Hold Time	1 min
Post Run	100 °C
Program	
#1 Rate	70 °C/min
#1 Value	280 °C
#1 Hold Time	6.43 min

Equilibration Time	1.5 min
Max Temperature	325 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled

ALS
Front Injector

Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	1
Sample Wash Volume	4 µL
Sample Pumps	2
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	6000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	6000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL

Solvent Wash Mode	A, B

BH
3-11-23

Back Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	2
Sample Wash Volume	8 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL
Solvent Wash Mode	A, B

Sample Overlap	
Mode	Sample overlap is not enabled

ALS Errors	Pause for user interaction

Front SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 12.023 psi
Total Flow	On 91.918 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	On 30 After 3 min mL/min
Split Ratio	80 :1
Split Flow	87.82 mL/min
Liner	A Liner has not been selected.

Back SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 10 psi
Total Flow	On 172.89 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	On 20 After 2 min mL/min
Split Ratio	50 :1
Split Flow	166.56 mL/min
Liner	A Liner has not been selected.

Thermal Aux 3 (MSD Transfer Line)	
Temperature	
Setpoint	On
(Initial)	280 °C

Column	
Column #1	
Flow	
Setpoint	Off

(Initial)	1.0978 mL/min
Post Run	0.57353 mL/min

BH
3-11-23

Column Information	Agilent 19091S-602
HP-1MS	
Temperature Range	-60 °C—325 °C (350 °C)
Dimensions	12.5 m x 200 µm x 0.33 µm (Calibrated)
Column lock	Locked
In	Front SS Inlet He
Out	MSD
(Initial)	100 °C
Pressure	12.023 psi
Flow	1.0978 mL/min
Average Velocity	60.532 cm/sec
Holdup Time	0.34417 min
Control Mode	Constant Flow

Column #2	
Pressure	
Setpoint	On
(Initial)	10 psi
Post Run	11.178 psi

Column Information	Agilent 19091S-913
HP-1MS	
Temperature Range	-60 °C—325 °C (325 °C)
Dimensions	15 m x 320 µm x 0.25 µm (Calibrated)
Column lock	Locked
In	Back SS Inlet He
Out	Back Detector FID
(Initial)	100 °C
Pressure	10 psi
Flow	3.3311 mL/min
Average Velocity	63.306 cm/sec
Holdup Time	0.39491 min
Control Mode	Constant Pressure

Column Outlet Pressure	0 psi

Back Detector FID	
Makeup	He
Column Compensation	Signal is modified by Column Compensation Curve #2
Heater	On 300 °C
H2 Flow	On 40 mL/min
Air Flow	On 400 mL/min
Makeup Flow (Combined)	On 25 mL/min
Carrier Gas Flow Correction	Column + Makeup = Constant
Flame	On

Aux EPC 1,2,3	
Aux EPC 1 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Aux EPC 2 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness ***Excluded from Affecting GC's Readiness State***

BH
3-11-23

Aux EPC 3 N2
Pressure
Setpoint Off
(Initial) 10 psi
Post Run 0 psi

Excluded from Readiness ***Excluded from Affecting GC's Readiness State***

Signals
Signal #1: Back Signal
Description Back Signal
Details Back Signal (FID)
Save On
Data Rate 50 Hz
Dual Injection Assignment Front Sample

Signal #2: Test Plot
Description Test Plot
Save Off
Data Rate 50 Hz
Dual Injection Assignment Back Sample

Signal #3: Test Plot
Description Test Plot
Save Off
Data Rate 50 Hz
Dual Injection Assignment Back Sample

Signal #4: Test Plot
Description Test Plot
Save Off
Data Rate 50 Hz
Dual Injection Assignment Back Sample

TUNE PARAMETERS for SN: US1648M021

Trace Ion Detection is OFF.

34.593	:	EMISSION
70.007	:	ENERGY
34.899	:	REPELLER
90.331	:	IONFOCUS
22.672	:	ENTRANCE_LENS
1360.190	:	EMVOLTS
1498.6	:	Actual EMV
1.00	:	GAIN FACTOR
2908.000	:	AMUGAIN
136.750	:	AMUOFFSET
1.000	:	FILAMENT
0.000	:	DCPOLARITY
12.032	:	ENTLENSOFFSET
0.000	:	Ion_Body
0.000	:	EXTLENS
442.000	:	MASSGAIN
-22.000	:	MASSOFFSET

END OF TUNE PARAMETERS

BH
3-11-23

END OF INSTRUMENT CONTROL PARAMETERS

DATA ANALYSIS PARAMETERS

Method Name: C:\MassHunter\GCMS\1\methods\ASGC100.M

Percent Report Settings

Sort By: Signal

Output Destination
    Screen: No
    Printer: Yes
    File: No

Integration Events: AutoIntegrate

Generate Report During Run Method: No

Signal Correlation Window: 0.020

Quantitative Report Settings

Report Type: Summary

Output Destination
    Screen: Yes
    Printer: No
    File: No

Generate Report During Run Method: No

Calibration Last Updated:

Reference Window: 10.00 Percent
Non-Reference Window: 5.00 Percent
Correlation Window: 0.02 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

Compound Information

END OF DATA ANALYSIS PARAMETERS

Fri Mar 10 14:50:26 2023

METHOD CONTROL PARAMETERS

BH
3-11-23

Method Information for: C:\MassHunter\GCMS\1\methods\ASGC100.M

Method Sections To Run:

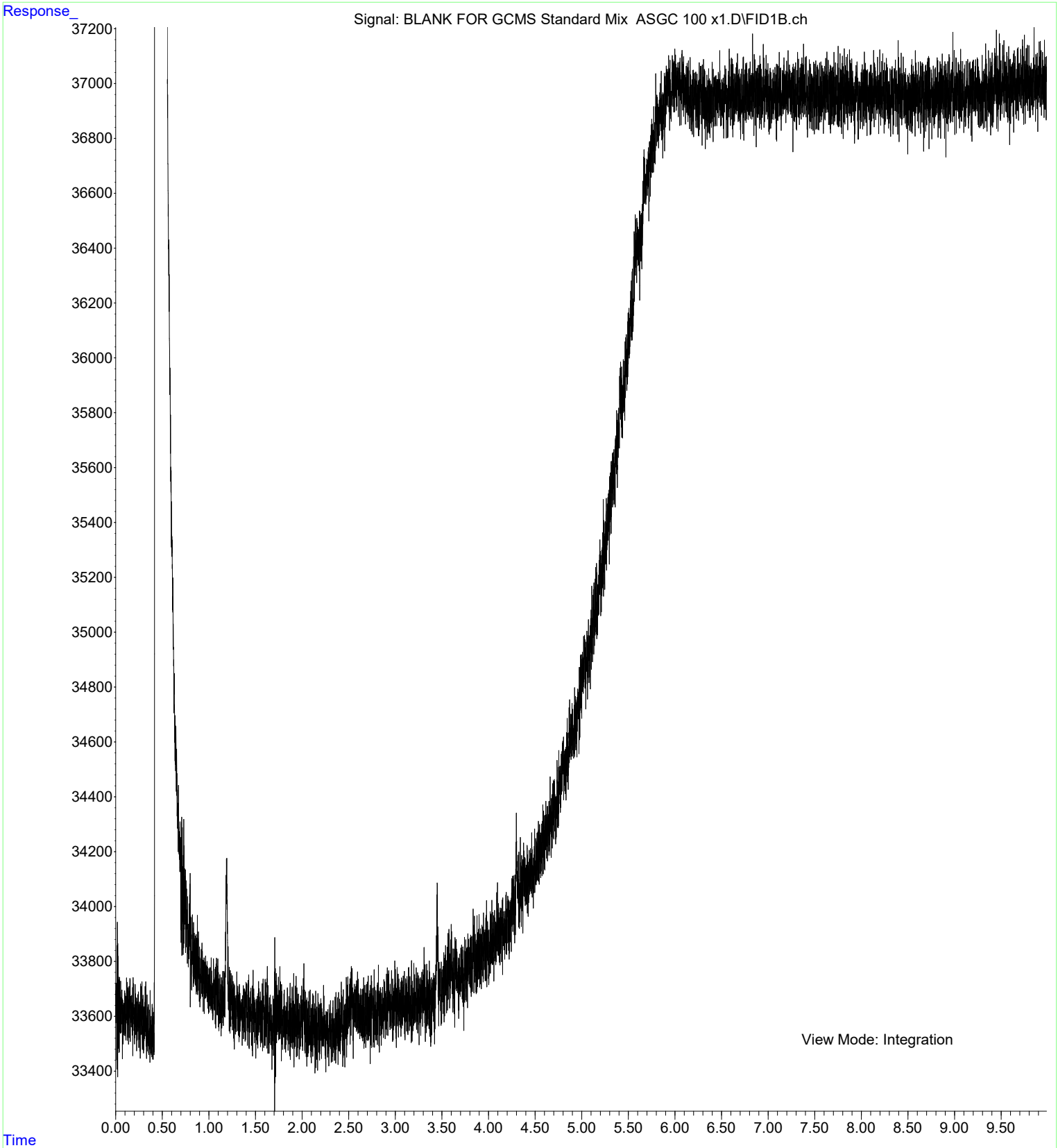
( ) Save Copy of Method With Data
( ) Instrument Control Pre-Run Cmd/Macro =
( ) Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
(X) Data Analysis
( ) Instrument Control Post-Run Cmd/Macro =
( ) Data Analysis Post-Run Cmd/Macro =

Method Comments:
ASGC100

END OF METHOD CONTROL PARAMETERS

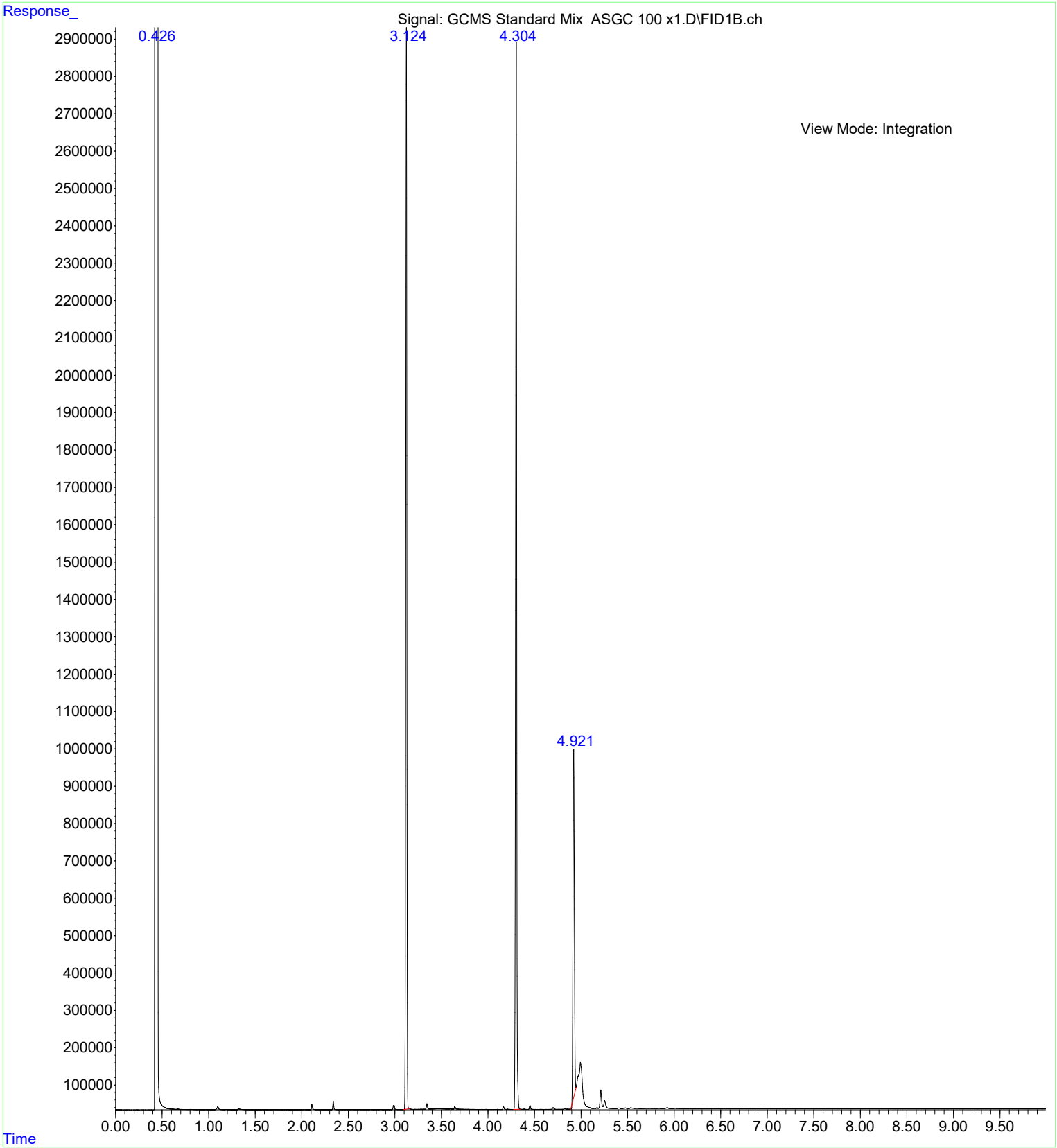
BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR GCMS Standard Mix ASGC 100 x1.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 00:03 using AcqMethod ASGC100.M
Sample Name: BLANK FOR GCMS Standard Mix ASGC 100 x1
Misc Info : METHANOL



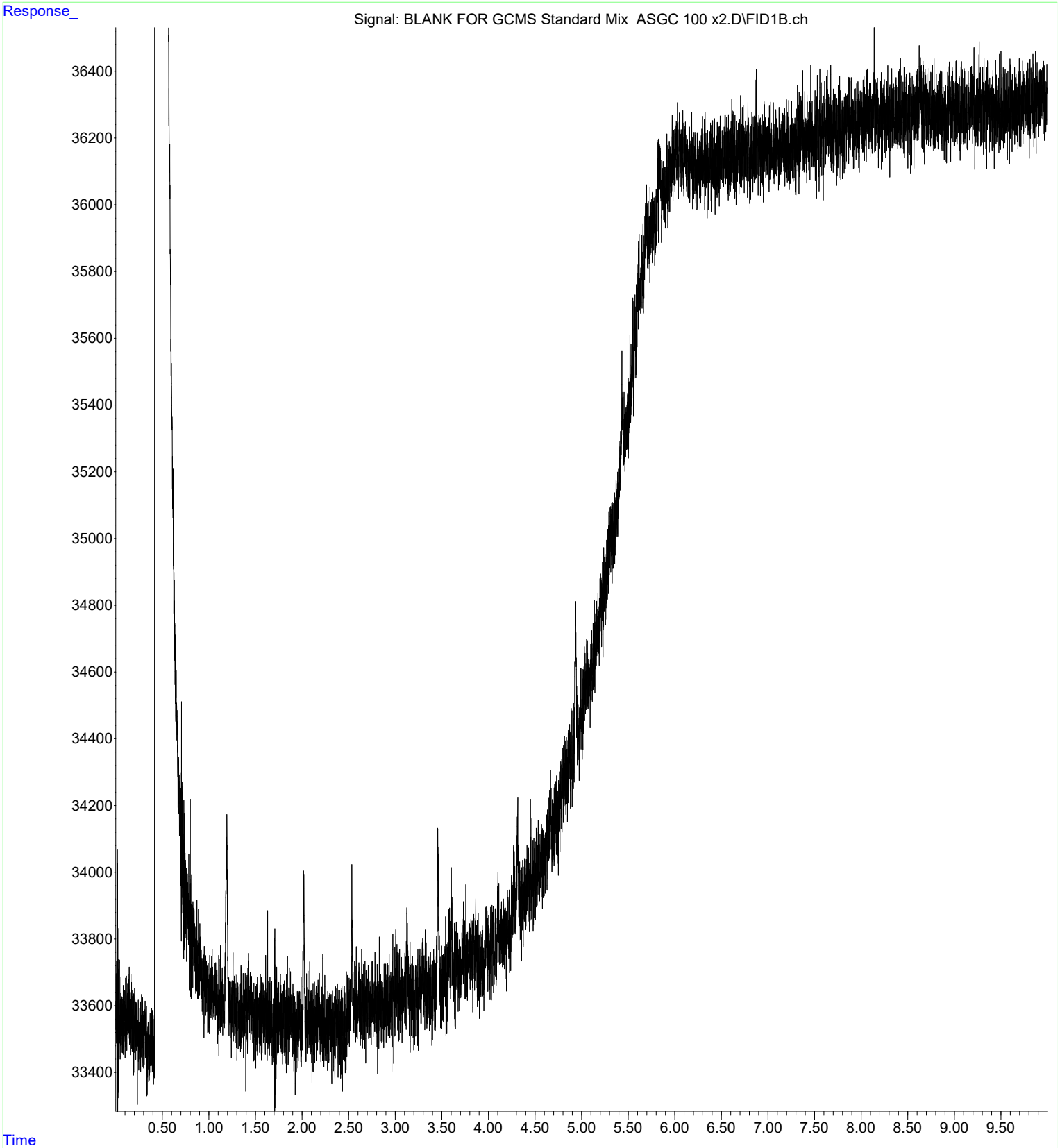
BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASGC 100 x1.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 00:18 using AcqMethod ASGC100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASGC 100 x1
Misc Info : METHANOL



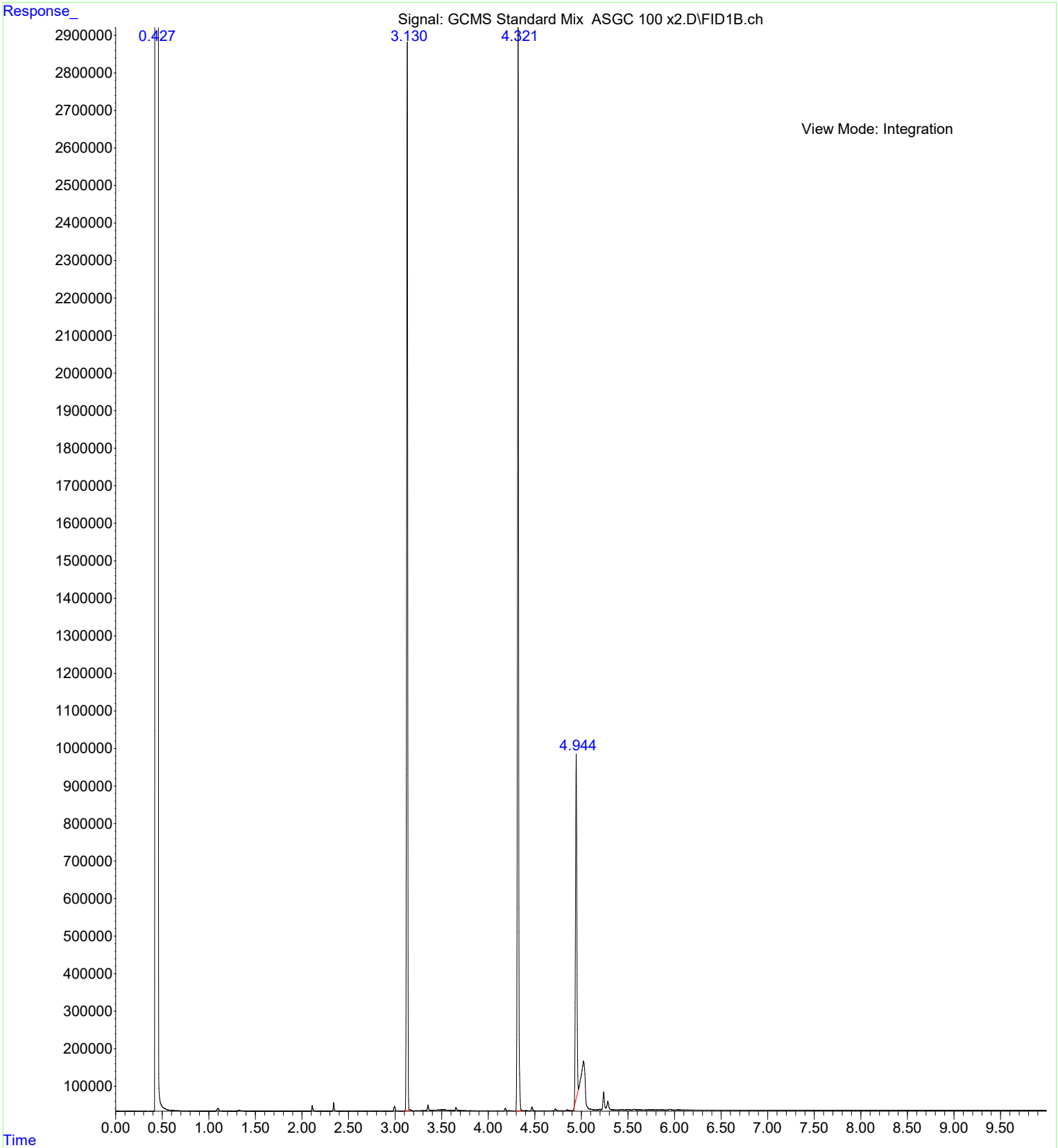
BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR GCMS Standard Mix ASGC 100 x2.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 00:47 using AcqMethod ASGC100.M
Sample Name: BLANK FOR GCMS Standard Mix ASGC 100 x2
Misc Info : METHANOL



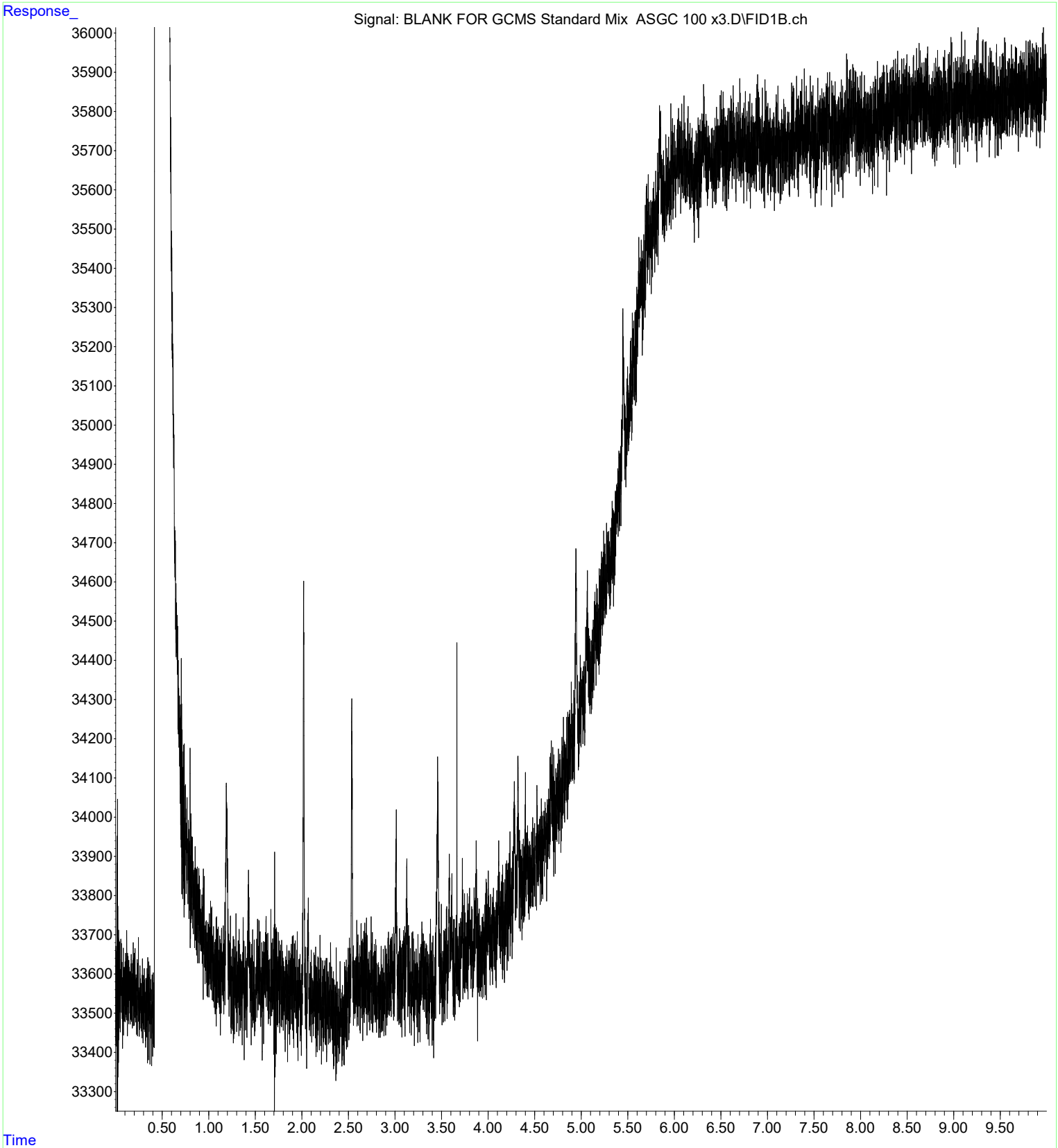
BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASGC 100 x2.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 01:01 using AcqMethod ASGC100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASGC 100 x2
Misc Info : METHANOL



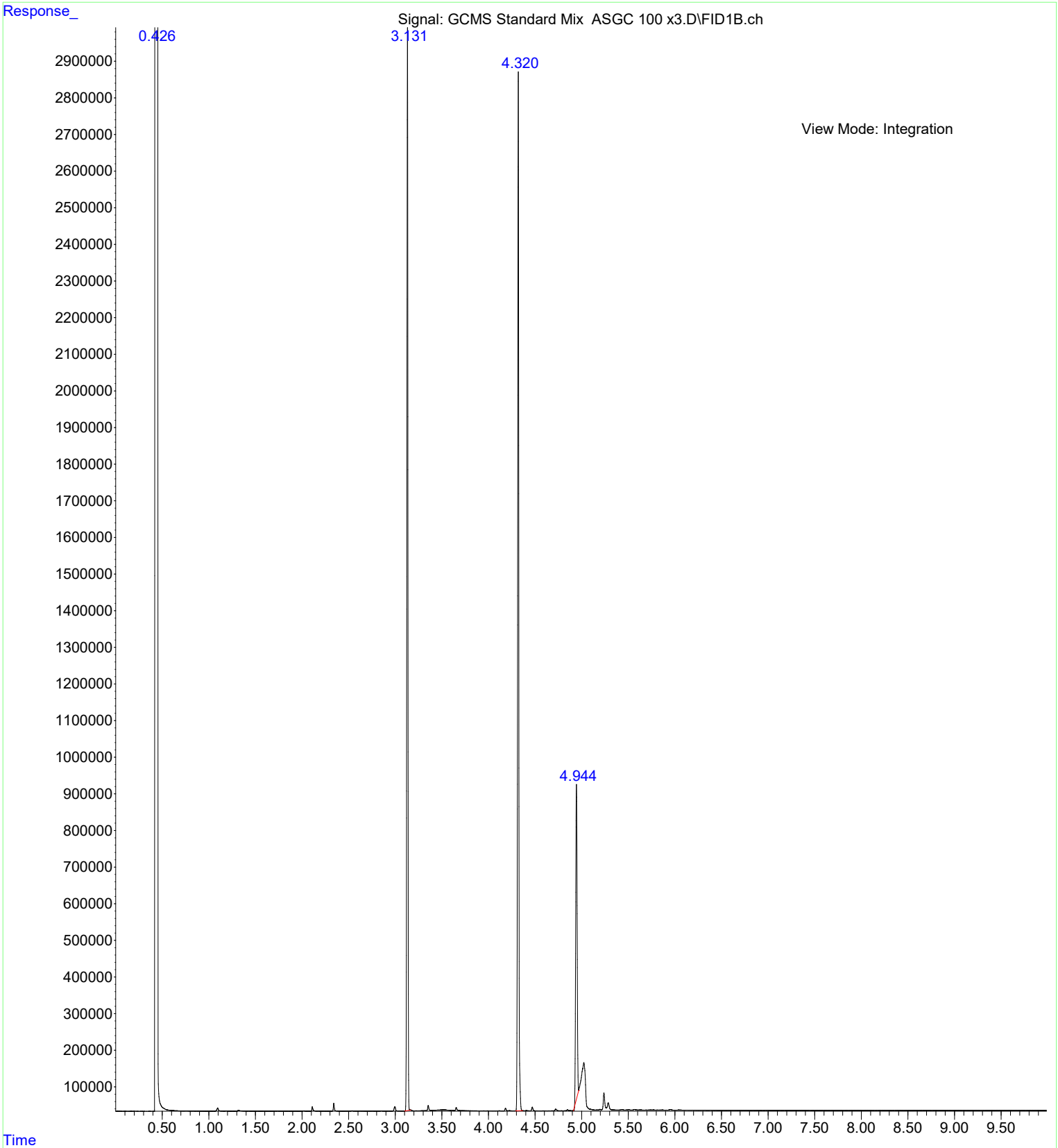
BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR GCMS Standard Mix ASGC 100 x3.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 01:30 using AcqMethod ASGC100.M
Sample Name: BLANK FOR GCMS Standard Mix ASGC 100 x3
Misc Info : METHANOL



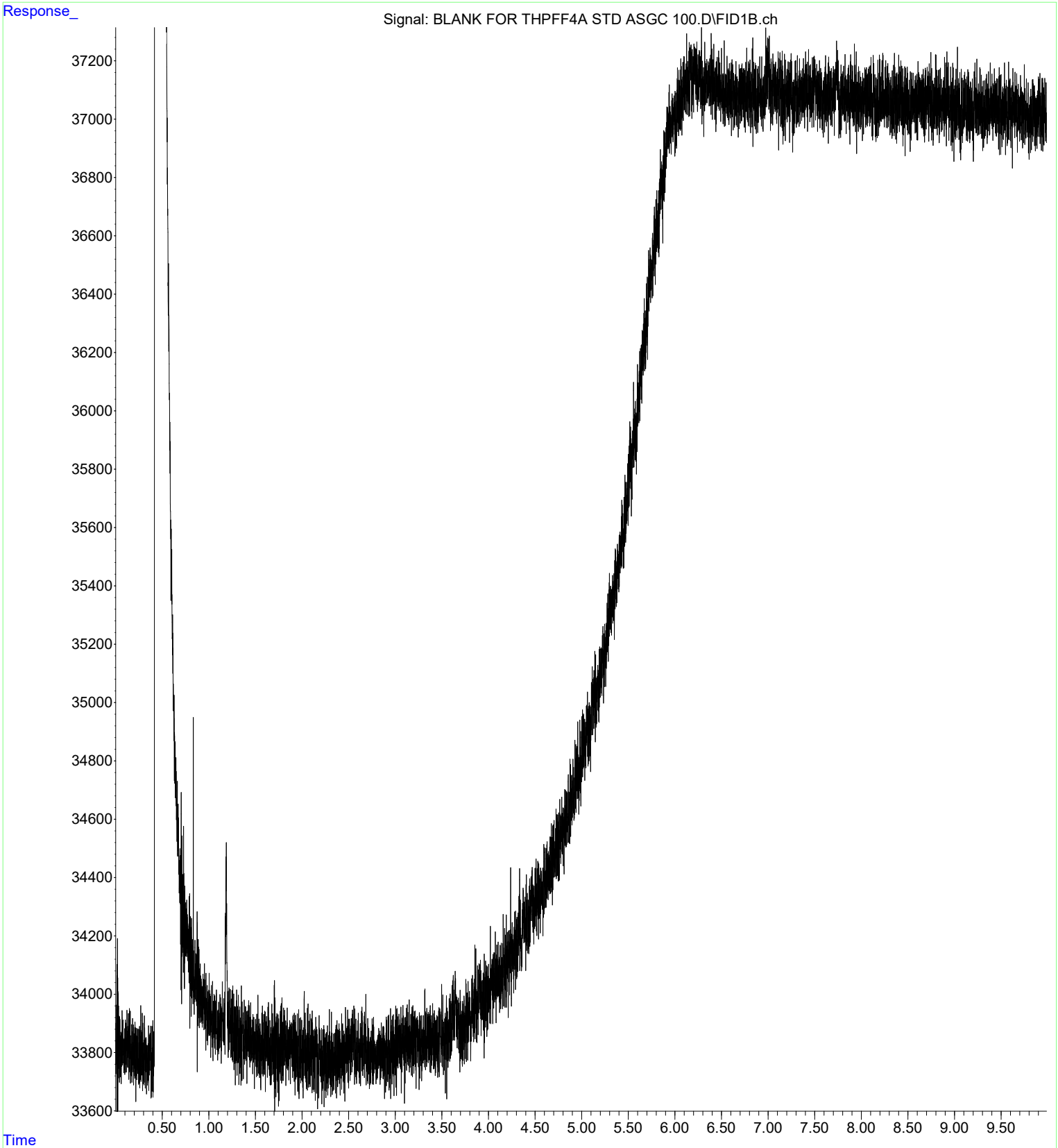
BH
3-11-23

```
File       :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
...         MS Standard Mix  ASGC 100 x3.D
Operator   :
Instrument :   Heisenberg
Acquired   : 11 Mar 2023  01:45     using AcqMethod ASGC100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASGC 100 x3
Misc Info  : METHANOL
```



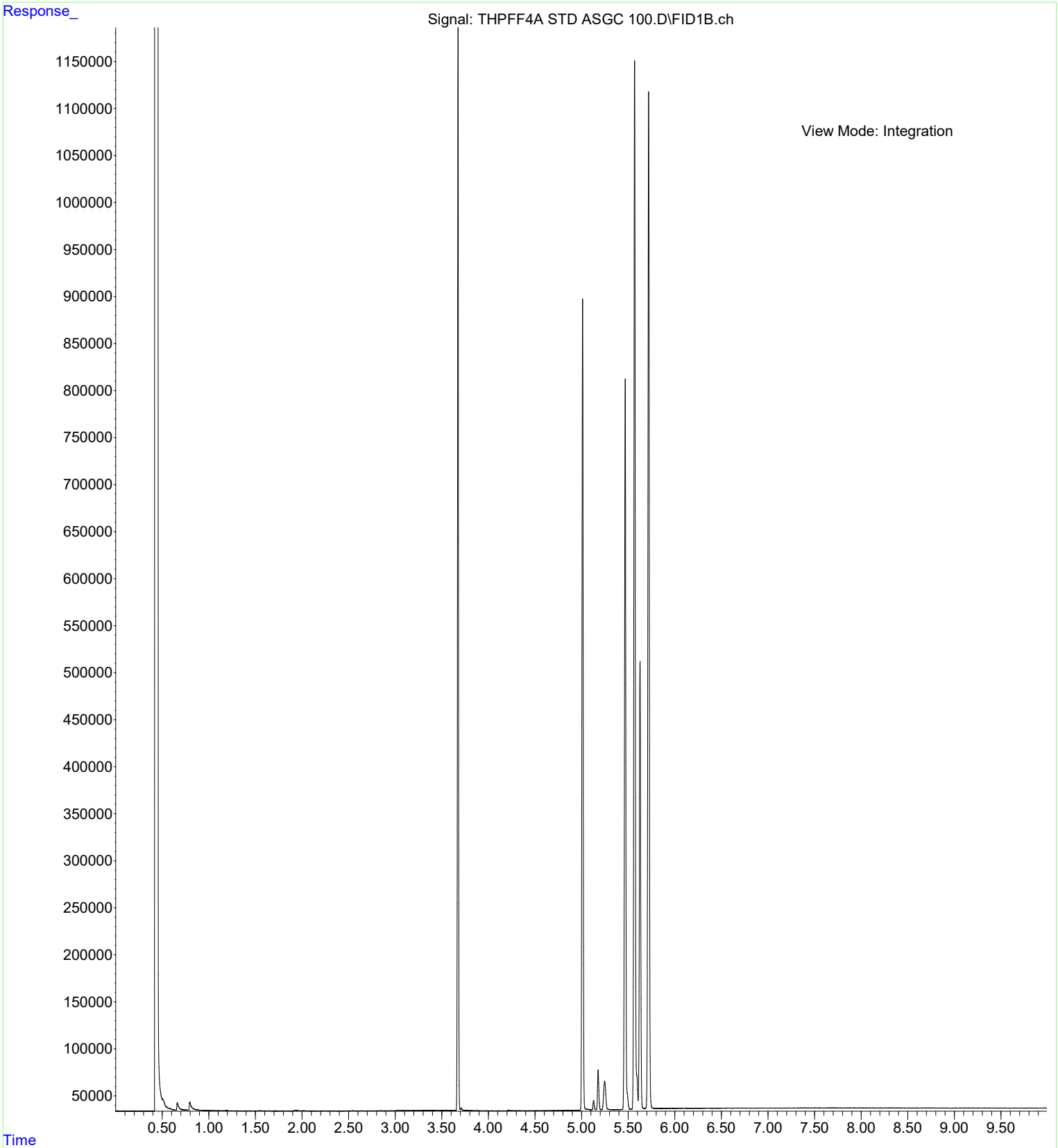
BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR THPFF4A STD ASGC 100.D
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 22:34 using AcqMethod ASGC100.M
Sample Name: BLANK FOR THPFF4A STD ASGC 100
Misc Info : METHANOL



BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASGC 100.D
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 22:49 using AcqMethod ASGC100.M
Sample Name: THPFF4A STD EXP. 10-20-23 ASGC 100
Misc Info : METHANOL



BH
3-11-23

C:\MassHunter\GCMS\1\methods\ASGC200.M
Fri Mar 10 21:41:19 2023

Control Information

Sample Inlet	: GC
Injection Source	: GC ALS
Injection Location:	Rear
Mass Spectrometer	: Disabled

No Sample Prep method has been assigned to this method.

GC

GC Summary

Run Time	10.003 min
Post Run Time	0 min

Oven

Temperature	
Setpoint	On
(Initial)	200 °C
Hold Time	1 min
Post Run	100 °C
Program	
#1 Rate	70 °C/min
#1 Value	280 °C
#1 Hold Time	7.86 min

Equilibration Time	1.5 min
Max Temperature	325 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled

ALS

Front Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	0
Solvent A Washes (PostInj)	0
Solvent A Volume	4 µL
Solvent B Washes (PreInj)	0
Solvent B Washes (PostInj)	0
Solvent B Volume	4 µL
Sample Washes	1
Sample Wash Volume	1 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0 µL

Solvent Wash Mode	A, B

BH
3-11-23

Back Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	2
Sample Wash Volume	8 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL
Solvent Wash Mode	A, B

Sample Overlap	
Mode	Sample overlap is not enabled

ALS Errors	Pause for user interaction

Front SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 17.921 psi
Total Flow	On 91.918 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	On 30 After 3 min mL/min
Split Ratio	80 :1
Split Flow	87.82 mL/min
Liner	A Liner has not been selected.

Back SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 10 psi
Total Flow	On 117.01 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	Off
Split Ratio	50 :1
Split Flow	111.77 mL/min
Liner	A Liner has not been selected.

Thermal Aux 3 (MSD Transfer Line)	
Temperature	
Setpoint	On
(Initial)	280 °C

Column	
Column #1	
Flow	
Setpoint	On

(Initial)	1.0978 mL/min
Post Run	0.57353 mL/min

BH
3-11-23

Column Information	Agilent 19091S-602
HP-1MS	
Temperature Range	-60 °C—325 °C (350 °C)
Dimensions	12.5 m x 200 µm x 0.33 µm (Calibrated)
Column lock	Locked
In	Front SS Inlet He
Out	MSD
(Initial)	200 °C
Pressure	17.921 psi
Flow	1.0978 mL/min
Average Velocity	62.876 cm/sec
Holdup Time	0.33134 min
Control Mode	Constant Flow

Column #2	
Pressure	
Setpoint	On
(Initial)	10 psi
Post Run	11.178 psi

Column Information	Agilent 19091S-913
HP-1MS	
Temperature Range	-60 °C—325 °C (325 °C)
Dimensions	15 m x 320 µm x 0.25 µm (Calibrated)
Column lock	Locked
In	Back SS Inlet He
Out	Back Detector FID
(Initial)	200 °C
Pressure	10 psi
Flow	2.2354 mL/min
Average Velocity	53.867 cm/sec
Holdup Time	0.4641 min
Control Mode	Constant Pressure

Column Outlet Pressure	0 psi

Back Detector FID	
Makeup	He
Heater	On 300 °C
H2 Flow	On 40 mL/min
Air Flow	On 400 mL/min
Makeup Flow (Combined)	On 25 mL/min
Carrier Gas Flow Correction	Column + Makeup = Constant
Flame	On

Aux EPC 1,2,3	
Aux EPC 1 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Aux EPC 2 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Aux EPC 3 N2
Pressure

Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Signals

Signal #1: Back Signal

Description	Back Signal
Details	Back Signal (FID)
Save	On
Data Rate	50 Hz
Dual Injection Assignment	Front Sample

Signal #2: Test Plot

Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

Signal #3: Test Plot

Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

Signal #4: Test Plot

Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

TUNE PARAMETERS for SN: US1648M021

Trace Ion Detection is OFF.

34.593	:	EMISSION
70.007	:	ENERGY
34.899	:	REPELLER
90.331	:	IONFOCUS
22.672	:	ENTRANCE_LENS
1360.190	:	EMVOLTS
1498.6	:	Actual EMV
1.00	:	GAIN FACTOR
2908.000	:	AMUGAIN
136.750	:	AMUOFFSET
1.000	:	FILAMENT
0.000	:	DCPOLARITY
12.032	:	ENTLENSOFFSET
0.000	:	Ion_Body
0.000	:	EXTLENS
442.000	:	MASSGAIN
-22.000	:	MASSOFFSET

END OF TUNE PARAMETERS

BH
3-11-23

END OF INSTRUMENT CONTROL PARAMETERS

DATA ANALYSIS PARAMETERS

Method Name: C:\MassHunter\GCMS\1\methods\ASGC200.M

Percent Report Settings

Sort By: Signal

Output Destination
    Screen: No
    Printer: Yes
    File: No

Integration Events: AutoIntegrate

Generate Report During Run Method: No

Signal Correlation Window: 0.020

Quantitative Report Settings

Report Type: Summary

Output Destination
    Screen: Yes
    Printer: No
    File: No

Generate Report During Run Method: No

Calibration Last Updated:

Reference Window: 10.00 Percent
Non-Reference Window: 5.00 Percent
Correlation Window: 0.02 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

Compound Information

END OF DATA ANALYSIS PARAMETERS

Fri Mar 10 21:41:38 2023

METHOD CONTROL PARAMETERS

BH
3-11-23

Method Information for: C:\MassHunter\GCMS\1\methods\ASGC200.M

Method Sections To Run:

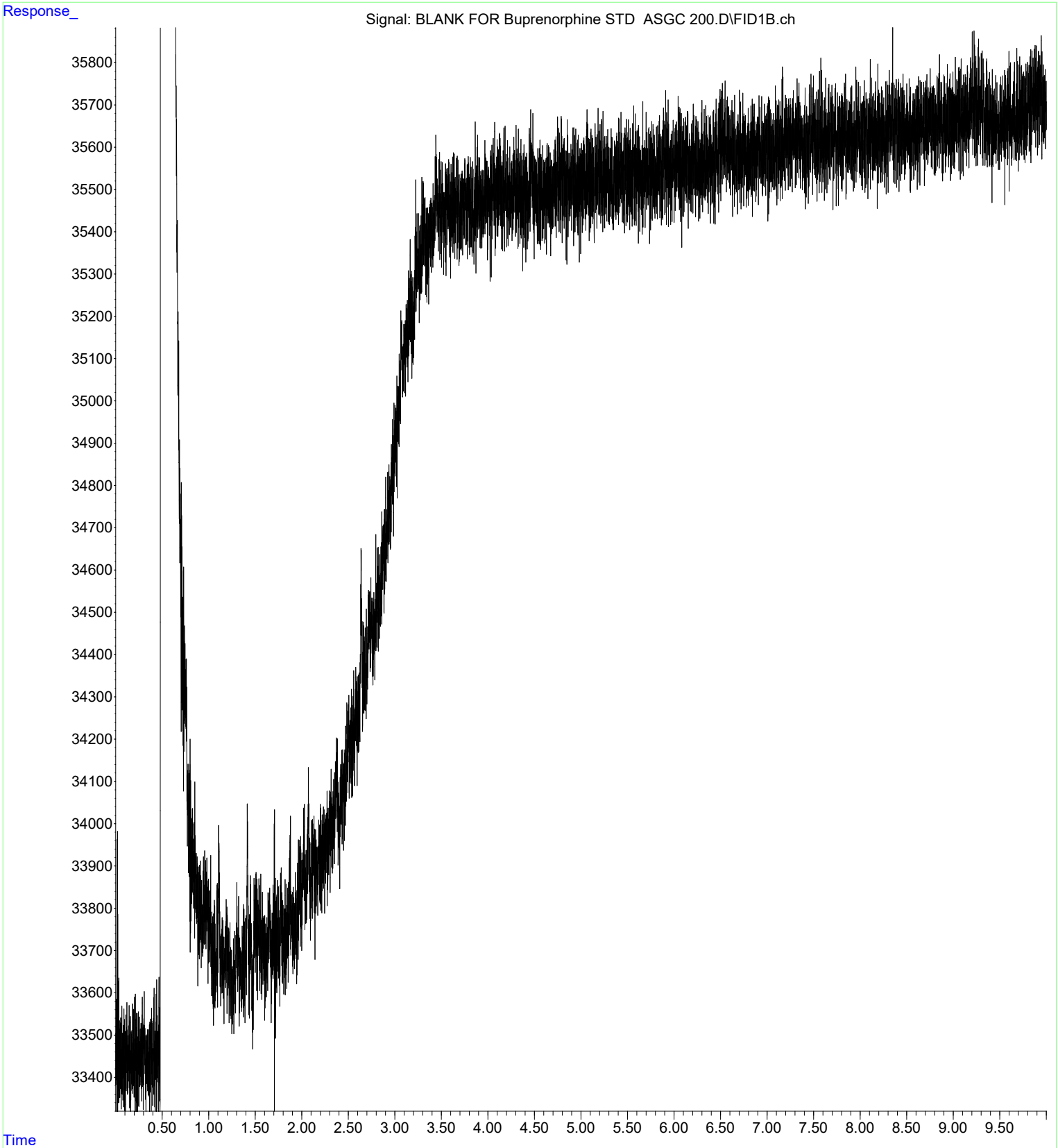
( ) Save Copy of Method With Data
( ) Instrument Control Pre-Run Cmd/Macro =
( ) Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
(X) Data Analysis
( ) Instrument Control Post-Run Cmd/Macro =
( ) Data Analysis Post-Run Cmd/Macro =

Method Comments:
ASGC200

END OF METHOD CONTROL PARAMETERS

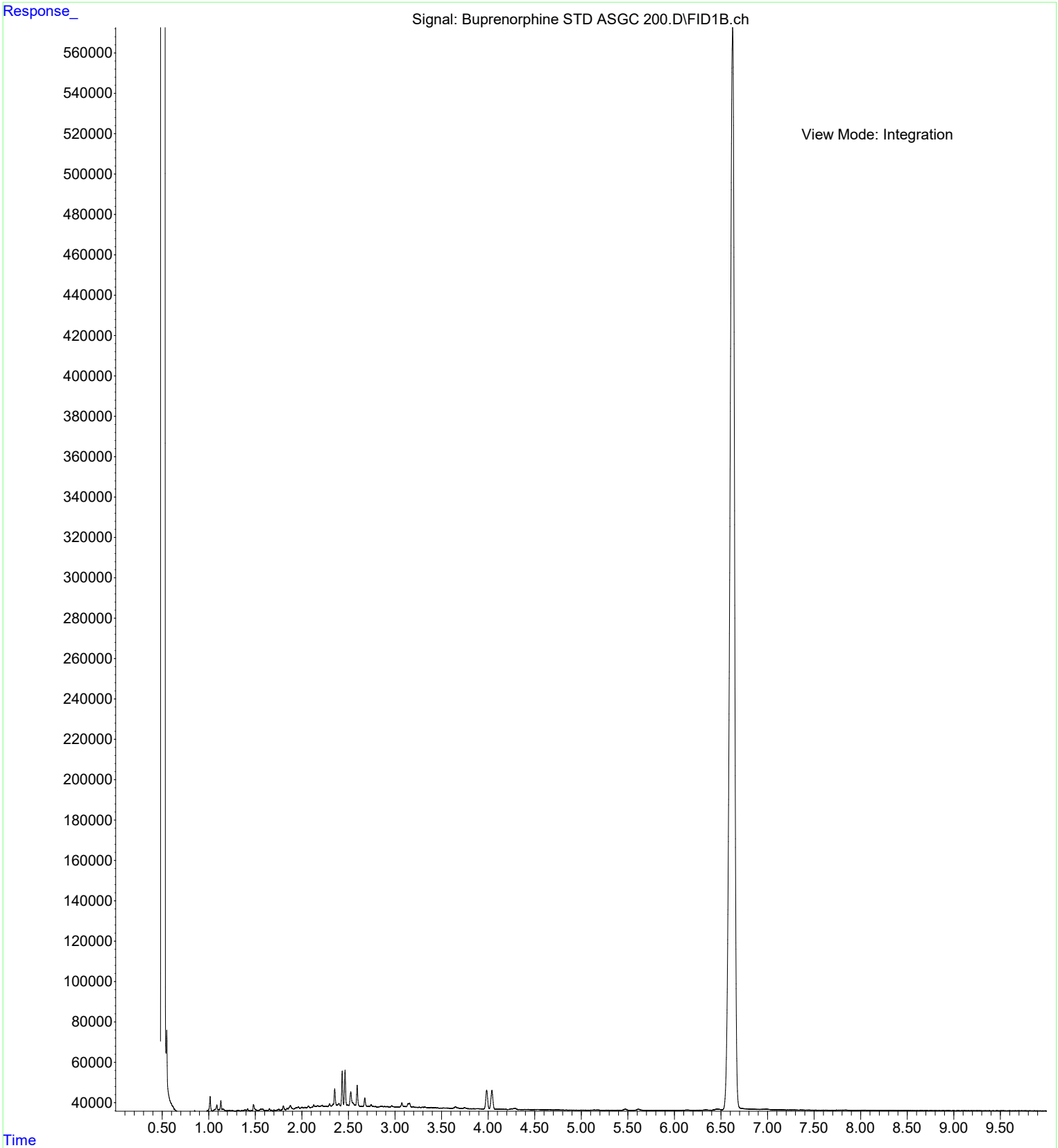
BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR Buprenorphine STD ASGC 200.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 02:15 using AcqMethod ASGC200.M
Sample Name: BLANK FOR Buprenorphine STD ASGC 200
Misc Info : METHANOL



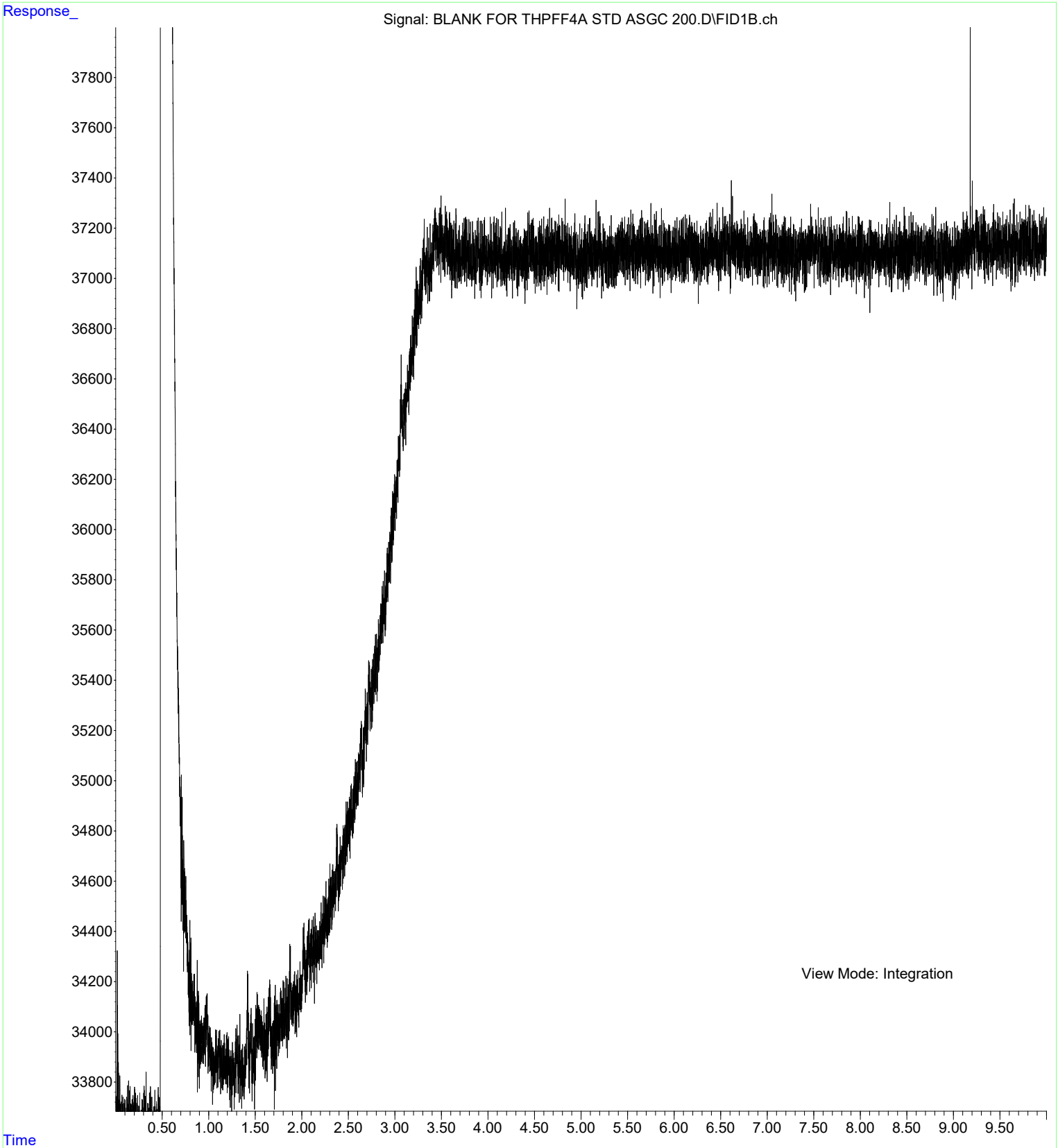
BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\Bu
... prenorphine STD ASGC 200.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 02:29 using AcqMethod ASGC200.M
Sample Name: Buprenorphine STD EXP. 6-2024 ASGC 200
Misc Info : METHANOL



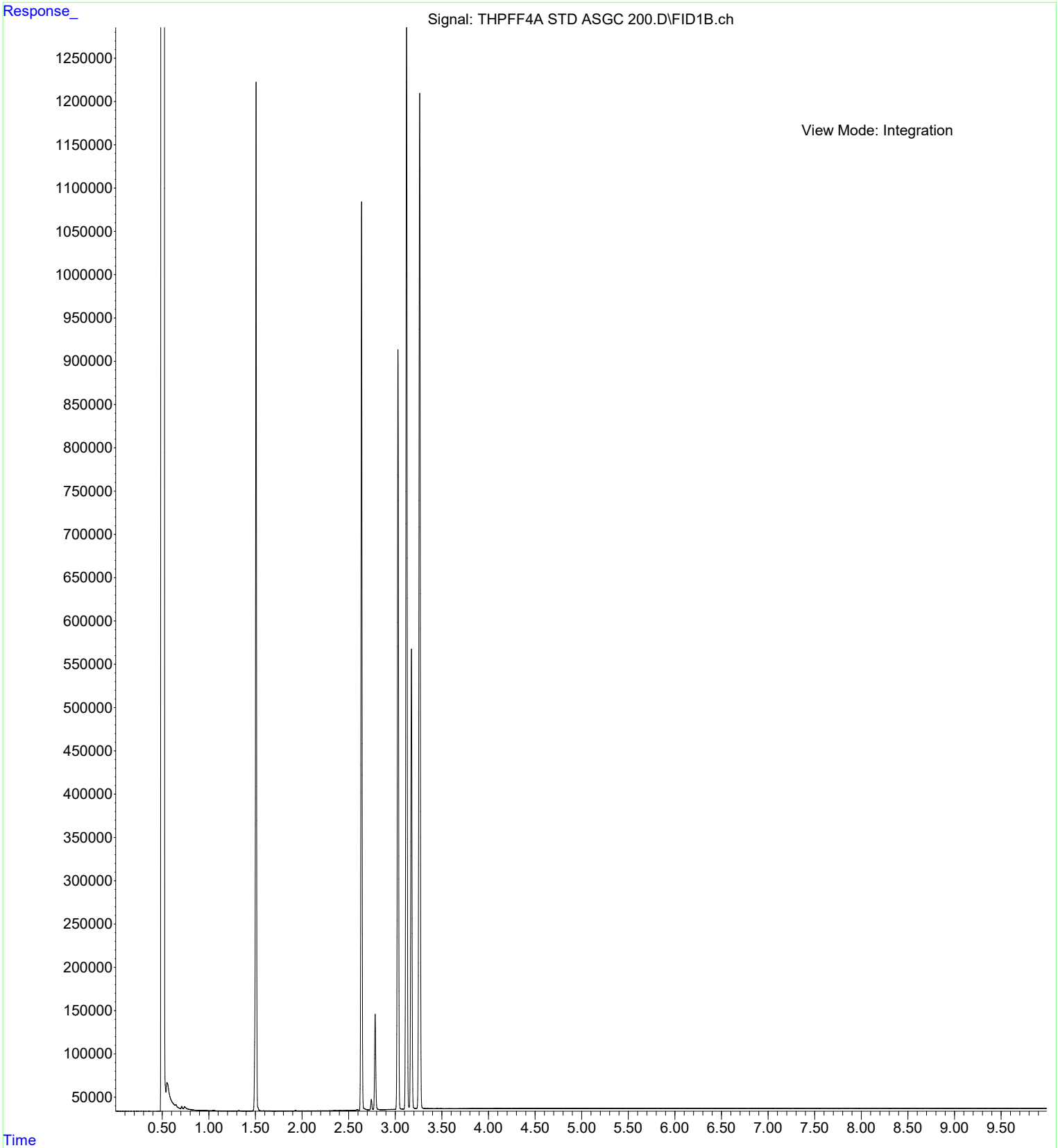
BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR THPFF4A STD ASGC 200.D
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 23:19 using AcqMethod ASGC200.M
Sample Name: BLANK FOR THPFF4A STD ASGC 200
Misc Info : METHANOL



BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASGC 200.D
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 23:33 using AcqMethod ASGC200.M
Sample Name: THPFF4A STD EXP. 10-20-23 ASGC 200
Misc Info : METHANOL



BH
3-11-23

C:\MassHunter\GCMS\1\methods\ASGC280ISOTI.M
Fri Mar 10 21:47:52 2023

Control Information

Sample Inlet : GC
Injection Source : GC ALS
Injection Location: Rear
Mass Spectrometer : Disabled

No Sample Prep method has been assigned to this method.

GC
GC Summary

Run Time	30 min
Post Run Time	0 min

Oven
Temperature

Setpoint	On
(Initial)	280 °C
Hold Time	30 min
Post Run	100 °C
Equilibration Time	1.5 min
Max Temperature	325 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled

ALS
Front Injector

Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	0
Solvent A Washes (PostInj)	0
Solvent A Volume	4 µL
Solvent B Washes (PreInj)	0
Solvent B Washes (PostInj)	0
Solvent B Volume	4 µL
Sample Washes	1
Sample Wash Volume	1 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0 µL
Solvent Wash Mode	A, B

Back Injector

Syringe Size	10 µL
Injection Volume	1 µL

BH
3-11-23

Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	1
Sample Wash Volume	4 µL
Sample Pumps	2
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	6000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	6000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL
Solvent Wash Mode	A, B

Sample Overlap

Mode	Sample overlap is not enabled

ALS Errors	Pause for user interaction

Front SS Inlet He

Mode	Split
Heater	On 250 °C
Pressure	On 15 psi
Total Flow	On 38.695 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	On 30 After 3 min mL/min
Split Ratio	50 :1
Split Flow	34.995 mL/min
Liner	A Liner has not been selected.

Back SS Inlet He

Mode	Split
Heater	On 250 °C
Pressure	On 10 psi
Total Flow	On 90.689 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	Off
Split Ratio	50 :1
Split Flow	85.97 mL/min
Liner	A Liner has not been selected.

Thermal Aux 3 (MSD Transfer Line)

Temperature	
Setpoint	On
(Initial)	280 °C

Column

Column #1

Flow	
Setpoint	On
(Initial)	0.69991 mL/min
Post Run	0.57353 mL/min

Column Information	Agilent 19091S-602 HP-1MS

Temperature Range	-60 °C—325 °C (350 °C)
Dimensions	12.5 m x 200 µm x 0.33 µm
Column lock	Unlocked
In	Front SS Inlet He
Out	MSD
(Initial)	280 °C
Pressure	15 psi
Flow	0.69991 mL/min
Average Velocity	51.477 cm/sec
Holdup Time	0.40472 min
Control Mode	Constant Flow

BH
3-11-23

Column #2
Pressure

Setpoint	On
(Initial)	10 psi
Post Run	11.178 psi

Column Information	Agilent 19091S-913

HP-1MS

Temperature Range	-60 °C—325 °C (325 °C)
Dimensions	15 m x 320 µm x 0.25 µm (Calibrated)
Column lock	Locked
In	Back SS Inlet He
Out	Back Detector FID
(Initial)	280 °C
Pressure	10 psi
Flow	1.7194 mL/min
Average Velocity	48.439 cm/sec
Holdup Time	0.51612 min
Control Mode	Constant Pressure

Column Outlet Pressure	0 psi

Back Detector FID

Makeup	He
Column Compensation	Signal is modified by Column Compensation Curve #2
Heater	On 300 °C
H2 Flow	On 40 mL/min
Air Flow	On 400 mL/min
Makeup Flow (Combined)	On 25 mL/min
Carrier Gas Flow Correction	Column + Makeup = Constant
Flame	On

Aux EPC 1,2,3
Aux EPC 1 N2
Pressure

Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Aux EPC 2 N2
Pressure

Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Aux EPC 3 N2
Pressure

Setpoint	Off

(Initial)	10 psi
Post Run	0 psi

BH
3-11-23

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Signals

Signal #1: Back Signal	
Description	Back Signal
Details	Back Signal (FID)
Save	On
Data Rate	50 Hz
Dual Injection Assignment	Front Sample
Signal #2: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample
Signal #3: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample
Signal #4: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

TUNE PARAMETERS for SN: US1648M021

Trace Ion Detection is OFF.

34.593	:	EMISSION
70.007	:	ENERGY
34.899	:	REPELLER
90.331	:	IONFOCUS
22.672	:	ENTRANCE_LENS
1360.190	:	EMVOLTS
1498.6	:	Actual EMV
1.00	:	GAIN FACTOR
2908.000	:	AMUGAIN
136.750	:	AMUOFFSET
1.000	:	FILAMENT
0.000	:	DCPOLARITY
12.032	:	ENTLENSOFFSET
0.000	:	Ion_Body
0.000	:	EXTLENS
442.000	:	MASSGAIN
-22.000	:	MASSOFFSET

END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

BH
3-11-23

DATA ANALYSIS PARAMETERS

Method Name: C:\MassHunter\GCMS\1\methods\ASGC280ISOTI.M

Percent Report Settings

Sort By: Signal

Output Destination
    Screen: No
    Printer: Yes
    File: No

Integration Events: AutoIntegrate

Generate Report During Run Method: No

Signal Correlation Window: 0.020

Quantitative Report Settings

Report Type: Summary

Output Destination
    Screen: Yes
    Printer: No
    File: No

Generate Report During Run Method: No

Calibration Last Updated:

Reference Window: 10.00 Percent
Non-Reference Window: 5.00 Percent
Correlation Window: 0.02 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

Compound Information

END OF DATA ANALYSIS PARAMETERS

Fri Mar 10 21:48:11 2023

METHOD CONTROL PARAMETERS

BH
3-11-23

Method Information for: C:\MassHunter\GCMS\1\methods\ASGC280ISOTI.M

Method Sections To Run:

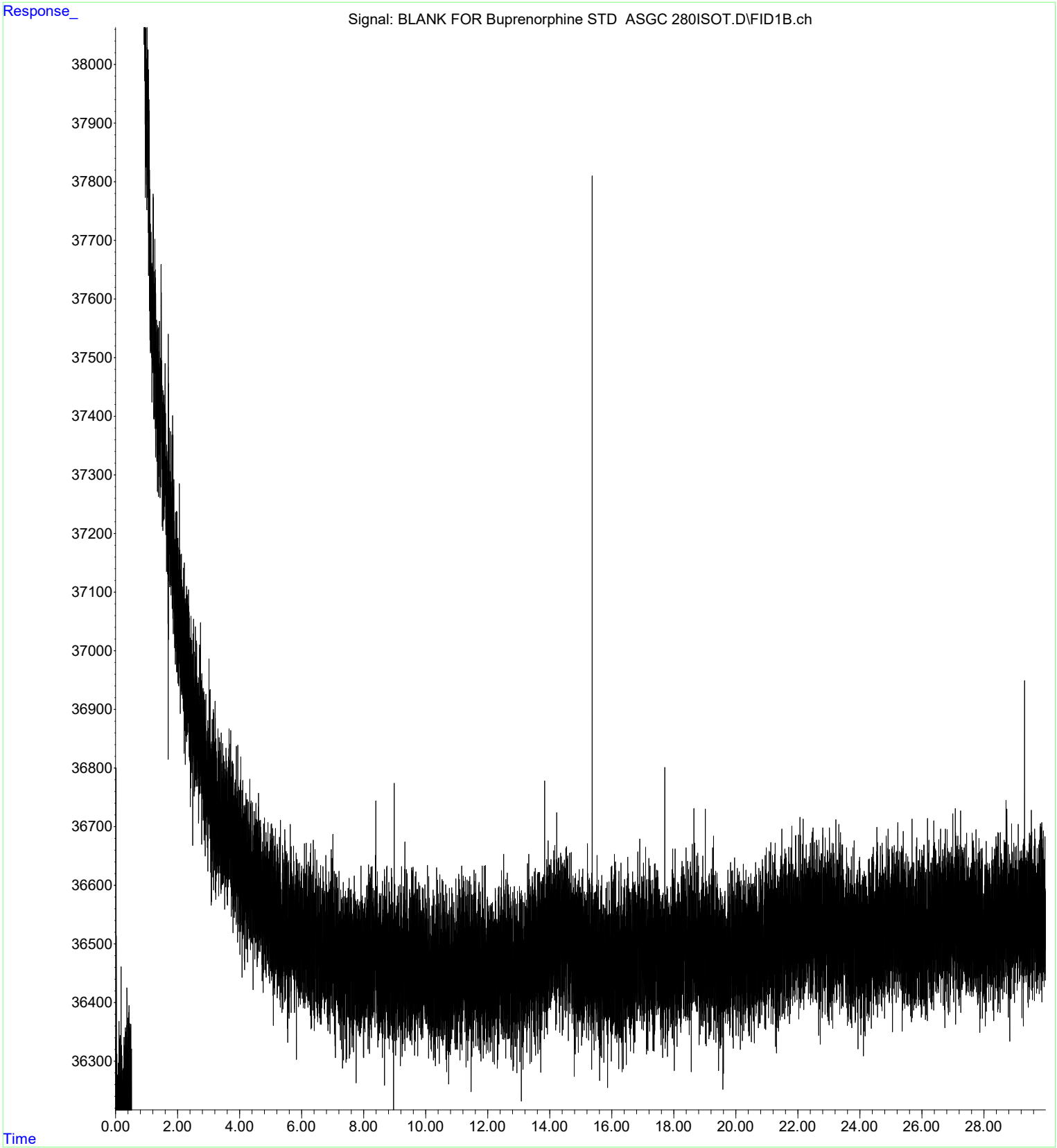
( ) Save Copy of Method With Data
( ) Instrument Control Pre-Run Cmd/Macro =
( ) Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
(X) Data Analysis
( ) Instrument Control Post-Run Cmd/Macro =
( ) Data Analysis Post-Run Cmd/Macro =

Method Comments:
ASGC280ISO

END OF METHOD CONTROL PARAMETERS

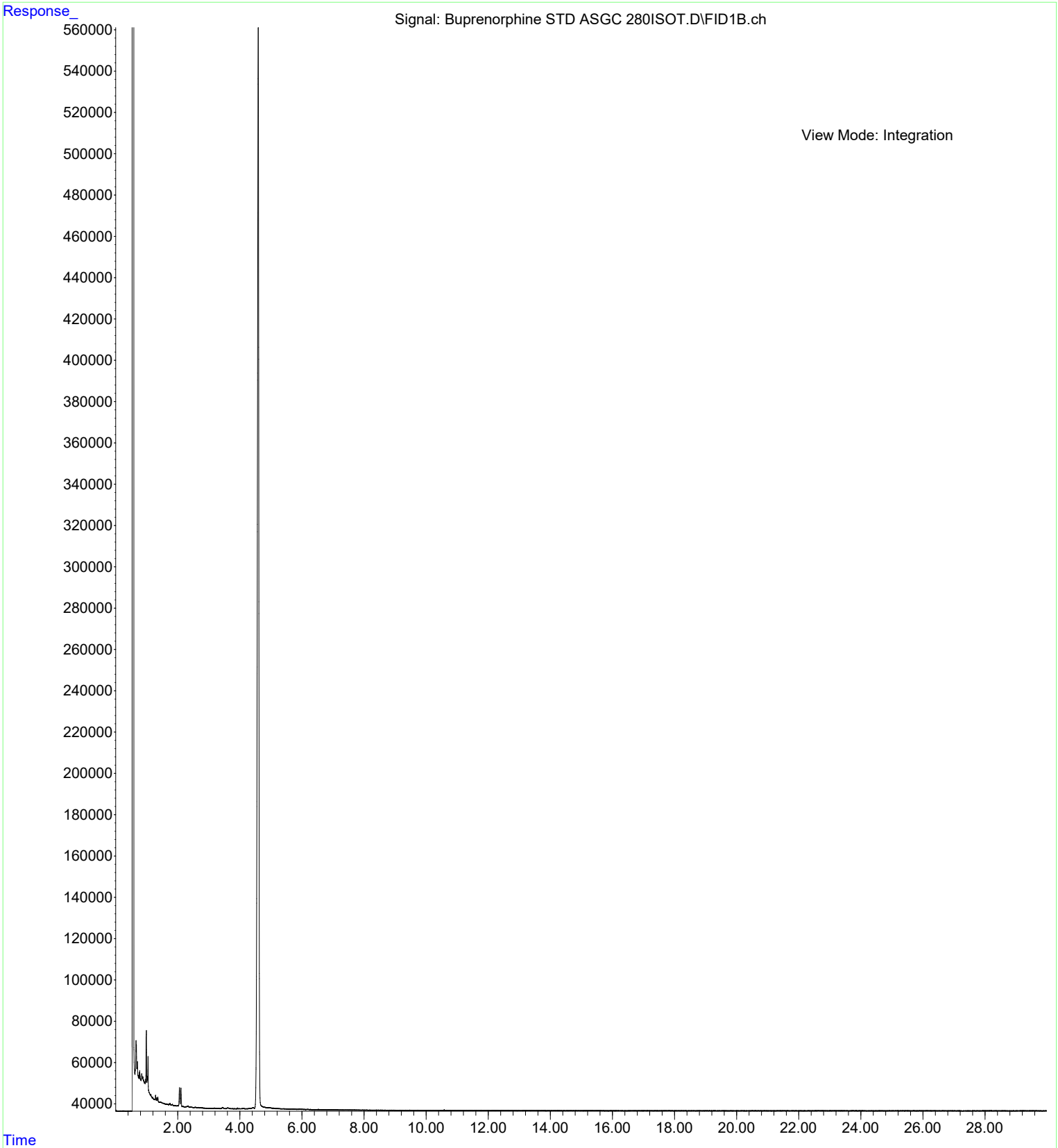
BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR Buprenorphine STD ASGC 280ISOT.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 04:33 using AcqMethod ASGC280ISOTI.M
Sample Name: BLANK FOR Buprenorphine STD ASGC 280ISOT
Misc Info : METHANOL



BH
3-11-23

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\Bu
... prenorphine STD ASGC 280ISOT.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 05:07 using AcqMethod ASGC280ISOTI.M
Sample Name: Buprenorphine STD EXP. 6-2024 ASGC 280ISOT
Misc Info : METHANOL



Single Quadrupole Acquisition Method - MS Parameters Report

Method file	C:\MassHunter\GCMS\1\methods\ASMSDRUGS60.M
Tune file	atune.u
Ion source	EI
Source temperature (°C)	230
Quad temperature (°C)	150
Fixed Electron energy (eV)	70.0
Acquisition Type	Scan
Stop time (min)	650.00
Solvent delay (min)	1.00
Trace Ion Detection	False
Gain Factor	10
EM Saver	False
EM Saver Limit	N/A

Scan Time Segments

Time	Start Mass	End Mass	Threshold	Scan Speed
1.00	40	550	150	6,250 [N=0]

Timed Events

Time	Type of Event	Parameter

Real-Time Plots

Type of Plot	Label	Low Mass	High Mass
Total Ion	N/A	N/A	N/A

Self-Cleaning Ion Source Parameters

Mode	No Cleaning

METHOD CONTROL PARAMETERS

BH
3-11-23

Method Information for: C:\MassHunter\GCMS\1\methods\ASMSDRUGS60.M

Method Sections To Run:

( ) Save Copy of Method With Data
( ) Instrument Control Pre-Run Cmd/Macro =
( ) Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
(X) Data Analysis
( ) Instrument Control Post-Run Cmd/Macro =
( ) Data Analysis Post-Run Cmd/Macro =

Method Comments:
ASMSDRUGS60

END OF METHOD CONTROL PARAMETERS

BH
3-11-23

C:\MassHunter\GCMS\1\methods\ASMSDRUGS60.M
Fri Mar 10 21:53:59 2023

Control Information

Sample Inlet : GC
Injection Source : GC ALS
Injection Location: Front
Mass Spectrometer : Enabled

No Sample Prep method has been assigned to this method.

GC
GC Summary

Run Time	10.003 min
Post Run Time	0 min

Oven
Temperature

Setpoint	On
(Initial)	60 °C
Hold Time	3 min
Post Run	100 °C
Program	
#1 Rate	70 °C/min
#1 Value	280 °C
#1 Hold Time	3.86 min

Equilibration Time	1.5 min
Max Temperature	325 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled

ALS
Front Injector

Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	2
Sample Wash Volume	4 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	6000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	6000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL

Solvent Wash Mode	A, B
Back Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	2
Sample Wash Volume	8 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL
Solvent Wash Mode	A, B
Sample Overlap	
Mode	Sample overlap is not enabled
ALS Errors	Pause for user interaction
Front SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 8.489 psi
Total Flow	On 54 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	On 30 After 3 min mL/min
Split Ratio	50 :1
Split Flow	50 mL/min
Liner	A Liner has not been selected.
Back SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 3.016 psi
Total Flow	On 79 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	Off
Split Ratio	75 :1
Split Flow	75 mL/min
Liner	A Liner has not been selected.
Thermal Aux 3 (MSD Transfer Line)	
Temperature	
Setpoint	On
(Initial)	280 °C
Column	
Column #1	
Flow	
Setpoint	On

(Initial)	1 mL/min
Post Run	0.57353 mL/min

BH
3-11-23

Column Information	Agilent 19091S-602
HP-1MS	
Temperature Range	-60 °C—325 °C (350 °C)
Dimensions	12.5 m x 200 µm x 0.33 µm (Calibrated)
Column lock	Locked
In	Front SS Inlet He
Out	MSD
(Initial)	60 °C
Pressure	8.489 psi
Flow	1 mL/min
Average Velocity	56.736 cm/sec
Holdup Time	0.3672 min
Control Mode	Constant Flow

Column #2	
Flow	
Setpoint	On
(Initial)	1 mL/min
Post Run	1 mL/min

Column Information	Agilent 19091S-913
HP-1MS	
Temperature Range	-60 °C—325 °C (325 °C)
Dimensions	15 m x 320 µm x 0.25 µm (Calibrated)
Column lock	Locked
In	Back SS Inlet He
Out	Back Detector FID
(Initial)	60 °C
Pressure	3.016 psi
Flow	1 mL/min
Average Velocity	21.006 cm/sec
Holdup Time	1.1901 min
Control Mode	Constant Flow

Column Outlet Pressure	0 psi

Back Detector FID	
Makeup	He
Column Compensation	Signal is modified by Column Compensation Curve #2
Heater	On 300 °C
H2 Flow	Off
Air Flow	Off
Makeup Flow	On 25 mL/min
Carrier Gas Flow Correction	Constant Makeup and Fuel Flow
Flame	Off

Aux EPC 1,2,3	
Aux EPC 1 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Aux EPC 2 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

BH
3-11-23

Aux EPC 3 N2 Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Signals

Signal #1:	
Description	None
Signal #2: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample
Signal #3: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample
Signal #4: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

TUNE PARAMETERS for SN: US1648M021

Trace Ion Detection is OFF.

34.593	:	EMISSION
70.007	:	ENERGY
34.899	:	REPELLER
90.331	:	IONFOCUS
22.672	:	ENTRANCE_LENS
1360.190	:	EMVOLTS
1498.6	:	Actual EMV
1.00	:	GAIN FACTOR
2908.000	:	AMUGAIN
136.750	:	AMUOFFSET
1.000	:	FILAMENT
0.000	:	DCPOLARITY
12.032	:	ENTLENSOFFSET
0.000	:	Ion_Body
0.000	:	EXTLENS
442.000	:	MASSGAIN
-22.000	:	MASSOFFSET

END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

DATA ANALYSIS PARAMETERS

Method Name: C:\MassHunter\GCMS\1\methods\ASMSDRUGS60.M

Percent Report Settings

Sort By: Signal

Output Destination
    Screen: No
    Printer: Yes
    File: No

Integration Events: AutoIntegrate

Generate Report During Run Method: No

Signal Correlation Window: 0.020

Qualitative Report Settings

Peak Location of Unknown: Apex

Library to Search	Minimum Quality
DEMO.L	0

Integration Events: AutoIntegrate

Report Type: Summary

Output Destination
    Screen: No
    Printer: Yes
    File: No

Generate Report During Run Method: No

Quantitative Report Settings

Report Type: Summary

Output Destination

Screen: Yes
Printer: No
File: No

BH
3-11-23

Generate Report During Run Method: No

Calibration Last Updated:

Reference Window: 10.00 Percent
Non-Reference Window: 5.00 Percent
Correlation Window: 0.02 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

Compound Information

*** Empty Quantitation Database ***

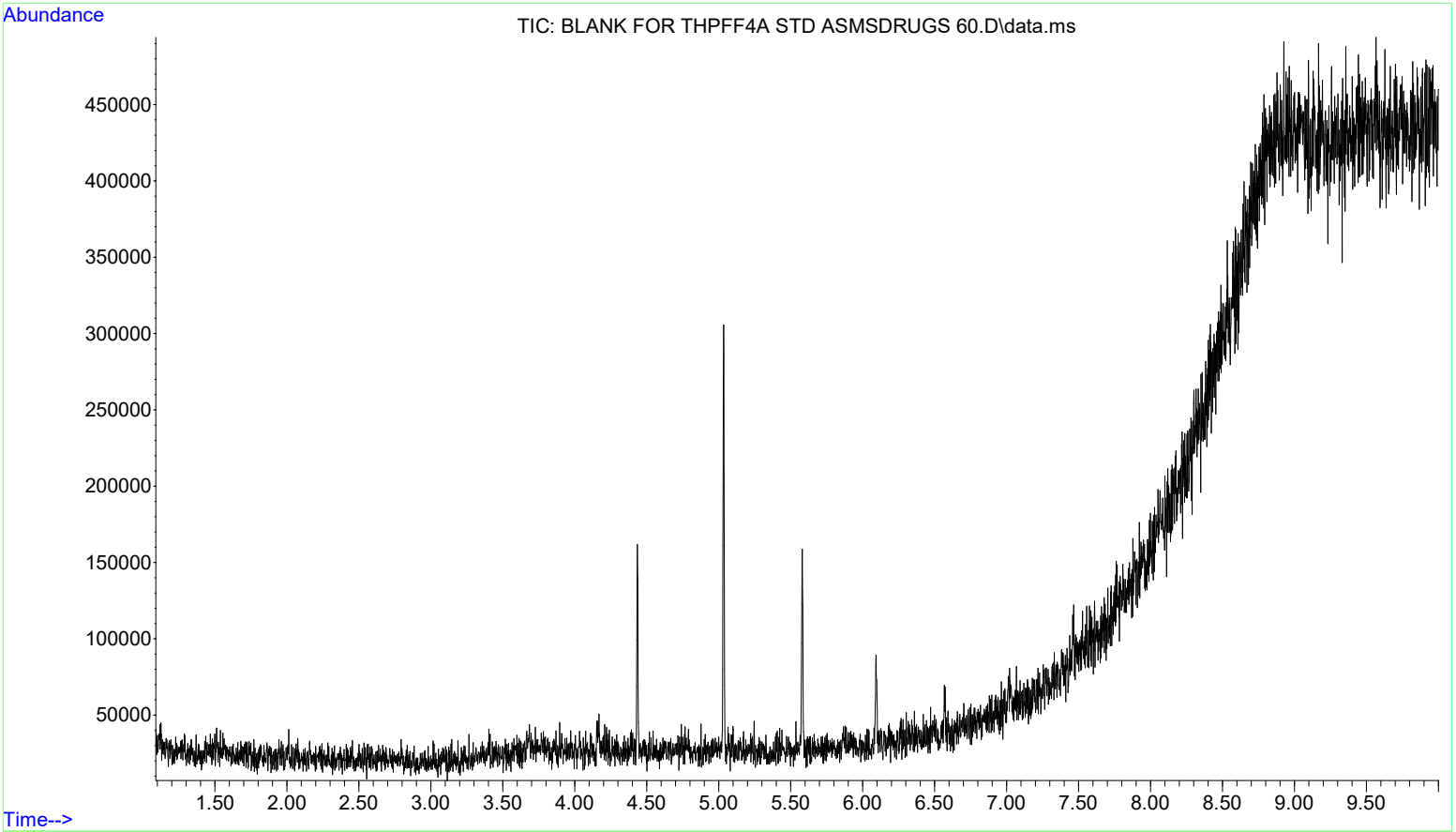
END OF DATA ANALYSIS PARAMETERS

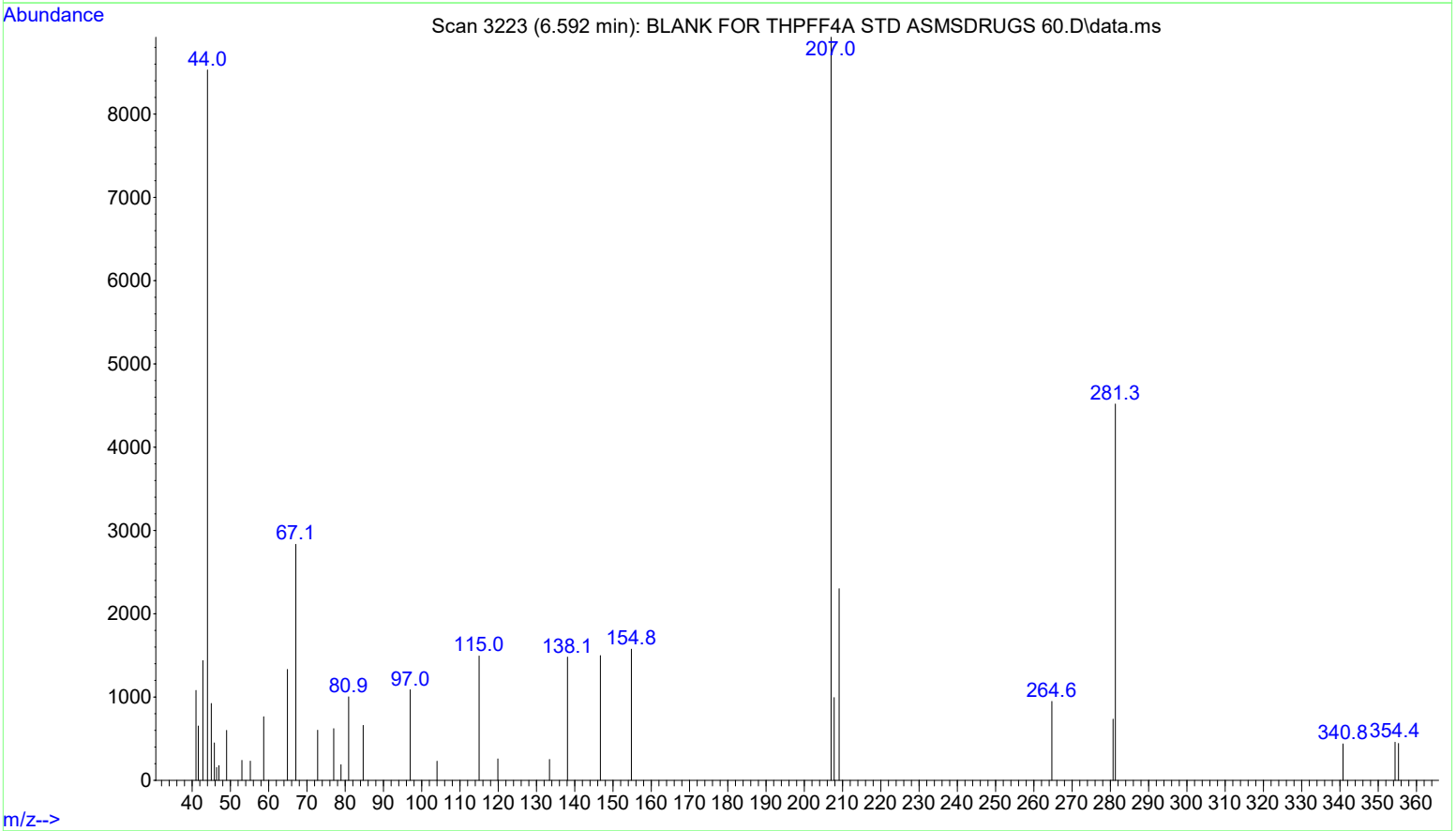
Fri Mar 10 21:54:25 2023

File :Y:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR THPFF4A STD ASMSDRUGS 60.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:34 using AcqMethod ASMSDRUGS60.M
Sample Name: BLANK FOR THPFF4A STD
Misc Info : METHANOL

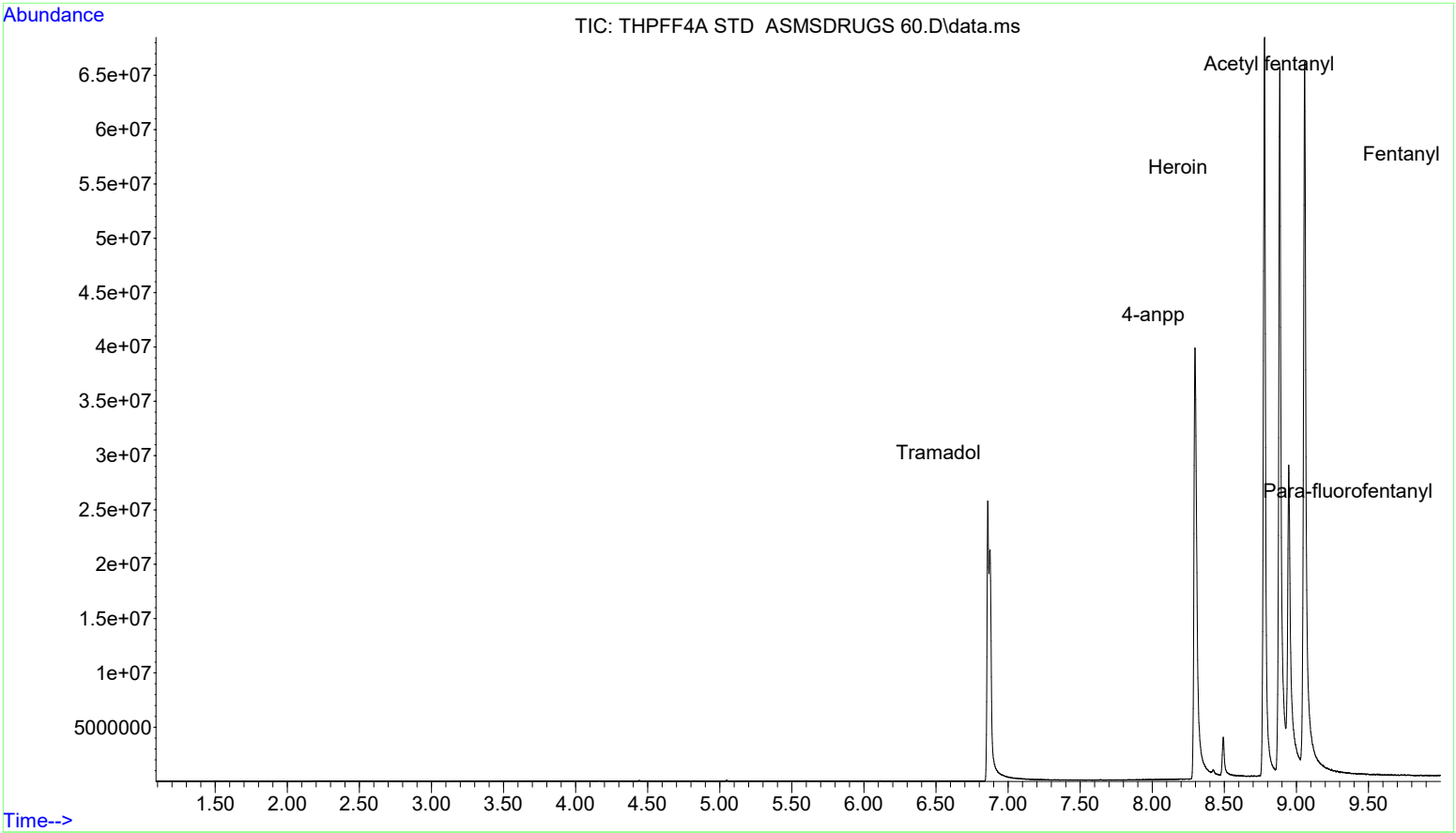


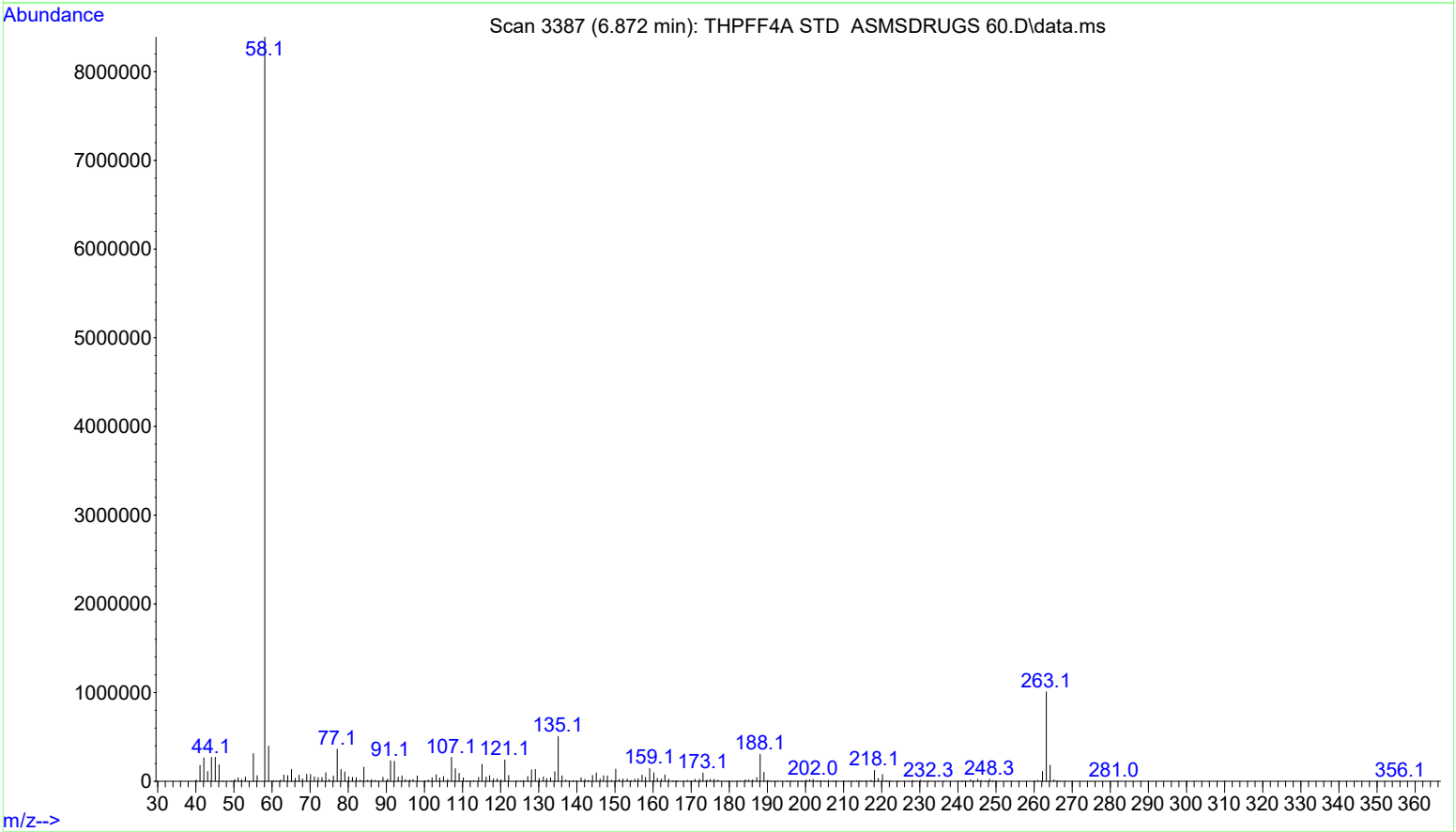


File :Y:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 60.D

BH
3-11-23

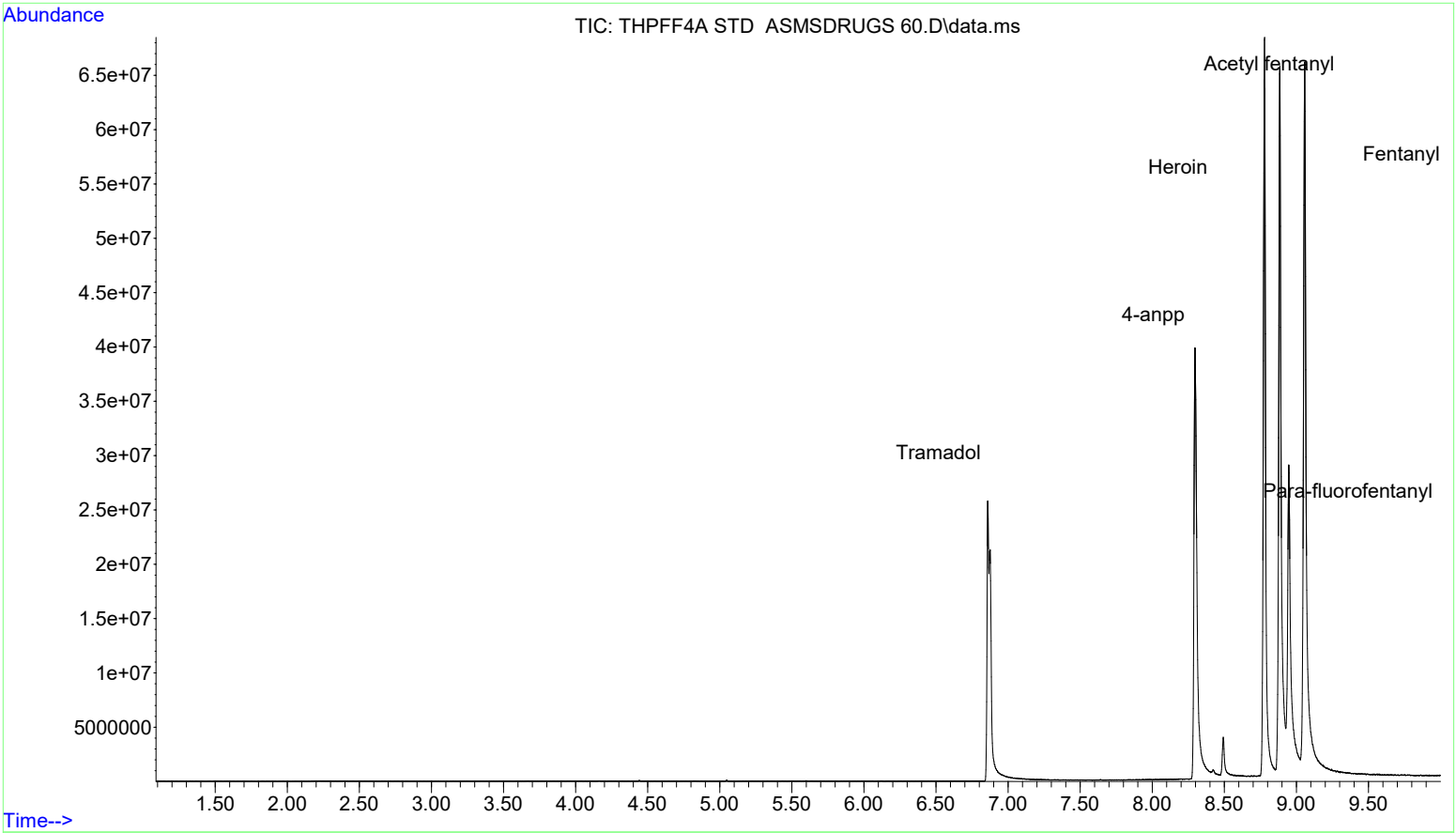
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:50 using AcqMethod ASMSDRUGS60.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

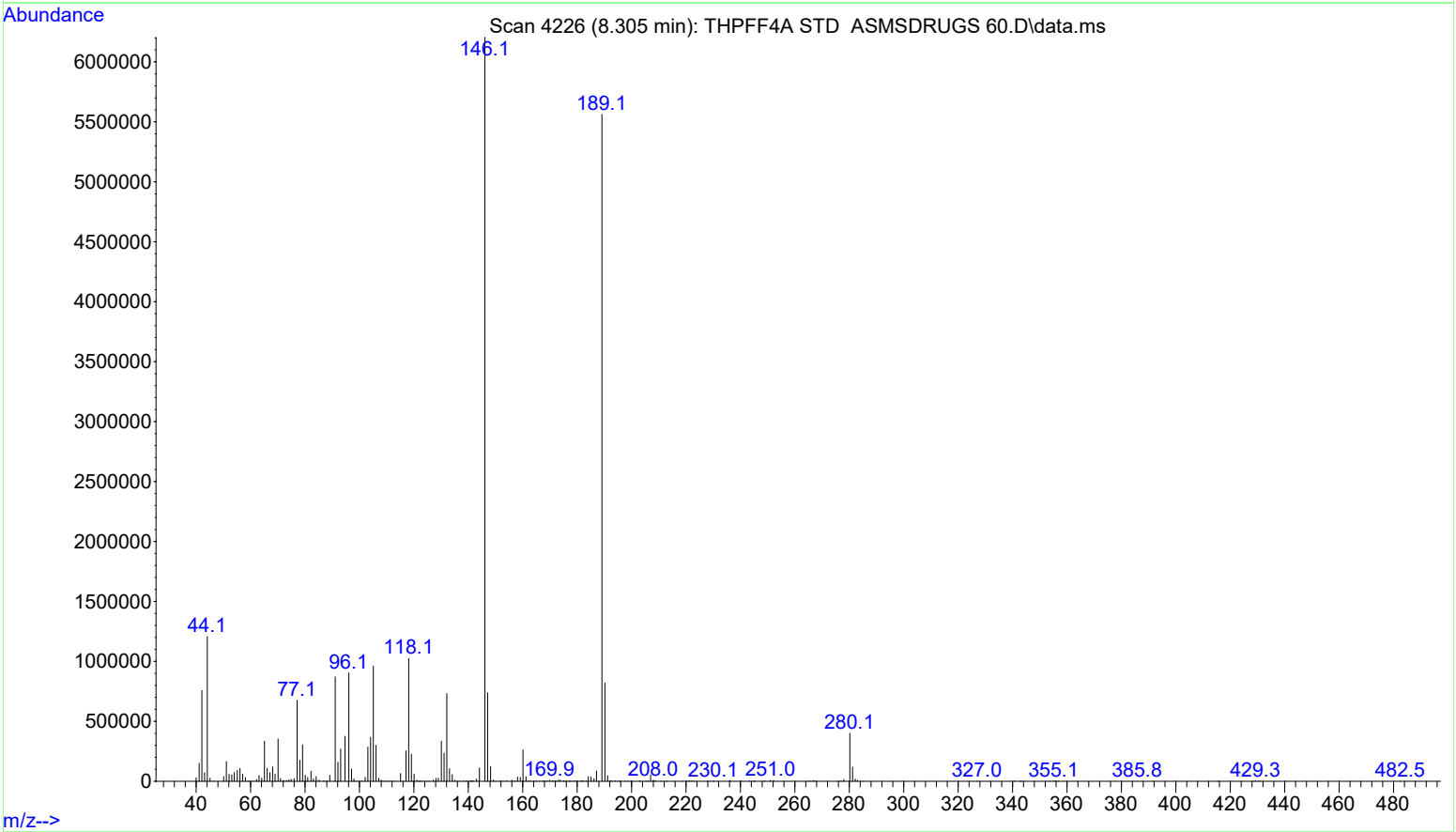




File :Y:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 60.D
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:50 using AcqMethod ASMSDRUGS60.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

BH
3-11-23

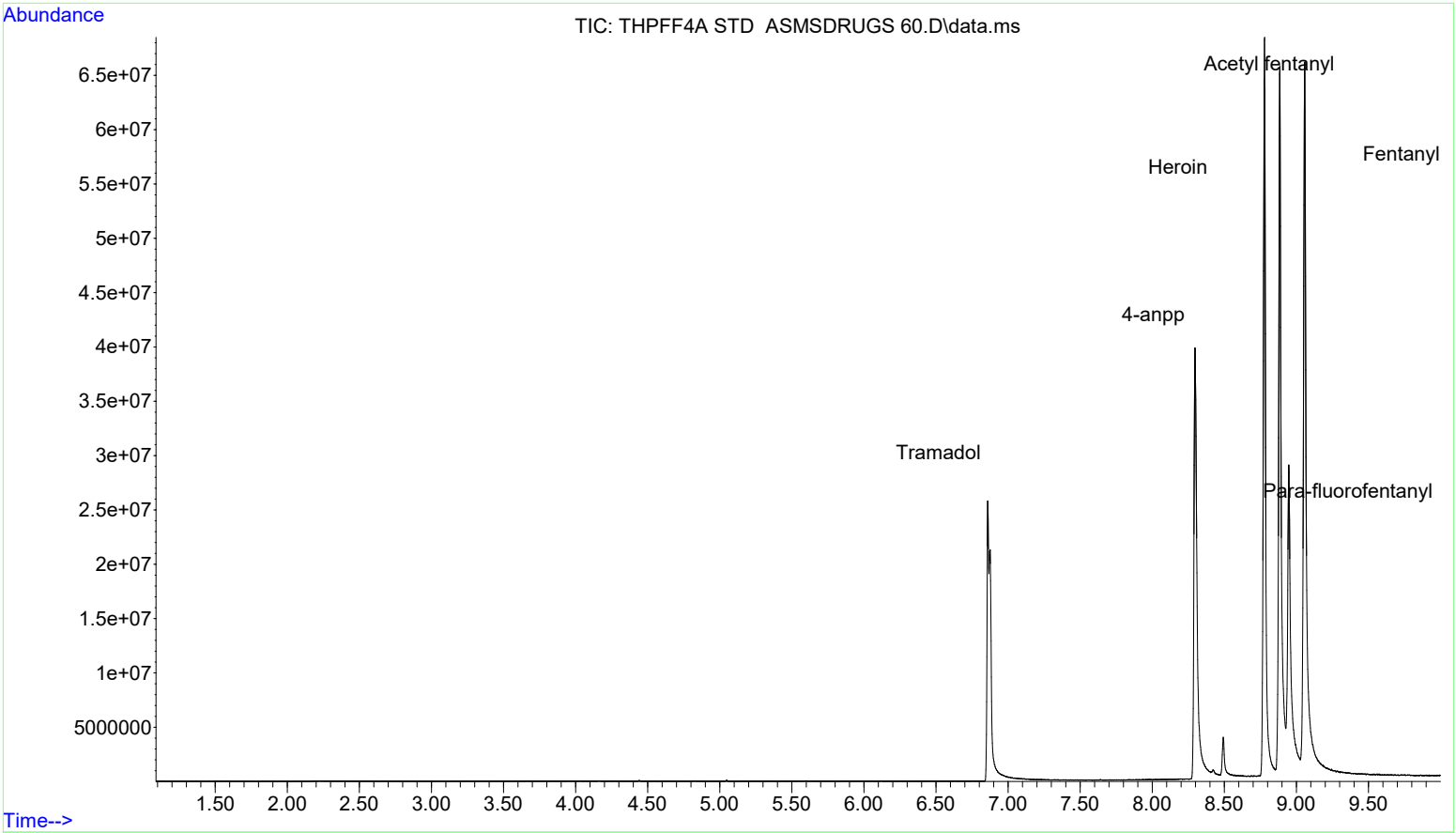


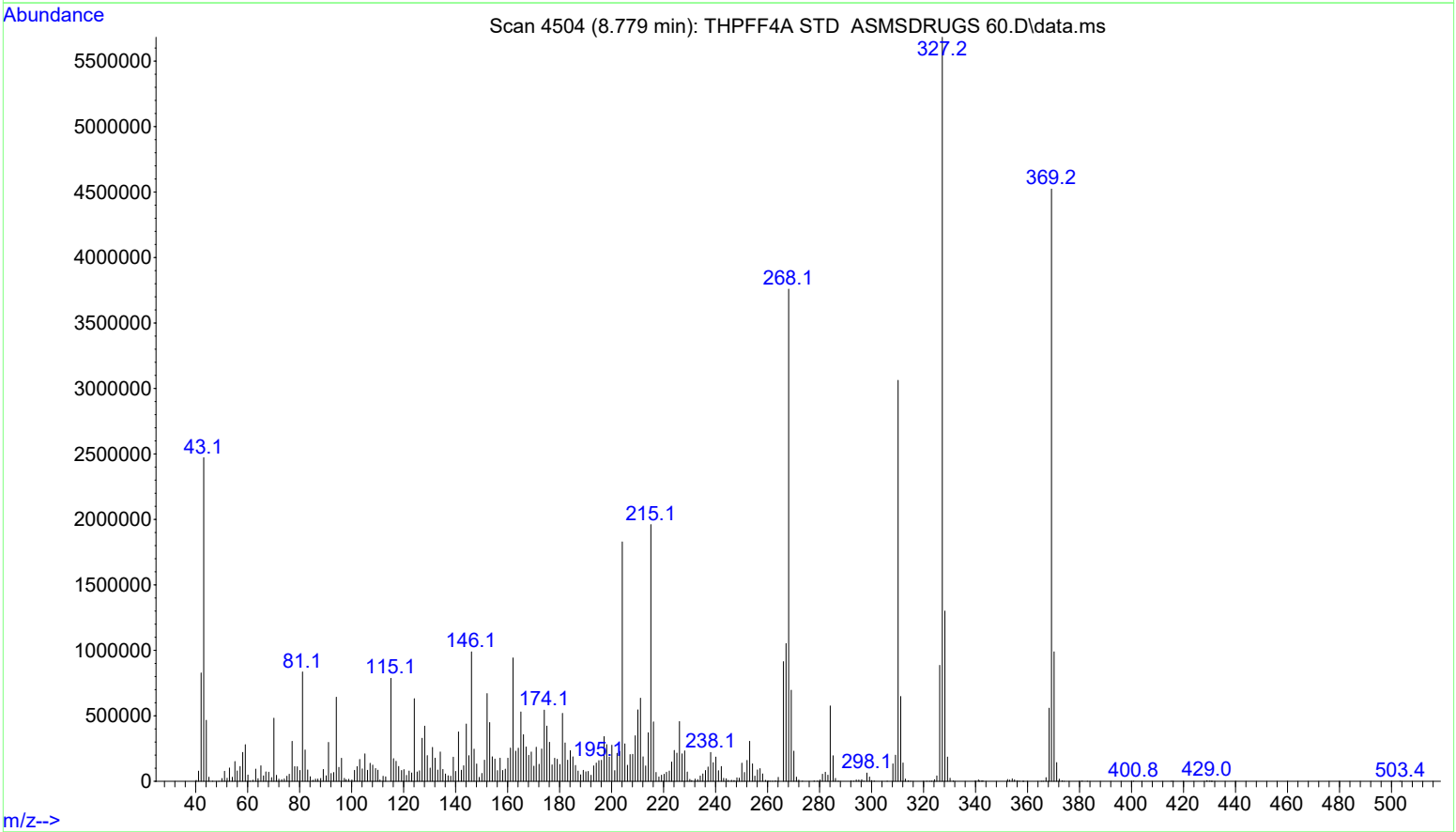


File :Y:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 60.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:50 using AcqMethod ASMSDRUGS60.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

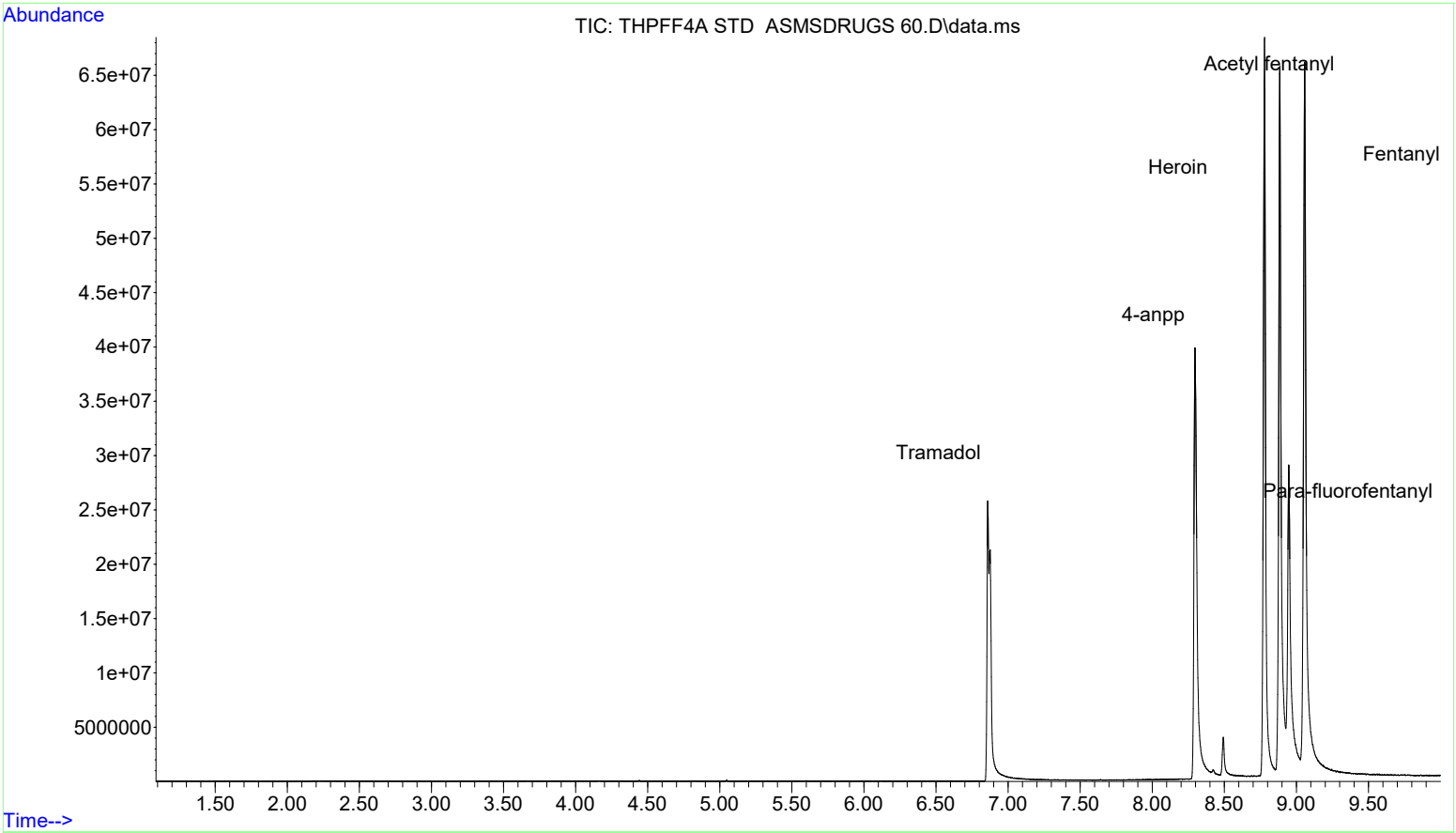


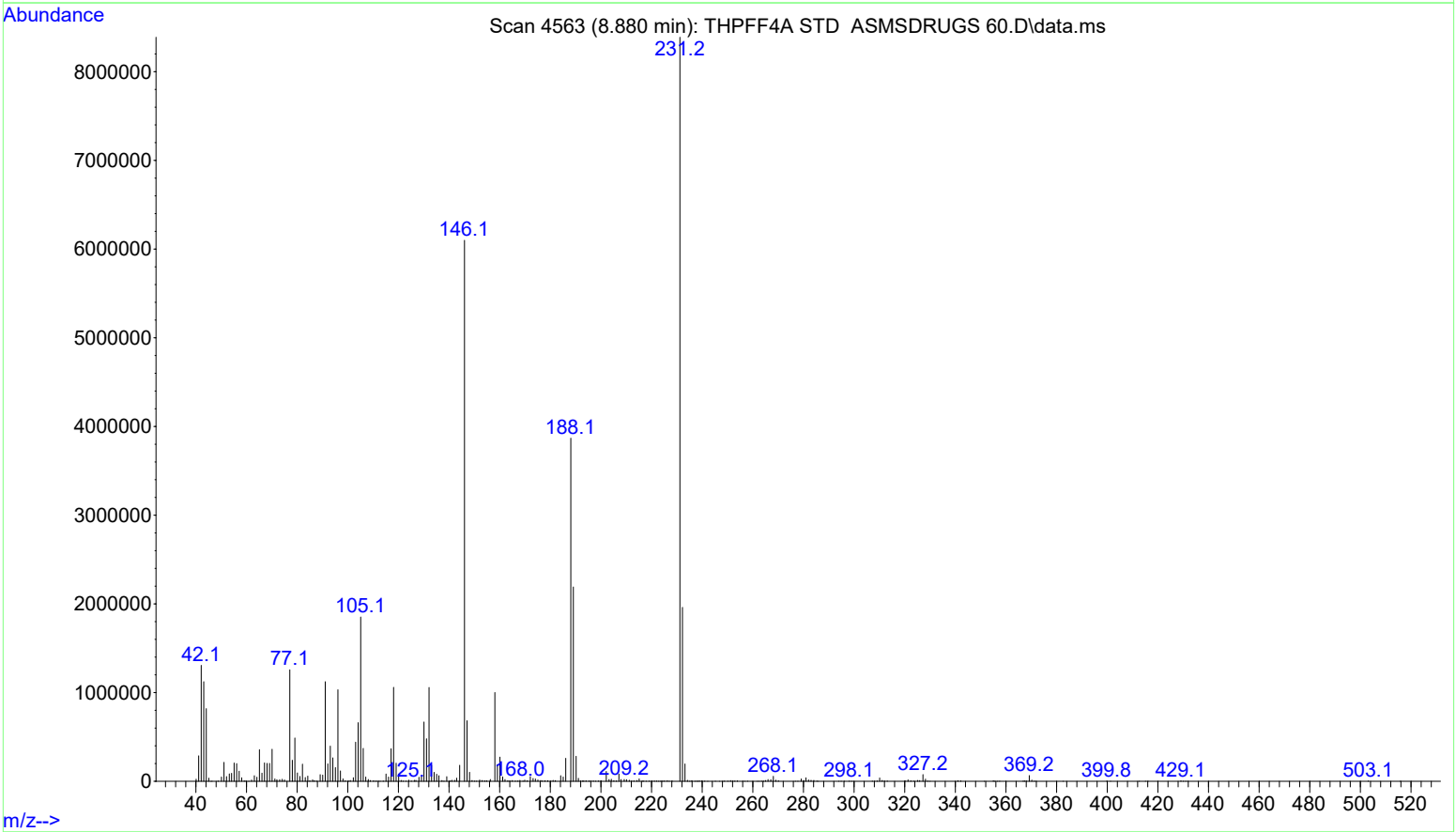


File :Y:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 60.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:50 using AcqMethod ASMSDRUGS60.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

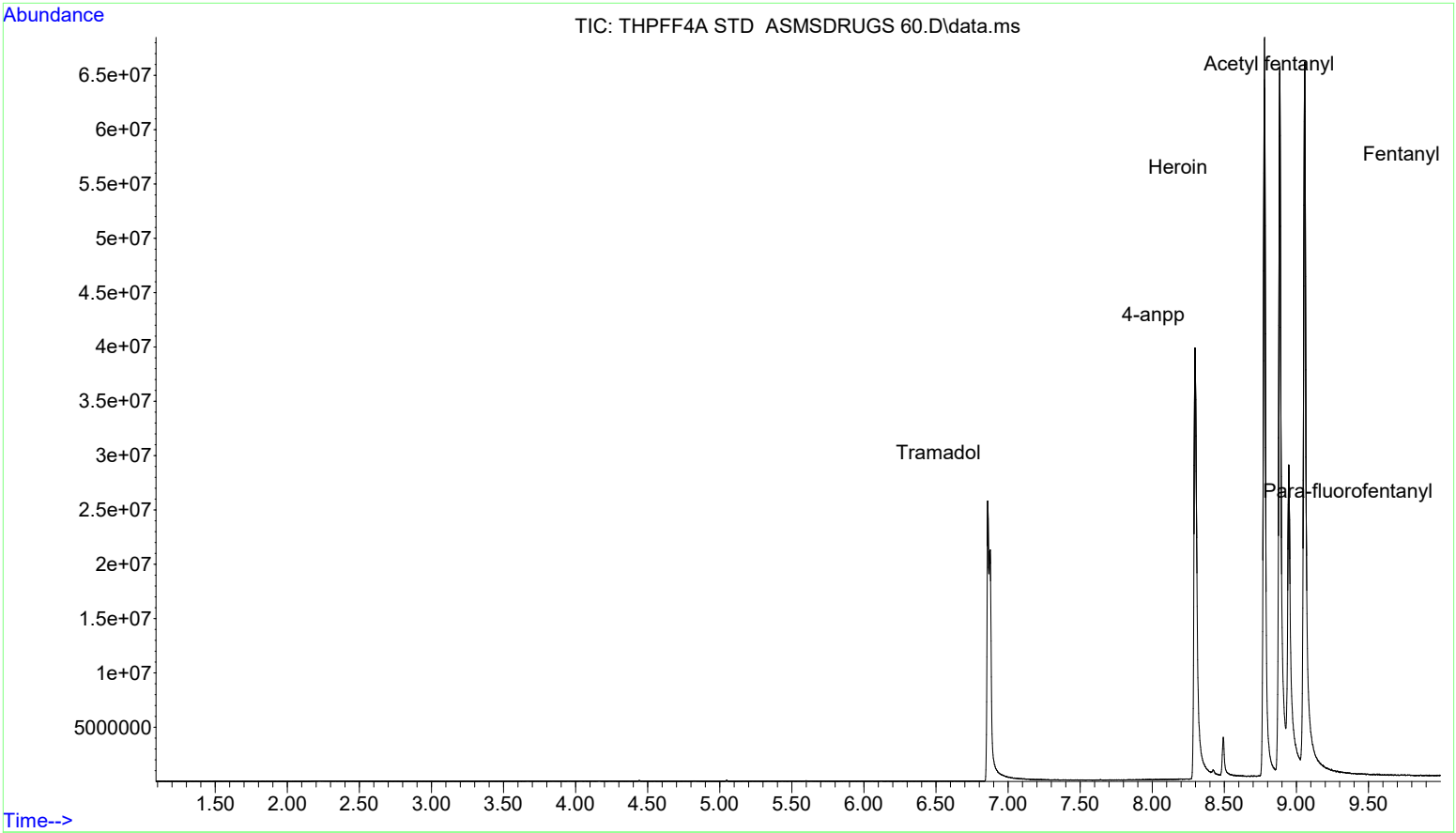


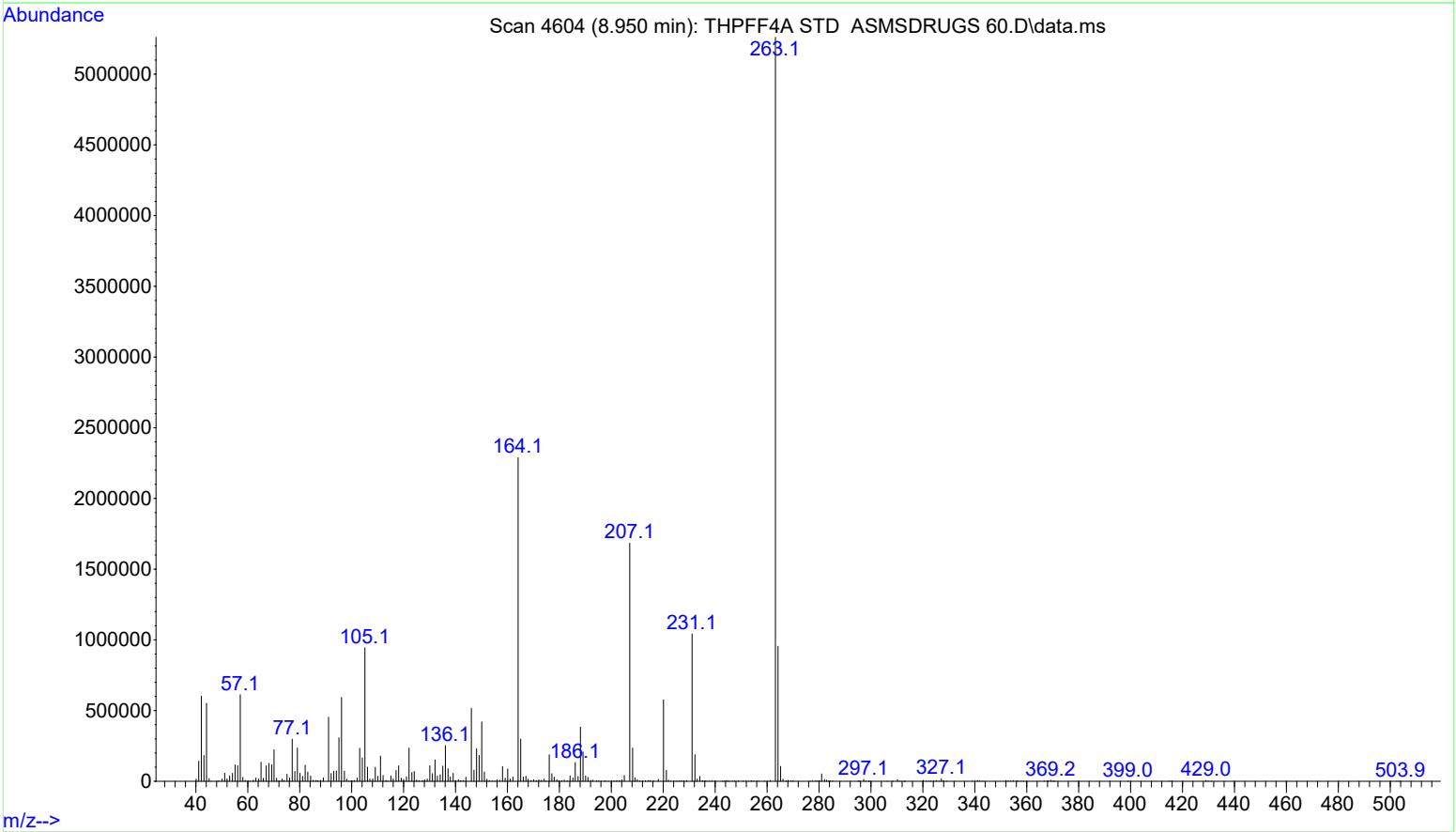


File :Y:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 60.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:50 using AcqMethod ASMSDRUGS60.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

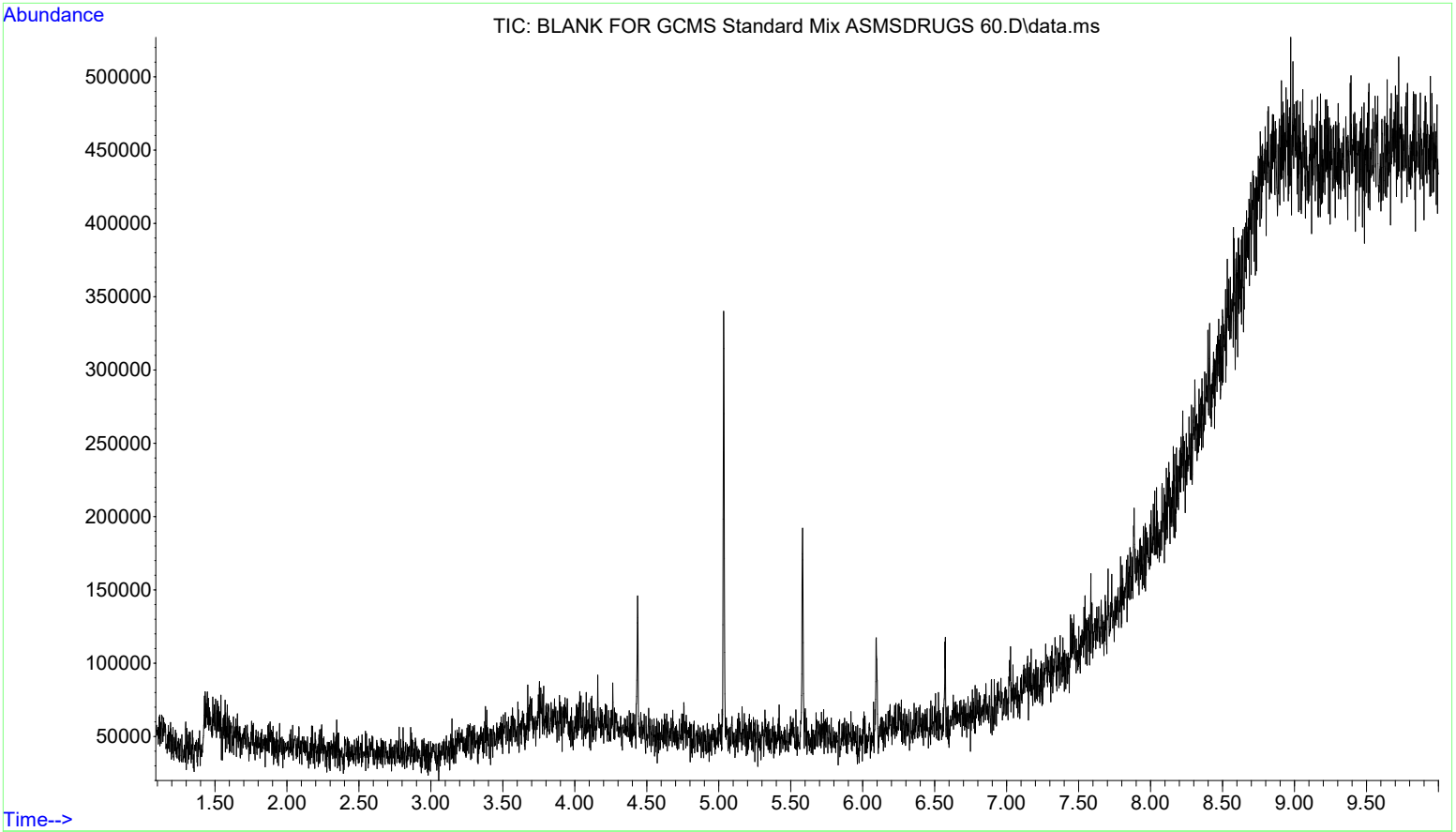


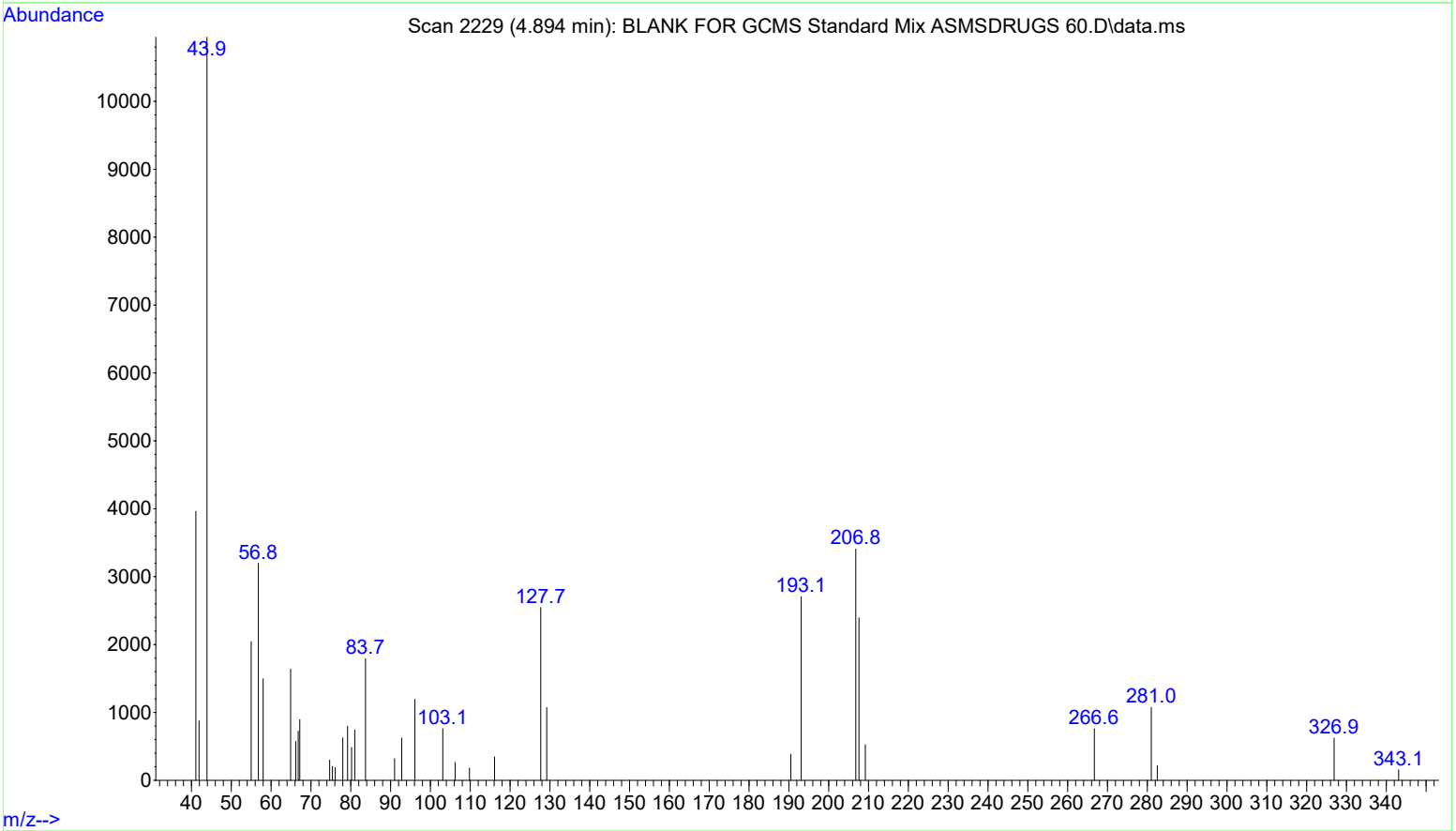


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR GCMS Standard Mix ASMSDRUGS 60.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 17:20 using AcqMethod ASMSDRUGS60.M
Sample Name: BLANK FOR GCMS Standard Mix ASMSDRUGS 60
Misc Info : METHANOL

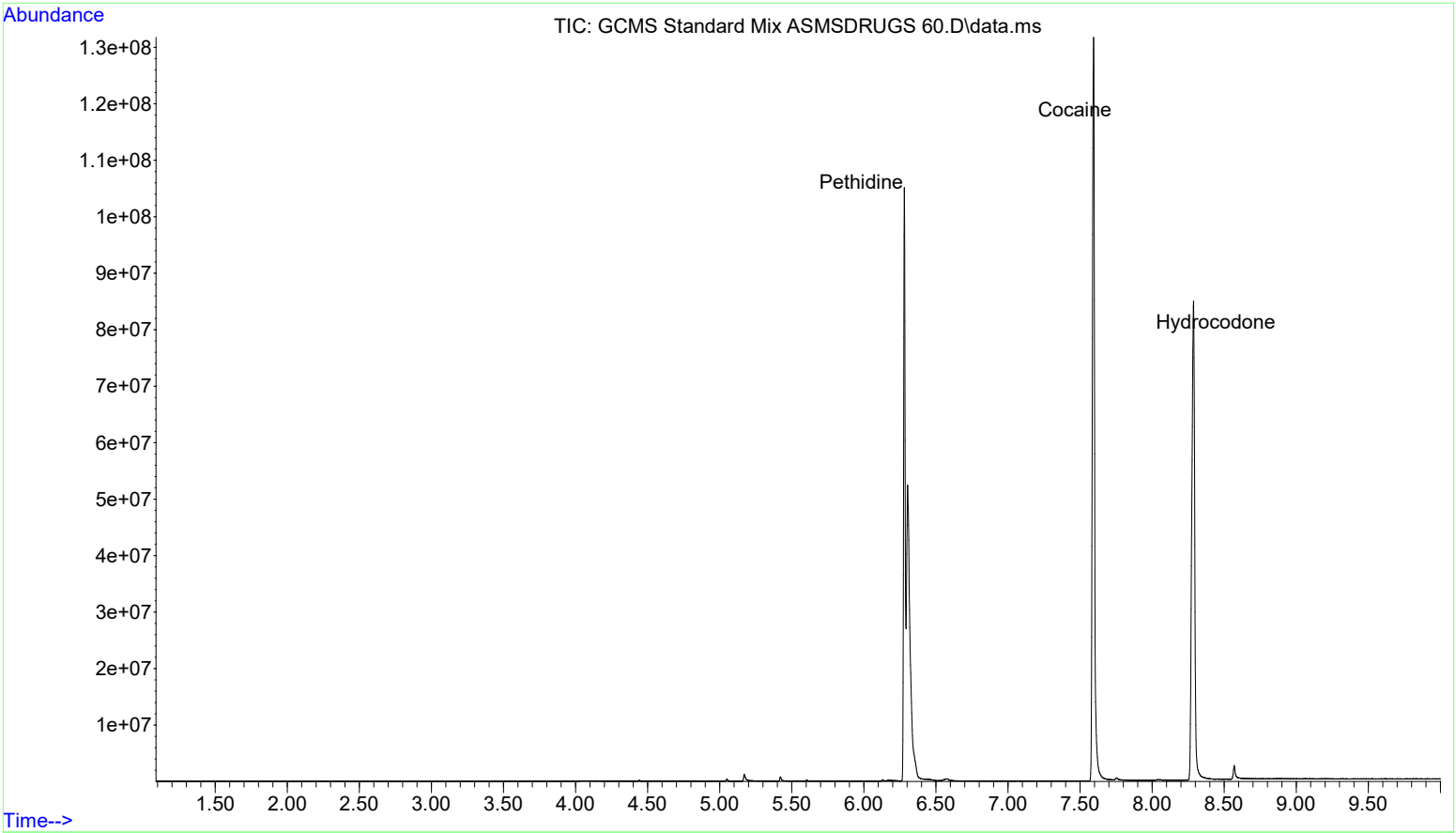


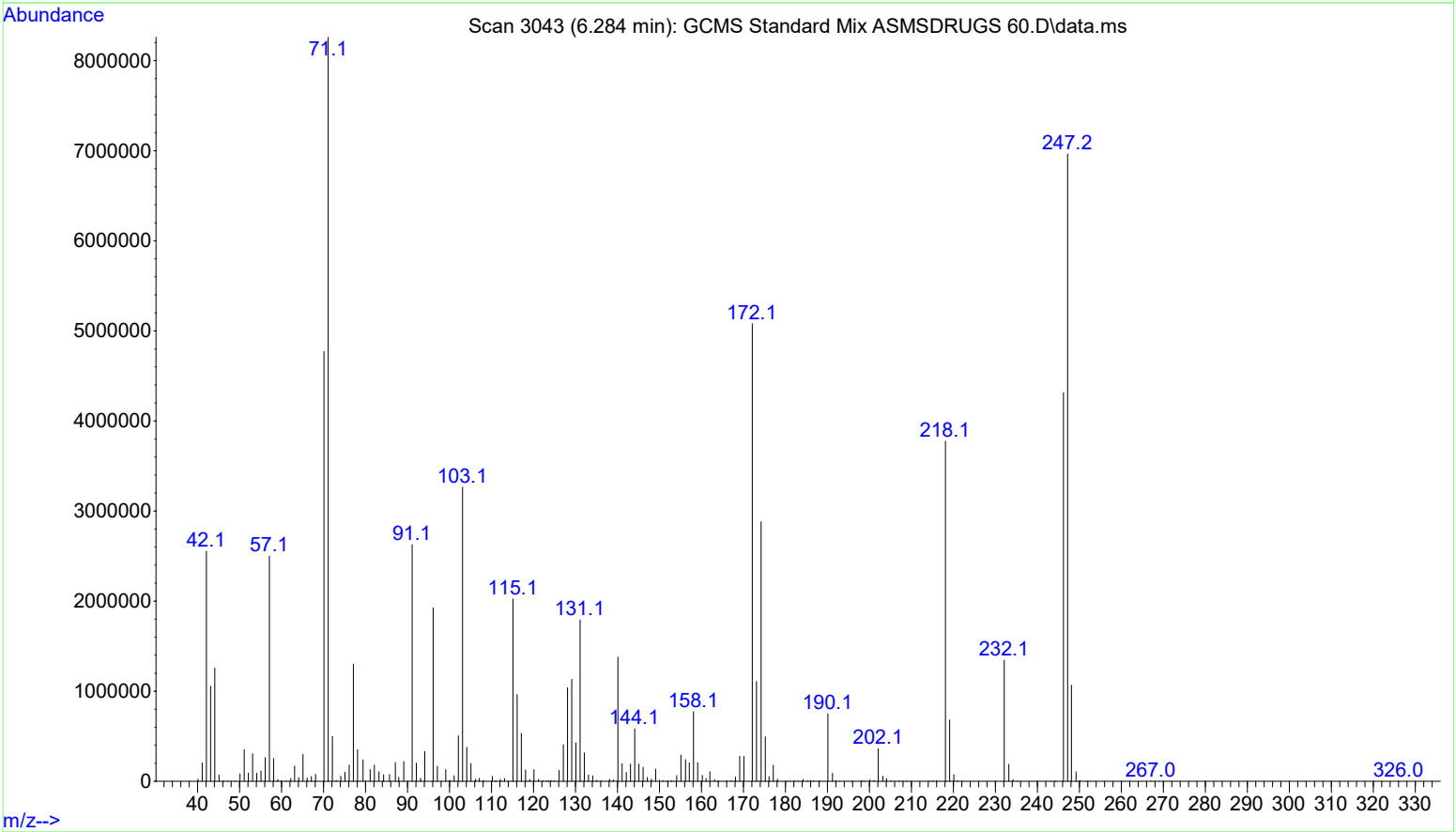


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS 60.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 17:35 using AcqMethod ASMSDRUGS60.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS 6
Misc Info : METHANOL

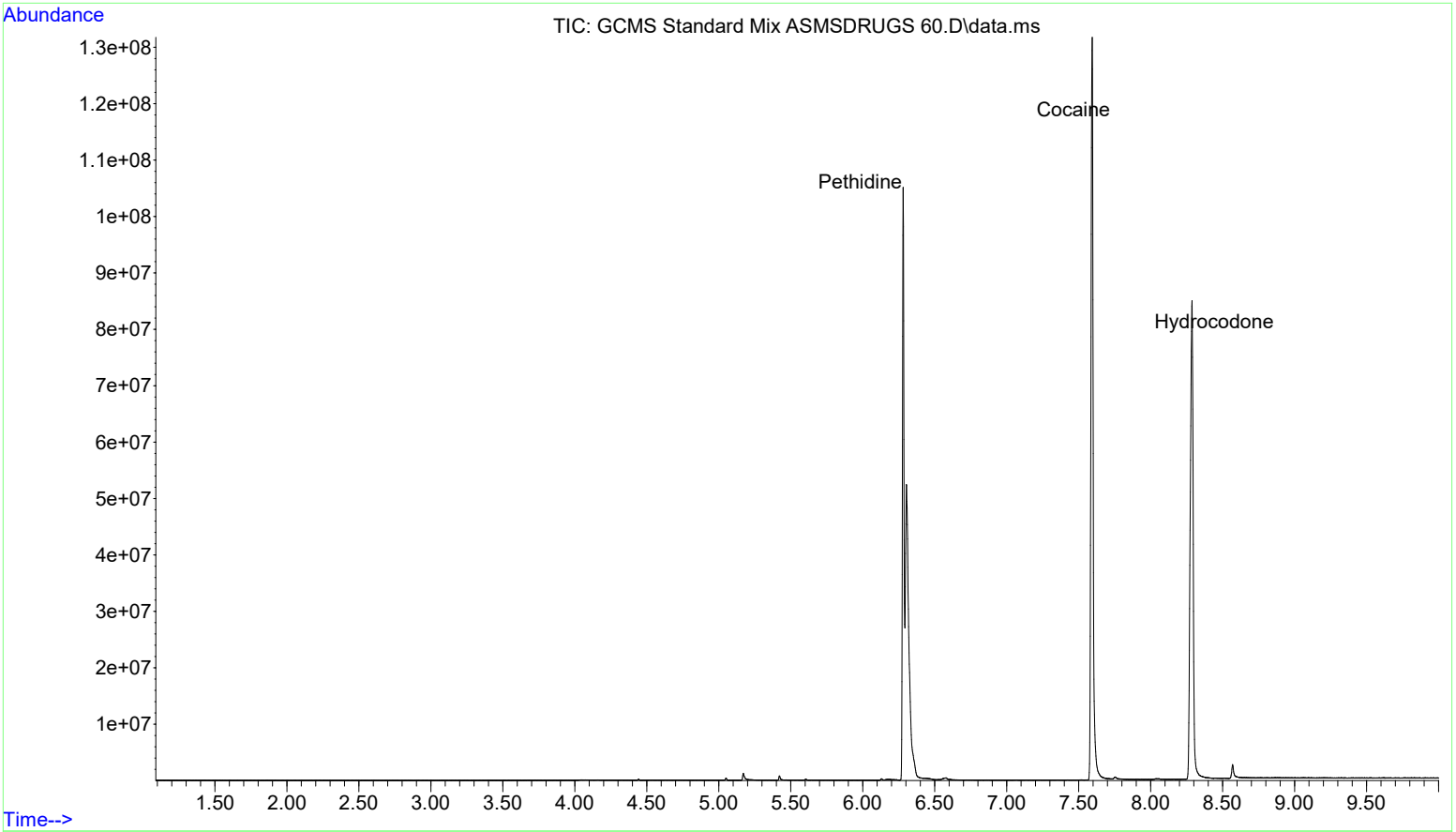


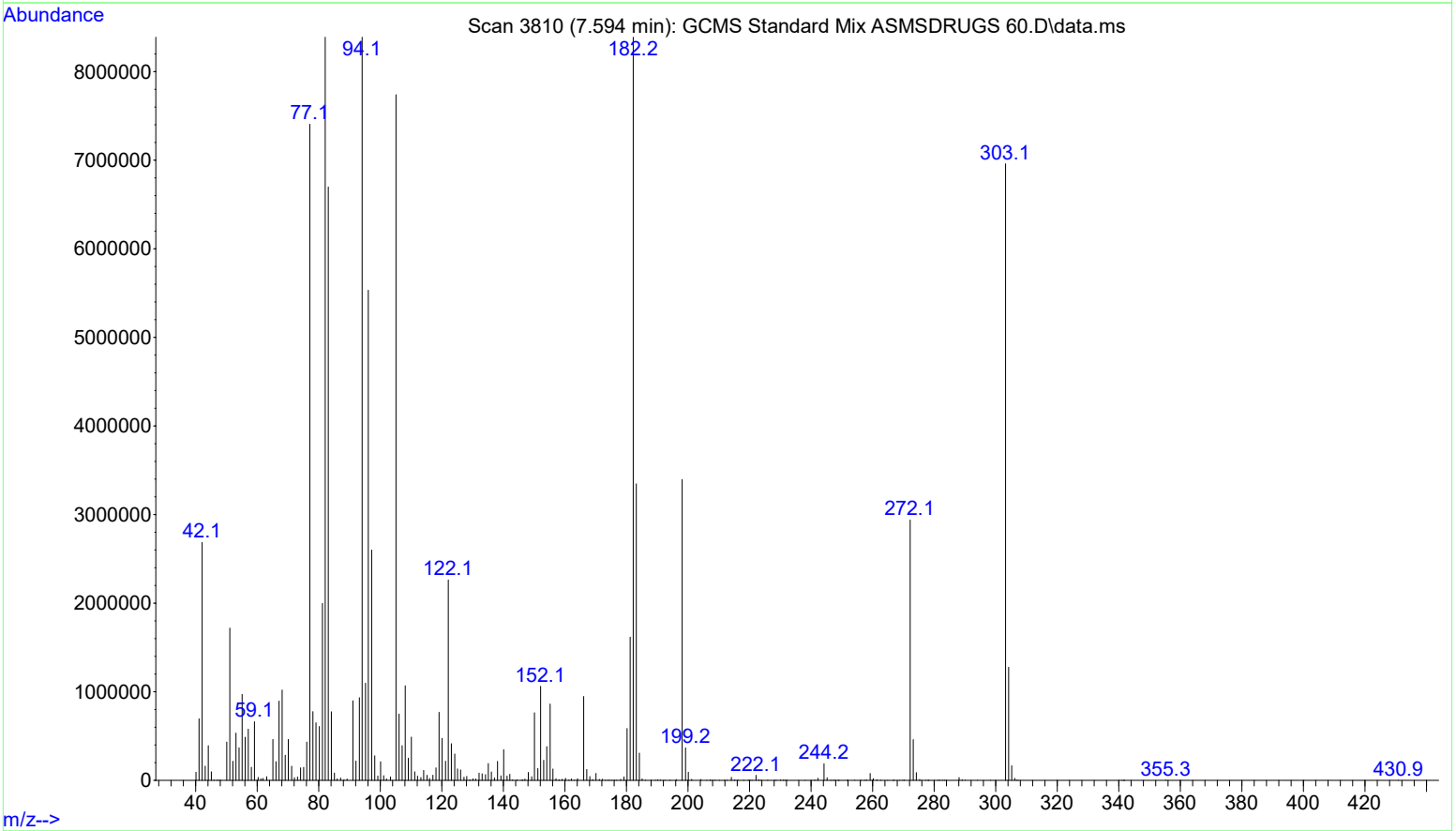


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS 60.D

BH
3-11-23

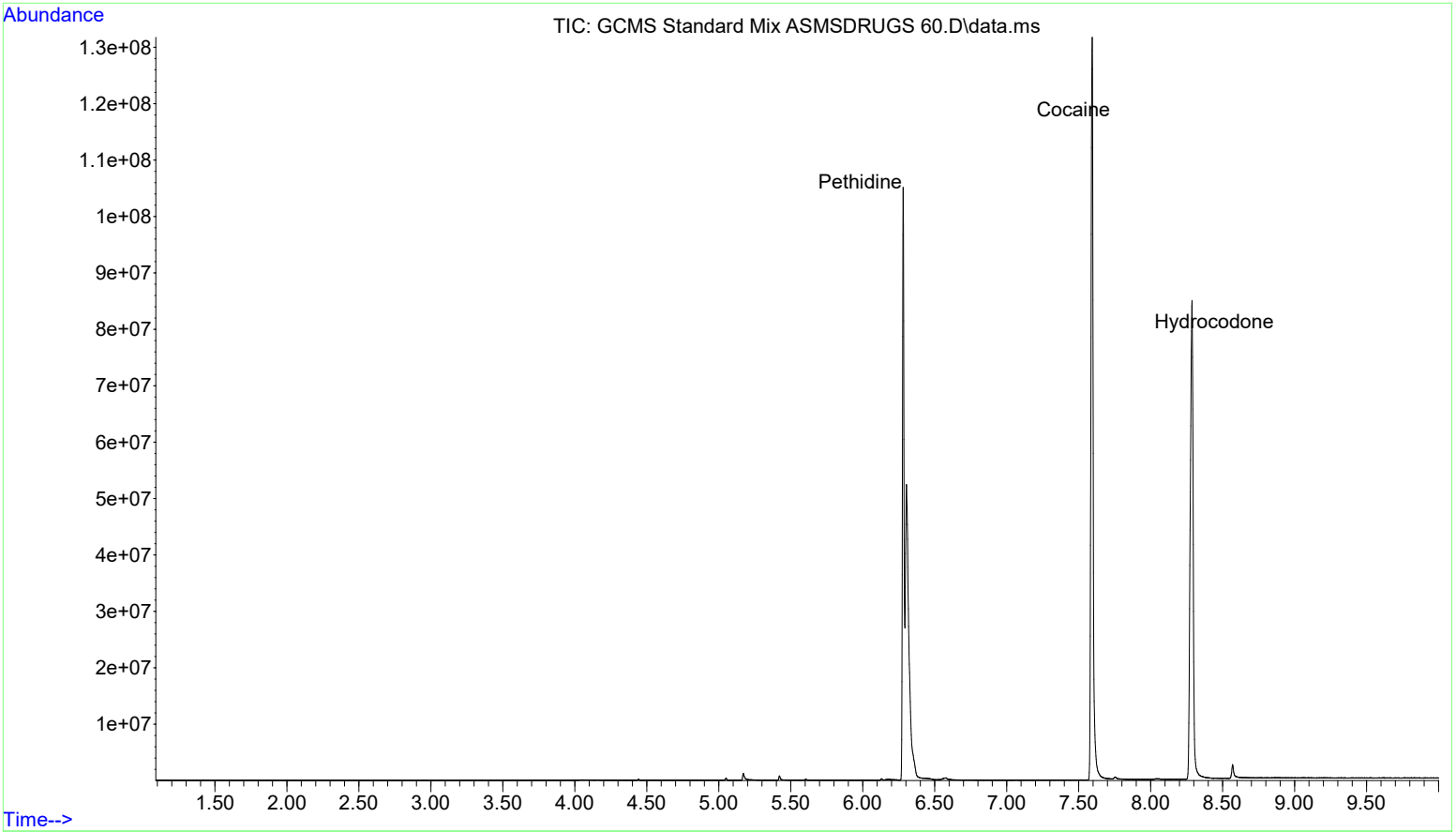
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 17:35 using AcqMethod ASMSDRUGS60.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS 6
Misc Info : METHANOL

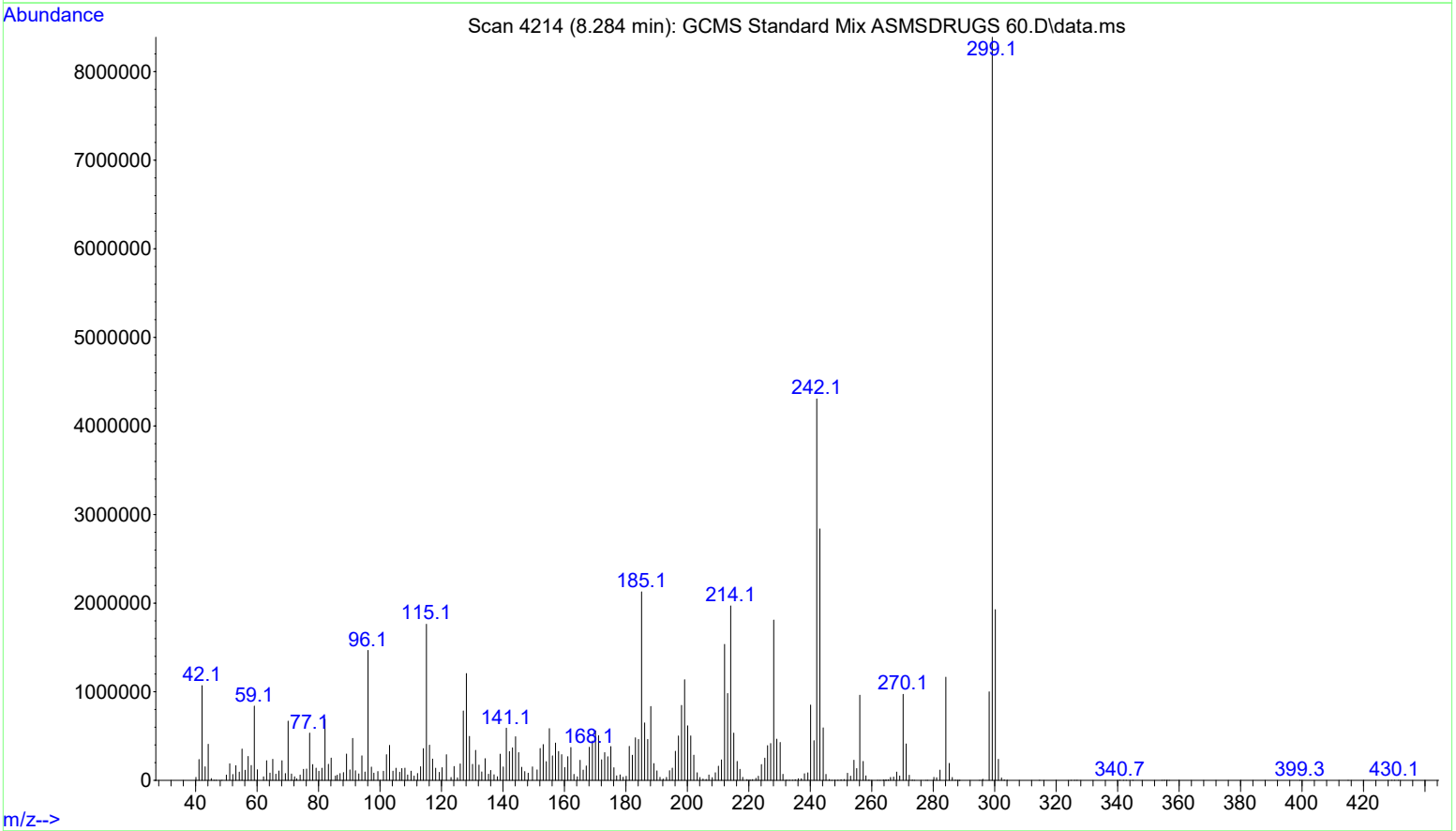




File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS 60.D
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 17:35 using AcqMethod ASMSDRUGS60.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS 6
Misc Info : METHANOL

BH
3-11-23





Single Quadrupole Acquisition Method - MS Parameters Report

Method file	C:\MassHunter\GCMS\1\methods\ASMSDRUGS100.M
Tune file	atune.u
Ion source	EI
Source temperature (°C)	230
Quad temperature (°C)	150
Fixed Electron energy (eV)	70.0
Acquisition Type	Scan
Stop time (min)	650.00
Solvent delay (min)	1.00
Trace Ion Detection	False
Gain Factor	1
EM Saver	False
EM Saver Limit	N/A

Scan Time Segments

Time	Start Mass	End Mass	Threshold	Scan Speed
1.00	40	550	150	6,250 [N=0]

Timed Events

Time	Type of Event	Parameter

Real-Time Plots

Type of Plot	Label	Low Mass	High Mass
Total Ion	N/A	N/A	N/A

Self-Cleaning Ion Source Parameters

Mode	No Cleaning

METHOD CONTROL PARAMETERS

BH
3-11-23

Method Information for: C:\MassHunter\GCMS\1\methods\ASMSDRUGS100.M

Method Sections To Run:

( ) Save Copy of Method With Data
( ) Instrument Control Pre-Run Cmd/Macro =
( ) Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
(X) Data Analysis
( ) Instrument Control Post-Run Cmd/Macro =
( ) Data Analysis Post-Run Cmd/Macro =

Method Comments:
ASMSDRUGS100

END OF METHOD CONTROL PARAMETERS

C:\MassHunter\GCMS\1\methods\ASMSDRUGS100.M
Fri Mar 10 21:57:01 2023

Control Information
------- -----------

Sample Inlet : GC
Injection Source : GC ALS
Injection Location: Front
Mass Spectrometer : Enabled

No Sample Prep method has been assigned to this method.

GC
GC Summary

Run Time	10.001 min
Post Run Time	0 min

Oven
Temperature

Setpoint	On
(Initial)	100 °C
Hold Time	1 min
Post Run	100 °C
Program	
#1 Rate	70 °C/min
#1 Value	280 °C
#1 Hold Time	6.43 min
Equilibration Time	1 min
Max Temperature	325 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled

ALS
Front Injector

Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	1
Sample Wash Volume	4 µL
Sample Pumps	2
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	6000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	6000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL

Solvent Wash Mode	A, B

BH
3-11-23

Back Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	0
Solvent A Washes (PostInj)	0
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	0
Solvent B Washes (PostInj)	0
Solvent B Volume	8 µL
Sample Washes	0
Sample Wash Volume	8 µL
Sample Pumps	6
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL
Solvent Wash Mode	A, B

Sample Overlap	
Mode	Sample overlap is not enabled

ALS Errors	Pause for user interaction

Front SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 10.806 psi
Total Flow	On 54 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	On 30 After 3 min mL/min
Split Ratio	50 :1
Split Flow	50 mL/min
Liner	A Liner has not been selected.

Back SS Inlet He	
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***
Mode	Split
Heater	On 250 °C
Pressure	On 3.5859 psi
Total Flow	On 79 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	Off
Split Ratio	75 :1
Split Flow	75 mL/min
Liner	A Liner has not been selected.

Thermal Aux 3 (MSD Transfer Line)	
Temperature	
Setpoint	On
(Initial)	280 °C

Column
Column #1
Flow

Setpoint	On
(Initial)	1 mL/min
Post Run	0.57353 mL/min

BH
3-11-23

Column Information	Agilent 19091S-602
HP-1MS	
Temperature Range	-60 °C—325 °C (350 °C)
Dimensions	12.5 m x 200 µm x 0.33 µm (Calibrated)
Column lock	Locked
In	Front SS Inlet He
Out	MSD
(Initial)	100 °C
Pressure	10.806 psi
Flow	1 mL/min
Average Velocity	57.774 cm/sec
Holdup Time	0.3606 min
Control Mode	Constant Flow

Column #2	
Flow	
Setpoint	On
(Initial)	1 mL/min
Post Run	1 mL/min

Column Information	Agilent 19091S-913
HP-1MS	
Temperature Range	-60 °C—325 °C (325 °C)
Dimensions	15 m x 320 µm x 0.25 µm (Calibrated)
Column lock	Locked
In	Back SS Inlet He
Out	Back Detector FID
(Initial)	100 °C
Pressure	3.5859 psi
Flow	1 mL/min
Average Velocity	23.097 cm/sec
Holdup Time	1.0824 min
Control Mode	Constant Flow

Column Outlet Pressure	0 psi

Back Detector FID	
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***
Makeup	He
Column Compensation	Signal is modified by Column Compensation Curve #2
Heater	On 300 °C
H2 Flow	Off
Air Flow	Off
Makeup Flow	On 25 mL/min
Carrier Gas Flow Correction	Constant Makeup and Fuel Flow
Flame	Off

Aux EPC 1,2,3	
Aux EPC 1 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Aux EPC 2 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi

Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State*** BH 3-11-23
Aux EPC 3 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Signals

Signal #1: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Front Sample
Signal #2: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample
Signal #3: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample
Signal #4: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

TUNE PARAMETERS for SN: US1648M021

Trace Ion Detection is OFF.

34.593	:	EMISSION
70.007	:	ENERGY
34.899	:	REPELLER
90.331	:	IONFOCUS
22.672	:	ENTRANCE_LENS
1360.190	:	EMVOLTS
1498.6	:	Actual EMV
1.00	:	GAIN FACTOR
2908.000	:	AMUGAIN
136.750	:	AMUOFFSET
1.000	:	FILAMENT
0.000	:	DCPOLARITY
12.032	:	ENTLENSOFFSET
0.000	:	Ion_Body
0.000	:	EXTLENS
442.000	:	MASSGAIN

-22.000 : MASSOFFSET

END OF TUNE PARAMETERS

BH
3-11-23

END OF INSTRUMENT CONTROL PARAMETERS

DATA ANALYSIS PARAMETERS

Method Name: C:\MassHunter\GCMS\1\methods\ASMSDRUGS100.M

Percent Report Settings

Sort By: Signal

Output Destination
    Screen: No
    Printer: Yes
    File: No

Integration Events: AutoIntegrate

Generate Report During Run Method: No

Signal Correlation Window: 0.020

Qualitative Report Settings

Peak Location of Unknown: Apex

Library to Search   Minimum Quality
D:\MassHunter\Library\TBI_DRUG.L 0
D:\MassHunter\Library\Cayman120417.L 0
D:\MassHunter\Library\SWGDRUG010616.L

Integration Events: AutoIntegrate

Report Type: Summary

Output Destination
    Screen: No
    Printer: Yes
    File: No

Generate Report During Run Method: No

Quantitative Report Settings

Report Type: Summary

Output Destination
    Screen: Yes
    Printer: No
    File: No

Generate Report During Run Method: No

Calibration Last Updated:

Reference Window: 10.00 Percent
Non-Reference Window: 5.00 Percent
Correlation Window: 0.02 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

Compound Information

*** Empty Quantitation Database ***

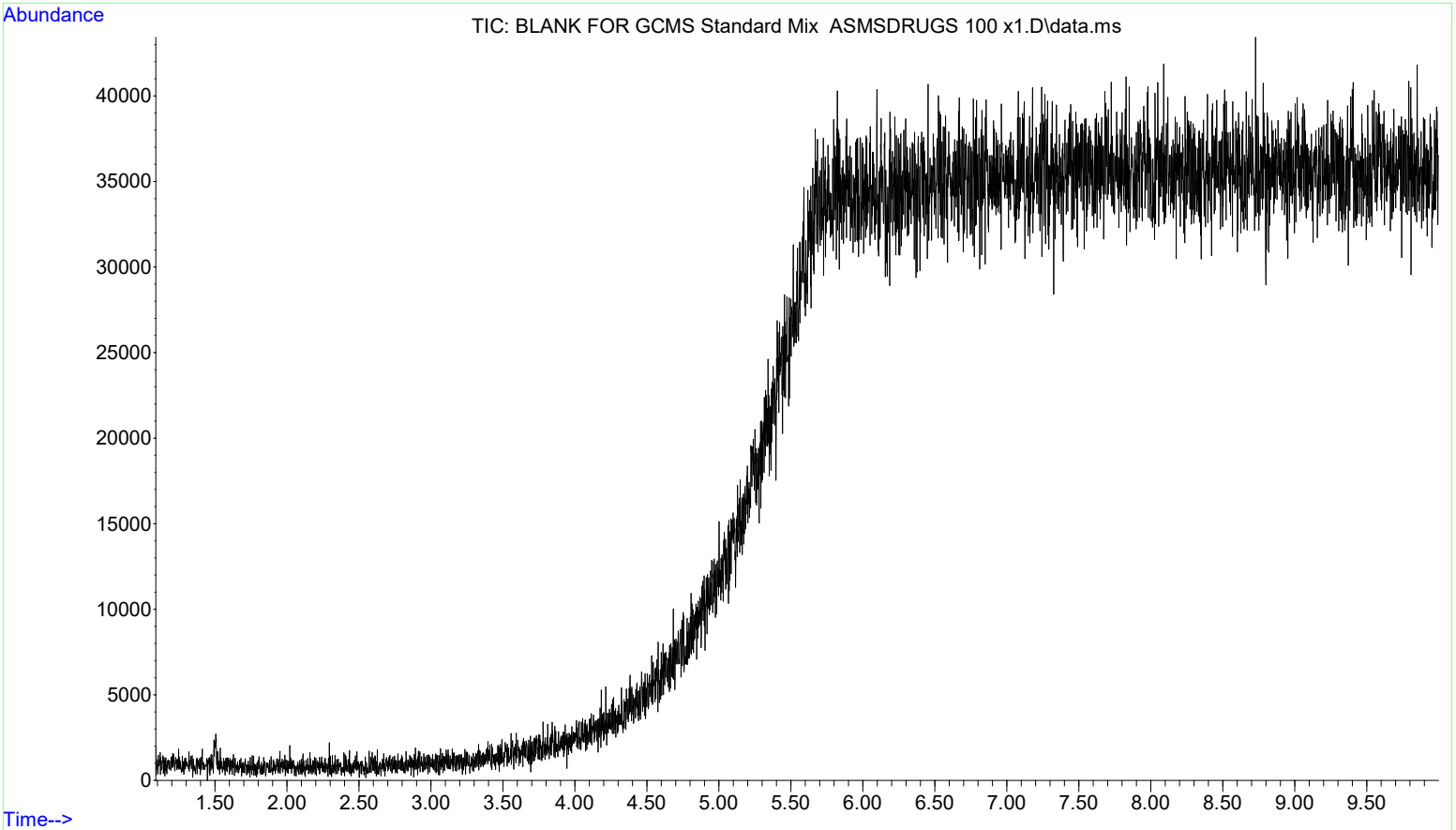
END OF DATA ANALYSIS PARAMETERS

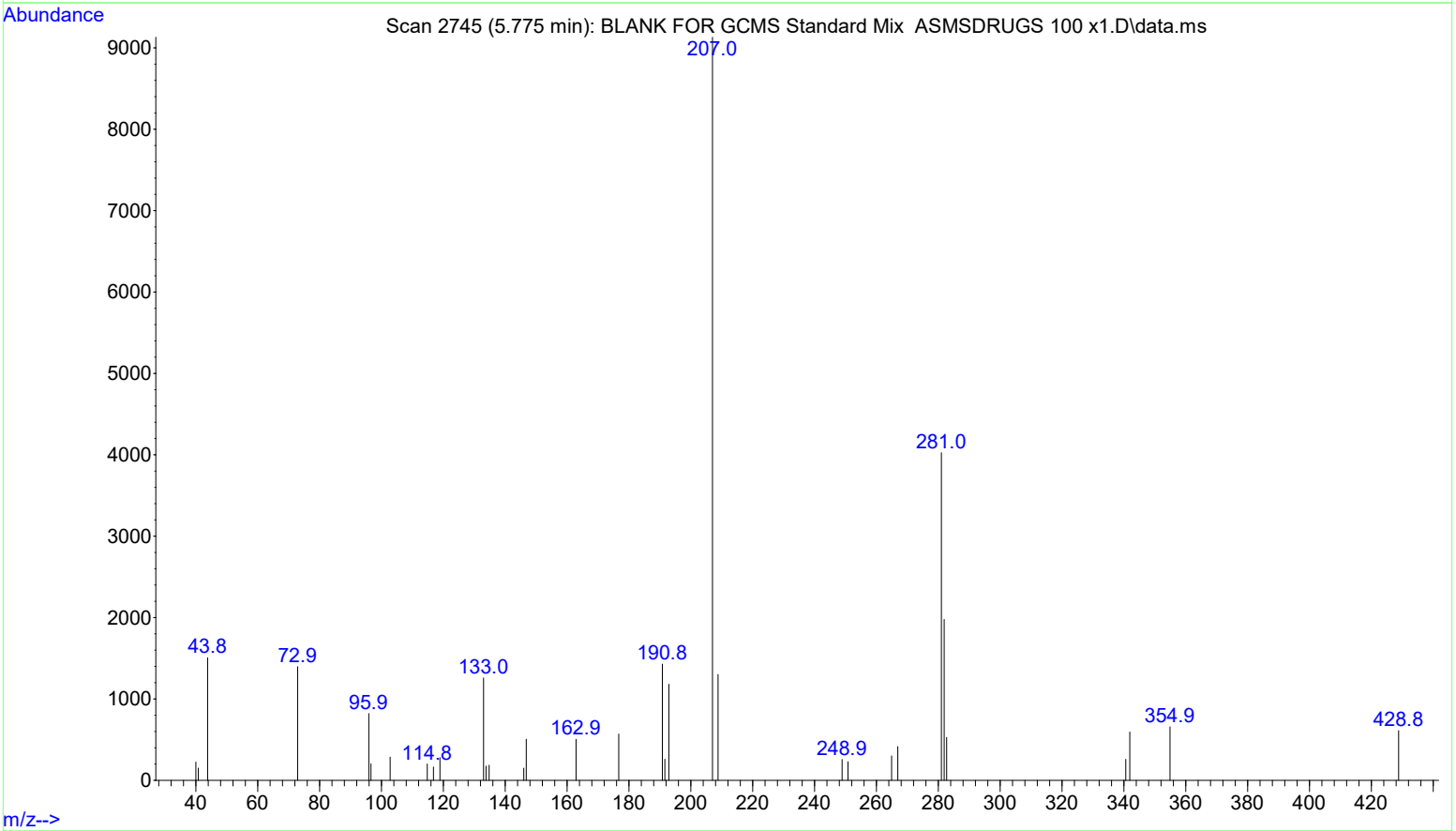
Fri Mar 10 21:57:27 2023

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR GCMS Standard Mix ASMSDRUGS 100 x1.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 15:14 using AcqMethod ASMSDRUGS100.M
Sample Name: BLANK FOR GCMS Standard Mix ASMSDRUGS100 x1
Misc Info : METHANOL

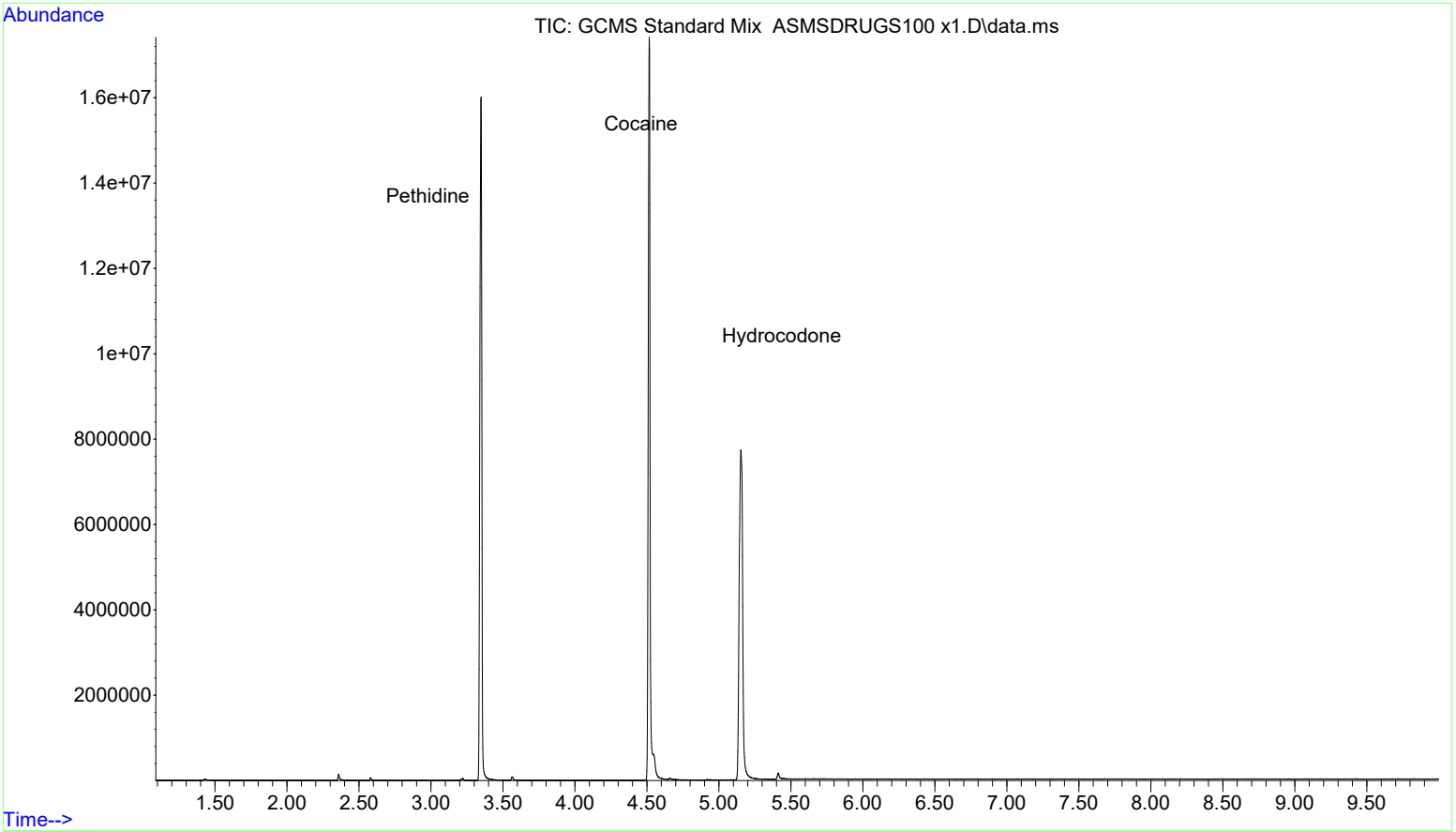


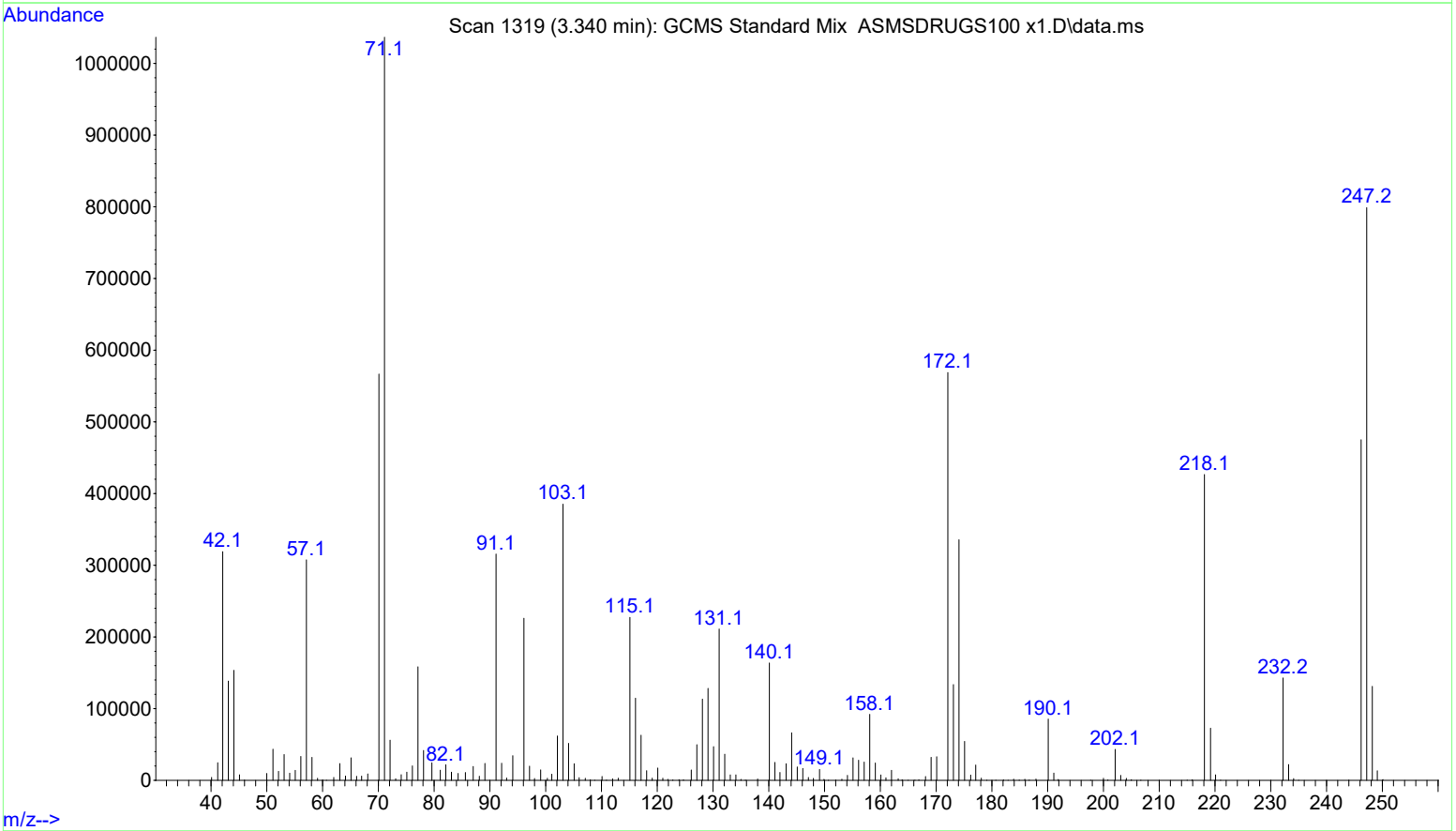


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS100 x1.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 15:28 using AcqMethod ASMSDRUGS100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS10
Misc Info : METHANOL

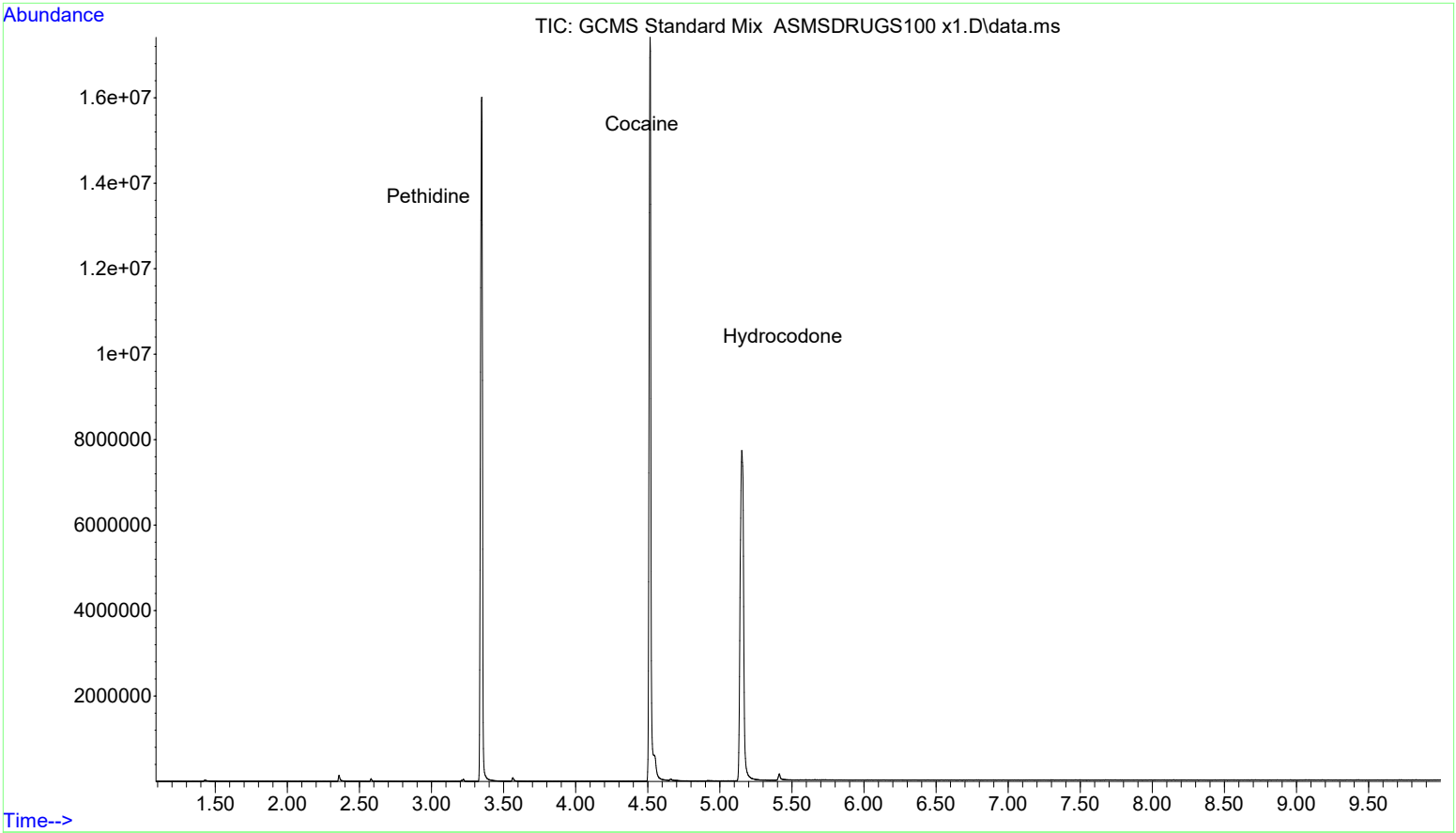


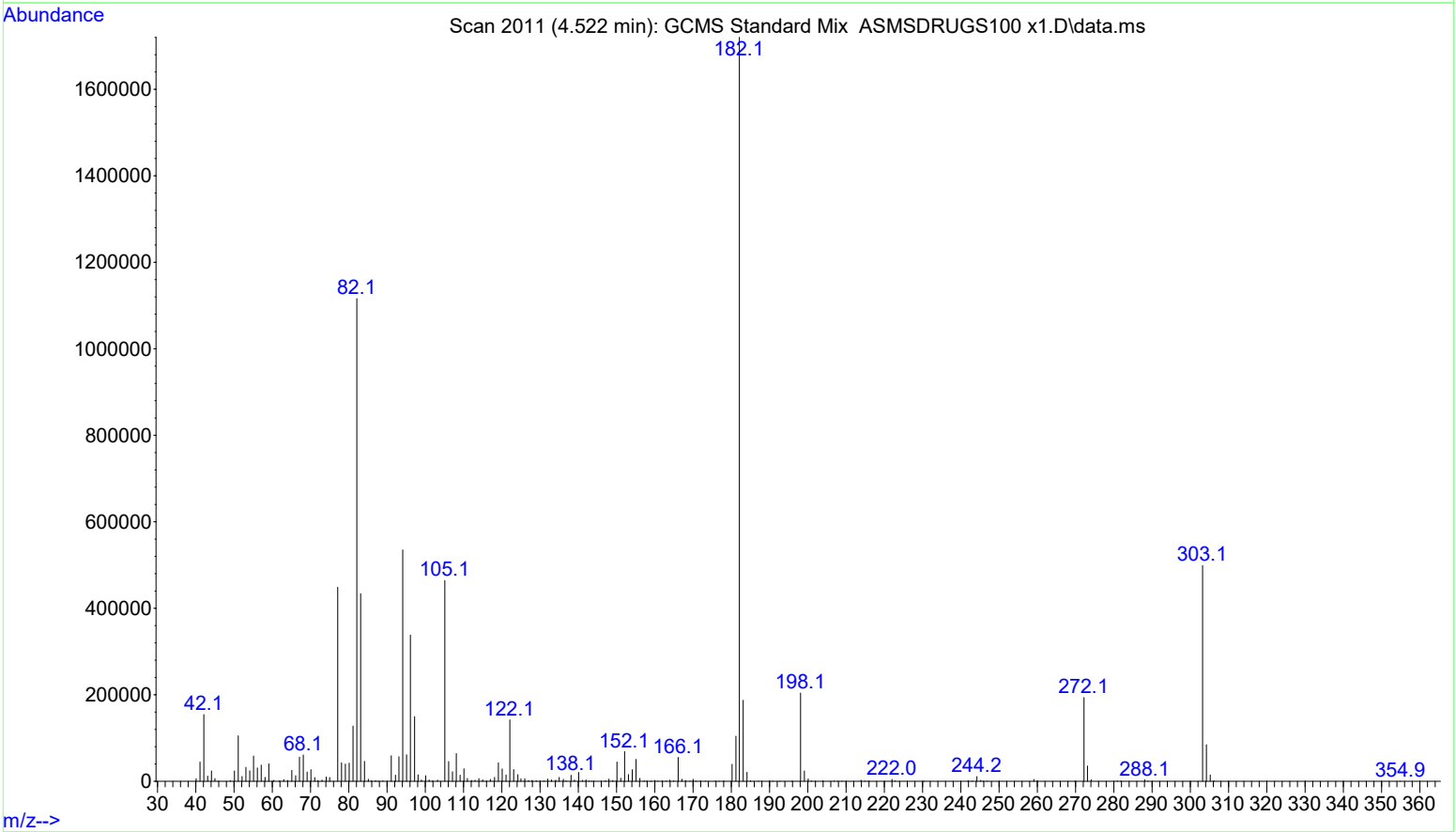


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS100 x1.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 15:28 using AcqMethod ASMSDRUGS100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS10
Misc Info : METHANOL

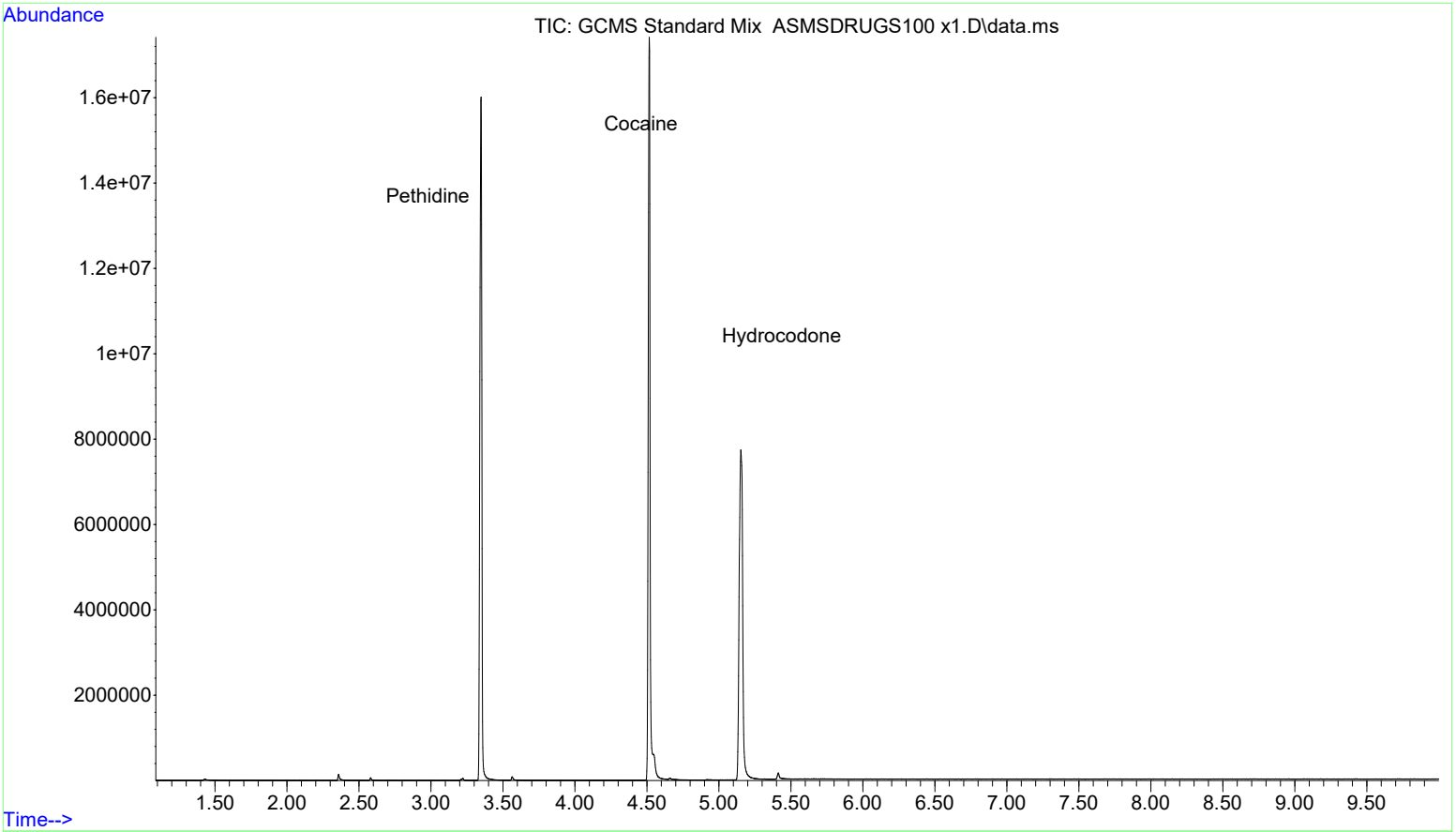


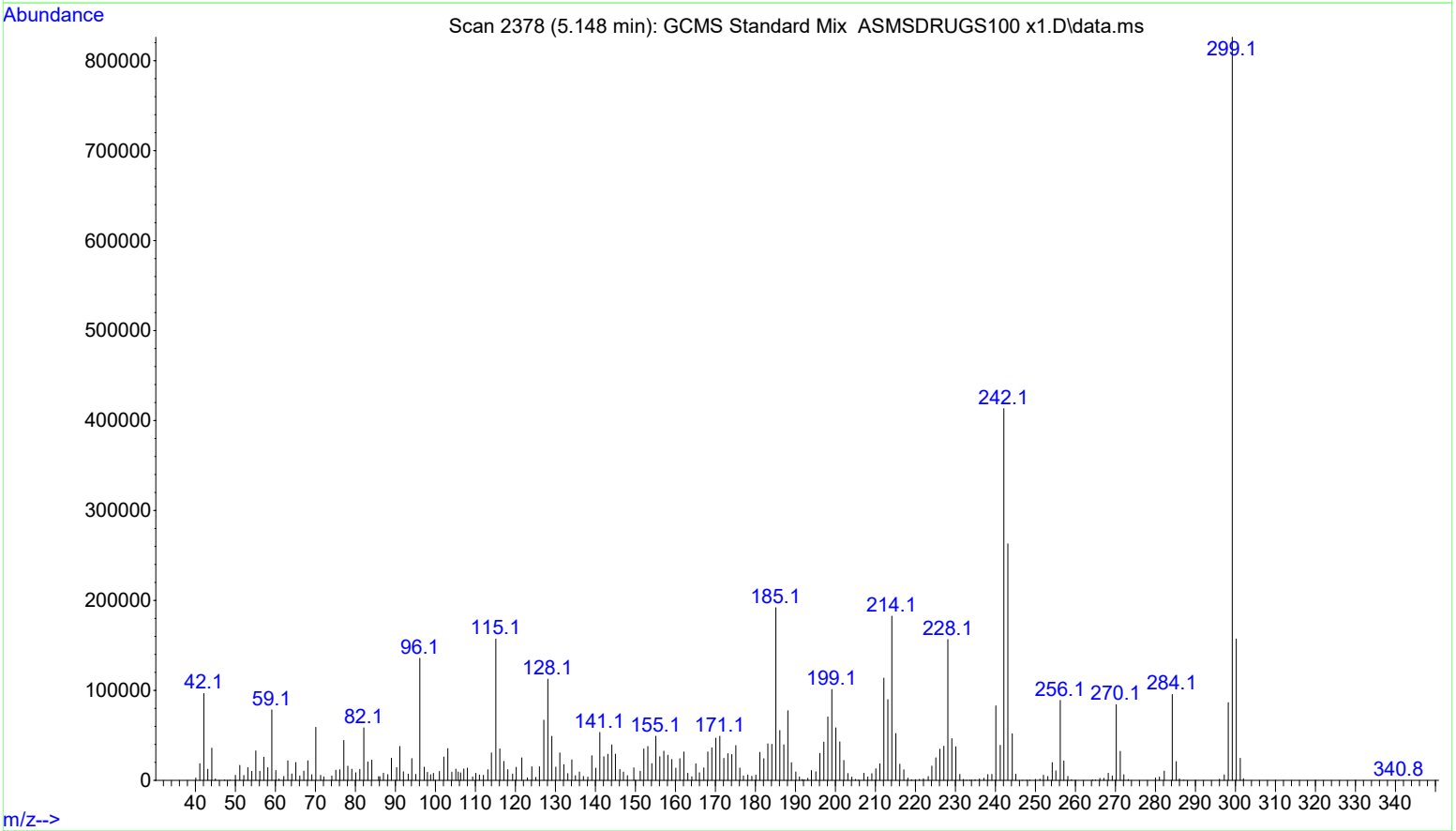


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS100 x1.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 15:28 using AcqMethod ASMSDRUGS100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS10
Misc Info : METHANOL

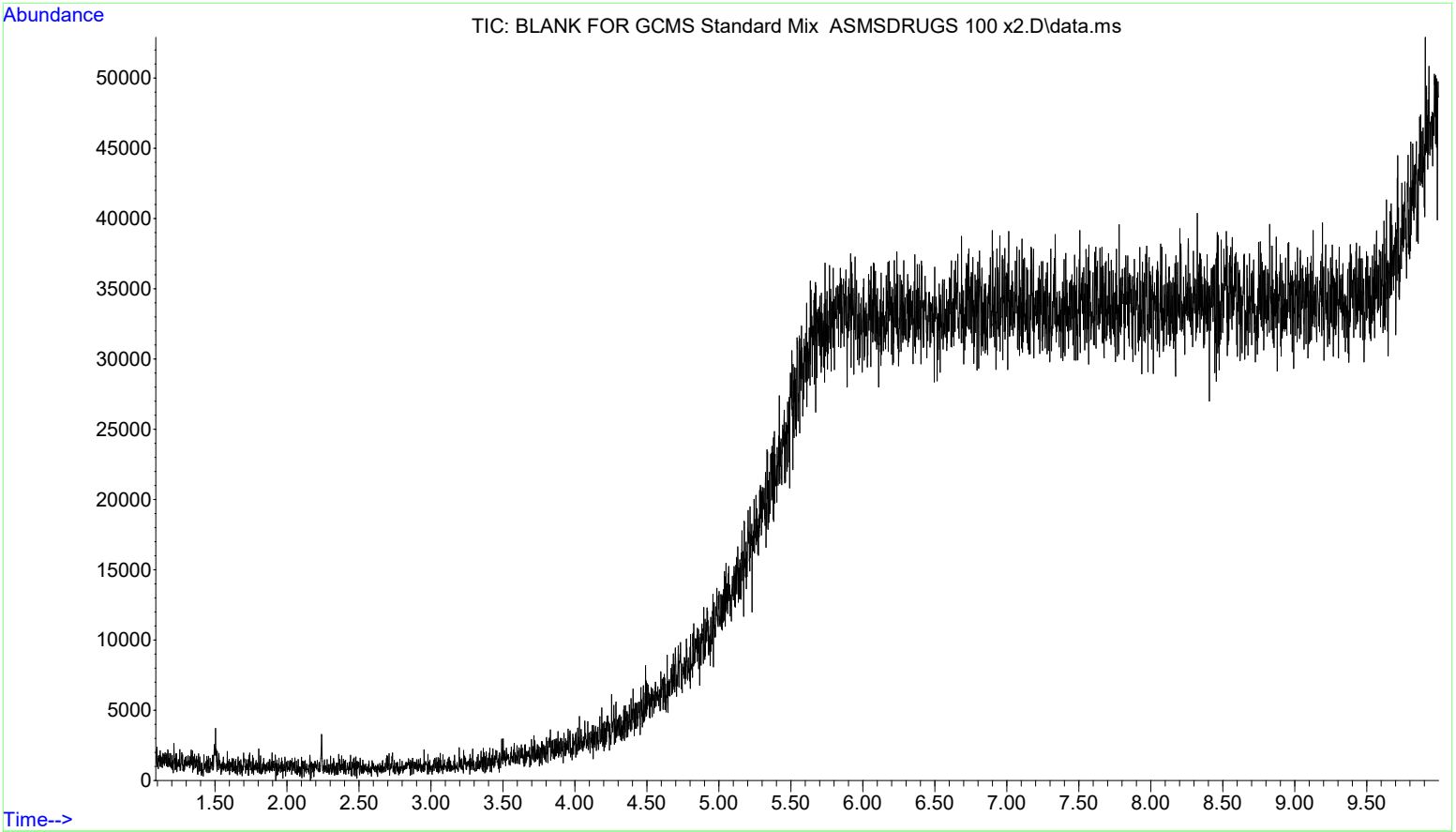


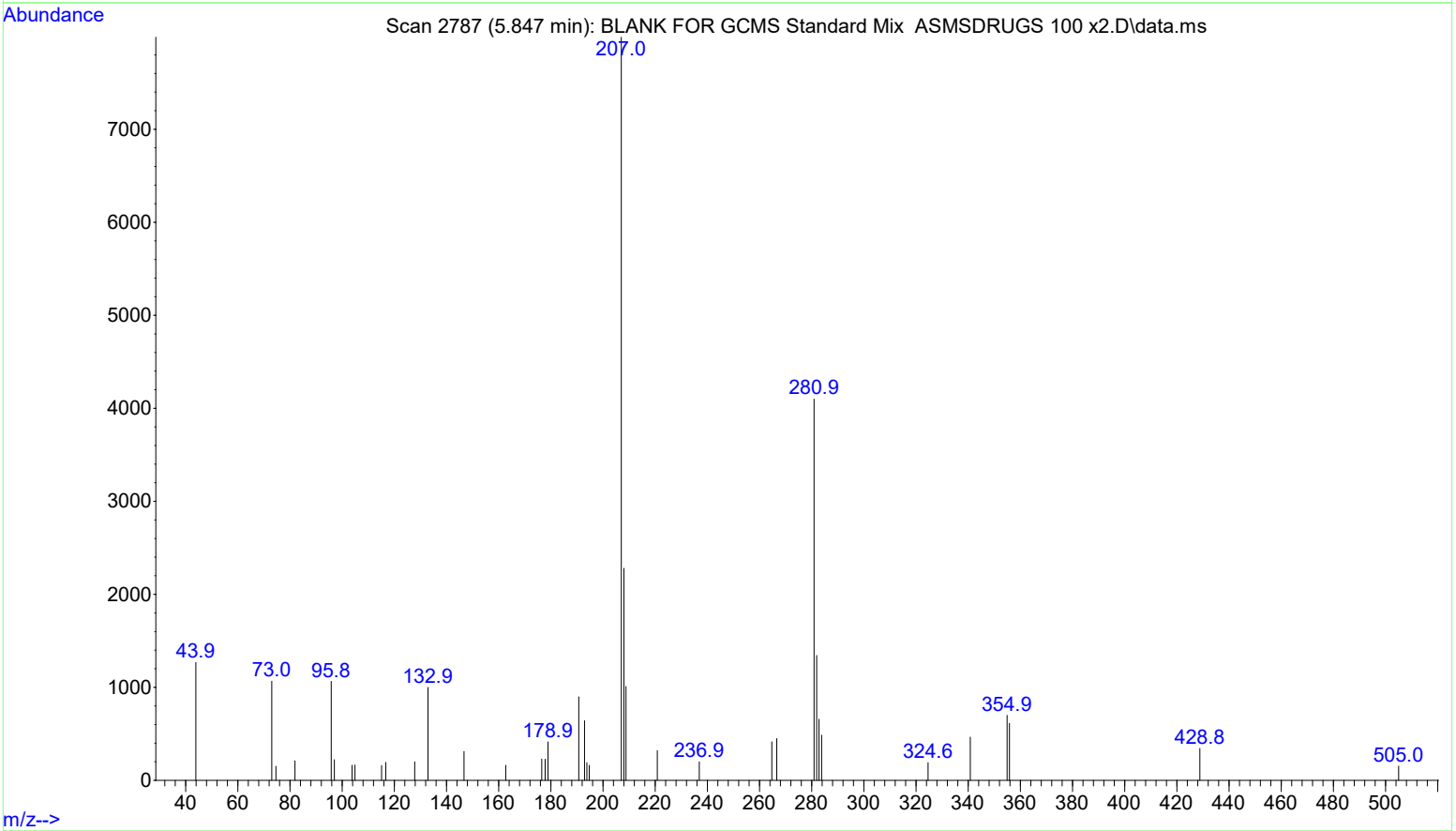


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR GCMS Standard Mix ASMSDRUGS 100 x2.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 15:56 using AcqMethod ASMSDRUGS100.M
Sample Name: BLANK FOR GCMS Standard Mix ASMSDRUGS 100 x2
Misc Info : METHANOL

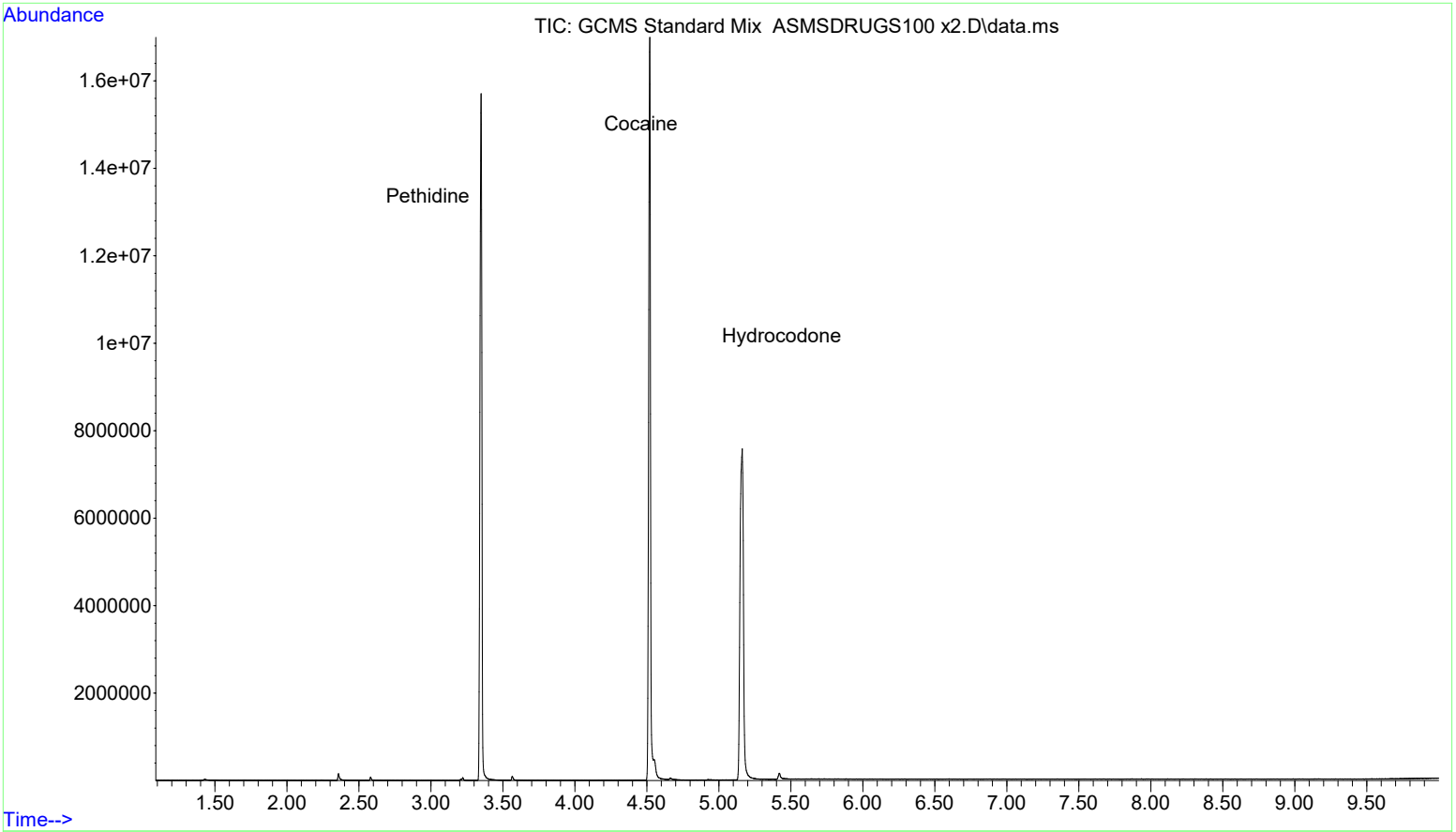


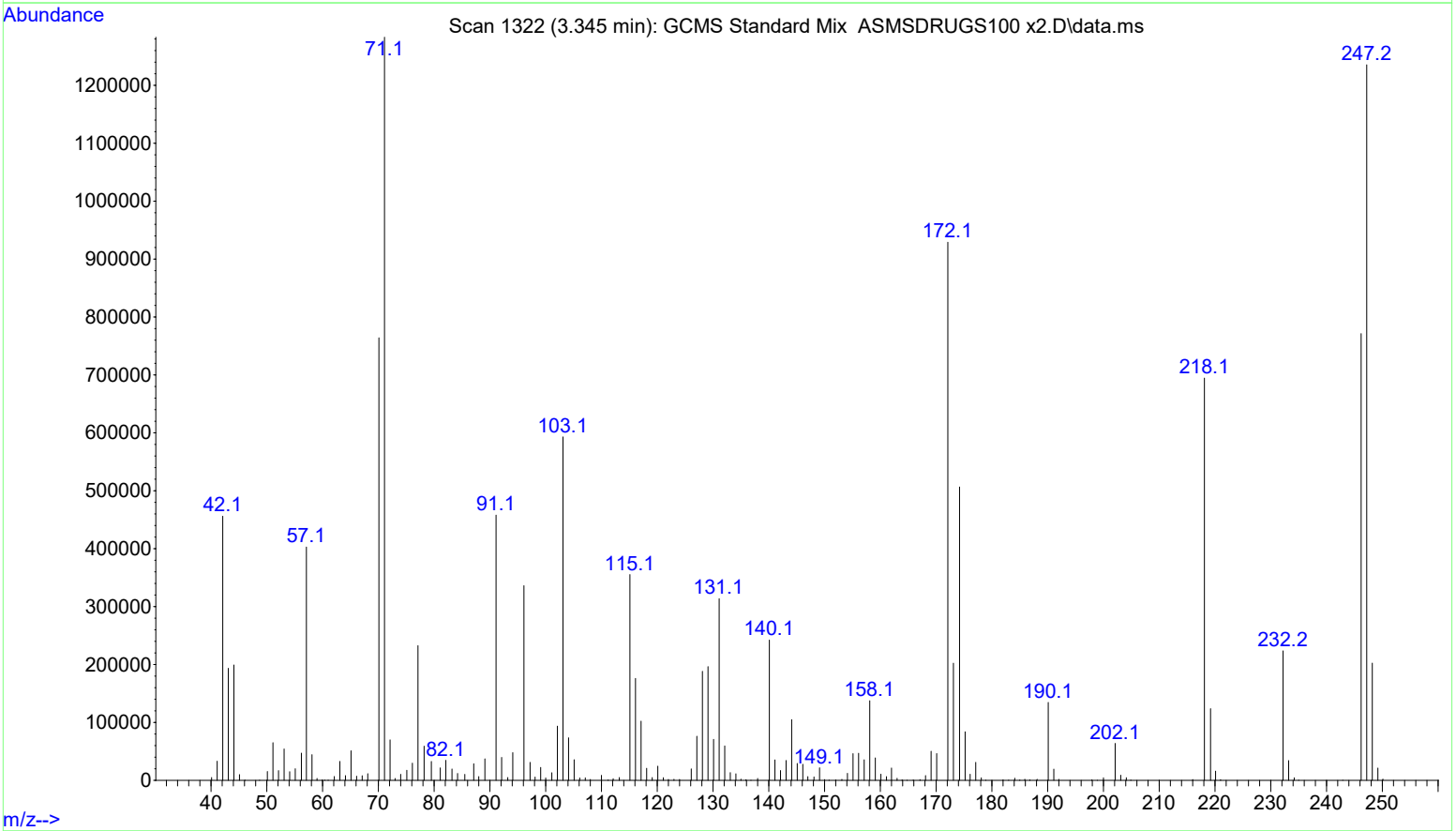


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS100 x2.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 16:09 using AcqMethod ASMSDRUGS100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS10
Misc Info : METHANOL

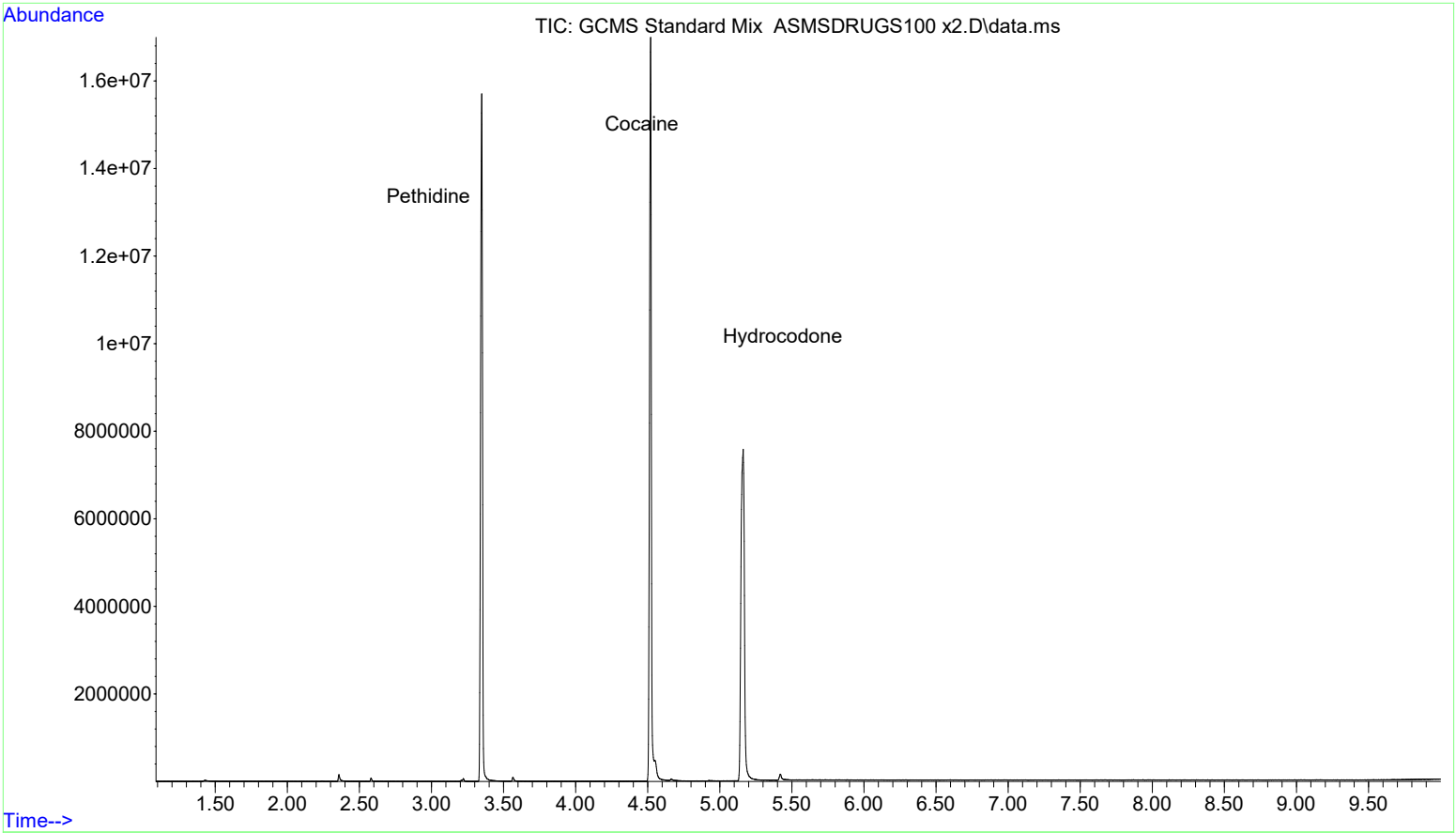


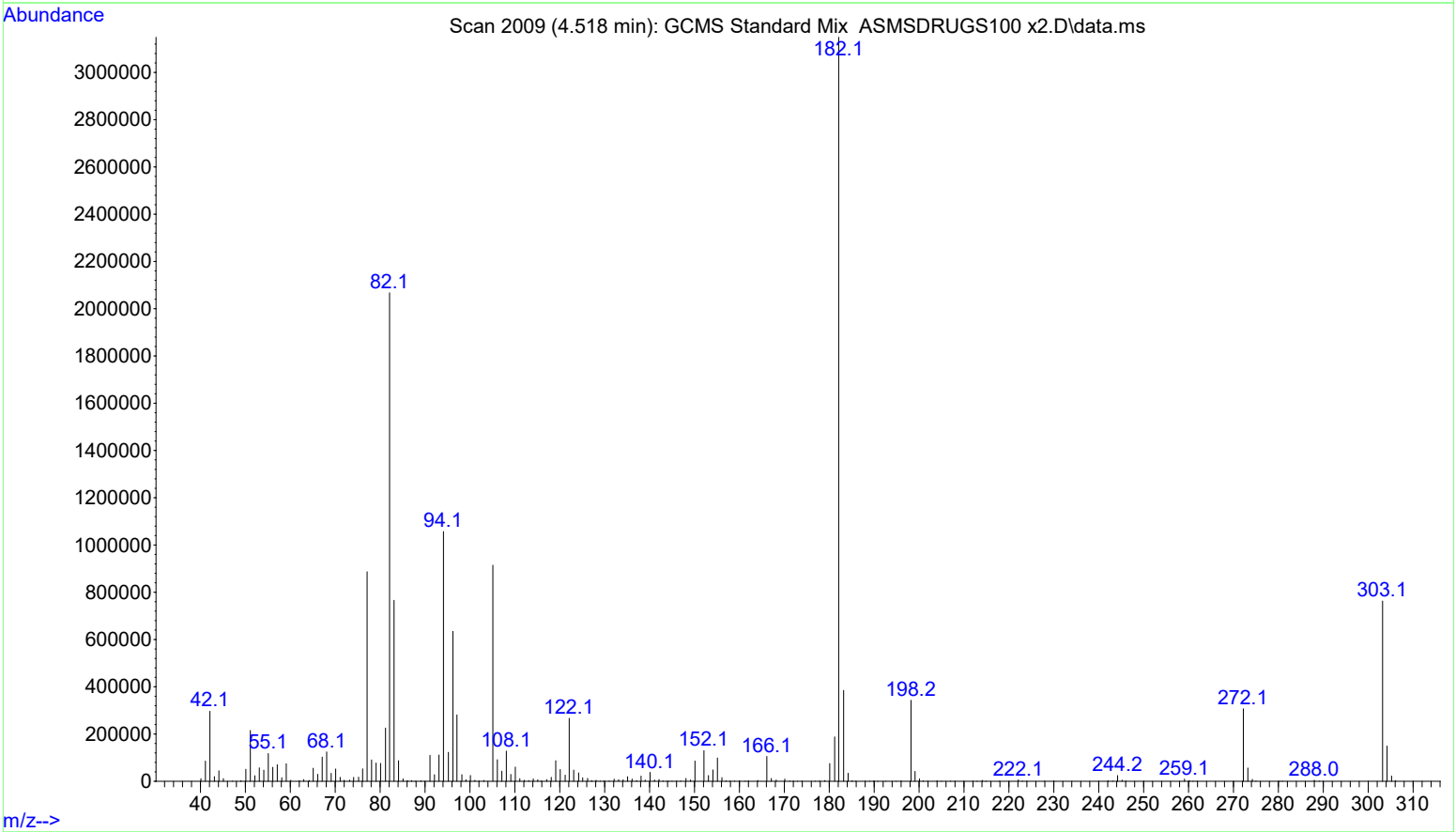


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS100 x2.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 16:09 using AcqMethod ASMSDRUGS100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS10
Misc Info : METHANOL

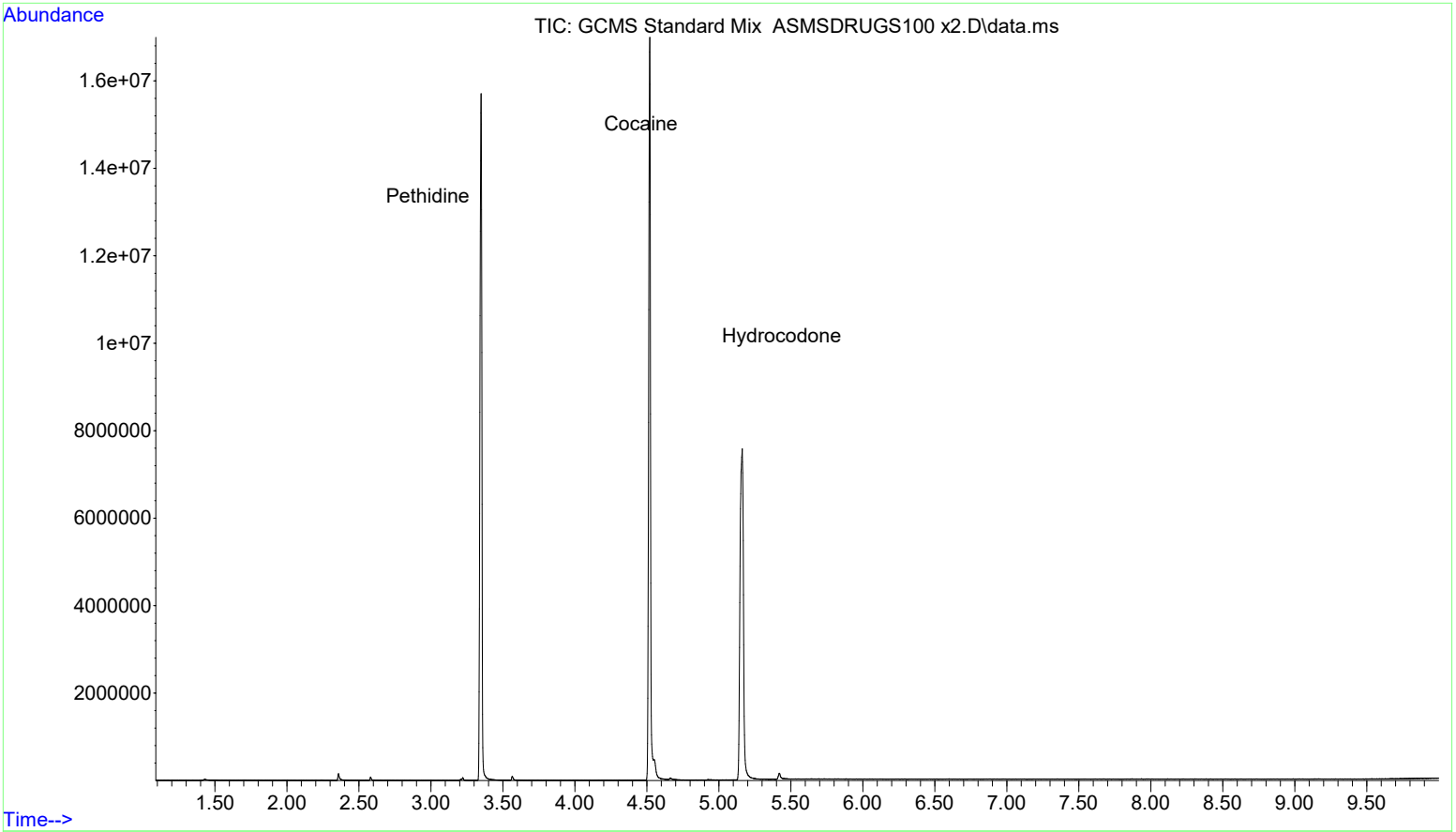


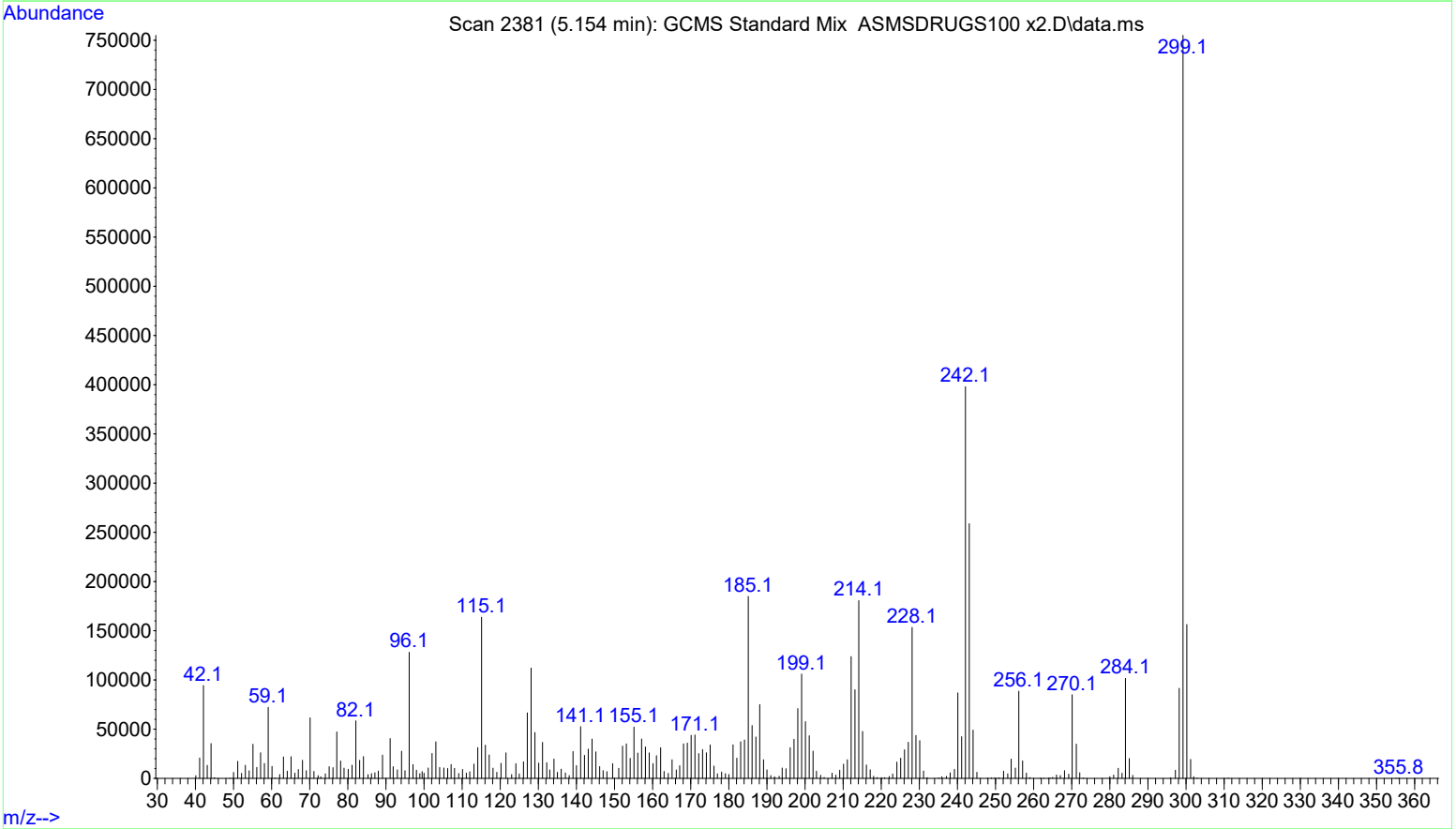


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS100 x2.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 16:09 using AcqMethod ASMSDRUGS100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS10
Misc Info : METHANOL

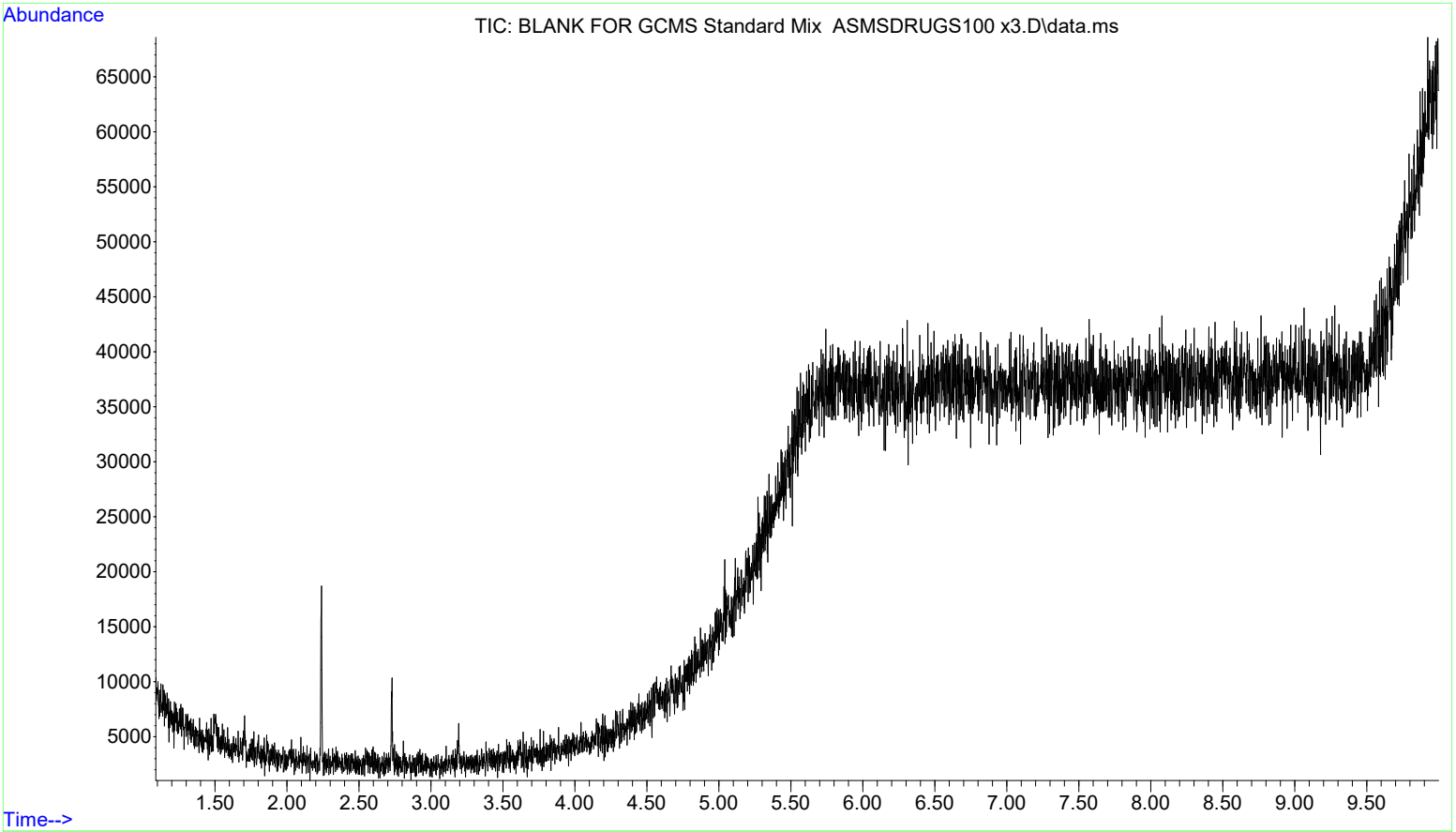


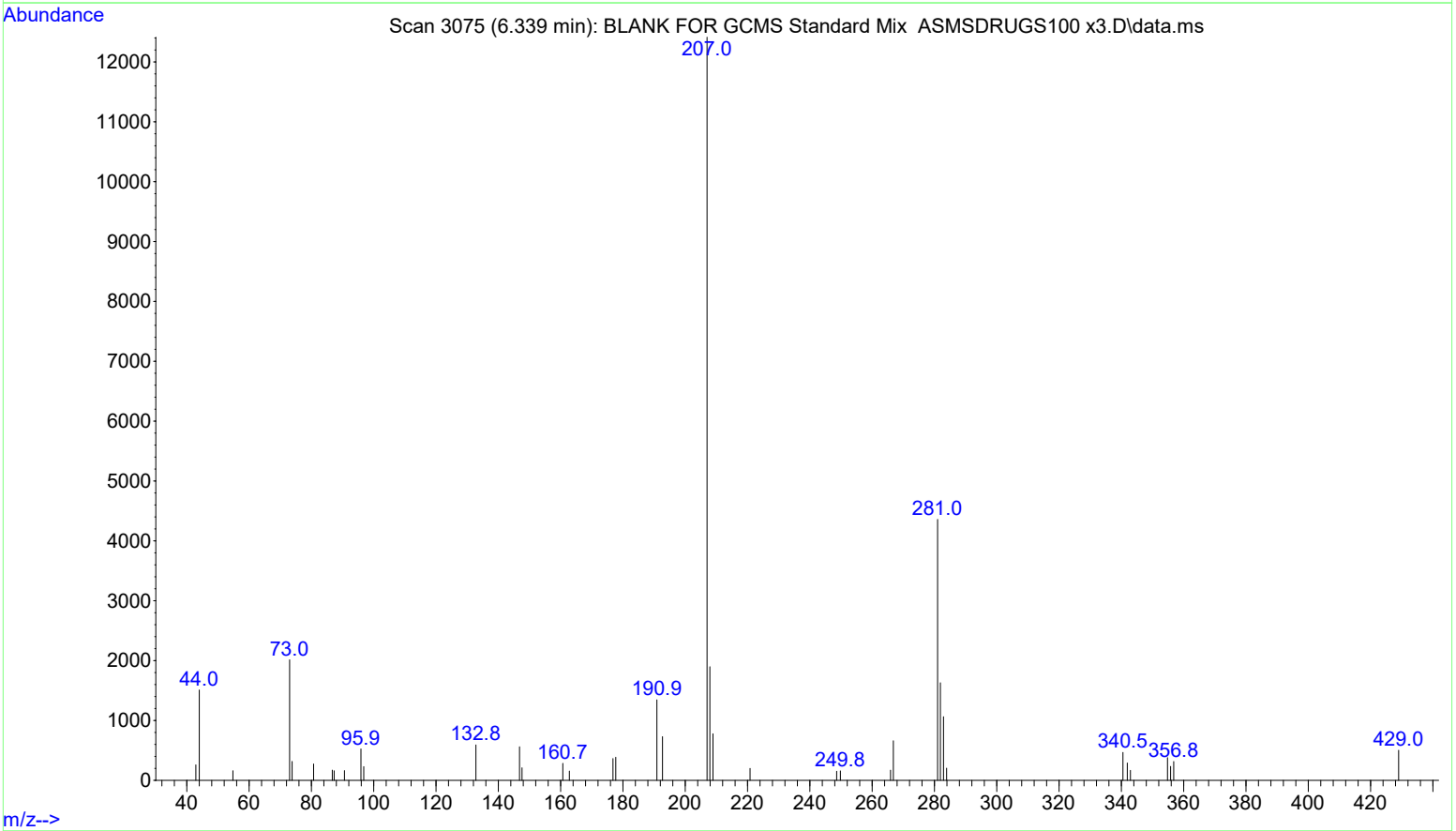


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR GCMS Standard Mix ASMSDRUGS100 x3.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 16:37 using AcqMethod ASMSDRUGS100.M
Sample Name: BLANK FOR GCMS Standard Mix ASMSDRUGS100 x3
Misc Info : METHANOL

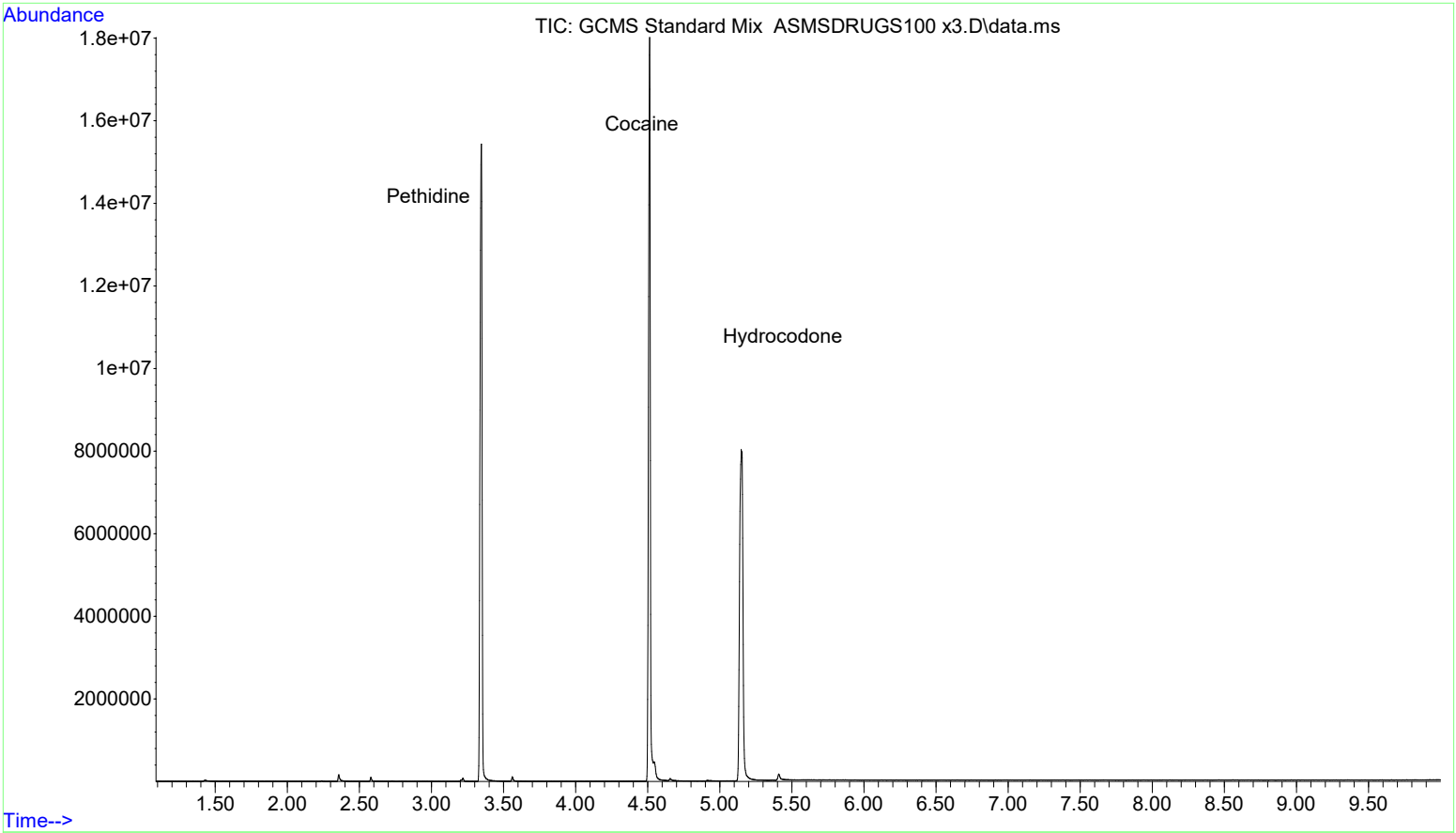


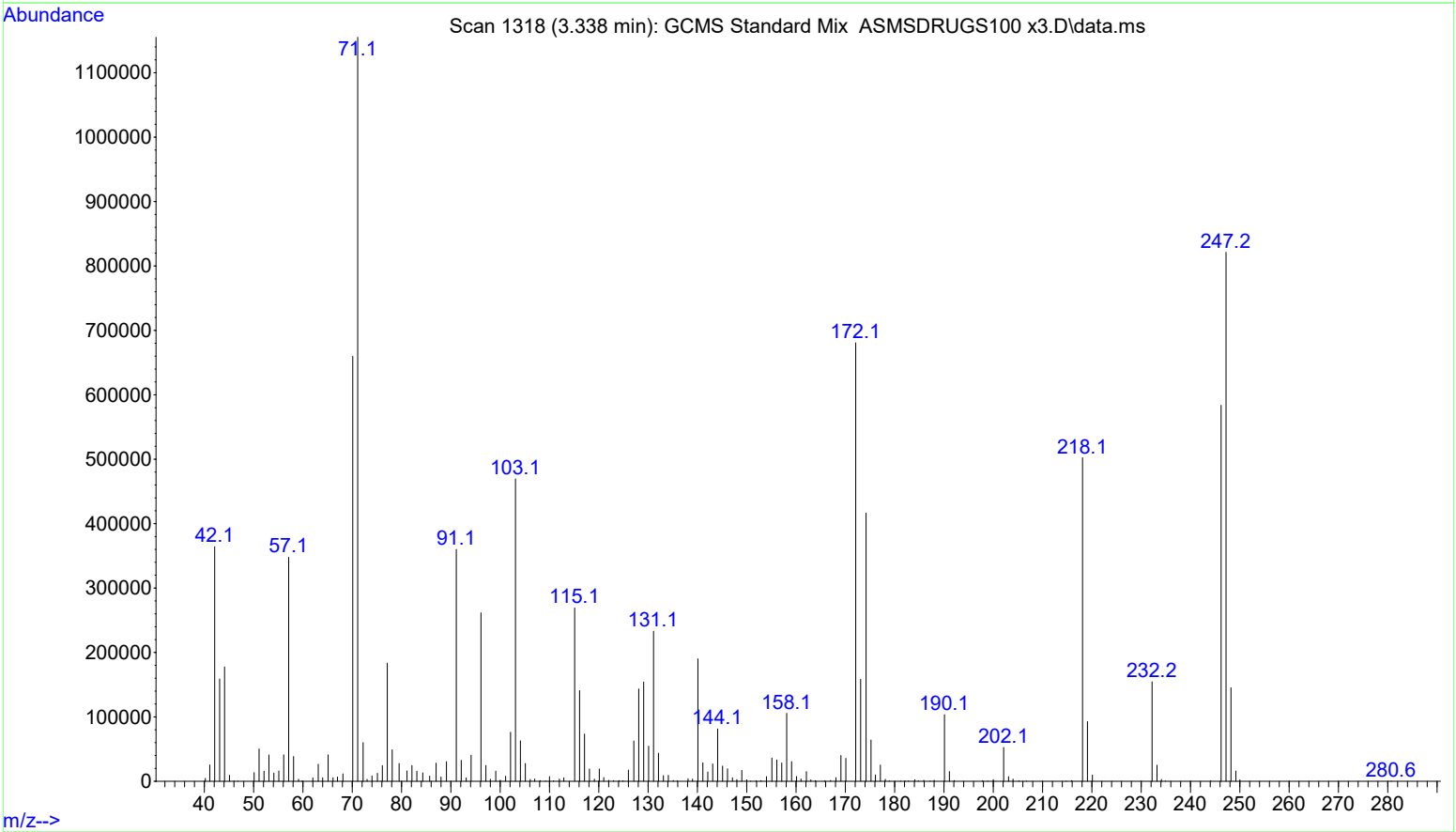


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS100 x3.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 16:51 using AcqMethod ASMSDRUGS100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS10
Misc Info : METHANOL

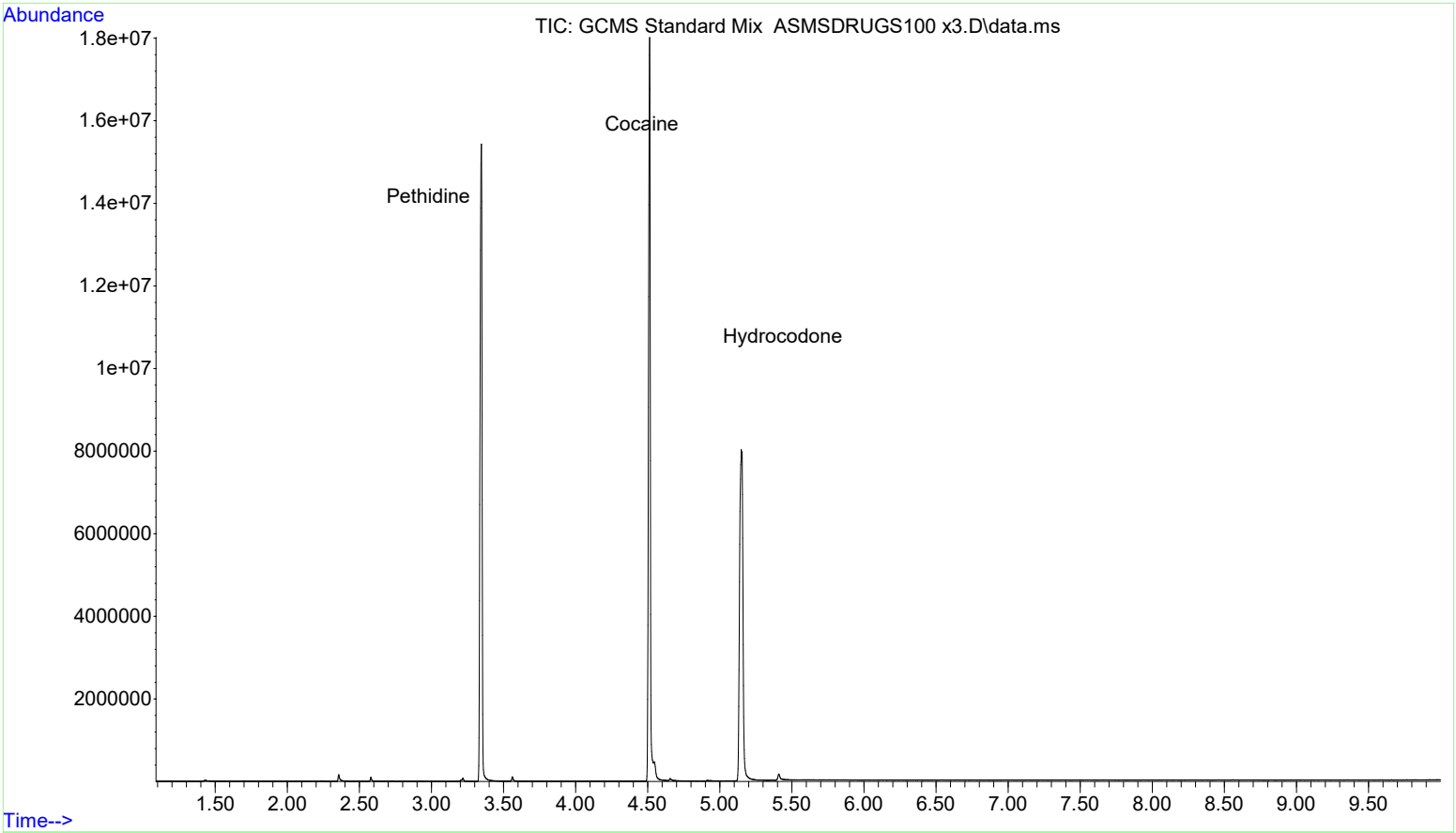


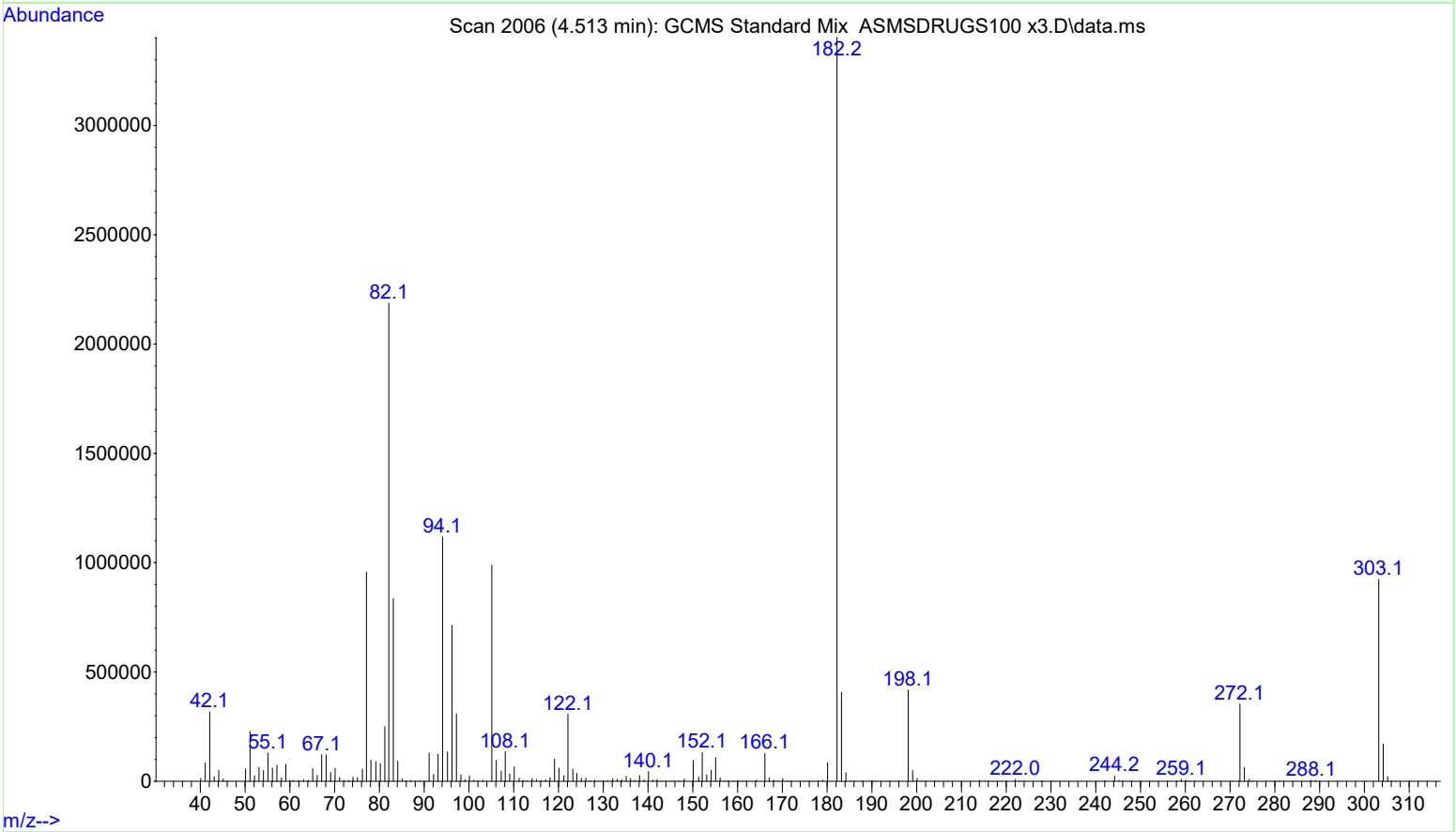


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS100 x3.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 16:51 using AcqMethod ASMSDRUGS100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS10
Misc Info : METHANOL

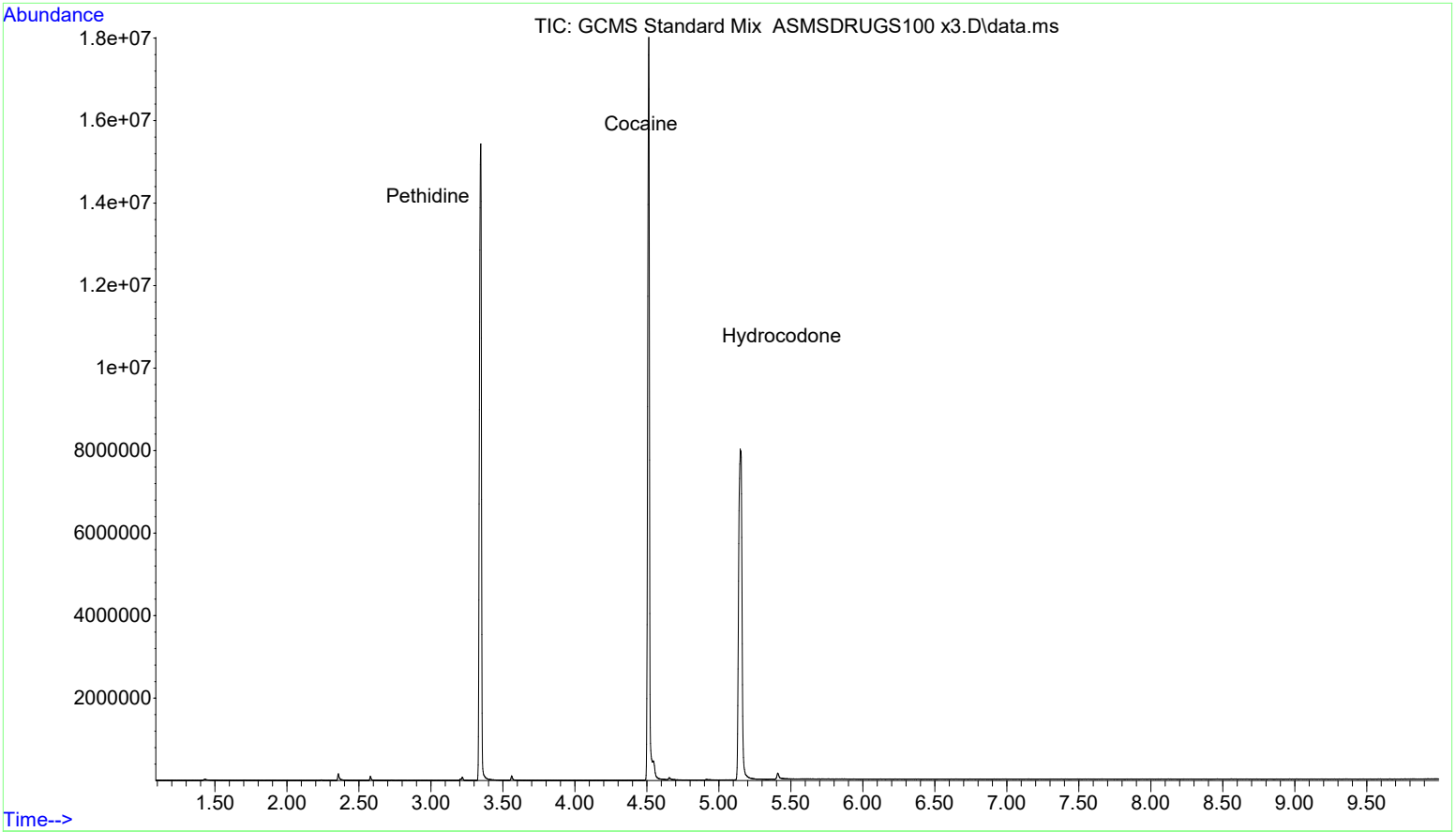


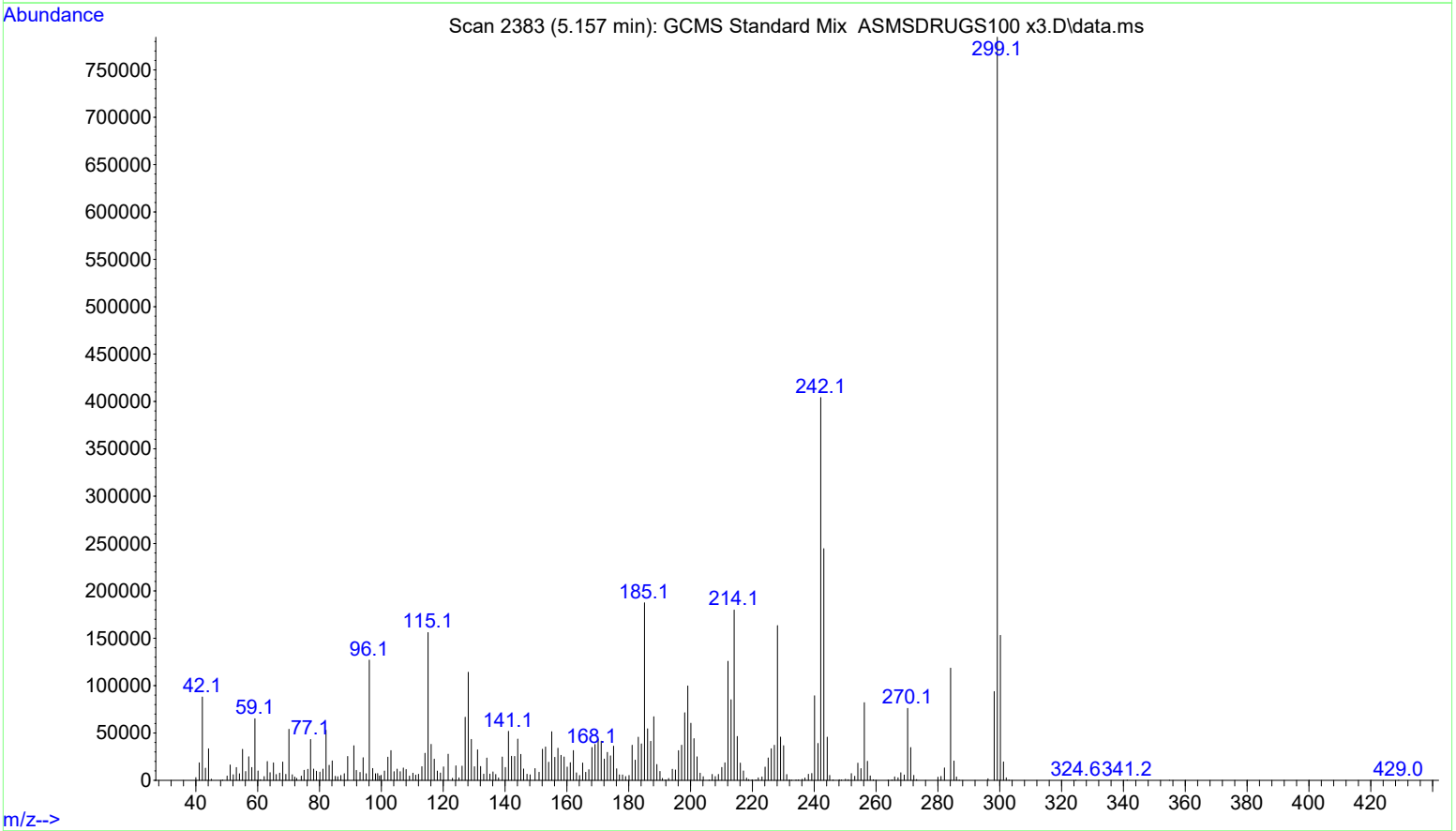


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\GC
... MS Standard Mix ASMSDRUGS100 x3.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 16:51 using AcqMethod ASMSDRUGS100.M
Sample Name: GCMS Standard Mix STD EXP. 5-2-23 ASMSDRUGS10
Misc Info : METHANOL

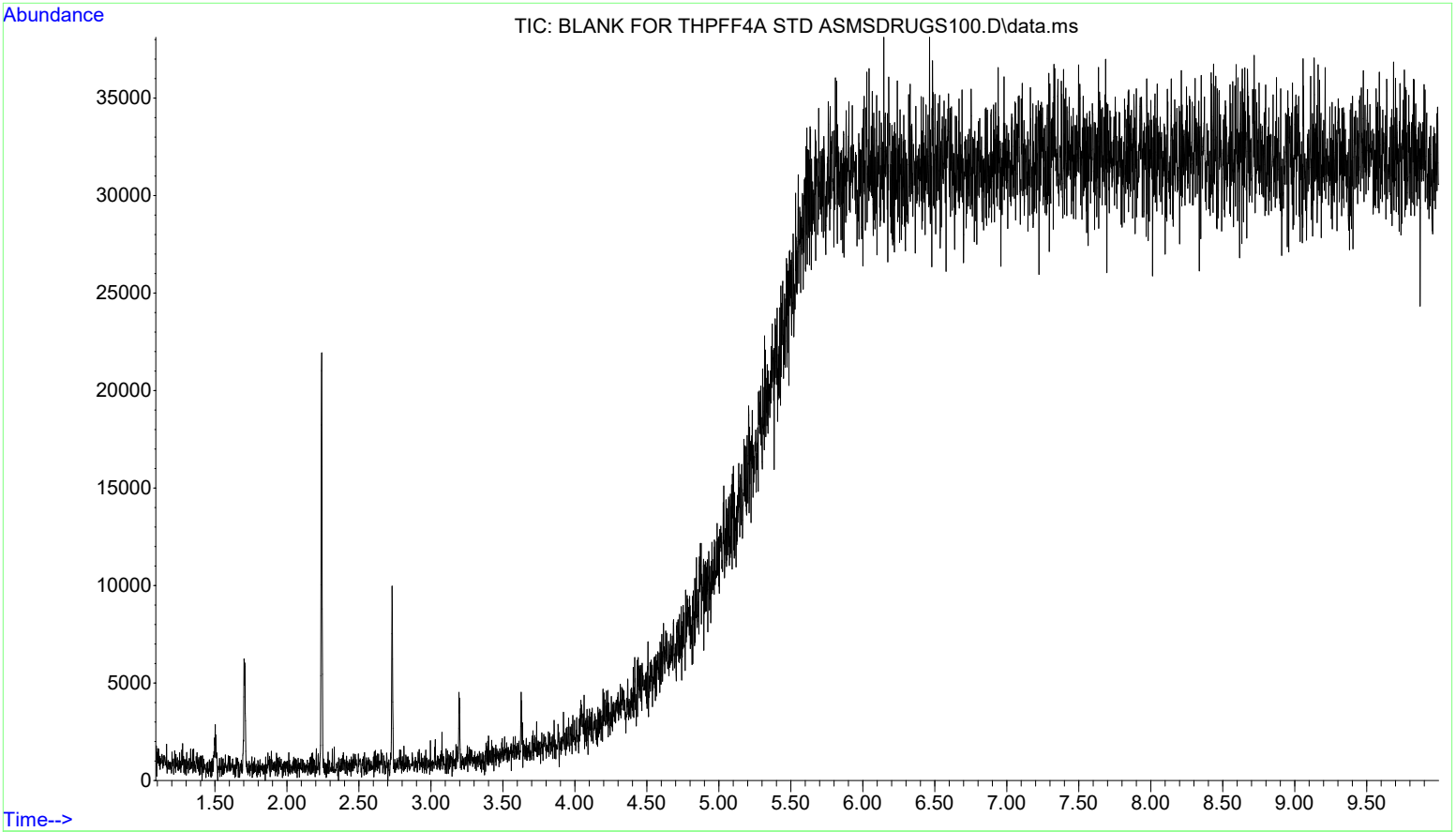


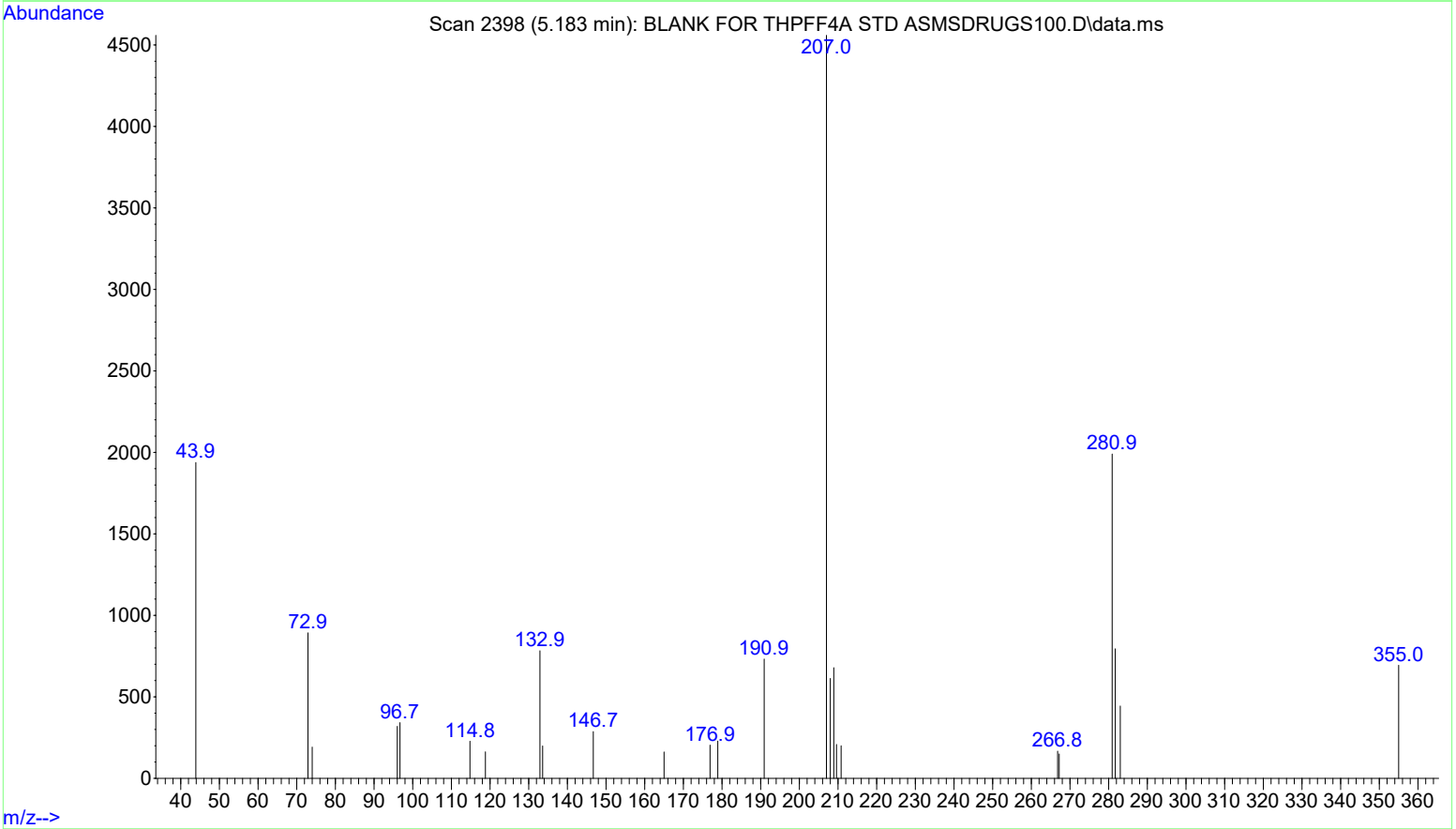


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR THPFF4A STD ASMSDRUGS100.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 12:51 using AcqMethod ASMSDRUGS100.M
Sample Name: BLANK FOR THPFF4A STD
Misc Info : METHANOL

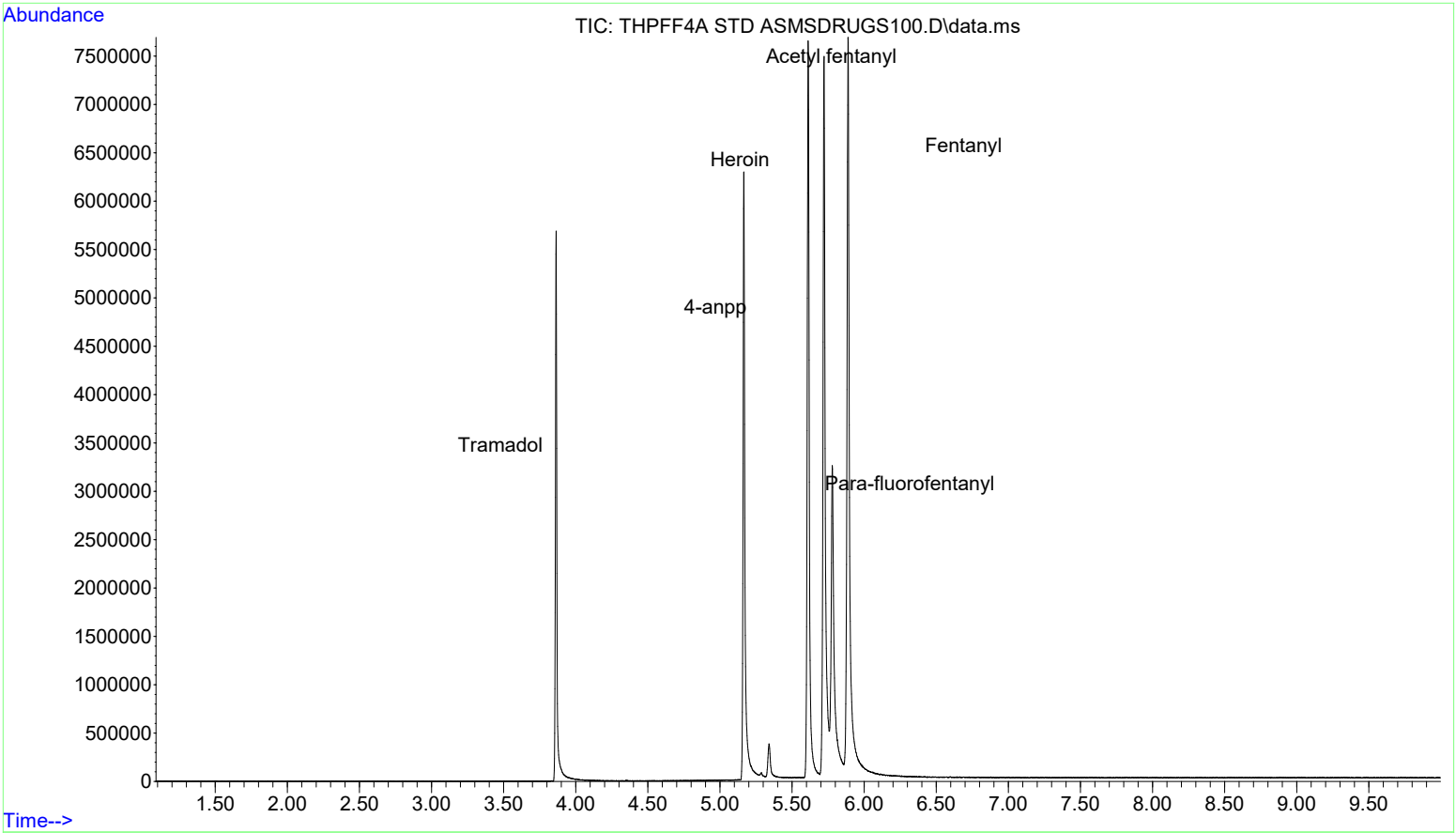


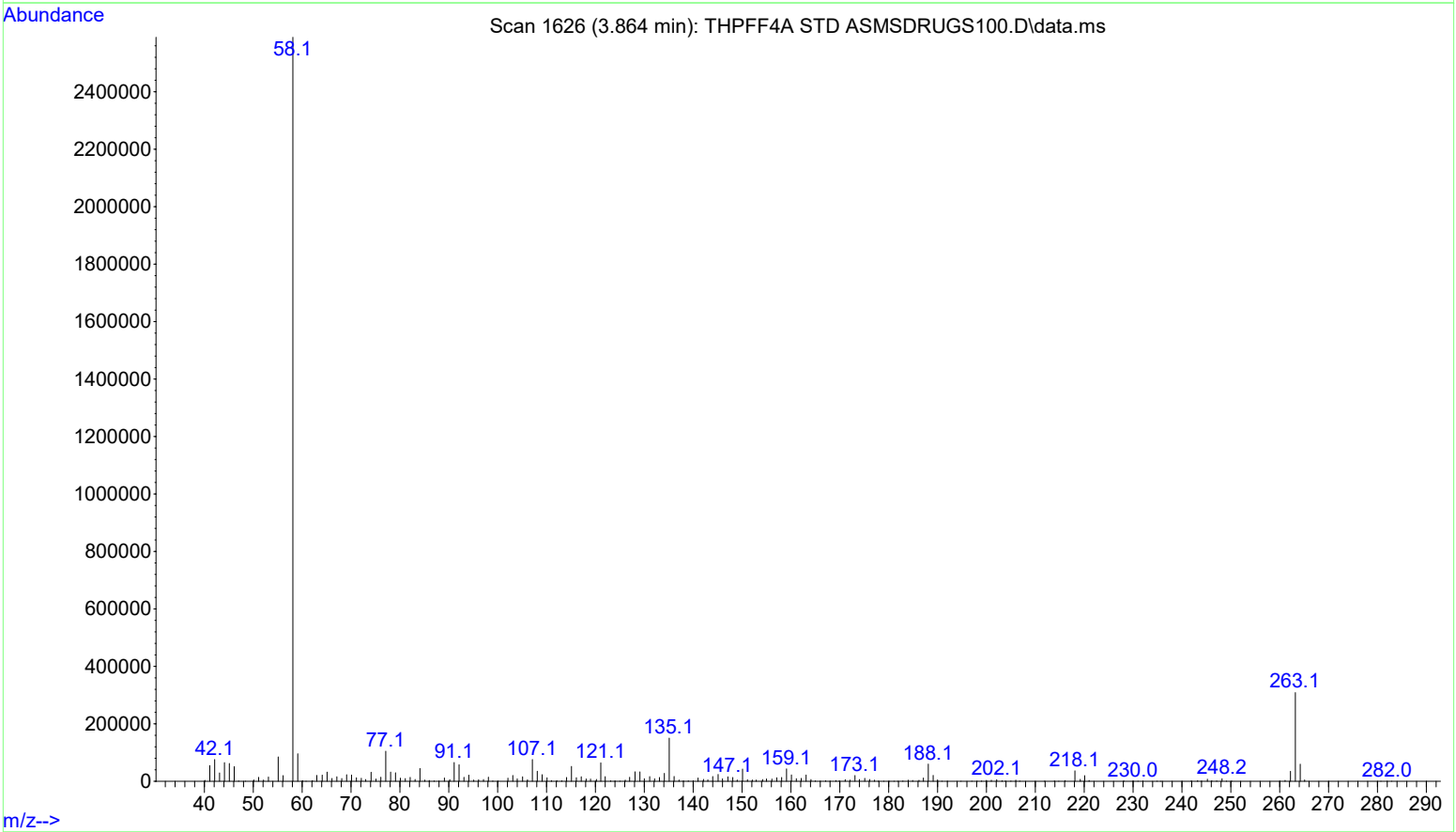


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS100.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:05 using AcqMethod ASMSDRUGS100.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

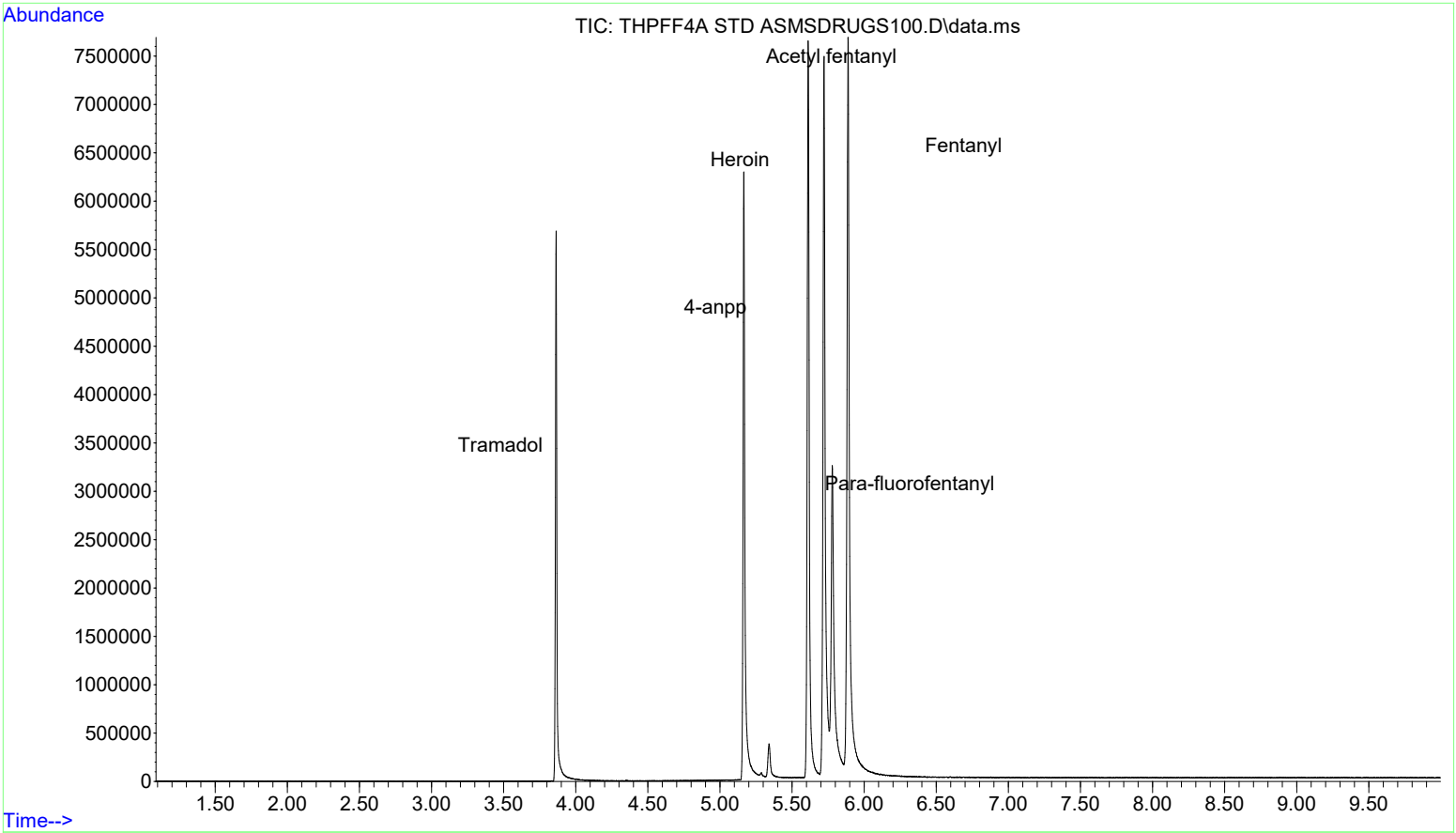


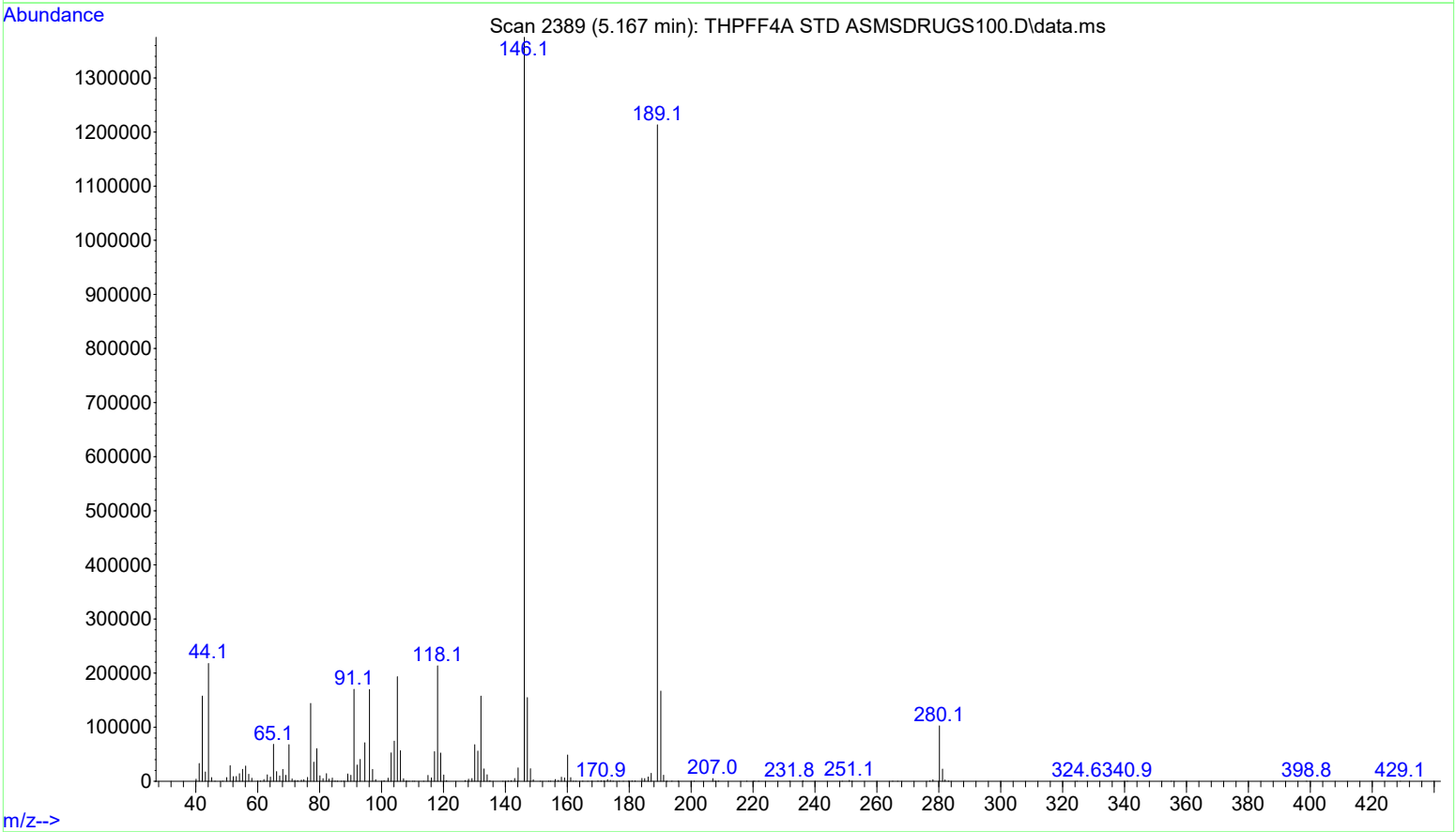


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS100.D

BH
3-11-23

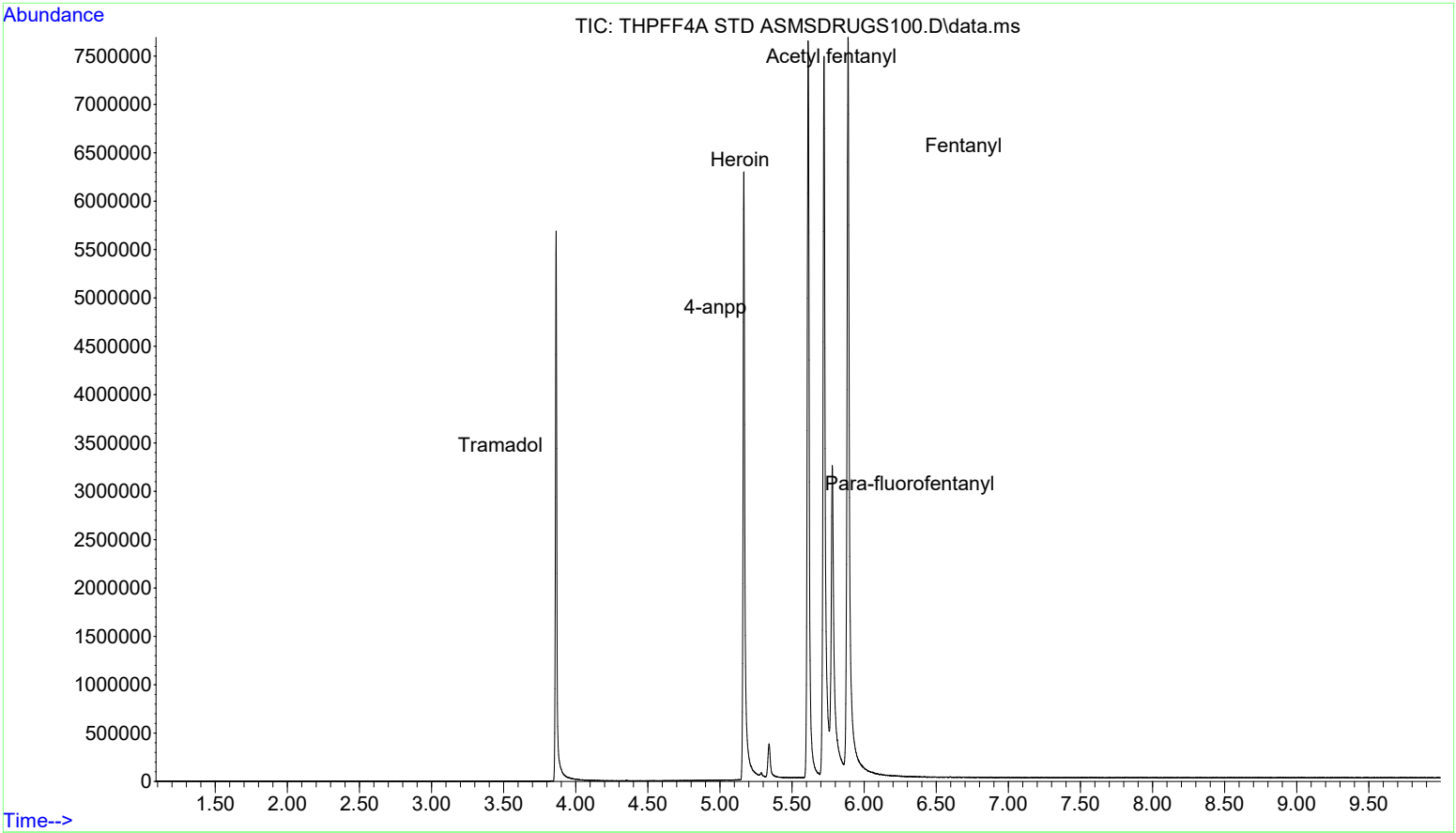
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:05 using AcqMethod ASMSDRUGS100.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

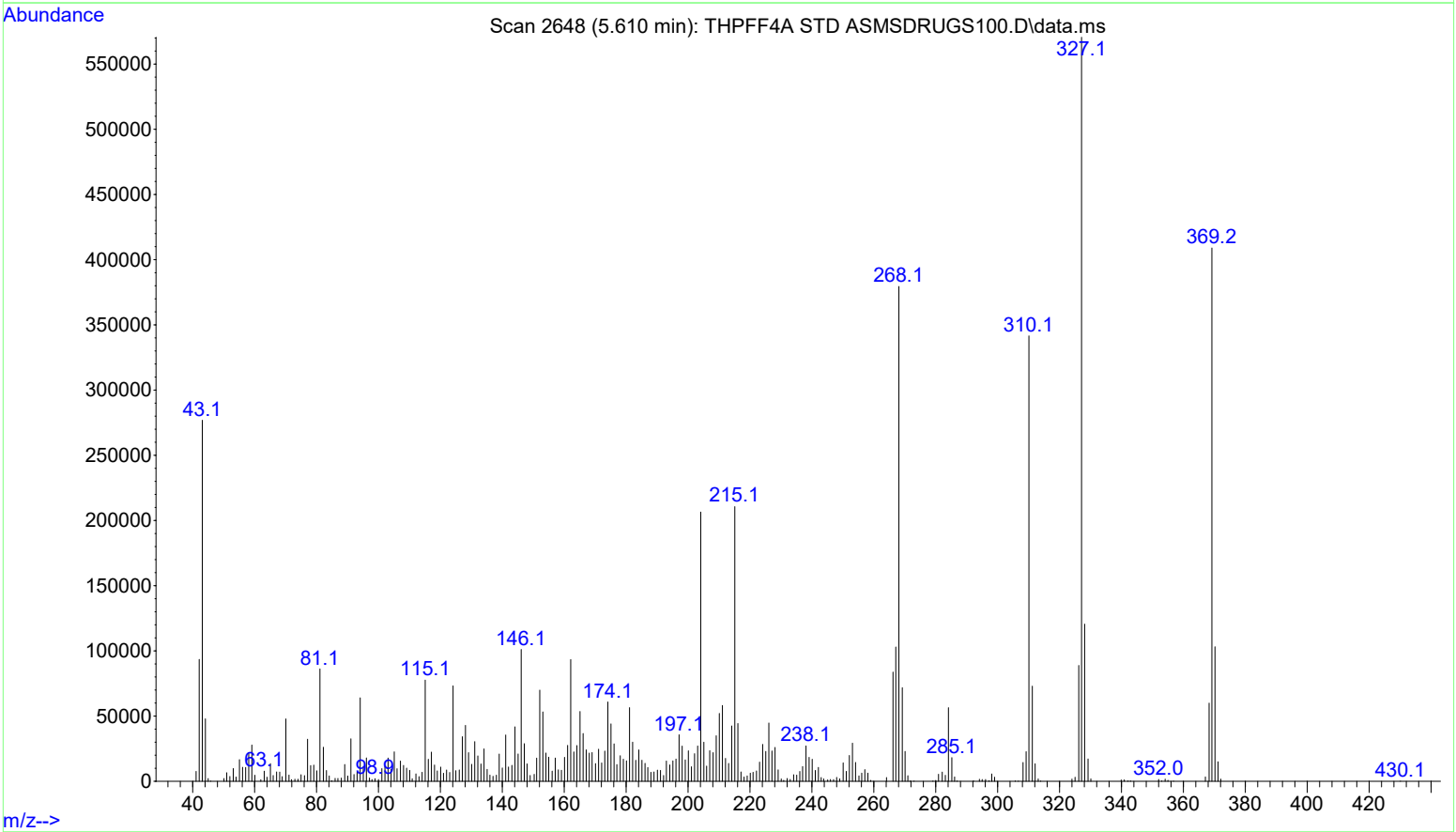




File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS100.D
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:05 using AcqMethod ASMSDRUGS100.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

BH
3-11-23

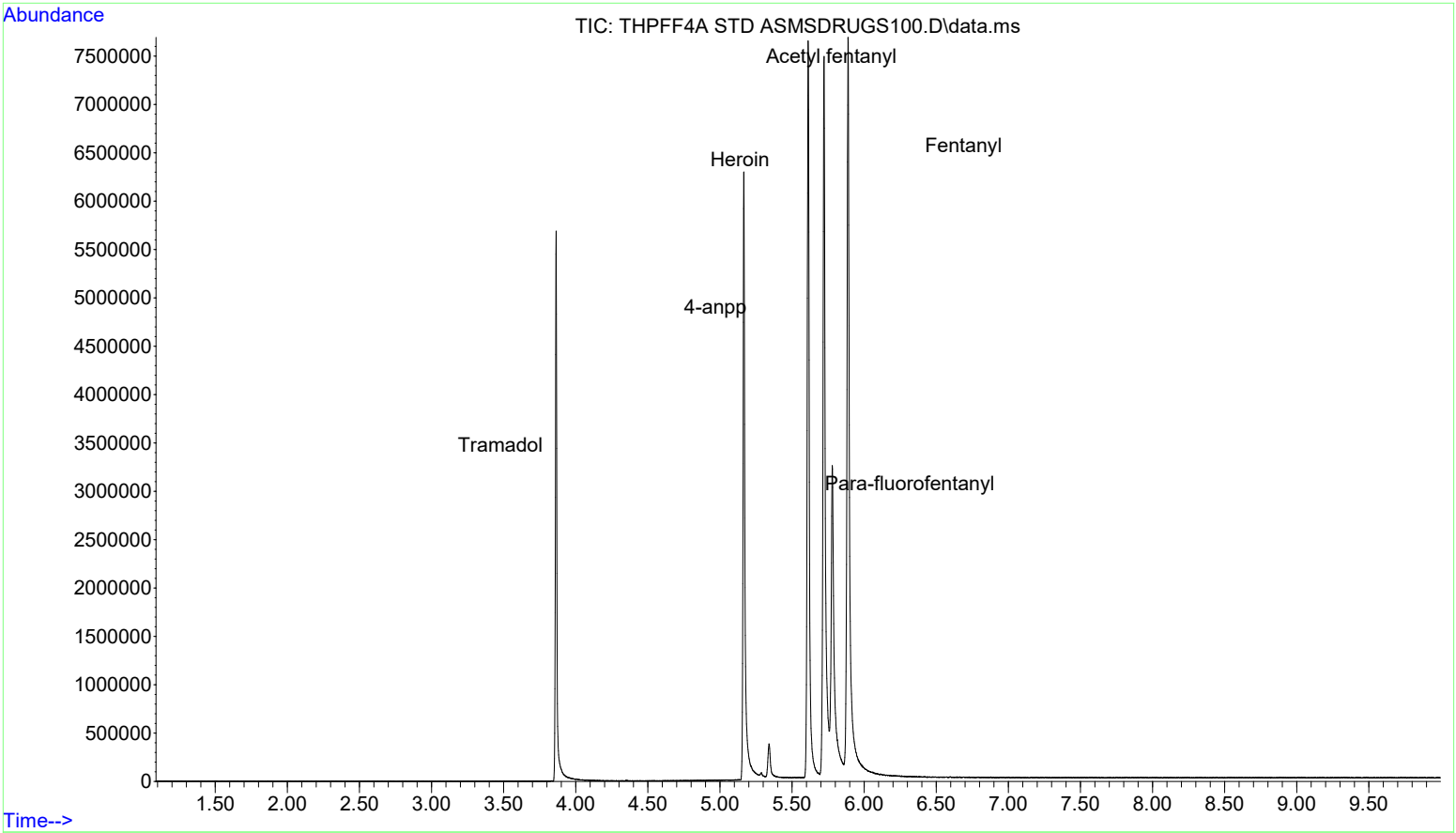


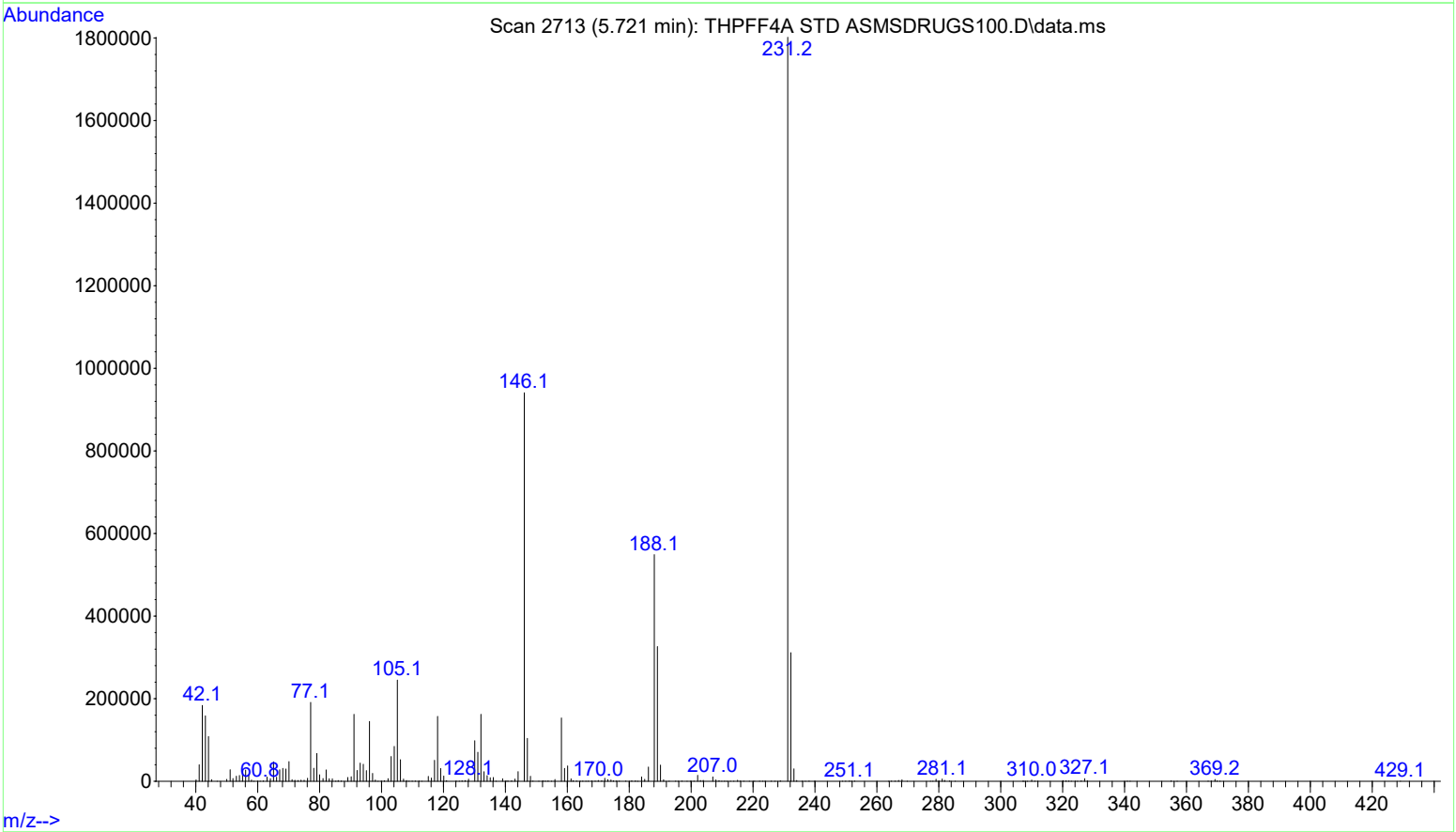


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS100.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:05 using AcqMethod ASMSDRUGS100.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

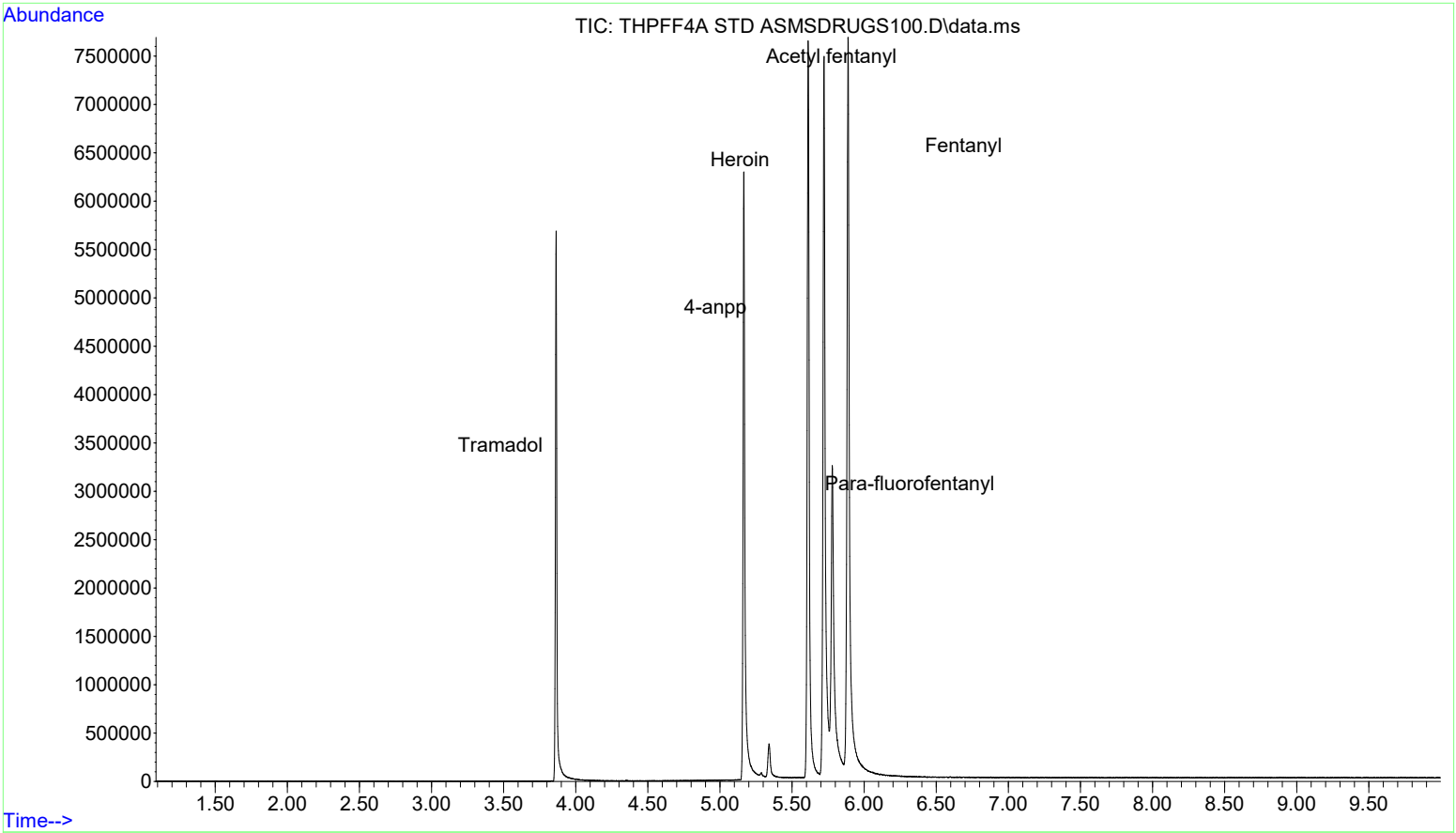


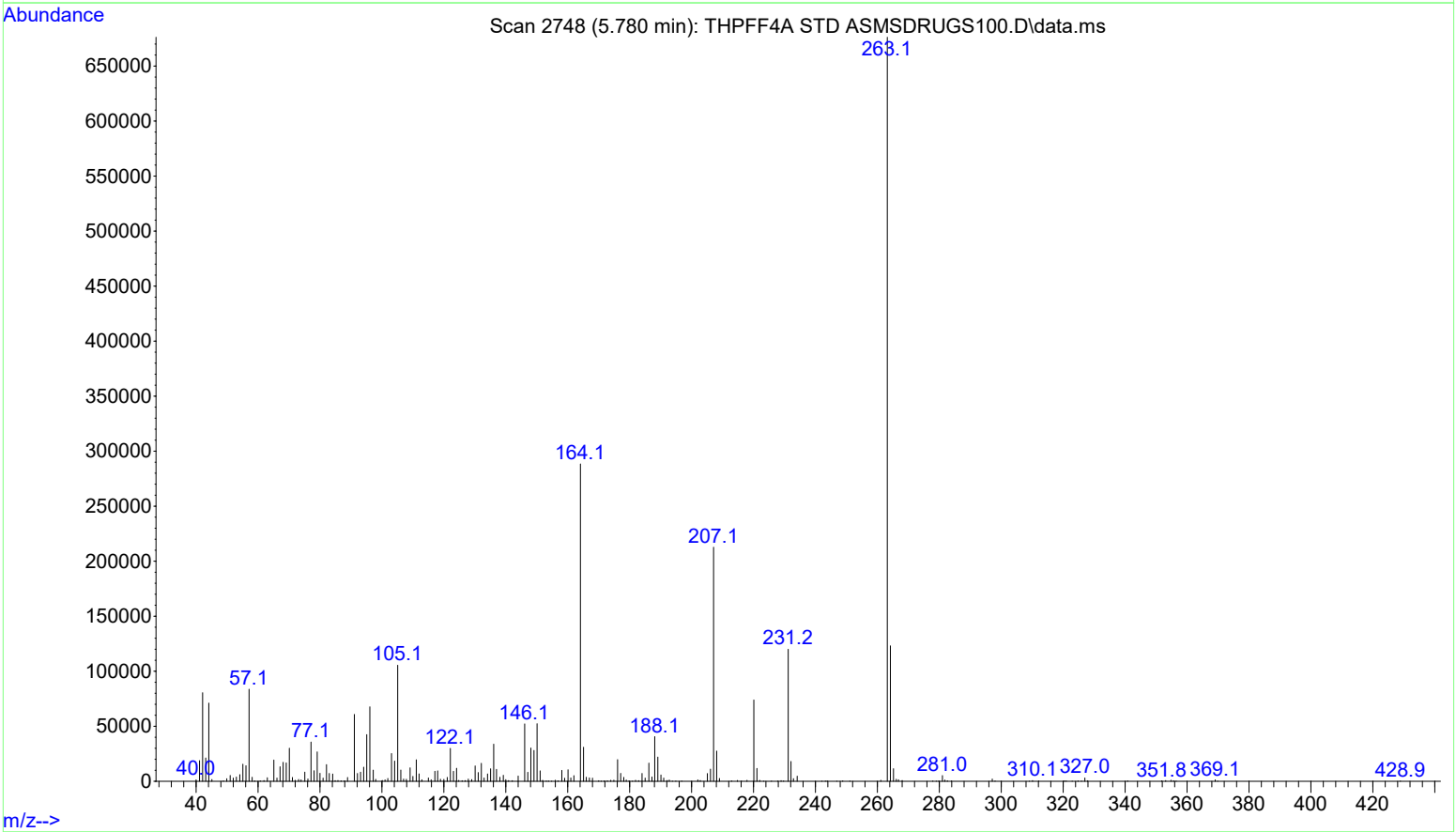


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS100.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:05 using AcqMethod ASMSDRUGS100.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

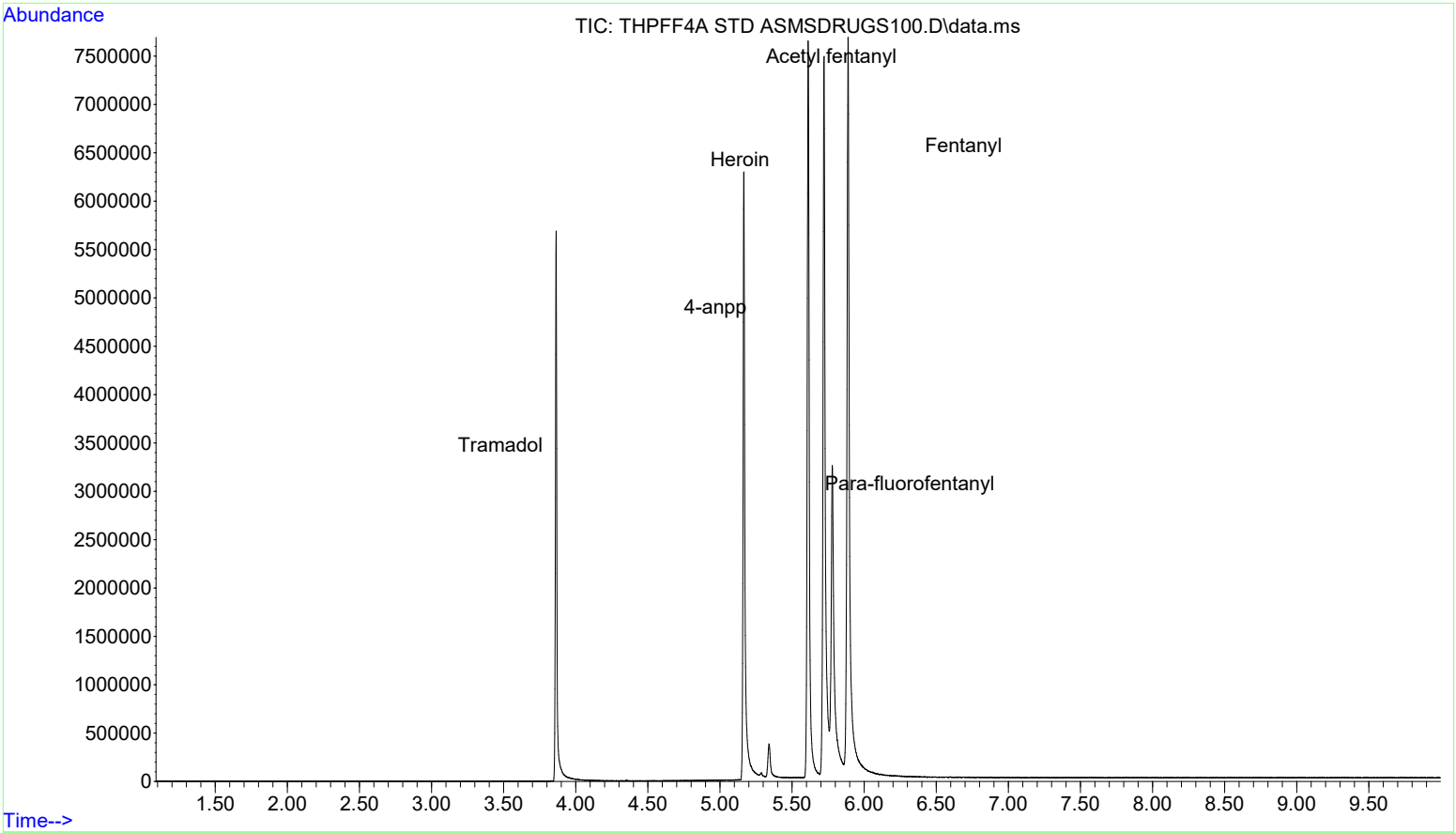


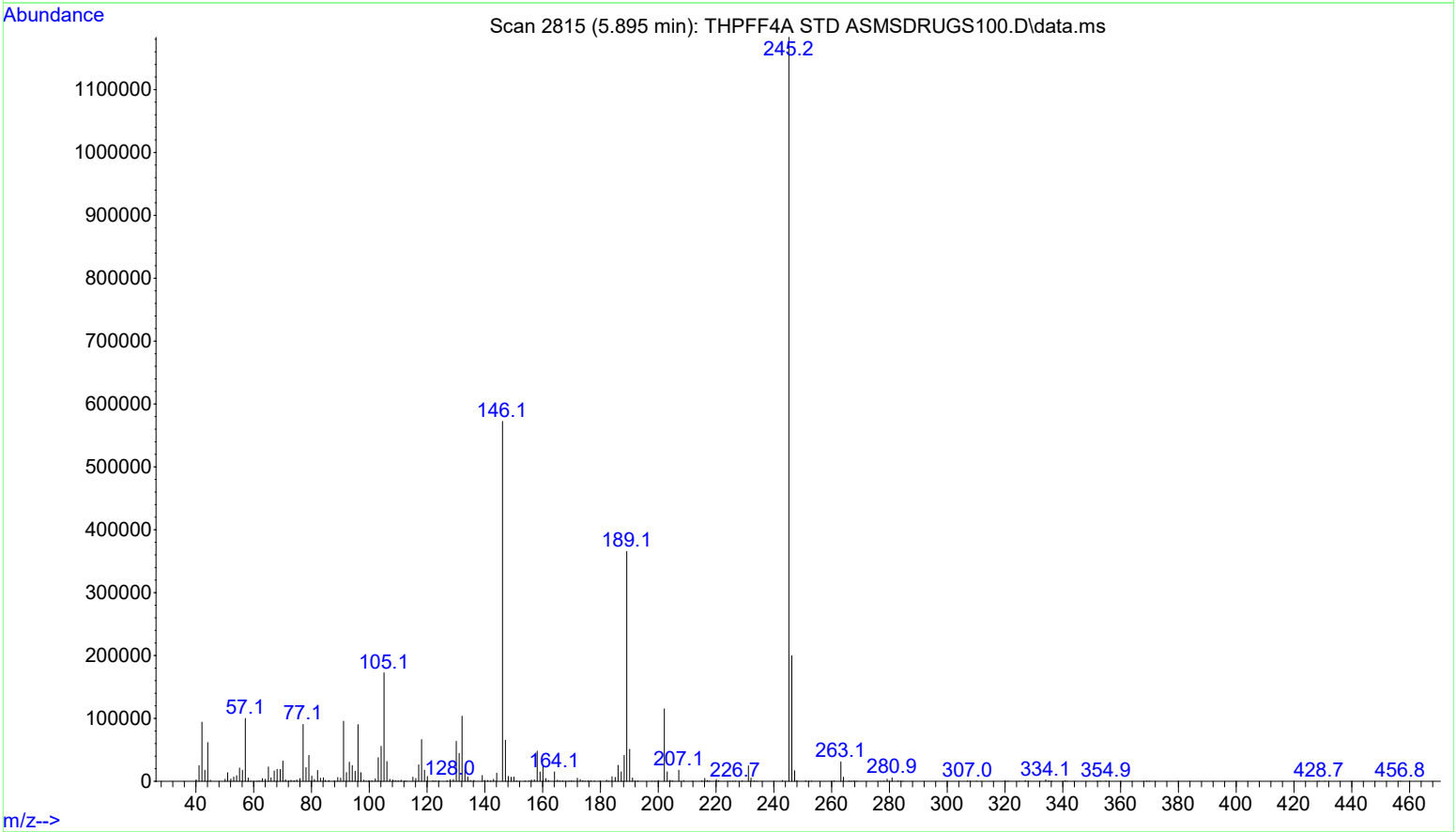


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS100.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 13:05 using AcqMethod ASMSDRUGS100.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL





Single Quadrupole Acquisition Method - MS Parameters Report

Method file	C:\MassHunter\GCMS\1\methods\ASMSDRUGS200.M
Tune file	atune.u
Ion source	EI
Source temperature (°C)	230
Quad temperature (°C)	150
Fixed Electron energy (eV)	70.0
Acquisition Type	Scan
Stop time (min)	650.00
Solvent delay (min)	1.00
Trace Ion Detection	False
Gain Factor	10
EM Saver	False
EM Saver Limit	N/A

Scan Time Segments

Time	Start Mass	End Mass	Threshold	Scan Speed
1.00	40	550	150	6,250 [N=0]

Timed Events

Time	Type of Event	Parameter

Real-Time Plots

Type of Plot	Label	Low Mass	High Mass
Total Ion	N/A	N/A	N/A

Self-Cleaning Ion Source Parameters

Mode	No Cleaning

METHOD CONTROL PARAMETERS

BH
3-11-23

Method Information for: C:\MassHunter\GCMS\1\methods\ASMSDRUGS200.M

Method Sections To Run:

( ) Save Copy of Method With Data
( ) Instrument Control Pre-Run Cmd/Macro =
( ) Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
(X) Data Analysis
( ) Instrument Control Post-Run Cmd/Macro =
( ) Data Analysis Post-Run Cmd/Macro =

Method Comments:
ASMSDRUGS200

END OF METHOD CONTROL PARAMETERS

C:\MassHunter\GCMS\1\methods\ASMSDRUGS200.M
Fri Mar 10 21:59:33 2023

Control Information
------- -----------

Sample Inlet : GC
Injection Source : GC ALS
Injection Location: Front
Mass Spectrometer : Enabled

No Sample Prep method has been assigned to this method.

GC
GC Summary

Run Time	10.003 min
Post Run Time	0 min

Oven
Temperature

Setpoint	On
(Initial)	200 °C
Hold Time	1 min
Post Run	200 °C
Program	
#1 Rate	70 °C/min
#1 Value	280 °C
#1 Hold Time	7.86 min
Equilibration Time	1.5 min
Max Temperature	325 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled

ALS
Front Injector

Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	1
Sample Wash Volume	4 µL
Sample Pumps	2
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	6000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	6000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL

Solvent Wash Mode	A, B

BH
3-11-23

Back Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	0
Solvent A Washes (PostInj)	0
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	0
Solvent B Washes (PostInj)	0
Solvent B Volume	8 µL
Sample Washes	0
Sample Wash Volume	8 µL
Sample Pumps	6
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL
Solvent Wash Mode	A, B

Sample Overlap	
Mode	Sample overlap is not enabled

ALS Errors	Pause for user interaction

Front SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 16.435 psi
Total Flow	On 79 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	On 30 After 3 min mL/min
Split Ratio	75 :1
Split Flow	75 mL/min
Liner	A Liner has not been selected.

Back SS Inlet He	
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***
Mode	Split
Heater	On 250 °C
Pressure	On 5.1078 psi
Total Flow	On 104 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	Off
Split Ratio	100 :1
Split Flow	100 mL/min
Liner	A Liner has not been selected.

Thermal Aux 3 (MSD Transfer Line)	
Temperature	
Setpoint	On
(Initial)	280 °C

Column
Column #1
Flow

Setpoint	On
(Initial)	1 mL/min
Post Run	0.57353 mL/min

BH
3-11-23

Column Information	Agilent 19091S-602
HP-1MS	
Temperature Range	-60 °C—325 °C (350 °C)
Dimensions	12.5 m x 200 µm x 0.33 µm (Calibrated)
Column lock	Locked
In	Front SS Inlet He
Out	MSD
(Initial)	200 °C
Pressure	16.435 psi
Flow	1 mL/min
Average Velocity	60.011 cm/sec
Holdup Time	0.34716 min
Control Mode	Constant Flow

Column #2	
Flow	
Setpoint	On
(Initial)	1 mL/min
Post Run	2.2354 mL/min

Column Information	Agilent 19091S-913
HP-1MS	
Temperature Range	-60 °C—325 °C (325 °C)
Dimensions	15 m x 320 µm x 0.25 µm (Calibrated)
Column lock	Locked
In	Back SS Inlet He
Out	Back Detector FID
(Initial)	200 °C
Pressure	5.1078 psi
Flow	1 mL/min
Average Velocity	27.902 cm/sec
Holdup Time	0.896 min
Control Mode	Constant Flow

Column Outlet Pressure	0 psi

Back Detector FID	
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***
Makeup	He
Column Compensation	Signal is modified by Column Compensation Curve #2
Heater	On 300 °C
H2 Flow	Off
Air Flow	Off
Makeup Flow	On 25 mL/min
Carrier Gas Flow Correction	Constant Makeup and Fuel Flow
Flame	Off

Aux EPC 1,2,3	
Aux EPC 1 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Aux EPC 2 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi

Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State*** BH 3-11-23

Aux EPC 3 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Signals

Signal #1: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Front Sample
Signal #2: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample
Signal #3: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample
Signal #4: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

TUNE PARAMETERS for SN: US1648M021

Trace Ion Detection is OFF.

34.593	:	EMISSION
70.007	:	ENERGY
34.899	:	REPELLER
90.331	:	IONFOCUS
22.672	:	ENTRANCE_LENS
1360.190	:	EMVOLTS
1498.6	:	Actual EMV
1.00	:	GAIN FACTOR
2908.000	:	AMUGAIN
136.750	:	AMUOFFSET
1.000	:	FILAMENT
0.000	:	DCPOLARITY
12.032	:	ENTLENSOFFSET
0.000	:	Ion_Body
0.000	:	EXTLENS
442.000	:	MASSGAIN

-22.000 : MASSOFFSET

END OF TUNE PARAMETERS

BH
3-11-23

END OF INSTRUMENT CONTROL PARAMETERS

DATA ANALYSIS PARAMETERS

Method Name: C:\MassHunter\GCMS\1\methods\ASMSDRUGS200.M

Percent Report Settings

Sort By: Signal

Output Destination
    Screen: No
    Printer: Yes
    File: No

Integration Events: AutoIntegrate

Generate Report During Run Method: No

Signal Correlation Window: 0.020

Qualitative Report Settings

Peak Location of Unknown: Apex

Library to Search	Minimum Quality
DEMO.L	0

Integration Events: AutoIntegrate

Report Type: Summary

Output Destination
    Screen: No
    Printer: Yes
    File: No

Generate Report During Run Method: No

Quantitative Report Settings

Report Type: Summary

Output Destination

Screen: Yes
Printer: No
File: No

BH
3-11-23

Generate Report During Run Method: No

Calibration Last Updated:

Reference Window: 10.00 Percent
Non-Reference Window: 5.00 Percent
Correlation Window: 0.02 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

Compound Information

*** Empty Quantitation Database ***

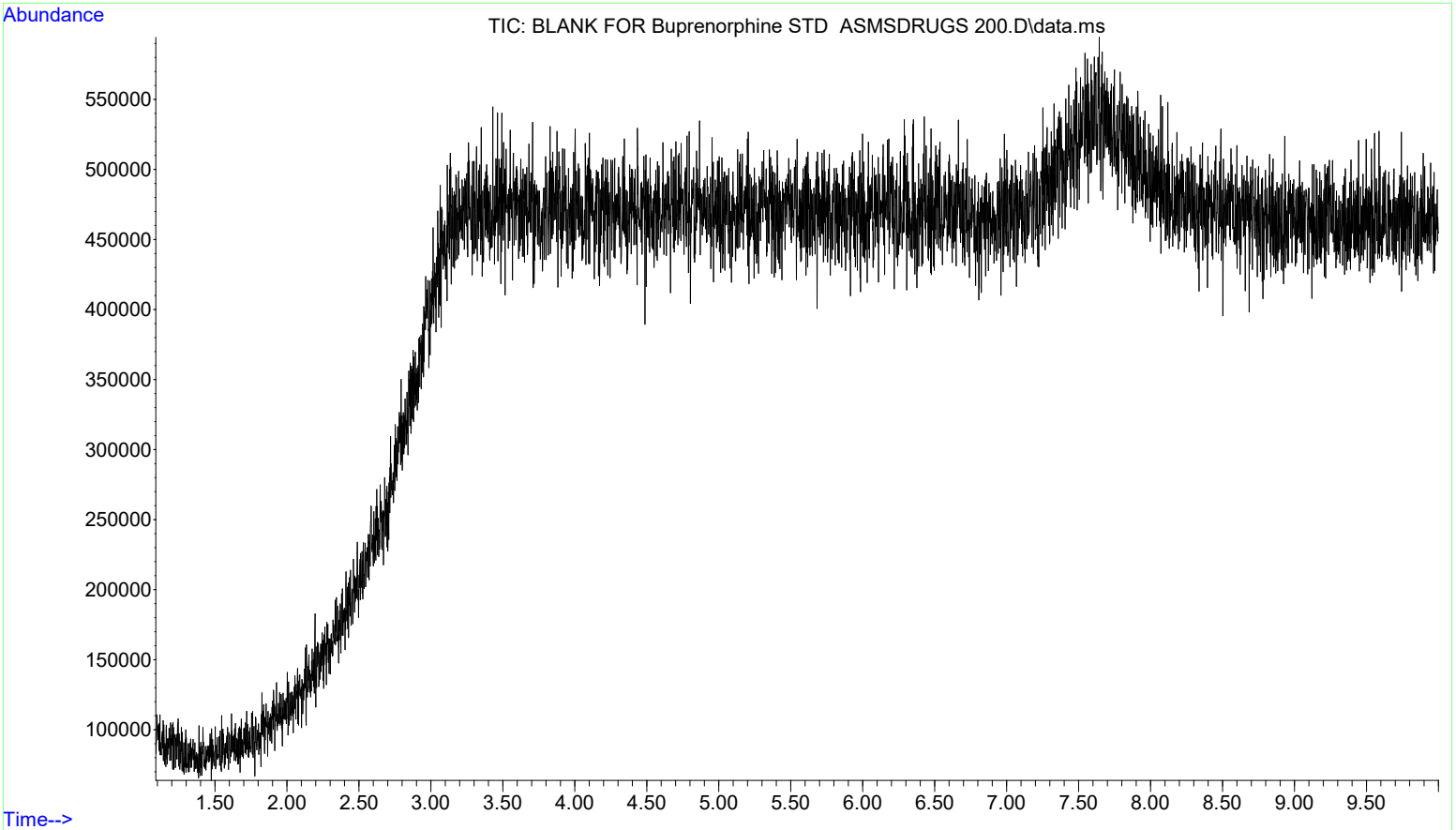
END OF DATA ANALYSIS PARAMETERS

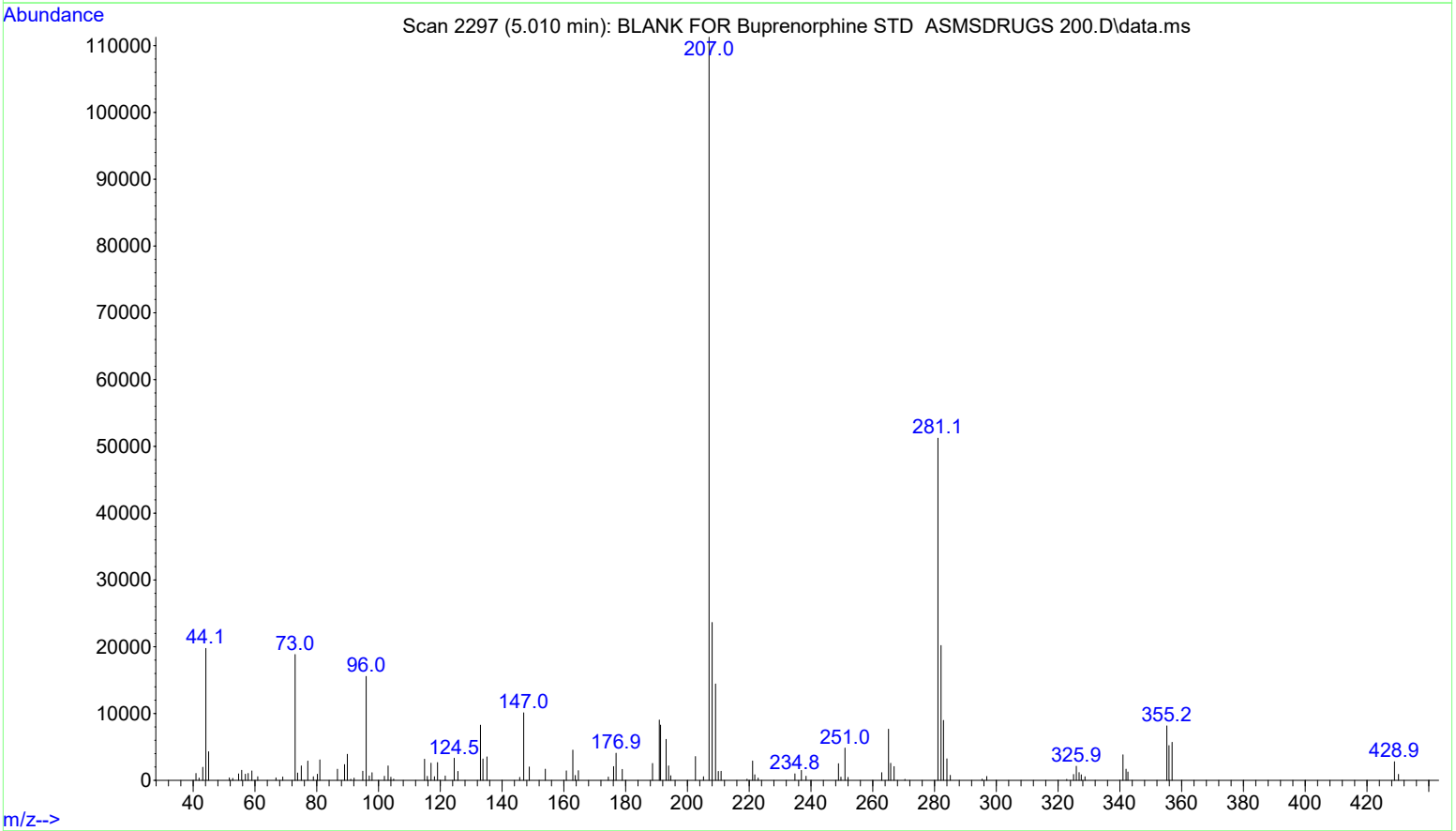
Fri Mar 10 22:00:00 2023

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR Buprenorphine STD ASMSDRUGS 200.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 18:03 using AcqMethod ASMSDRUGS200.M
Sample Name: BLANK FOR Buprenorphine STD ASMSDRUGS 200
Misc Info : METHANOL

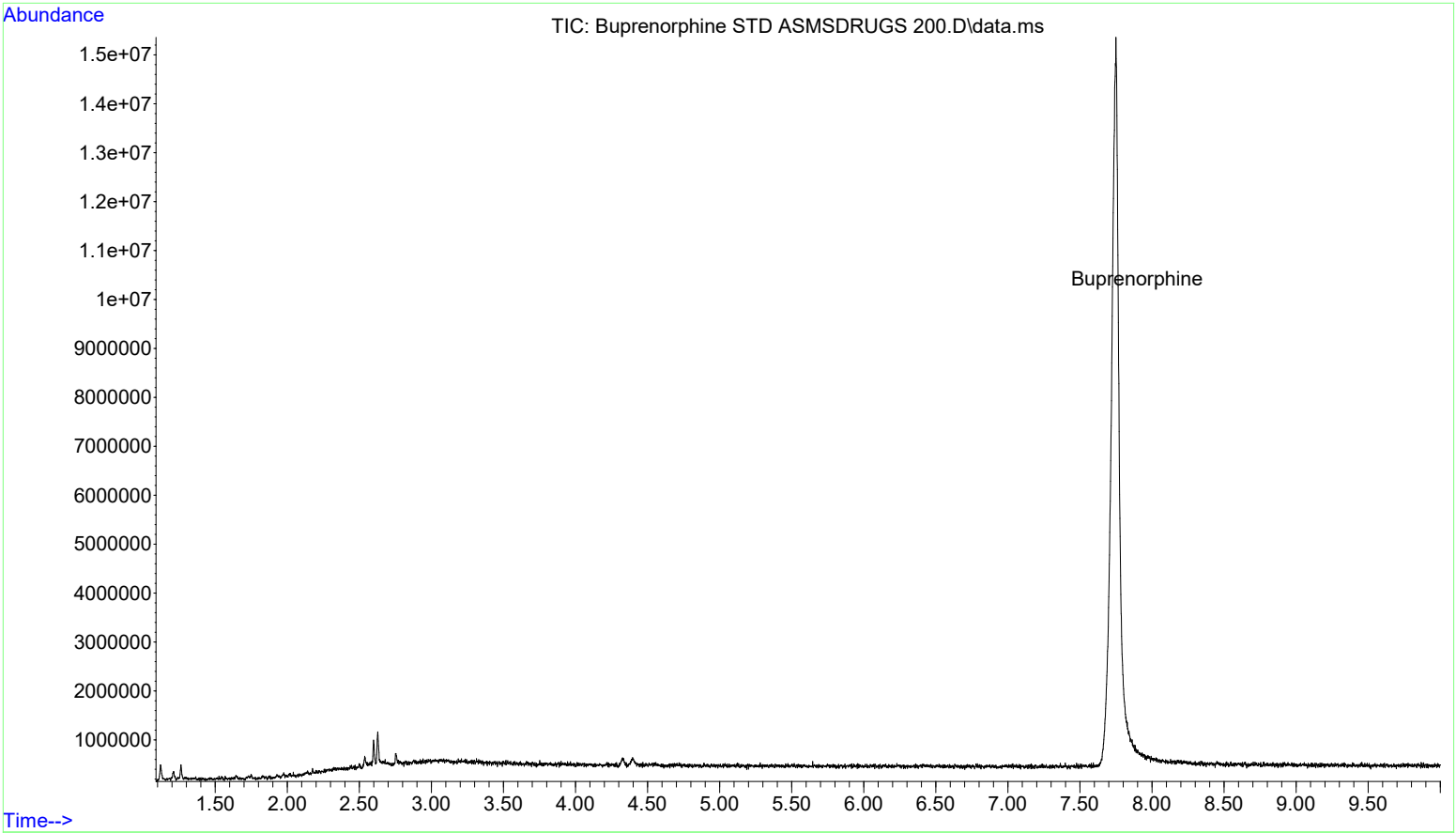


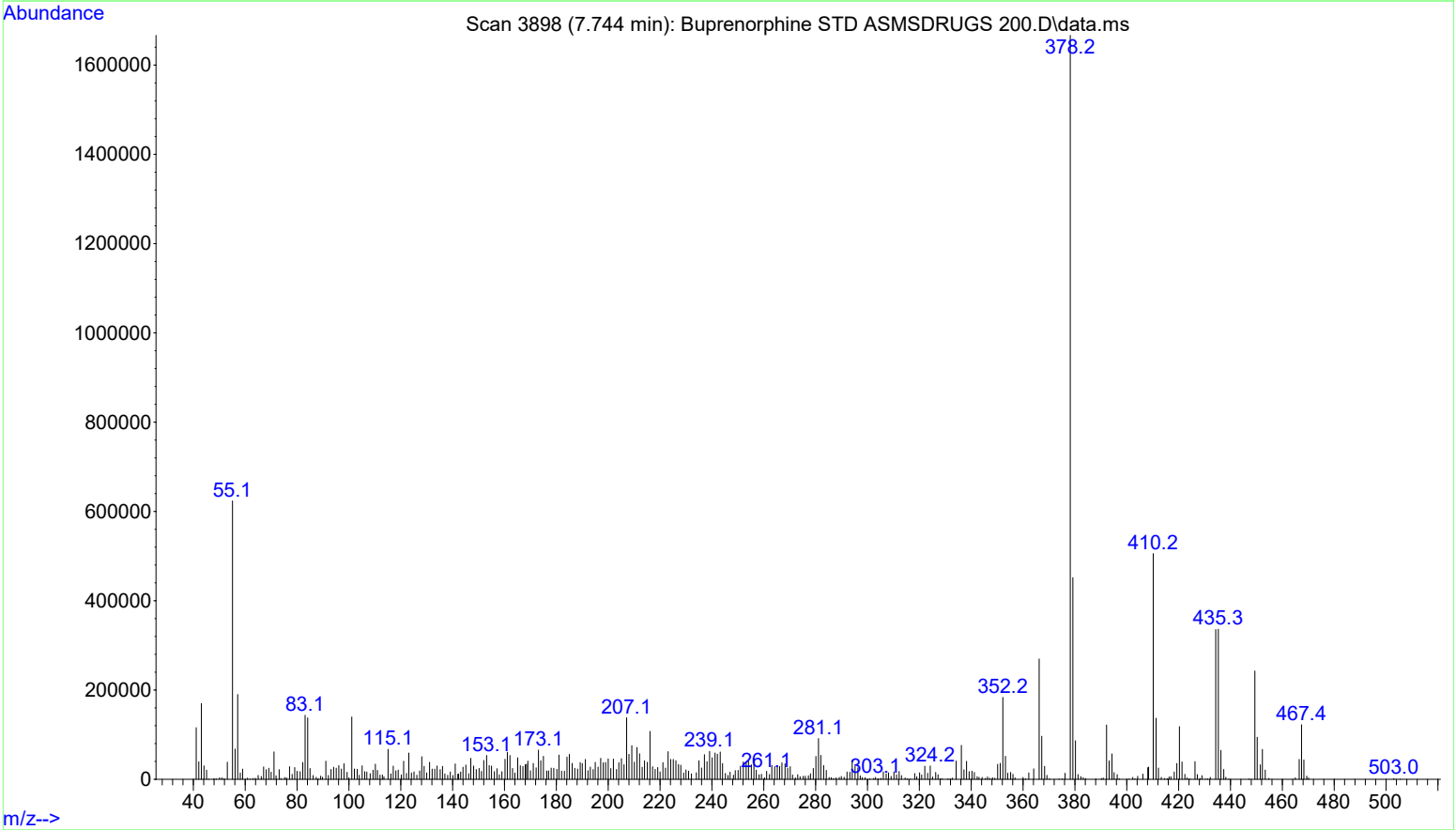


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\Bu
... prenorphine STD ASMSDRUGS 200.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 18:17 using AcqMethod ASMSDRUGS200.M
Sample Name: Buprenorphine STD EXP. 6-2024 ASMSDRUGS 200
Misc Info : METHANOL

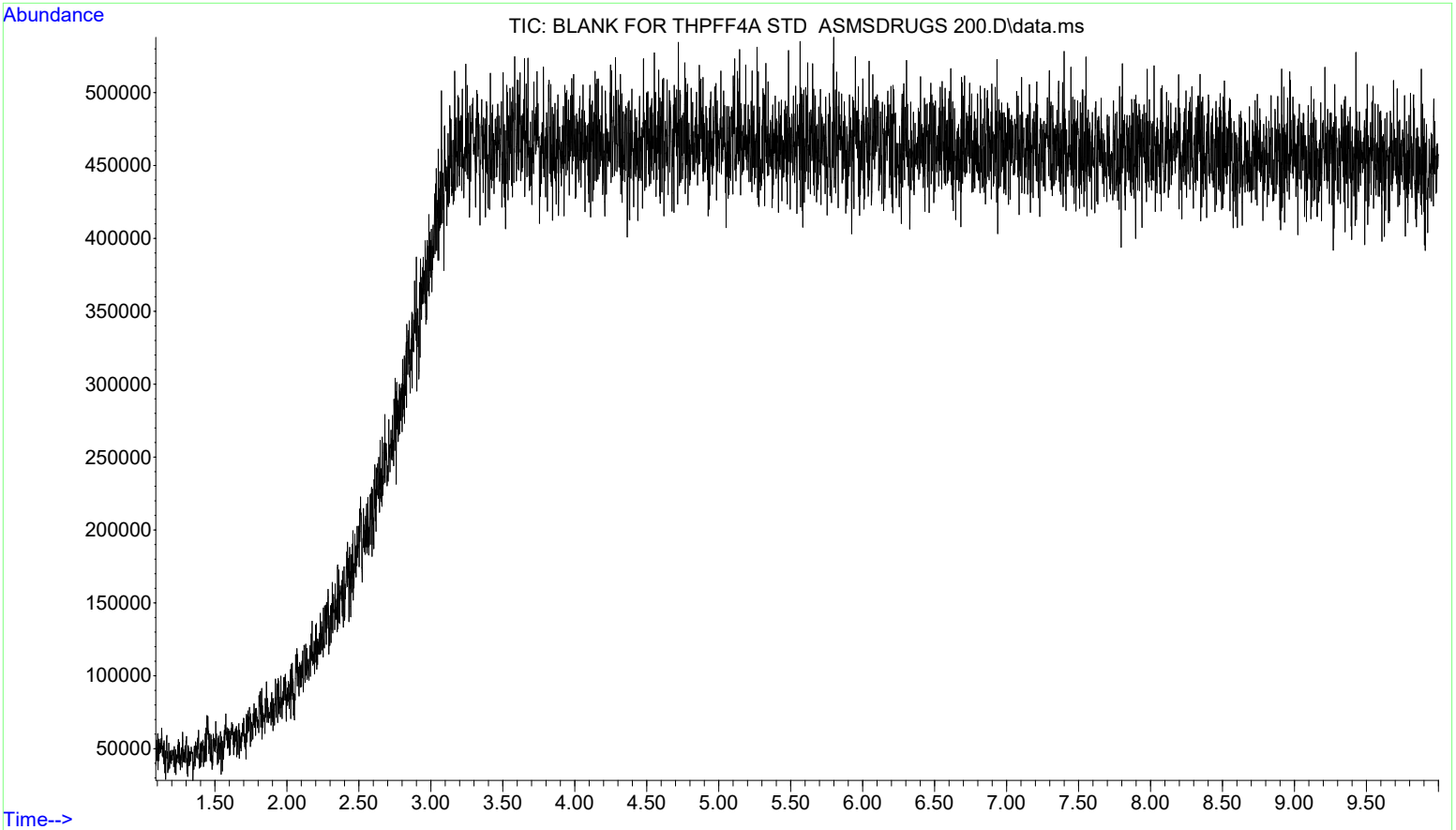


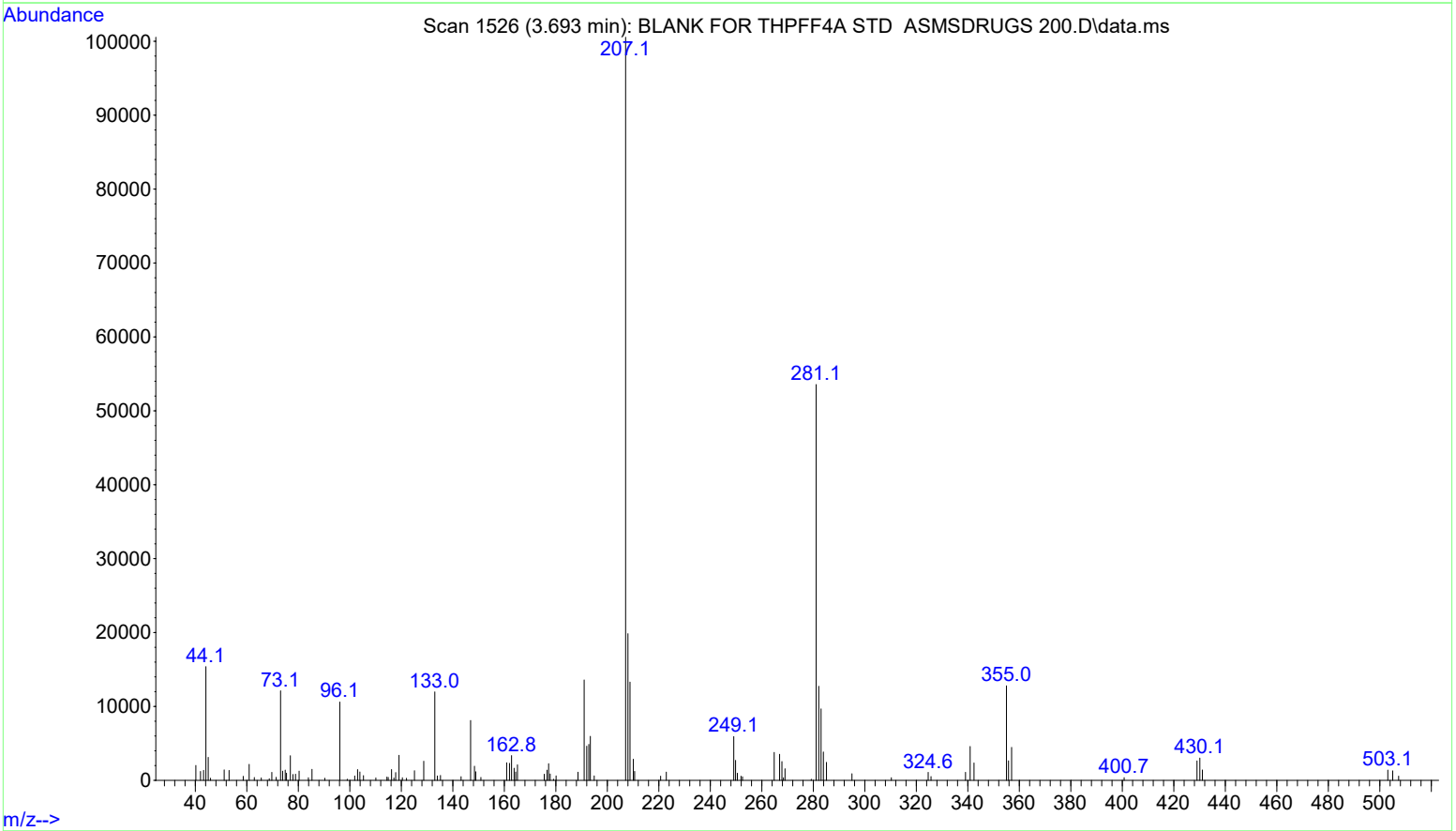


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR THPFF4A STD ASMSDRUGS 200.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 14:17 using AcqMethod ASMSDRUGS200.M
Sample Name: BLANK FOR THPFF4A STD asms 200
Misc Info : METHANOL

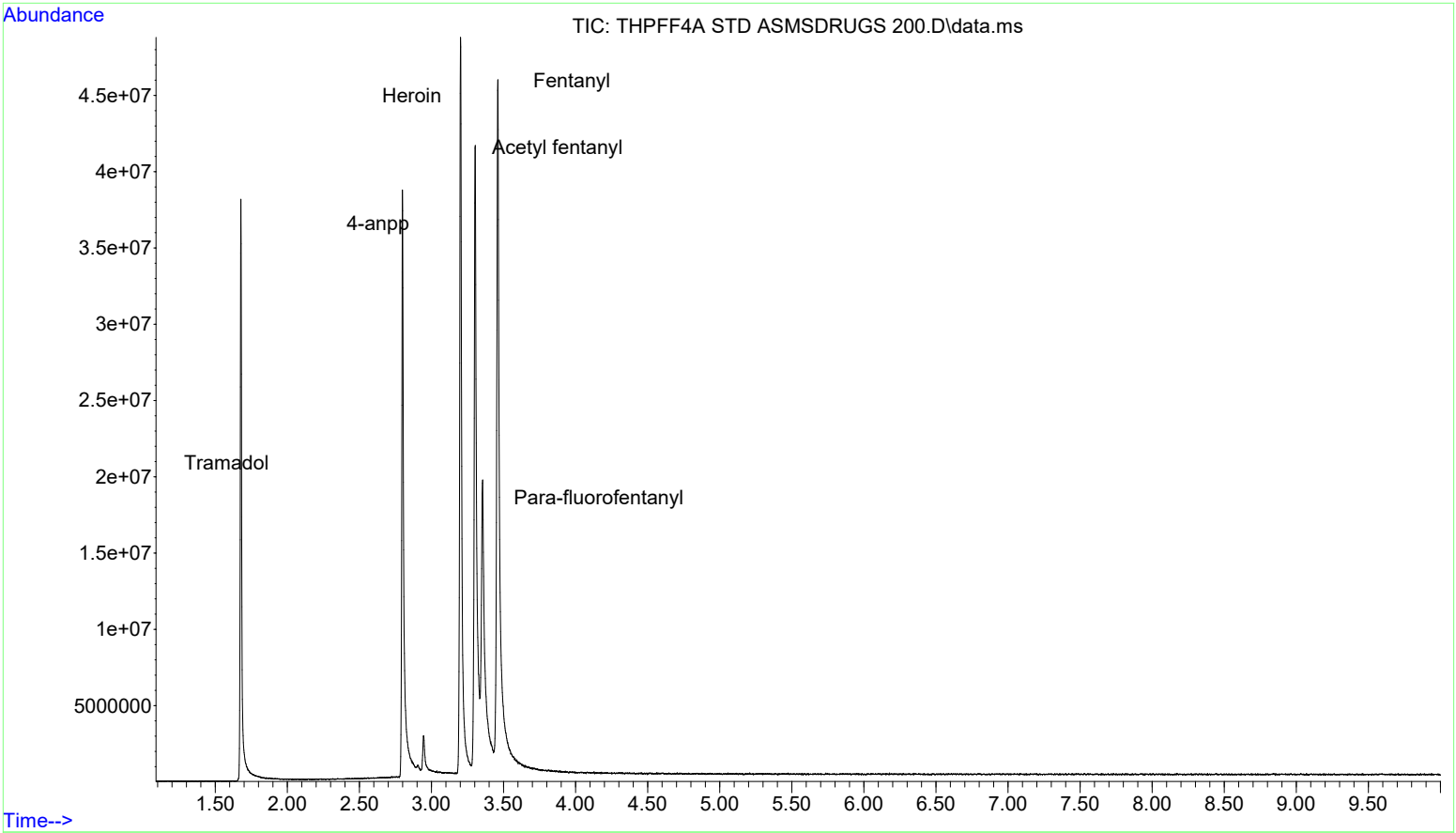


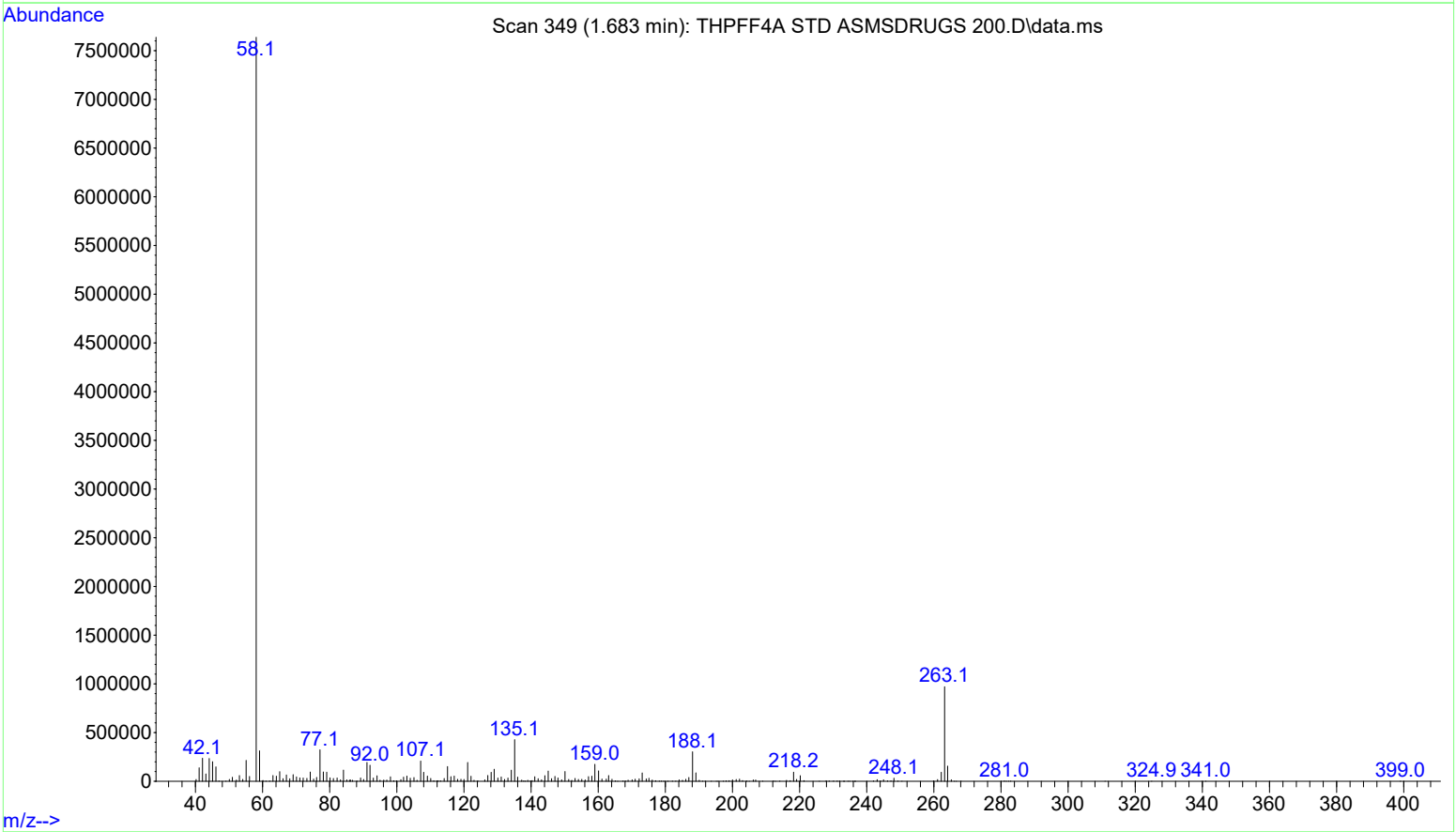


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 200.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 14:31 using AcqMethod ASMSDRUGS200.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

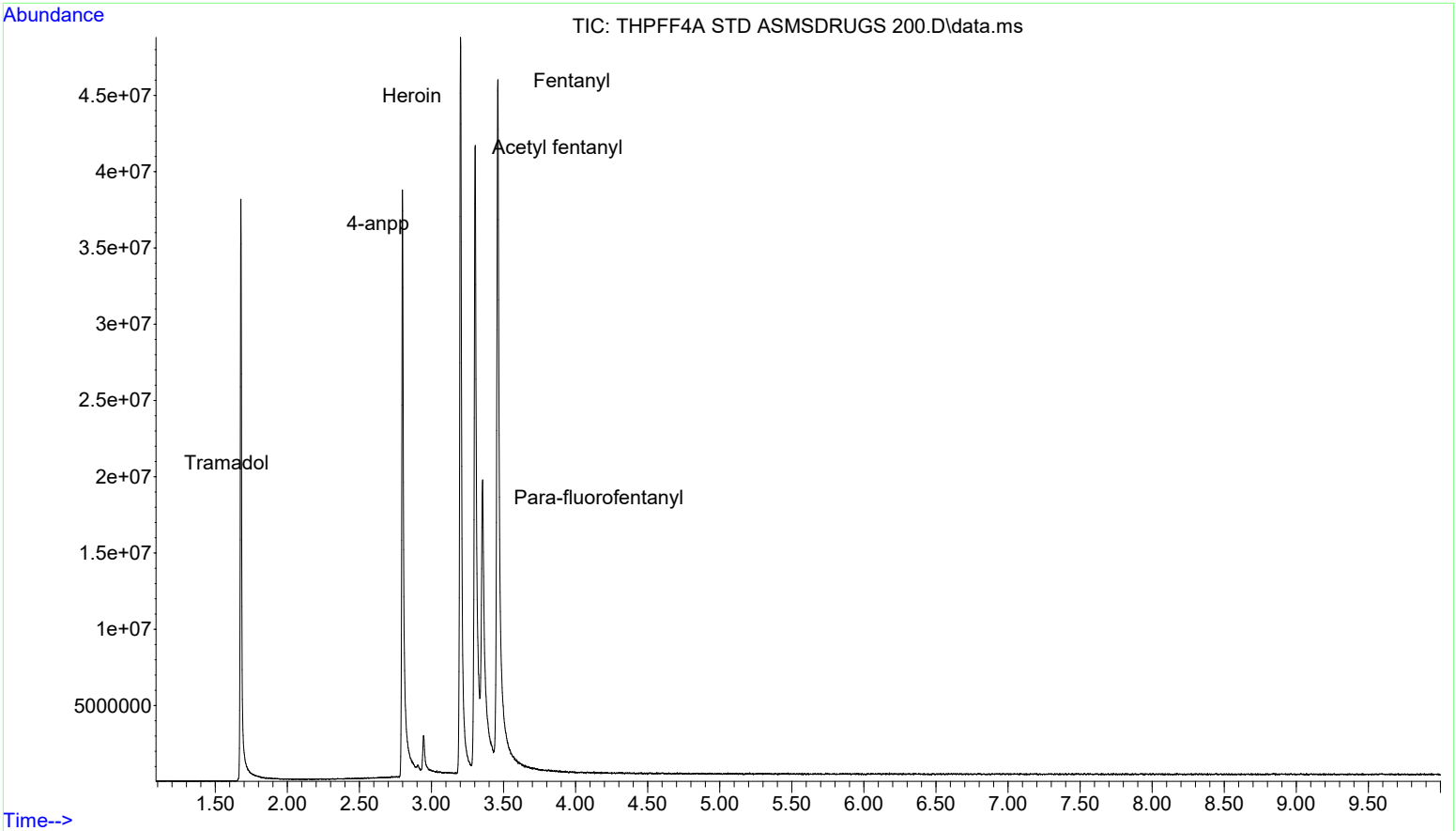


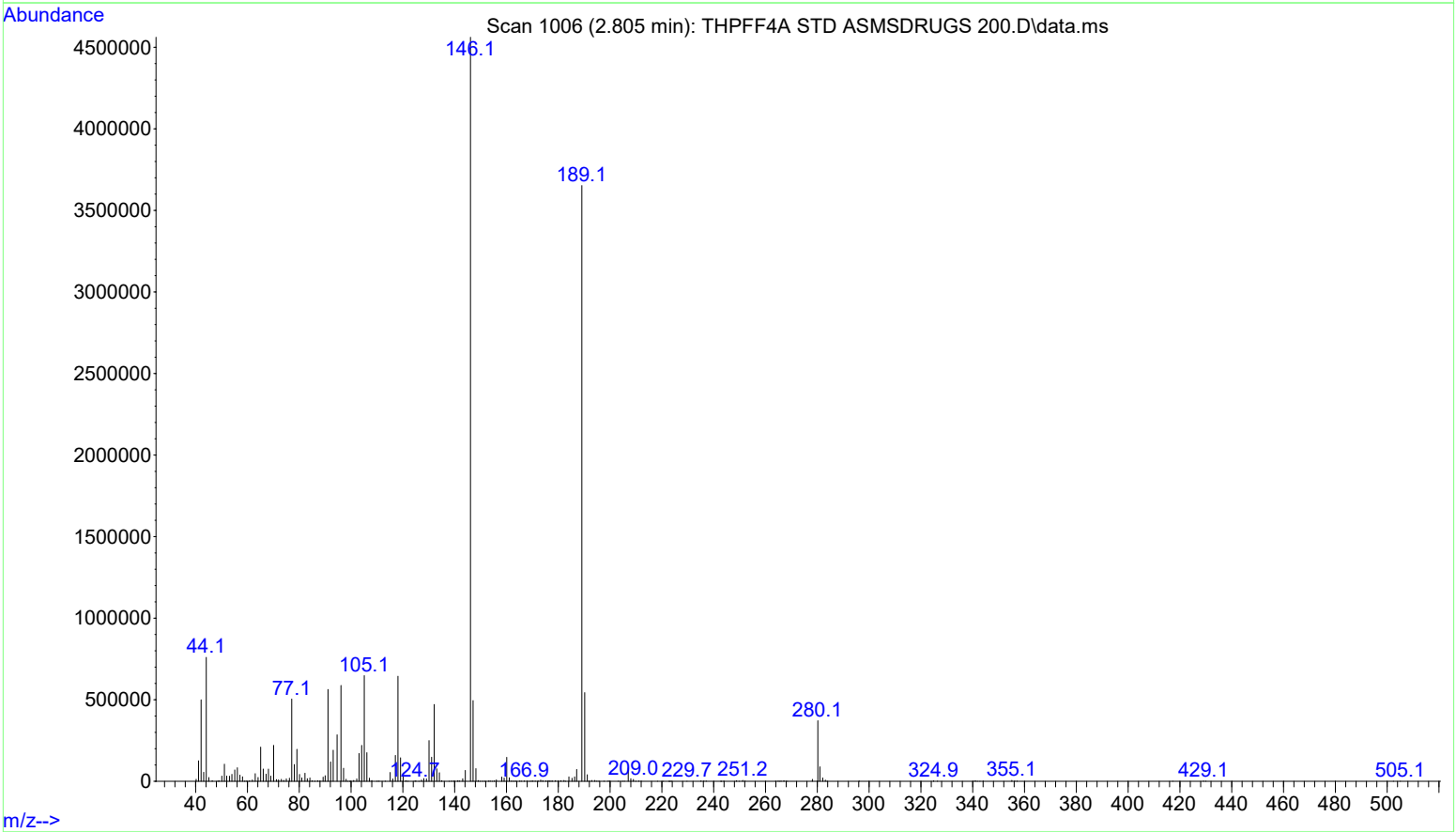


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 200.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 14:31 using AcqMethod ASMSDRUGS200.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

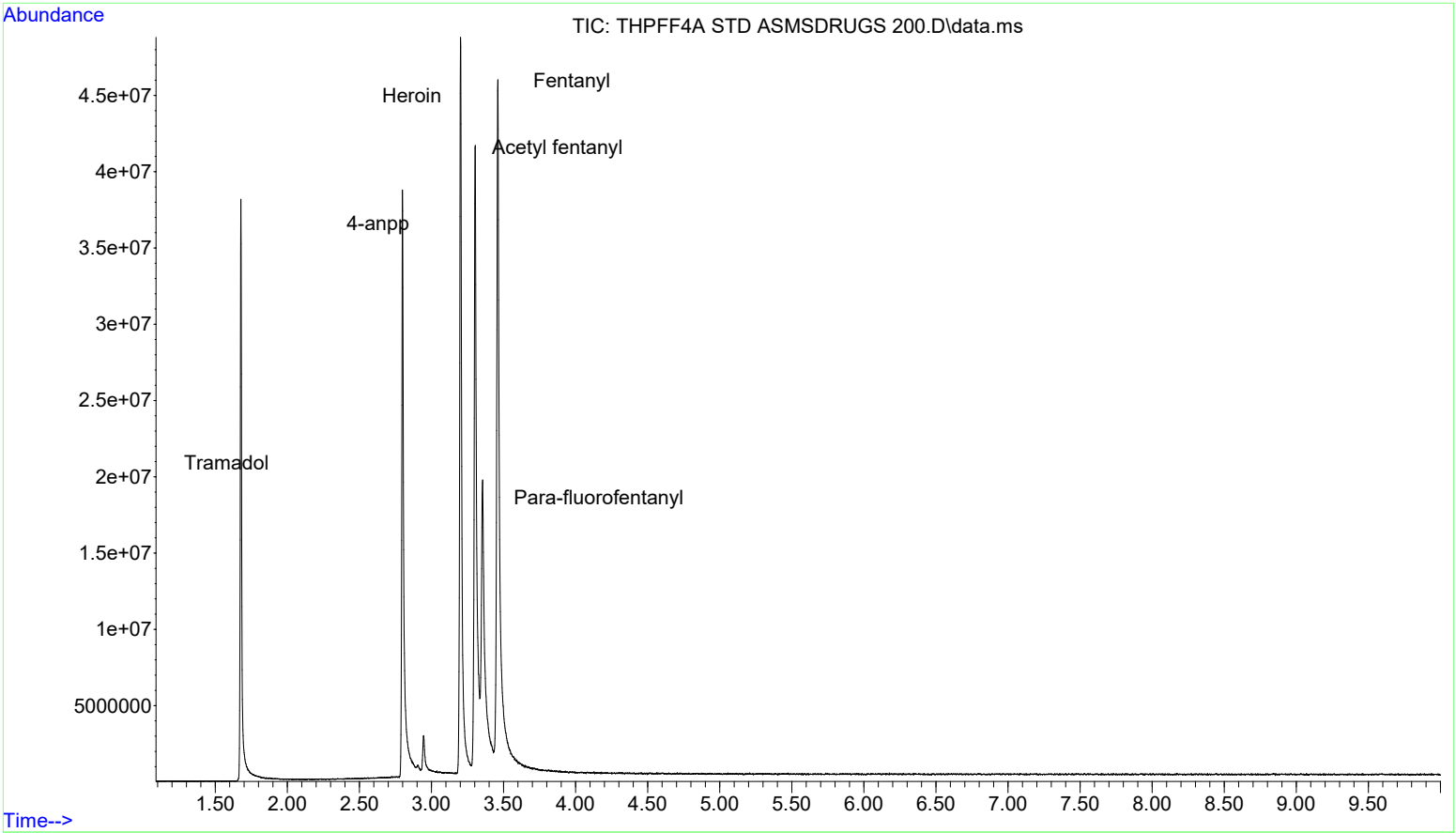


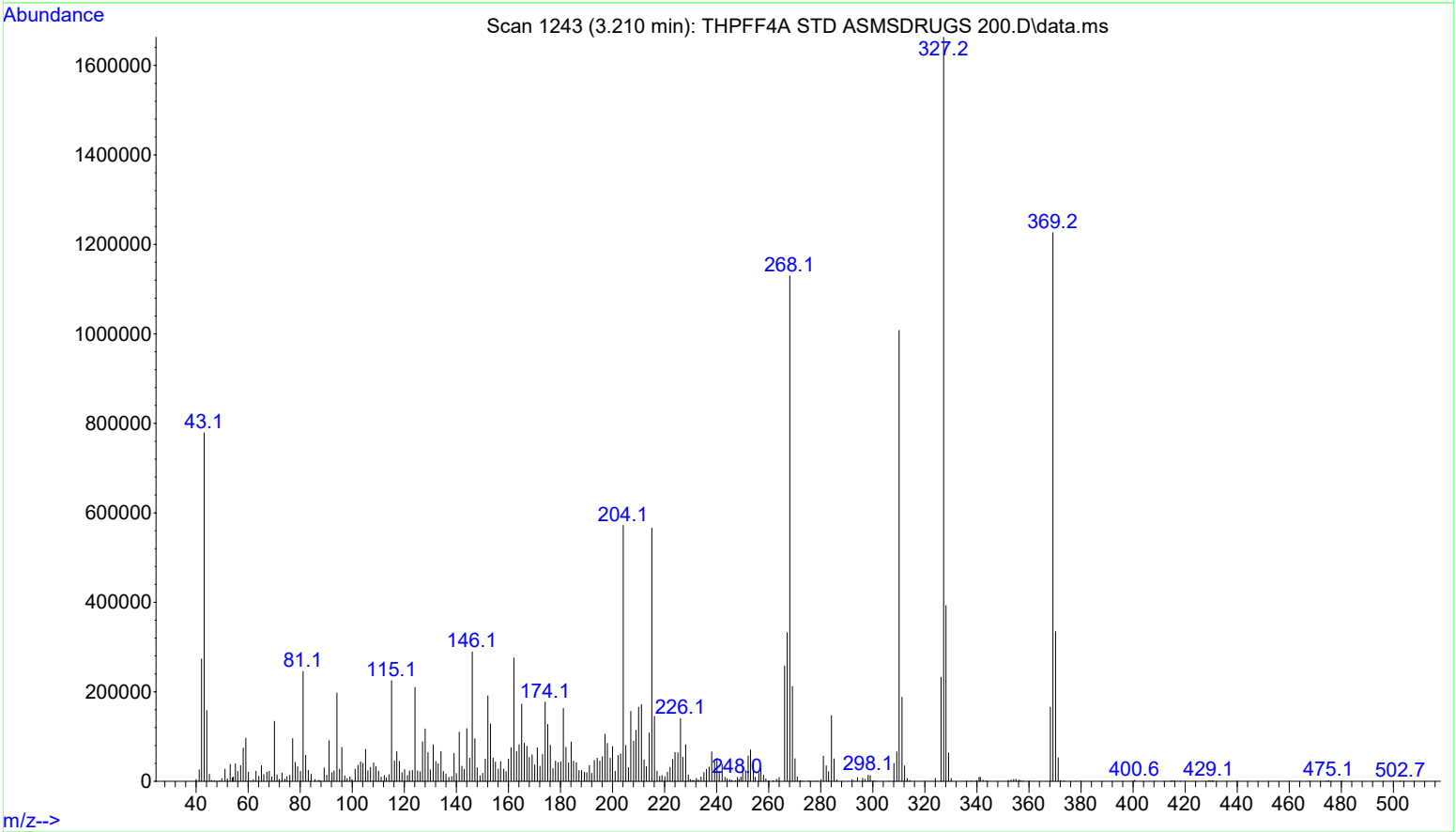


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 200.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 14:31 using AcqMethod ASMSDRUGS200.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

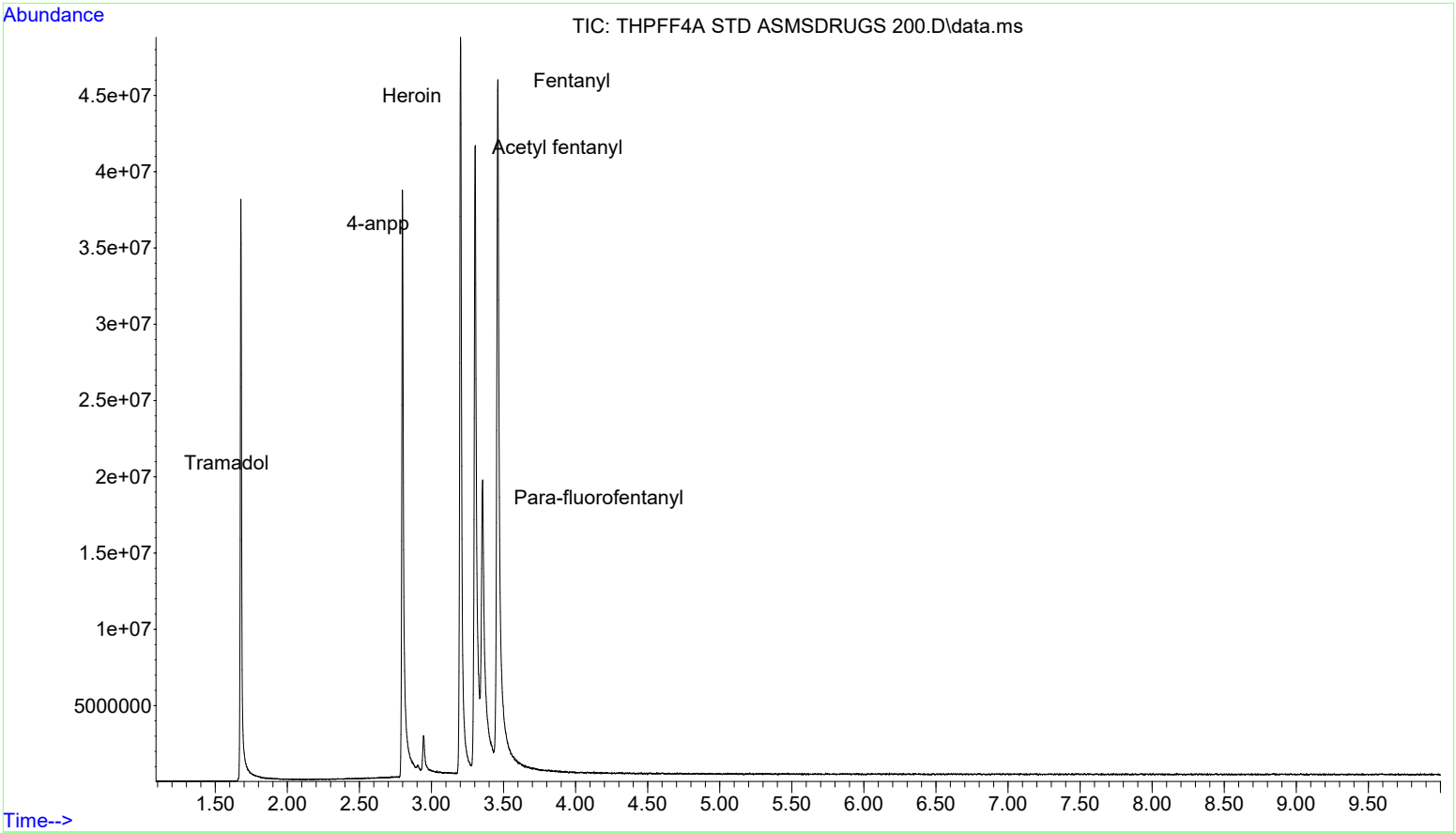


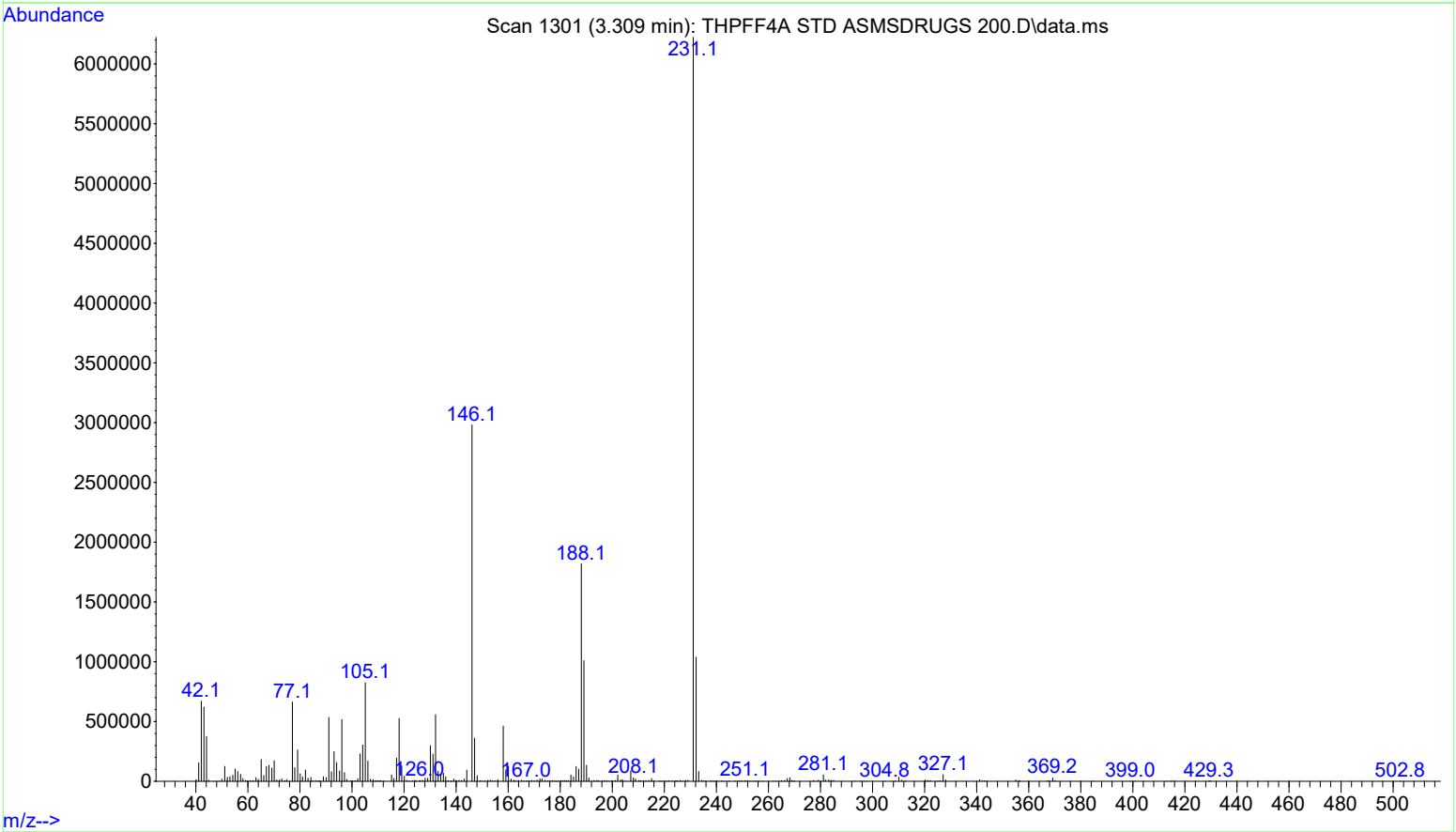


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 200.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 14:31 using AcqMethod ASMSDRUGS200.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

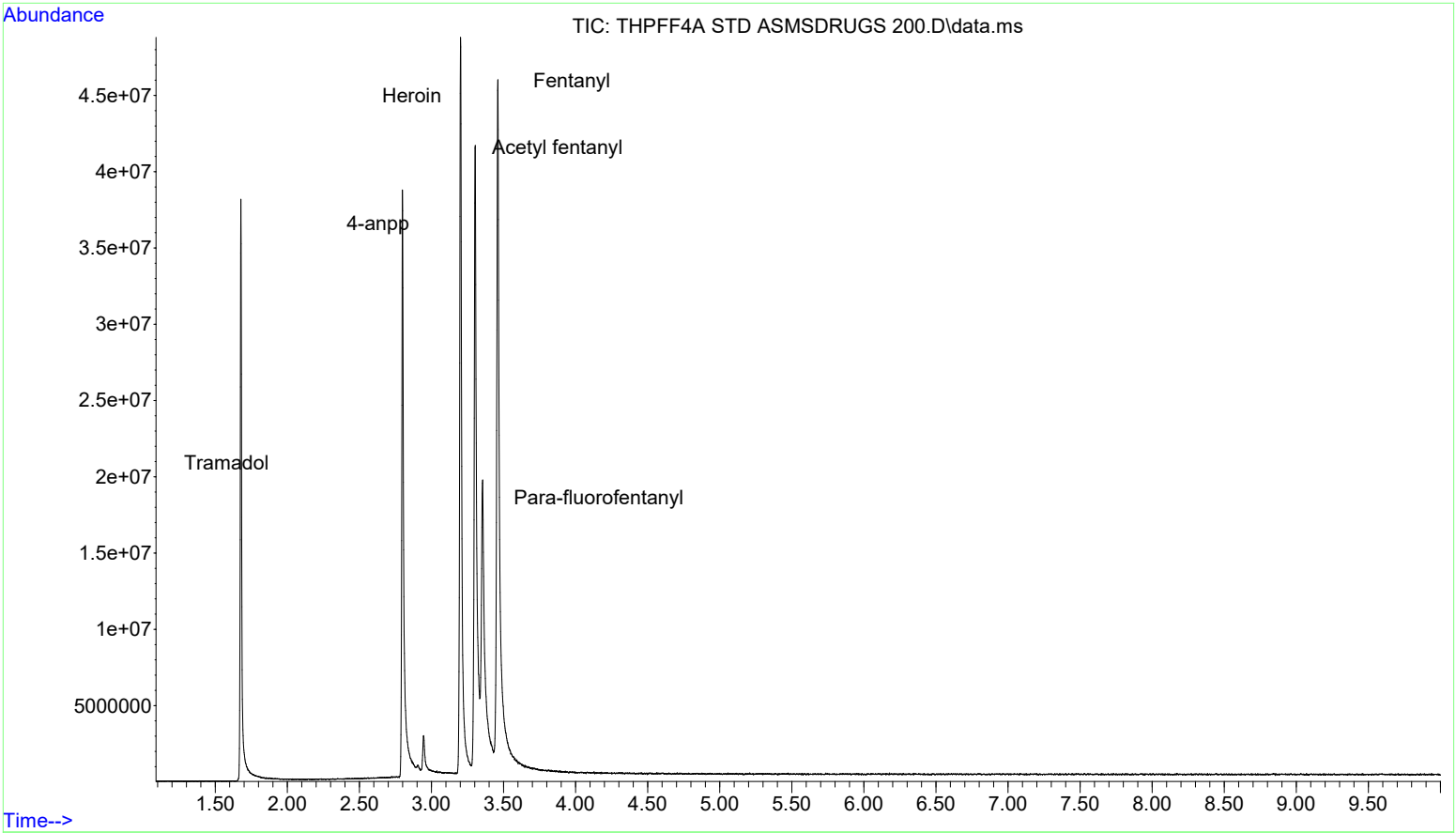


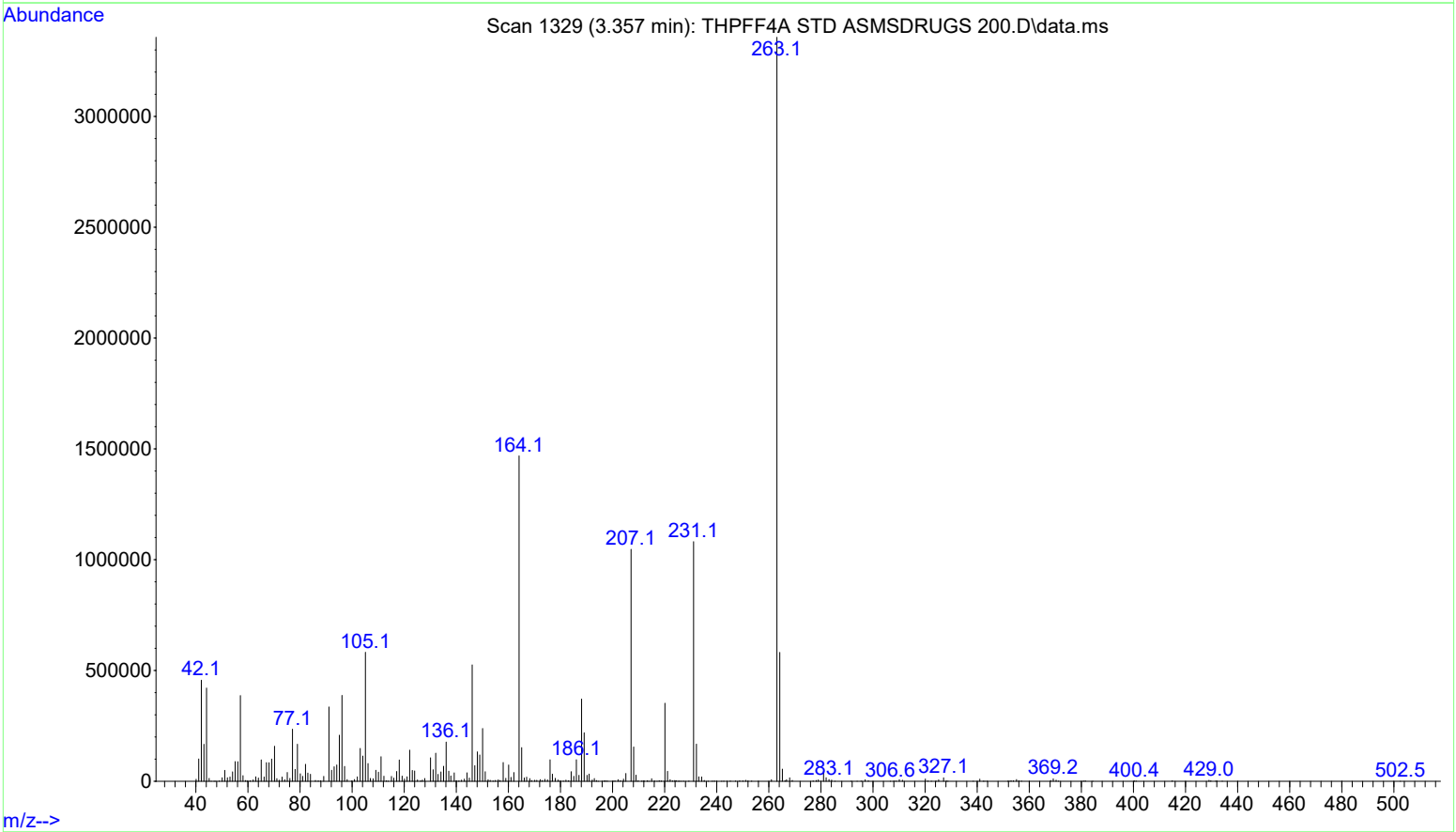


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 200.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 14:31 using AcqMethod ASMSDRUGS200.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL

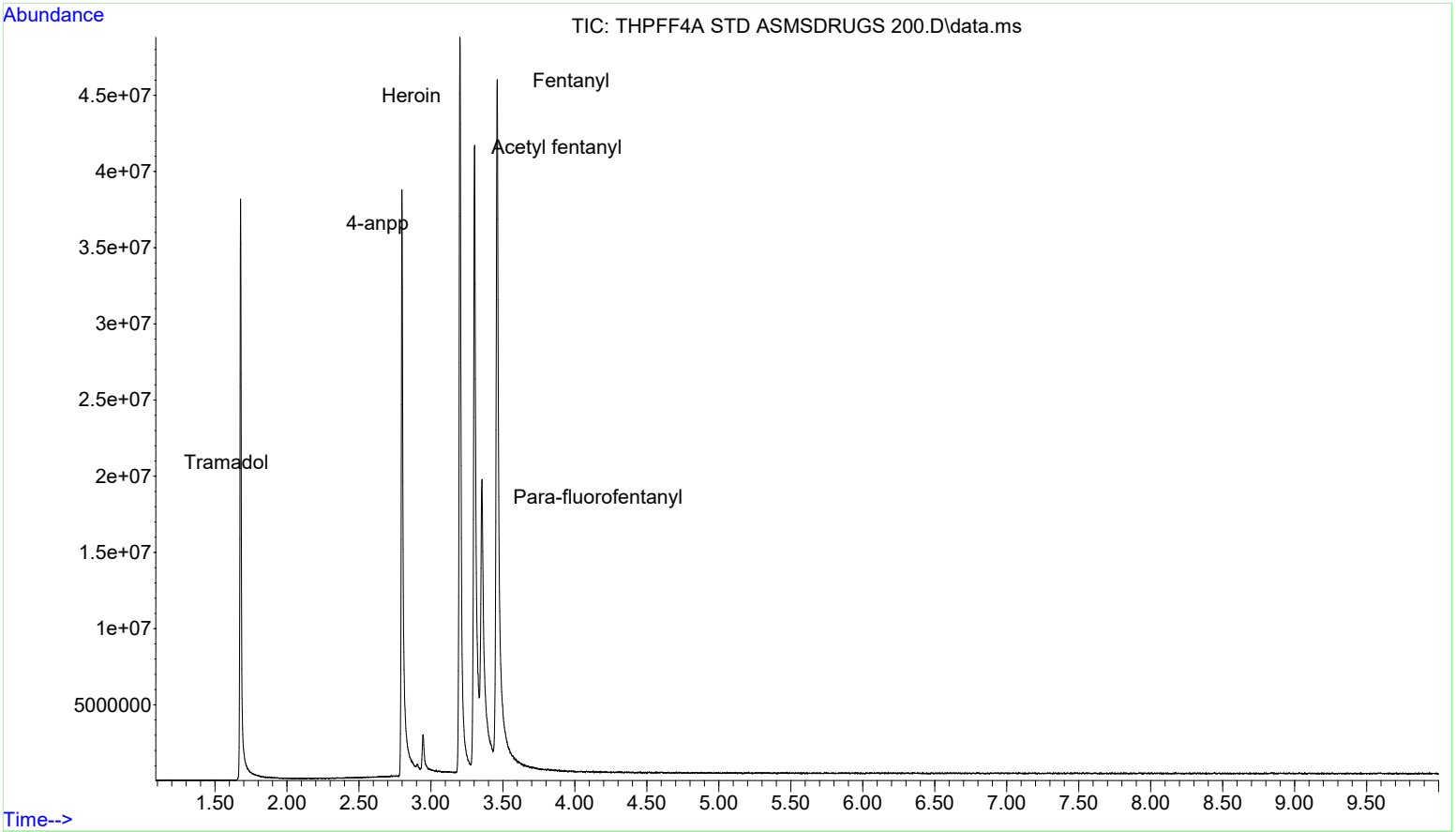


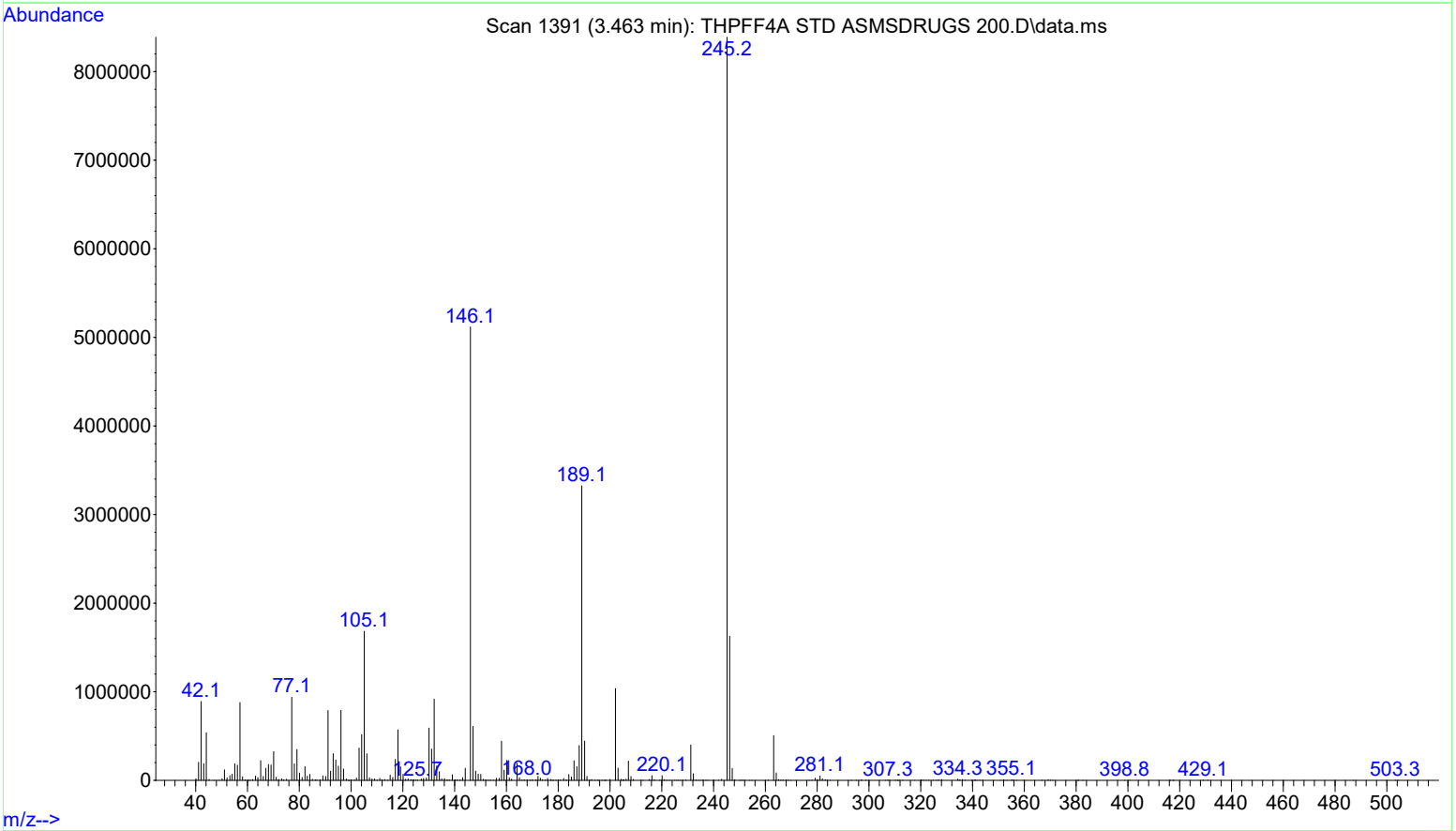


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGS 200.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 14:31 using AcqMethod ASMSDRUGS200.M
Sample Name: THPFF4A STD EXP. 10-20-23
Misc Info : METHANOL





Single Quadrupole Acquisition Method - MS Parameters Report

Method file	C:\MassHunter\GCMS\1\methods\ASMSDRUGSTI.M
Tune file	atune.u
Ion source	EI
Source temperature (°C)	230
Quad temperature (°C)	150
Fixed Electron energy (eV)	70.0
Acquisition Type	Scan
Stop time (min)	650.00
Solvent delay (min)	1.00
Trace Ion Detection	False
Gain Factor	10
EM Saver	False
EM Saver Limit	N/A

Scan Time Segments

Time	Start Mass	End Mass	Threshold	Scan Speed
1.00	40	550	150	6,250 [N=0]

Timed Events

Time	Type of Event	Parameter

Real-Time Plots

Type of Plot	Label	Low Mass	High Mass
Total Ion	N/A	N/A	N/A

Self-Cleaning Ion Source Parameters

Mode	No Cleaning

METHOD CONTROL PARAMETERS

BH
3-11-23

Method Information for: C:\MassHunter\GCMS\1\methods\ASMSDRUGSTI.M

Method Sections To Run:

( ) Save Copy of Method With Data
( ) Instrument Control Pre-Run Cmd/Macro =
( ) Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
(X) Data Analysis
( ) Instrument Control Post-Run Cmd/Macro =
( ) Data Analysis Post-Run Cmd/Macro =

Method Comments:
ASMSDRUGSTI

END OF METHOD CONTROL PARAMETERS

C:\MassHunter\GCMS\1\methods\ASMSDRUGSTI.M
Fri Mar 10 22:05:04 2023

Control Information
------- -----------

Sample Inlet : GC
Injection Source : GC ALS
Injection Location: Front
Mass Spectrometer : Enabled

No Sample Prep method has been assigned to this method.

GC
GC Summary

Run Time	30.001 min
Post Run Time	0 min

Oven

Temperature	
Setpoint	On
(Initial)	100 °C
Hold Time	1 min
Post Run	100 °C
Program	
#1 Rate	70 °C/min
#1 Value	280 °C
#1 Hold Time	26.43 min
Equilibration Time	1.5 min
Max Temperature	325 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled

ALS

Front Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	2
Sample Wash Volume	8 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	6000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	6000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL

BH
3-11-23

Solvent Wash Mode	A, B
Back Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	2
Sample Wash Volume	8 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL
Solvent Wash Mode	A, B
Sample Overlap	
Mode	Sample overlap is not enabled
ALS Errors	Pause for user interaction
Front SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 10.806 psi
Total Flow	On 79 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	On 30 After 3 min mL/min
Split Ratio	75 :1
Split Flow	75 mL/min
Liner	A Liner has not been selected.
Back SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 3.5859 psi
Total Flow	On 79 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	Off
Split Ratio	75 :1
Split Flow	75 mL/min
Liner	A Liner has not been selected.
Thermal Aux 3 (MSD Transfer Line)	
Temperature	
Setpoint	On
(Initial)	280 °C
Column	
Column #1	
Flow	
Setpoint	On

(Initial)	1 mL/min
Post Run	0.57353 mL/min

BH
3-11-23

Column Information	Agilent 19091S-602
HP-1MS	
Temperature Range	-60 °C—325 °C (350 °C)
Dimensions	12.5 m x 200 µm x 0.33 µm (Calibrated)
Column lock	Locked
In	Front SS Inlet He
Out	MSD
(Initial)	100 °C
Pressure	10.806 psi
Flow	1 mL/min
Average Velocity	57.774 cm/sec
Holdup Time	0.3606 min
Control Mode	Constant Flow

Column #2	
Flow	
Setpoint	On
(Initial)	1 mL/min
Post Run	1 mL/min

Column Information	Agilent 19091S-913
HP-1MS	
Temperature Range	-60 °C—325 °C (325 °C)
Dimensions	15 m x 320 µm x 0.25 µm (Calibrated)
Column lock	Locked
In	Back SS Inlet He
Out	Back Detector FID
(Initial)	100 °C
Pressure	3.5859 psi
Flow	1 mL/min
Average Velocity	23.097 cm/sec
Holdup Time	1.0824 min
Control Mode	Constant Flow

Column Outlet Pressure	0 psi

Back Detector FID	
Makeup	He
Column Compensation	Signal is modified by Column Compensation Curve #2
Heater	On 300 °C
H2 Flow	Off
Air Flow	Off
Makeup Flow	On 25 mL/min
Carrier Gas Flow Correction	Constant Makeup and Fuel Flow
Flame	Off

Aux EPC 1,2,3	
Aux EPC 1 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Aux EPC 2 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi

Excluded from Readiness ***Excluded from Affecting GC's Readiness State***

BH
3-11-23

Aux EPC 3 N2
Pressure
Setpoint Off
(Initial) 10 psi
Post Run 0 psi

Excluded from Readiness ***Excluded from Affecting GC's Readiness State***

Signals
Signal #1:
Description None

Signal #2: Test Plot
Description Test Plot
Save Off
Data Rate 50 Hz
Dual Injection Assignment Back Sample

Signal #3: Test Plot
Description Test Plot
Save Off
Data Rate 50 Hz
Dual Injection Assignment Back Sample

Signal #4: Test Plot
Description Test Plot
Save Off
Data Rate 50 Hz
Dual Injection Assignment Back Sample

TUNE PARAMETERS for SN: US1648M021

Trace Ion Detection is OFF.

34.593	:	EMISSION
70.007	:	ENERGY
34.899	:	REPELLER
90.331	:	IONFOCUS
22.672	:	ENTRANCE_LENS
1360.190	:	EMVOLTS
1498.6	:	Actual EMV
1.00	:	GAIN FACTOR
2908.000	:	AMUGAIN
136.750	:	AMUOFFSET
1.000	:	FILAMENT
0.000	:	DCPOLARITY
12.032	:	ENTLENSOFFSET
0.000	:	Ion_Body
0.000	:	EXTLENS
442.000	:	MASSGAIN
-22.000	:	MASSOFFSET

END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

DATA ANALYSIS PARAMETERS

Method Name: C:\MassHunter\GCMS\1\methods\ASMSDRUGSTI.M

Percent Report Settings

Sort By: Signal

Output Destination
    Screen: No
    Printer: Yes
    File: No

Integration Events: AutoIntegrate

Generate Report During Run Method: No

Signal Correlation Window: 0.020

Qualitative Report Settings

Peak Location of Unknown: Apex

Library to Search	Minimum Quality
DEMO.L	0

Integration Events: AutoIntegrate

Report Type: Summary

Output Destination
    Screen: No
    Printer: Yes
    File: No

Generate Report During Run Method: No

Quantitative Report Settings

Report Type: Summary

Output Destination

Screen: Yes
Printer: No
File: No

BH
3-11-23

Generate Report During Run Method: No

Calibration Last Updated:

Reference Window: 10.00 Percent
Non-Reference Window: 5.00 Percent
Correlation Window: 0.02 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

Compound Information

*** Empty Quantitation Database ***

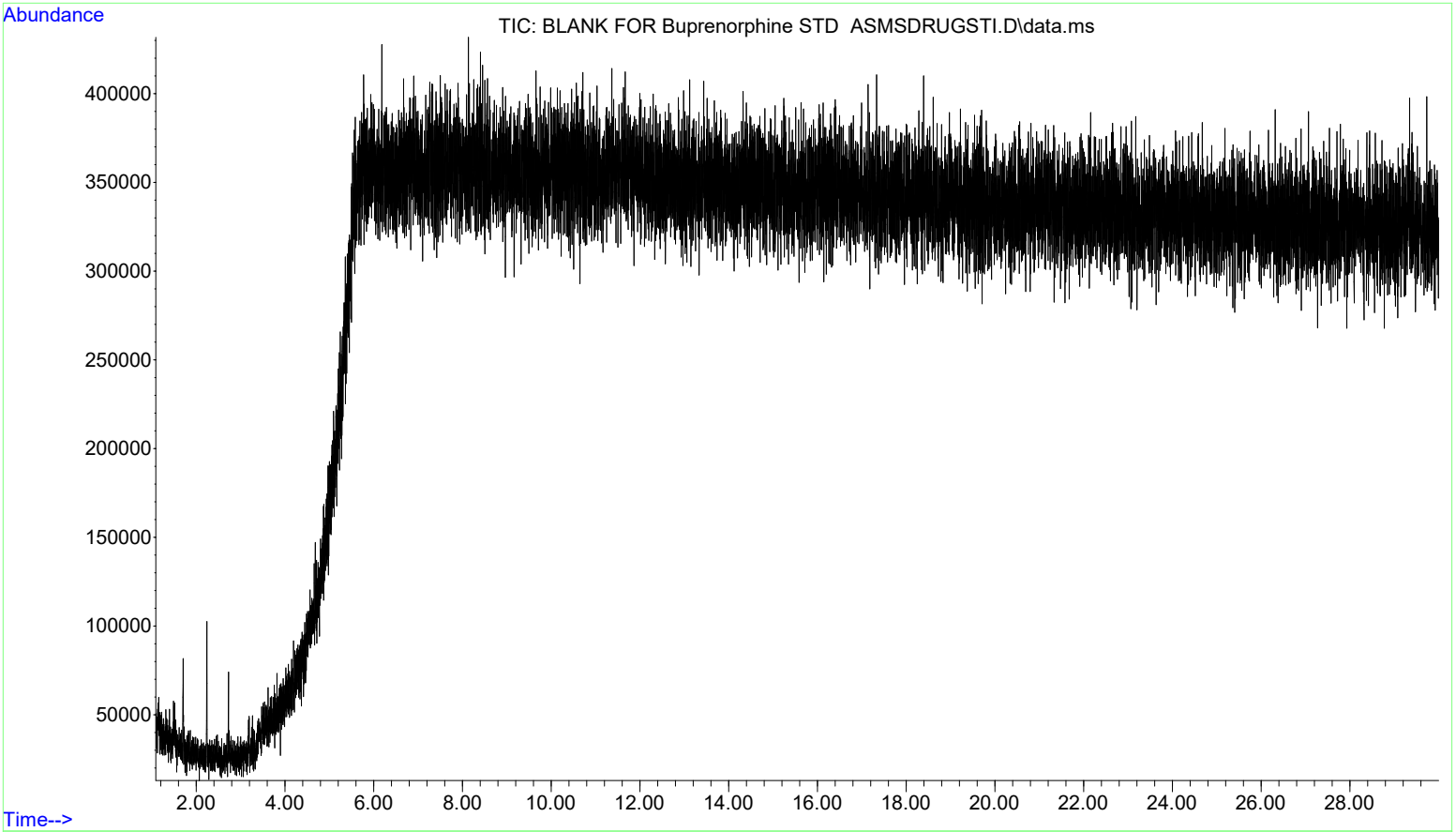
END OF DATA ANALYSIS PARAMETERS

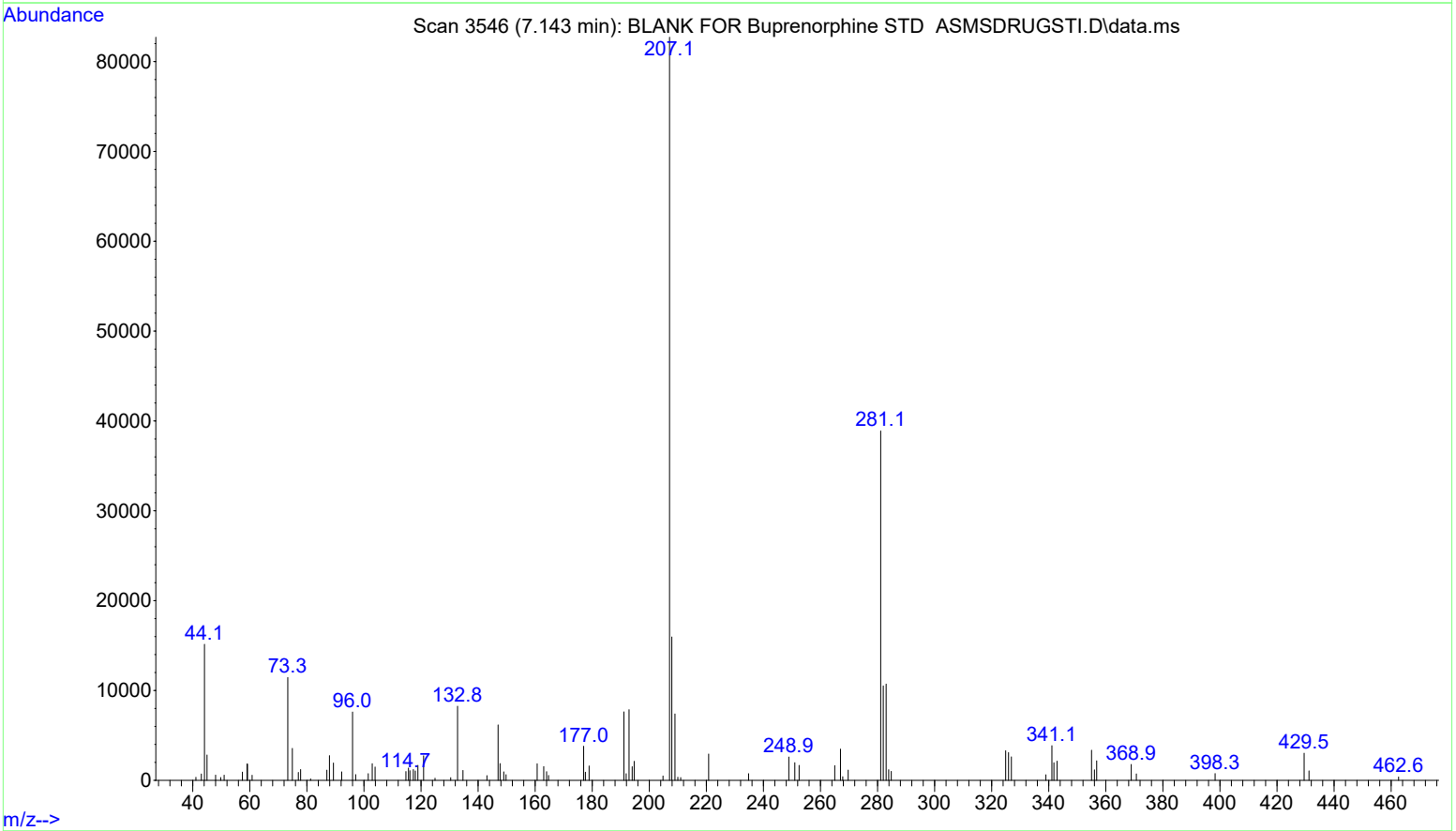
Fri Mar 10 22:05:30 2023

File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR Buprenorphine STD ASMSDRUGSTI.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 20:08 using AcqMethod ASMSDRUGSTI.M
Sample Name: BLANK FOR Buprenorphine STD ASMSDRUGSTI
Misc Info : METHANOL

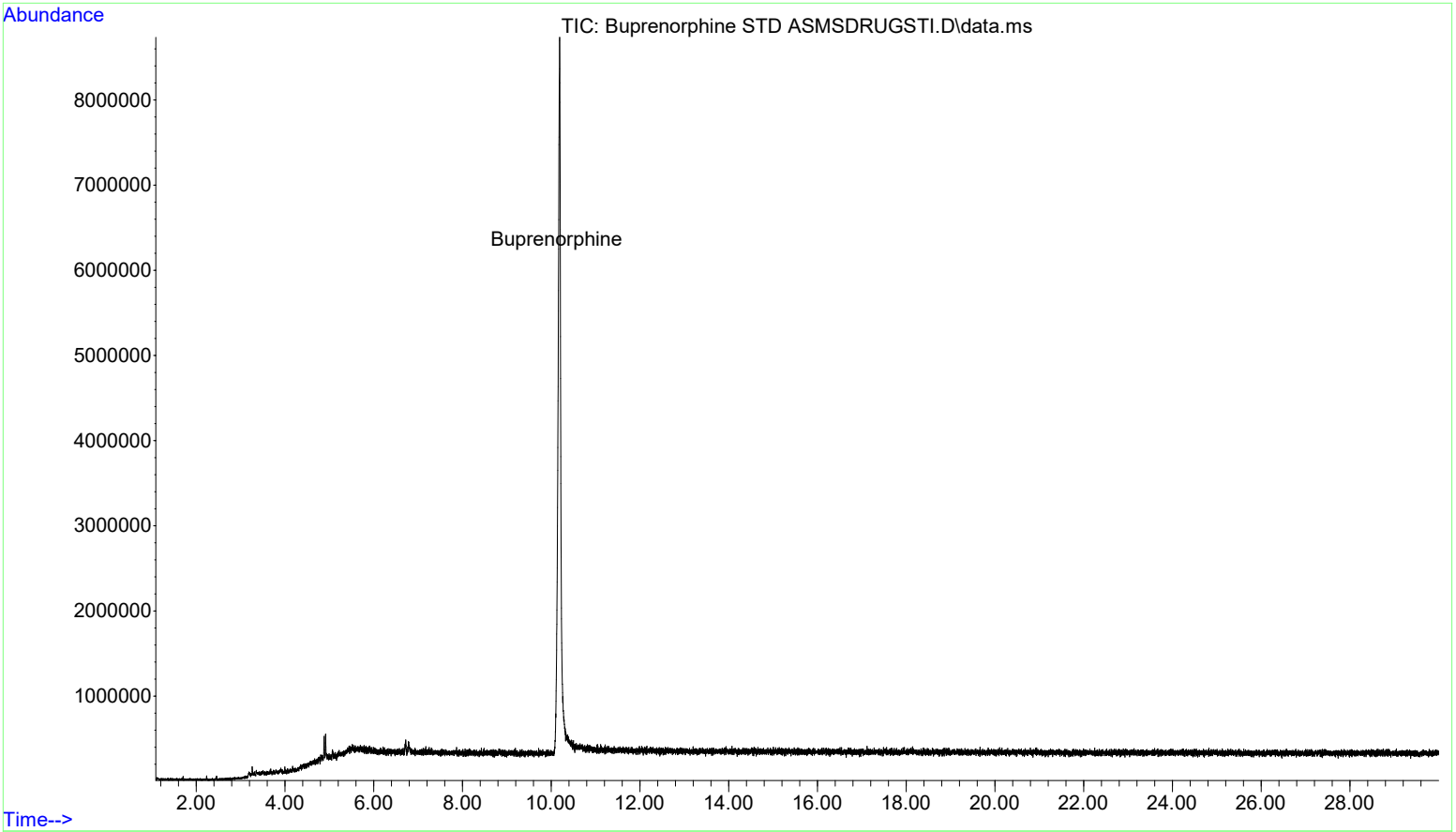


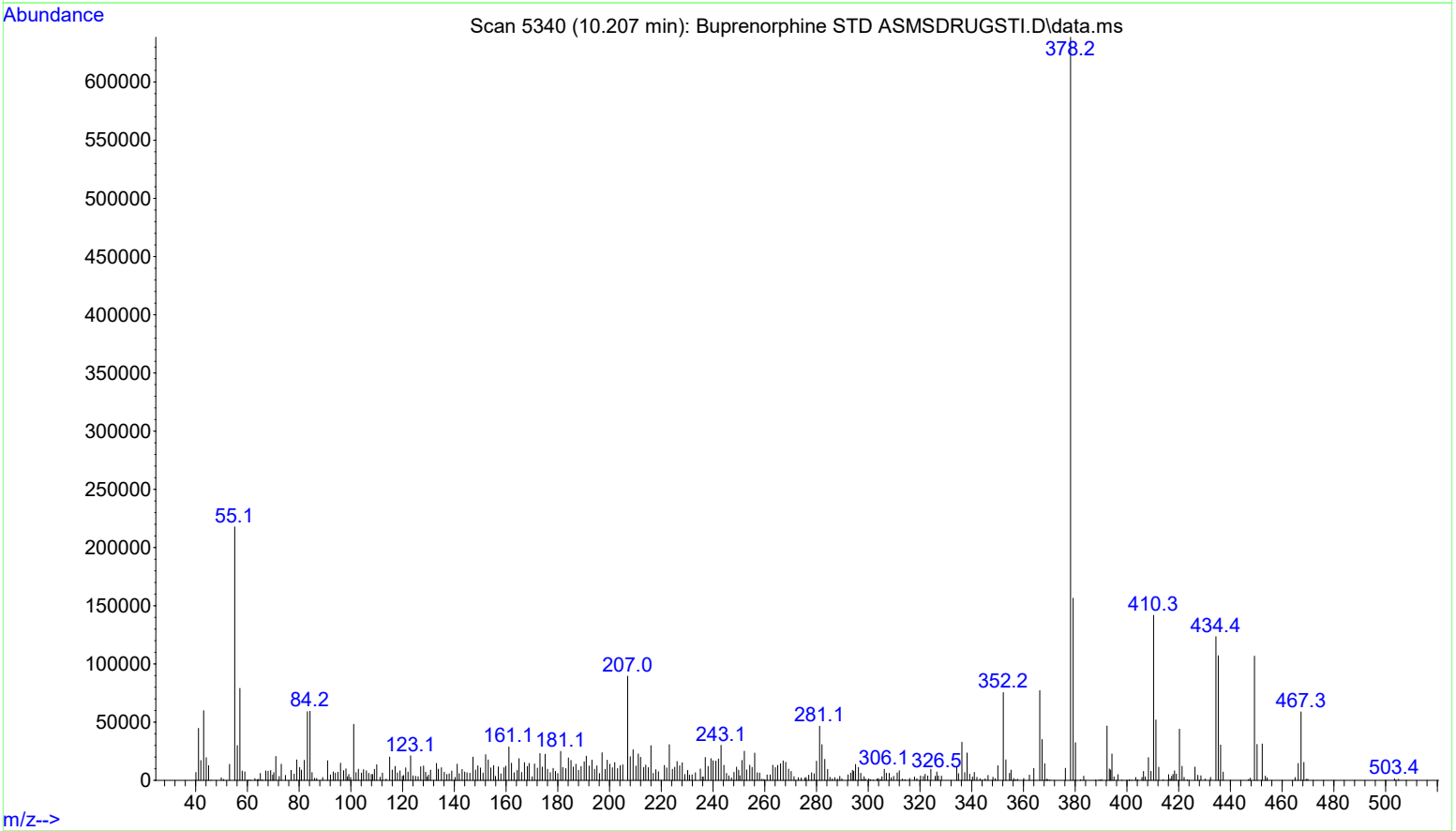


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\Bu
... prenorphine STD ASMSDRUGSTI.D

BH
3-11-23

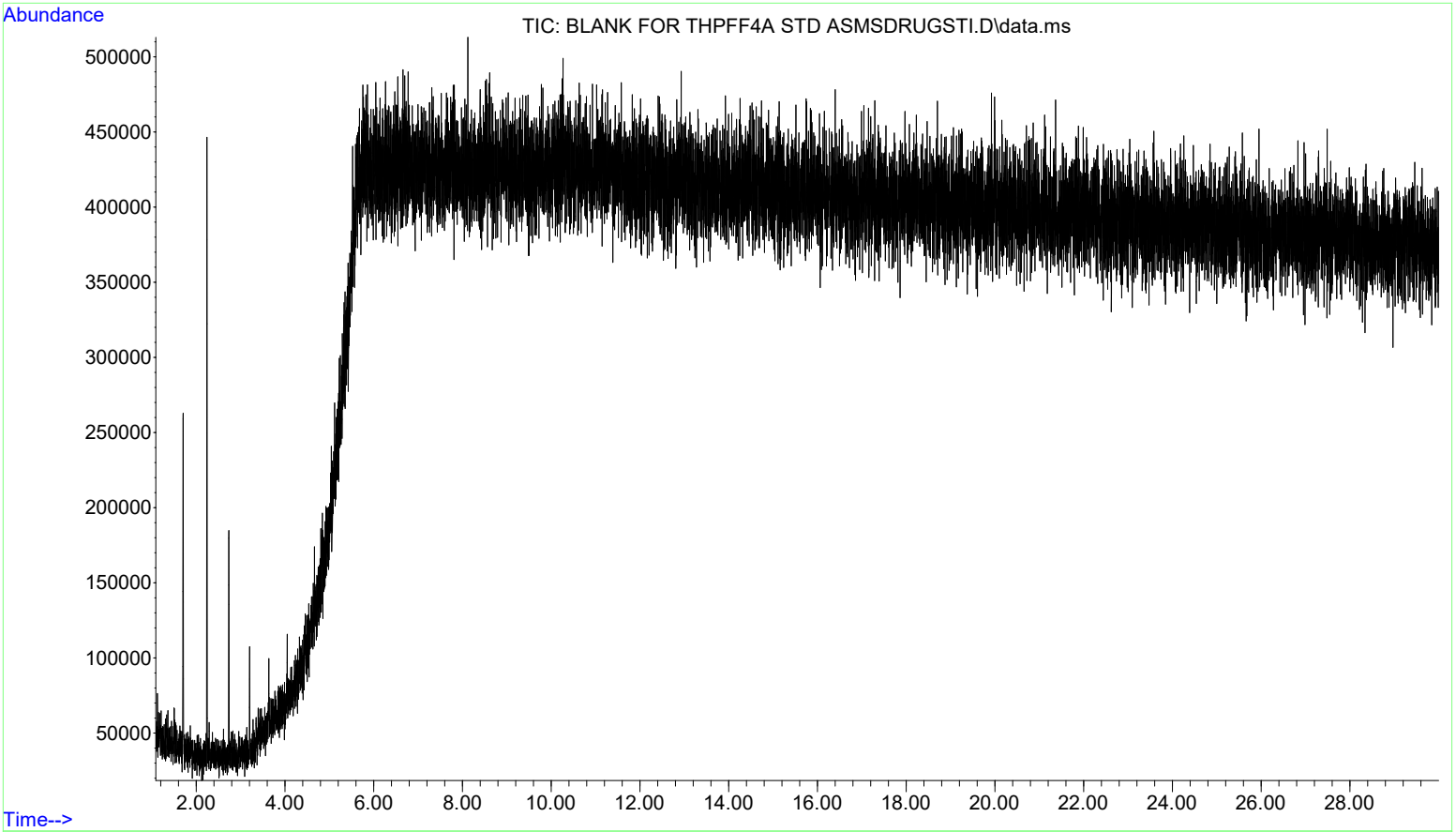
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 20:43 using AcqMethod ASMSDRUGSTI.M
Sample Name: Buprenorphine STD EXP. 6-2024 ASMSDRUGSTI
Misc Info : METHANOL

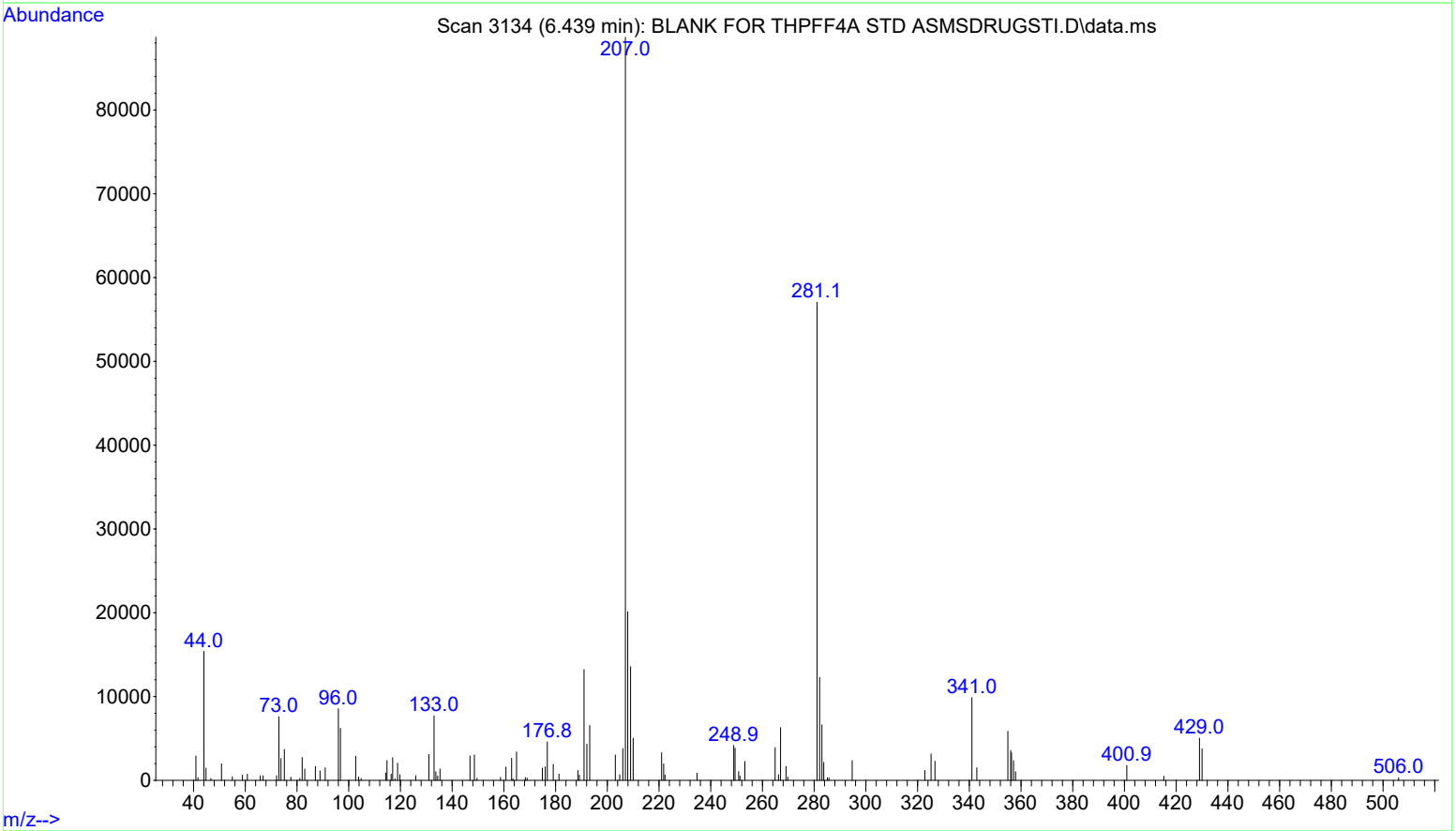




File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\BL
... ANK FOR THPFF4A STD ASMSDRUGSTI.D
Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 18:45 using AcqMethod ASMSDRUGSTI.M
Sample Name: BLANK FOR THPFF4A STD ASMSDRUGSTI
Misc Info : METHANOL

BH
3-11-23

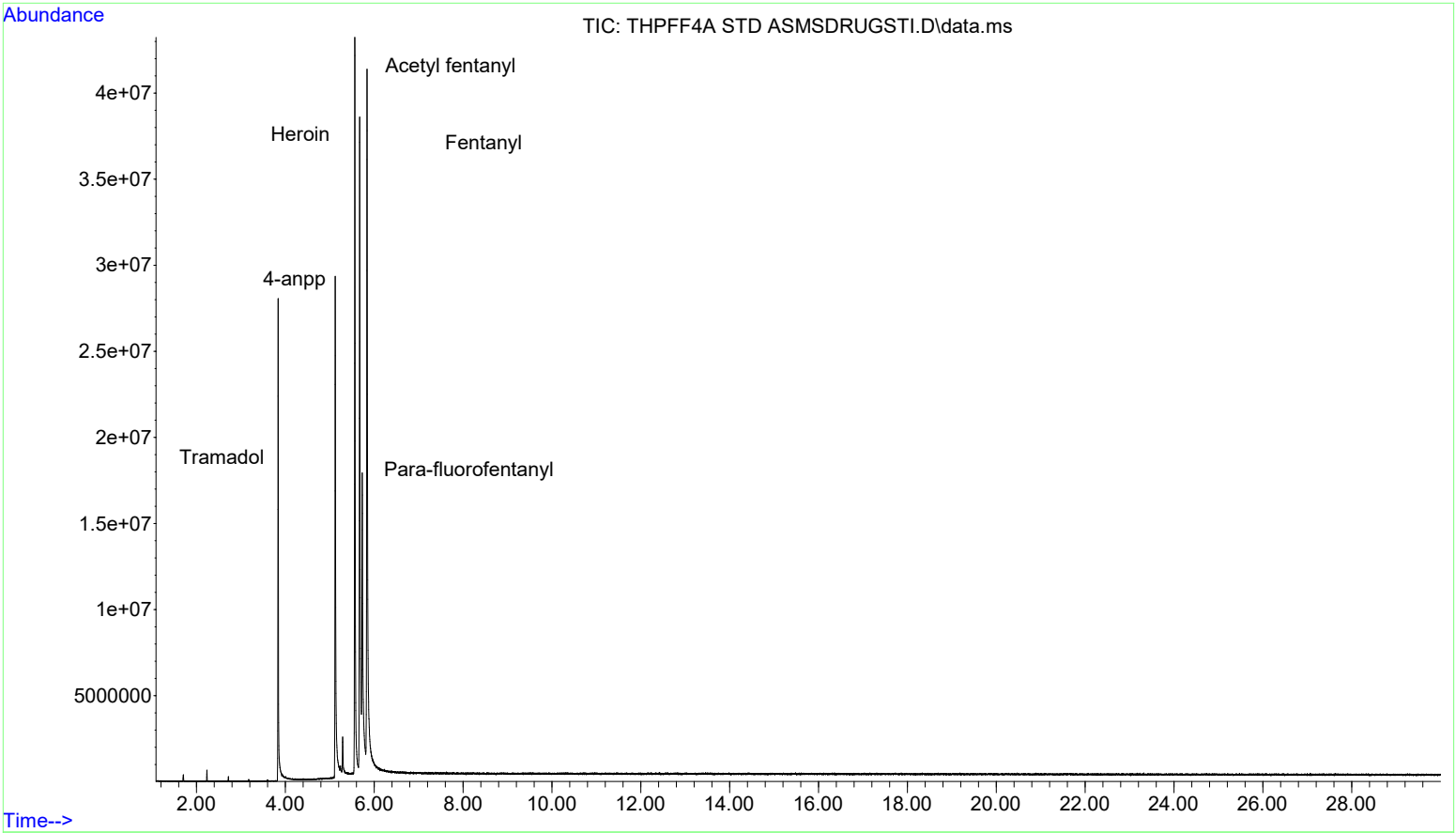


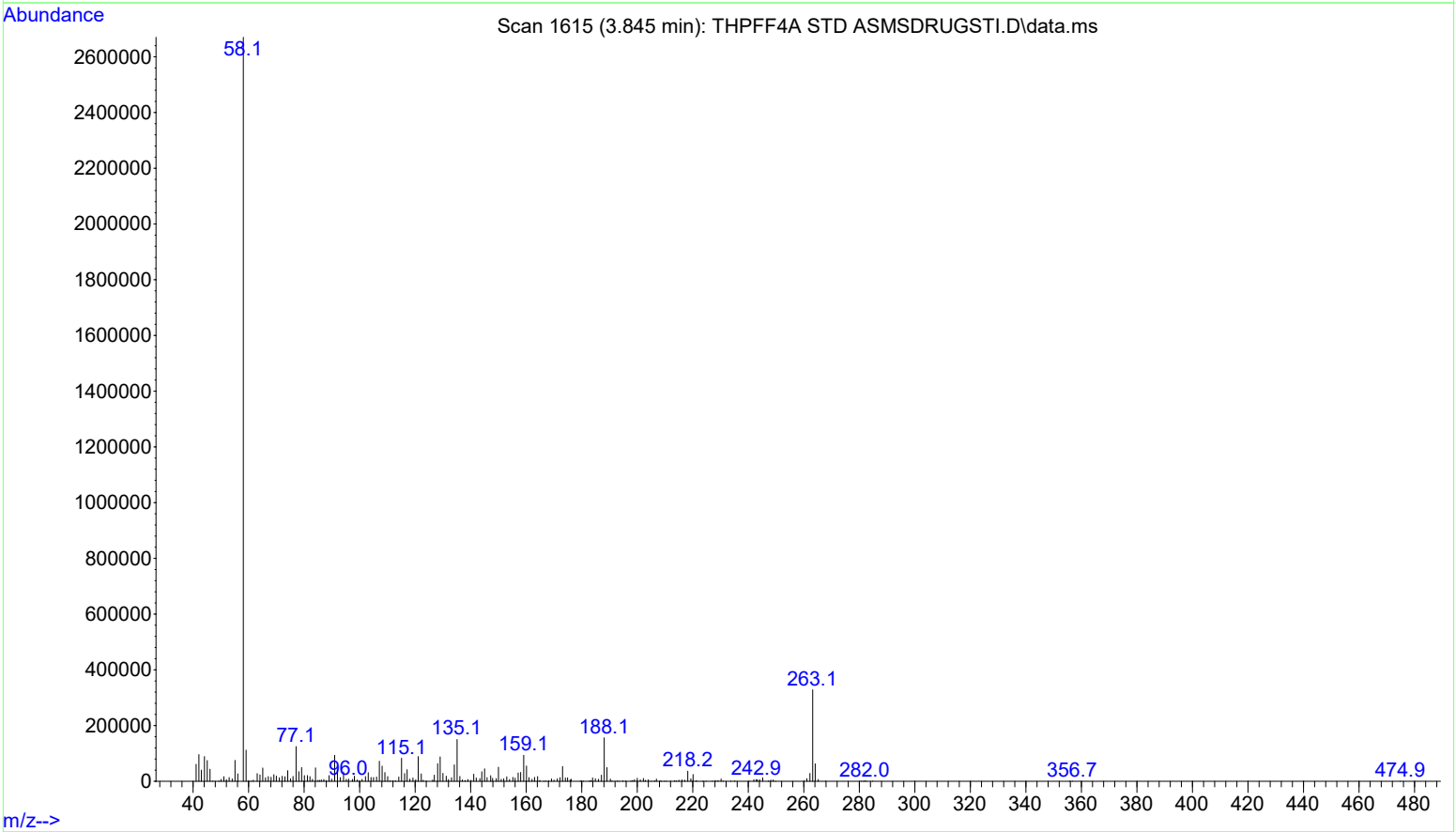


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGSTI.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 19:20 using AcqMethod ASMSDRUGSTI.M
Sample Name: THPFF4A STD EXP. 10-20-23 ASMSDRUGSTI
Misc Info : METHANOL

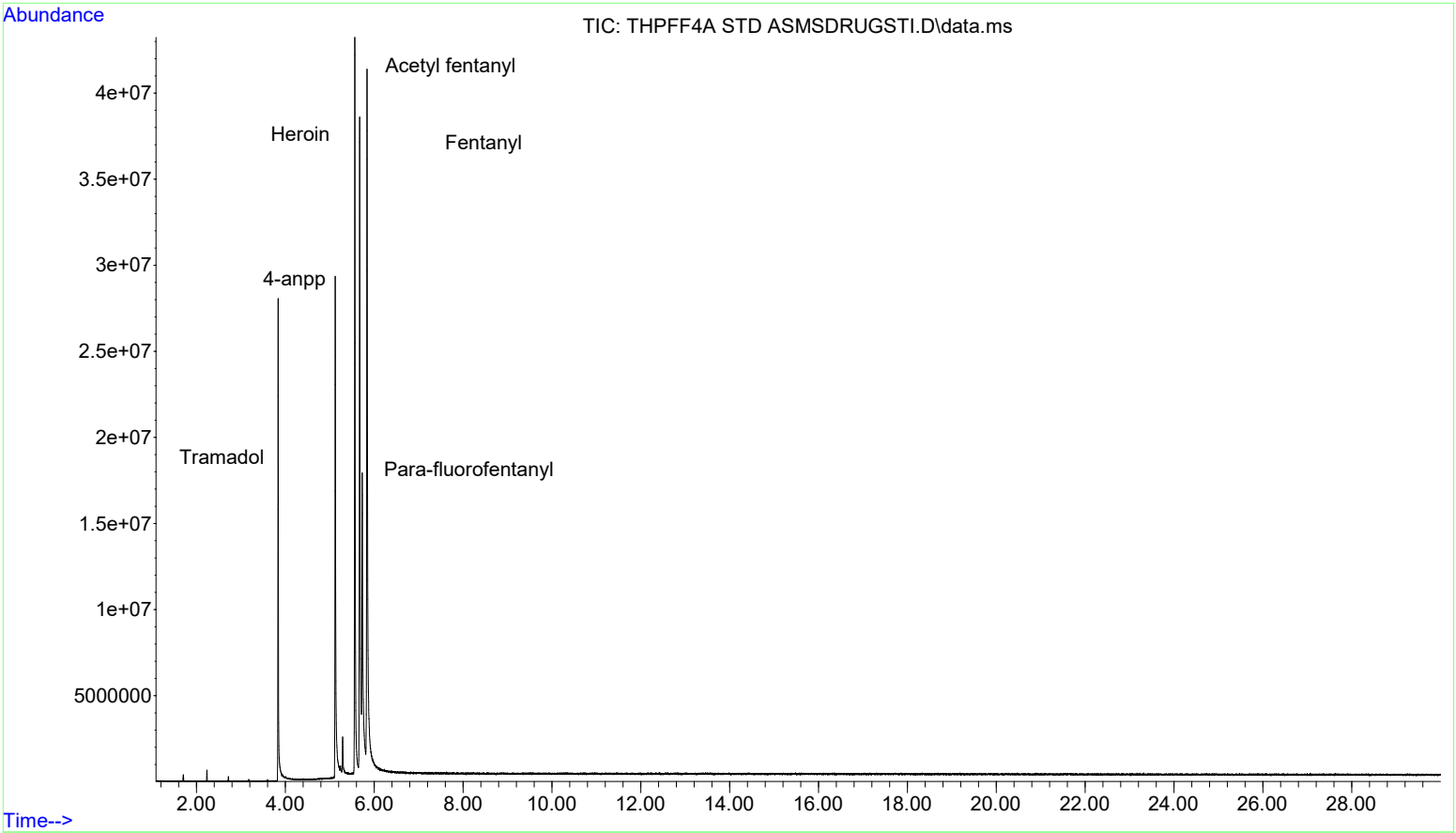


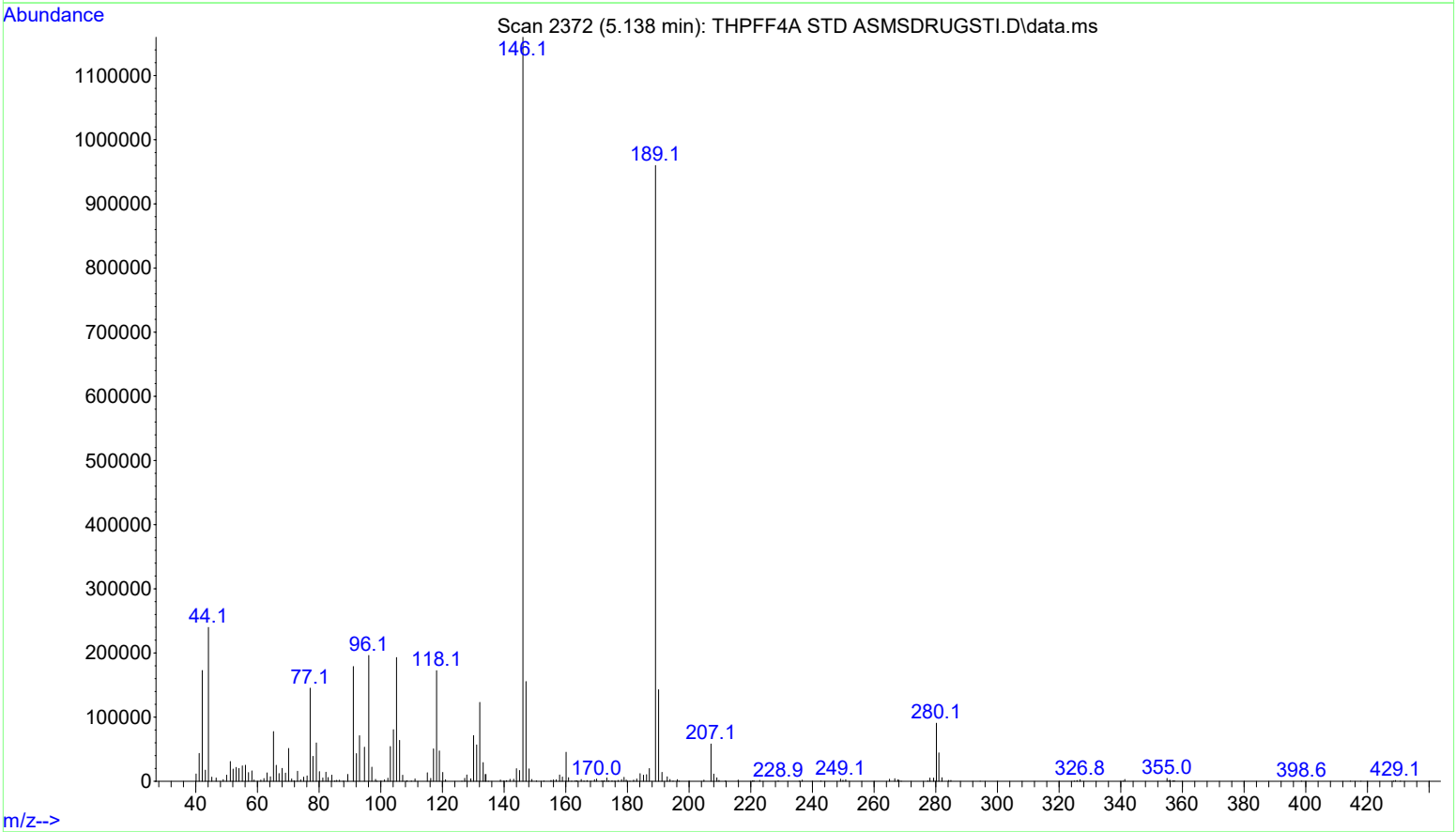


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGSTI.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 19:20 using AcqMethod ASMSDRUGSTI.M
Sample Name: THPFF4A STD EXP. 10-20-23 ASMSDRUGSTI
Misc Info : METHANOL

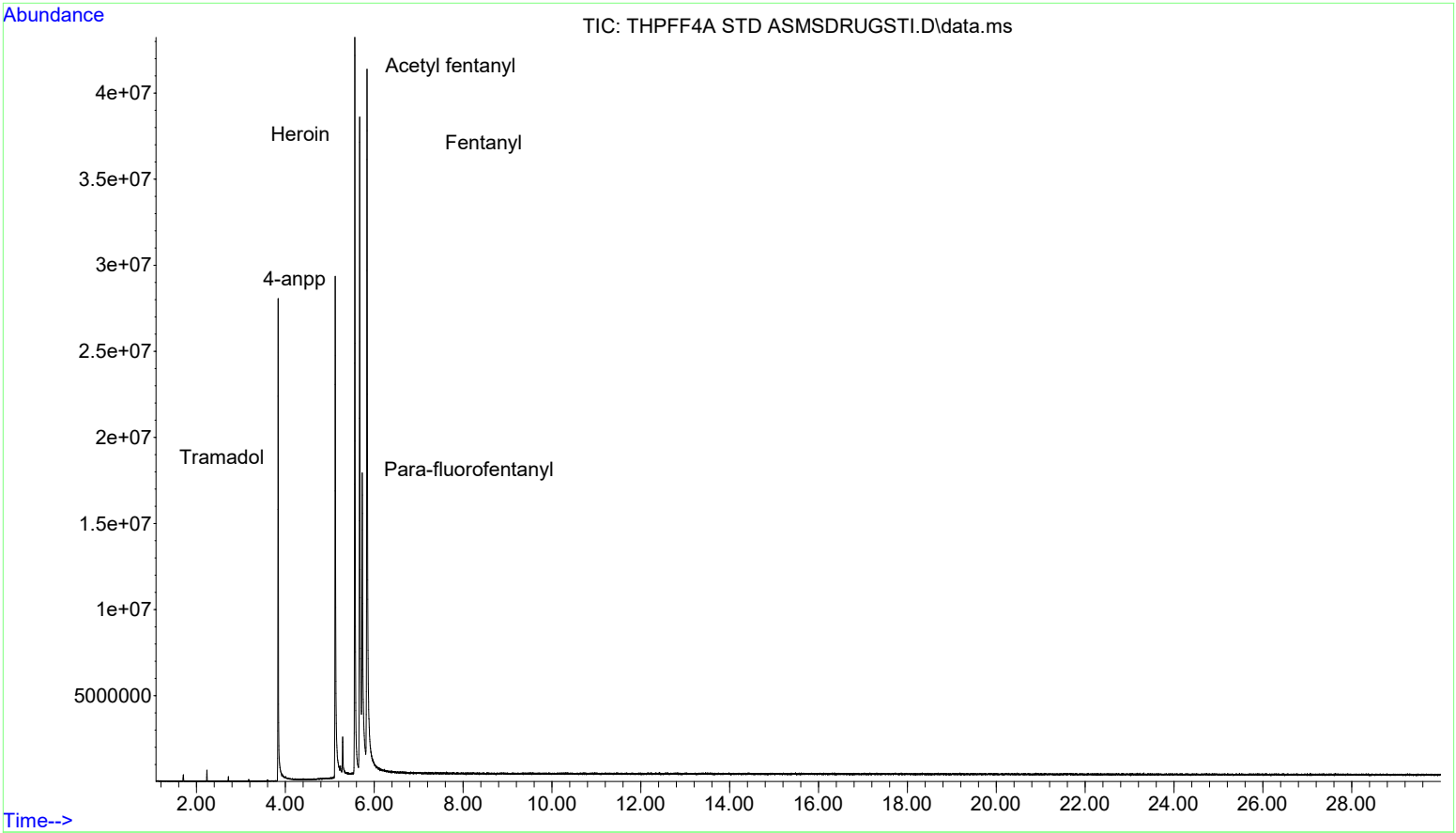


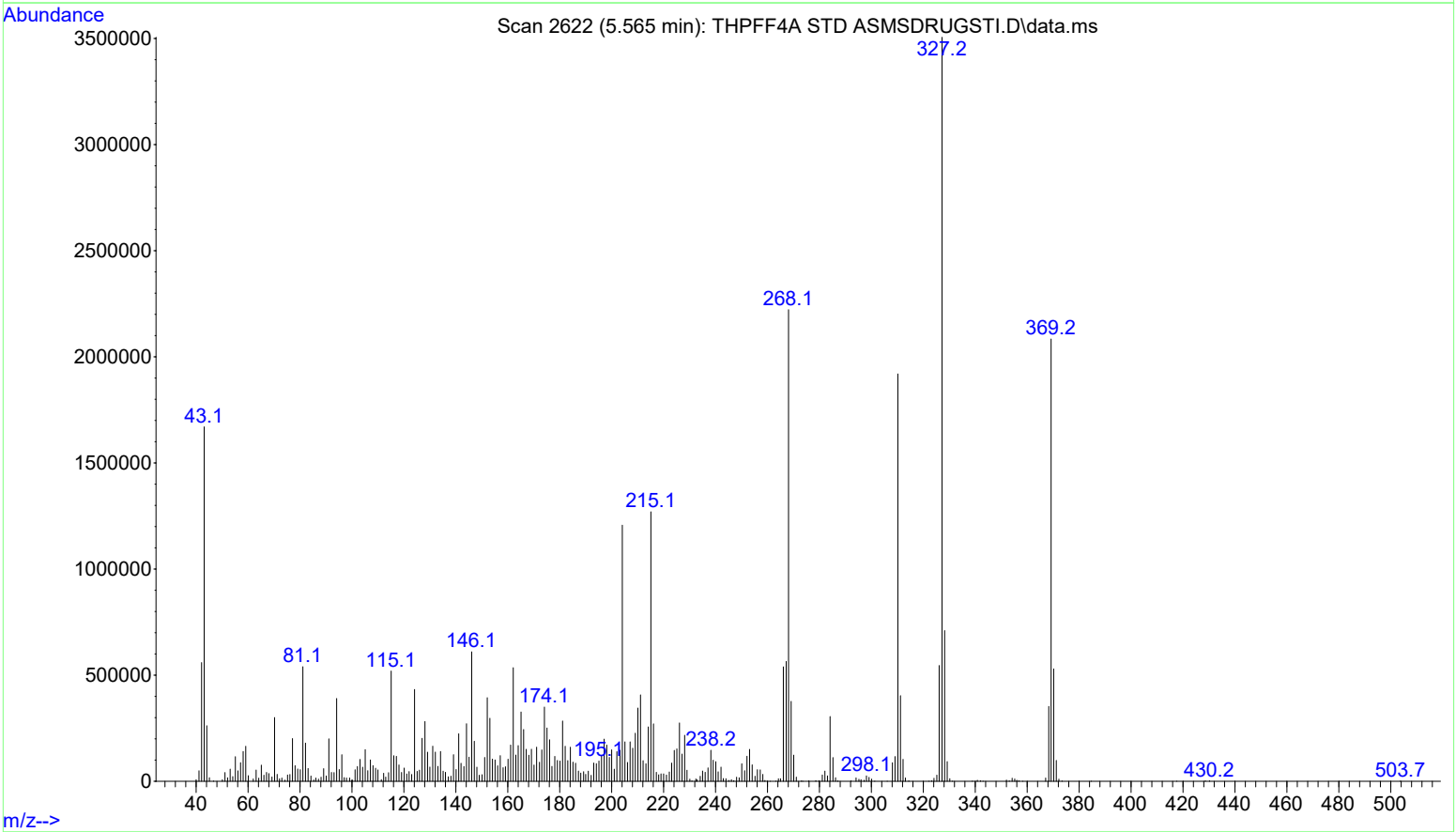


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGSTI.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 19:20 using AcqMethod ASMSDRUGSTI.M
Sample Name: THPFF4A STD EXP. 10-20-23 ASMSDRUGSTI
Misc Info : METHANOL

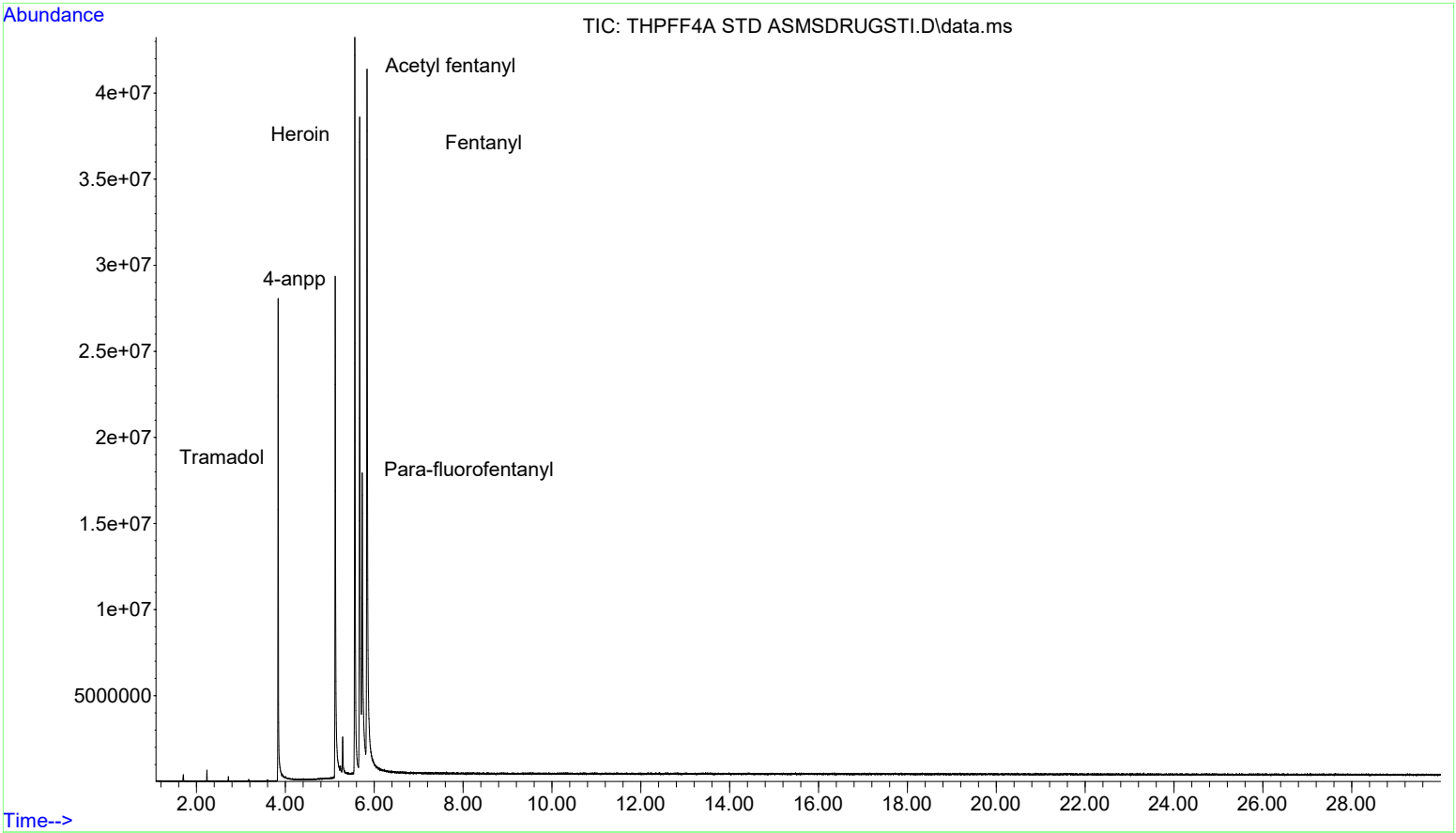


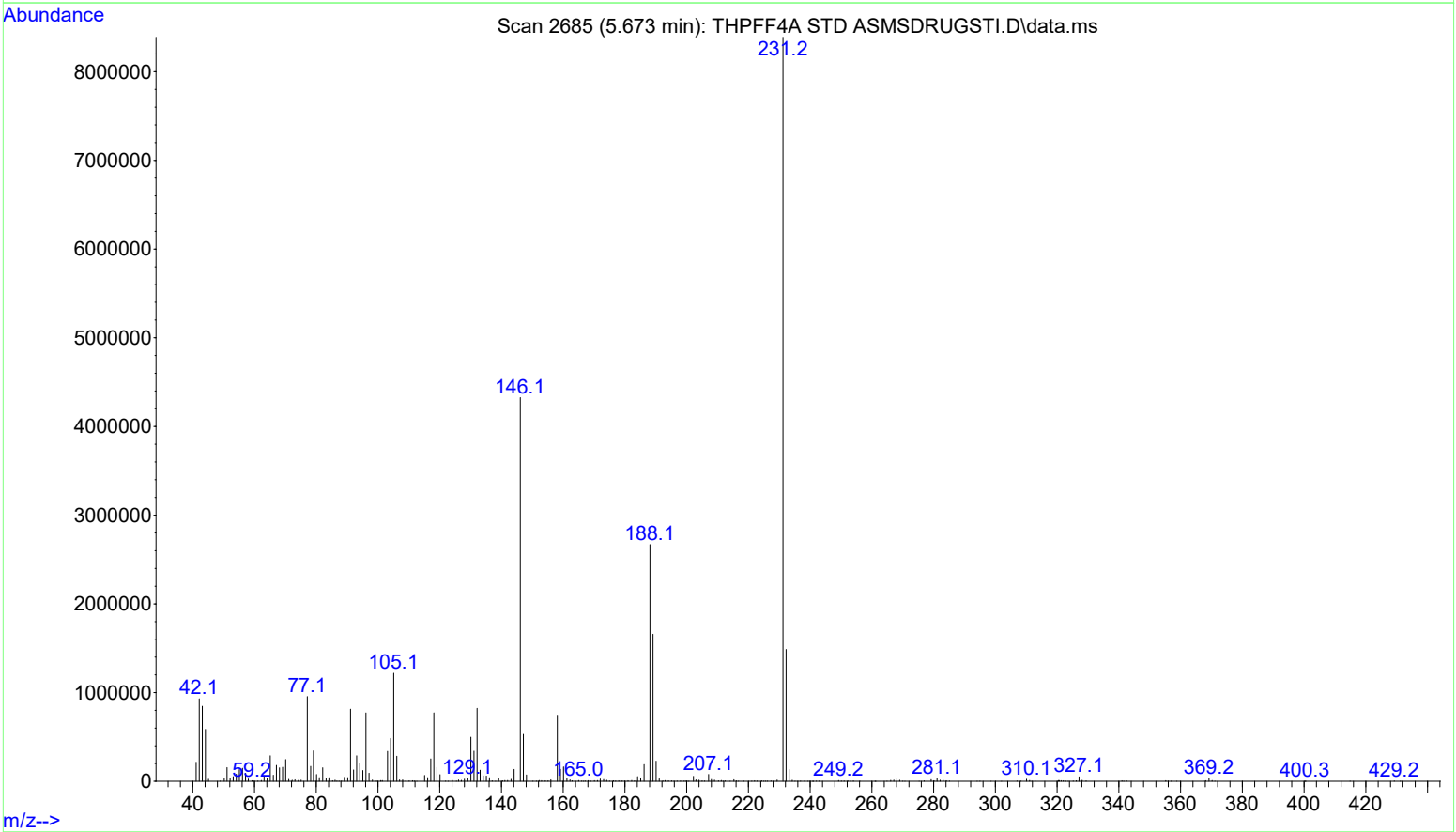


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGSTI.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 19:20 using AcqMethod ASMSDRUGSTI.M
Sample Name: THPFF4A STD EXP. 10-20-23 ASMSDRUGSTI
Misc Info : METHANOL

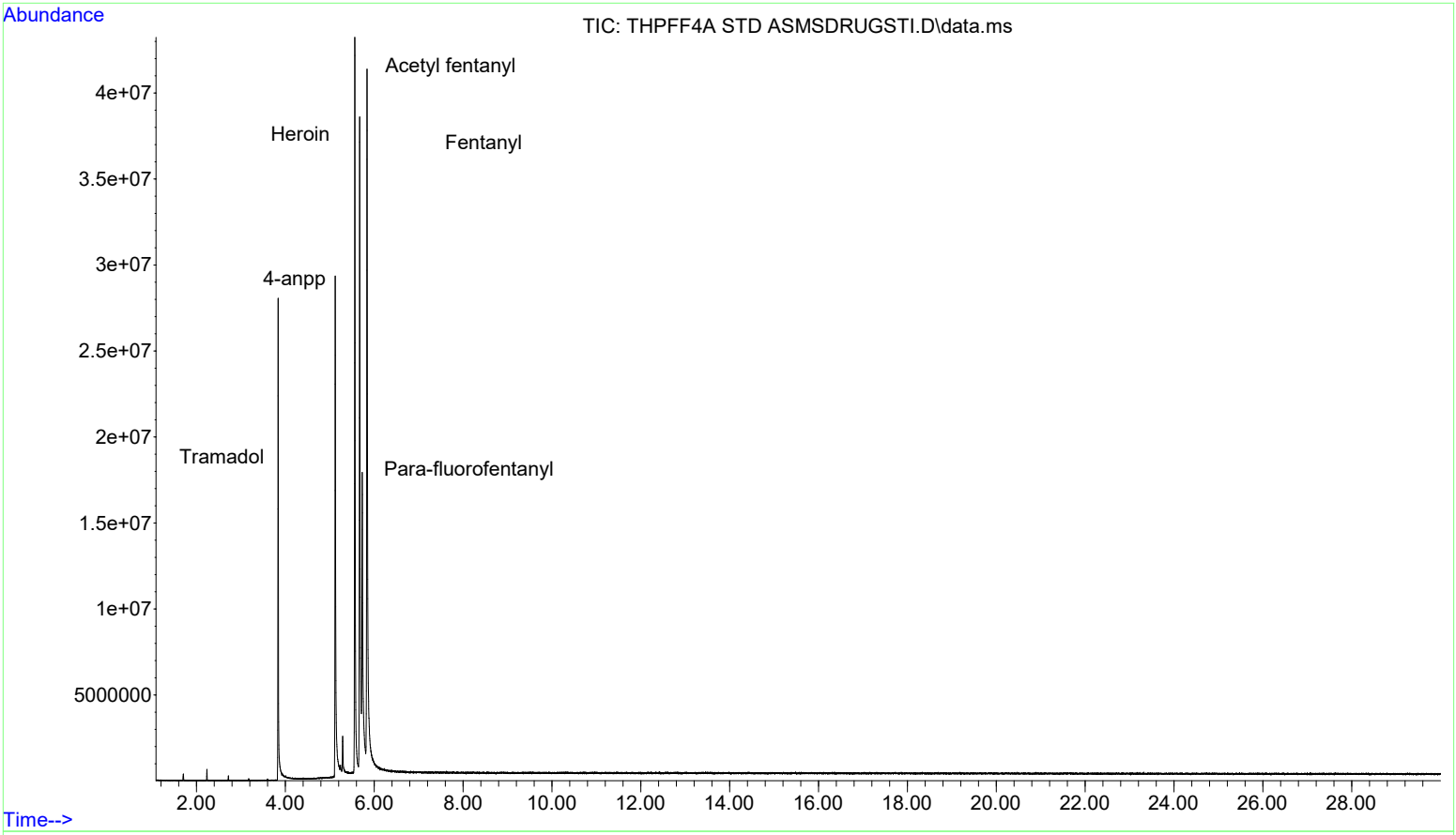


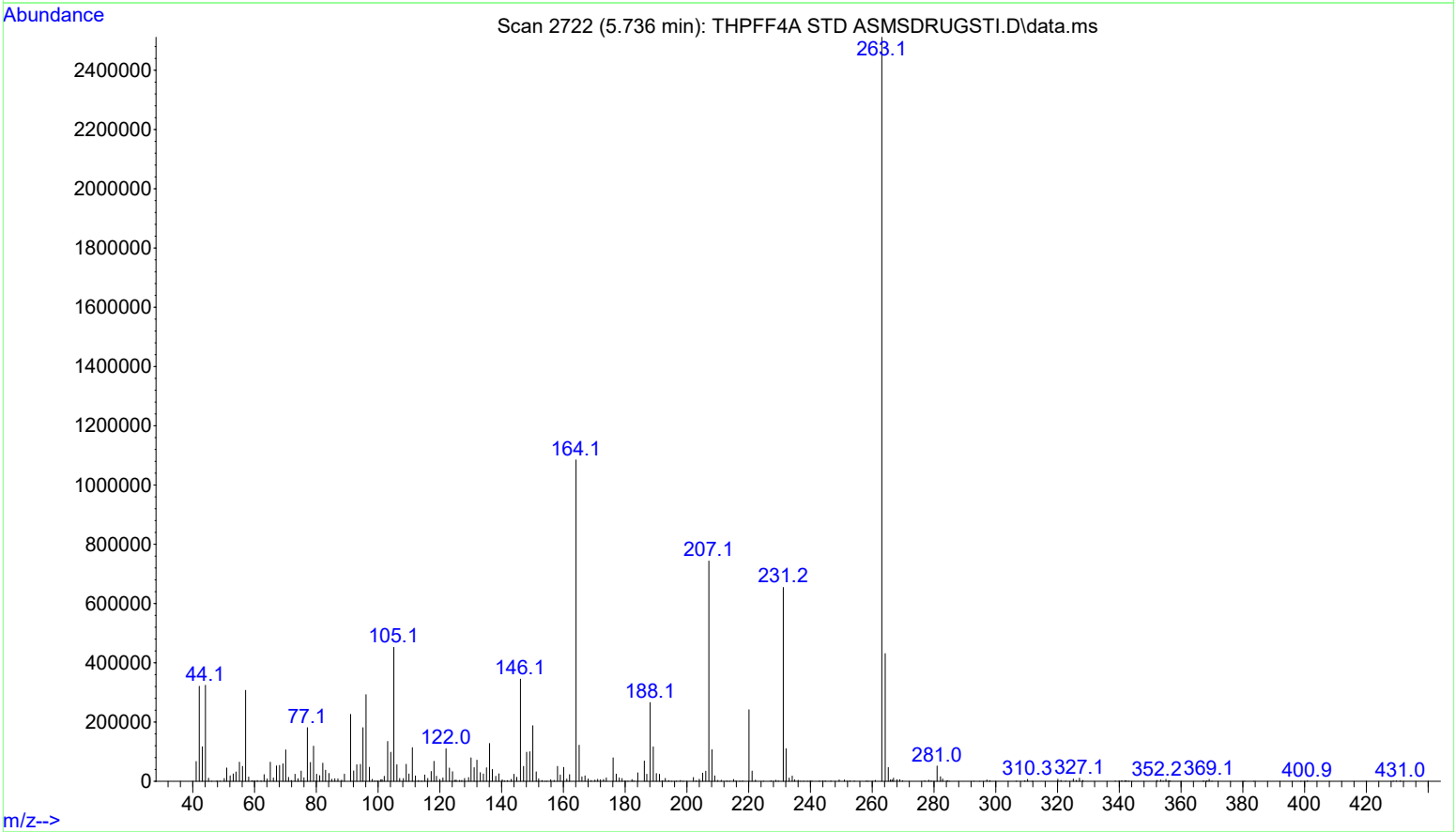


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGSTI.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 19:20 using AcqMethod ASMSDRUGSTI.M
Sample Name: THPFF4A STD EXP. 10-20-23 ASMSDRUGSTI
Misc Info : METHANOL

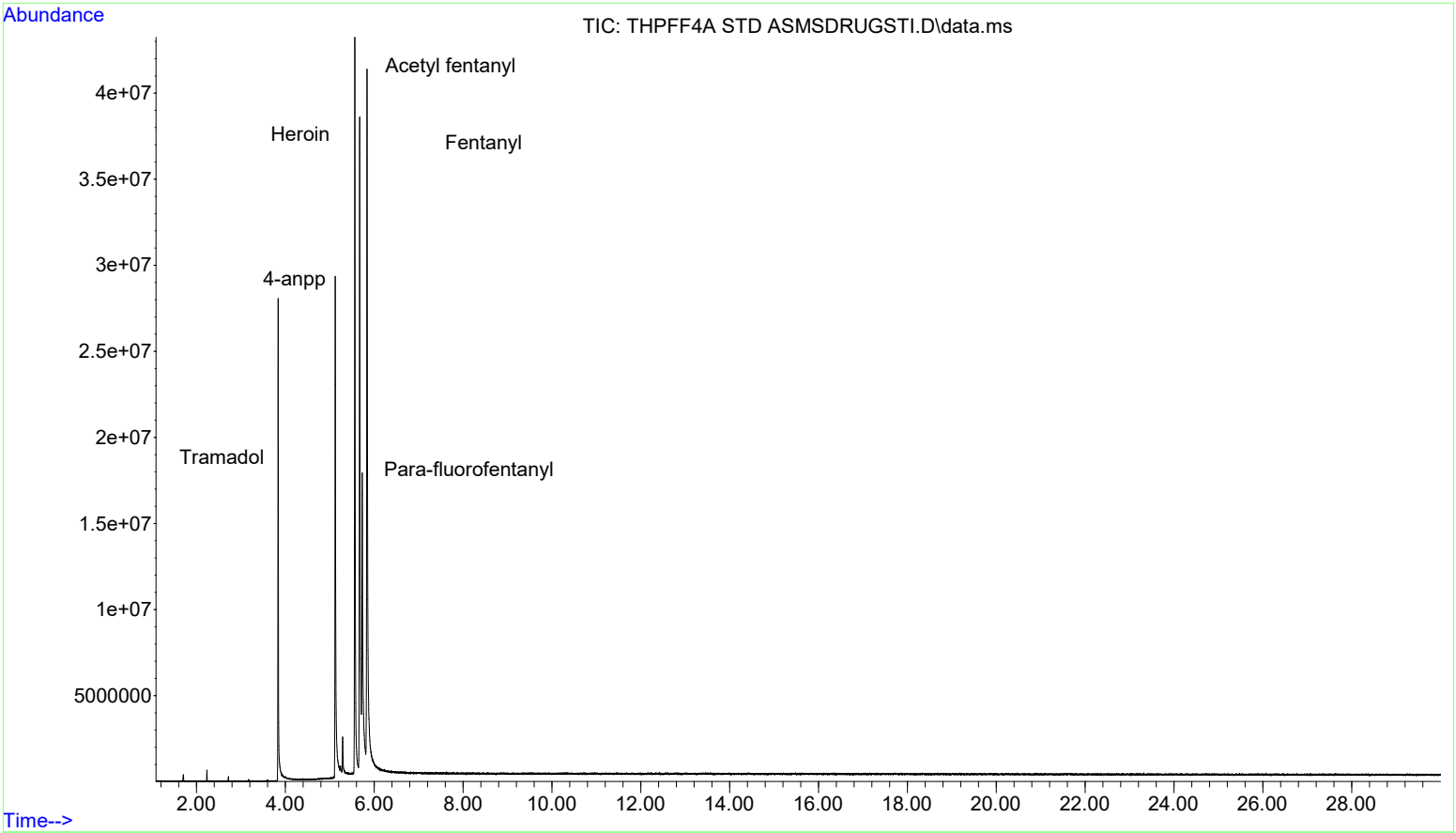


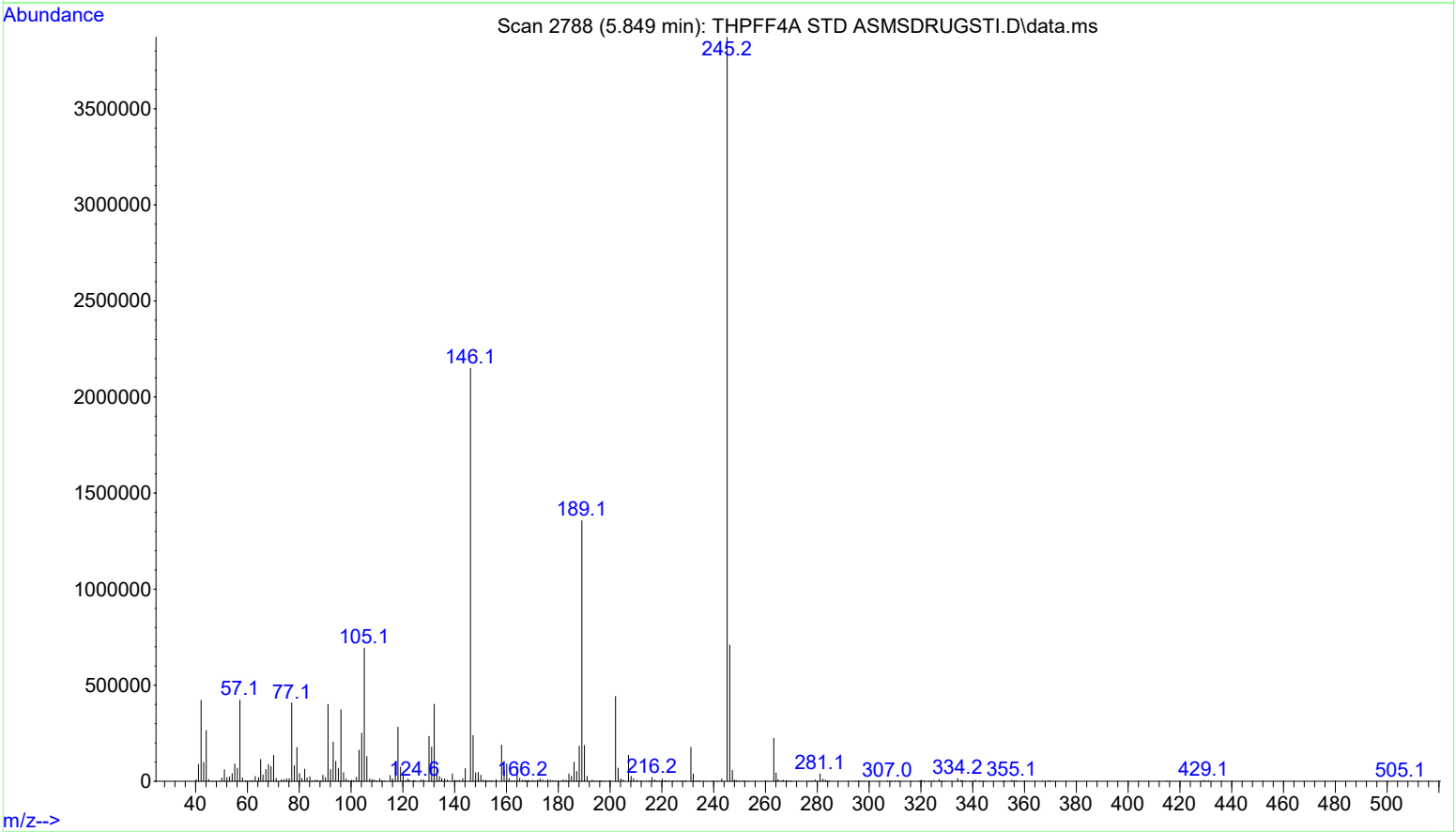


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGSTI.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 19:20 using AcqMethod ASMSDRUGSTI.M
Sample Name: THPFF4A STD EXP. 10-20-23 ASMSDRUGSTI
Misc Info : METHANOL

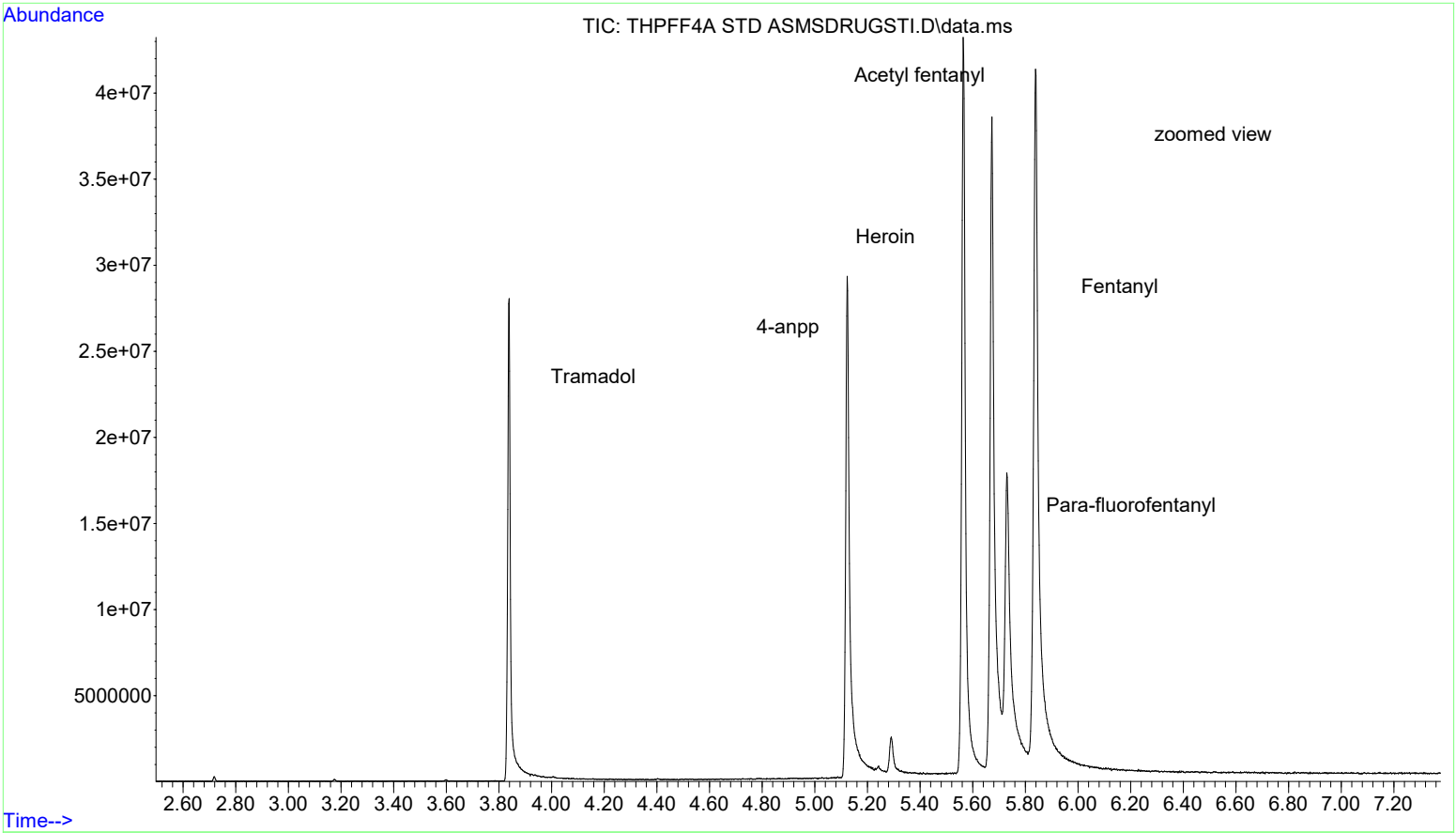


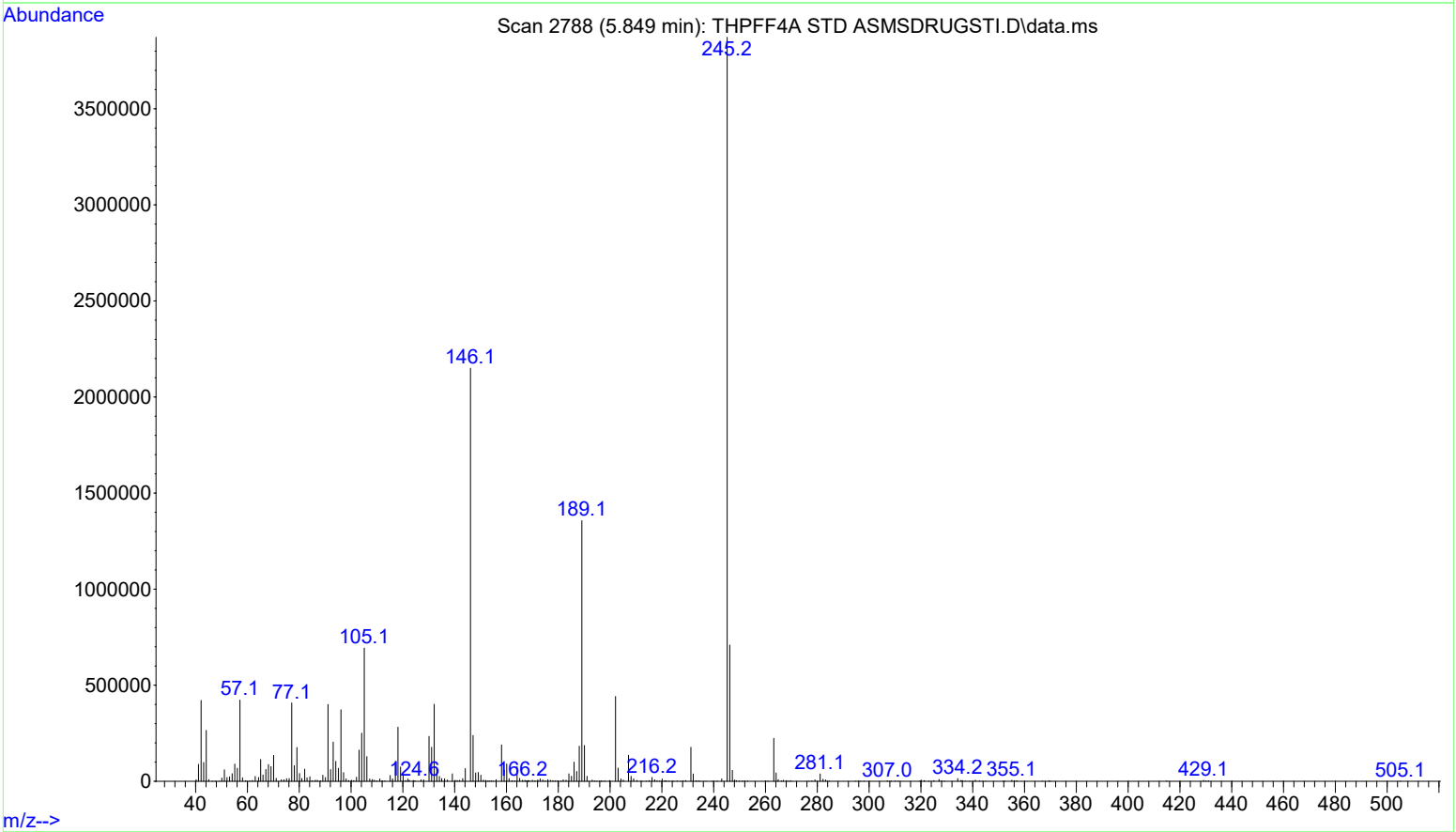


File :Z:\Instruments\GCMS\Heisenberg\2023\BH\3-10-23 validation\TH
... PFF4A STD ASMSDRUGSTI.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 10 Mar 2023 19:20 using AcqMethod ASMSDRUGSTI.M
Sample Name: THPFF4A STD EXP. 10-20-23 ASMSDRUGSTI
Misc Info : METHANOL





Single Quadrupole Acquisition Method - MS Parameters Report

Method file	C:\MassHunter\GCMS\1\methods\MSDRUGS100.M
Tune file	ATUNE.U
Ion source	EI
Source temperature (°C)	230
Quad temperature (°C)	150
Fixed Electron energy (eV)	70.0
Acquisition Type	Scan
Stop time (min)	650.00
Solvent delay (min)	1.00
Trace Ion Detection	False
Gain Factor	1
EM Saver	False
EM Saver Limit	N/A

Scan Time Segments

Time	Start Mass	End Mass	Threshold	Scan Speed
1.00	40	550	150	6,250 [N=0]

Timed Events

Time	Type of Event	Parameter

Real-Time Plots

Type of Plot	Label	Low Mass	High Mass
Total Ion	N/A	N/A	N/A
Spectrum	N/A	N/A	N/A
Extracted Ion	Scan 1-1	50	550

Self-Cleaning Ion Source Parameters

Mode	No Cleaning

METHOD CONTROL PARAMETERS

BH
3-11-23

Method Information for: C:\MassHunter\GCMS\1\methods\MSDRUGS100.M

Method Sections To Run:

( ) Save Copy of Method With Data
( ) Instrument Control Pre-Run Cmd/Macro =
( ) Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
(X) Data Analysis
( ) Instrument Control Post-Run Cmd/Macro =
( ) Data Analysis Post-Run Cmd/Macro =

Method Comments:
MSDRUGS100

END OF METHOD CONTROL PARAMETERS

C:\MassHunter\GCMS\1\methods\MSDRUGS100.M
Fri Mar 10 22:12:35 2023

Control Information
------- -----------

Sample Inlet	: GC
Injection Source	: Manual
Mass Spectrometer	: Enabled

No Sample Prep method has been assigned to this method.

GC
GC Summary

Run Time	10.001 min
Post Run Time	0 min

Oven

Temperature	
Setpoint	On
(Initial)	100 °C
Hold Time	1 min
Post Run	100 °C
Program	
#1 Rate	70 °C/min
#1 Value	280 °C
#1 Hold Time	6.43 min
Equilibration Time	1 min
Max Temperature	325 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled

ALS

Front Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	0
Solvent A Washes (PostInj)	0
Solvent A Volume	4 µL
Solvent B Washes (PreInj)	0
Solvent B Washes (PostInj)	0
Solvent B Volume	4 µL
Sample Washes	1
Sample Wash Volume	1 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0 µL
Solvent Wash Mode	A, B

Back Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	2
Sample Wash Volume	8 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL
Solvent Wash Mode	A, B
Sample Overlap	
Mode	Sample overlap is not enabled
ALS Errors	Pause for user interaction
Front SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 10.806 psi
Total Flow	On 79 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	Off
Split Ratio	75 :1
Split Flow	75 mL/min
Liner	A Liner has not been selected.
Back SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 10 psi
Total Flow	On 256.16 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	On 20 After 2 min mL/min
Split Ratio	75 :1
Split Flow	249.83 mL/min
Liner	A Liner has not been selected.
Thermal Aux 3 (MSD Transfer Line)	
Temperature	
Setpoint	On
(Initial)	280 °C
Column	
Column #1	
Flow	
Setpoint	On
(Initial)	1 mL/min

Post Run	0.57353 mL/min
Column Information	Agilent 19091S-602
HP-1MS	
Temperature Range	-60 °C—325 °C (350 °C)
Dimensions	12.5 m x 200 µm x 0.33 µm (Calibrated)
Column lock	Locked
In	Front SS Inlet He
Out	MSD
(Initial)	100 °C
Pressure	10.806 psi
Flow	1 mL/min
Average Velocity	57.774 cm/sec
Holdup Time	0.3606 min
Control Mode	Constant Flow
Column #2	
Pressure	
Setpoint	On
(Initial)	10 psi
Post Run	3.5859 psi
Column Information	Agilent 19091S-913
HP-1MS	
Temperature Range	-60 °C—325 °C (325 °C)
Dimensions	15 m x 320 µm x 0.25 µm (Calibrated)
Column lock	Locked
In	Back SS Inlet He
Out	Back Detector FID
(Initial)	100 °C
Pressure	10 psi
Flow	3.3311 mL/min
Average Velocity	63.306 cm/sec
Holdup Time	0.39491 min
Control Mode	Constant Pressure
Column Outlet Pressure	0 psi
Back Detector FID	
Makeup	He
Column Compensation	Signal is modified by Column Compensation Curve #2
Heater	On 300 °C
H2 Flow	Off
Air Flow	Off
Makeup Flow (Combined)	Off
Carrier Gas Flow Correction	Column + Makeup = Constant
Flame	Off
Aux EPC 1,2,3	
Aux EPC 1 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***
Aux EPC 2 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

BH
3-11-23

BH
3-11-23

Aux EPC 3 N2 Pressure Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Signals

Signal #1: Description	None
Signal #2: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample
Signal #3: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample
Signal #4: Test Plot	
Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

TUNE PARAMETERS for SN: US1648M021

Trace Ion Detection is OFF.

34.593	:	EMISSION
70.007	:	ENERGY
34.899	:	REPELLER
90.331	:	IONFOCUS
22.672	:	ENTRANCE_LENS
1360.190	:	EMVOLTS
1498.6	:	Actual EMV
1.00	:	GAIN FACTOR
2908.000	:	AMUGAIN
136.750	:	AMUOFFSET
1.000	:	FILAMENT
0.000	:	DCPOLARITY
12.032	:	ENTLENSOFFSET
0.000	:	Ion_Body
0.000	:	EXTLENS
442.000	:	MASSGAIN
-22.000	:	MASSOFFSET

END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

BH
3-11-23

DATA ANALYSIS PARAMETERS

Method Name: C:\MassHunter\GCMS\1\methods\MSDRUGS100.M

Percent Report Settings

Sort By: Signal

Output Destination
    Screen: No
    Printer: Yes
    File: No

Integration Events: AutoIntegrate

Generate Report During Run Method: No

Signal Correlation Window: 0.020

Qualitative Report Settings

Peak Location of Unknown: Apex

Library to Search	Minimum Quality
D:\MassHunter\Library\TBI_DRUG.L	50
D:\MassHunter\Library\CaymanSpectralLibrary 9-29-22.L	50
D:\MassHunter\Library\SWGDRUG 3.10.L	

Integration Events: AutoIntegrate

Report Type: Summary

Output Destination
    Screen: No
    Printer: Yes
    File: No

Generate Report During Run Method: Yes

Quantitative Report Settings

Report Type: Summary

Output Destination
    Screen: Yes
    Printer: No
    File: No

Generate Report During Run Method: No

Calibration Last Updated:

Reference Window: 10.00 Percent
Non-Reference Window: 5.00 Percent
Correlation Window: 0.02 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

Compound Information

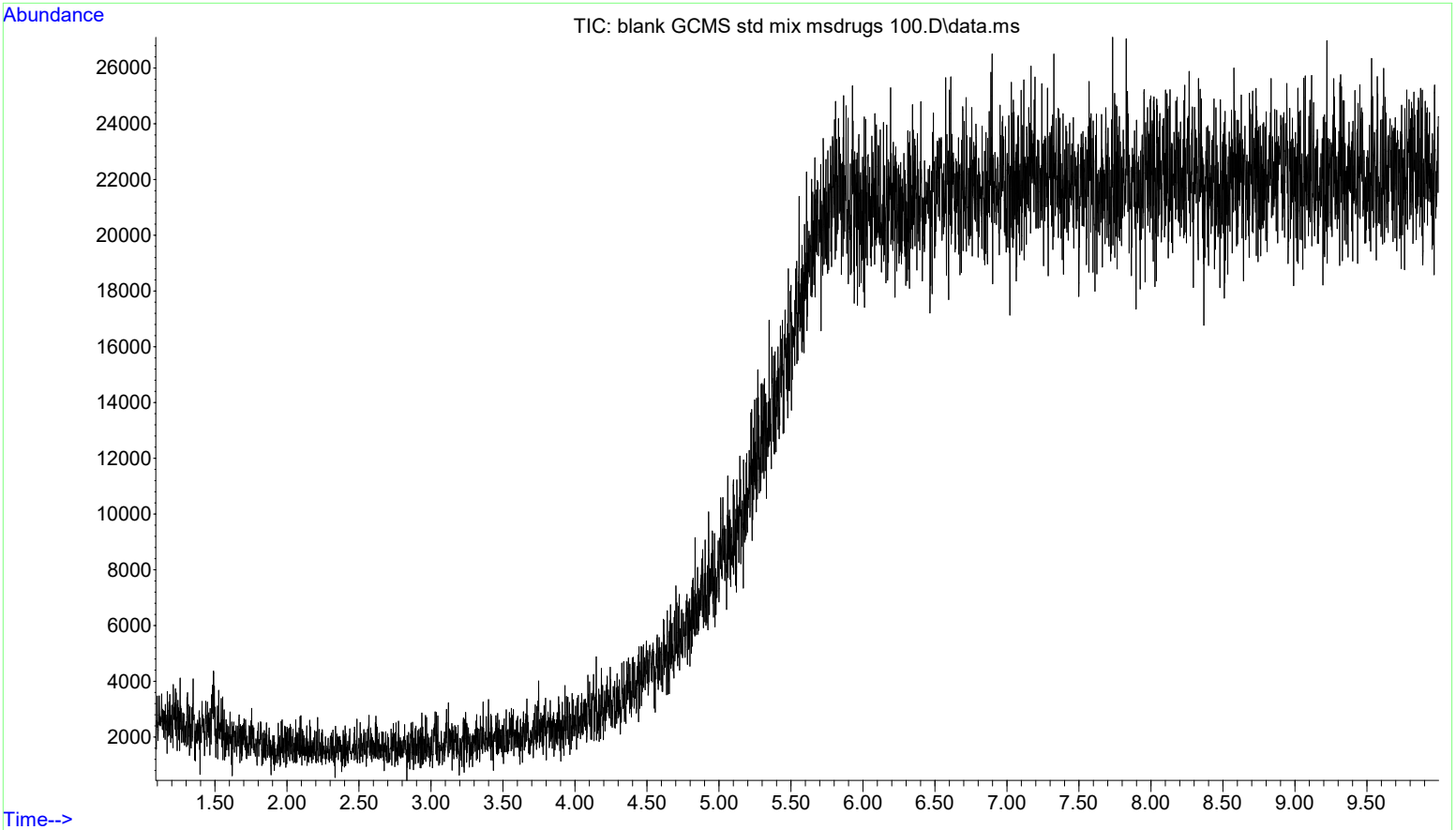
*** Empty Quantitation Database ***

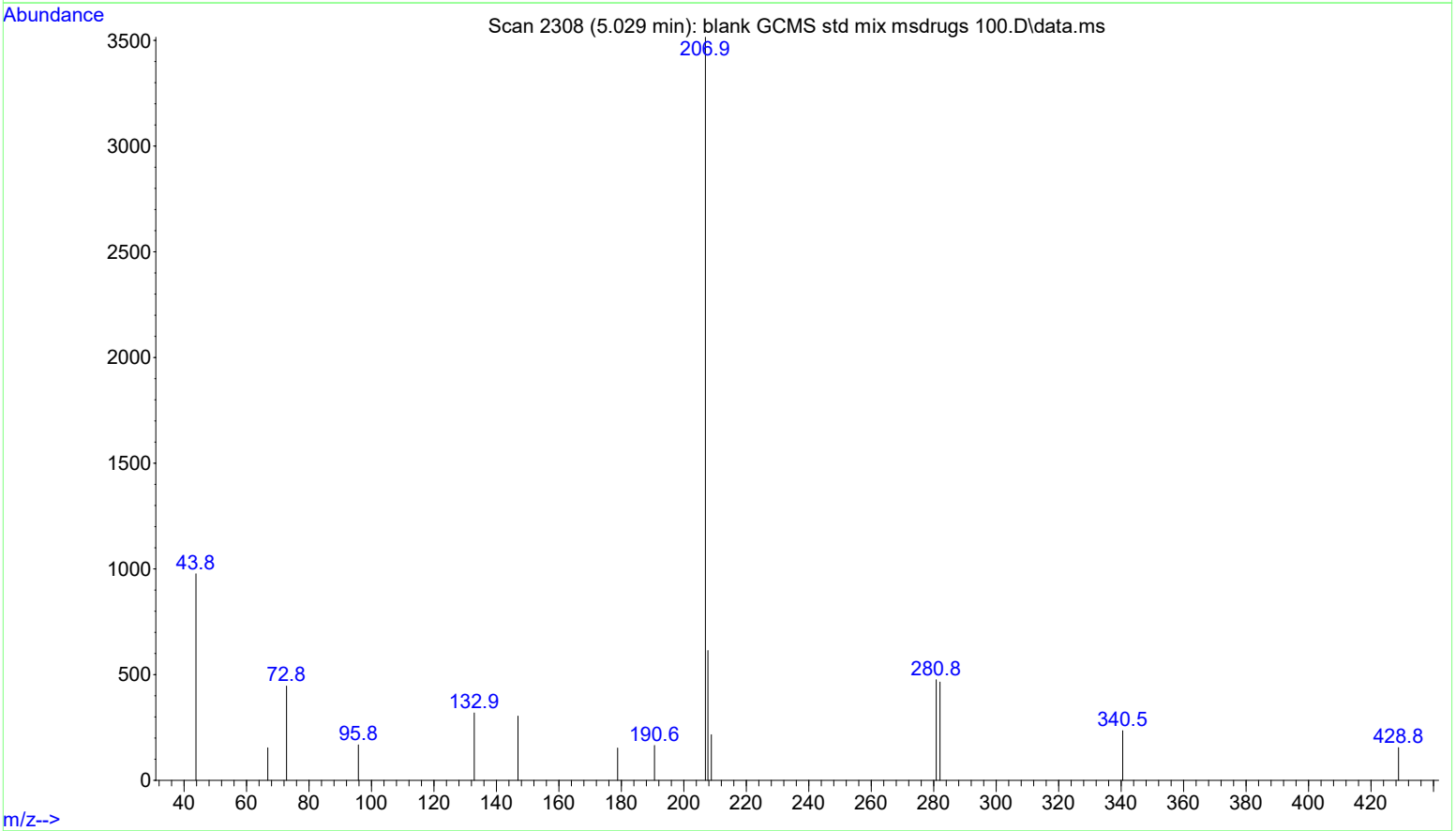
END OF DATA ANALYSIS PARAMETERS

Fri Mar 10 22:13:02 2023

File :Y:\Instruments\GCMS\Heisenberg\2023\BH\03-11-23 val\blank GC
... MS std mix msdrugs 100.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 10:49 using AcqMethod MSDRUGS100.M
Sample Name: blank GCMS std mix msdrugs 100
Misc Info : MEOH

BH
3-11-23

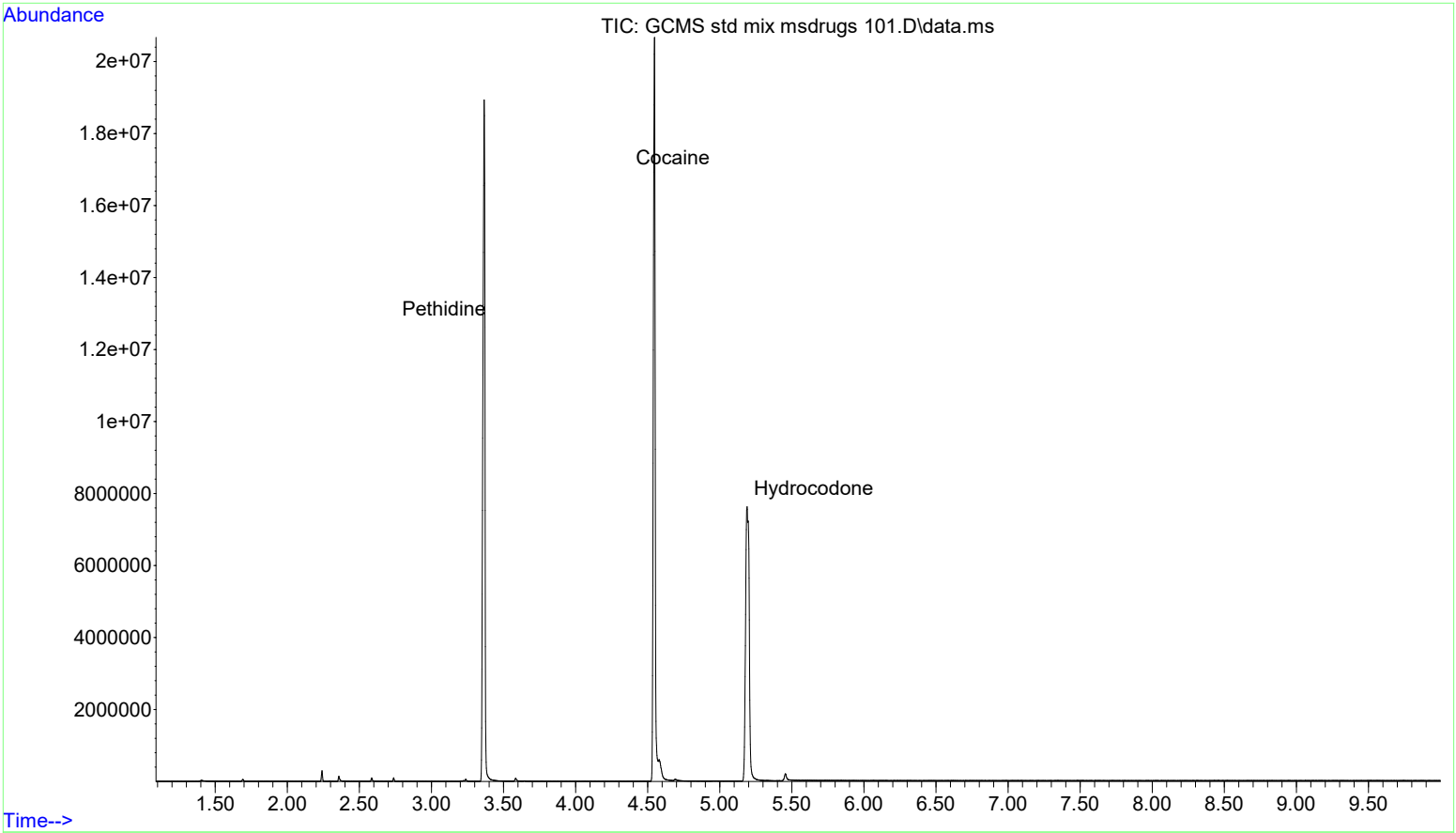


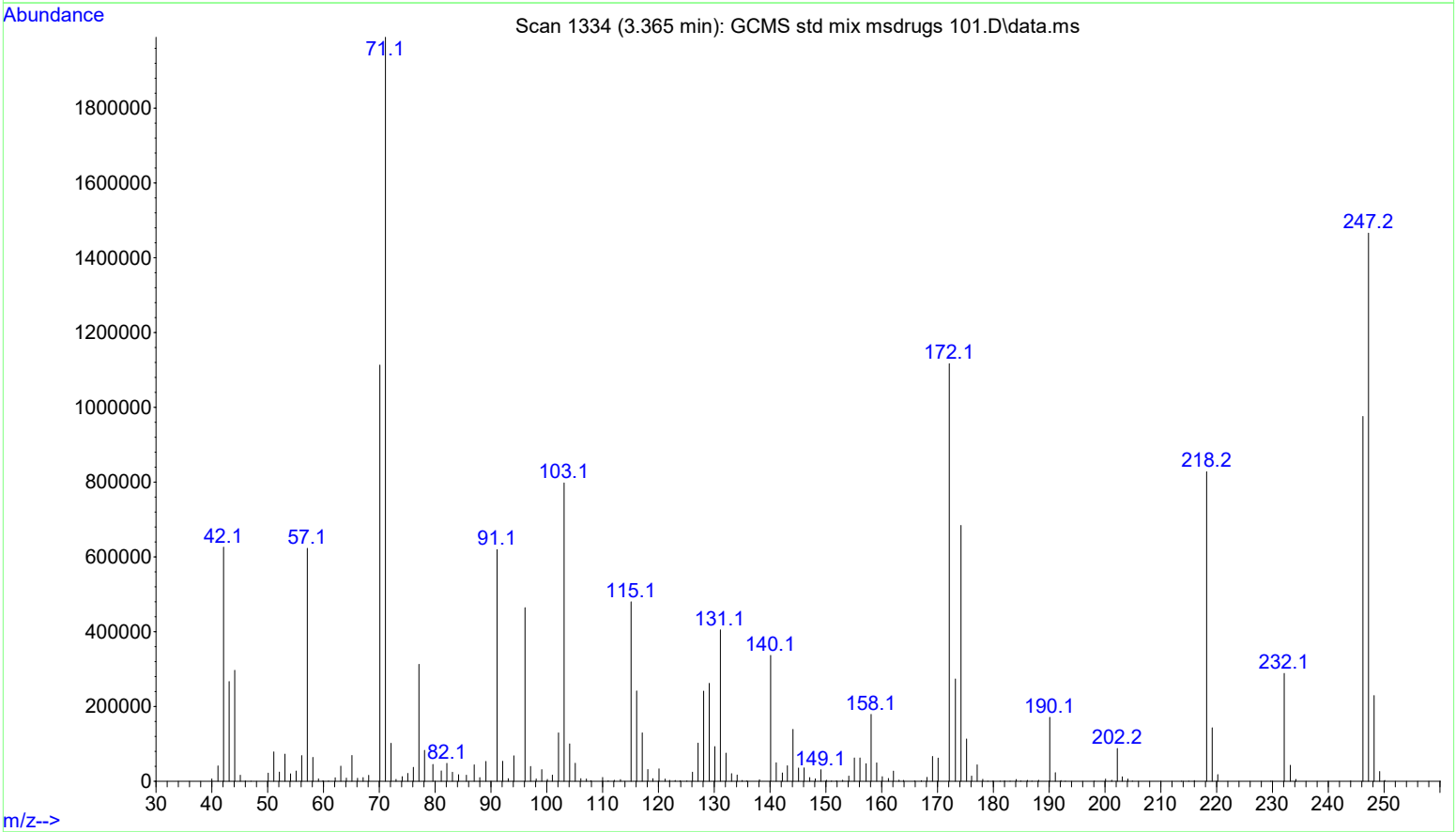


File :Y:\Instruments\GCMS\Heisenberg\2023\BH\03-11-23 val\GCMS std mix msdrugs 101.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 11:03 using AcqMethod MSDRUGS100.M
Sample Name: GCMS std mix msdrugs 100
Misc Info : MEOH

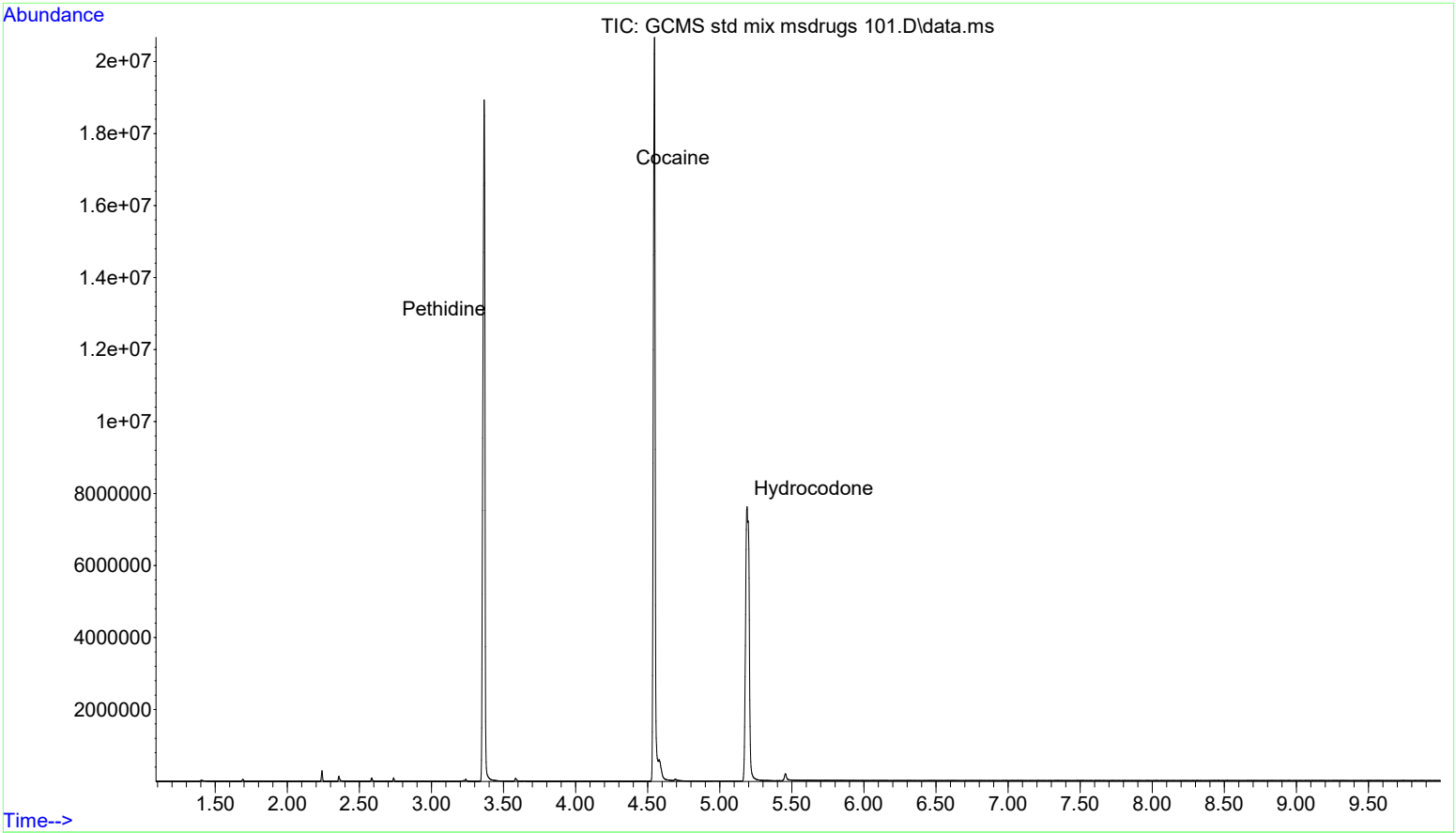


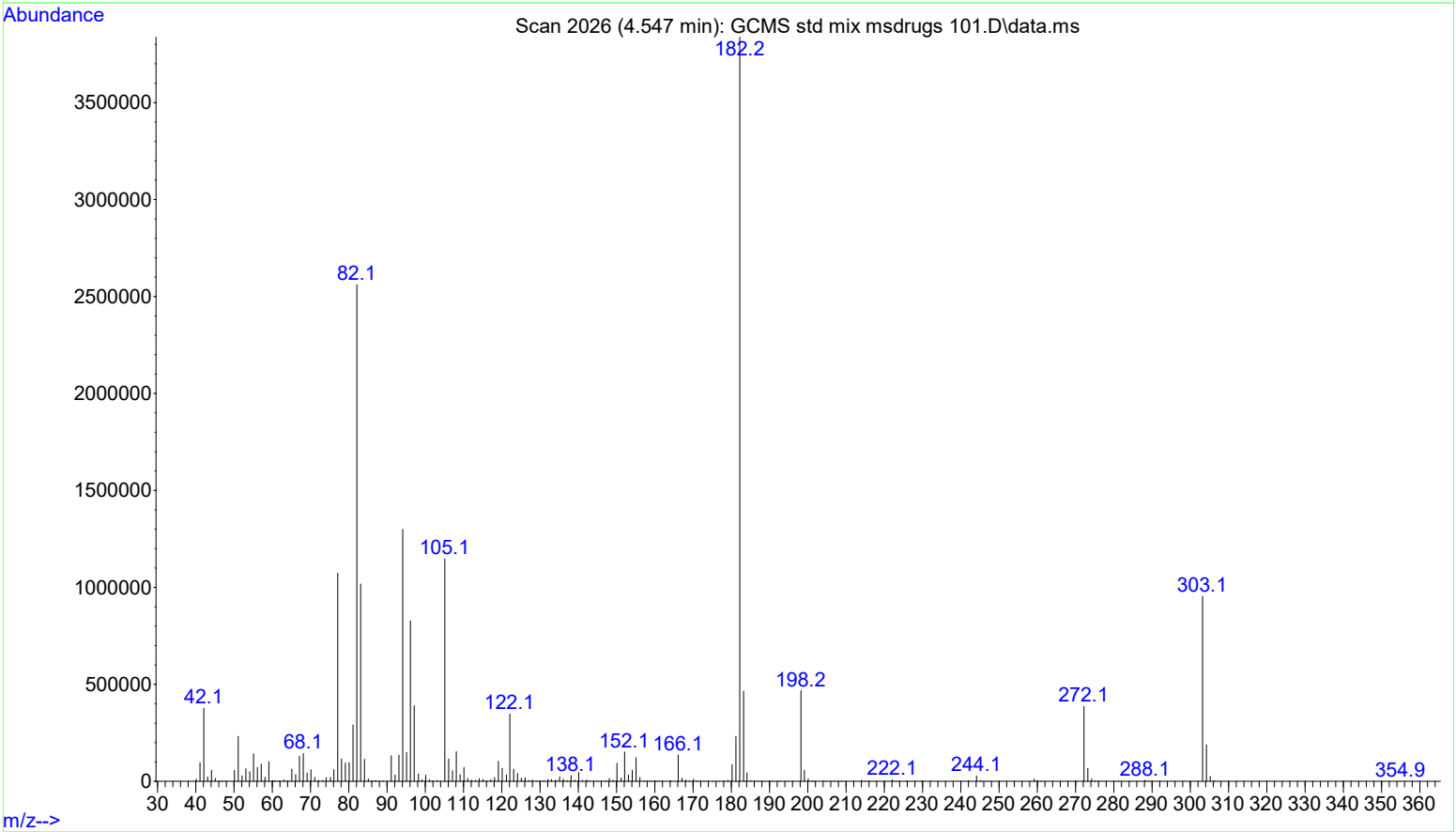


File :Y:\Instruments\GCMS\Heisenberg\2023\BH\03-11-23 val\GCMS std mix msdrugs 101.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 11:03 using AcqMethod MSDRUGS100.M
Sample Name: GCMS std mix msdrugs 100
Misc Info : MEOH

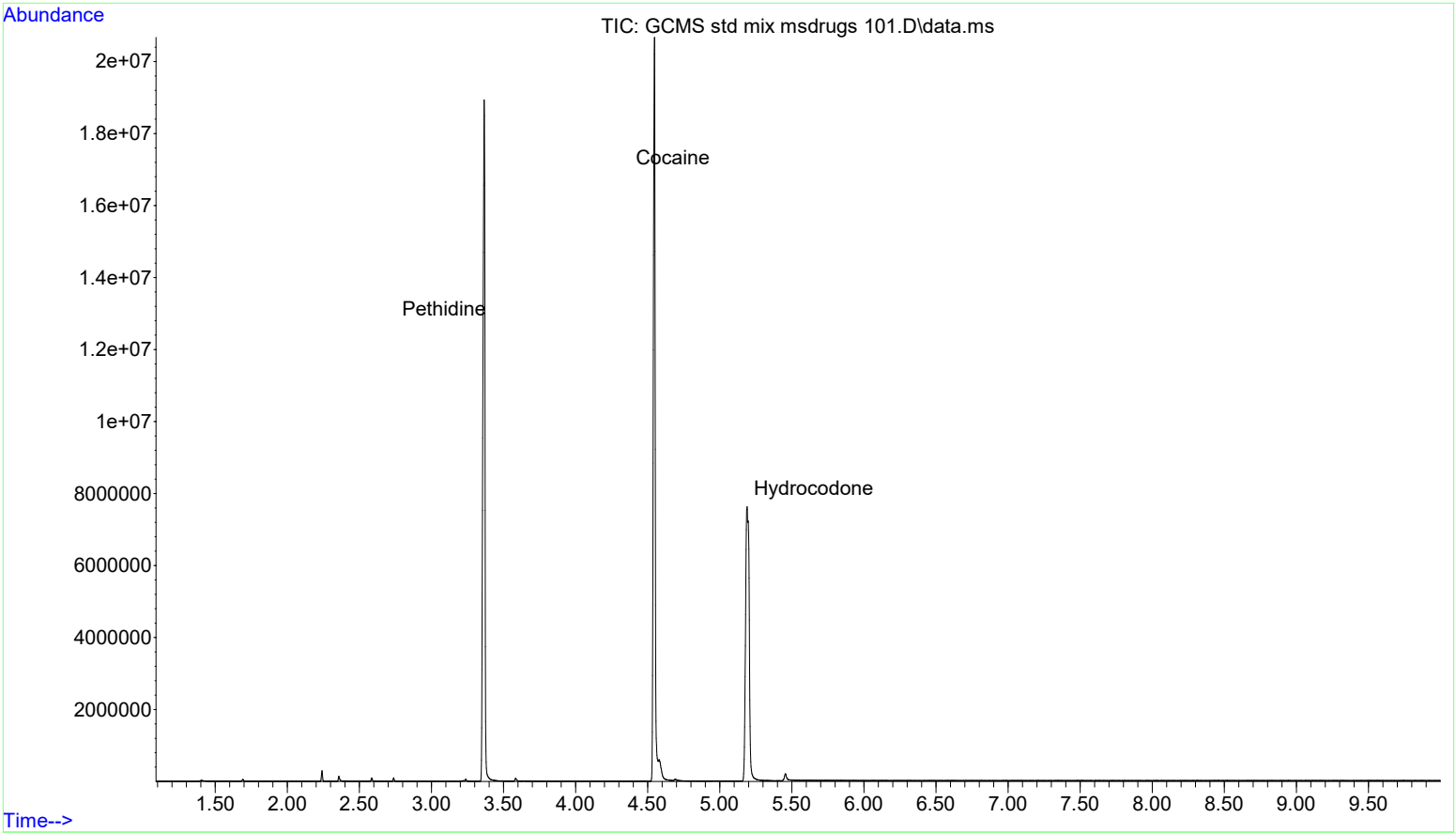


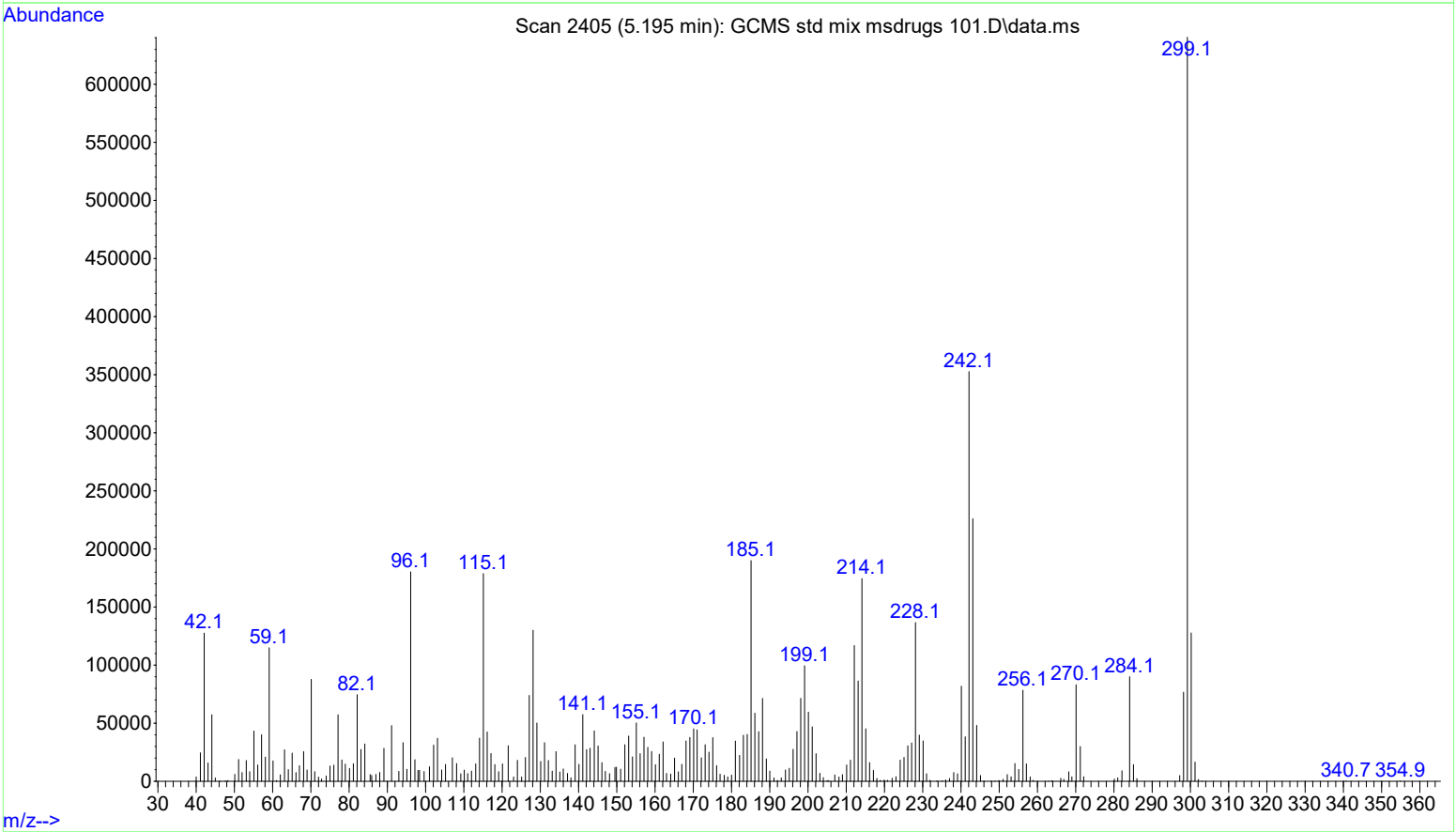


File :Y:\Instruments\GCMS\Heisenberg\2023\BH\03-11-23 val\GCMS std mix msdrugs 101.D

BH
3-11-23

Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 11:03 using AcqMethod MSDRUGS100.M
Sample Name: GCMS std mix msdrugs 100
Misc Info : MEOH





METHOD CONTROL PARAMETERS

BH
3-11-23

Method Information for: C:\MassHunter\GCMS\1\methods\GC100.M

Method Sections To Run:

( ) Save Copy of Method With Data
( ) Instrument Control Pre-Run Cmd/Macro =
( ) Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
(X) Data Analysis
( ) Instrument Control Post-Run Cmd/Macro =
( ) Data Analysis Post-Run Cmd/Macro =

Method Comments:
GC100

END OF METHOD CONTROL PARAMETERS

BH
3-11-23

C:\MassHunter\GCMS\1\methods\GC100.M
Fri Mar 10 22:08:17 2023

Control Information
------- -----------

Sample Inlet : GC
Injection Source : Manual
Mass Spectrometer : Disabled

No Sample Prep method has been assigned to this method.

GC
GC Summary

Run Time	10.001 min
Post Run Time	0 min

Oven
Temperature

Setpoint	On
(Initial)	100 °C
Hold Time	1 min
Post Run	100 °C

Program

#1 Rate	70 °C/min
#1 Value	280 °C
#1 Hold Time	6.43 min

Equilibration Time	1 min
Max Temperature	325 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled

ALS
Front Injector

Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	1
Sample Wash Volume	4 µL
Sample Pumps	2
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	6000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	6000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL
Solvent Wash Mode	A, B

Back Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (PreInj)	3
Solvent A Washes (PostInj)	3
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	3
Solvent B Washes (PostInj)	3
Solvent B Volume	8 µL
Sample Washes	2
Sample Wash Volume	8 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	3000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	3000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Injection Type	Standard
L1 Airgap	0.2 µL
Solvent Wash Mode	A, B
Sample Overlap	
Mode	Sample overlap is not enabled
ALS Errors	Pause for user interaction
Front SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 10.806 psi
Total Flow	On 79 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	Off
Split Ratio	75 :1
Split Flow	75 mL/min
Liner	A Liner has not been selected.
Back SS Inlet He	
Mode	Split
Heater	On 250 °C
Pressure	On 10 psi
Total Flow	On 256.16 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	On 20 After 2 min mL/min
Split Ratio	75 :1
Split Flow	249.83 mL/min
Liner	A Liner has not been selected.
Thermal Aux 3 (MSD Transfer Line)	
Temperature	
Setpoint	On
(Initial)	280 °C
Column	
Column #1	
Flow	
Setpoint	On
(Initial)	1 mL/min

Post Run	0.57353 mL/min
Column Information	Agilent 19091S-602
HP-1MS	
Temperature Range	-60 °C—325 °C (350 °C)
Dimensions	12.5 m x 200 µm x 0.33 µm (Calibrated)
Column lock	Locked
In	Front SS Inlet He
Out	MSD
(Initial)	100 °C
Pressure	10.806 psi
Flow	1 mL/min
Average Velocity	57.774 cm/sec
Holdup Time	0.3606 min
Control Mode	Constant Flow
Column #2	
Pressure	
Setpoint	On
(Initial)	10 psi
Post Run	3.5859 psi
Column Information	Agilent 19091S-913
HP-1MS	
Temperature Range	-60 °C—325 °C (325 °C)
Dimensions	15 m x 320 µm x 0.25 µm (Calibrated)
Column lock	Locked
In	Back SS Inlet He
Out	Back Detector FID
(Initial)	100 °C
Pressure	10 psi
Flow	3.3311 mL/min
Average Velocity	63.306 cm/sec
Holdup Time	0.39491 min
Control Mode	Constant Pressure
Column Outlet Pressure	0 psi
Back Detector FID	
Makeup	He
Column Compensation	Signal is modified by Column Compensation Curve #2
Heater	On 300 °C
H2 Flow	On 40 mL/min
Air Flow	On 400 mL/min
Makeup Flow (Combined)	On 25 mL/min
Carrier Gas Flow Correction	Column + Makeup = Constant
Flame	On
Aux EPC 1,2,3	
Aux EPC 1 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***
Aux EPC 2 N2	
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

BH
3-11-23

Aux EPC 3 N2
Pressure

Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Excluded from Readiness	***Excluded from Affecting GC's Readiness State***

Signals

Signal #1: Back Signal

Description	Back Signal
Details	Back Signal (FID)
Save	On
Data Rate	50 Hz
Dual Injection Assignment	Front Sample

Signal #2: Test Plot

Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

Signal #3: Test Plot

Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

Signal #4: Test Plot

Description	Test Plot
Save	Off
Data Rate	50 Hz
Dual Injection Assignment	Back Sample

TUNE PARAMETERS for SN: US1648M021

Trace Ion Detection is OFF.

35.000	:	EMISSION
70.000	:	ENERGY
25.900	:	REPELLER
90.200	:	IONFOCUS
28.500	:	ENTRANCE_LENS
1200.000	:	EMVOLTS
	1498.6	: Actual EMV
	54.93	: GAIN FACTOR
1800.000	:	AMUGAIN
120.000	:	AMUOFFSET
1.000	:	FILAMENT
0.000	:	DCPOLARITY
13.550	:	ENTLENSOFFSET
0.000	:	Ion_Body
0.000	:	EXTLENS
0.000	:	MASSGAIN
0.000	:	MASSOFFSET

END OF TUNE PARAMETERS

BH
3-11-23

END OF INSTRUMENT CONTROL PARAMETERS

DATA ANALYSIS PARAMETERS

Method Name: C:\MassHunter\GCMS\1\methods\GC100.M

Percent Report Settings

Sort By: Signal

Output Destination
    Screen: No
    Printer: Yes
    File: No

Integration Events: AutoIntegrate

Generate Report During Run Method: Yes

Signal Correlation Window: 0.020

Quantitative Report Settings

Report Type: Summary

Output Destination
    Screen: Yes
    Printer: No
    File: No

Generate Report During Run Method: No

Calibration Last Updated:

Reference Window: 10.00 Percent
Non-Reference Window: 5.00 Percent
Correlation Window: 0.02 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

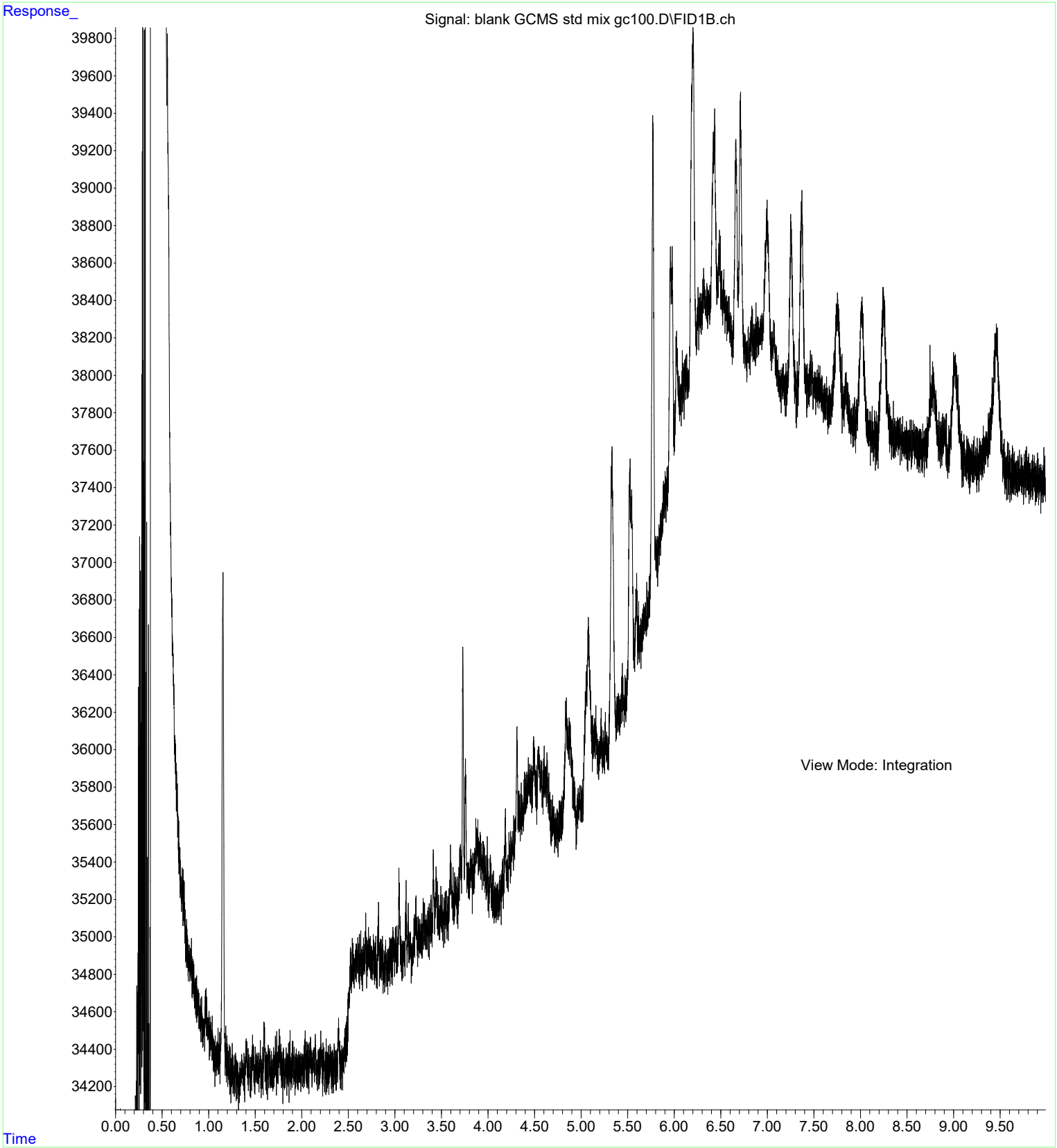
Compound Information

END OF DATA ANALYSIS PARAMETERS

Fri Mar 10 22:08:37 2023

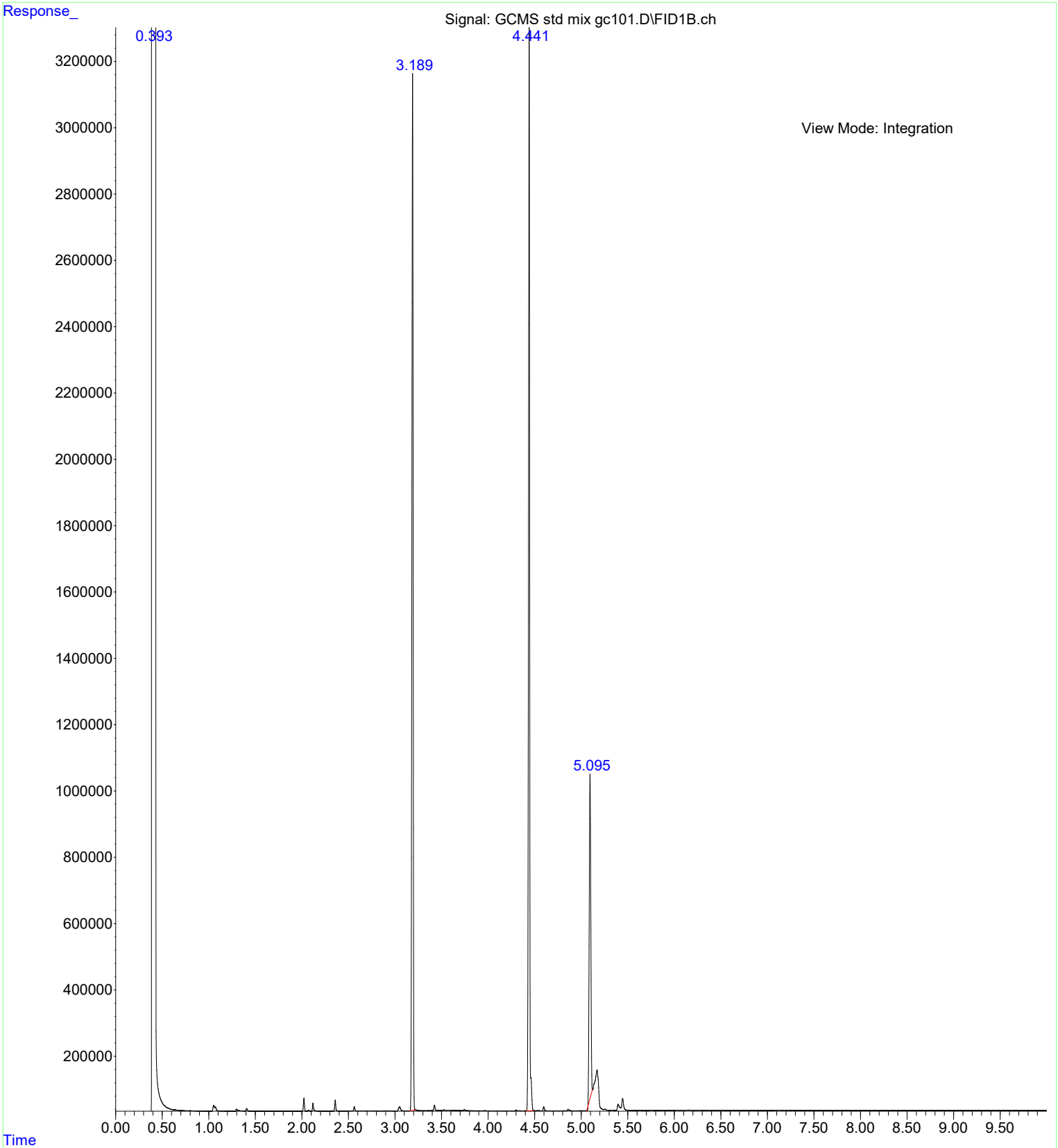
BH
3-11-23

File :Y:\Instruments\GCMS\Heisenberg\2023\BH\03-11-23 val\blank GC
... MS std mix gc100.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 10:01 using AcqMethod GC100.M
Sample Name: blank GCMS std mix gc100
Misc Info : MEOH



BH
3-11-23

File :Y:\Instruments\GCMS\Heisenberg\2023\BH\03-11-23 val\GCMS std
... mix gc101.D
Operator :
Instrument : Heisenberg
Acquired : 11 Mar 2023 10:20 using AcqMethod GC100.M
Sample Name: GCMS std mix gc100
Misc Info : MEOH



BH
3-11-23

Autotune - 5977

Tune timestamp: 3/10/2023 11:00 AM (UTC-06:00) Heisenberg

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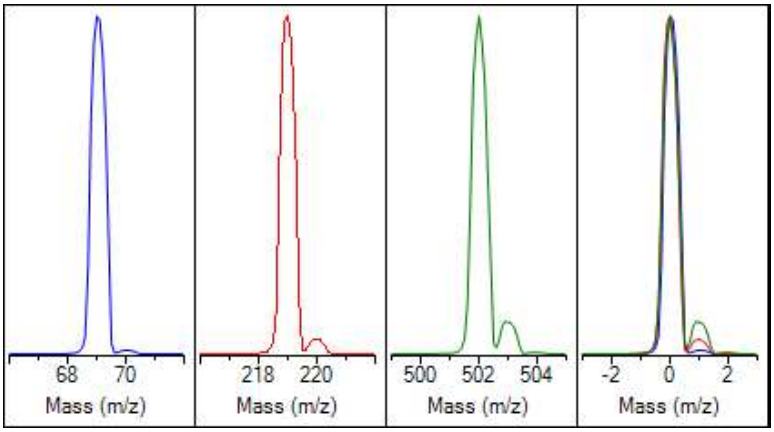
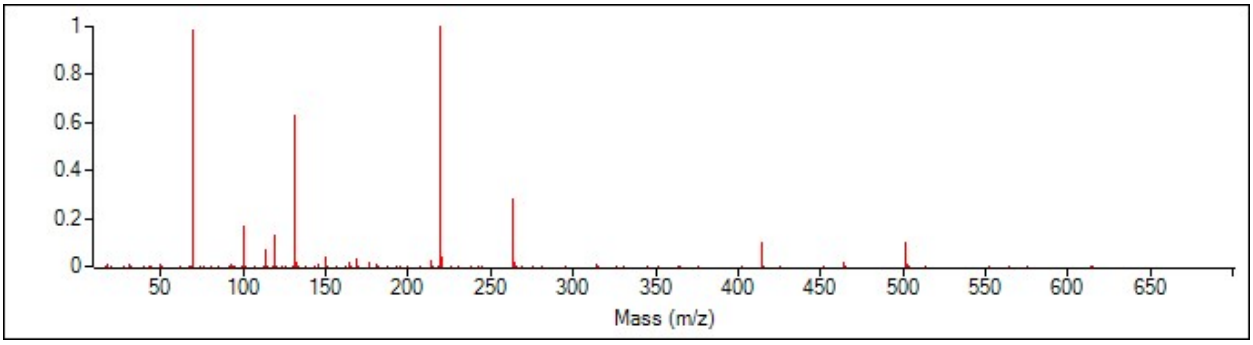


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	442
Electron Energy	70.0	Mass Offset	-22
Filament	1	Amu Gain	2908
Repeller	34.90	Amu Offset	136.75
Ion Focus	90.3	Width219	-0.017
Entrance Lens	22.7	DC Polarity	Pos
Ent Lens Offset	12.03	HED Enable	On
Ion Body	0.00	EM Volts	1360.2
Post Extractor 1	0	Extractor Lens	0.00
Post Extractor 2	0	Scan Speed	3
JetClean Flow Actual/[Setpoint]	0.00 [0.00]	Averages	3

Actual m/z	Abund	Rel Abund	Pw50
69.00	460,536	100.0%	0.60
219.00	470,585	102.2%	0.60
502.00	49,896	10.8%	0.60

Temperatures and Pressures			
MS Source	230	Turbo Speed	100.0
MS Quad	150	Hi Vac	6.61e-06

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	108	219.00	459,712	1,789,092



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio
69.00	69.00	453,952	100.0%	70.00	4,837	1.1%
219.00	219.00	459,712	101.3%	220.00	20,504	4.5%
502.00	502.00	47,784	10.5%	503.00	4,743	9.9%

Air/Water Check: H20 ~1.1% N2 ~0.7% O2 ~0.3% CO2 ~0.1% N2/H20 ~60.5%

Column(1) Flow: 0.72 Column(2): 1.00 ml/min Interface Temp: 280

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 40720.122

Repeller maximum 35 volts using ion 219; Gain Factor 0.4072

Mass Gain Values(Scan Speed): 445(3) 455(2) 465(1) 479(0) 558(FS1) 523(FS2)

TARGET MASS:	50	69	131	219	414	502	1050
Amu Offset	136.8	136.8	136.8	136.8	136.8	136.8	136.8
Entrance Lens Offset	12.0	12.0	12.0	12.0	12.0	12.0	12.0

Report Created: 3/10/2023 11:01 AM (UTC-06:00)

BH
3-11-23

Autotune - 5977

Tune timestamp: 3/11/2023 8:52 AM (UTC-06:00) Heisenberg

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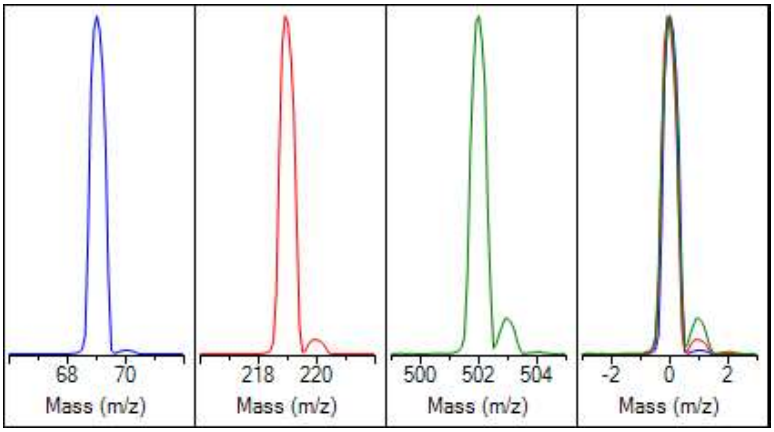
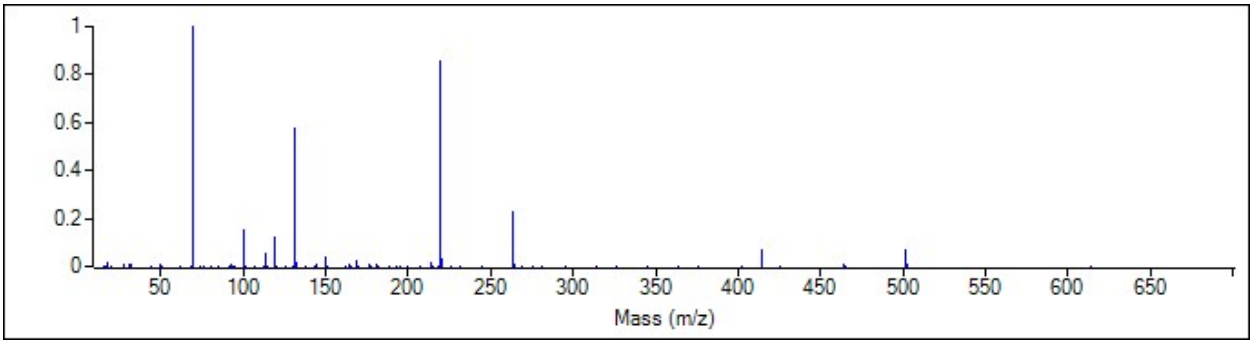


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	441
Electron Energy	70.0	Mass Offset	-23
Filament	1	Amu Gain	2906
Repeller	29.12	Amu Offset	136.25
Ion Focus	90.3	Width219	-0.023
Entrance Lens	20.2	DC Polarity	Pos
Ent Lens Offset	12.19	HED Enable	On
Ion Body	0.00	EM Volts	1395.3
Post Extractor 1	0	Extractor Lens	0.00
Post Extractor 2	0	Scan Speed	3
JetClean Flow Actual/[Setpoint]	0.00 [0.00]	Averages	3

Actual m/z	Abund	Rel Abund	Pw50
69.00	496,564	100.0%	0.60
218.90	426,063	85.8%	0.59
502.00	34,897	7.0%	0.61

Temperatures and Pressures			
MS Source	230	Turbo Speed	100.0
MS Quad	150	Hi Vac	7.87e-06

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	111	69.00	484,288	1,702,837



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio
69.00	69.00	484,288	100.0%	70.00	5,304	1.1%
219.00	219.00	414,656	85.6%	220.00	17,968	4.3%
502.00	502.00	34,288	7.1%	503.00	3,607	10.5%

Air/Water Check: H20 ~1.8% N2 ~0.9% O2 ~0.4% CO2 ~0.1% N2/H20 ~48.5%

Column(1) Flow: 1.00 Column(2): 3.33 ml/min Interface Temp: 280

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 57106.660

Repeller maximum 35 volts using ion 219; Gain Factor 0.5711

Mass Gain Values(Scan Speed): 447(3) 452(2) 466(1) 489(0) 576(FS1) 541(FS2)

TARGET MASS:	50	69	131	219	414	502	1050
Amu Offset	136.3	136.3	136.3	136.3	136.3	136.3	136.3
Entrance Lens Offset	12.2	12.2	12.2	12.2	12.2	12.2	12.2

Report Created: 3/11/2023 8:56 AM (UTC-06:00)

BH
3-11-23

Autotune - 5977

Tune timestamp: 3/11/2023 12:10 PM (UTC-06:00) Heisenberg

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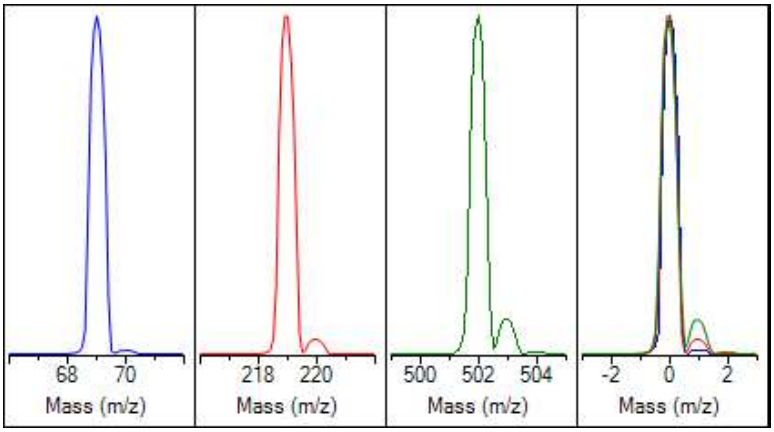
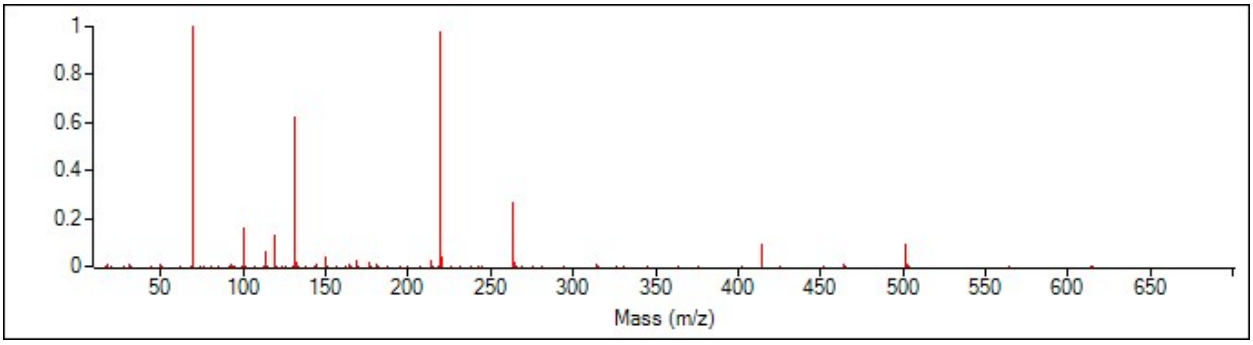


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	440
Electron Energy	70.0	Mass Offset	-24
Filament	1	Amu Gain	2905
Repeller	30.52	Amu Offset	136.25
Ion Focus	90.3	Width219	-0.026
Entrance Lens	20.2	DC Polarity	Pos
Ent Lens Offset	12.19	HED Enable	On
Ion Body	0.00	EM Volts	1388.6
Post Extractor 1	0	Extractor Lens	0.00
Post Extractor 2	0	Scan Speed	3
JetClean Flow Actual/[Setpoint]	0.00 [0.00]	Averages	3

Actual m/z	Abund	Rel Abund	Pw50
69.00	470,576	100.0%	0.60
218.90	458,847	97.5%	0.60
502.00	46,366	9.9%	0.59

Temperatures and Pressures			
MS Source	230	Turbo Speed	100.0
MS Quad	150	Hi Vac	8.52e-06

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	108	69.00	459,200	1,758,198



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio
69.00	69.00	459,200	100.0%	70.00	5,111	1.1%
219.00	219.00	450,304	98.1%	220.00	19,568	4.3%
502.00	502.00	44,760	9.7%	503.00	4,629	10.3%

Air/Water Check: H20 ~1.3% N2 ~0.6% O2 ~0.3% CO2 ~0.1% N2/H20 ~47.3%

Column(1) Flow: 1.00 Column(2): 3.33 ml/min Interface Temp: 280

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 50504.708

Repeller maximum 35 volts using ion 219; Gain Factor 0.5050

Mass Gain Values(Scan Speed): 450(3) 455(2) 467(1) 491(0) 570(FS1) 570(FS2)

TARGET MASS:	50	69	131	219	414	502	1050
Amu Offset	136.3	136.3	136.3	136.3	136.3	136.3	136.3
Entrance Lens Offset	12.2	12.2	12.2	12.2	12.2	12.2	12.2

Report Created: 3/11/2023 12:11 PM (UTC-06:00)