

Performance Check of Buttercup

by: Madison Talley



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Buttercup

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ABSTRACT & VALIDATION OVERVIEW

Agilent 8890 GC System – Serial # US2320A022

Agilent 5977C GC/MSD – Serial # US2313MA09

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The following documentation validates gas chromatograph / mass spectrometer instrumentation acquisitioned from Agilent Technologies for analytical utilization in the Forensic Chemistry Unit (FCU) of the Tennessee Bureau of Investigation Crime Laboratory in Knoxville, Tennessee. Method establishment with parametric consideration of the following parameters-- system temperature (inlet, GC oven ramping and duration, transfer line, MS source, MS quad), column, pressure (inlet, column), flow rates (column, split/split-less), split ratio, liners and autosample tower specifications and adjustments-- inaugurates performance verification of Agilent 8890 GC System and 5977C GC/MSD utilizing a variety of controlled substance analytical standards. These standards ranged in molecular weight and resulting retention time. Because this system is procedurally like GC/MS systems currently in use from Agilent Technologies and validated within the FCU, analysis of analytical standards in the initial method configuration guided subsequent manipulation of parameters to the final establishment of method parameters. Methods were verified as acceptable with performance data of total ion chromatographs, spectral analysis of the mass spectrometer, and chromatographic retention time. Also, during the entire process, inlet maintenance, autotune (atune), and analysis of the calibration standard mix (pethidine, cocaine and hydrocodone) for the GCMS were routinely performed to monitor and assess system functionality. The concluding recommendations from the review of method parameters, functionality, and data of specified analytical standards for specified GC and MS methods is for this Agilent 8890 GC System and 5977C GC/MSD, Buttercup, to be utilized for the analysis of controlled substances in the Forensic Chemistry Unit.

INSTRUMENT AND COMPONENT SPECIFICATIONS

Agilent 8890 GC System – Serial # US2320A022

Agilent 5977C GC/MSD – Serial # US2313MA09

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GAS CHROMATOGRAPH

Agilent 8890 GC System (G3540A)

Serial #US2320A022

MASS SPECTROMETER

Agilent 5977C GC/MSD (G7077C)

Serial #US2313MA09

AUTOSAMPLER TRAY

Agilent G4514A

Serial #R023107021

AUTOSAMPLER TOWERS

MS: Agilent G4513A

Serial #R023025123

GC: Agilent G4513A

Serial #R023035004

COLUMNS

MS: Agilent J&W DB-1MS

Part #128-0112, 12 meters, 0.200 mm diameter, 0.33 μ film thickness

Serial #US3215342A

COMPUTER OPERATING SYSTEM

Device specifications:

Model name	HP Z2 SFF G9 Workstation Desktop PC
Device name	DESKTOP-JSM0SOJ
Processor	12 th Gen Intel® Core™ i5-12500 3.00GHz
Installed RAM	16.0 GB (15.7 GB usable)
Device ID	C9A82879-2C7E-4939-B158-AA7BF4B27567
Product ID	00335-63189-72909-AAOEM
System type	64-bit operating system, x64-based

Windows Specifications:

Edition	Windows 11 Pro
Version	21H2
Installed on	5/5/2023
OS build	22000.194
Experience	Windows Feature Experience Pack 1000.22000.194.0

Productivity tools:

Enhanced ChemStation

MSD ChemStation F.01.03.2365

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Agilent MassHunter Workstation

GC/MS Data Acquisition

Version 10.2.524.1

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PURPOSE OF VALIDATION

Agilent 8890 GC System – Serial # US2320A022

Agilent 5977C GC/MSD – Serial # US2313MA09

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Gas Chromatograph / Mass Spectrometry is critically relied upon within the Forensic Chemistry Unit (FCU) for the analysis of controlled substances. Due to adulterants and multiple controlled substances within samples, chromatographic methodology is a necessity for separation, isolation and identification of these compounds. Historically, Agilent Technologies GC/MS systems have been utilized in the FCU for the past twenty-two years with ChemStation software that is familiar across each 6890/5973, 6890N/5973 inert, 6890N/5975, 7890A/5975C 7890B/5977B and 8890B/5977C GC/MS systems. Therefore, the purpose of this study is to establish method parameters for both gas chromatograph and mass spectrometer utilizing autosample mode of analysis. The methods will then be tested for function and practicality by injecting a variety of analytical standards to demonstrate detection at varying oven temperature initial set points and duration with ramped end points.

TRAINING REQUIREMENTS

Agilent 8890 GC System – Serial # US2320A022

Agilent 5977C GC/MSD – Serial # US2313MA09

Buttercup

The Agilent 8890 GC System and Agilent 5977C GC/MSD performs in concert with ChemStation and MassHunter engine and data analysis software consistent with that of Agilent's 6890/5973, 6890N/5973, 6890N/5975, 7890A/5975C, 7890/5977B and 8890/5977C. Each analyst within the Forensic Chemistry Unit has training and familiarity navigating this system; therefore, no special training is necessary for utilizing this system for analytical casework.

VALIDATION PROCEDURE

Agilent 8890 GC System – Serial # US2320A022

Agilent 5977C GC/MSD – Serial # US2313MA09

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Instrument Setup

The initial instrument setup and check-out procedure was performed by Agilent technical representative Christian Randall. All electrical requirements and performance gases (helium, hydrogen and air) were in place as specified prior to installation.

Maintenance

Throughout the validation procedure, regular inlet maintenance, autotunes, and analysis of the GC/MS Calibration Standard Mix will be performed. Note: this will not necessarily be performed on a weekly basis but in conjunction with time devoted to the development, testing and establishment of the methods.

Establishing Method Parameters

Utilizing the ChemStation software, method construction begins with loading the system's default.m method and referencing established TBI FCU GC/MS methods to first construct DRUG1. From the DRUG1 method, all parameters of the remaining methods will be constructed, named and saved.

General Screening Methods – The GC/MS Calibration Standard Mix (pethidine, cocaine and hydrocodone) and P-MOX standard (phentermine, methamphetamine, xylazine, 4-ANPP, heroin, para-fluorofentanyl, and fentanyl) were analyzed on all general screening methods (DRUG1, STERIOD, XLDRUGS). Additional standards spanning the range of screening analysis were analyzed for the DRUG1 method.

Extended Analysis Methods – Standards of substances known to come out later in extended analysis methods were analyzed on the STERIOD and XLDRUGS method. For STERIOD:

testosterone propionate, and buprenorphine. For XLDRUGS: buprenorphine, isotanitazene, testosterone propionate, and sildenafil.

Drug Specific Methods – Two methods were created for specific drugs/drug classes. Standards that correlate to these methods were analyzed.

For OPIATE: the P-MOX standard mix containing Phentermine, Methamphetamine, Xylazine, 4-ANPP, Heroin, para-Fluorofentanyl, and Fentanyl

For GHB: the GHB standard

Increased Sensitivity Method – A method was created for increased sensitivity as needed for weak or trace amount samples. A diluted version of the P-MOX standard was analyzed on the DRUG1LC method. The same diluted standard was analyzed on the DRUG1 method for comparison.

Evaluation

Acquired data from the aforementioned methods were considered in the establishment of methods, ensuring detection, chromatographic quality, total ion chromatograph and ion abundance as well as baseline separation of standard mixtures such as the GC/MS Calibration Standard Mix (pethidine, cocaine, hydrocodone), the GC/IR Standard Mix (amphetamine, methamphetamine and phentermine) and the P-MOX standard (phentermine, methamphetamine, xylazine, 4-ANPP, heroin, fentanyl, para-fluorofentanyl).

ANALYTICAL STANDARD SPECIFICATIONS

Agilent 8890 GC System – Serial # US2320A022

Agilent 5977C GC/MSD – Serial # US2313MA09

Buttercup

STANDARDS ANALYZED

Alprazolam STD

MEOH (Fisher lot# 198477 Bottle #3/4 exp. u/c)

(Sigma# 117K4017)

Made by ZJ 3/25/22

Reverified by LMM 3/3/23 exp. 3/3/24

Buprenorphine HCl

MEOH (Fisher lot# 197710 Bottle #2/4 exp. u/c)

(Sigma# SLBN0684V)

Made by LMM 9-8-22 exp. 9-8-23

GCIR Standard Mix

CHCl₃ (ACROS lot# B0542909B Bottle #1/4 exp. u/c)

W/ DI H₂O cap + NH₄OH (BDH 3014-500 MLP, lot# 2014061276 exp. u/c)

Amphetamine (Sigma# 79H0603)

Methamphetamine (Sigma# 50H02161)

Phentermine HCl (Sigma# 074K1059)

Made by ZJ 2/2/23 exp. 2/1/24

GHB STD

MEOH (Fisher lot# 217364 Bottle 4/4 exp. u/c)

(Sigma# 089H3410)

Made by CNS 6/14/23 exp. 6/14/24

Isotonitazene STD

MeOH (Fisher lot# 217364 Bottle 4/4 exp. u/c)

(Cayman# 0586760-21)

Made by ZJ 6/1/23 exp. 6/1/24

P-MOX STD

CHCl₃ (ACROS lot# B0542909B Bottle #1/4 exp. u/c)

w/ DI H₂O + base cap NH₄OH (BDH lot# 3014-500MLP)

Phentermine (Sigma# 074K1059)

Methamphetamine (Sigma# 071K1580)

Xylazine (Cayman# 0471462-19)

Heroin (Cayman# 0559235-10)

Para-Fluorofentanyl (Cayman# 0541563-43)

Fentanyl (Cayman# 0549959-44)

4-ANPP (Cayman# 0540831-18)

Made by NAH 6/13/23 exp. 6/12/24

Standard Mix

CHCl₃ (ACROS Fisher lot# B0542909B exp. u/c)

w/ DI H₂O + base cap NH₄OH (BDH lot# 2014042806 exp. u/c)

Pethidine (S.B. Penick# 413NMN-027)

Cocaine (Sigma# 69H1240)

Hydrocodone (Cayman Chem# 0524561-22-STD 1/2)

Hydrocodone (Cayman Chem# 0524561-22-STD 2/2)

Made by LMM 5/19/23 exp. 5/19/24

Sildenafil STD

MeOH (Fisher lot# 217364 Bottle 4/4 exp. u/c)

(Cayman# 0464768-1)

Made by CNS 6/15/23 exp. 6/14/24

Testosterone Propionate STD

MEOH (Fisher lot# 223204 exp. u/c)

(Sigma# 034K0695)

Made by CES 5/24/23 exp. 5/24/24

METHODS AND STANDARDS ANALYZED

Agilent 8890 GC System – Serial # US2320A022

Agilent 5977C GC/MSD – Serial # US2313MA09

Buttercup

MASS SPEC – AUTO SAMPLE INJECTION

DRUG1

ALPRAZOLAM STD
BUPRENORPHINE STD
GCIR STD MIX
GC/MS CALIBRATION MIX
ISOTONITAZENE STD
P-MOX STD

OPIATE

GC/MS CALIBRATION MIX
P-MOX STD

DRUG1LC

P-MOX STD (DILUTED)

GHB

GHB STD

XLDRUG

BURPRENORPHINE STD
GC/MS CALIBRATION MIX
ISOTONITAZENE STD
P-MOX STD
SILDENAFIL STD
TESTOSTERONE PROPIONATE STD

STEROID

BUPRENORPHINE STD
GC/MS CALIBRATION MIX
P-MOX STD
TESTOSTERONE PROPINATE STD

METHOD CONTROL PARAMETERS

Method Information for: D:\MassHunter\GCMS\1\methods\DRUG1.M

Method Sections To Run:

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

Method Comments:

Profile method

END OF METHOD CONTROL PARAMETERS

Single Quadrupole Acquisition Method - MS Parameters Report

Method file	D:\MassHunter\GCMS\1\methods\DRUG1.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)	10.00
Solvent delay (min)	2.50
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
2.50	40	500	150	1,562 [N=2]

Timed Events

Time	Type of Event	Parameter
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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

Self-Cleaning Ion Source Parameters

Mode	No Cleaning
------	-------------

D:\MassHunter\GCMS\1\methods\DRUG1.M

Thu Aug 24 15:38:38 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 14.667 min
Post Run Time 0 min

Oven
Temperature
Setpoint On
(Initial) 80 °C
Hold Time 1.5 min
Post Run 0 °C
Program
#1 Rate 30 °C/min
#1 Value 280 °C
#1 Hold Time 6.5 min

Equilibration Time 1 min
Max Temperature 350 °C
Maximum Temperature Override Disabled
Slow Fan Disabled

ALS
Front Injector
Syringe Size 10 µL
Injection Volume 1 µL
Solvent A Washes (PreInj) 1
Solvent A Washes (PostInj) 1
Solvent A Volume 8 µL
Solvent B Washes (PreInj) 1
Solvent B Washes (PostInj) 1
Solvent B Volume 8 µL
Sample Washes 1
Sample Wash Volume 8 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 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
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	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	
Helium Conservation Controlled Mode	Off
Heater	Split
Pressure	On 250 °C
Total Flow	On 9 psi
Septum Purge Flow	On 58.248 mL/min
Pre-Run Flow Test	On 3 mL/min
Gas Saver	Off
Split Ratio	On 20 mL/min after 2 min
Split Flow	55 :1
Liner	54.261 mL/min
	Agilent 5190-2271: 900 µL (Splitless, single taper, wool, c
Back SS Inlet He	
Helium Conservation Controlled Mode	Off
Heater	Split
Pressure	Off
Total Flow	Off
Septum Purge Flow	Off
Pre-Run Flow Test	Off
Liner	Off
	A Liner has not been selected.
Column	
Column #1	
Flow	
Setpoint	On
(Initial)	0.98657 mL/min
Post Run	1 mL/min
Column Information	Agilent 128-0112: 1
Description	DB-1ms

Temperature Range	-60 °C-340 °C (350 °C)
Dimensions	12 m x 200 µm x 0.33 µm (Calibrated)
Heater	Oven
Column lock	Unlocked
In	Front SS Inlet He
Out	MSD
(Initial)	80 °C
Pressure	9 psi
Flow	0.98657 mL/min
Average Velocity	58.054 cm/sec
Holdup Time	0.3445 min
Control Mode	Constant Flow
Column Outlet Pressure	0 psi
Front Detector FID	
Makeup	He
Heater	Off
H2 Flow	Off
Air Flow	Off
Makeup Flow	Off
Carrier Gas Flow Correction	Constant Makeup and Fuel Flow
Flame	Off
Blank Evaluation Setpoints	
Perform Blank Evaluation Test	Off
Helium Conservation	
Helium Valve	Off
Nitrogen Valve	Off
Detector Evaluation	
Perform Detector Evaluation Test	Off
MSD Transfer Line	
Temperature	
Setpoint	On
(Initial)	280 °C
Signals	
Signal #1:	
Description	None
Signal #2:	
Description	None
Signal #3:	
Description	None
Signal #4:	
Description	None
Signal #5:	
Description	None
Signal #6:	
Description	None
Signal #7:	
Description	None
Signal #8:	
Description	None

TUNE PARAMETERS for SN: US2313MA09

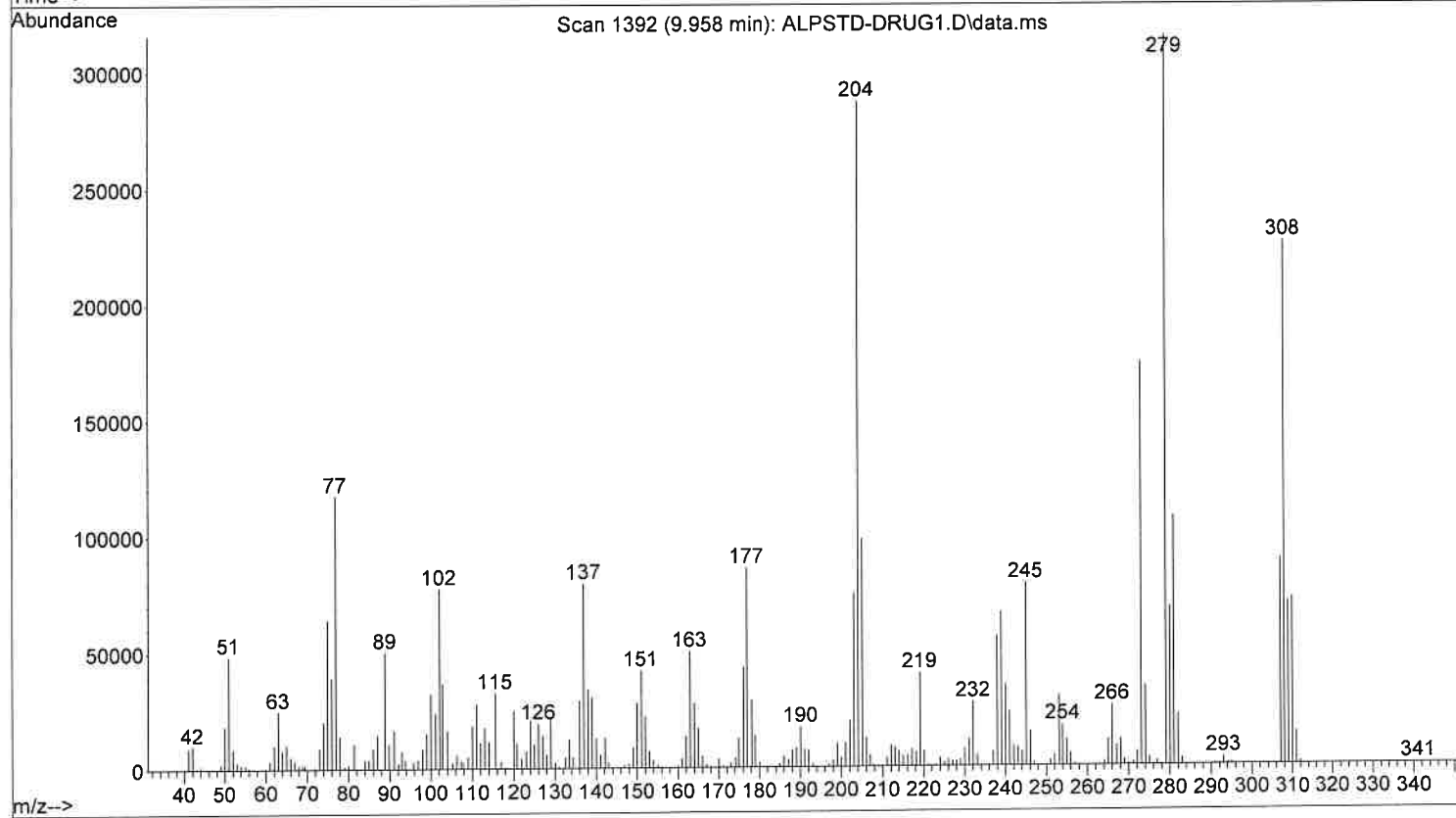
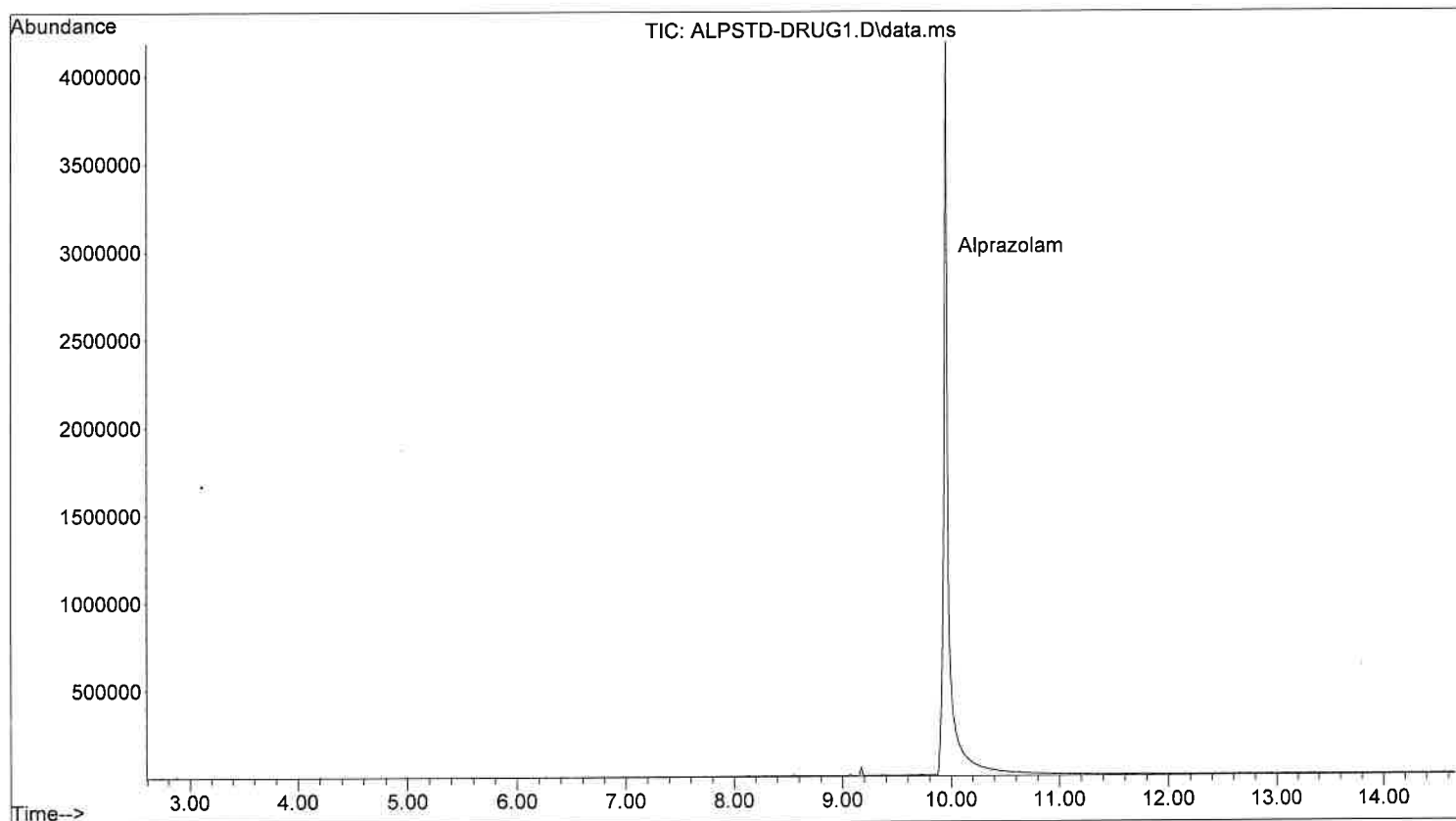
Trace Ion Detection is OFF.

34.593	:	EMISSION	
70.007	:	ENERGY	
29.919	:	REPELLER	
90.331	:	IONFOCUS	
25.226	:	ENTRANCE_LENS	
925.472	:	EMVOLTS	
		951.5	: Actual EMV
		1.00	: GAIN FACTOR
2896.000	:	AMUGAIN	
134.625	:	AMUOFFSET	
1.000	:	FILAMENT	
0.000	:	DCPOLARITY	
10.822	:	ENTLENSOFFSET	
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-23.000	:	MASSOFFSET	

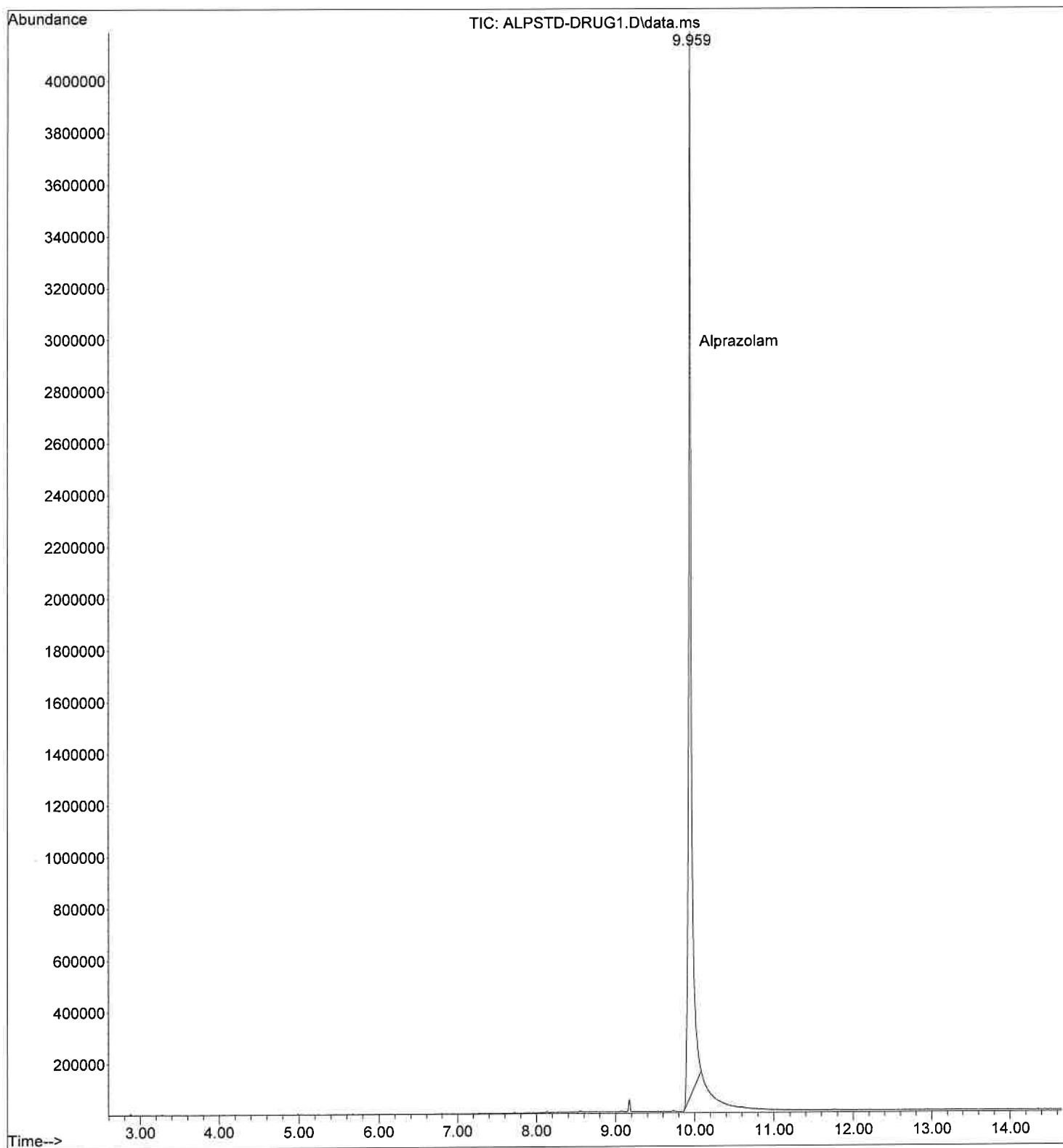
END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

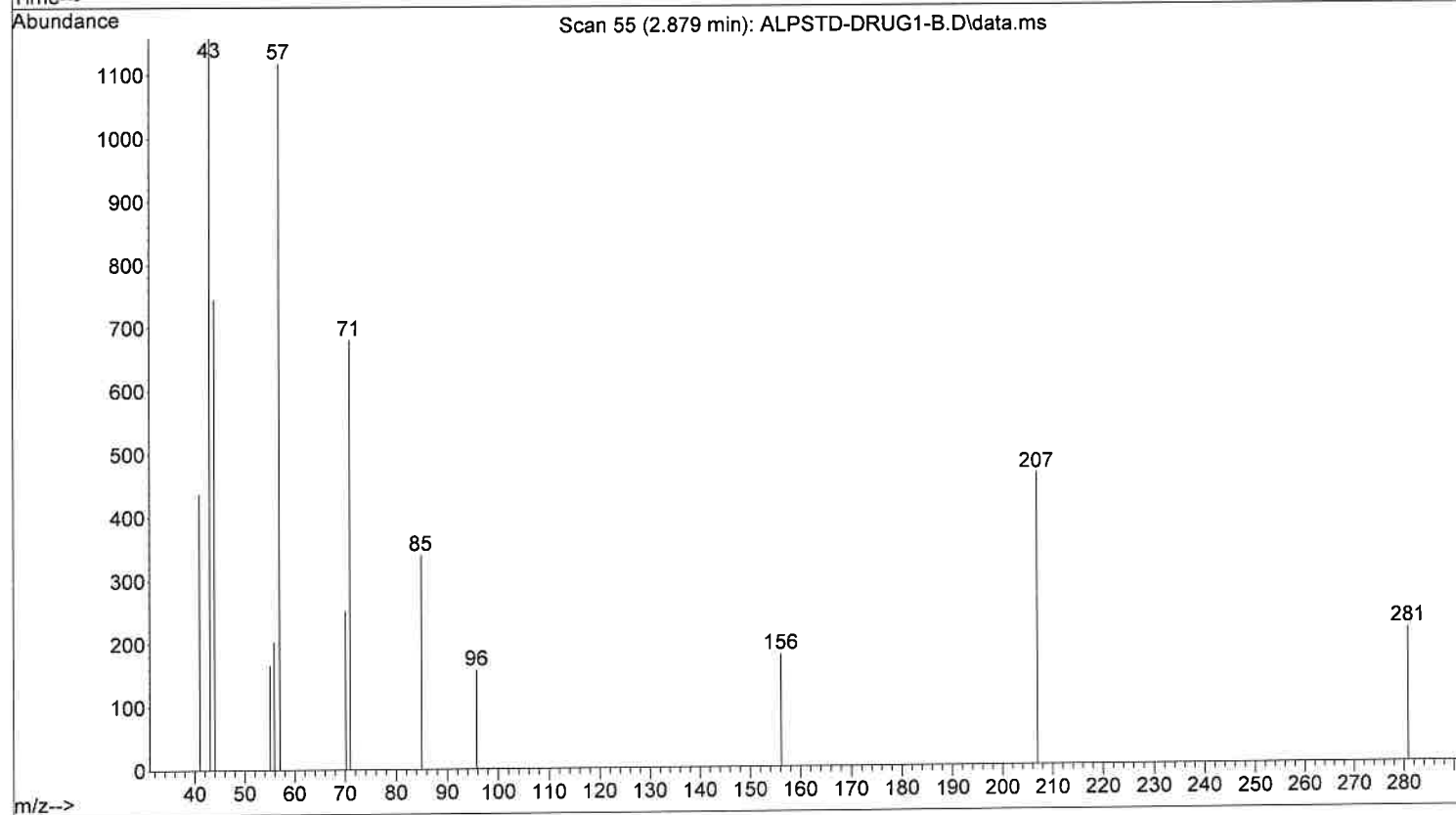
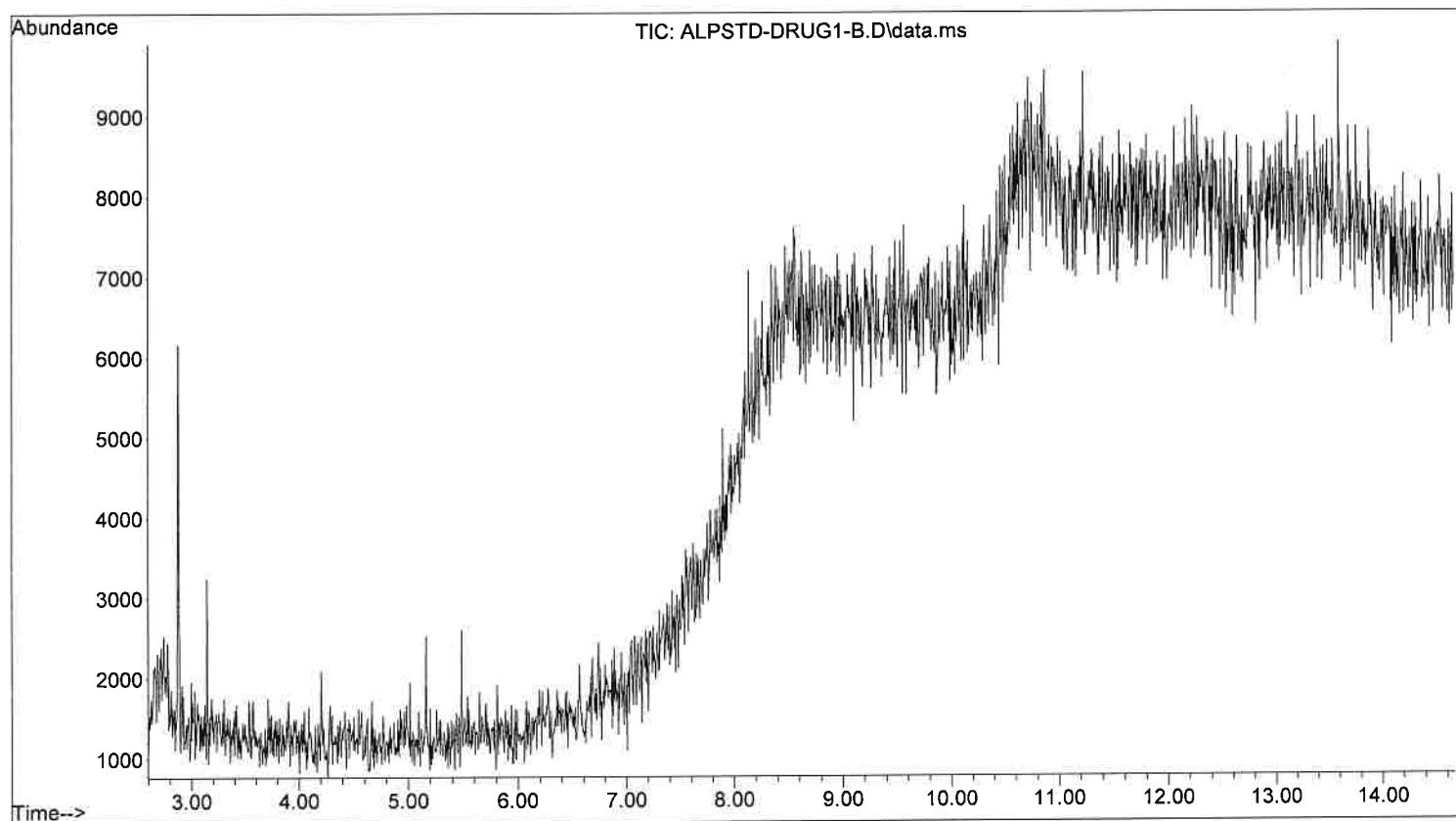
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Acquired : 18 Aug 2023 13:05 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Alprazolam Standard
Misc Info : in Methanol
Vial Number: 146



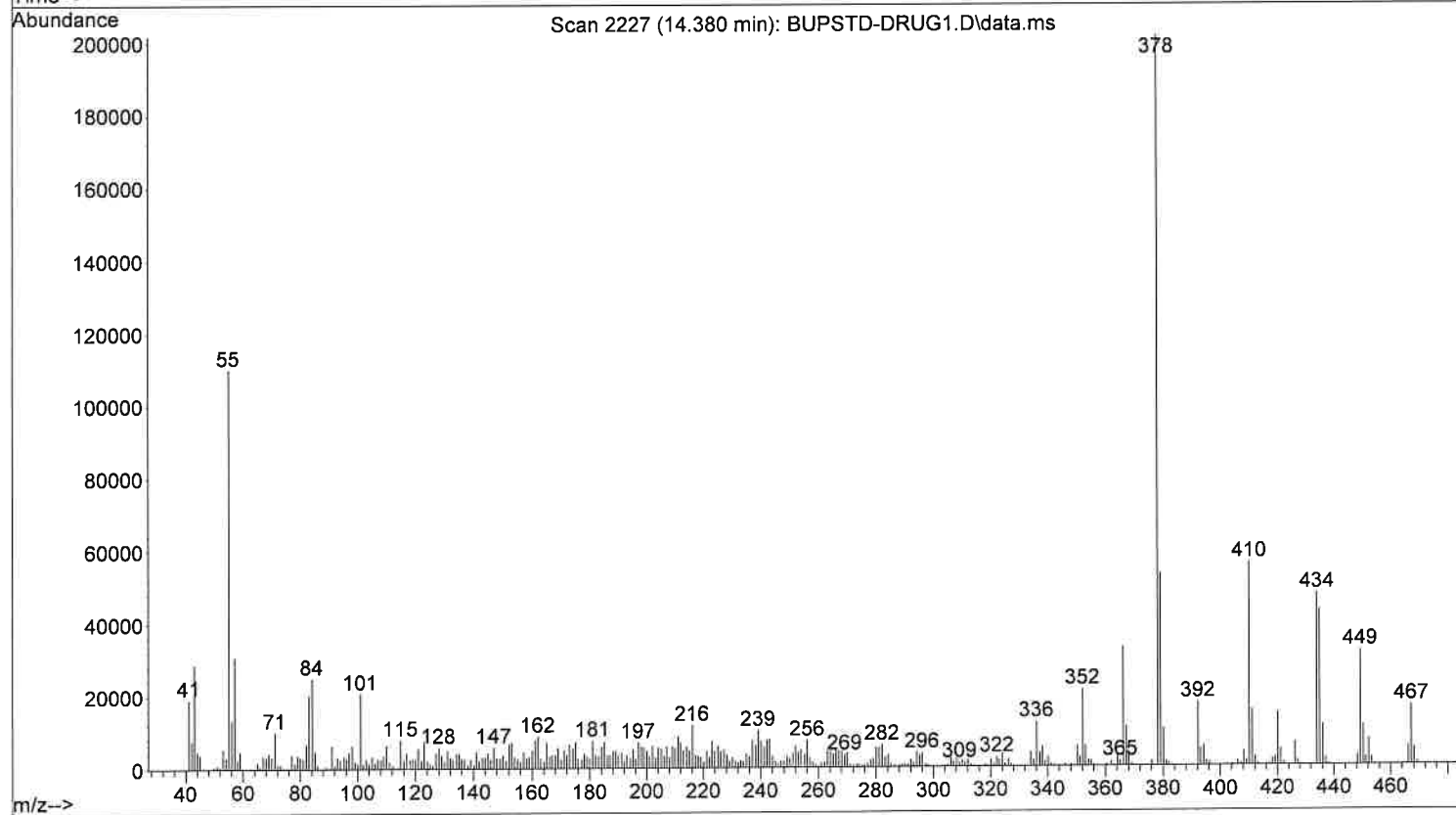
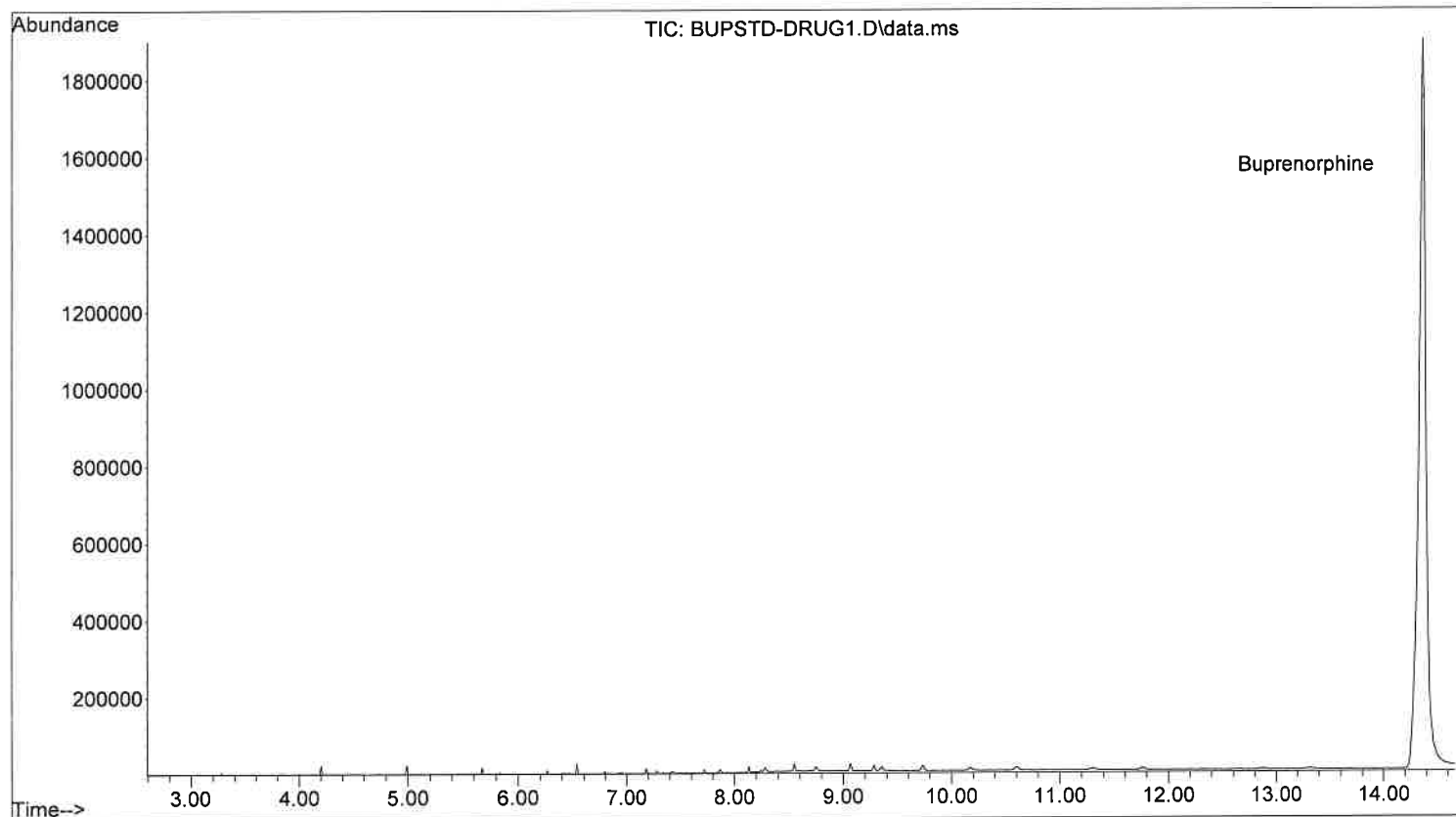
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Instrument : Buttercup
Sample Name: Alprazolam Standard
Misc Info : in Methanol
Vial Number: 146



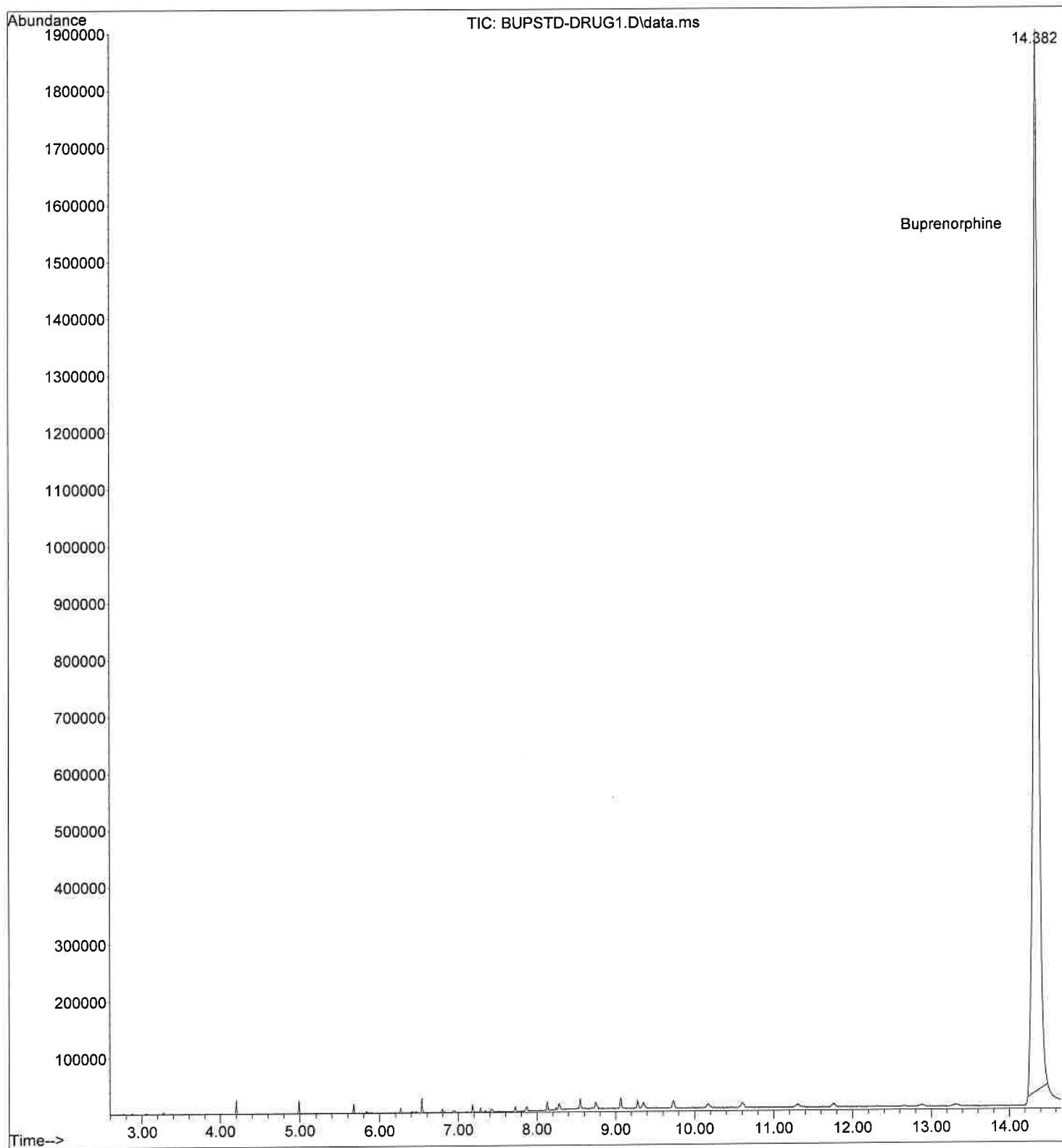
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Instrument : Buttercup
Sample Name: Methanol blank
Misc Info : for Alprazolam Standard
Vial Number: 141



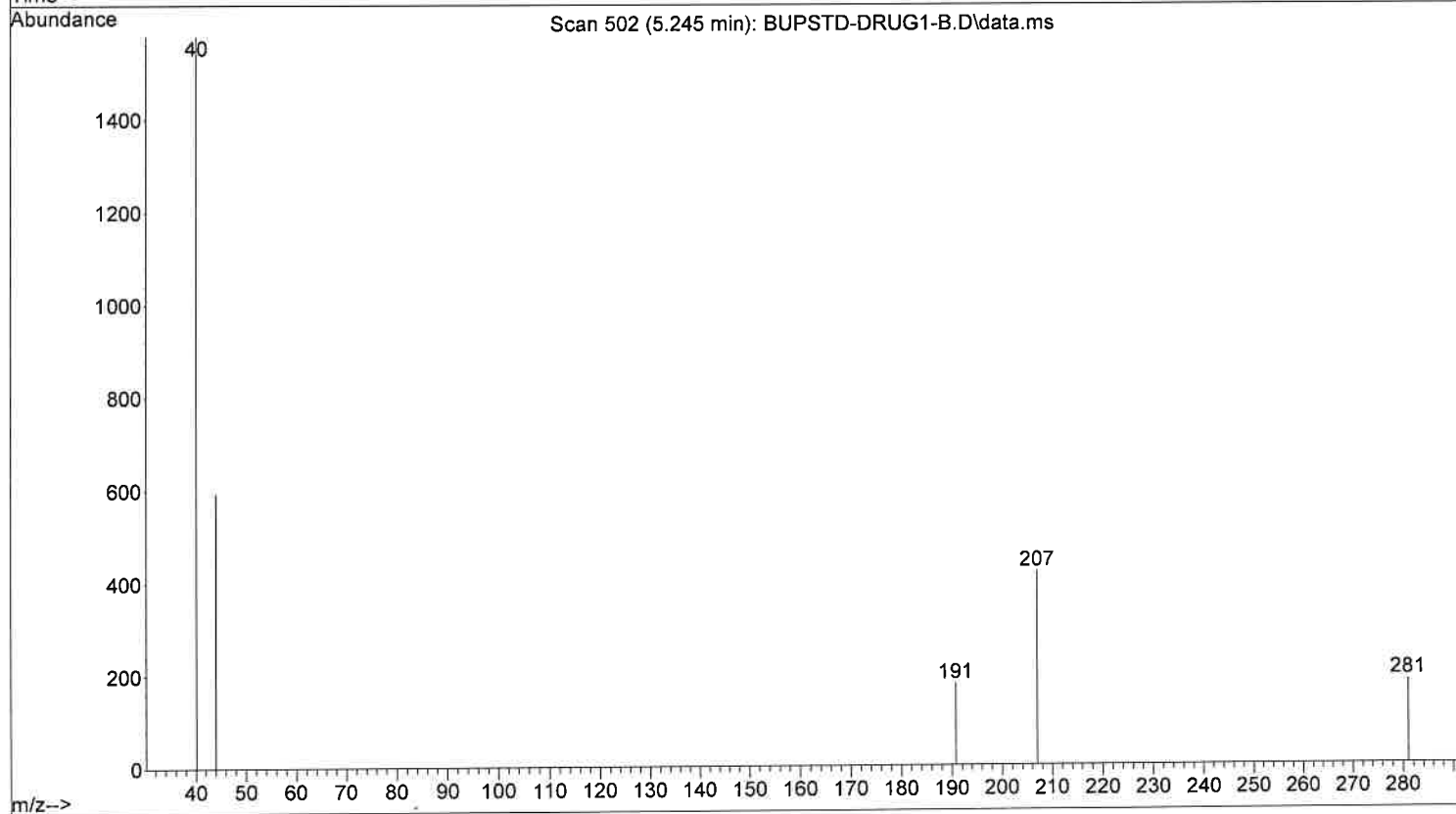
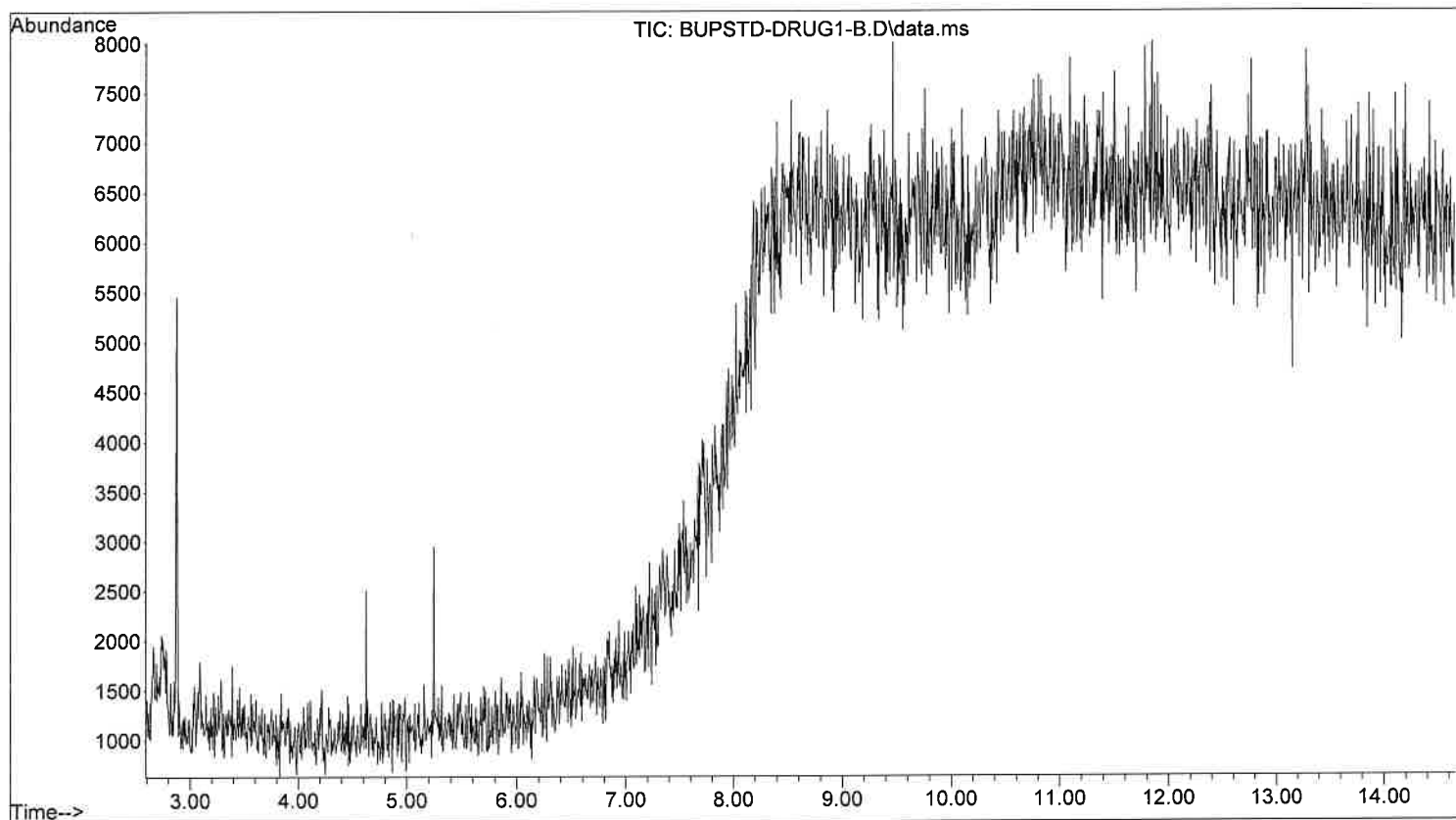
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Instrument : Buttercup
Sample Name: Buprenorphine Standard
Misc Info : in Methanol
Vial Number: 147



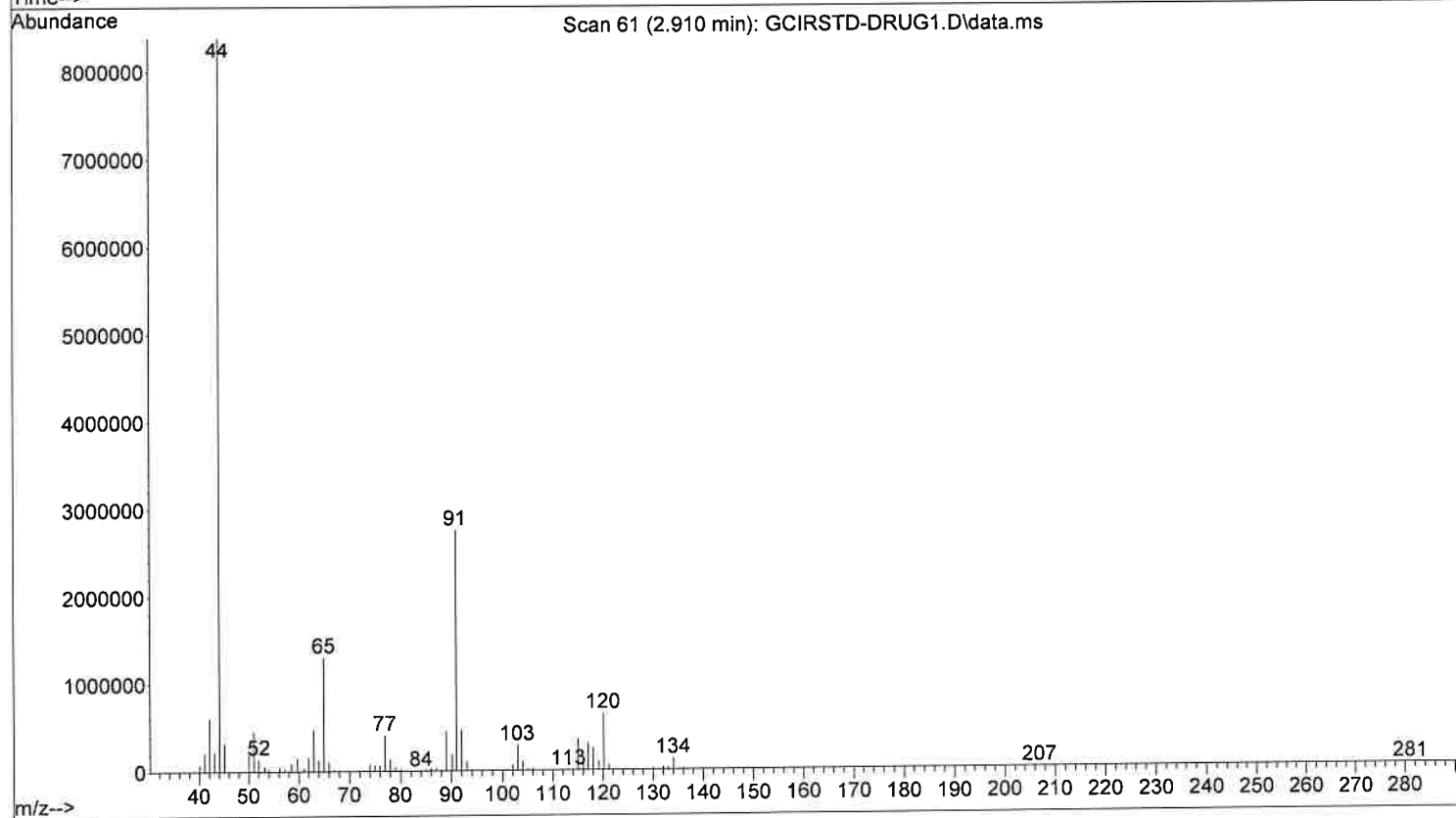
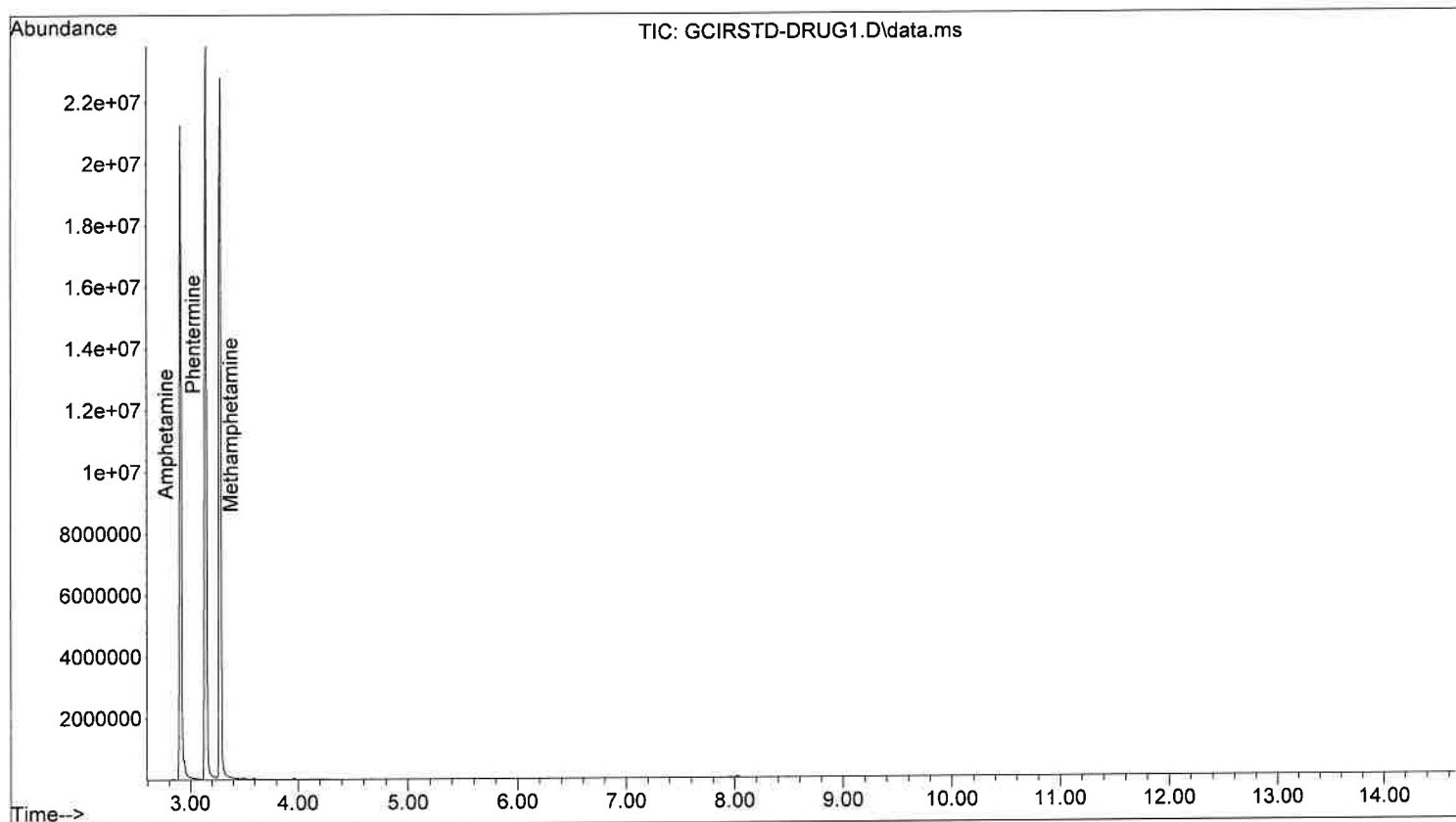
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Operator : KLAB
Acquired : 18 Aug 2023 13:52 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Buprenorphine Standard
Misc Info : in Methanol
Vial Number: 147



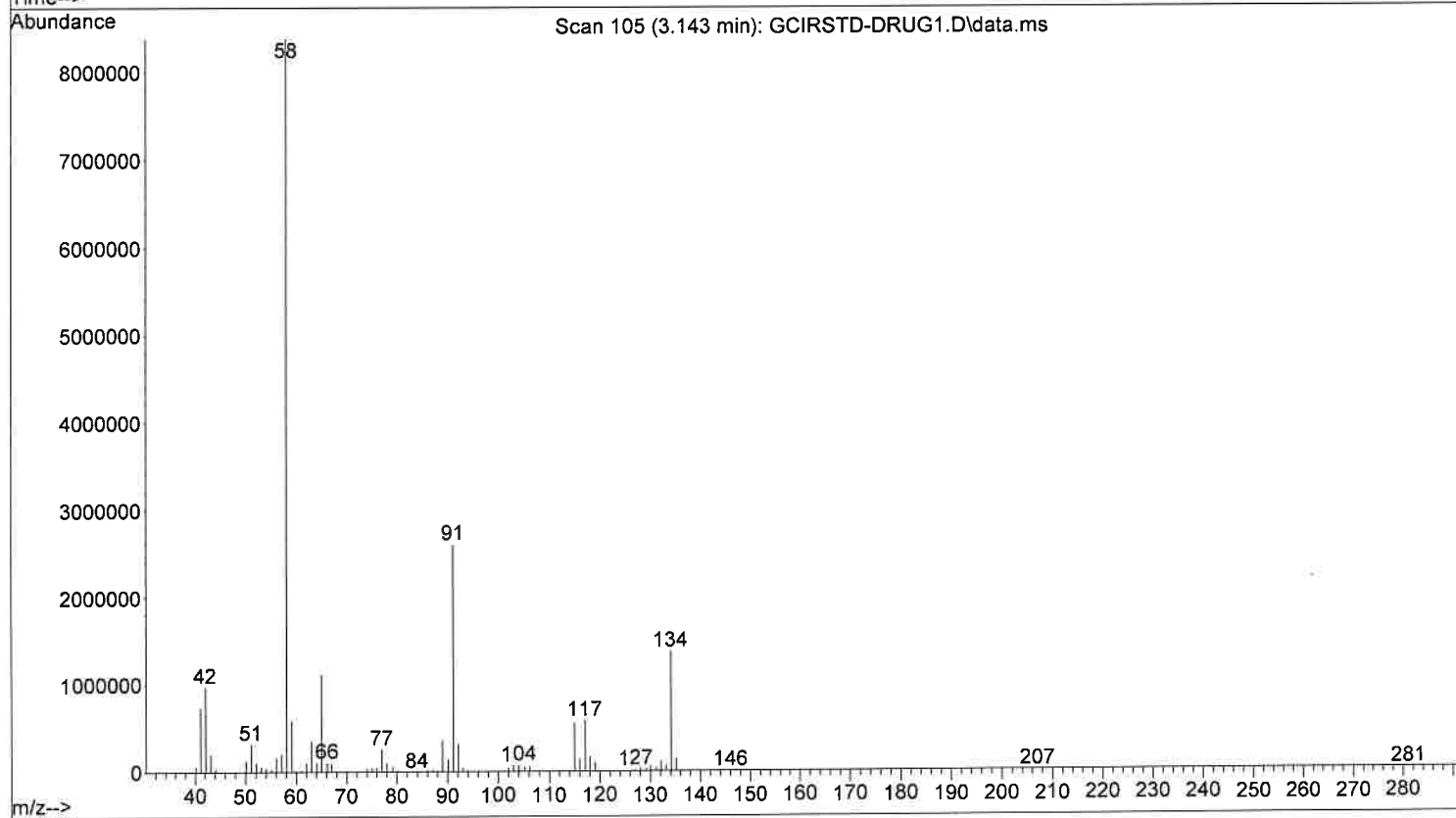
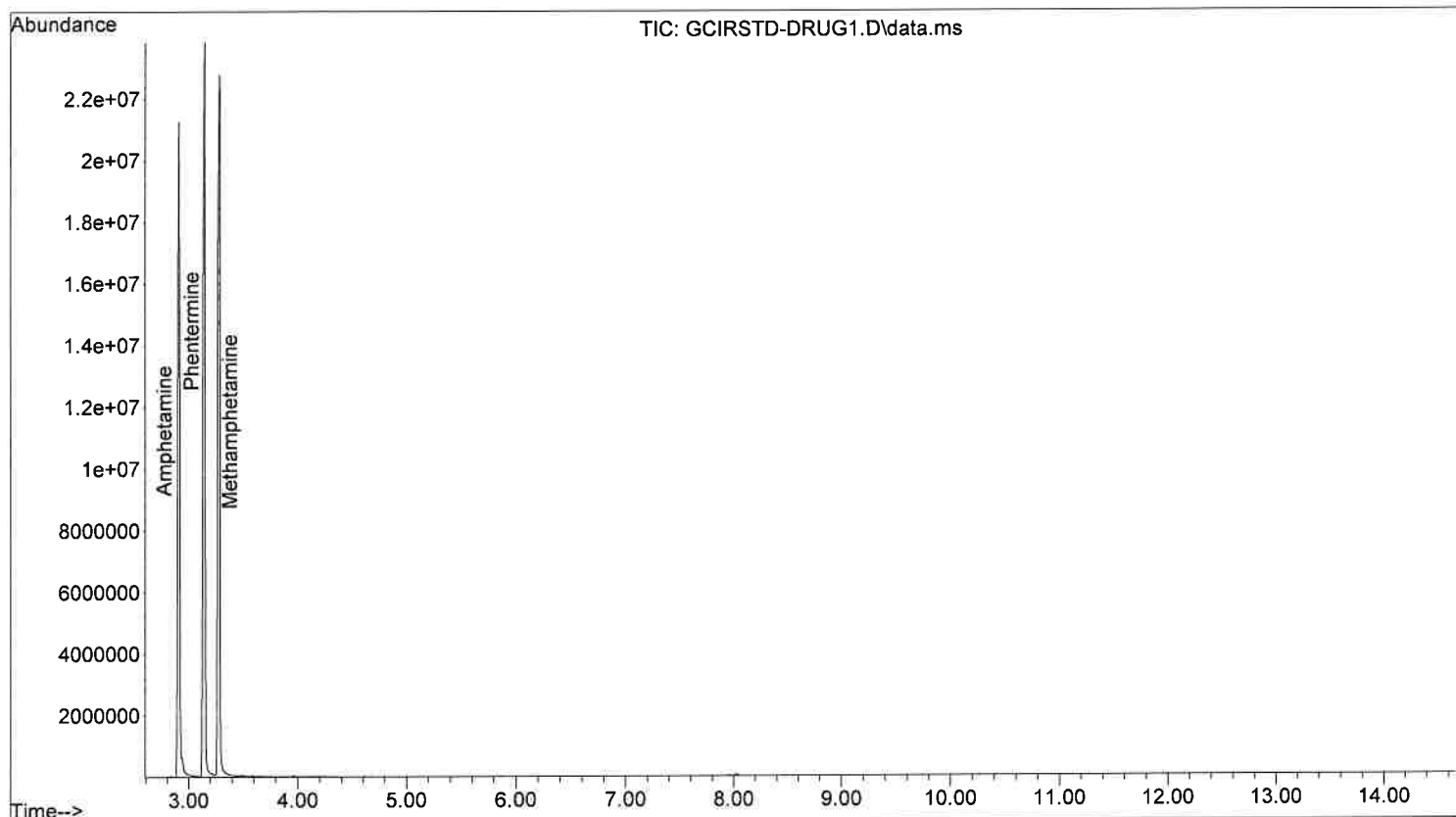
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Instrument : Buttercup
Sample Name: Methanol blank
Misc Info : for Buprenorphine Standard
Vial Number: 141



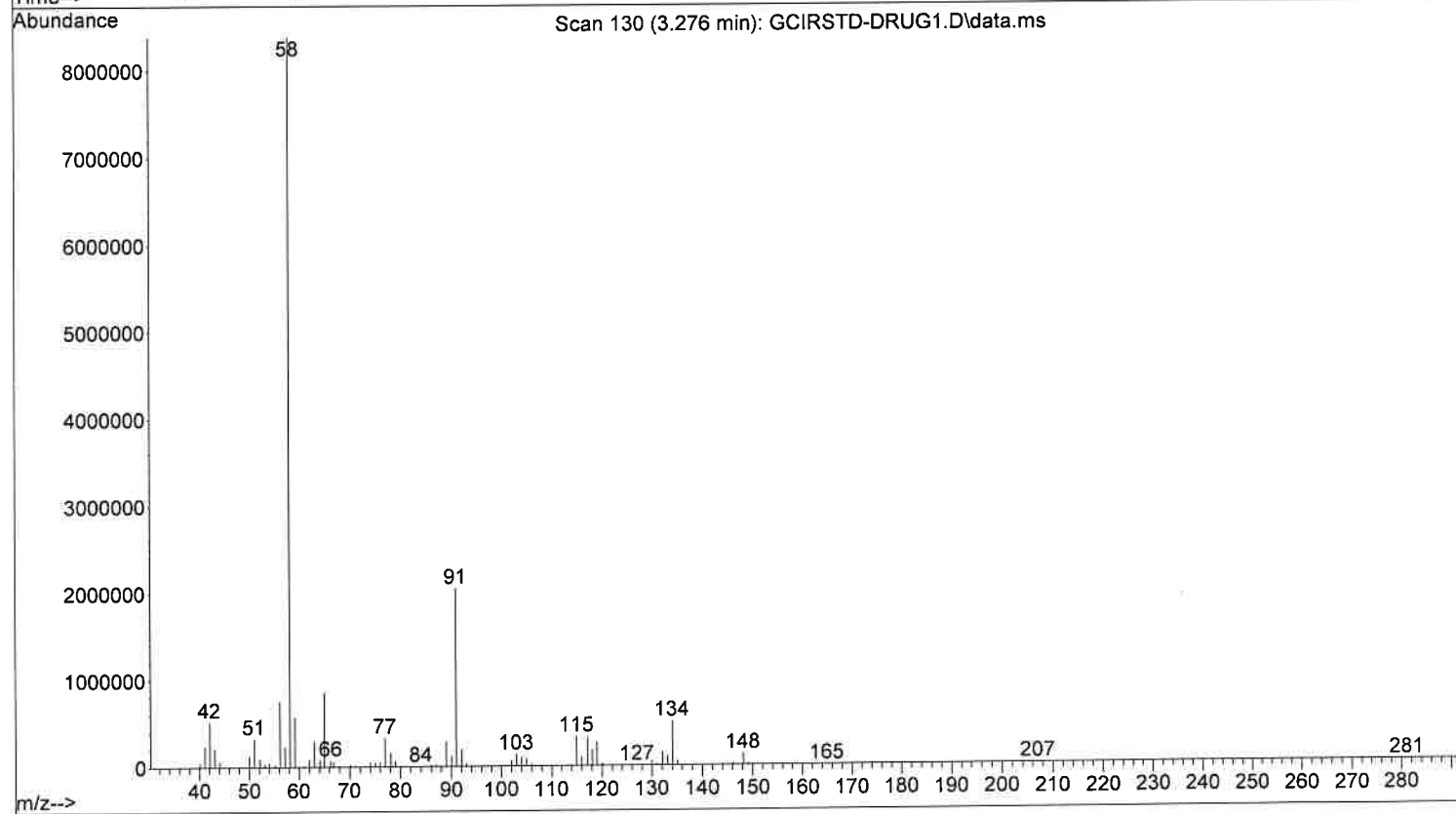
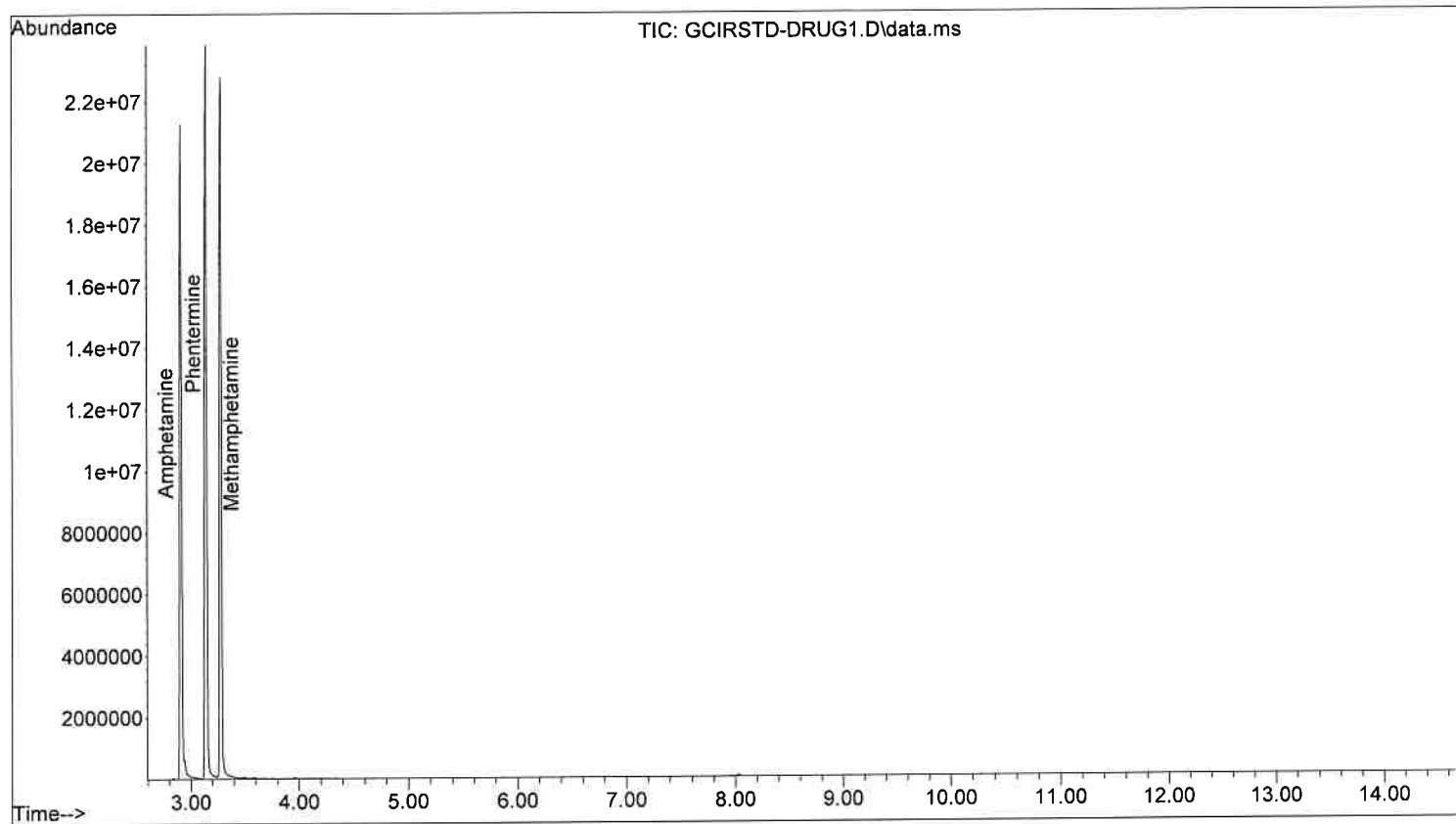
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Instrument : Buttercup
Sample Name: GCIR Standard
Misc Info : in Chloroform
Vial Number: 143



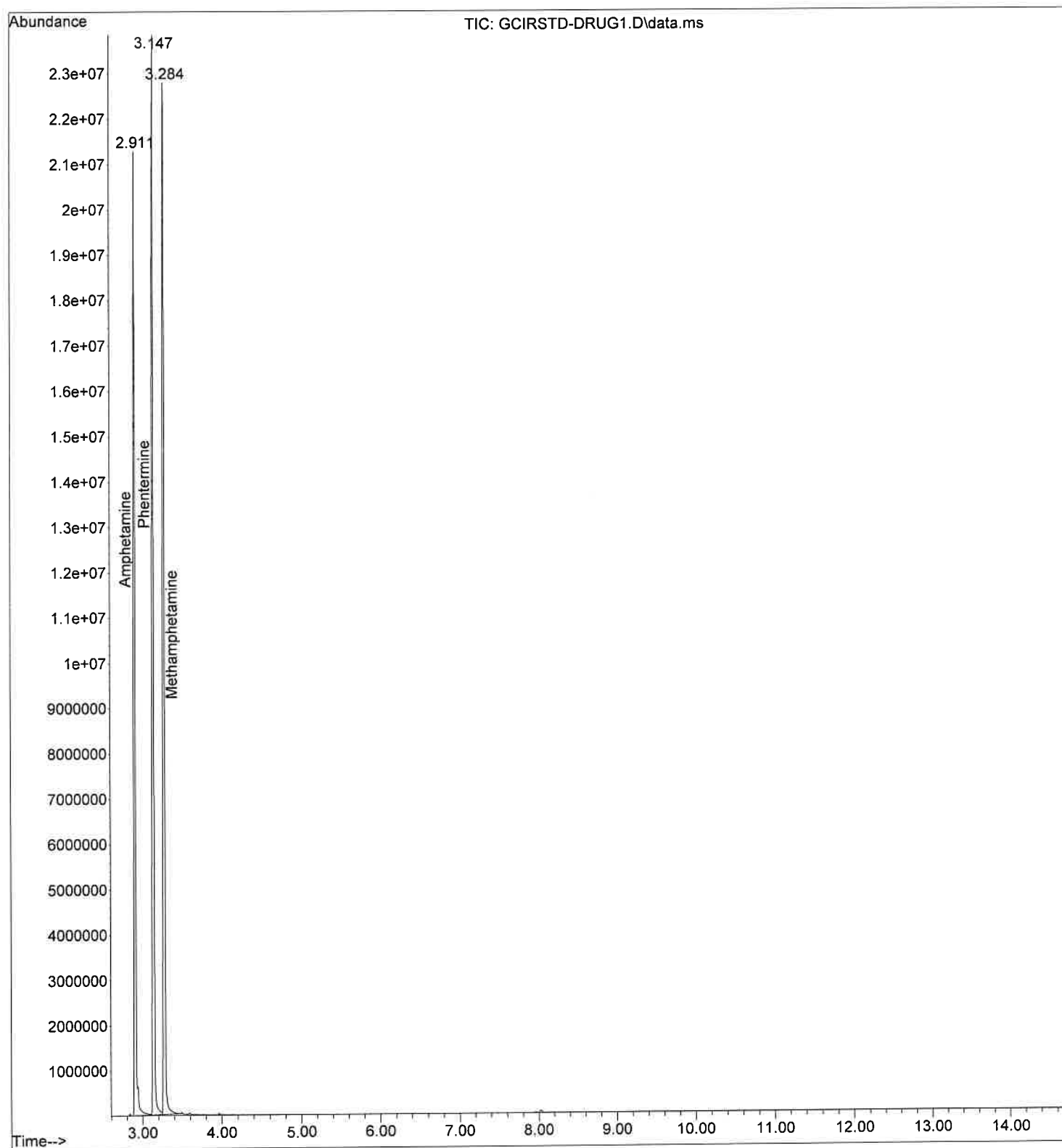
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Operator : KLAB
Acquired : 18 Aug 2023 10:47 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: GCIR Standard
Misc Info : in Chloroform
Vial Number: 143



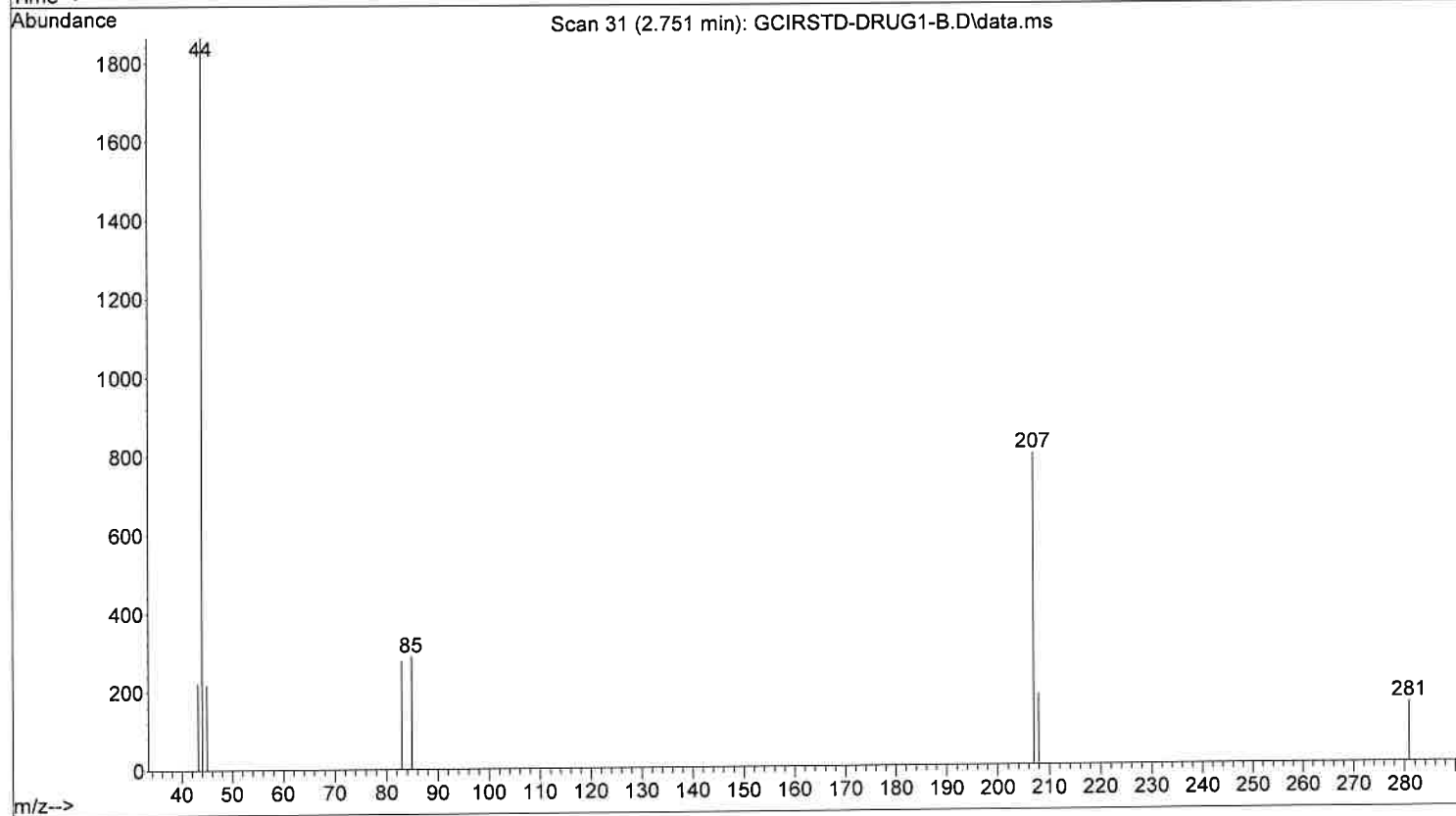
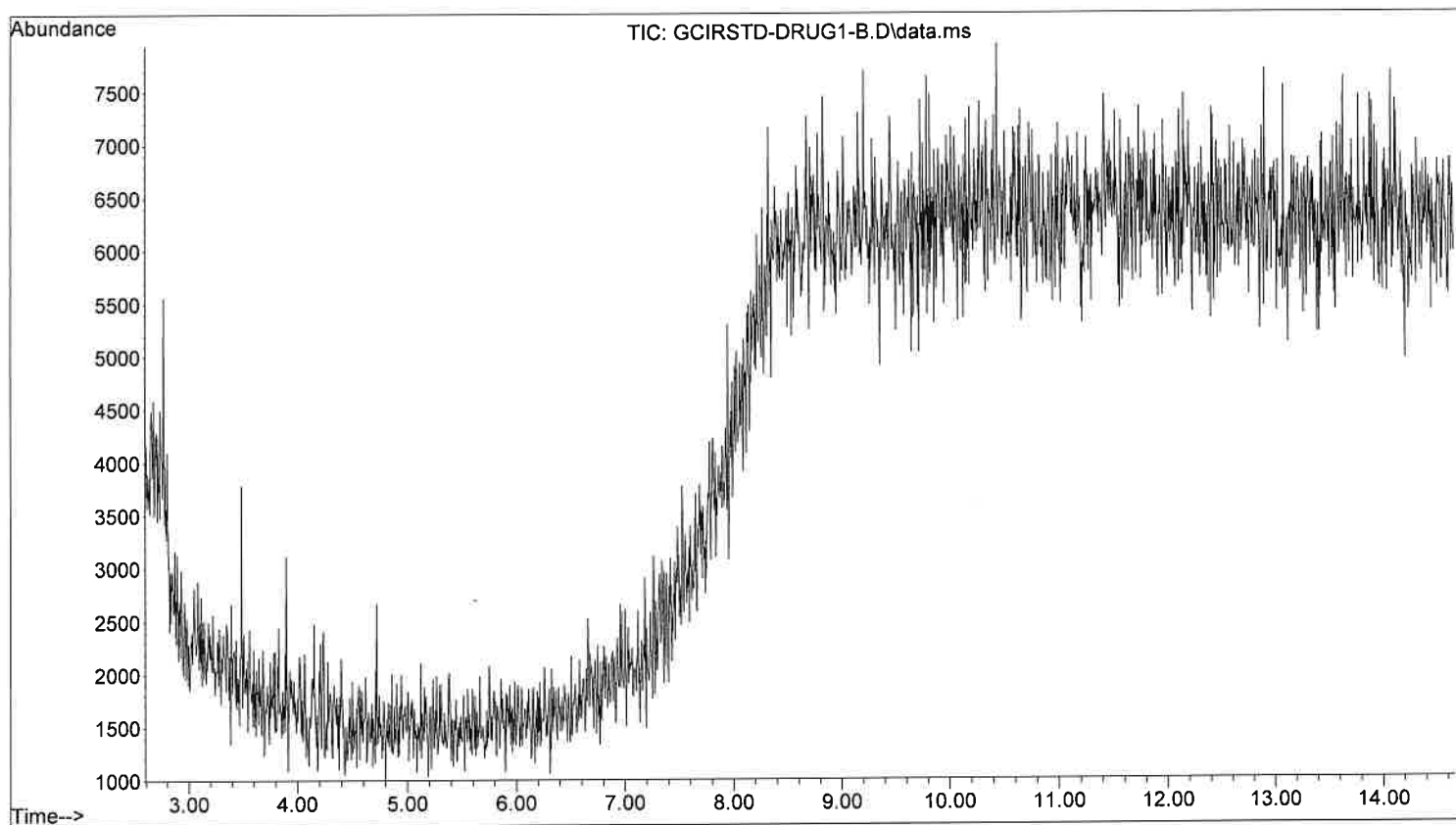
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Instrument : Buttercup
Sample Name: GCIR Standard
Misc Info : in Chloroform
Vial Number: 143



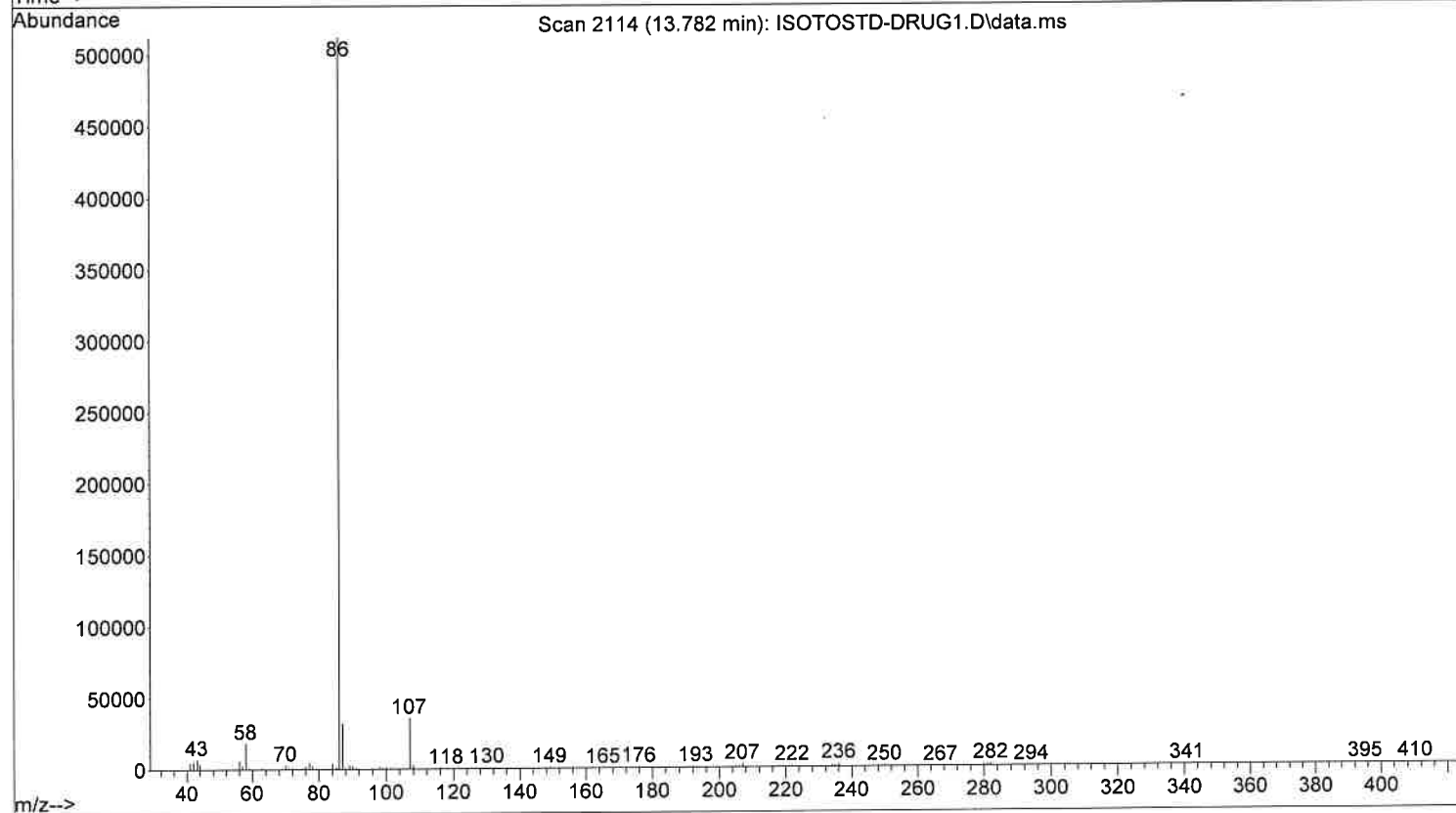
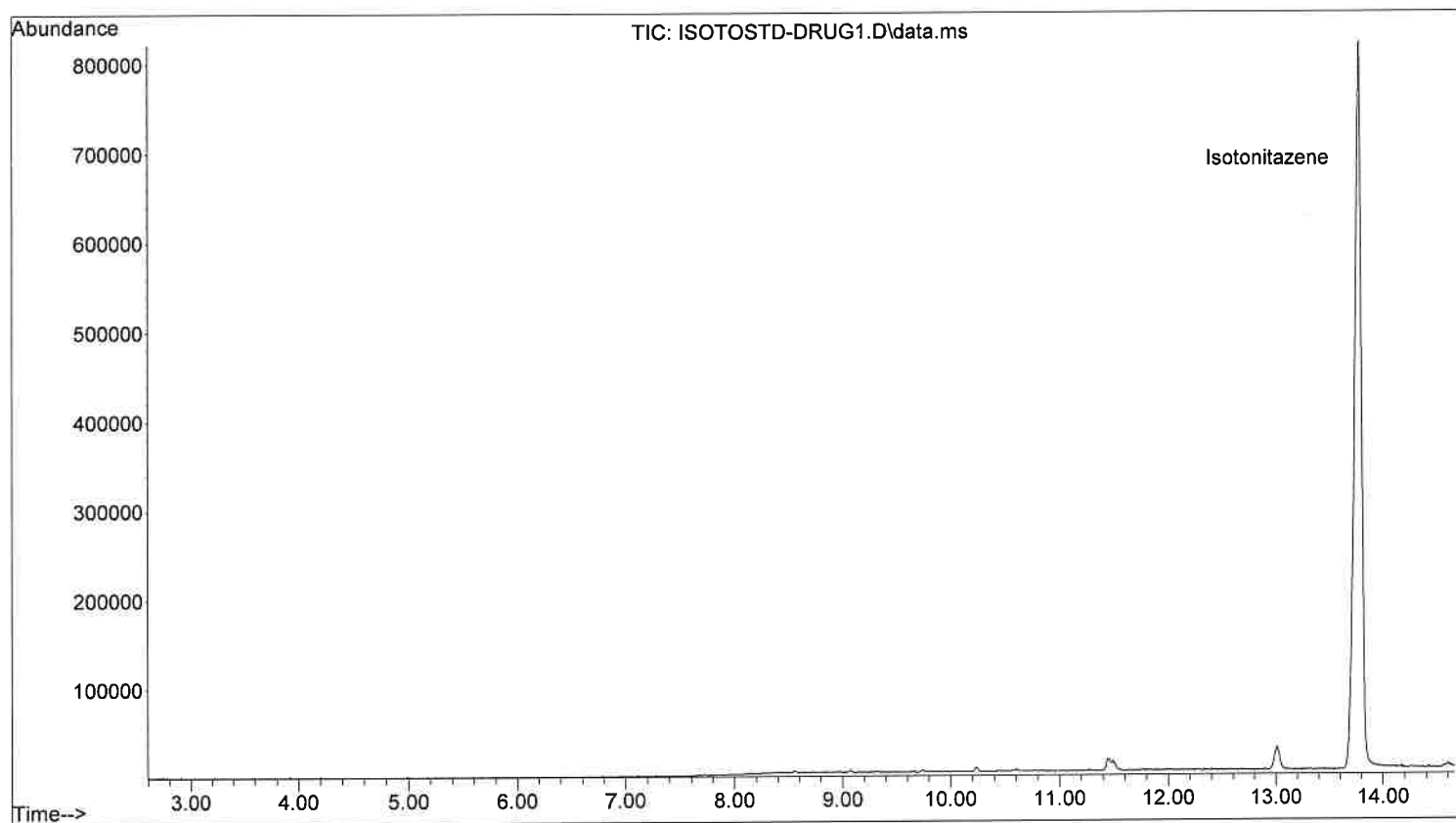
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\GCIRSTD-DRUG1.D
Operator : KLAB
Acquired : 18 Aug 2023 10:47 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: GCIR Standard
Misc Info : in Chloroform
Vial Number: 143



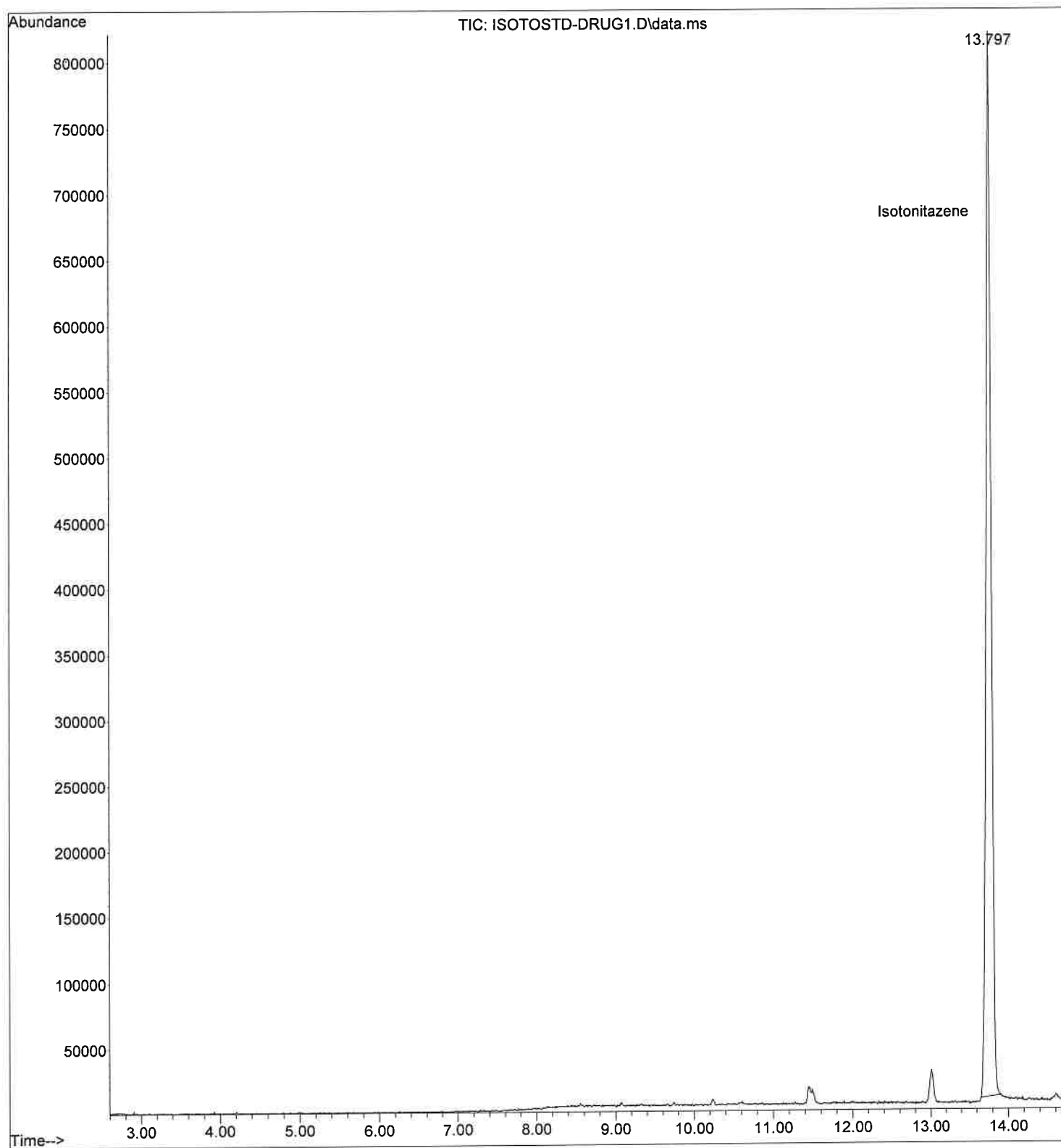
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\GCIRSTD-DRUG1-
... B.D
Operator : KLAB
Acquired : 18 Aug 2023 10:28 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : for GCIR Standard
Vial Number: 142



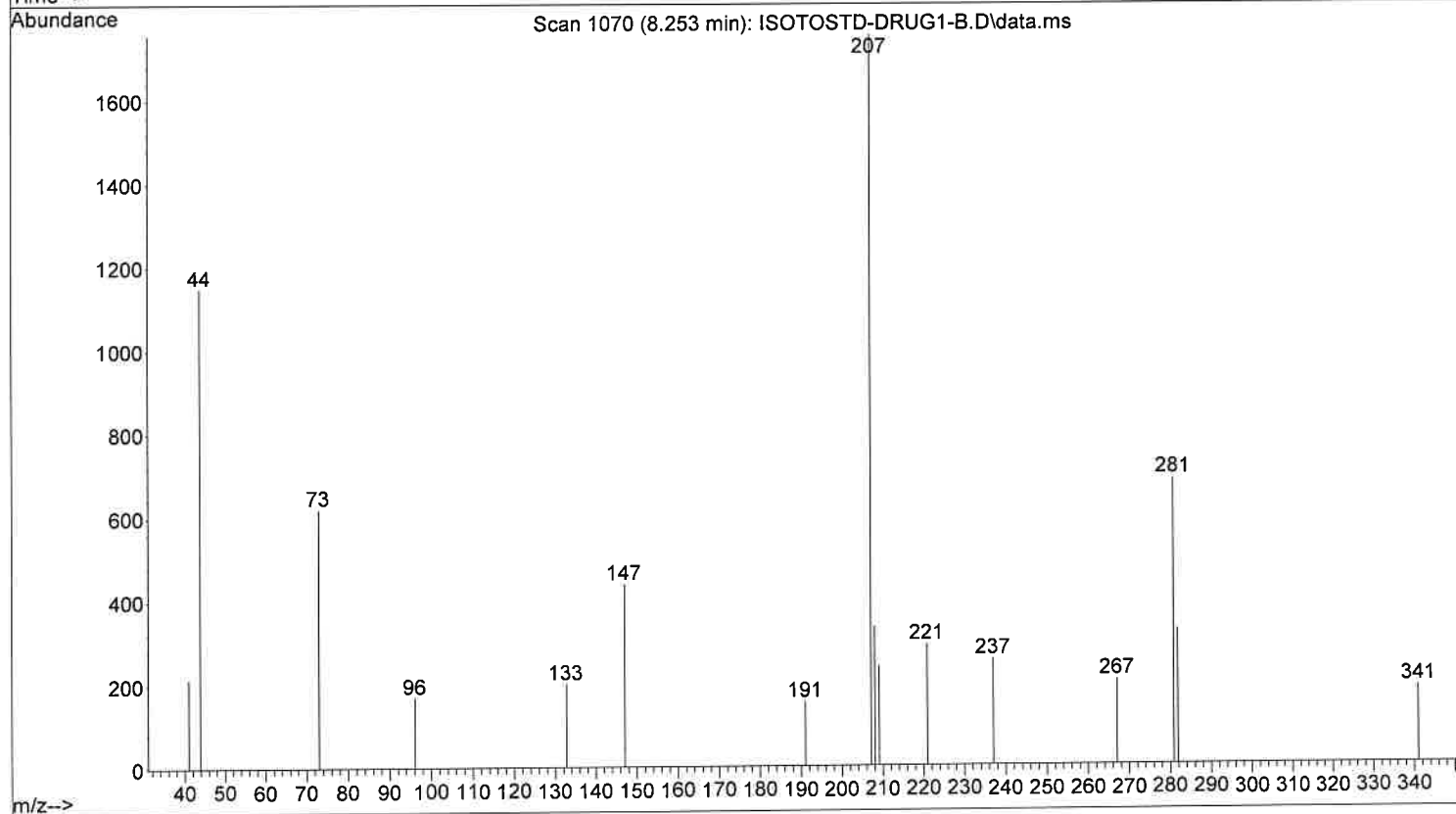
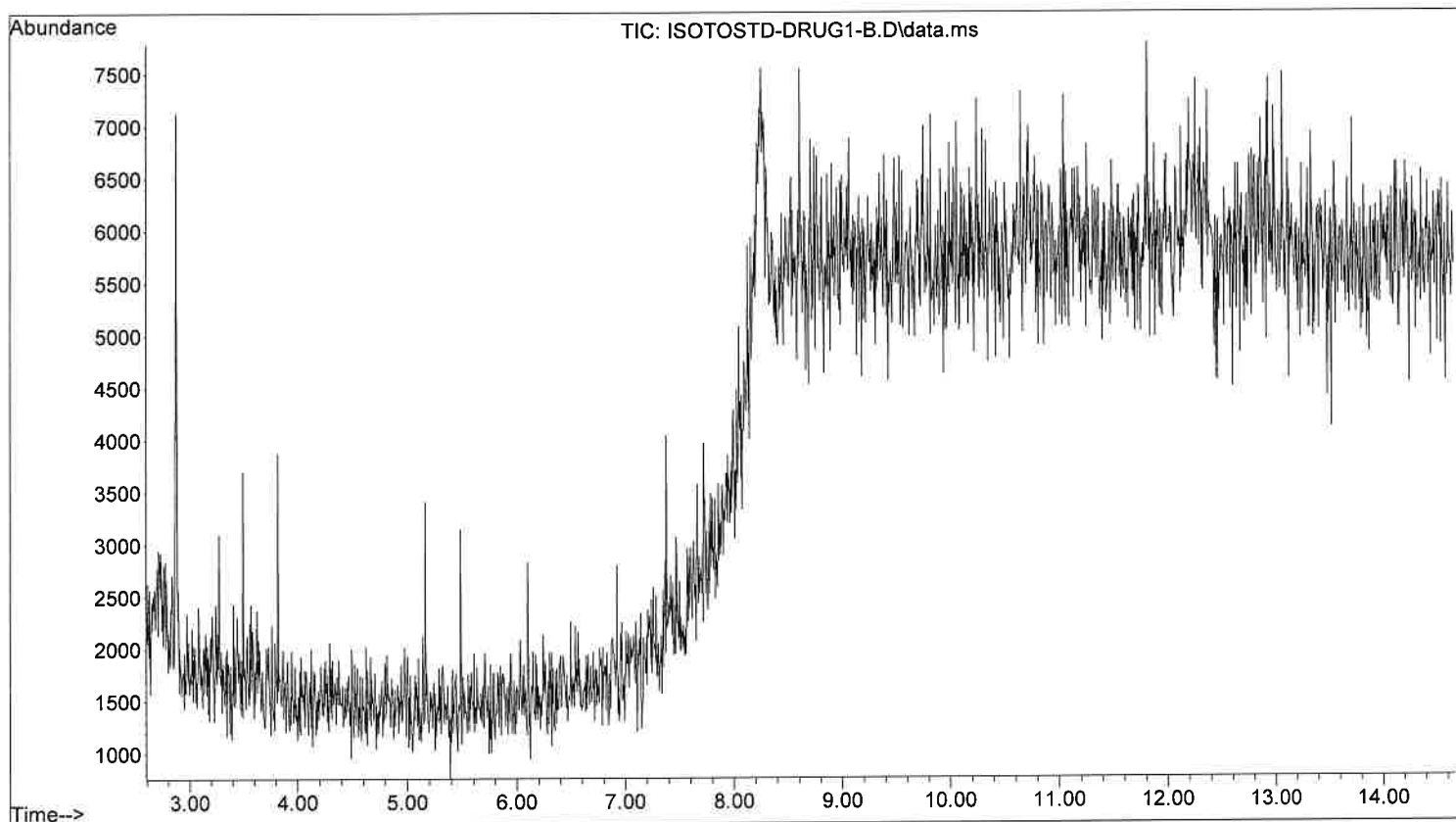
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\ISOTOSTD-DRUG1
... .D
Operator : KLAB
Acquired : 18 Aug 2023 14:37 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Isotonitazene Standard
Misc Info : in Methanol
Vial Number: 148



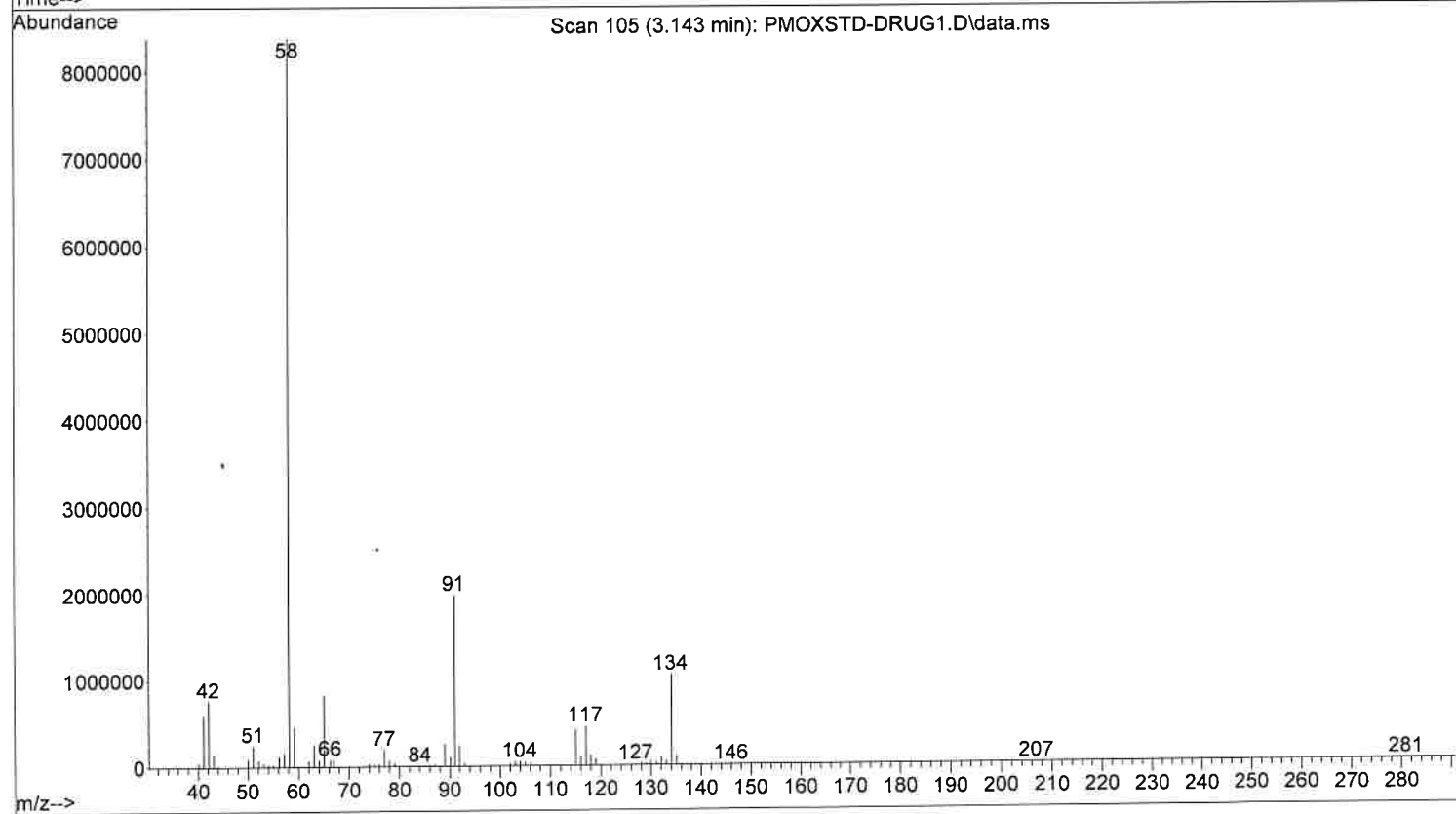
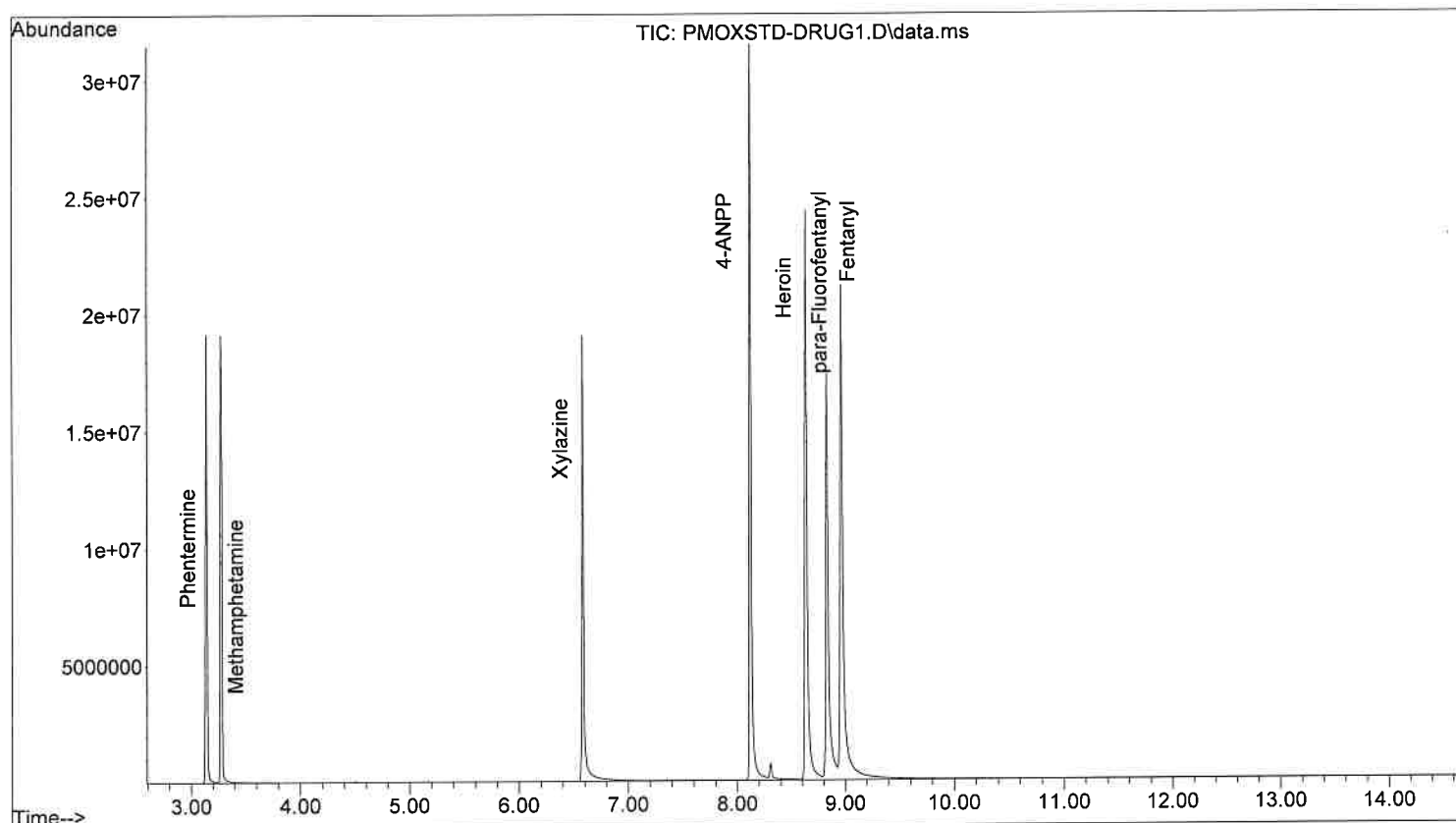
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\ISOTOSTD-DRUG1
... .D
Operator : KLAB
Instrument : Buttercup
Acquired : 18 Aug 2023 14:37 using AcqMethod DRUG1.M
Sample Name: Isotonitazene Standard
Misc Info : in Methanol



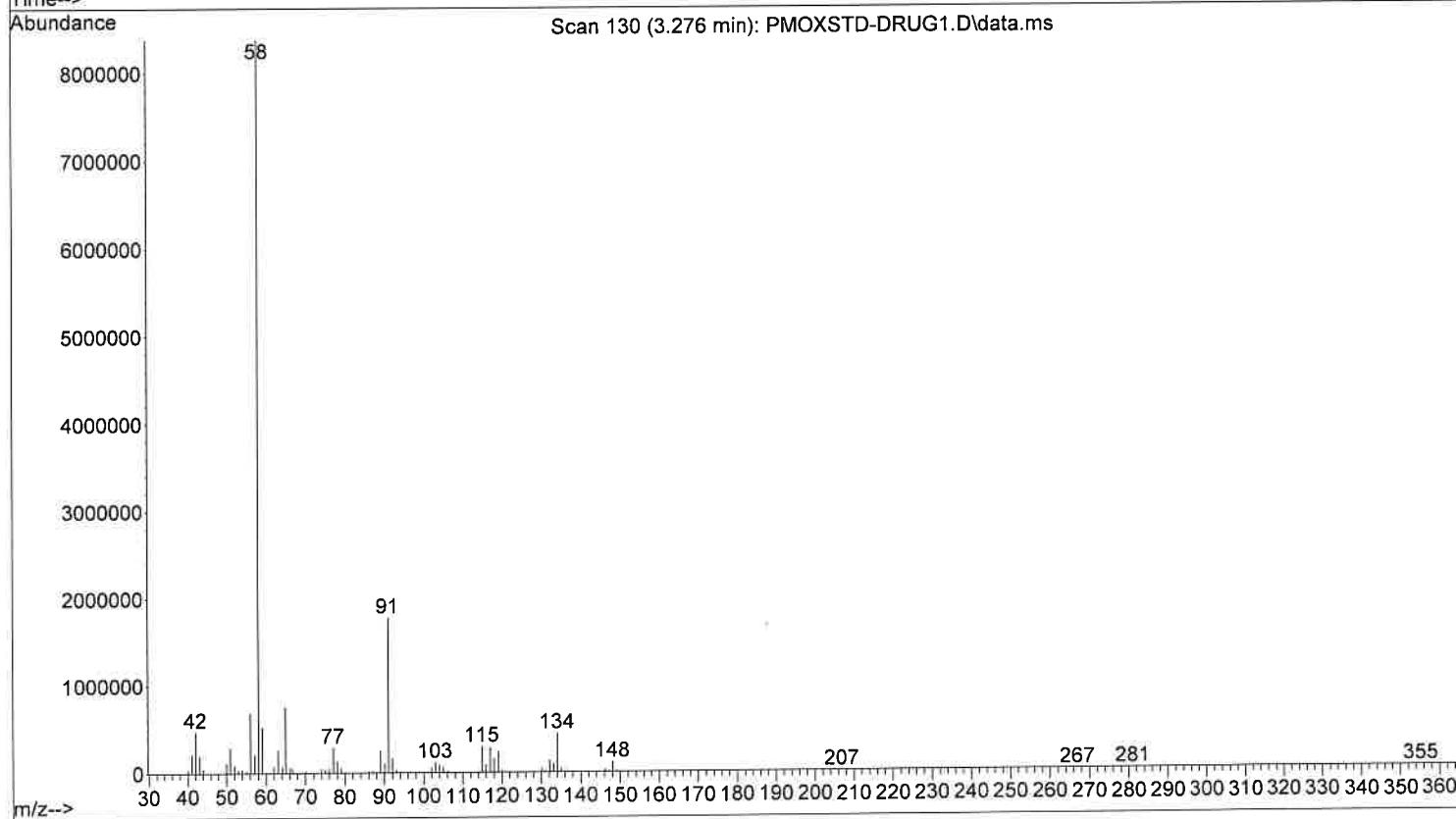
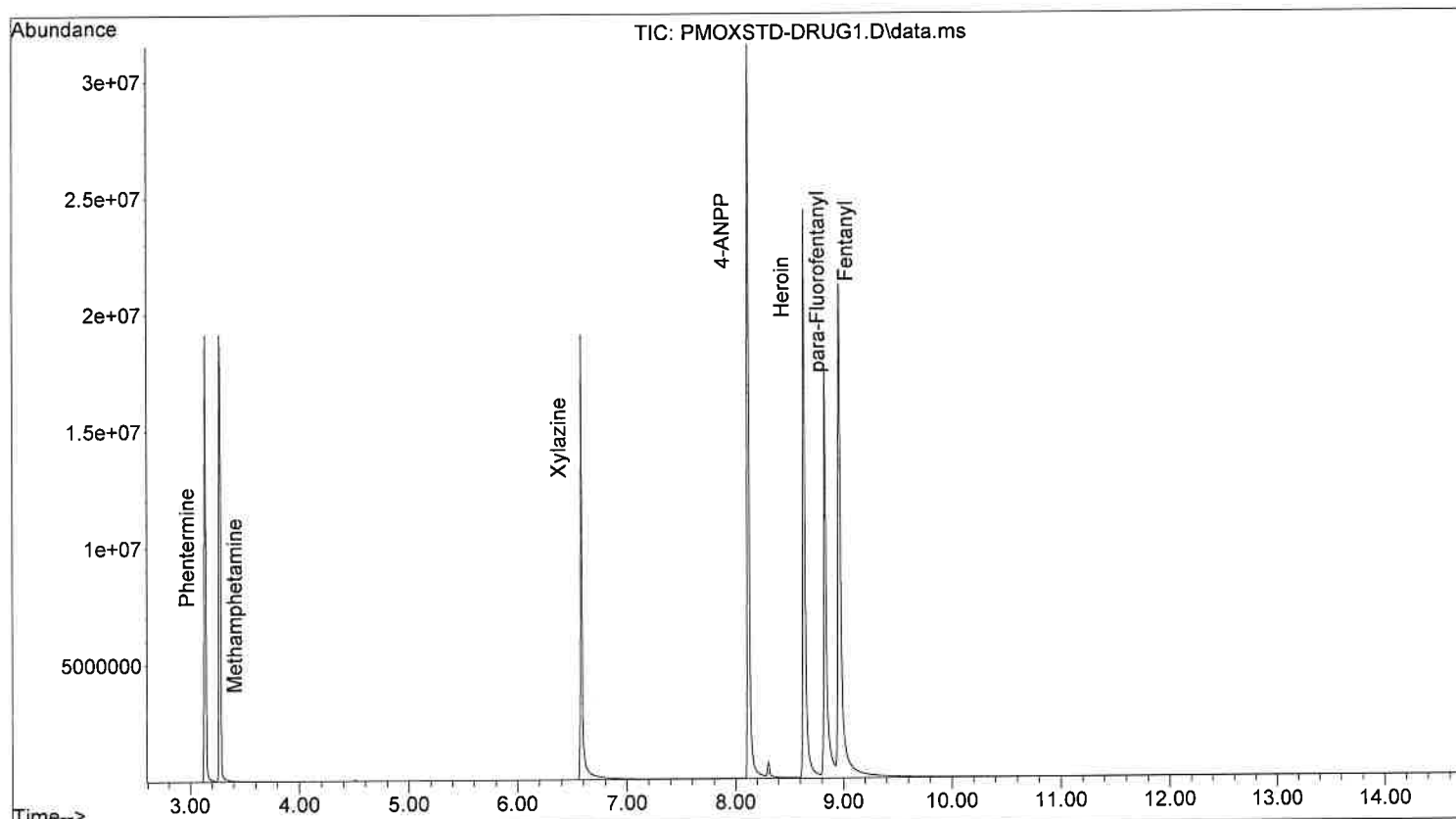
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... -B.D
Operator : KLAB
Acquired : 18 Aug 2023 14:19 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Methanol blank
Misc Info : for Isotonitazene Standard
Vial Number: 141



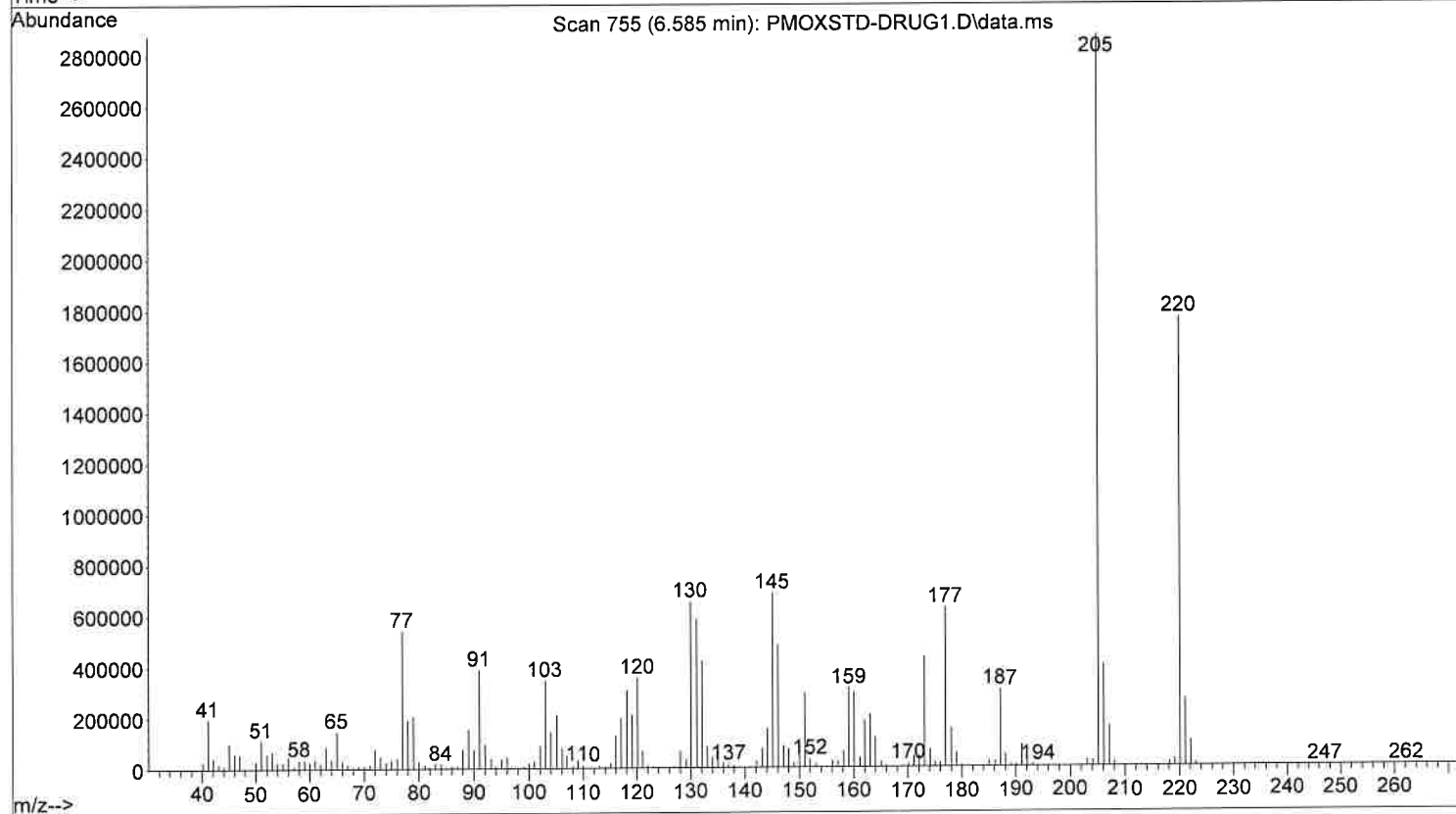
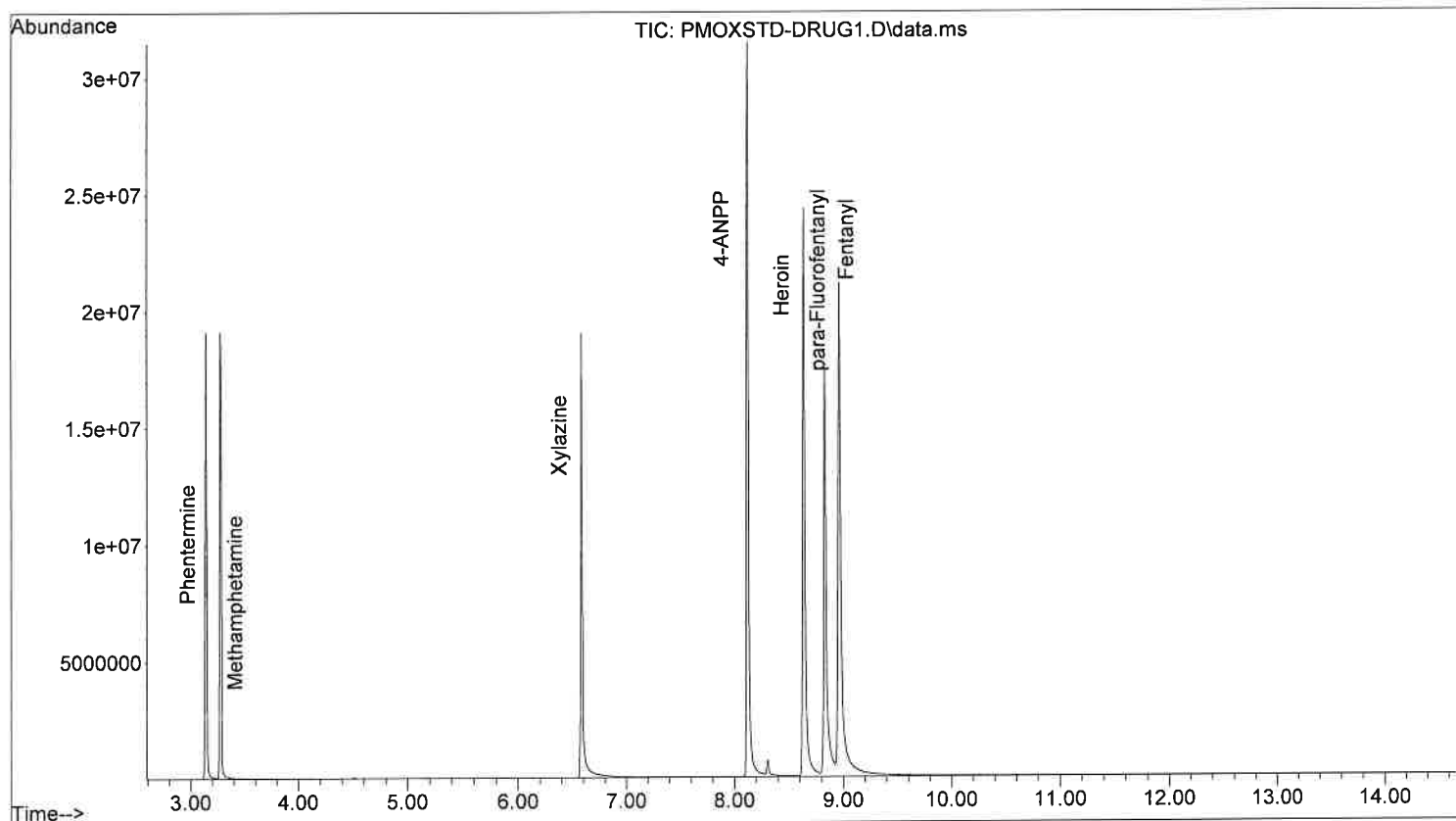
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Operator : KLAB
Acquired : 18 Aug 2023 11:34 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : in Chloroform
Vial Number: 144



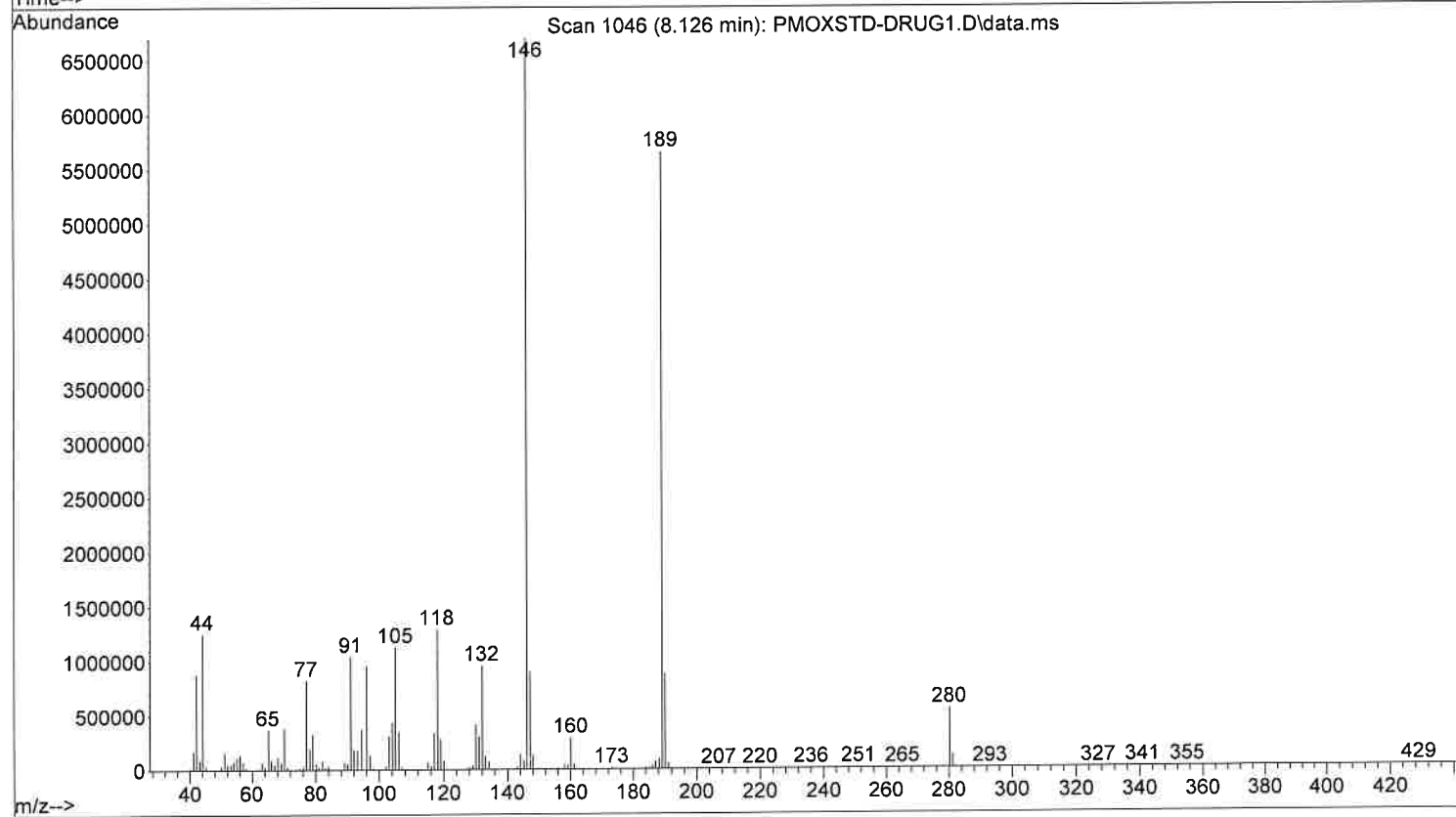
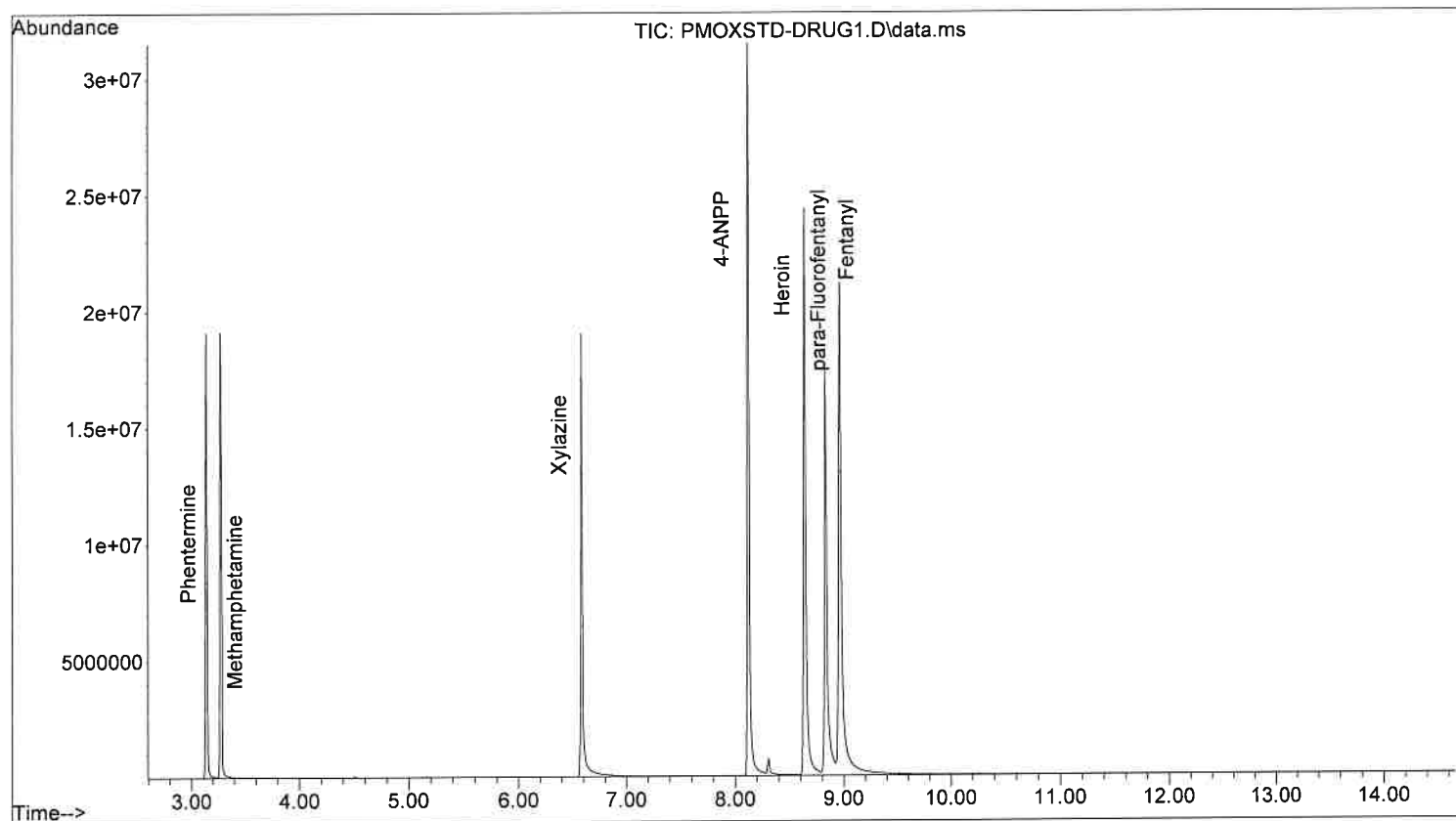
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Operator : KLAB
Acquired : 18 Aug 2023 11:34 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : in Chloroform
Vial Number: 144



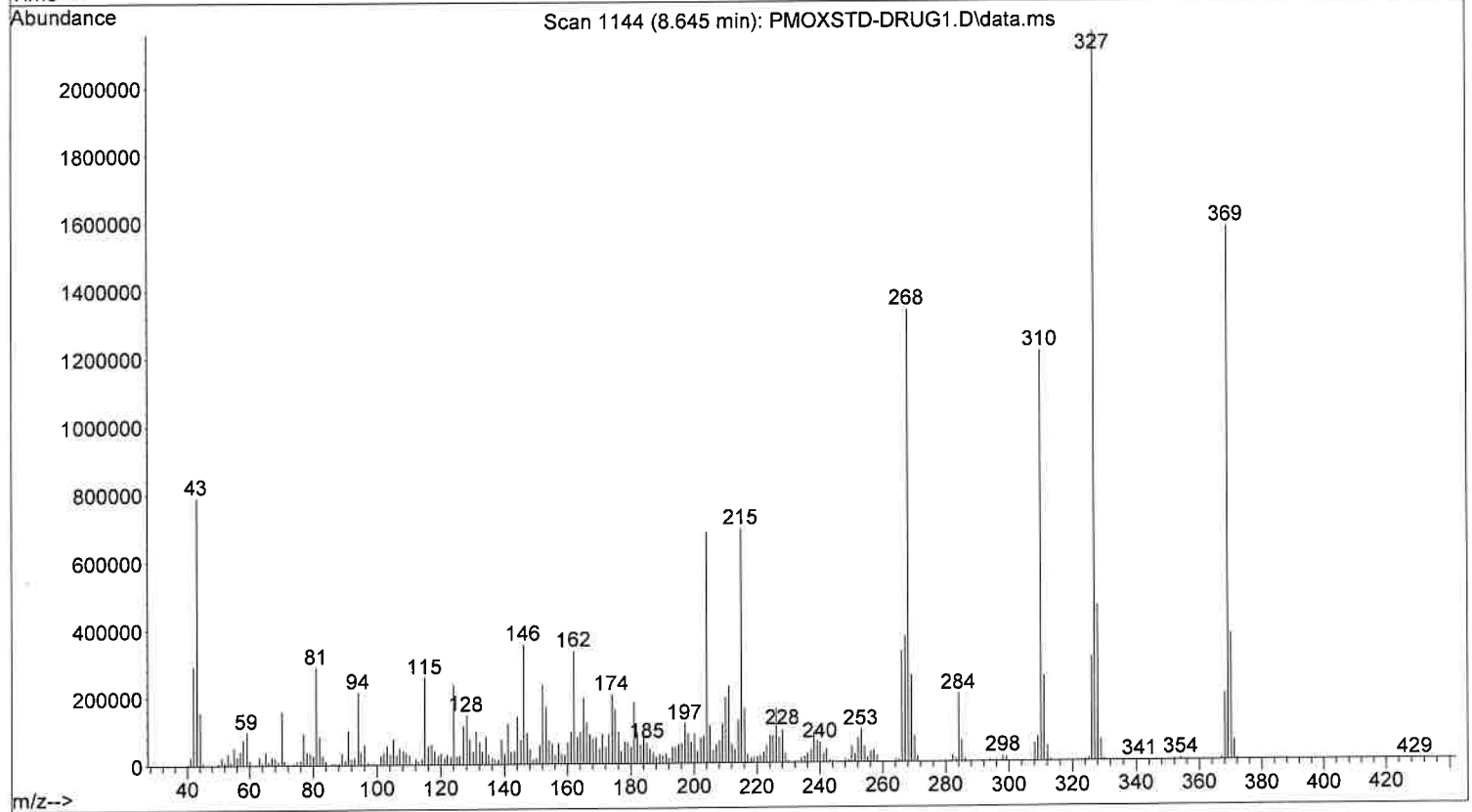
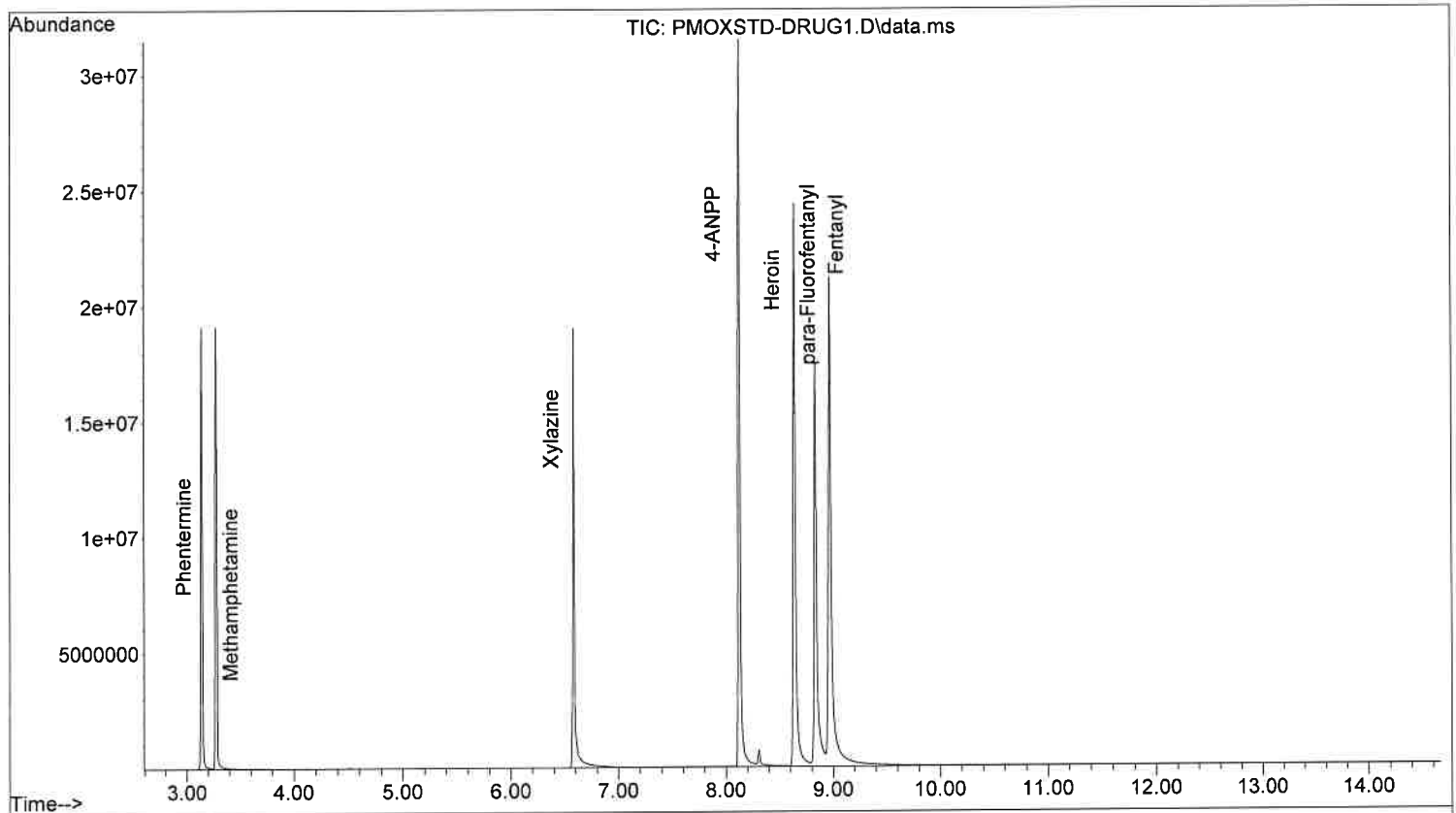
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Operator : KLAB
Acquired : 18 Aug 2023 11:34 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : in Chloroform
Vial Number: 144



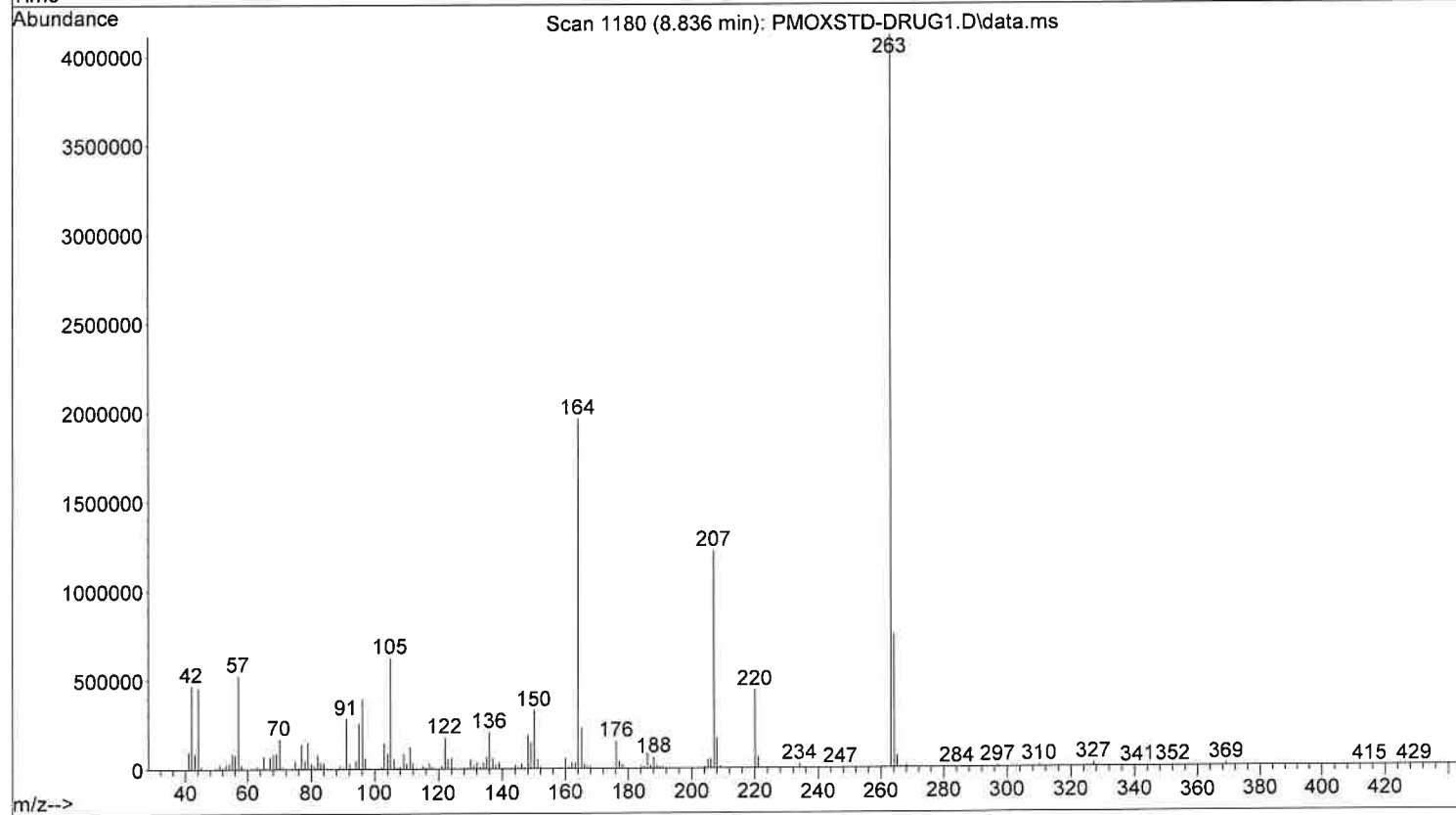
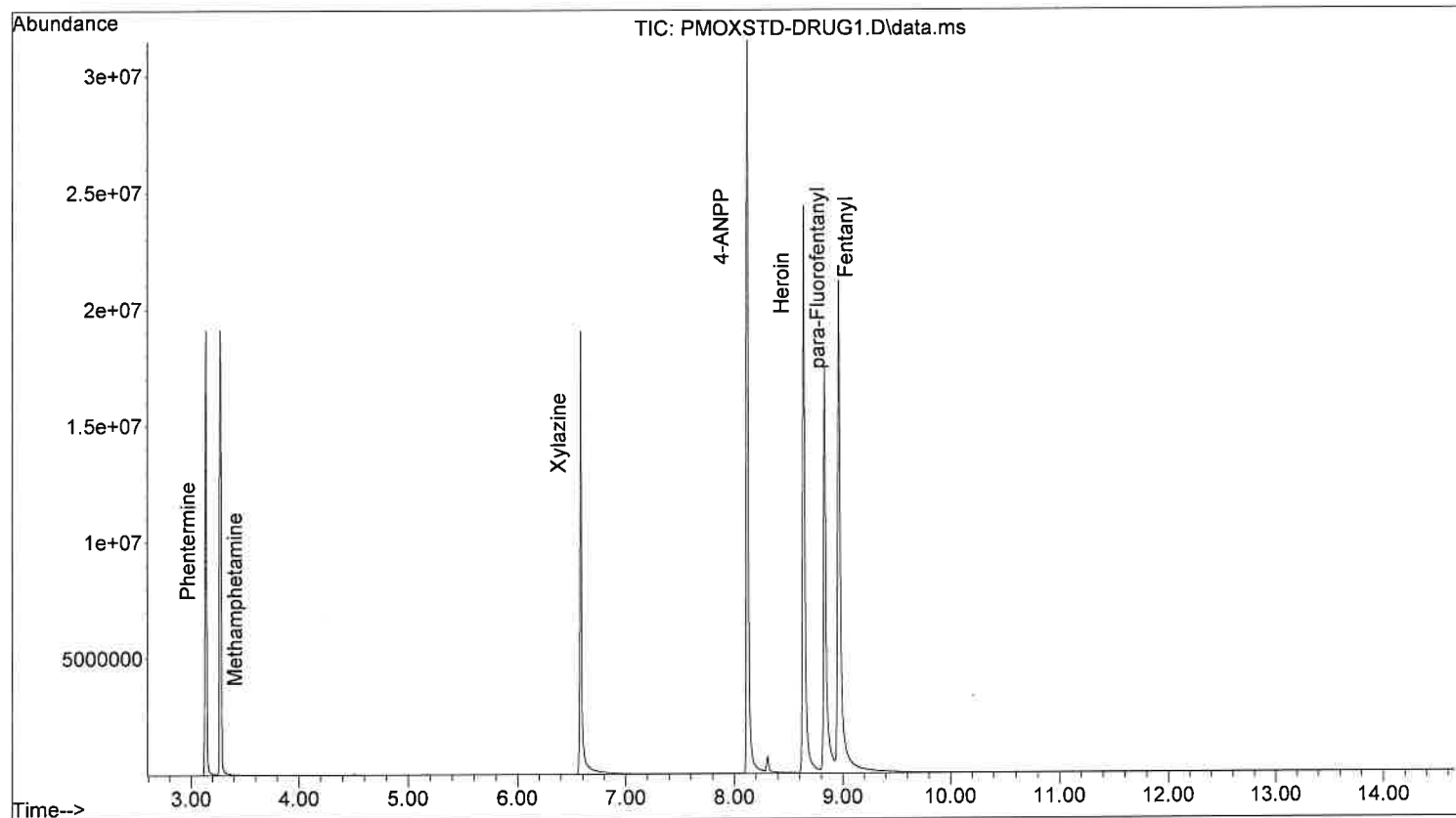
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Operator : KLAB
Acquired : 18 Aug 2023 11:34 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : in Chloroform
Vial Number: 144



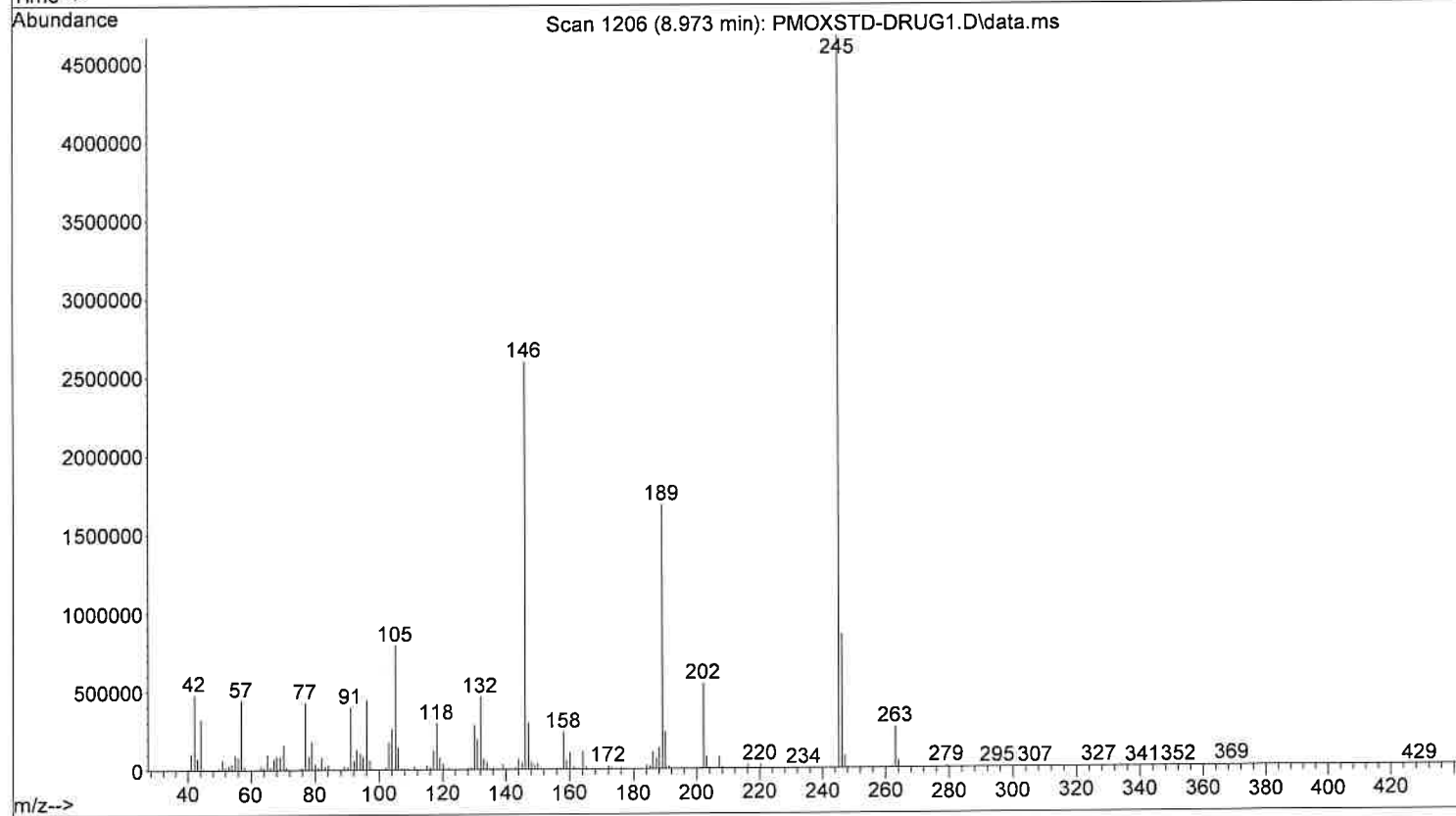
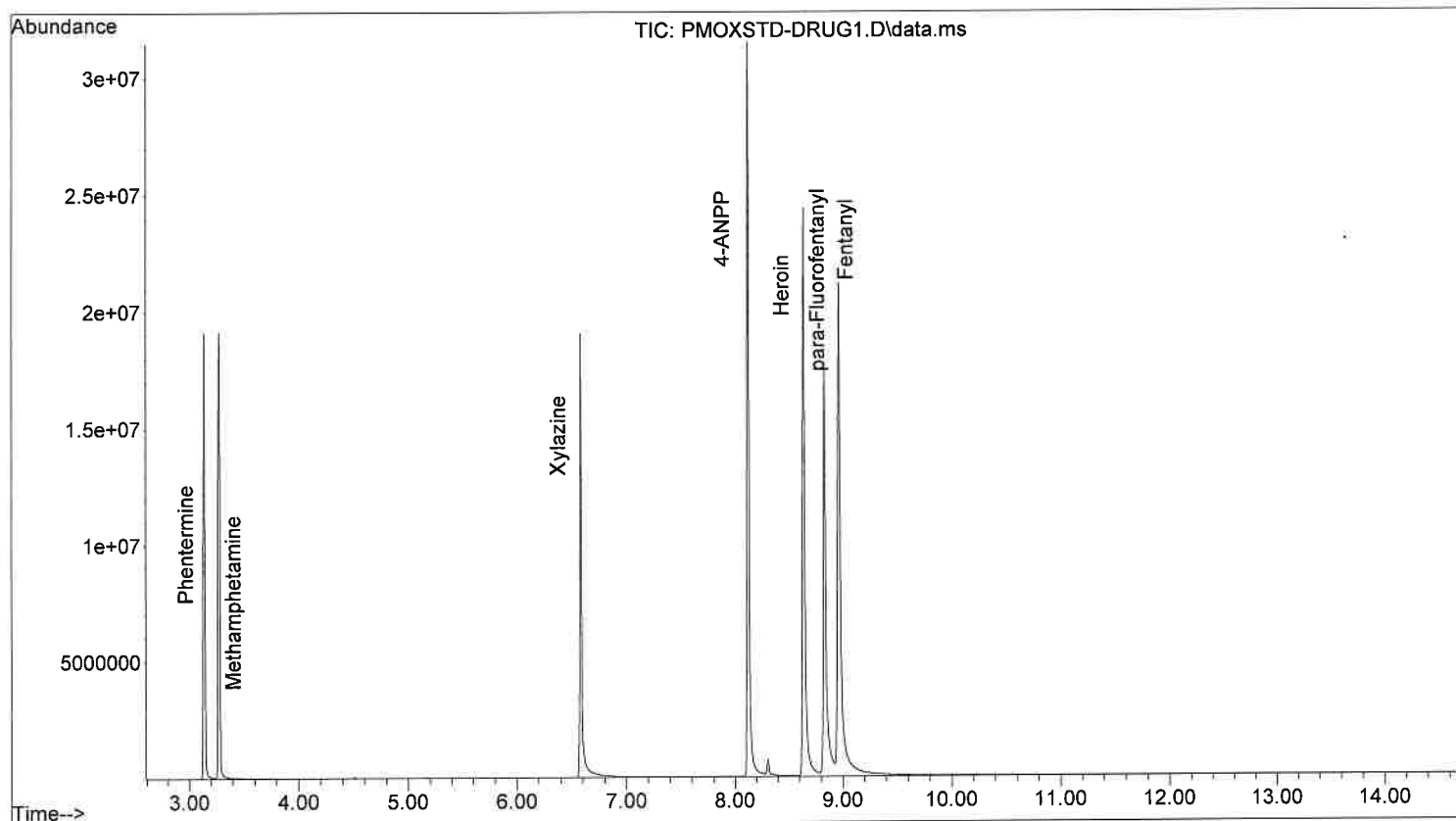
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\PMOXSTD-DRUG1.D
Operator : KLAB
Acquired : 18 Aug 2023 11:34 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : in Chloroform
Vial Number: 144



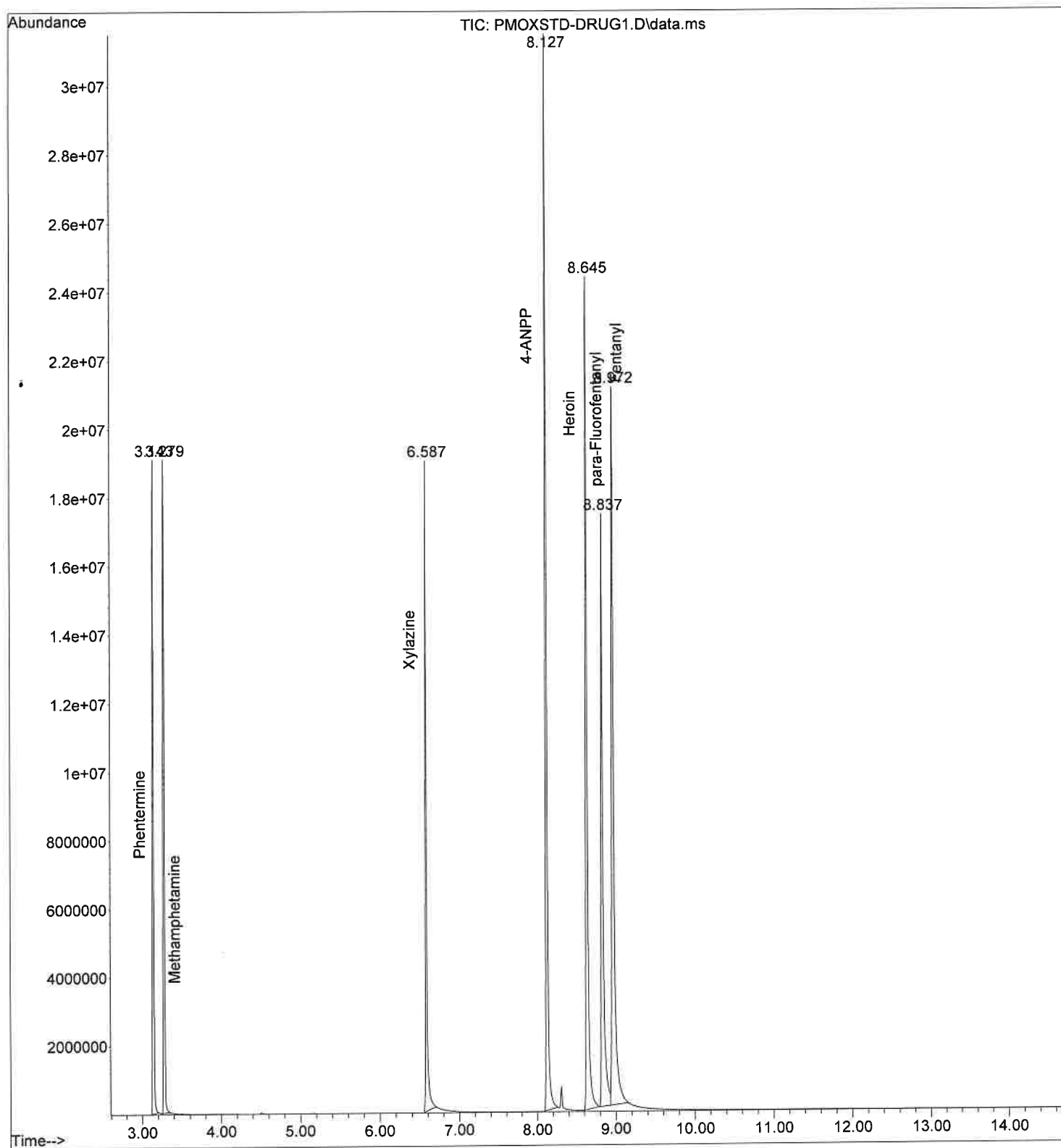
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\PMOXSTD-DRUG1.D
Operator : KLAB
Acquired : 18 Aug 2023 11:34 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : in Chloroform
Vial Number: 144



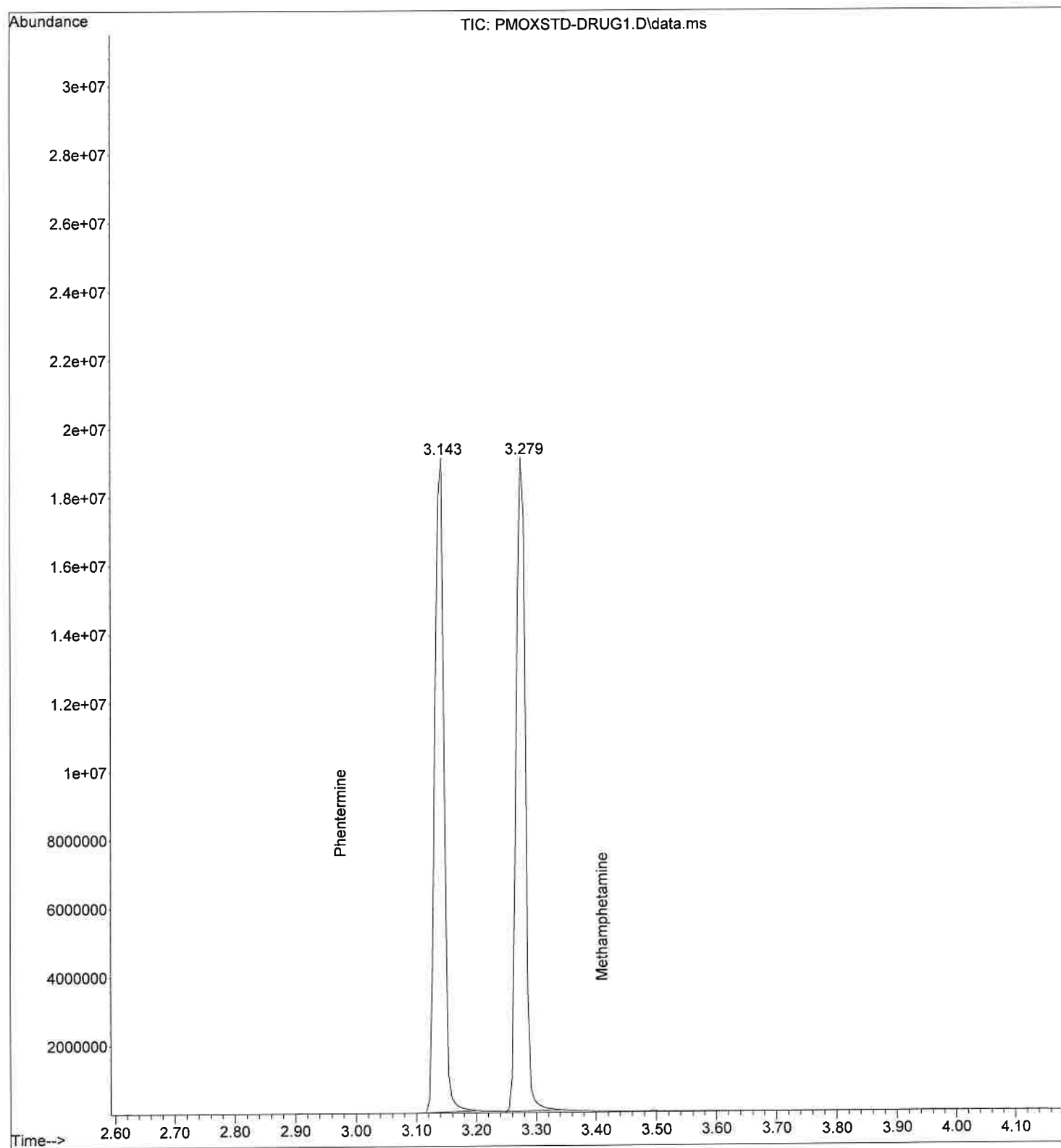
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\PMOXSTD-DRUG1.D
Operator : KLAB
Acquired : 18 Aug 2023 11:34 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : in Chloroform
Vial Number: 144



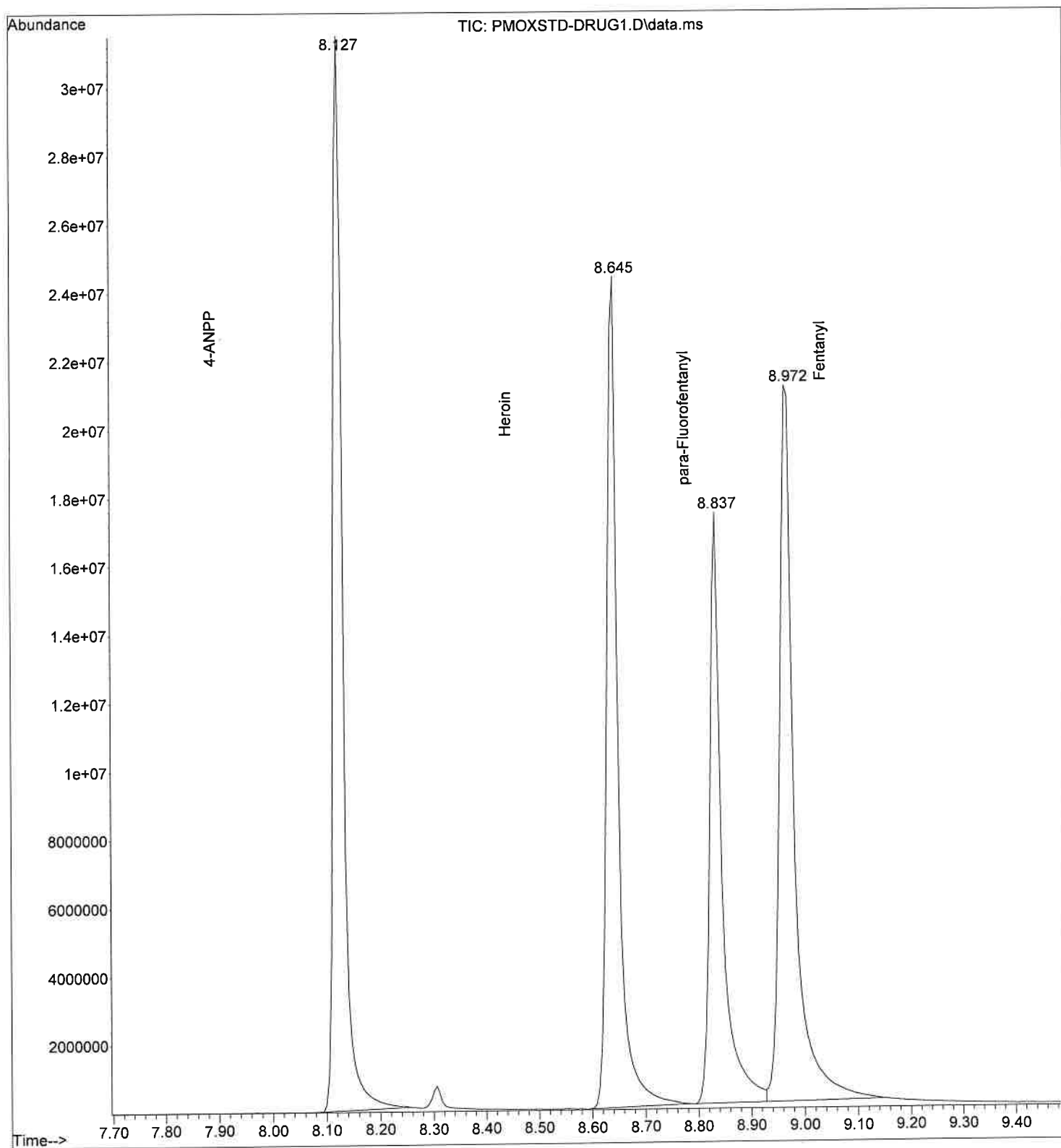
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\PMOXSTD-DRUG1.D
Operator : KLAB
Acquired : 18 Aug 2023 11:34 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : in Chloroform
Vial Number: 144



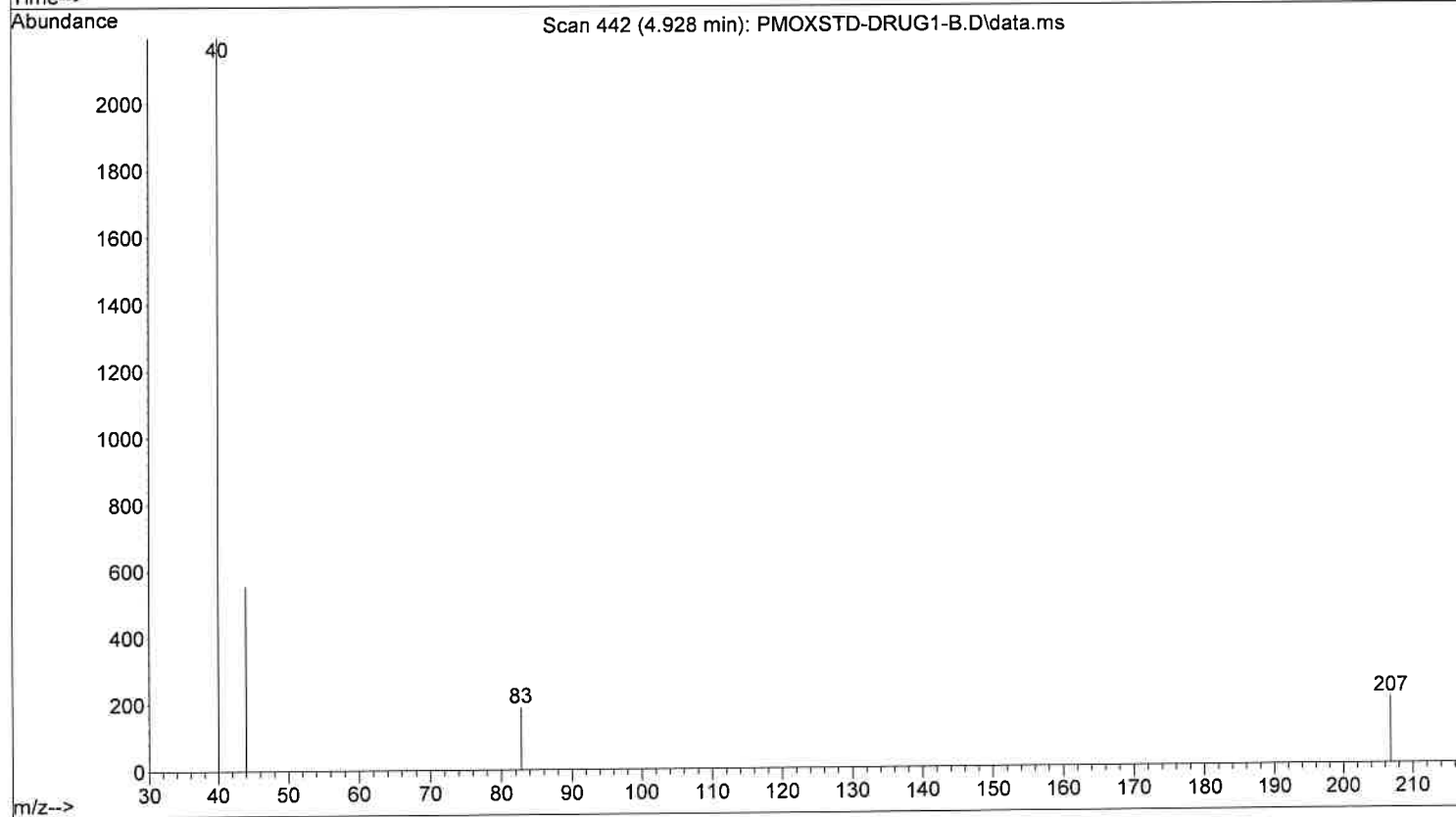
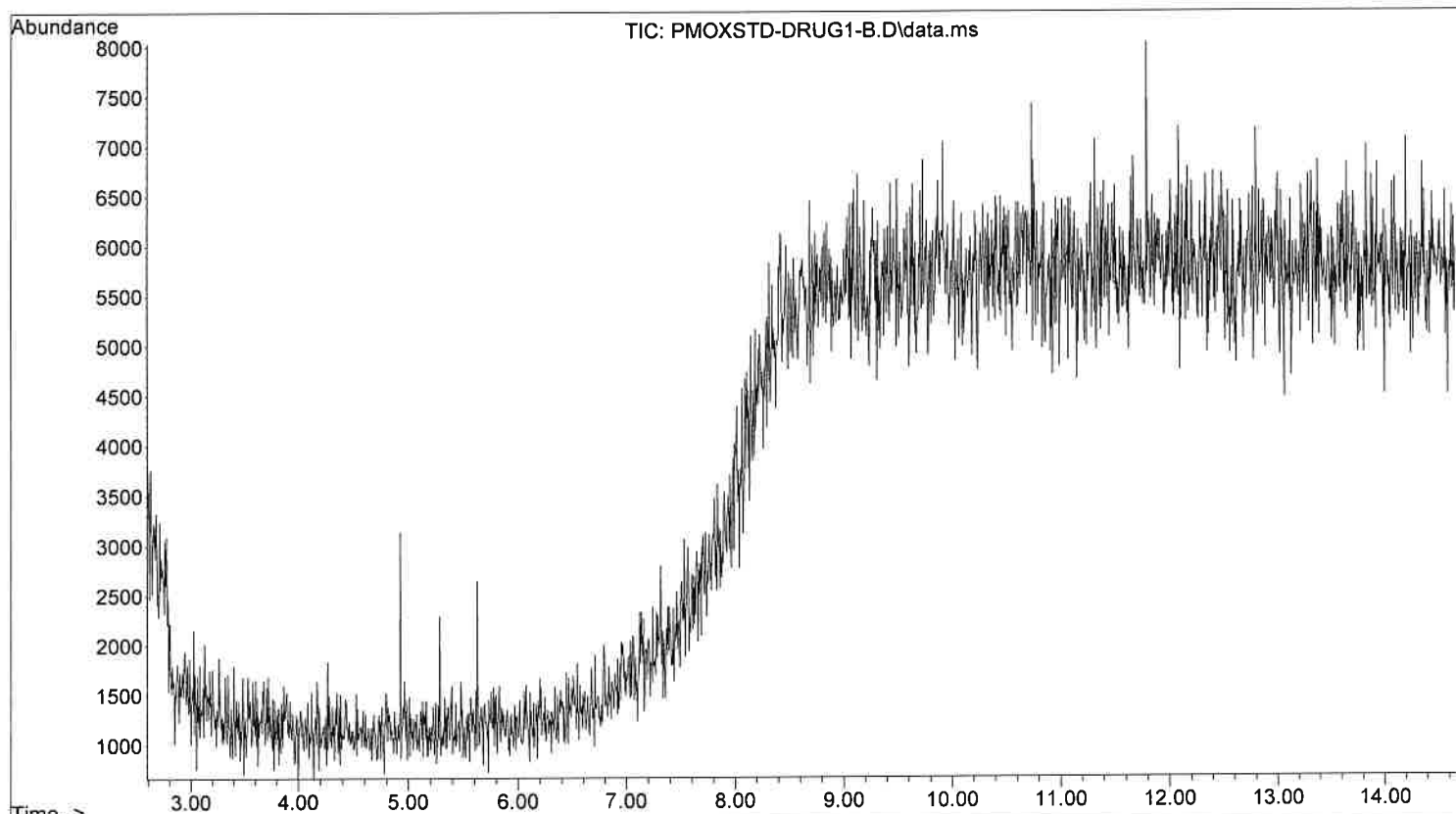
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\PMOXSTD-DRUG1.D
Operator : KLAB
Acquired : 18 Aug 2023 11:34 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : in Chloroform
Vial Number: 144



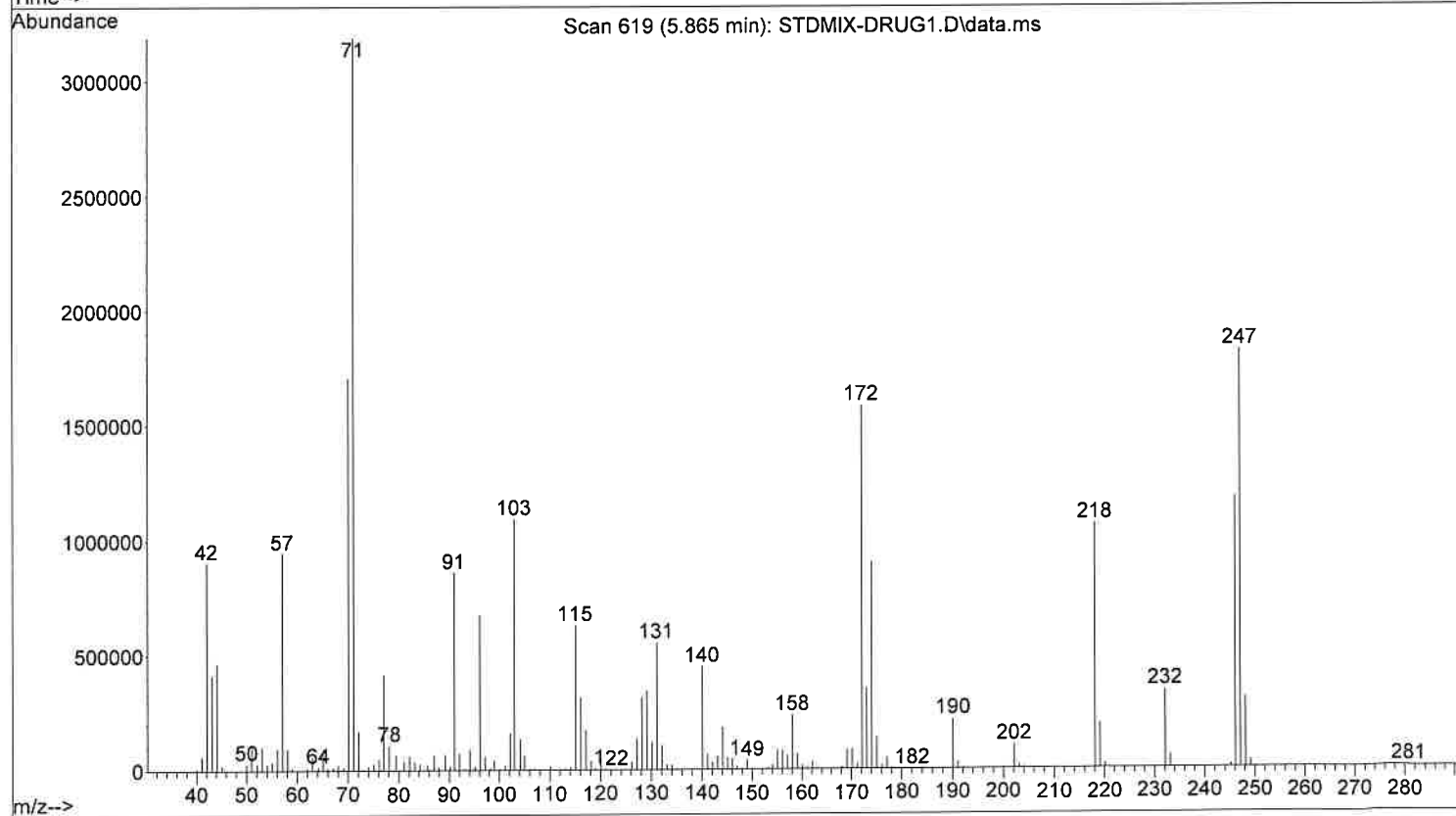
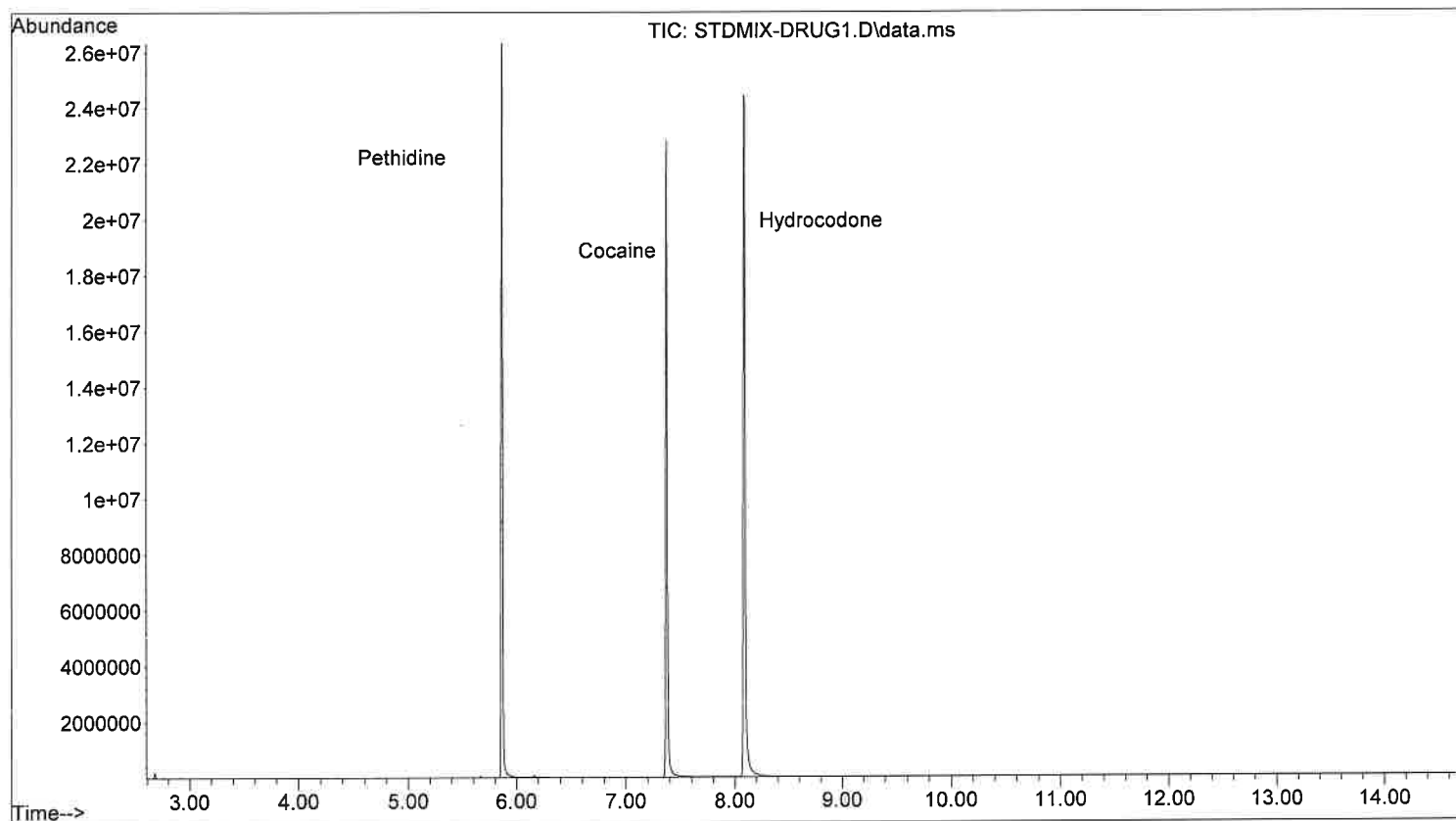
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\PMOXSTD-DRUG1.D
Operator : KLAB
Acquired : 18 Aug 2023 11:34 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : in Chloroform
Vial Number: 144



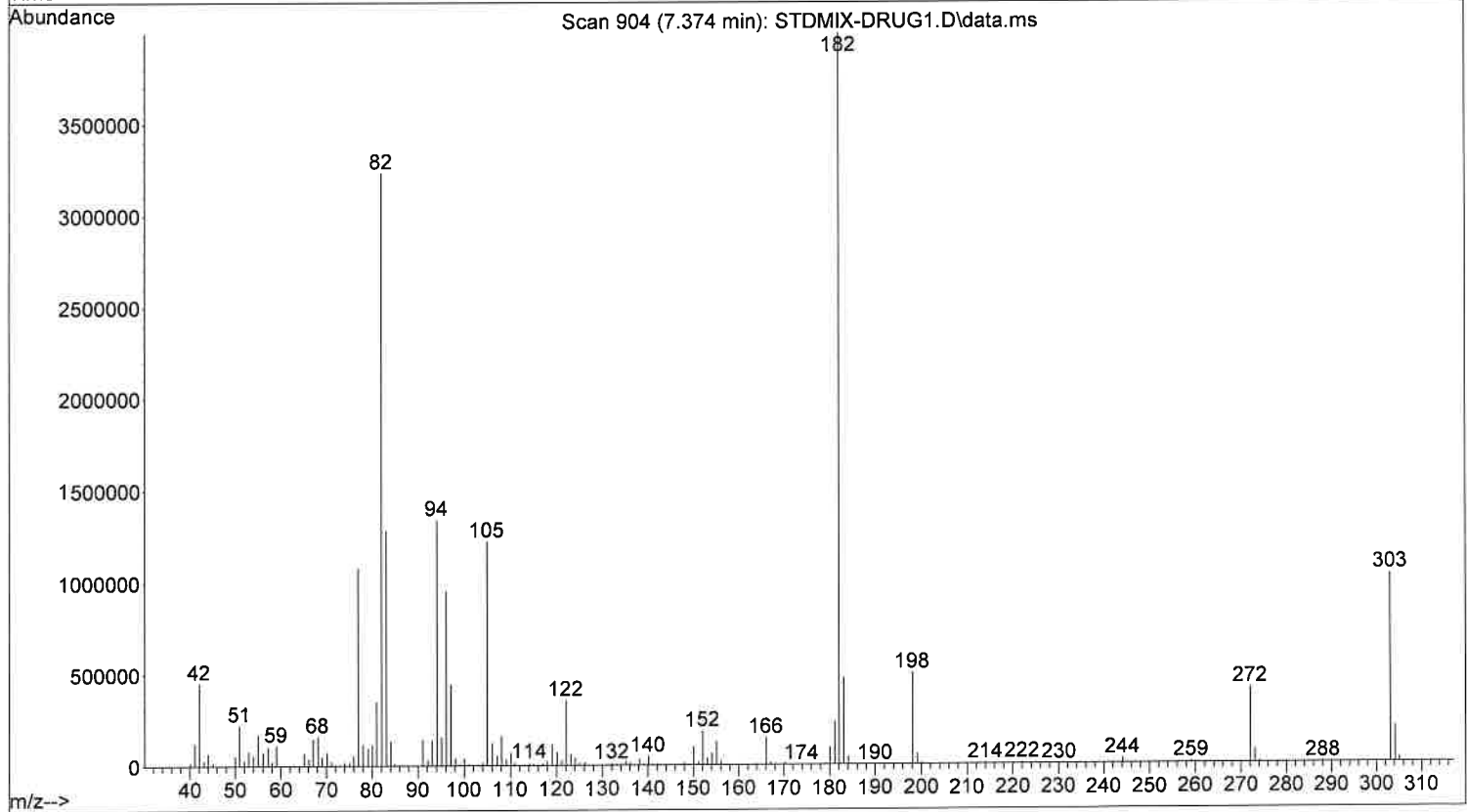
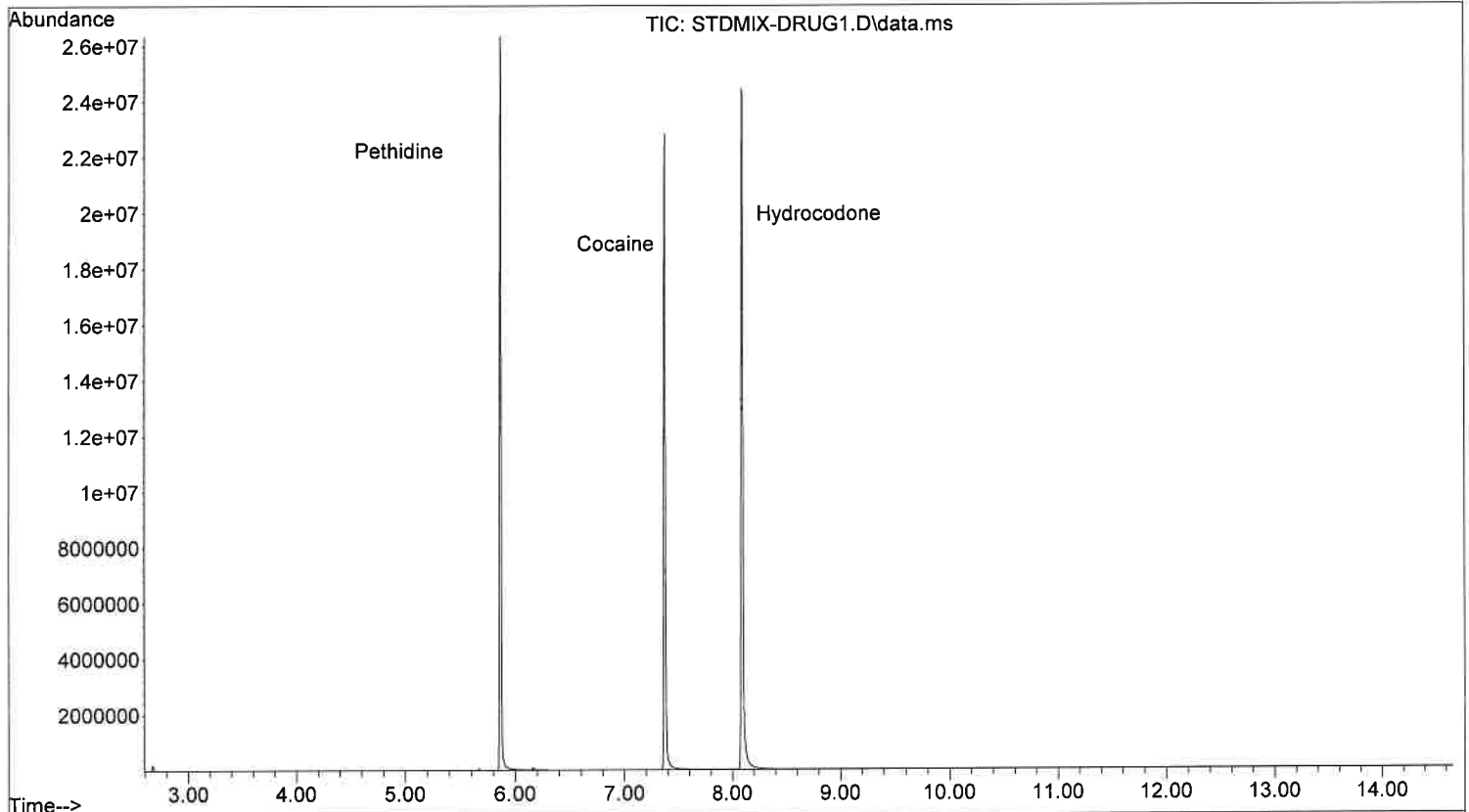
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\PMOXSTD-DRUG1-
... B.D
Operator : KLAB
Acquired : 18 Aug 2023 11:15 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : for P-MOX Standard
Vial Number: 142



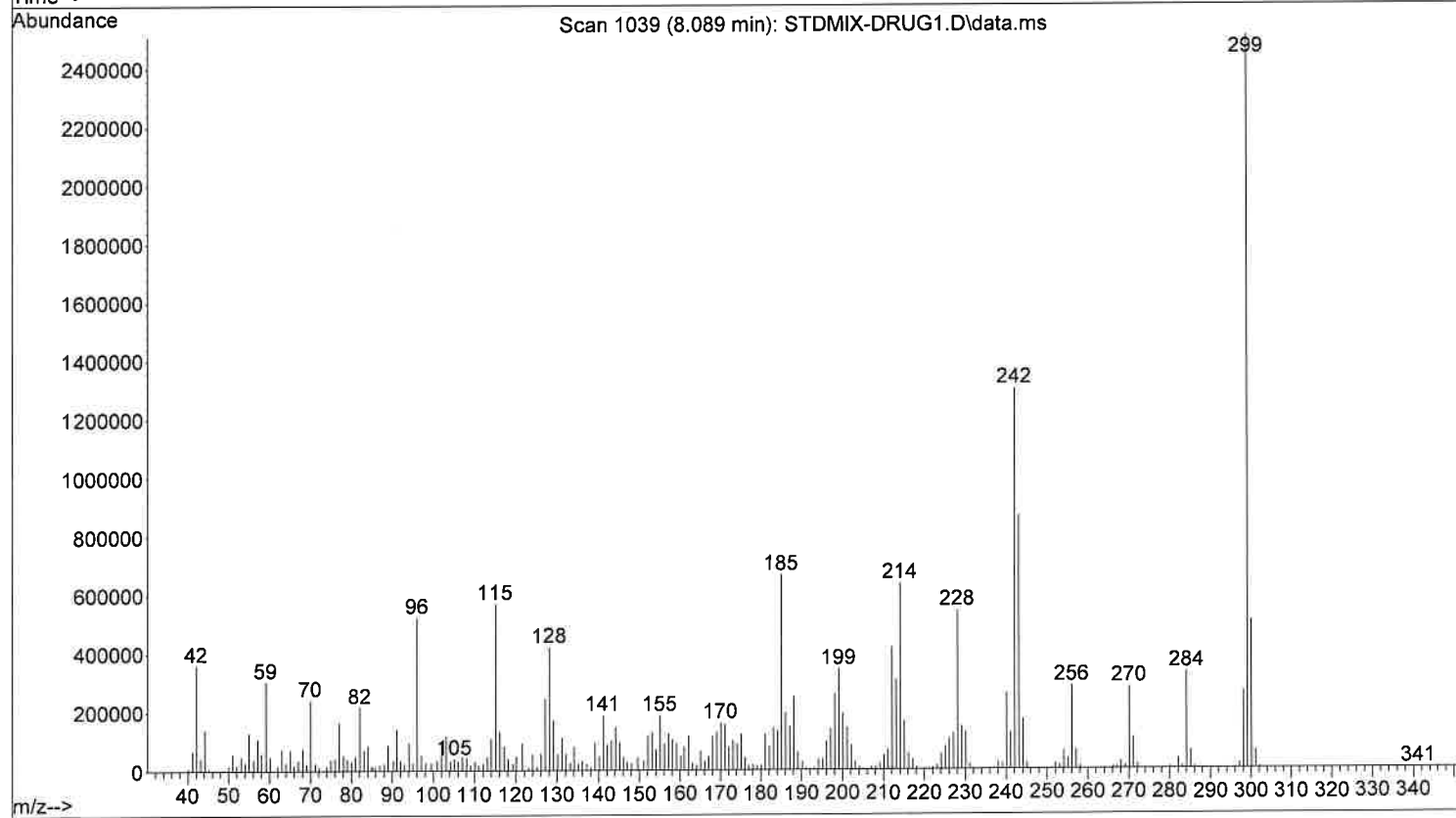
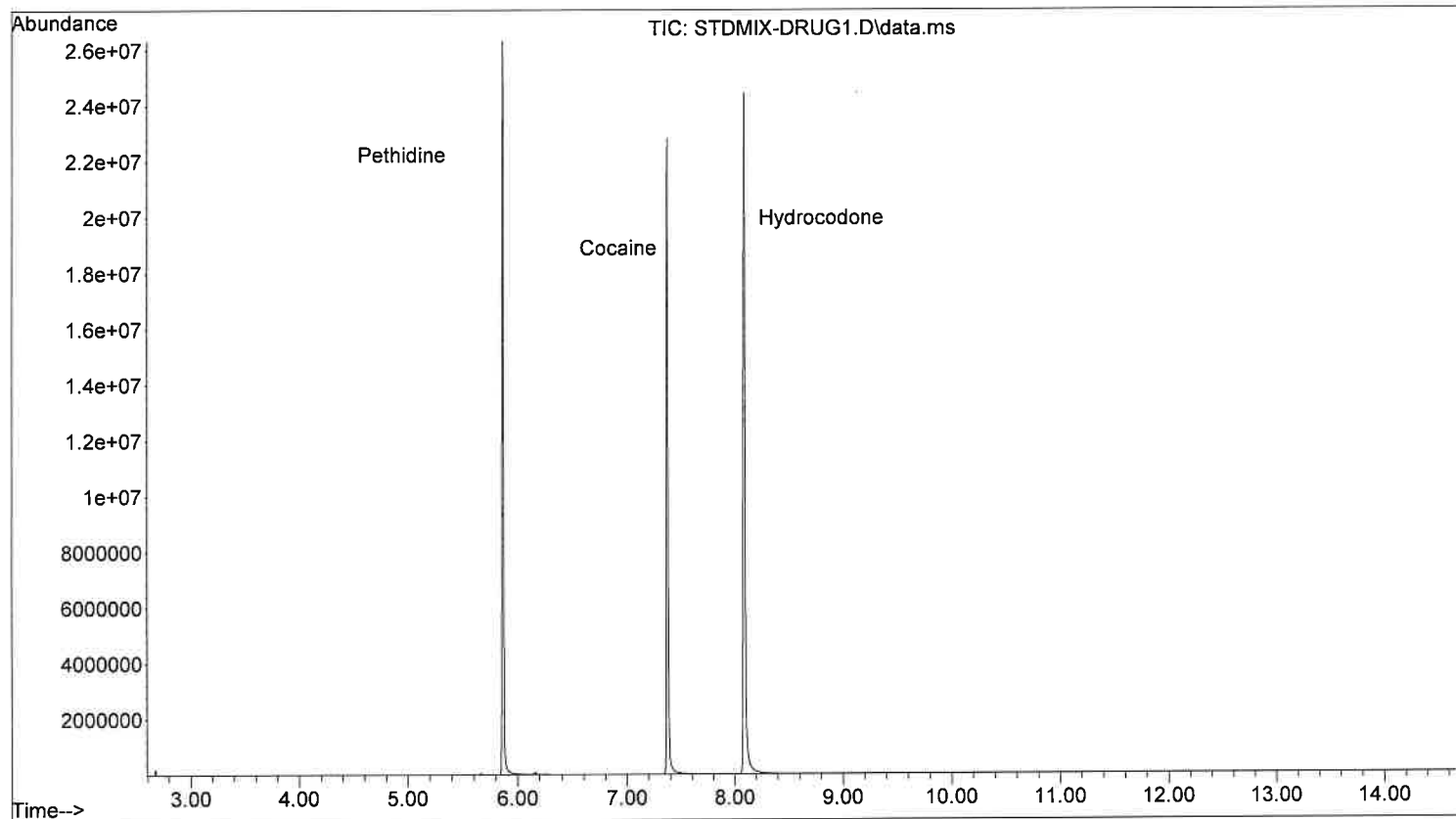
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\STDMIX-DRUG1.D
Operator : KLAB
Acquired : 18 Aug 2023 12:19 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : in Chloroform
Vial Number: 145



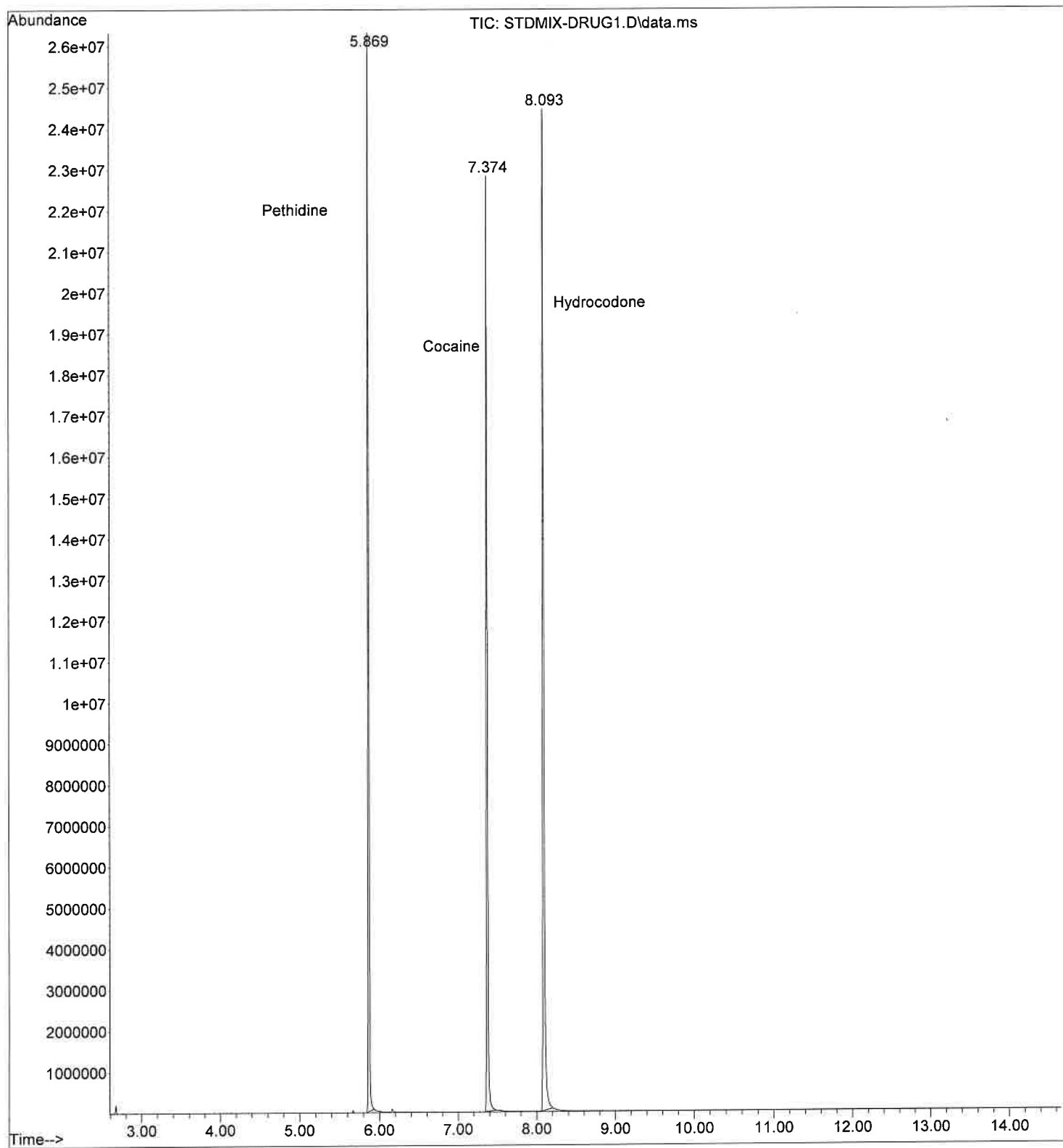
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\STDMIX-DRUG1.D
Operator : KLAB
Acquired : 18 Aug 2023 12:19 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : in Chloroform
Vial Number: 145



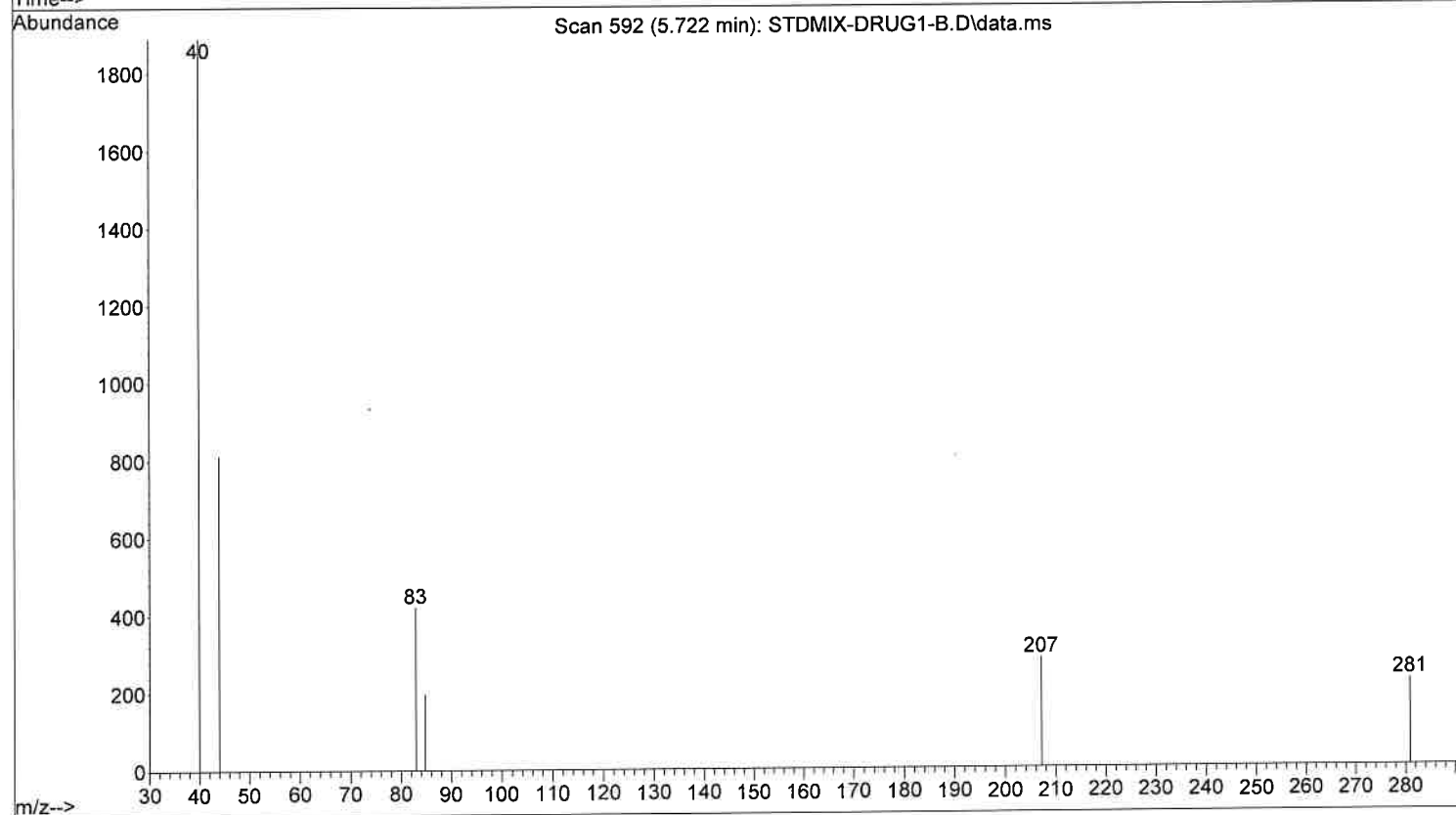
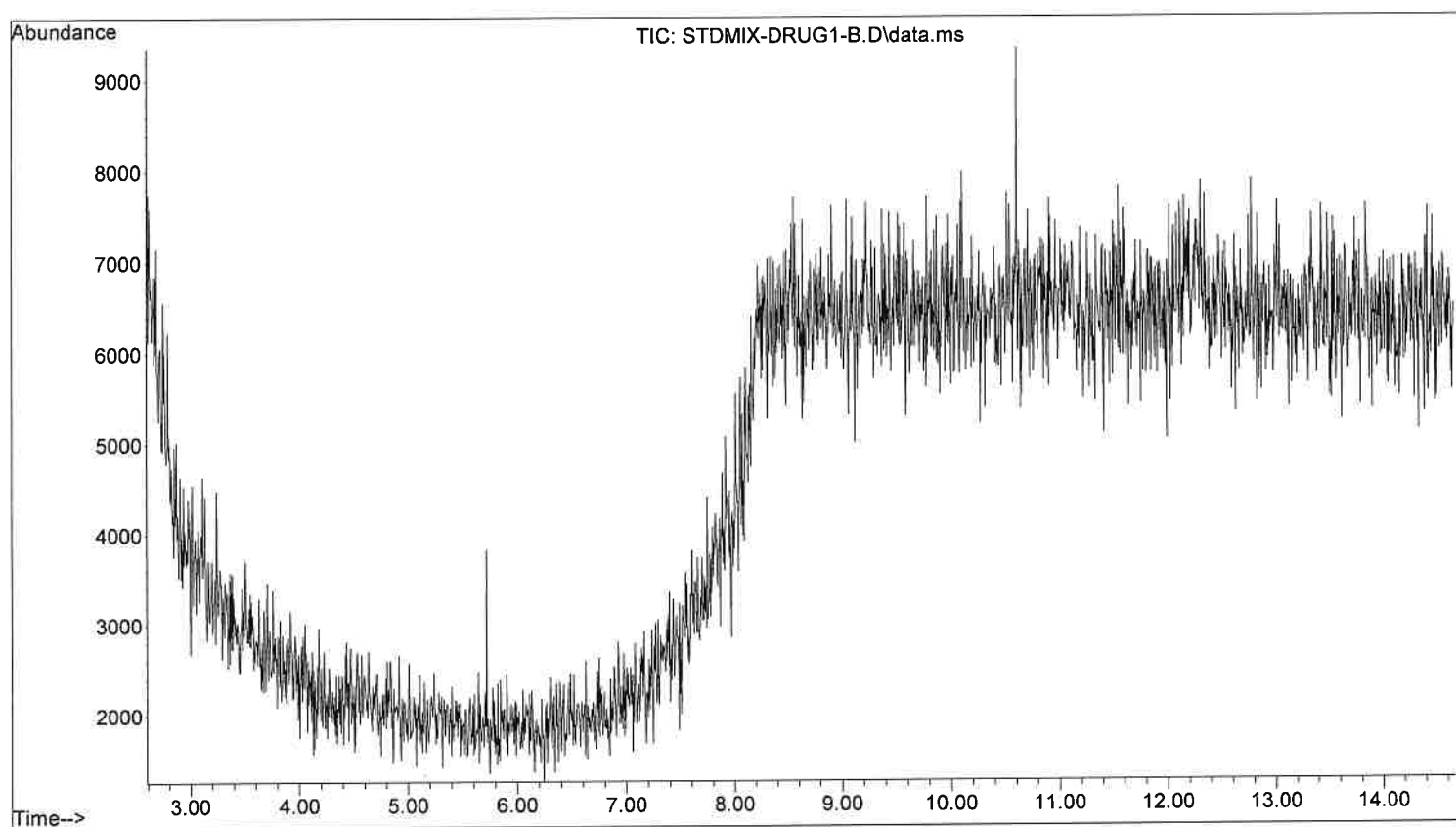
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Operator : KLAB
Acquired : 18 Aug 2023 12:19 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : in Chloroform
Vial Number: 145



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\STDMIX-DRUG1.D
Operator : KLAB
Acquired : 18 Aug 2023 12:19 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : in Chloroform
Vial Number: 145



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC081823\STDMIX-DRUG1-B
... .D
Operator : KLAB
Acquired : 18 Aug 2023 12:01 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : for Standard Mix
Vial Number: 142



METHOD CONTROL PARAMETERS

Method Information for: D:\MassHunter\GCMS\1\methods\OPIATE.M

Method Sections To Run:

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

Method Comments:

OPIATE

END OF METHOD CONTROL PARAMETERS

Single Quadrupole Acquisition Method - MS Parameters Report

Method file	D:\MassHunter\GCMS\1\methods\OPIATE.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)	10.00
Solvent delay (min)	2.50
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
2.50	40	550	150	1,562 [N=2]

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

Self-Cleaning Ion Source Parameters

Mode	No Cleaning
------	-------------

D:\MassHunter\GCMS\1\methods\OPIATE.M
Thu Aug 24 15:42:20 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 6.6667 min
Post Run Time 0 min

Oven
Temperature
Setpoint On
(Initial) 200 °C
Hold Time 1 min
Post Run 80 °C
Program
#1 Rate 30 °C/min
#1 Value 280 °C
#1 Hold Time 3 min

Equilibration Time 0 min
Max Temperature 350 °C
Maximum Temperature Override Disabled
Slow Fan Disabled

ALS
Front Injector
Syringe Size 10 µL
Injection Volume 1 µL
Solvent A Washes (PreInj) 1
Solvent A Washes (PostInj) 1
Solvent A Volume 8 µL
Solvent B Washes (PreInj) 1
Solvent B Washes (PostInj) 1
Solvent B Volume 8 µL
Sample Washes 0
Sample Wash Volume 8 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 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
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	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	
Helium Conservation Controlled Mode	Off
Heater	Split
Pressure	On 250 °C
Total Flow	On 9.1 psi
Septum Purge Flow	On 58.386 mL/min
Pre-Run Flow Test	On 3 mL/min
Gas Saver	Off
Split Ratio	On 20 mL/min after 2 min
Split Flow	90 :1
Liner	54.777 mL/min
	Agilent 5190-2271: 900 µL (Splitless, single taper, wool, c
Back SS Inlet He	
Helium Conservation Controlled Mode	Off
Heater	Split
Pressure	Off
Total Flow	Off
Septum Purge Flow	Off
Pre-Run Flow Test	Off
Liner	A Liner has not been selected.
Column	
Column #1	
Flow	
Setpoint	On
(Initial)	0.60864 mL/min
Post Run	1 mL/min
Column Information	Agilent 128-0112: 1
Description	DB-1ms

Temperature Range	-60 °C-340 °C (350 °C)
Dimensions	12 m x 200 µm x 0.33 µm (Calibrated)
Heater	Oven
Column lock	Unlocked
In	Front SS Inlet He
Out	MSD
(Initial)	200 °C
Pressure	9.1 psi
Flow	0.60864 mL/min
Average Velocity	47.783 cm/sec
Holdup Time	0.41855 min
Control Mode	Constant Flow
Column Outlet Pressure	0 psi
Front Detector FID	
Makeup	He
Heater	Off
H2 Flow	Off
Air Flow	Off
Makeup Flow	Off
Carrier Gas Flow Correction	Constant Makeup and Fuel Flow
Flame	Off
Blank Evaluation Setpoints	
Perform Blank Evaluation Test	Off
Helium Conservation	
Helium Valve	Off
Nitrogen Valve	Off
Detector Evaluation	
Perform Detector Evaluation Test	Off
MSD Transfer Line	
Temperature	
Setpoint	On
(Initial)	280 °C
Signals	
Signal #1:	
Description	None
Signal #2:	
Description	None
Signal #3:	
Description	None
Signal #4:	
Description	None
Signal #5:	
Description	None
Signal #6:	
Description	None
Signal #7:	
Description	None
Signal #8:	
Description	None

TUNE PARAMETERS for SN: US2313MA09

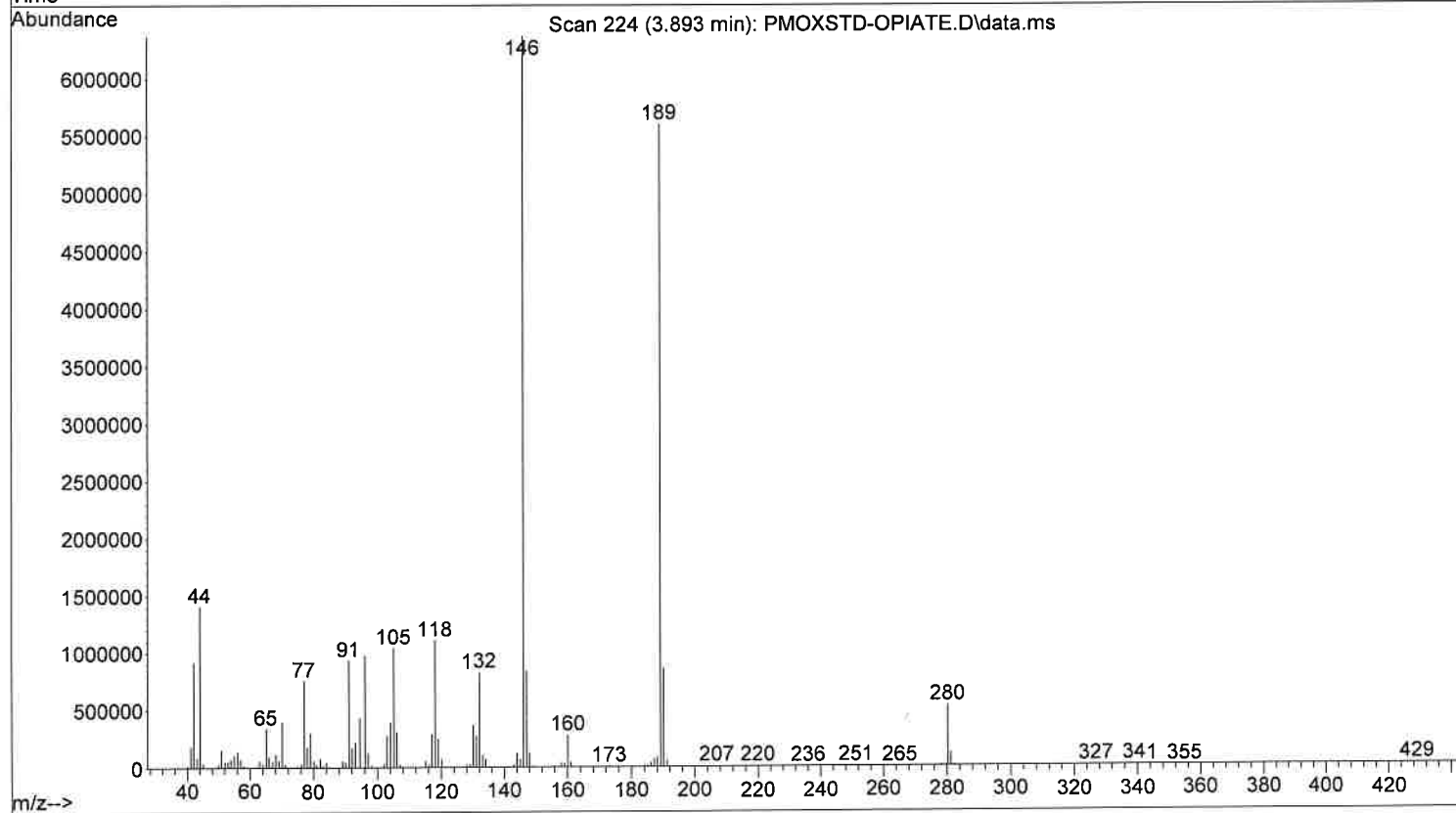
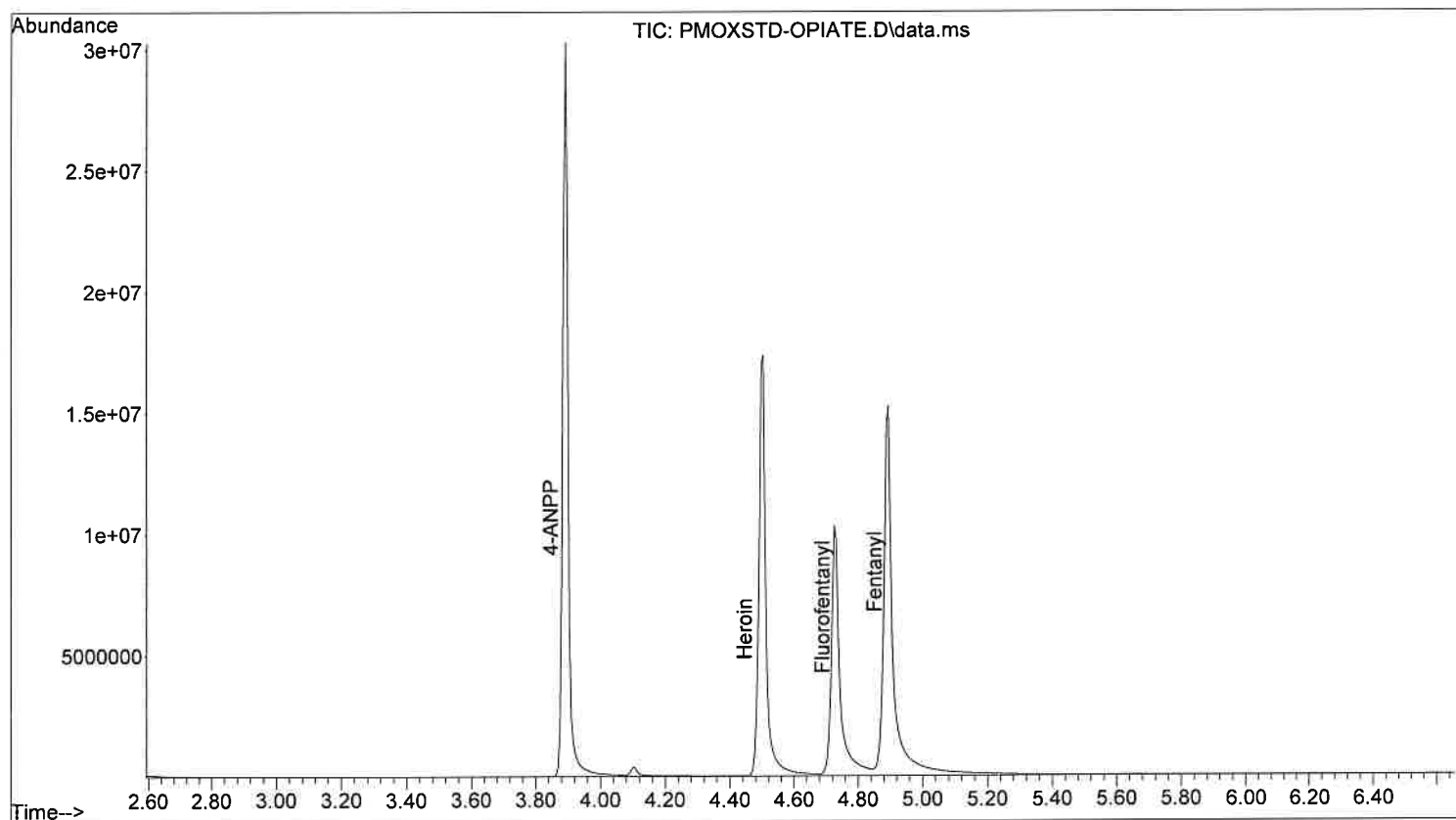
Trace Ion Detection is OFF.

34.593	:	EMISSION	
70.007	:	ENERGY	
29.919	:	REPELLER	
90.331	:	IONFOCUS	
25.226	:	ENTRANCE_LENS	
925.472	:	EMVOLTS	
		951.5	: Actual EMV
		1.00	: GAIN FACTOR
2896.000	:	AMUGAIN	
134.625	:	AMUOFFSET	
1.000	:	FILAMENT	
0.000	:	DCPOLARITY	
10.822	:	ENTLENSOFFSET	
0.000	:	Ion_Body	
0.000	:	EXTLENS	
257.000	:	MASSGAIN	
-23.000	:	MASSOFFSET	

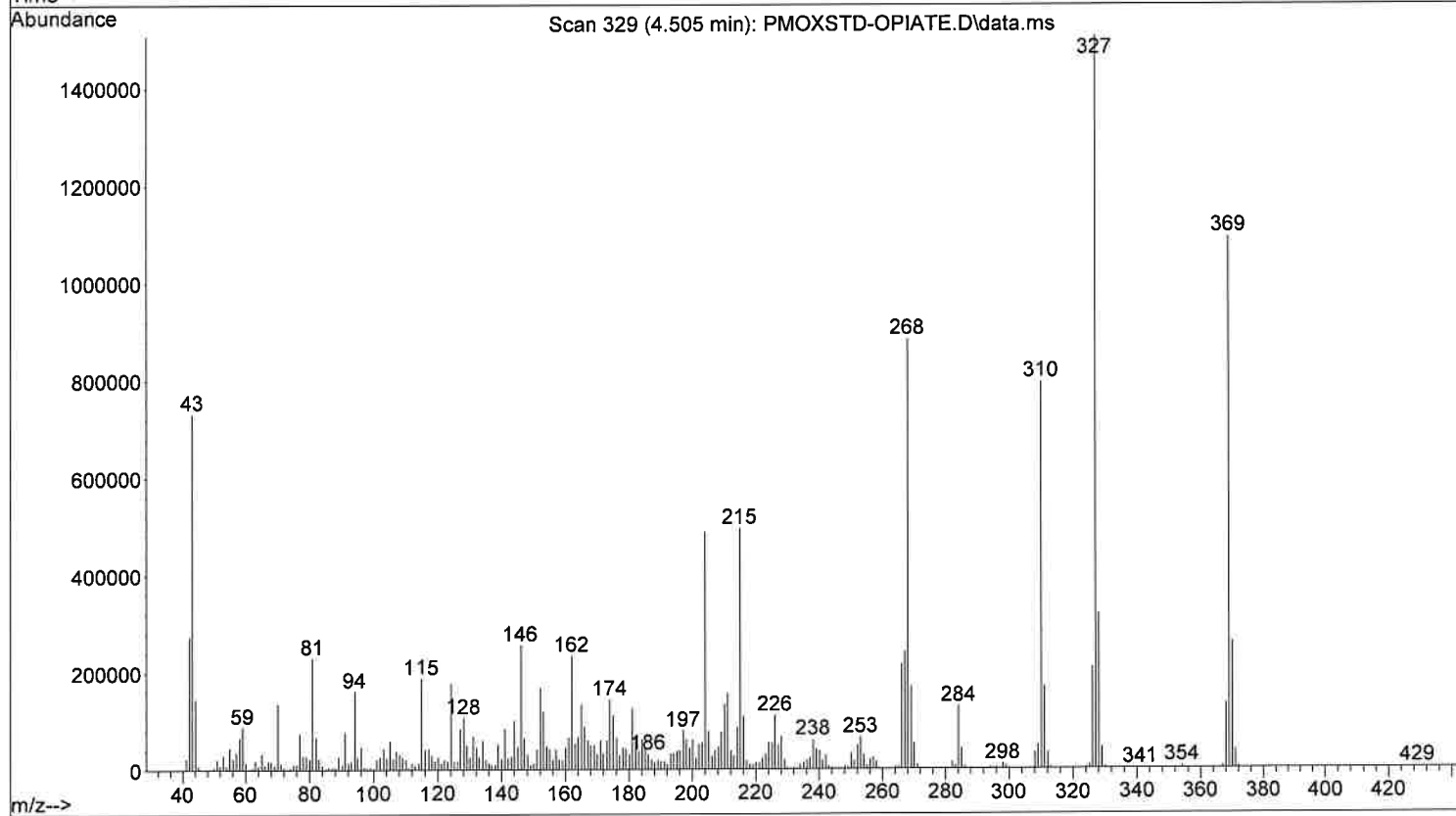
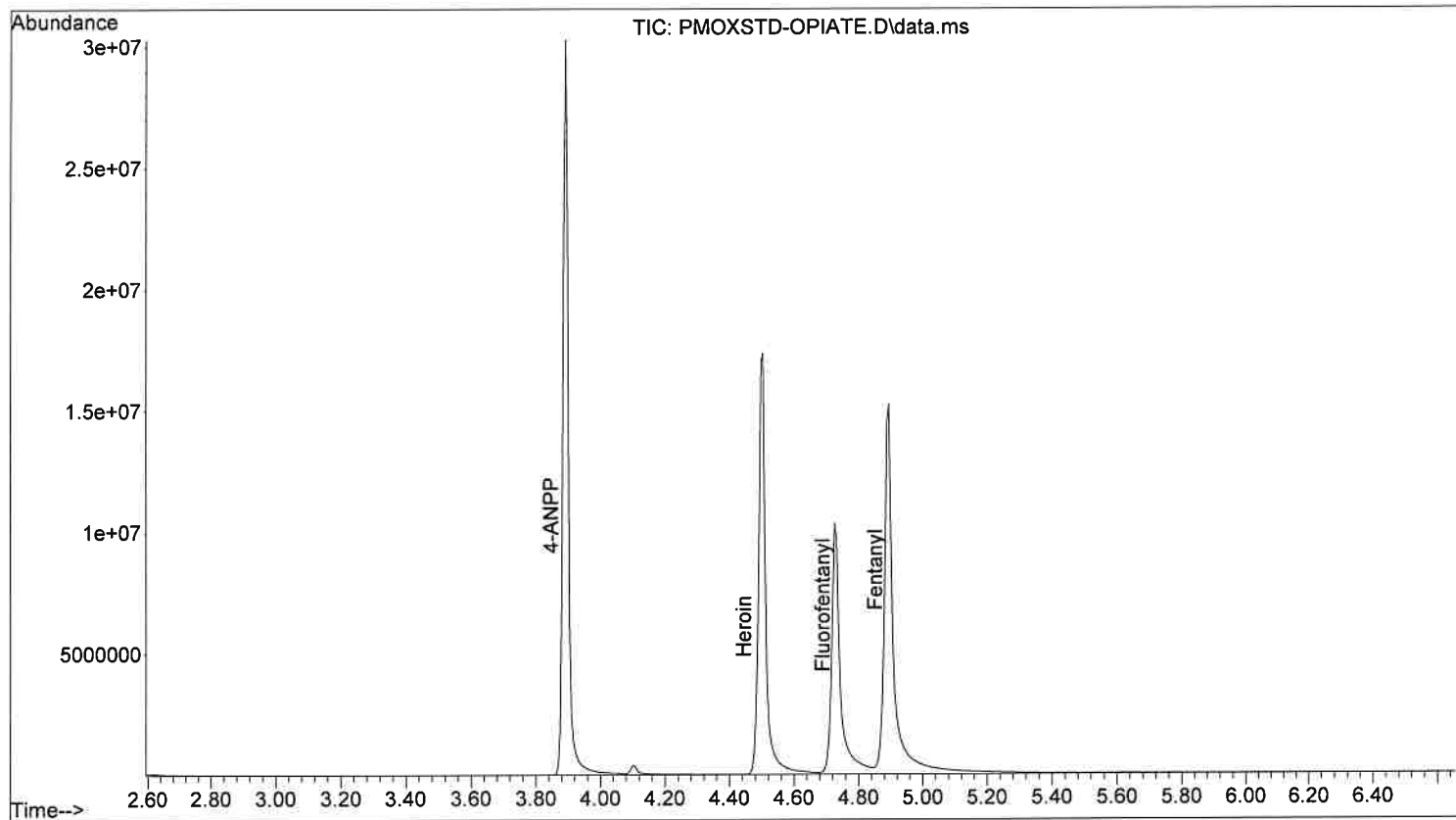
END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

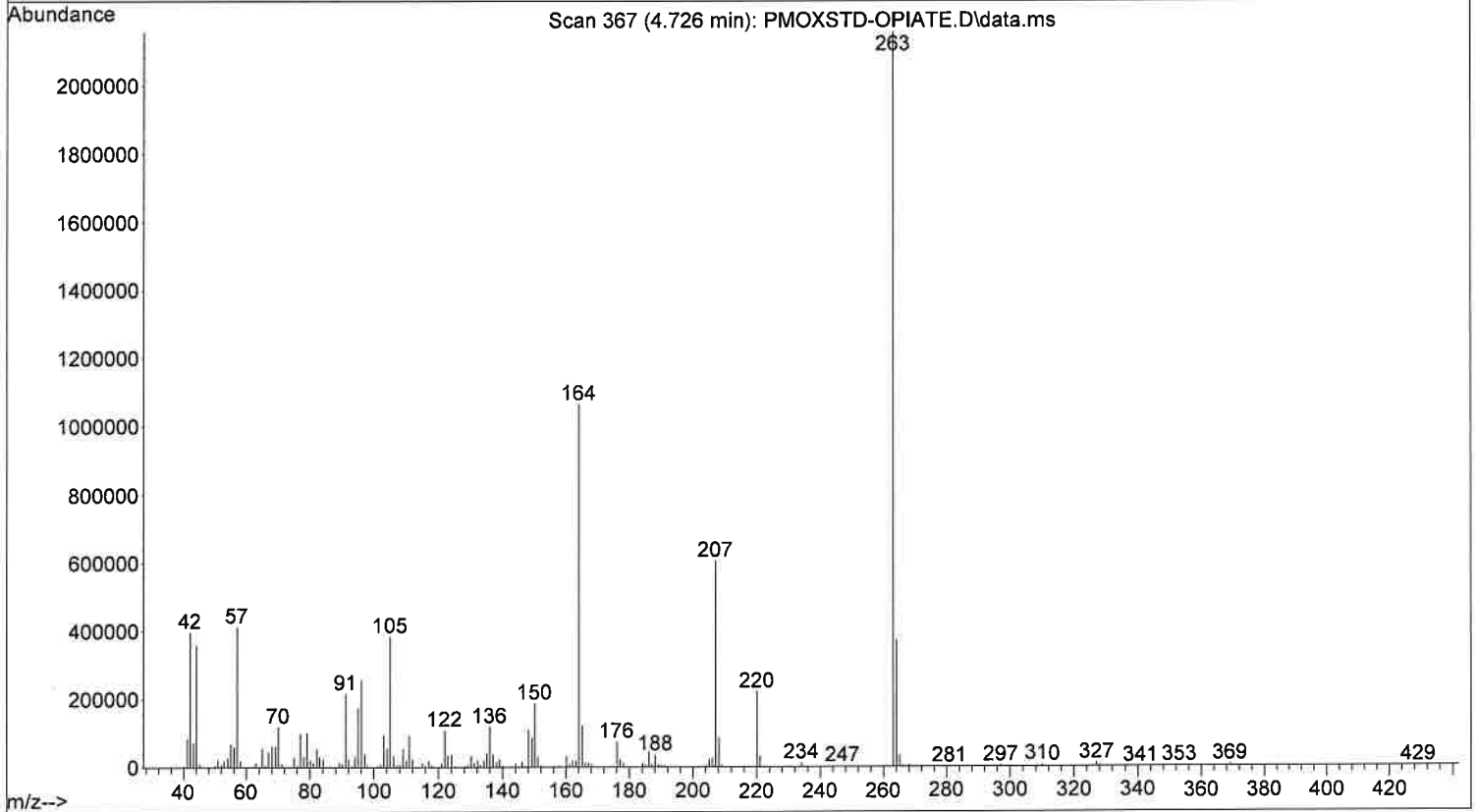
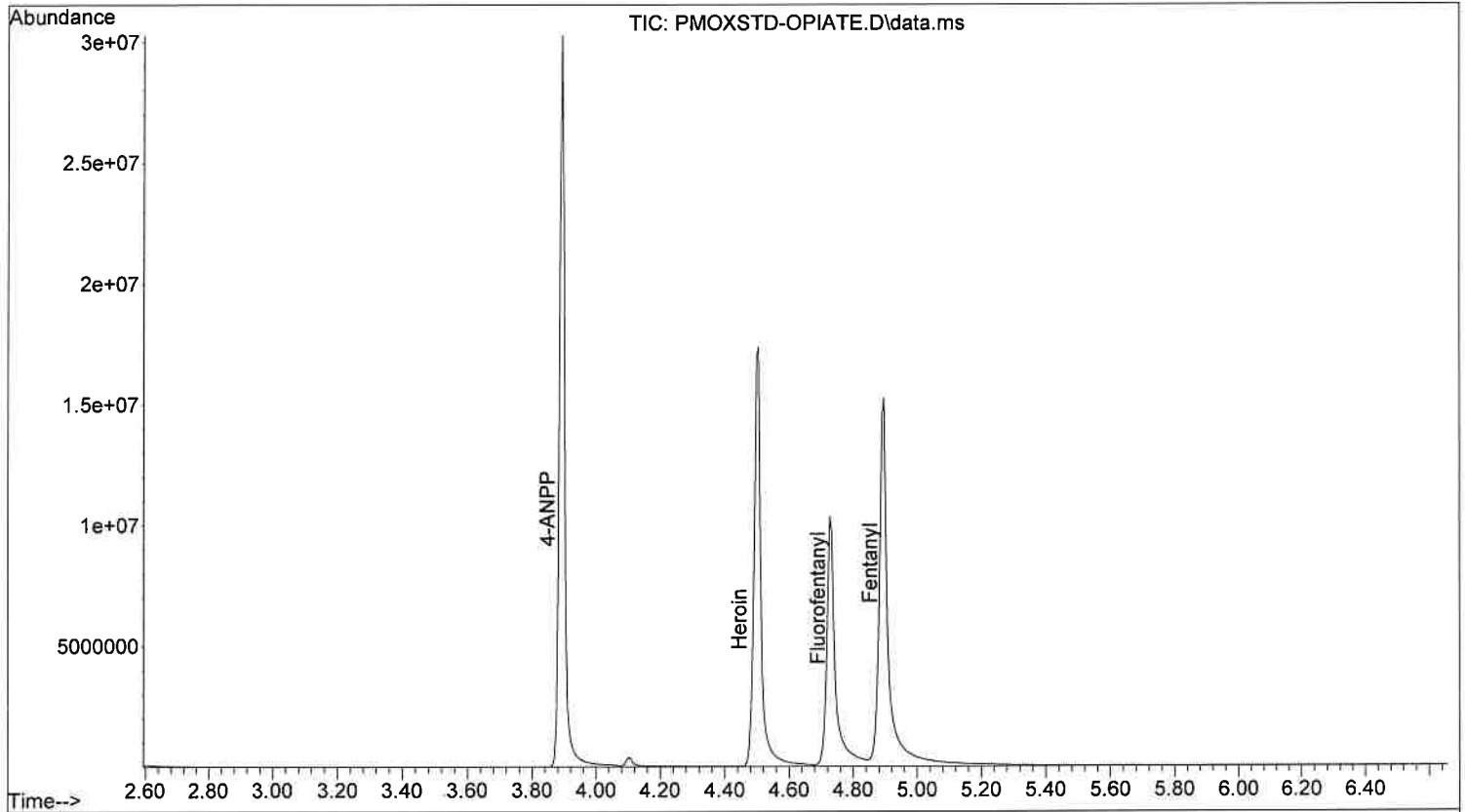
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Operator : KLAB
Acquired : 21 Aug 2023 12:43 using AcqMethod OPIATE.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



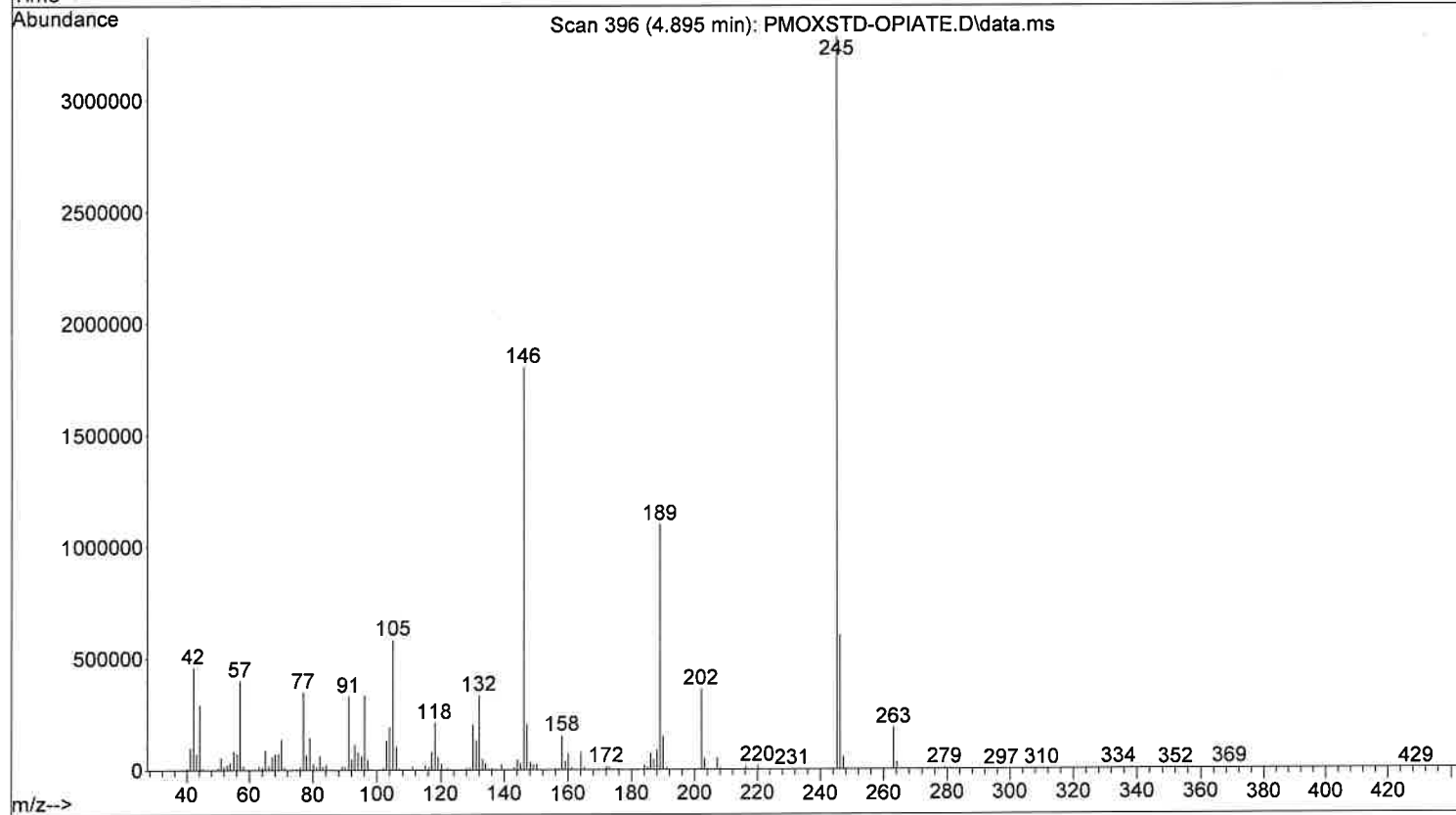
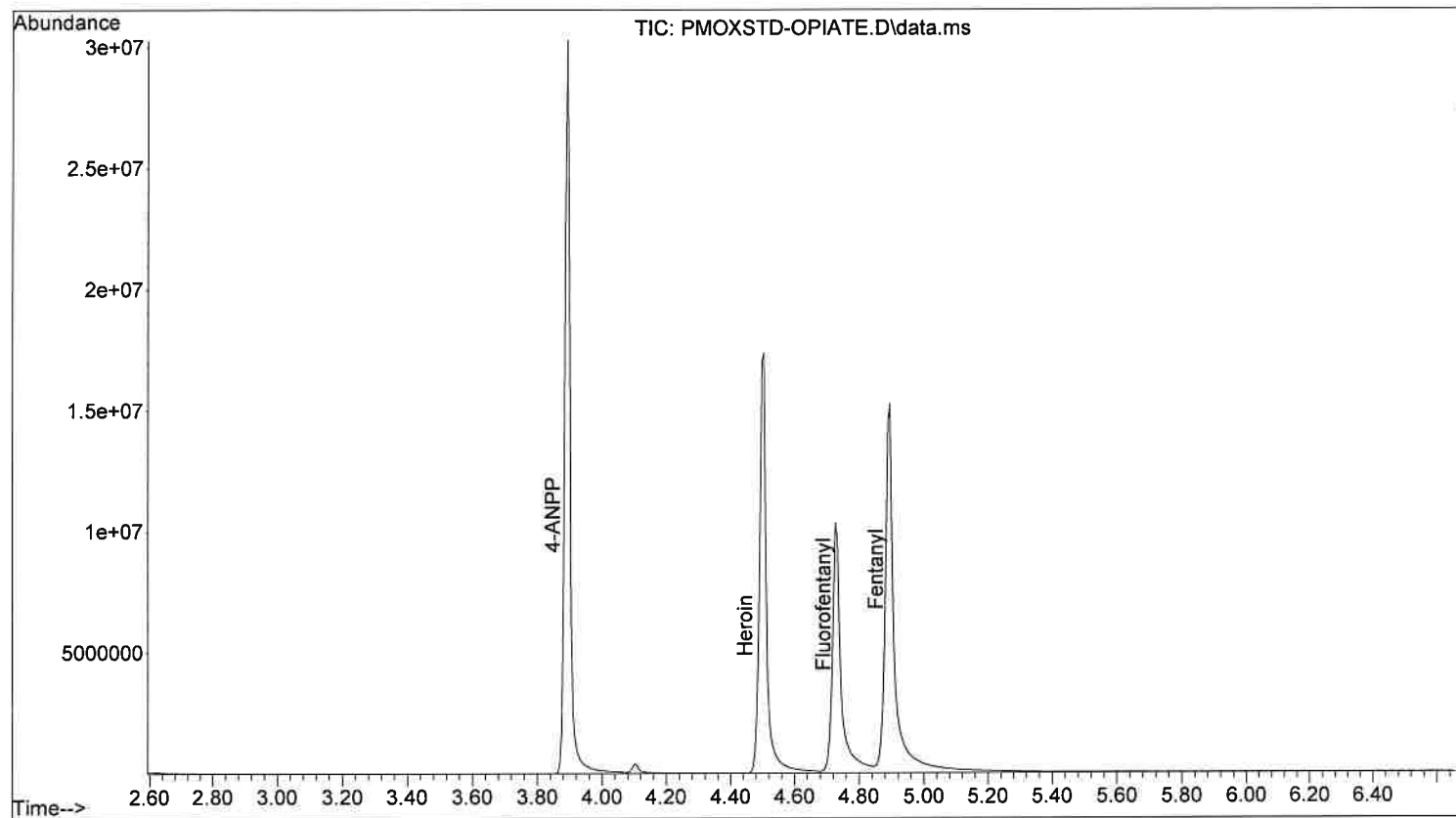
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Operator : KLAB
Acquired : 21 Aug 2023 12:43 using AcqMethod OPIATE.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



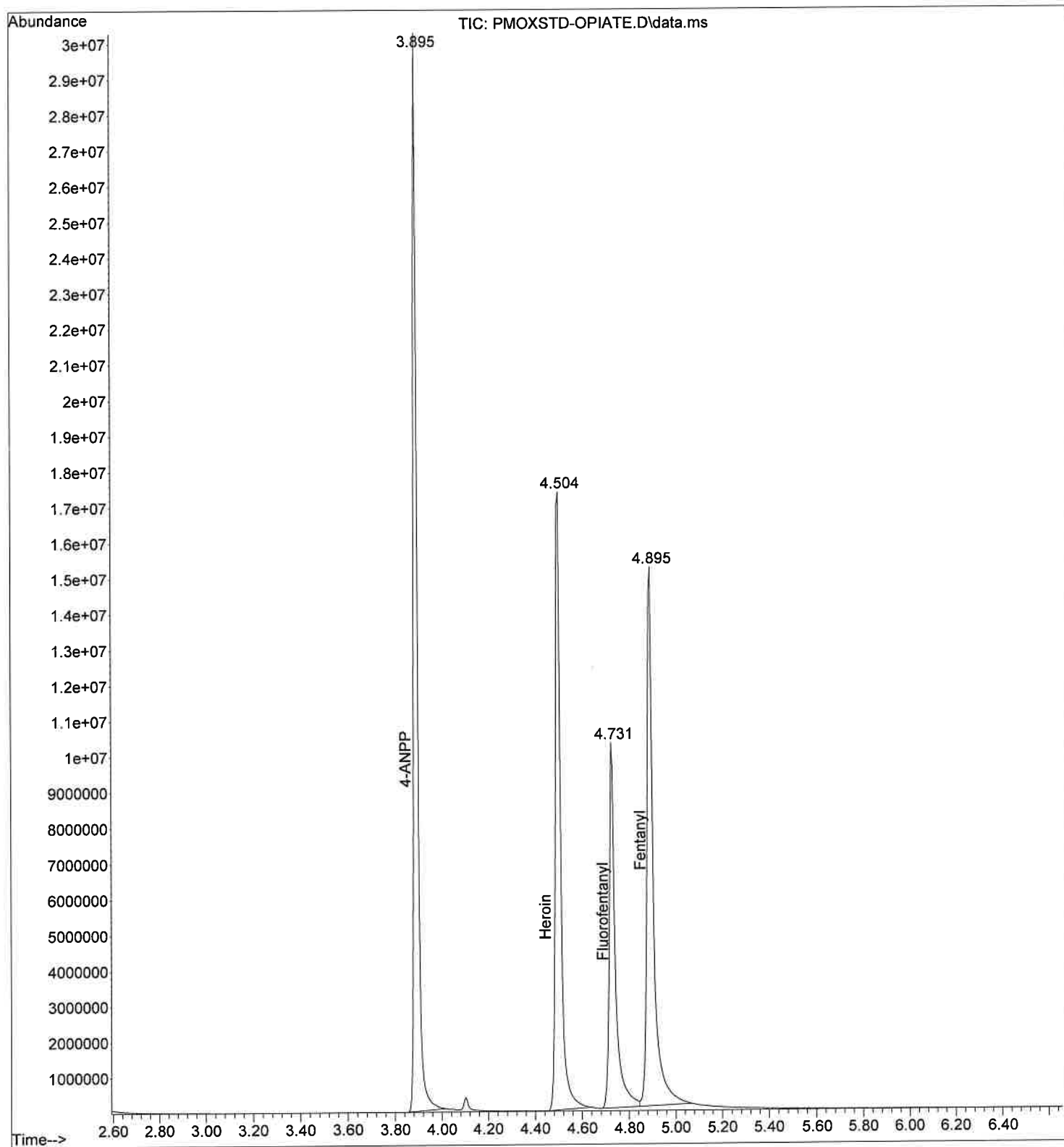
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PMOXSTD-OPIATE.D
Operator : KLAB
Acquired : 21 Aug 2023 12:43 using AcqMethod OPIATE.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



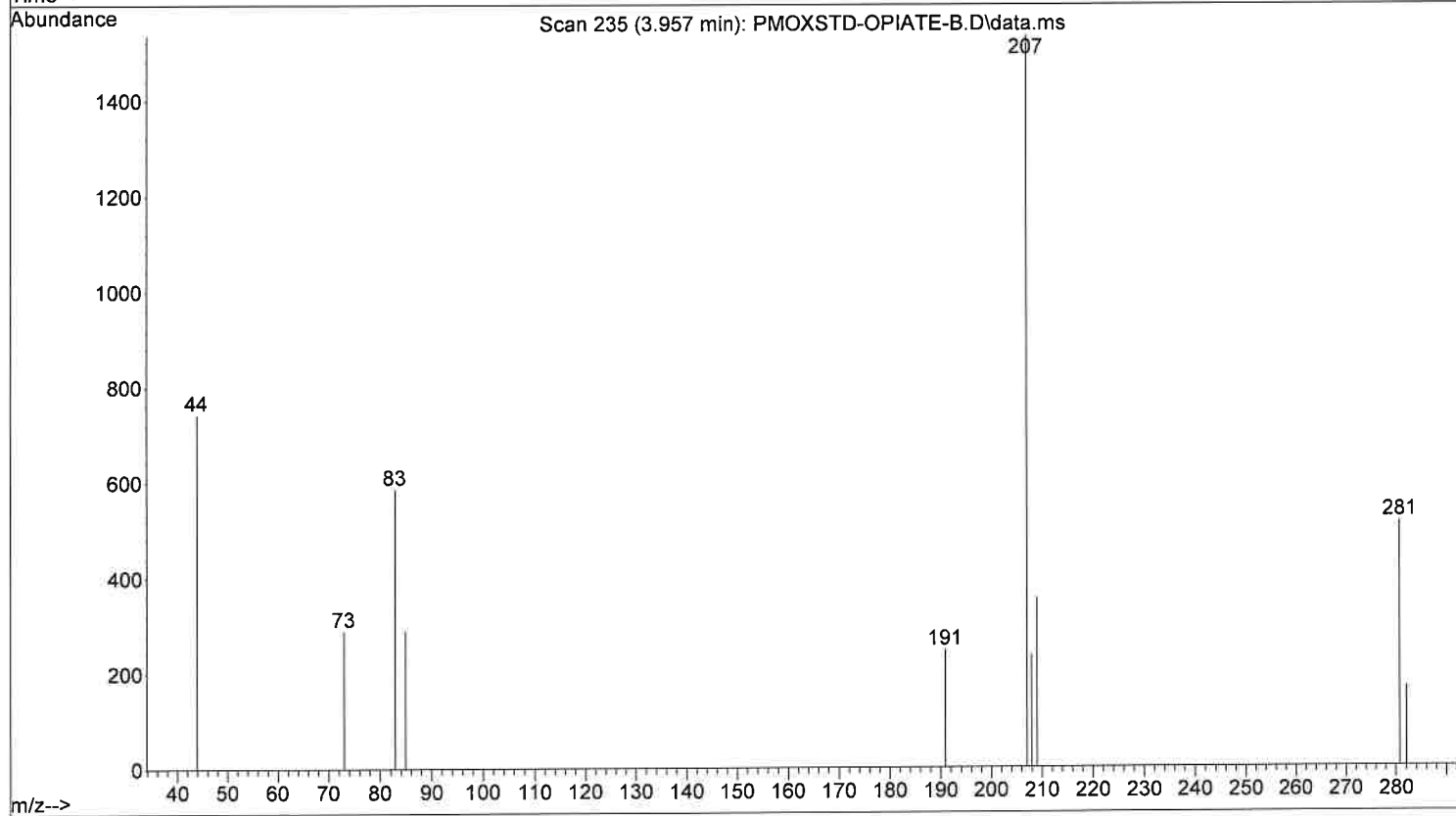
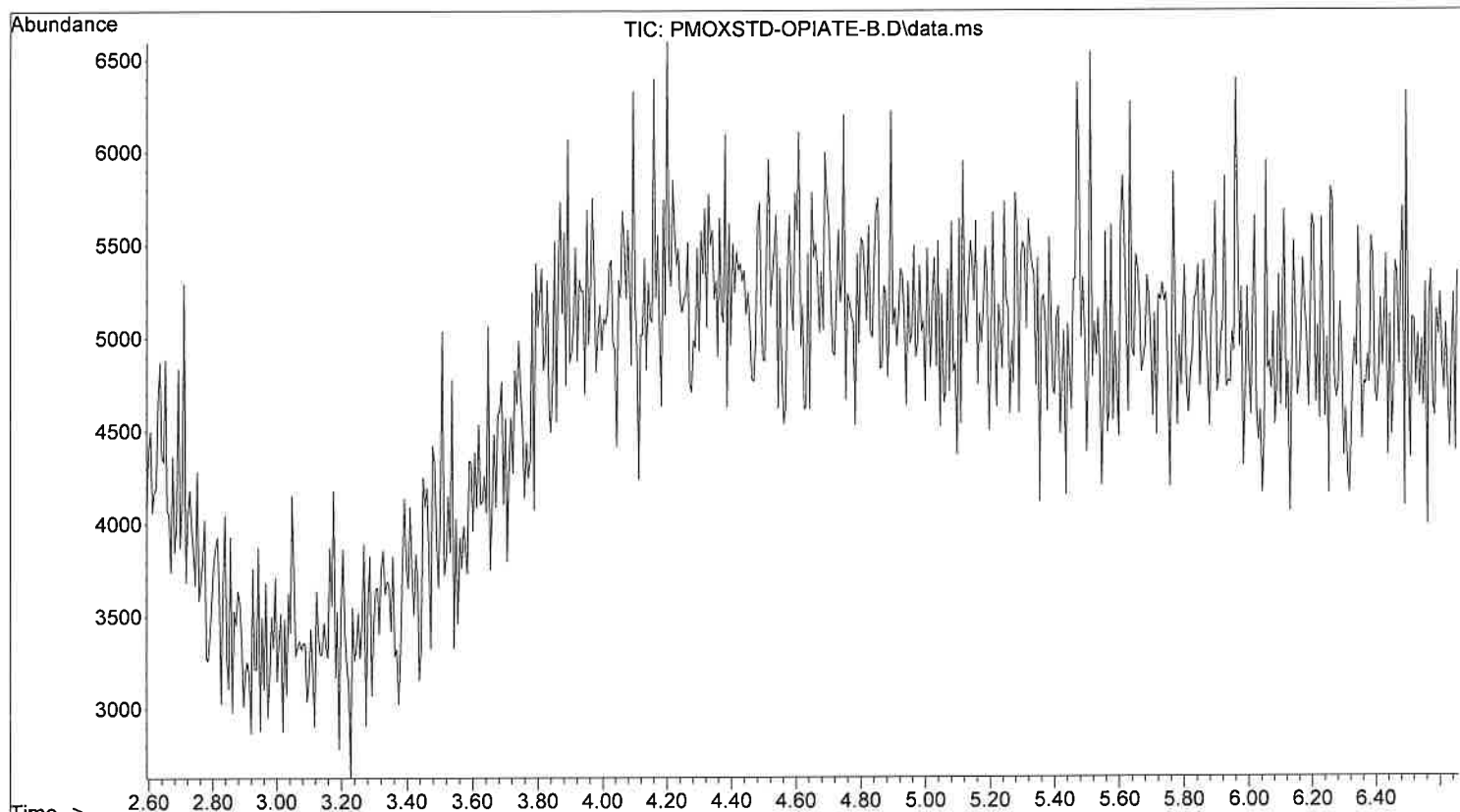
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PMOXSTD-OPIATE.D
Operator : KLAB
Acquired : 21 Aug 2023 12:43 using AcqMethod OPIATE.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



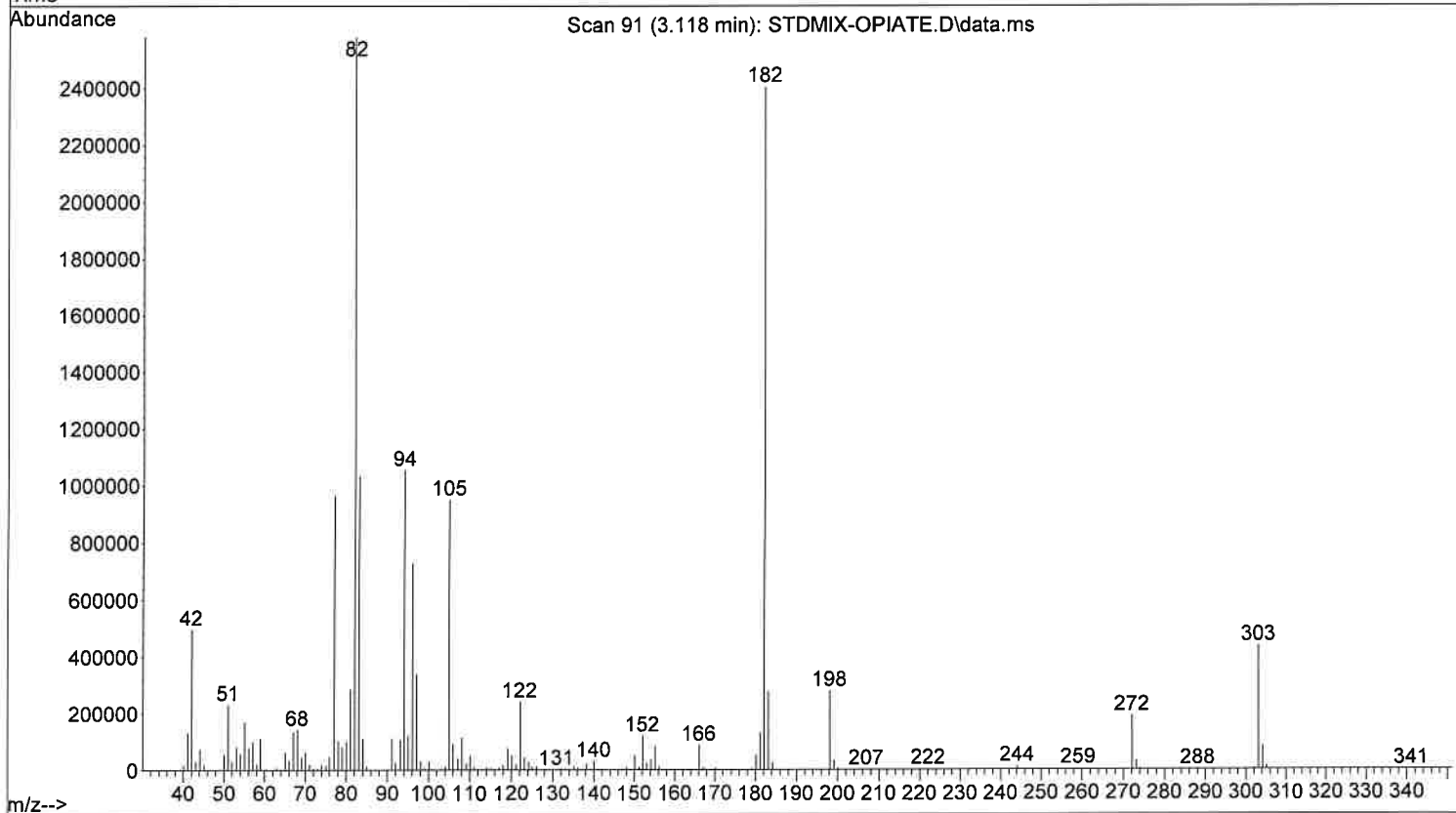
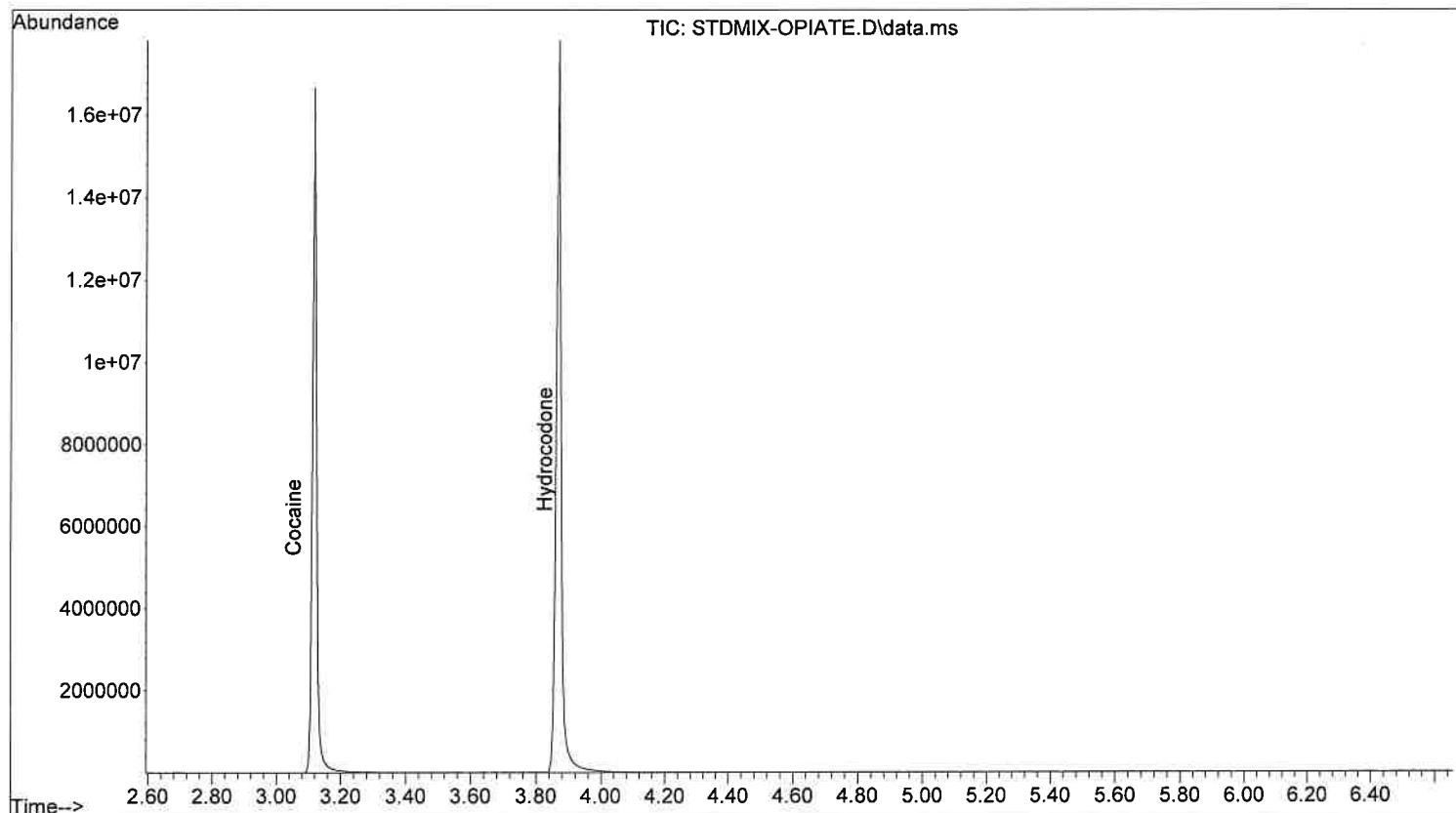
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PMOXSTD-OPIATE.D
Operator : KLAB
Acquired : 21 Aug 2023 12:43 using AcqMethod OPIATE.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



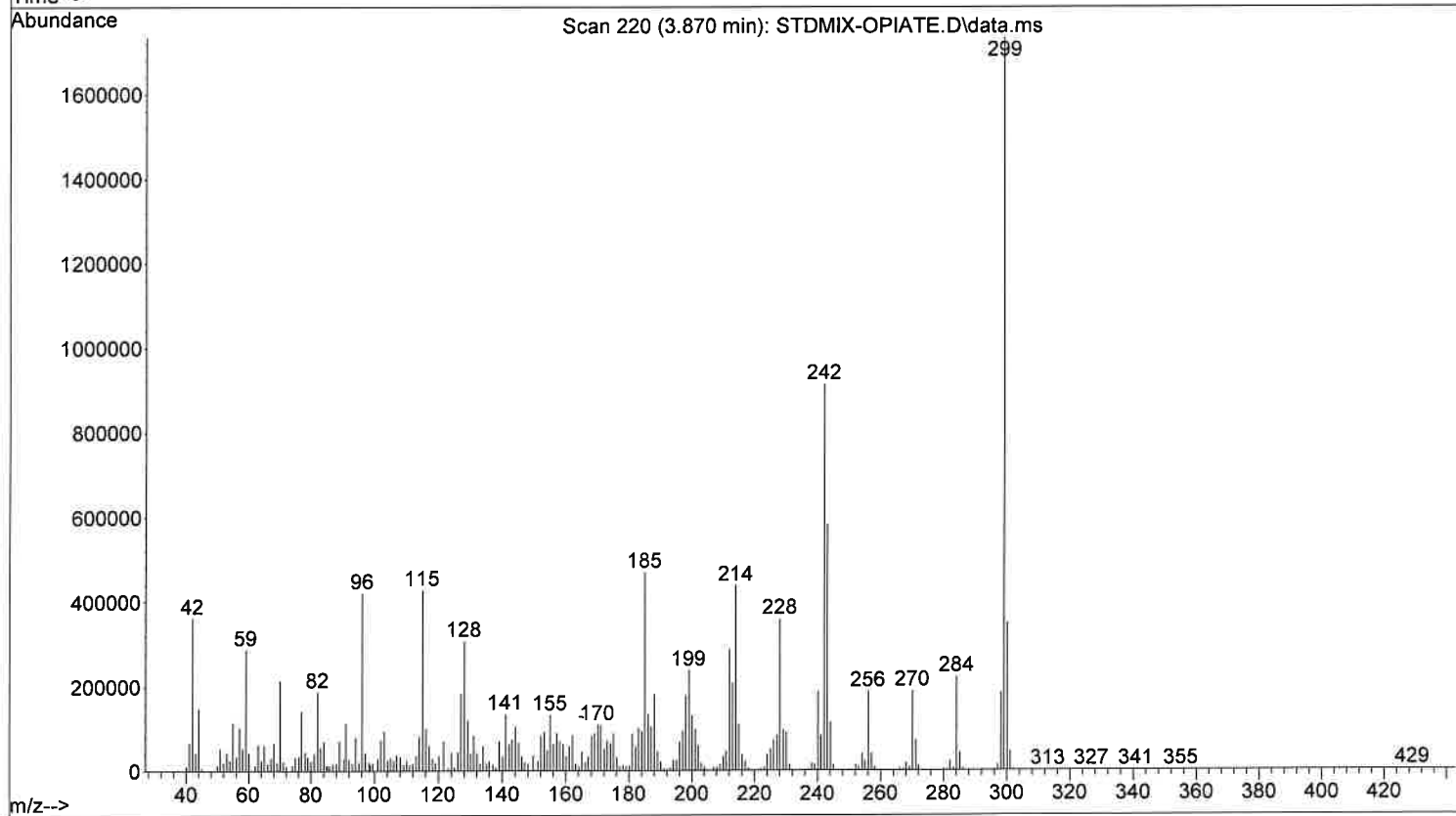
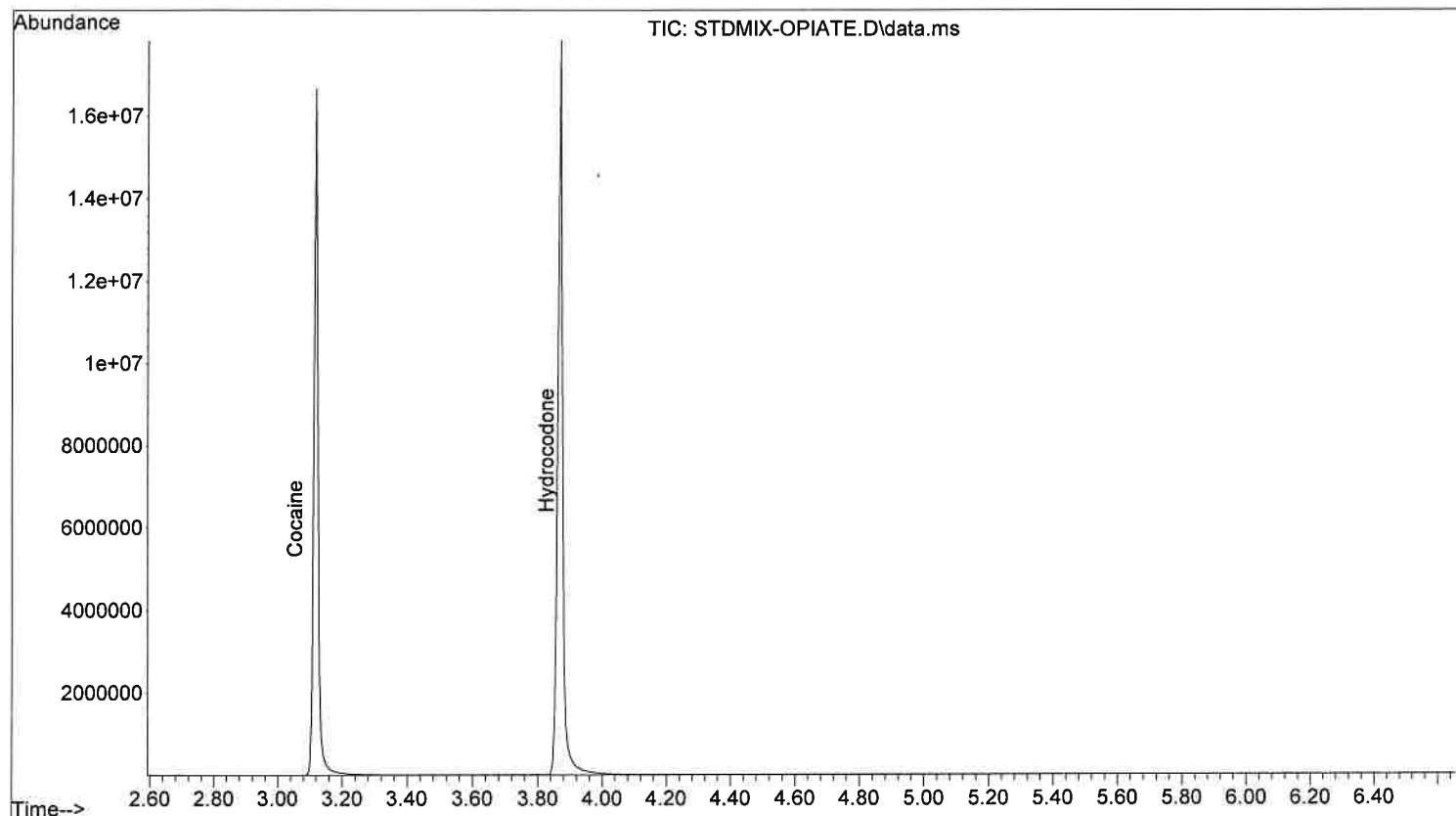
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PMOXSTD-OPIATE-B.D
Operator : KLAB
Acquired : 21 Aug 2023 12:35 using AcqMethod OPIATE.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : For P-MOX
Vial Number: 52



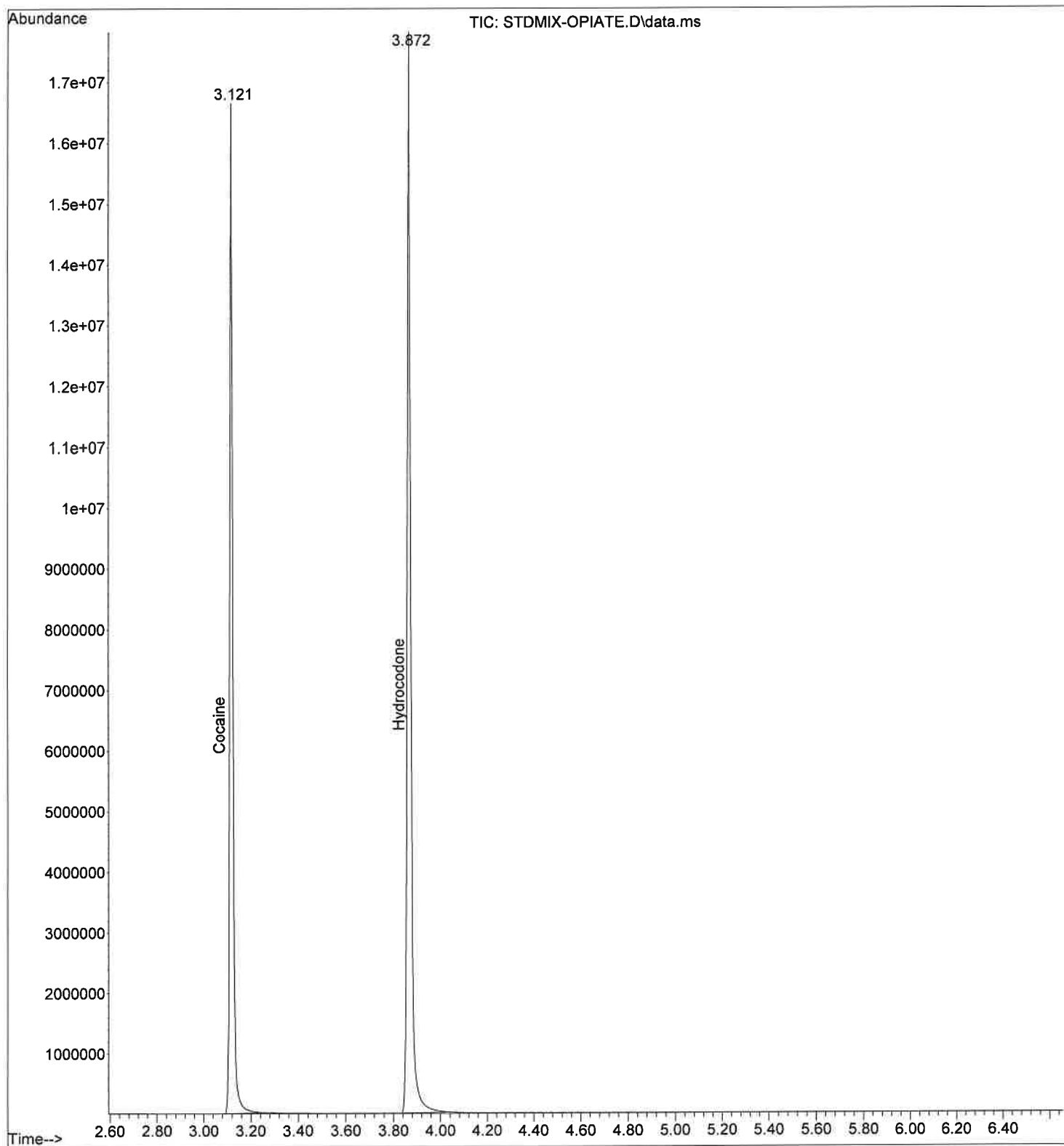
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\STDMIX-OPIATE.D
Operator : KLAB
Acquired : 22 Aug 2023 13:19 using AcqMethod OPIATE.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : CHCl3
Vial Number: 3



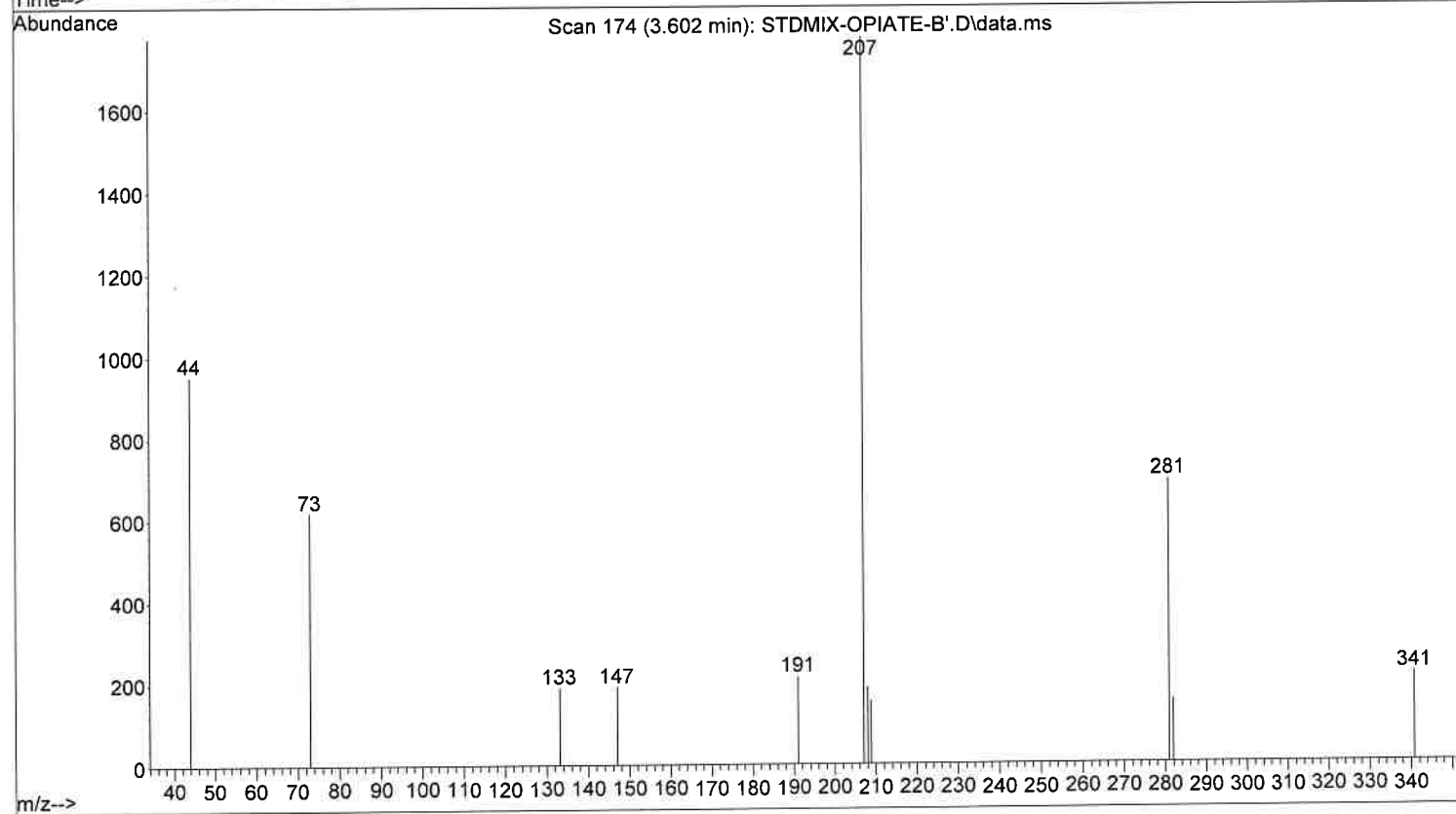
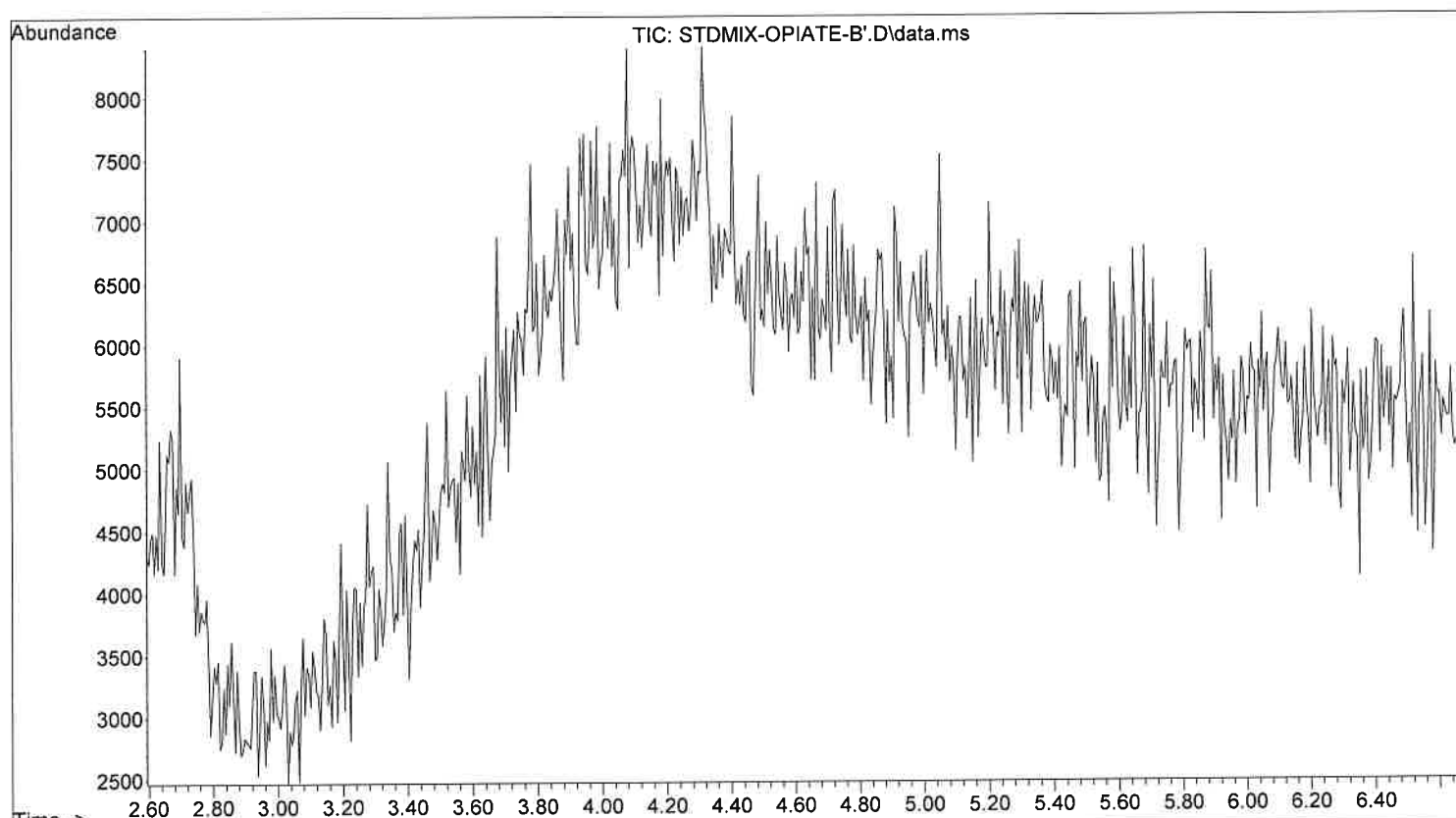
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\STDMIX-OPIATE.D
Operator : KLAB
Acquired : 22 Aug 2023 13:19 using AcqMethod OPIATE.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : CHCl3
Vial Number: 3



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\STDMIX-OPIATE.D
Operator : KLAB
Acquired : 22 Aug 2023 13:19 using AcqMethod OPIATE.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : CHCl3
Vial Number: 3



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\STDMIX-OPIATE-B'
... .D
Operator : KLAB
Acquired : 22 Aug 2023 13:11 using AcqMethod OPIATE.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : For Standard Mix
Vial Number: 2



METHOD CONTROL PARAMETERS

Method Information for: D:\MassHunter\GCMS\1\methods\DRUG1LC.M

Method Sections To Run:

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

Method Comments:

LOW CON

END OF METHOD CONTROL PARAMETERS

Single Quadrupole Acquisition Method - MS Parameters Report

Method file	D:\MassHunter\GCMS\1\methods\DRUG1LC.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)	10.00
Solvent delay (min)	2.50
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
2.50	40	550	150	1,562 [N=2]

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

Self-Cleaning Ion Source Parameters

Mode	No Cleaning
------	-------------

D:\MassHunter\GCMS\1\methods\DRUG1LC.M
Thu Aug 24 15:43:34 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 14.667 min
Post Run Time 0 min

Oven
Temperature
Setpoint On
(Initial) 80 °C
Hold Time 1.5 min
Post Run 0 °C
Program
#1 Rate 30 °C/min
#1 Value 280 °C
#1 Hold Time 6.5 min

Equilibration Time 0 min
Max Temperature 350 °C
Maximum Temperature Override Disabled
Slow Fan Disabled

ALS
Front Injector
Syringe Size 10 µL
Injection Volume 1 µL
Solvent A Washes (PreInj) 1
Solvent A Washes (PostInj) 1
Solvent A Volume 8 µL
Solvent B Washes (PreInj) 1
Solvent B Washes (PostInj) 1
Solvent B Volume 8 µL
Sample Washes 0
Sample Wash Volume 8 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 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
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	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	
Helium Conservation Controlled Mode	Off
Heater	Split
Pressure	On 250 °C
Total Flow	On 12 psi
Septum Purge Flow	On 5.5044 mL/min
Pre-Run Flow Test	On 3 mL/min
Gas Saver	Off
Split Ratio	On 20 mL/min after 2 min
Split Flow	1 : 1
Liner	1.2522 mL/min
	Agilent 5190-2271: 900 µL (Splitless, single taper, wool, 0
Back SS Inlet He	
Helium Conservation Controlled Mode	Off
Heater	Split
Pressure	Off
Total Flow	Off
Septum Purge Flow	Off
Pre-Run Flow Test	Off
Liner	A Liner has not been selected.
Column	
Column #1	
Flow	
Setpoint	On
(Initial)	1.2522 mL/min
Post Run	1 mL/min
Column Information	Agilent 128-0112: 1
Description	DB-1ms

Temperature Range	-60 °C-340 °C (350 °C)
Dimensions	12 m x 200 µm x 0.33 µm (Calibrated)
Heater	Oven
Column lock	Unlocked
In	Front SS Inlet He
Out	MSD
(Initial)	80 °C
Pressure	12 psi
Flow	1.2522 mL/min
Average Velocity	65.404 cm/sec
Holdup Time	0.30579 min
Control Mode	Constant Flow
Column Outlet Pressure	0 psi
Front Detector FID	
Makeup	He
Heater	Off
H2 Flow	Off
Air Flow	Off
Makeup Flow	Off
Carrier Gas Flow Correction	Constant Makeup and Fuel Flow
Flame	Off
Blank Evaluation Setpoints	
Perform Blank Evaluation Test	Off
Helium Conservation	
Helium Valve	Off
Nitrogen Valve	Off
Detector Evaluation	
Perform Detector Evaluation Test	Off
MSD Transfer Line	
Temperature	
Setpoint	On
(Initial)	280 °C
Signals	
Signal #1:	
Description	None
Signal #2:	
Description	None
Signal #3:	
Description	None
Signal #4:	
Description	None
Signal #5:	
Description	None
Signal #6:	
Description	None
Signal #7:	
Description	None
Signal #8:	
Description	None

TUNE PARAMETERS for SN: US2313MA09

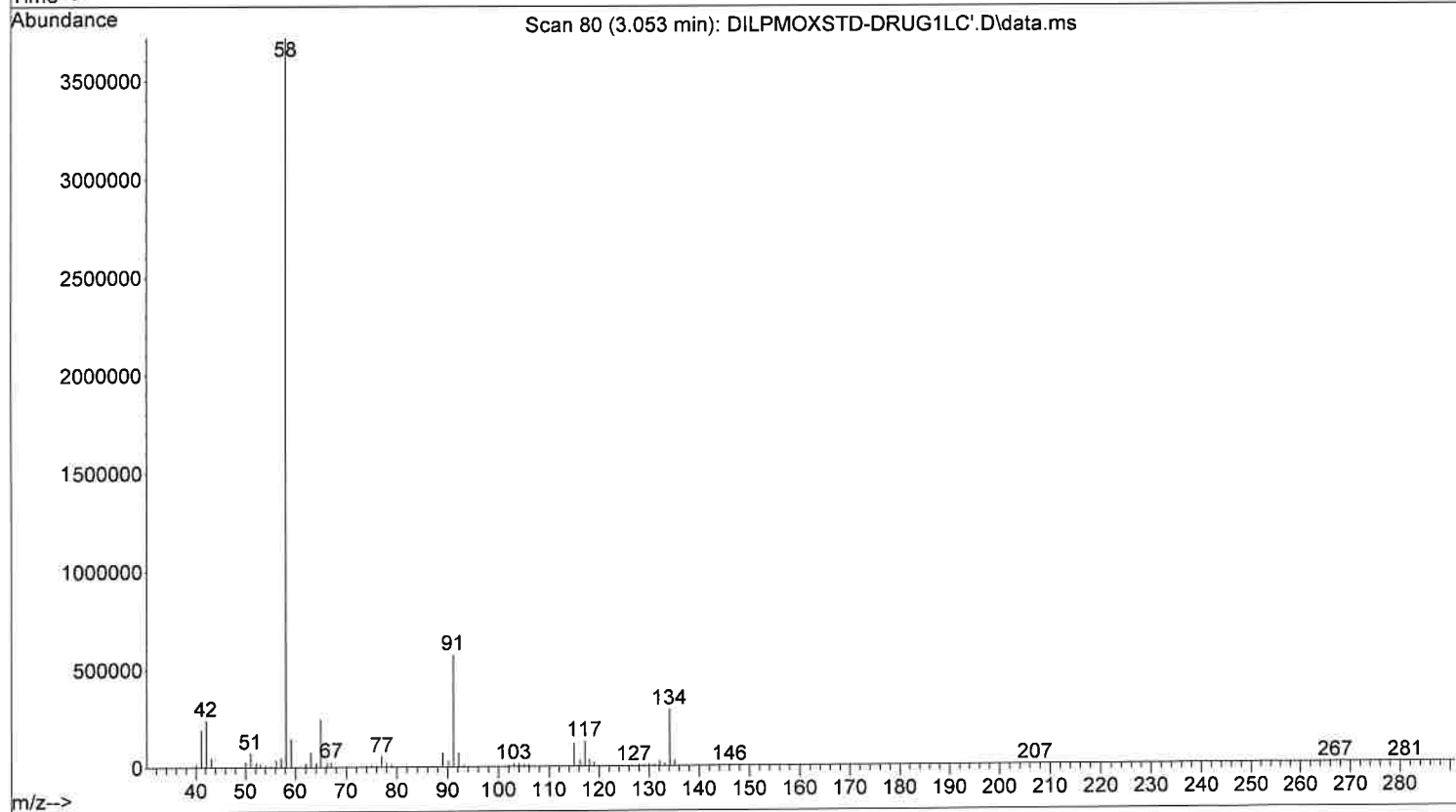
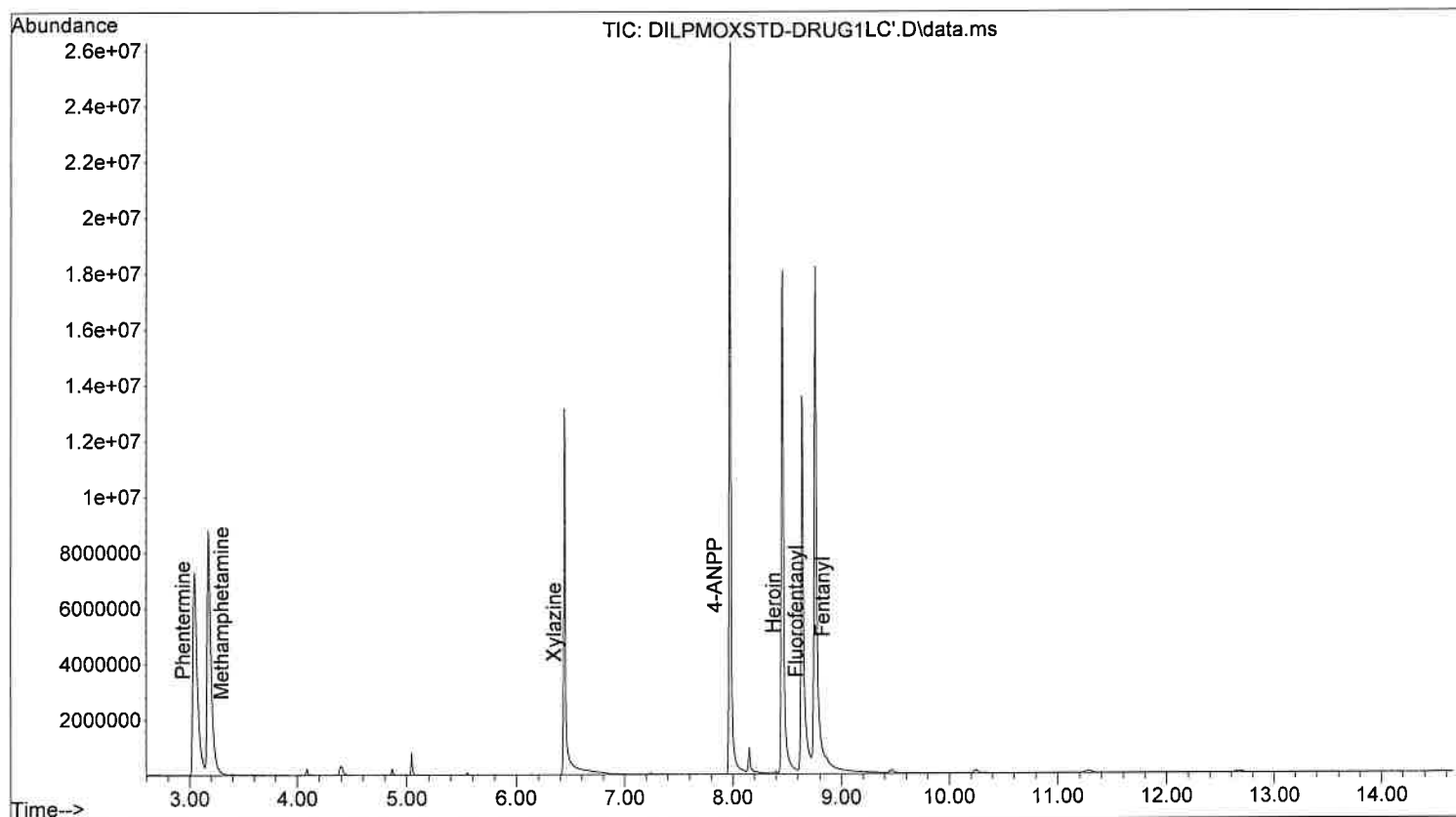
Trace Ion Detection is OFF.

34.593	:	EMISSION	
70.007	:	ENERGY	
29.919	:	REPELLER	
90.331	:	IONFOCUS	
25.226	:	ENTRANCE_LENS	
925.472	:	EMVOLTS	
		951.5	: Actual EMV
		1.00	: GAIN FACTOR
2896.000	:	AMUGAIN	
134.625	:	AMUOFFSET	
1.000	:	FILAMENT	
0.000	:	DCPOLARITY	
10.822	:	ENTLENSOFFSET	
0.000	:	Ion_Body	
0.000	:	EXTLENS	
257.000	:	MASSGAIN	
-23.000	:	MASSOFFSET	

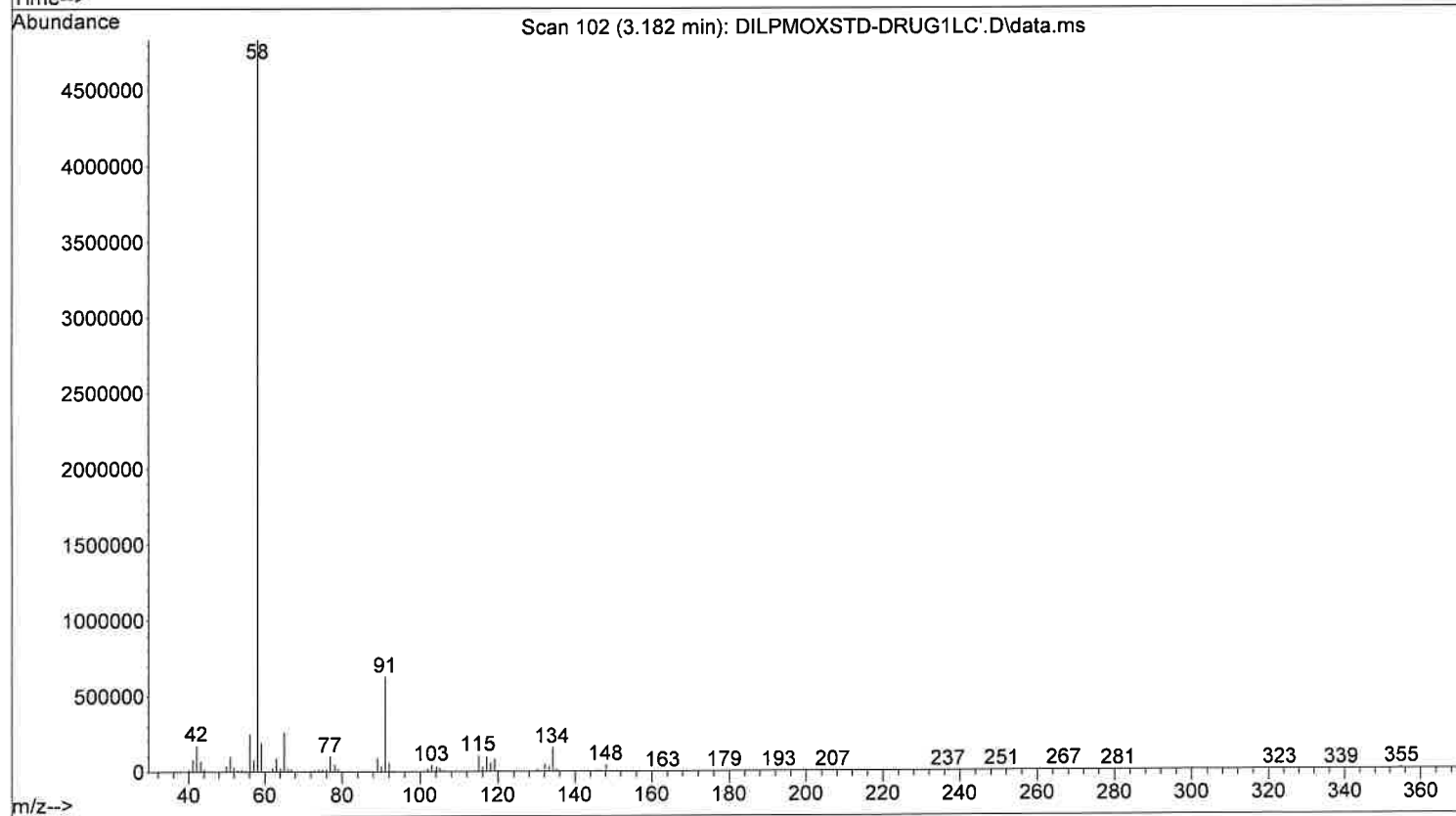
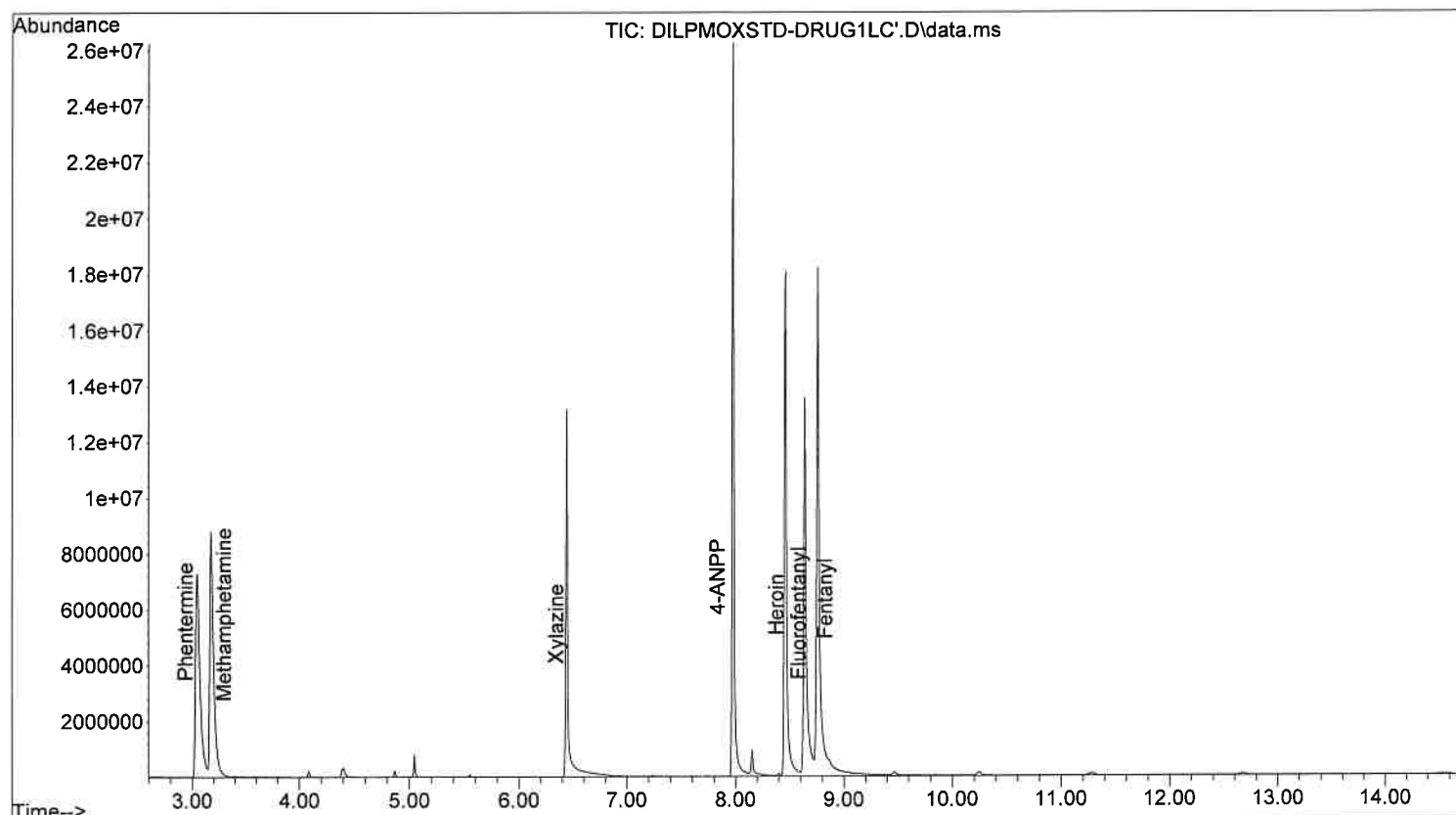
END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

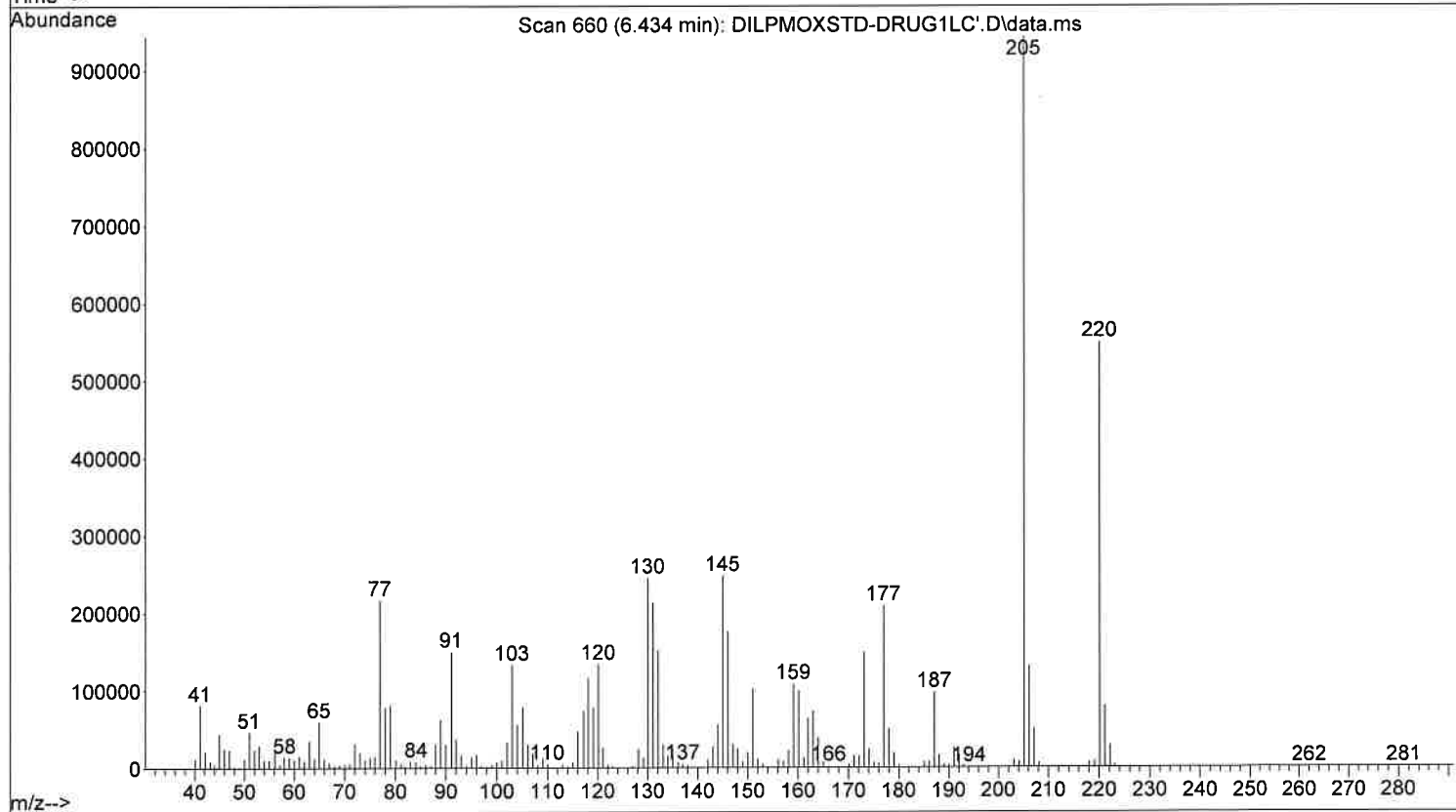
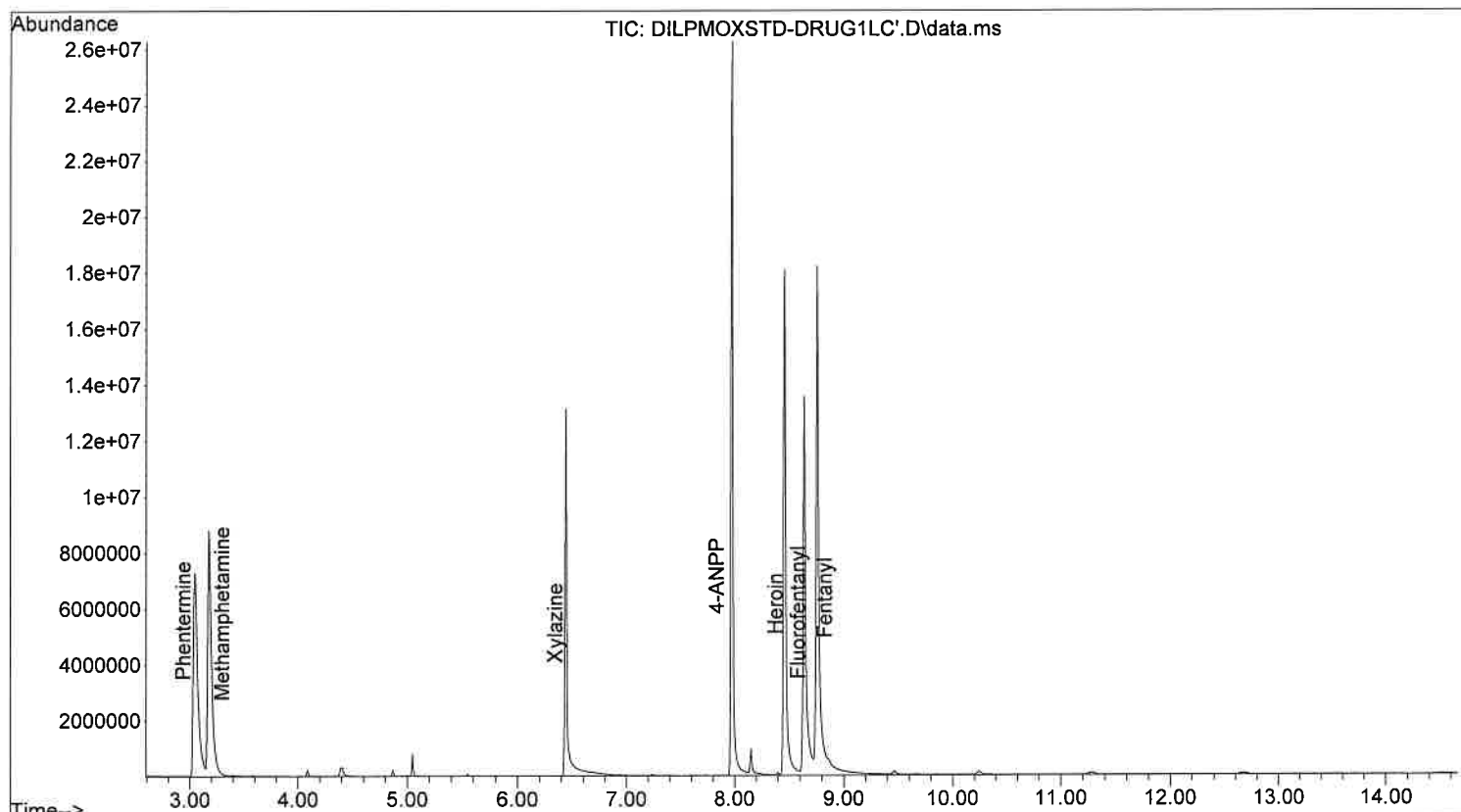
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... LC'.D
Operator : KLAB
Acquired : 24 Aug 2023 14:08 using AcqMethod DRUG1LC.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



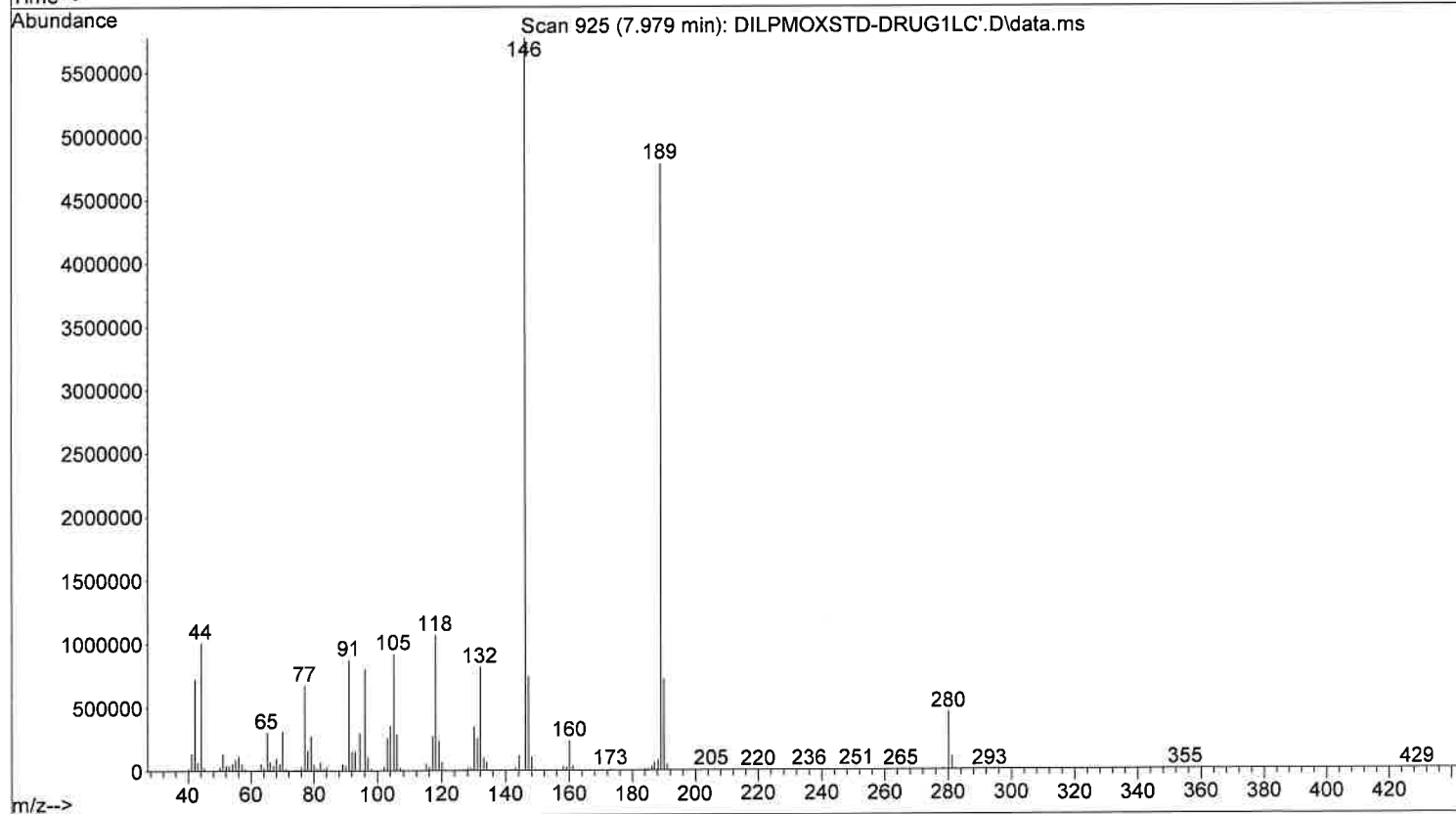
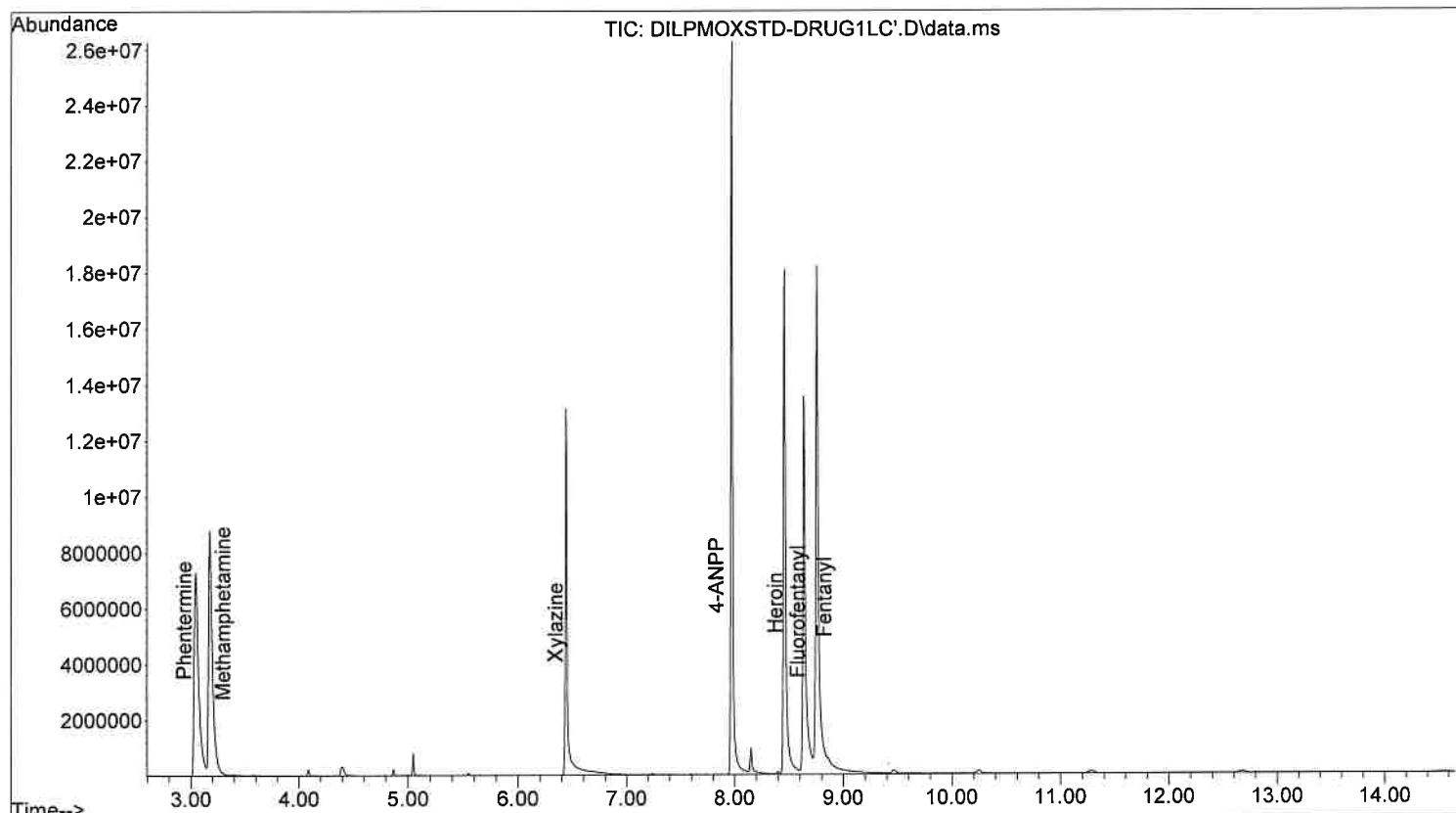
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... LC'.D
Operator : KLAB
Acquired : 24 Aug 2023 14:08 using AcqMethod DRUG1LC.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



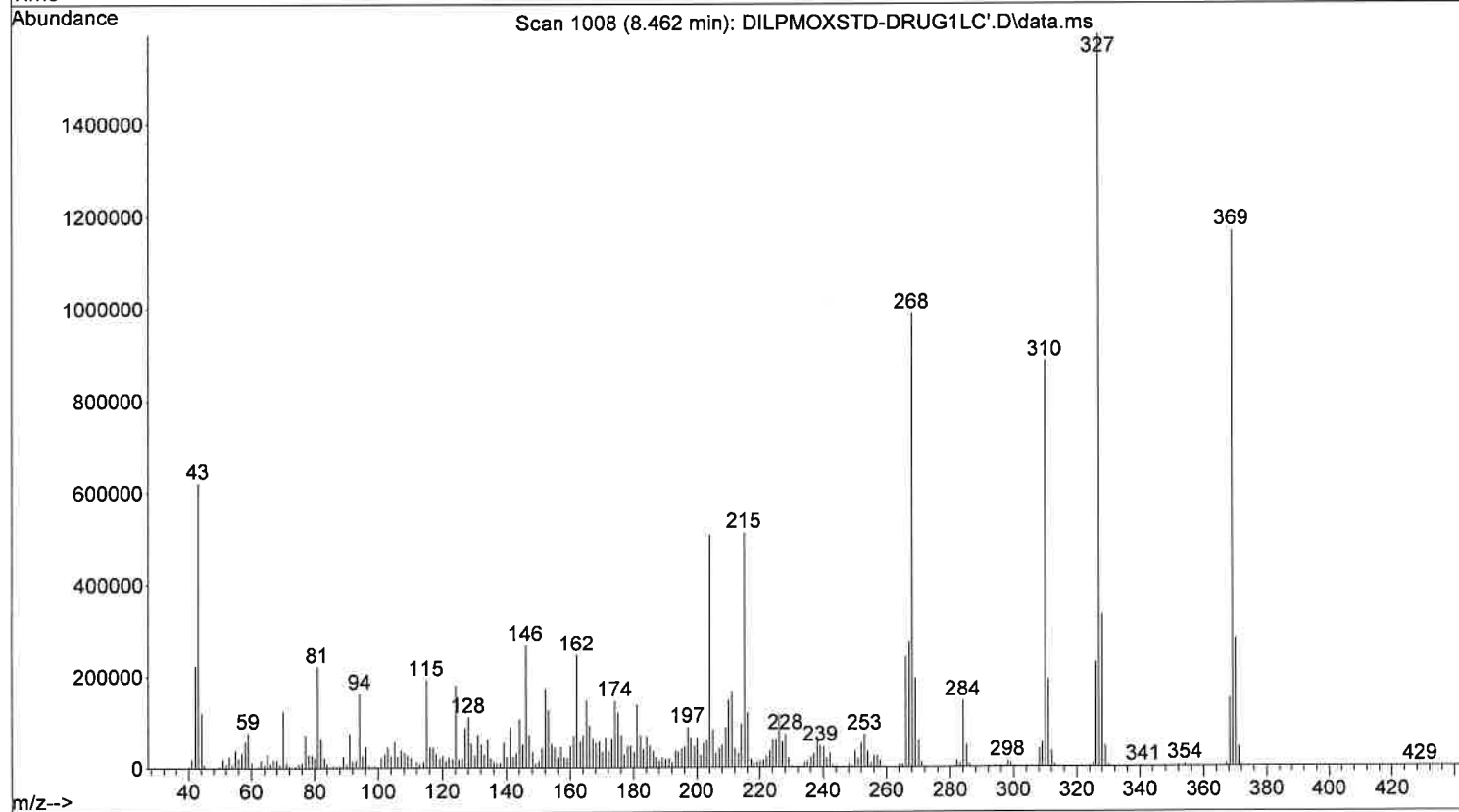
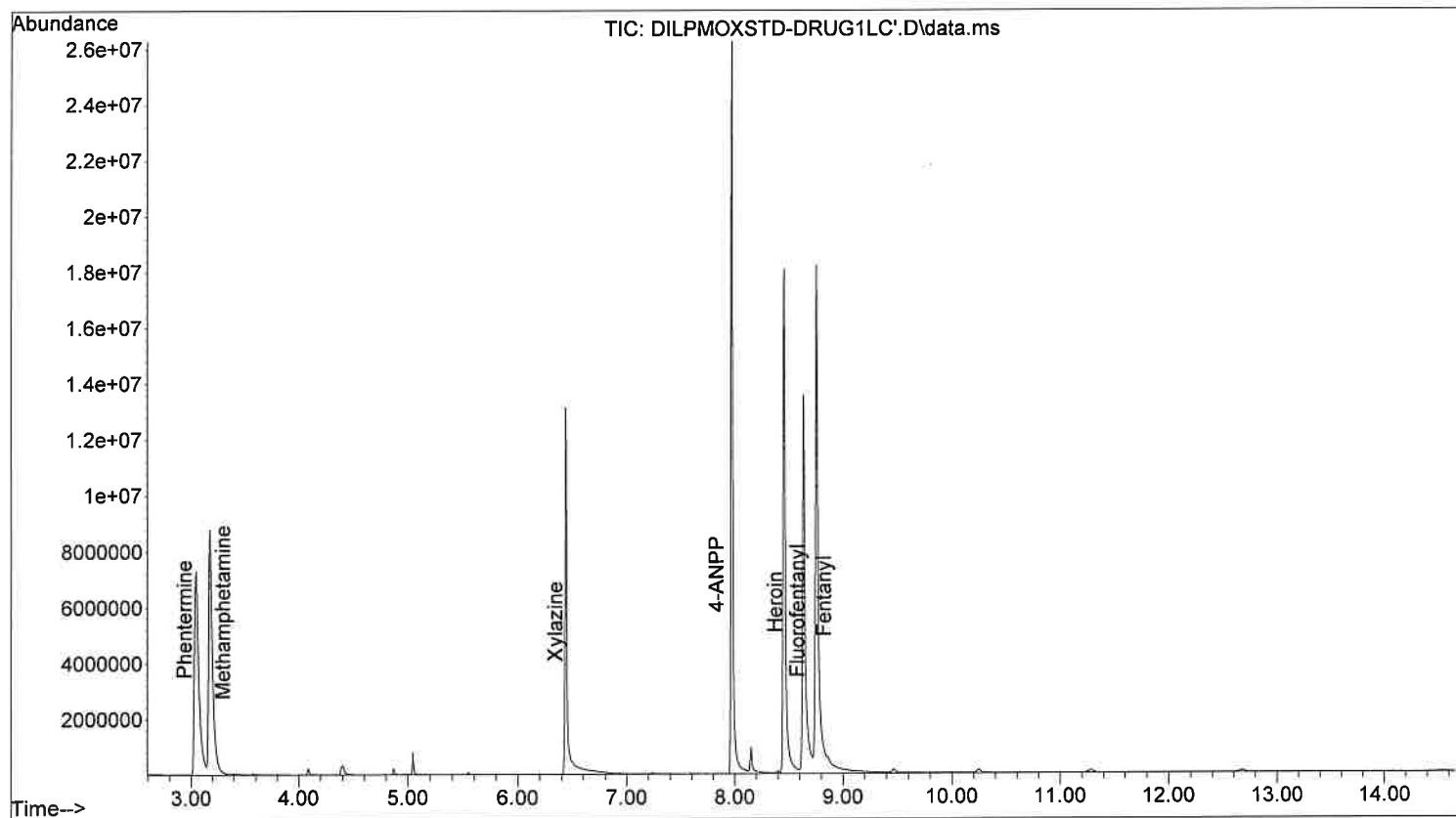
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... LC'.D
Operator : KLAB
Acquired : 24 Aug 2023 14:08 using AcqMethod DRUG1LC.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



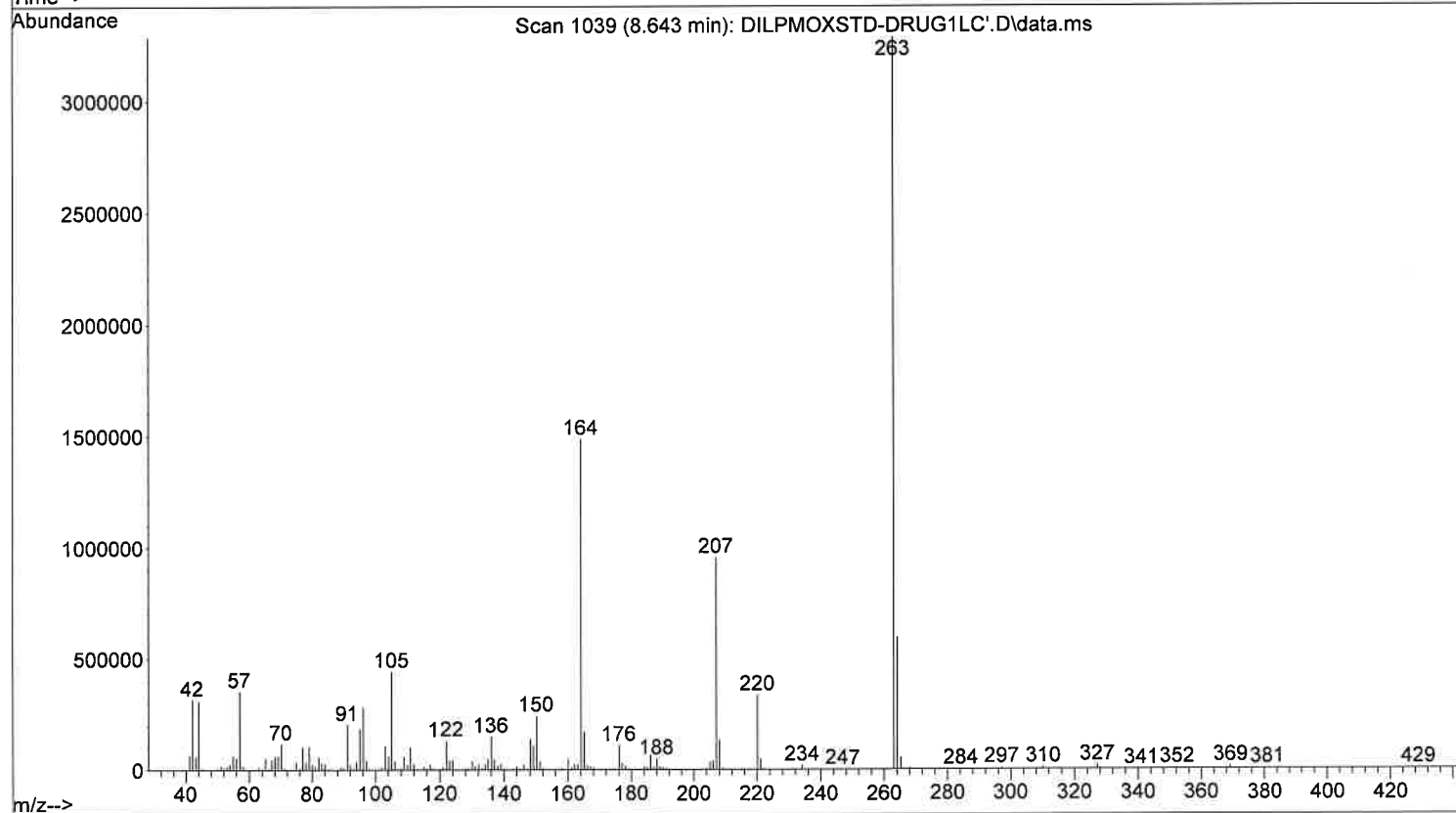
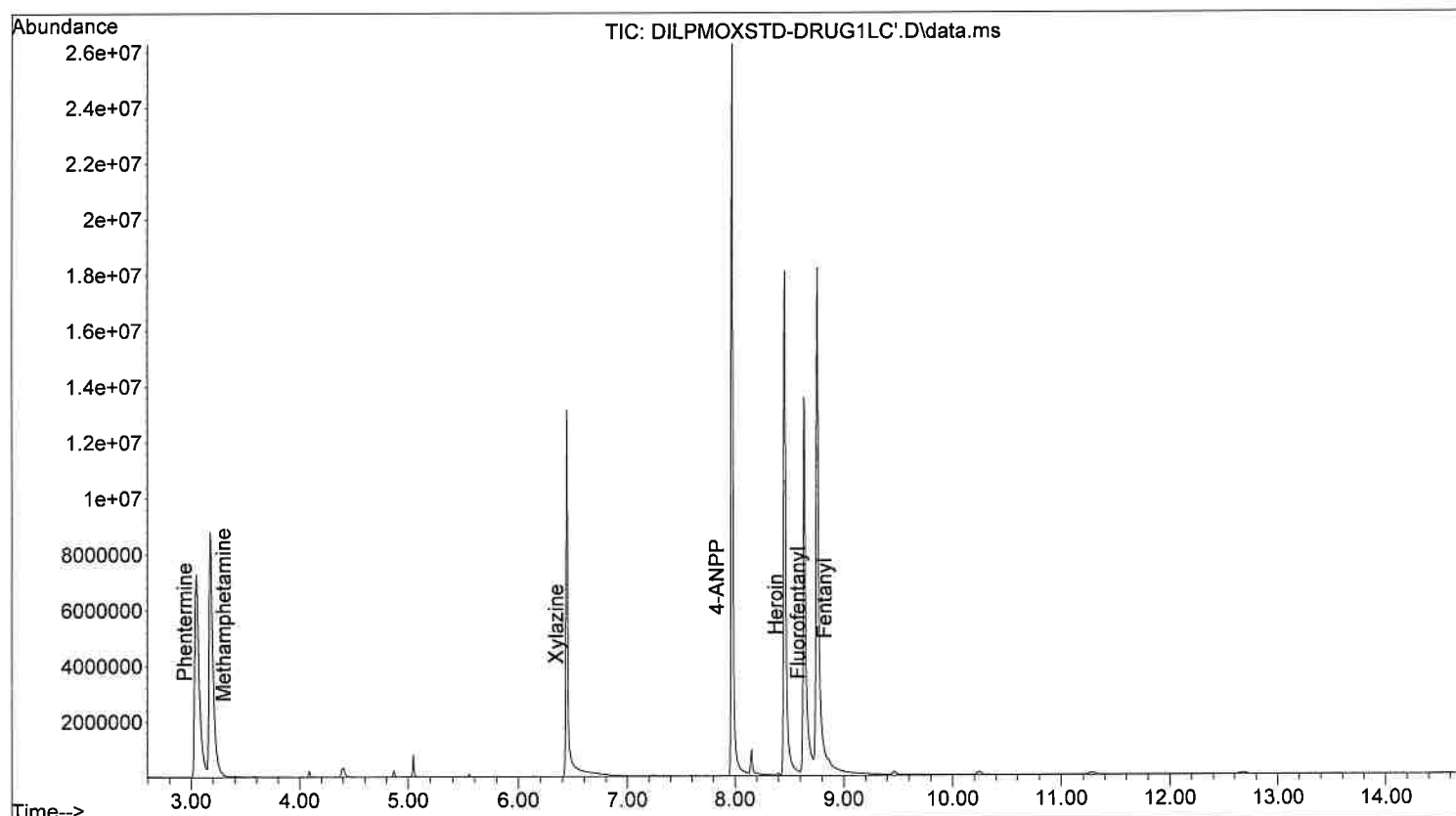
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... LC'.D
Operator : KLAB
Acquired : 24 Aug 2023 14:08 using AcqMethod DRUG1LC.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



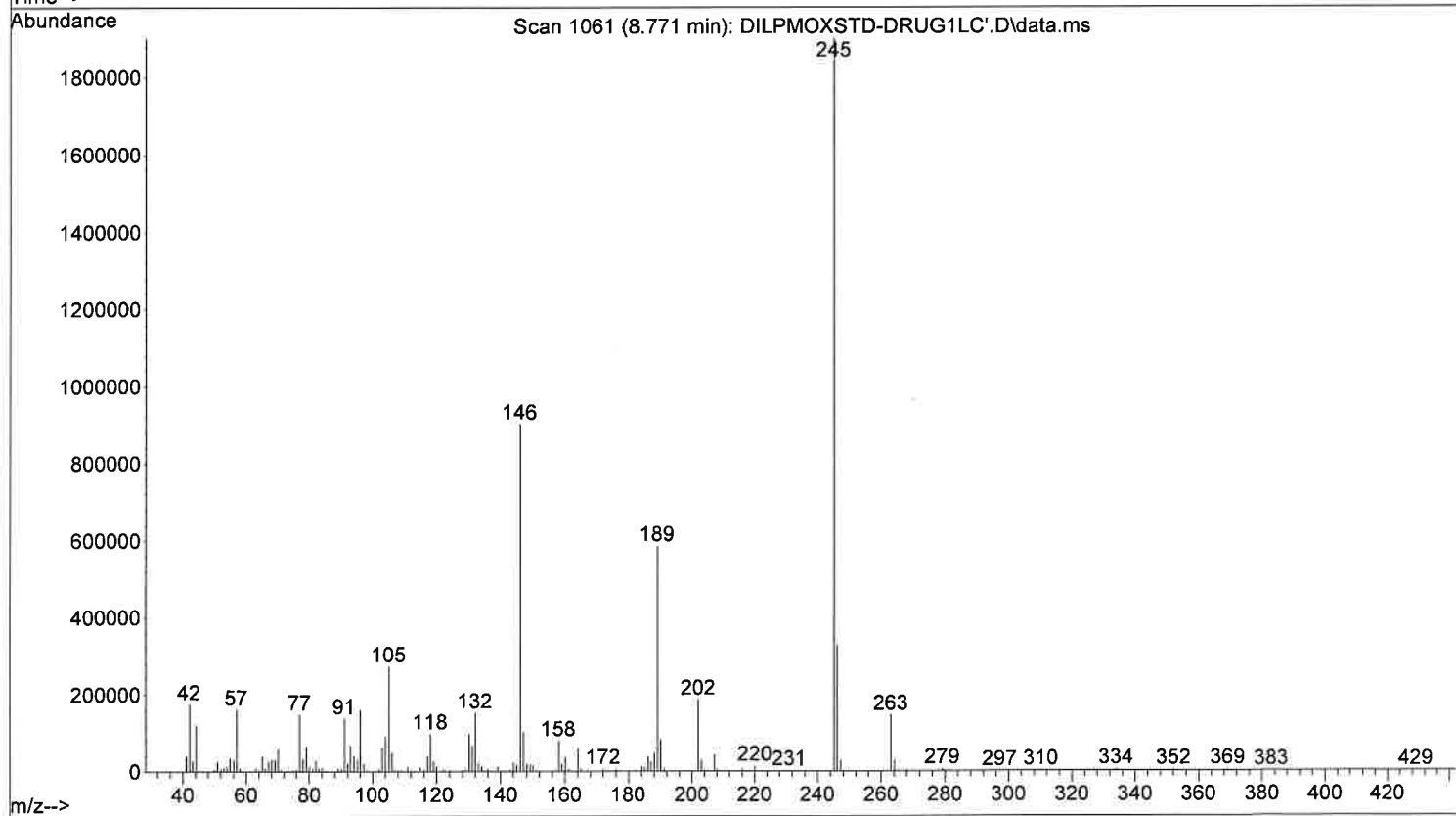
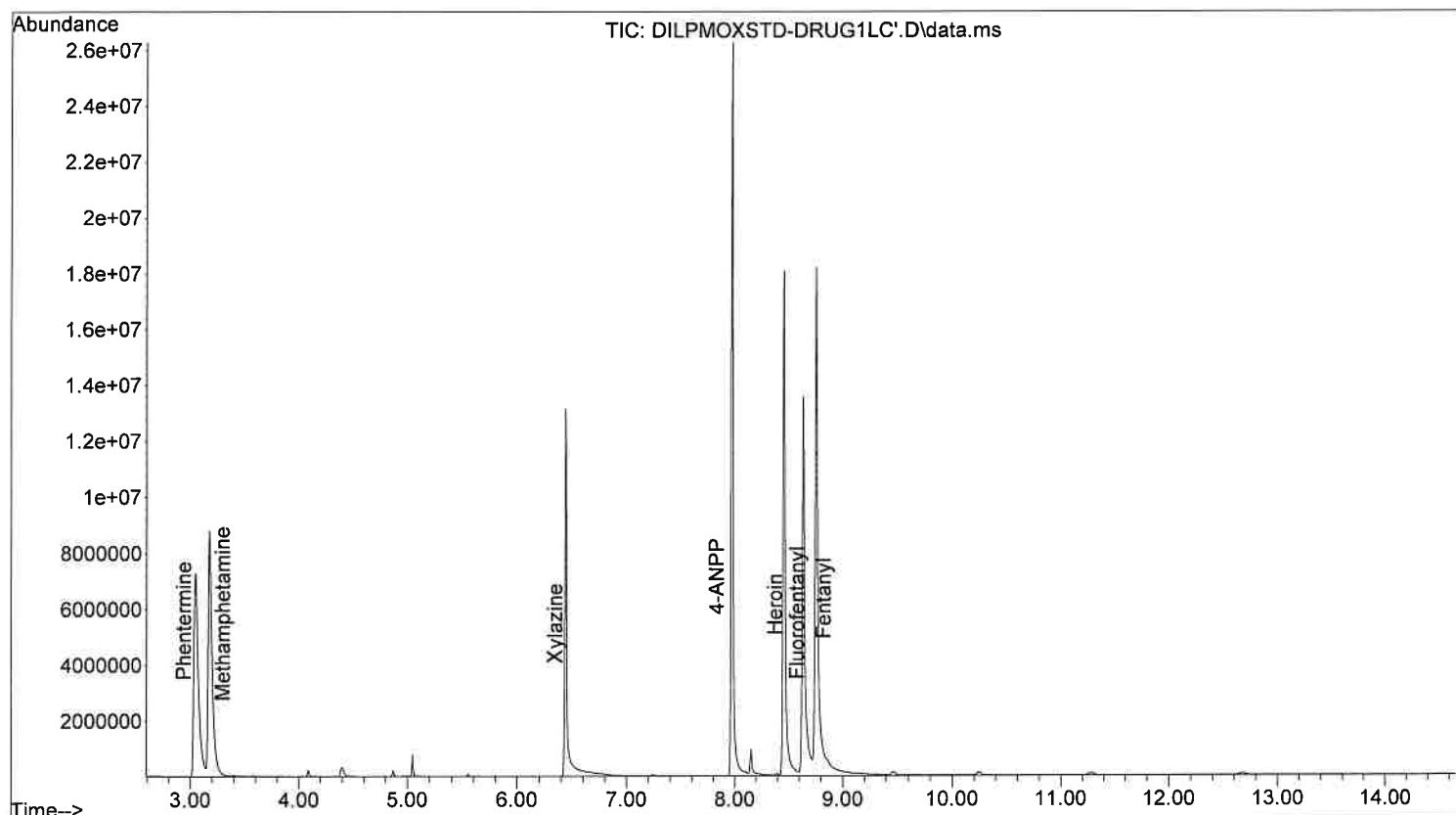
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... LC'.D
Operator : KLAB
Acquired : 24 Aug 2023 14:08 using AcqMethod DRUG1LC.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



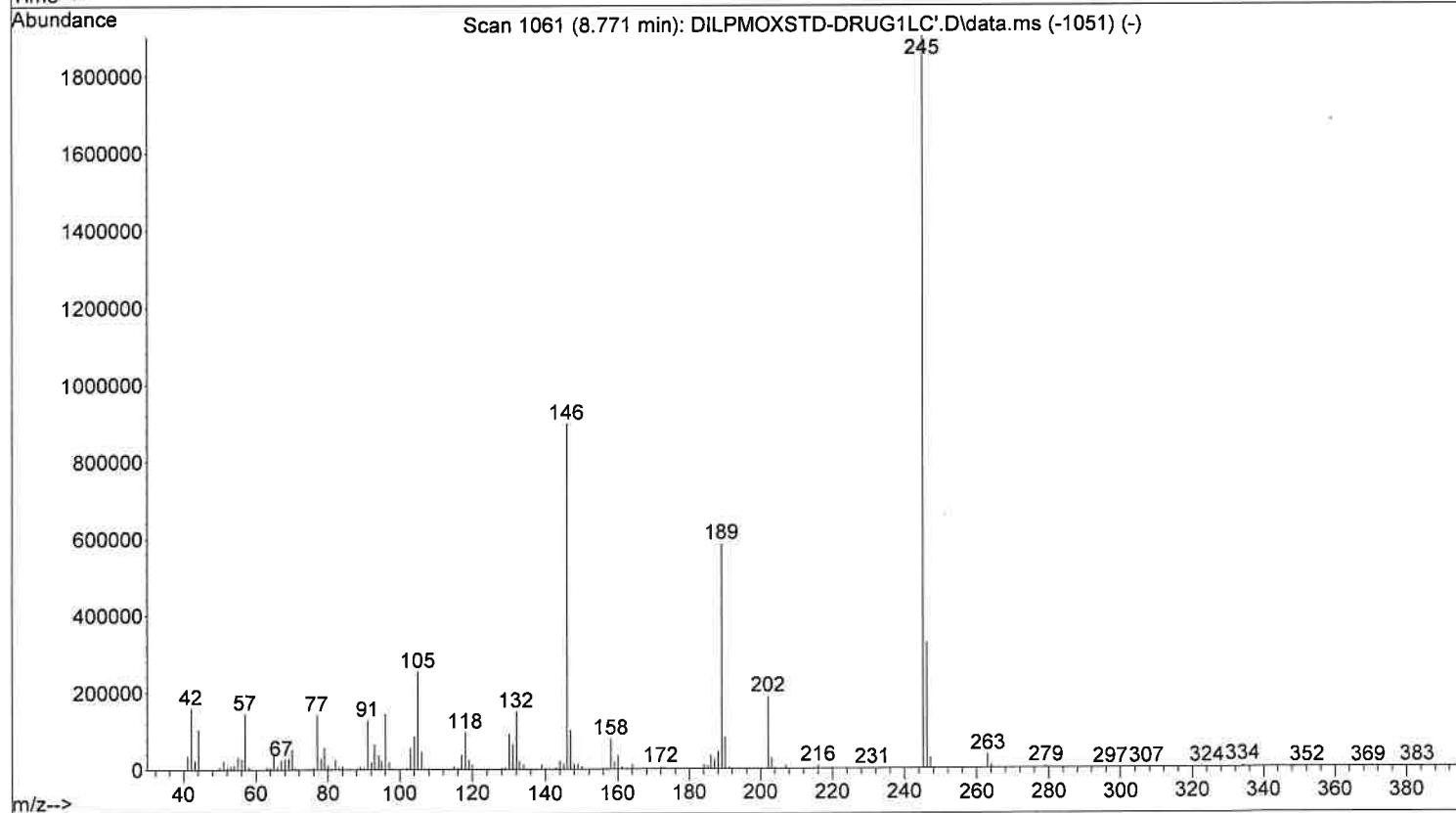
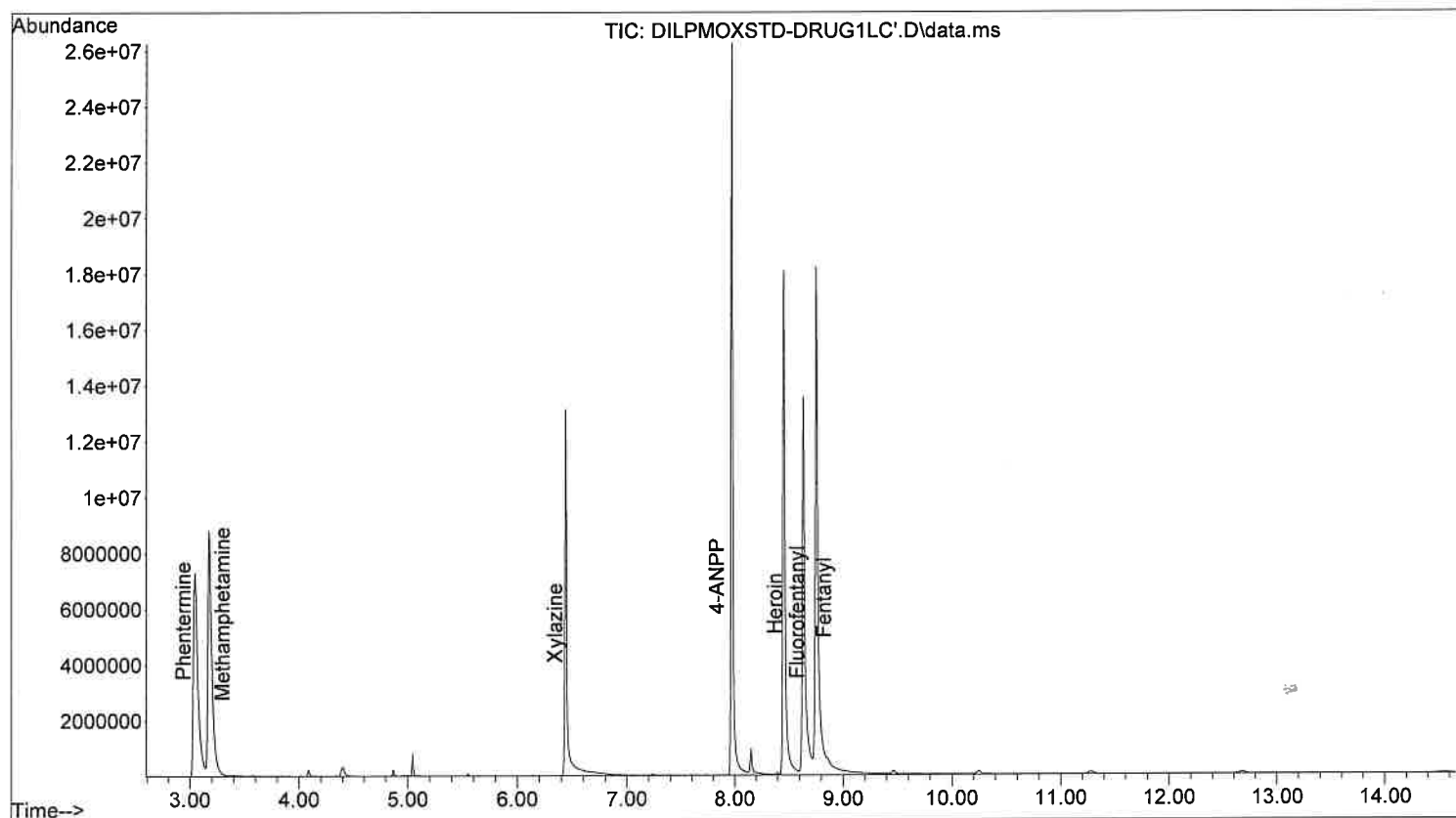
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... LC'.D
Operator : KLAB
Acquired : 24 Aug 2023 14:08 using AcqMethod DRUG1LC.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



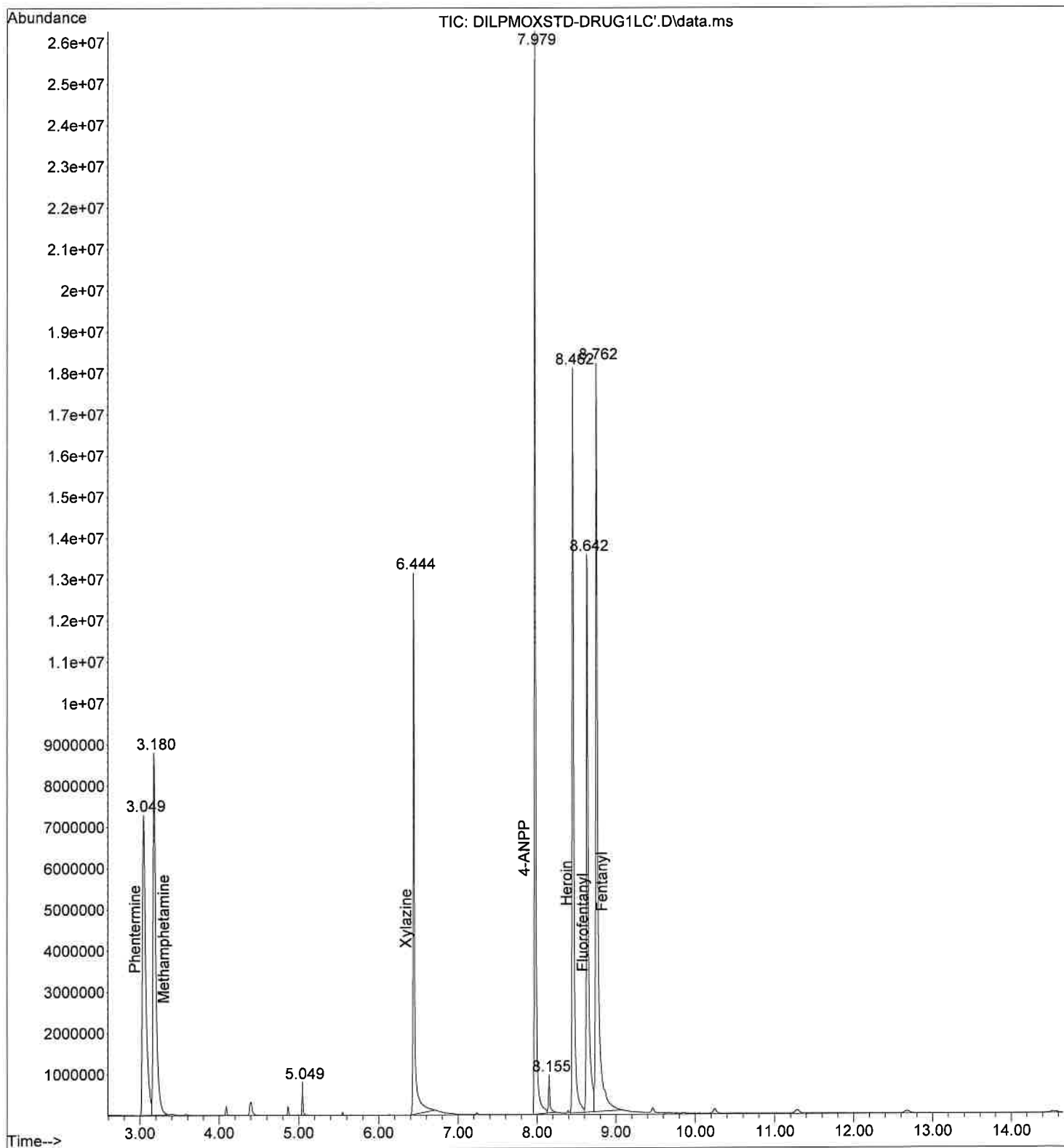
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... LC'.D
Operator : KLAB
Acquired : 24 Aug 2023 14:08 using AcqMethod DRUG1LC.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



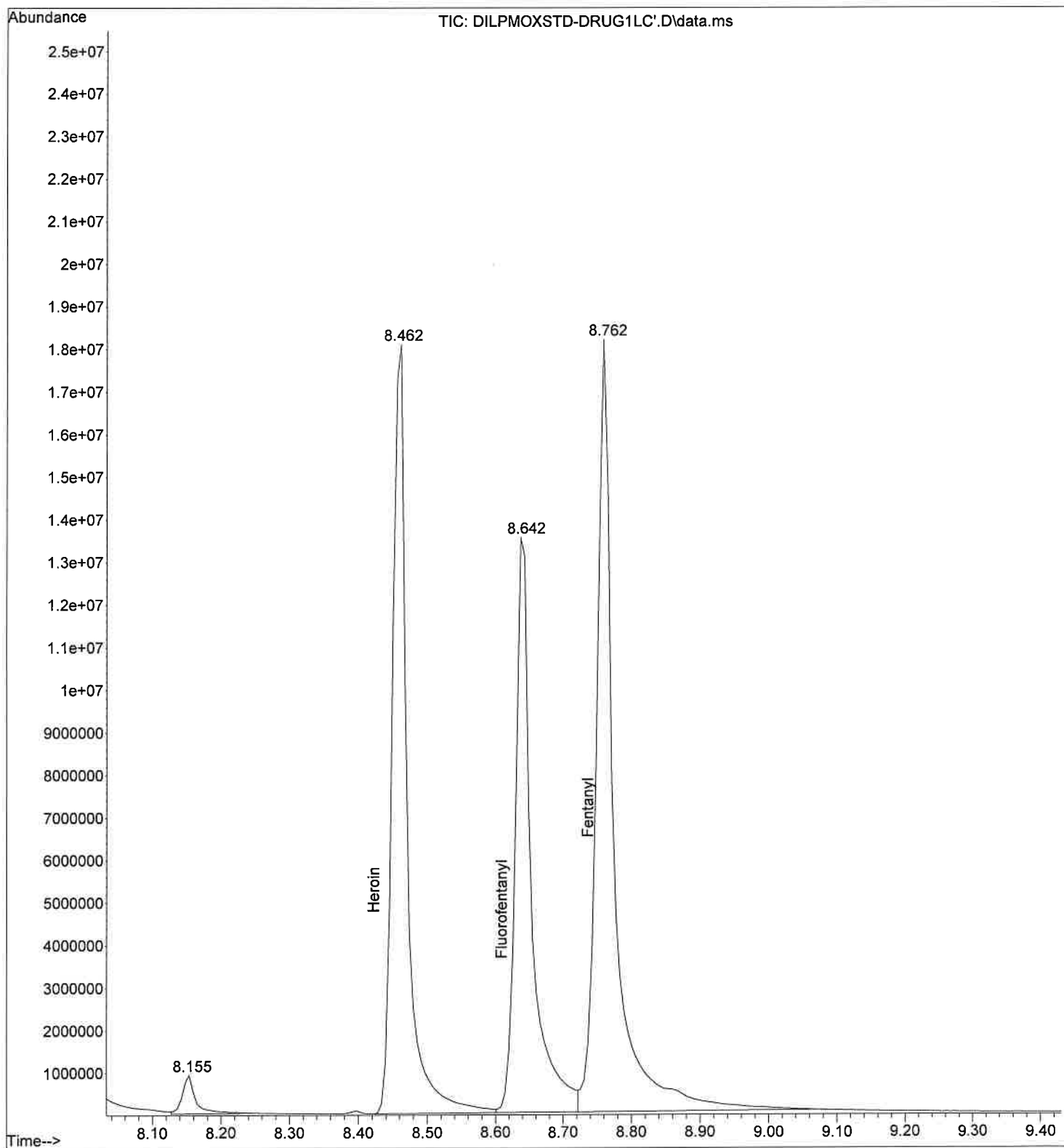
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... LC'.D
Operator : KLAB
Acquired : 24 Aug 2023 14:08 using AcqMethod DRUG1LC.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



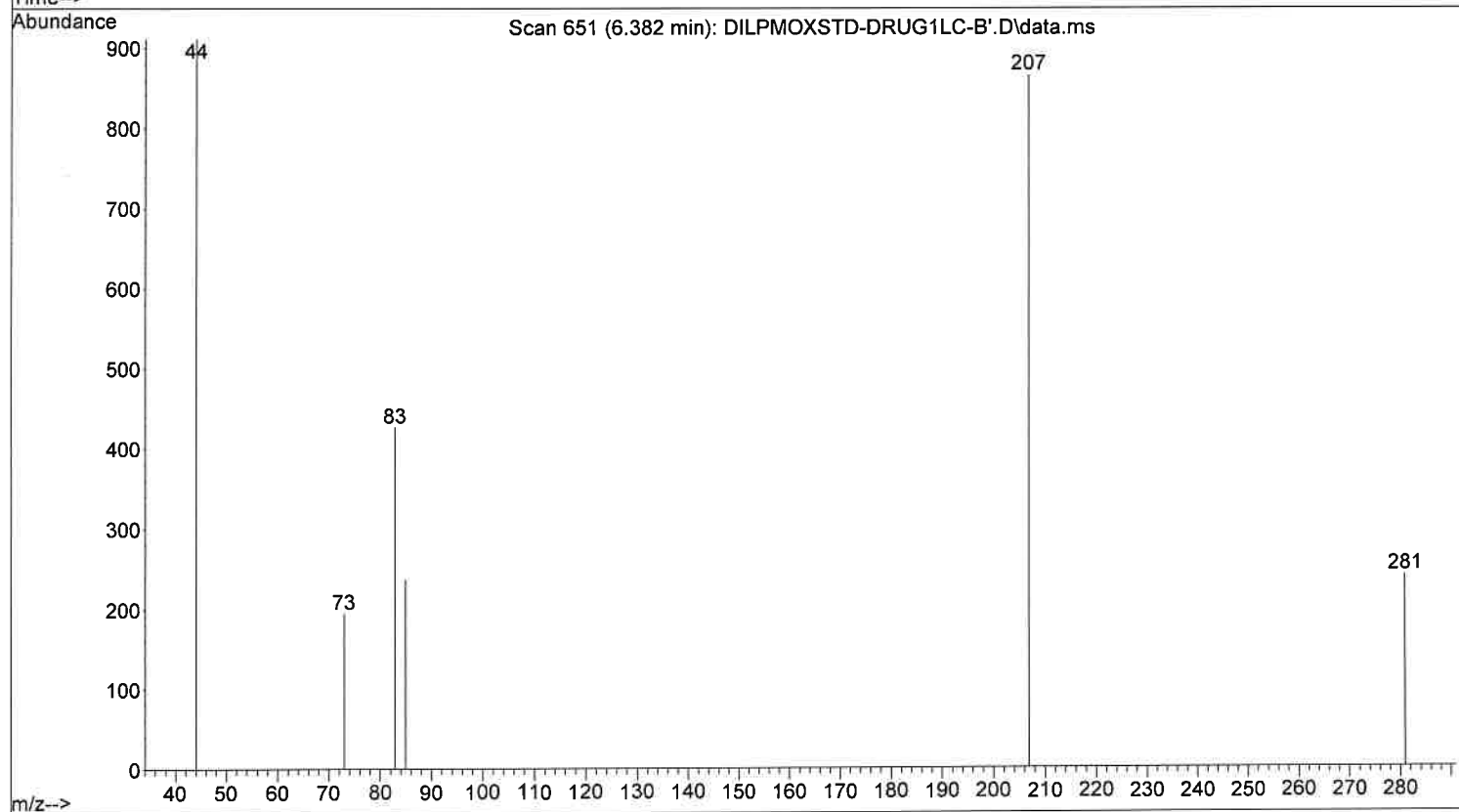
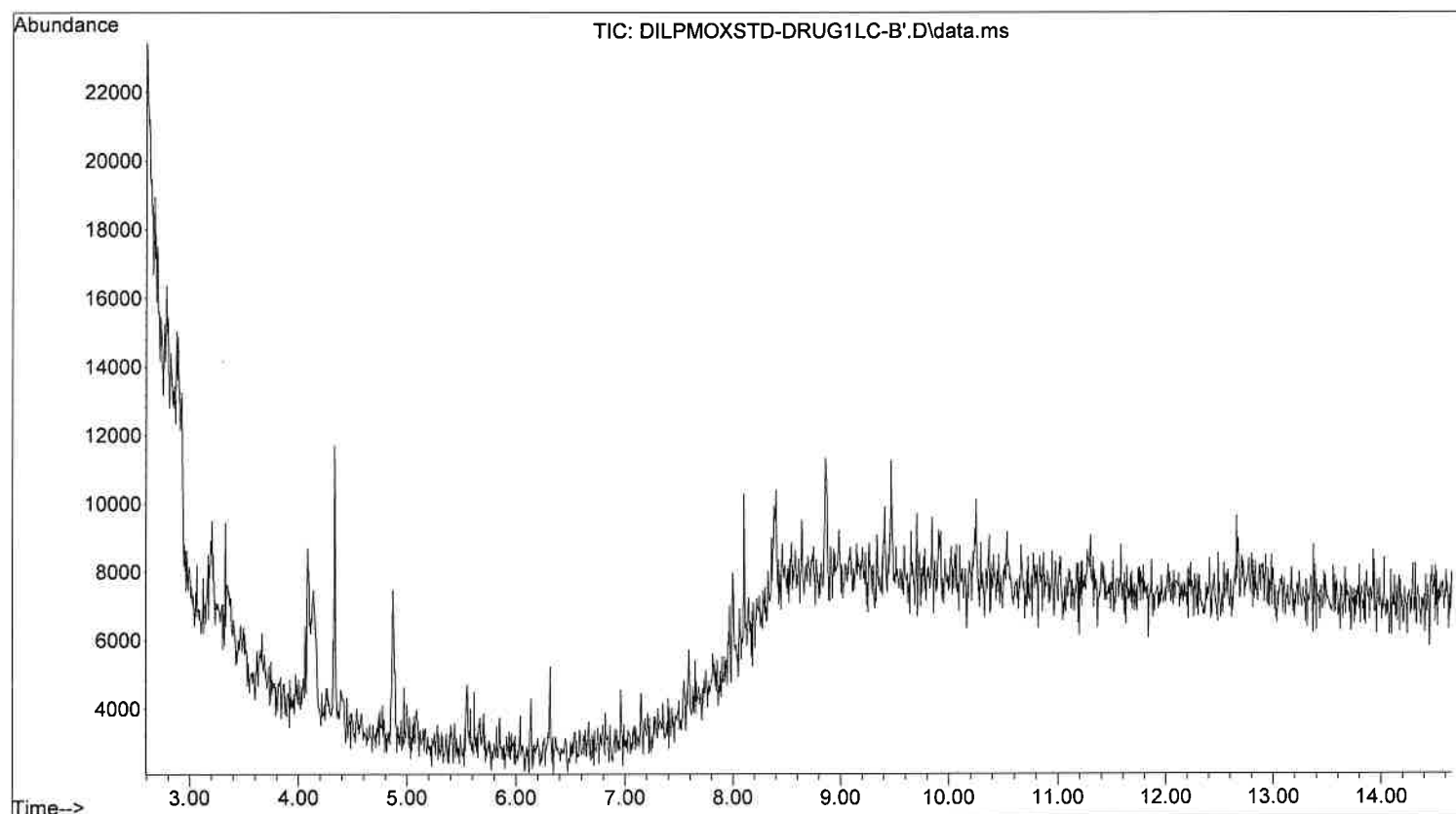
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... LC'.D
Operator : KLAB
Instrument : Buttercup
Acquired : 24 Aug 2023 14:08 using AcqMethod DRUG1LC.M
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3



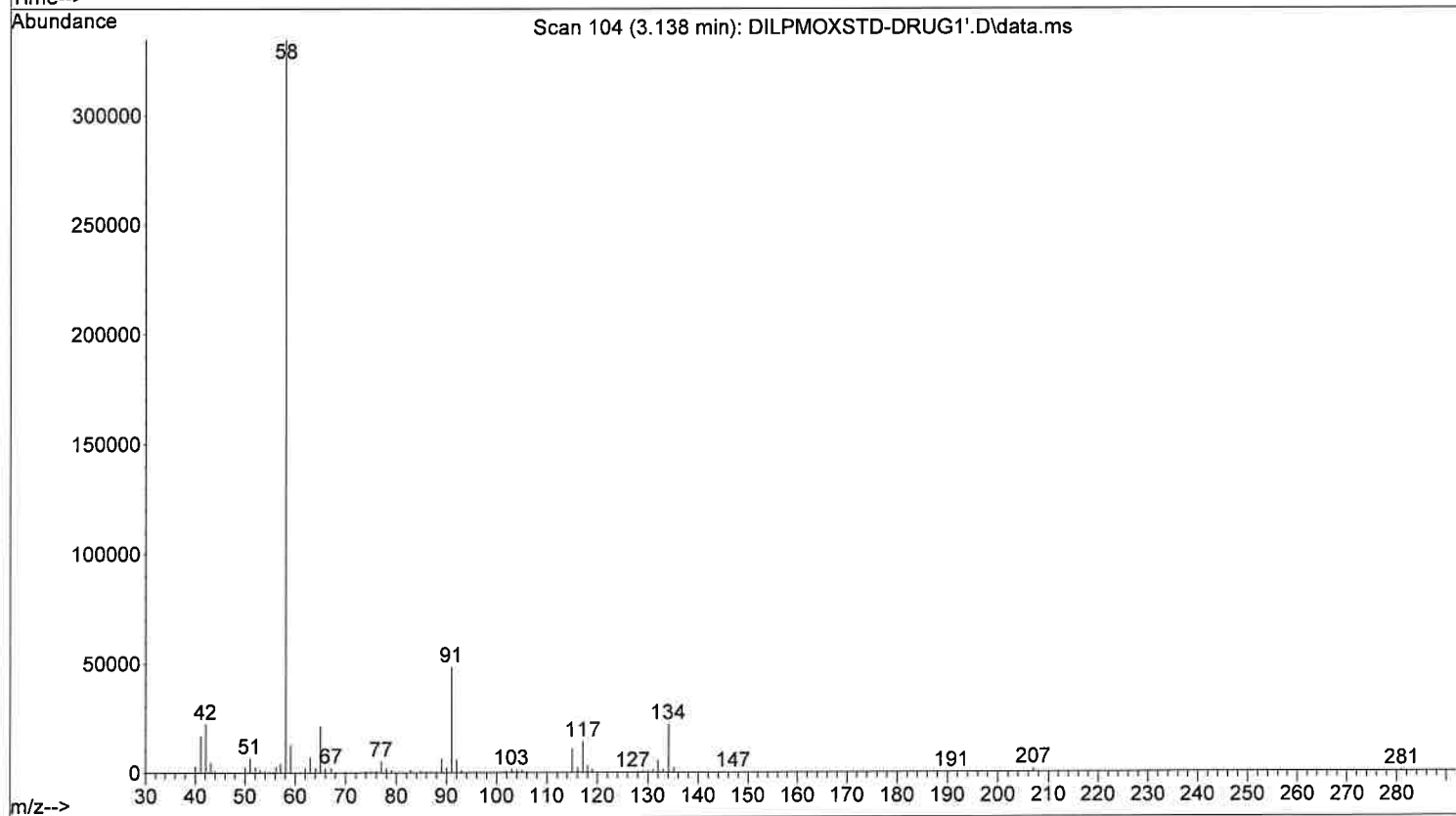
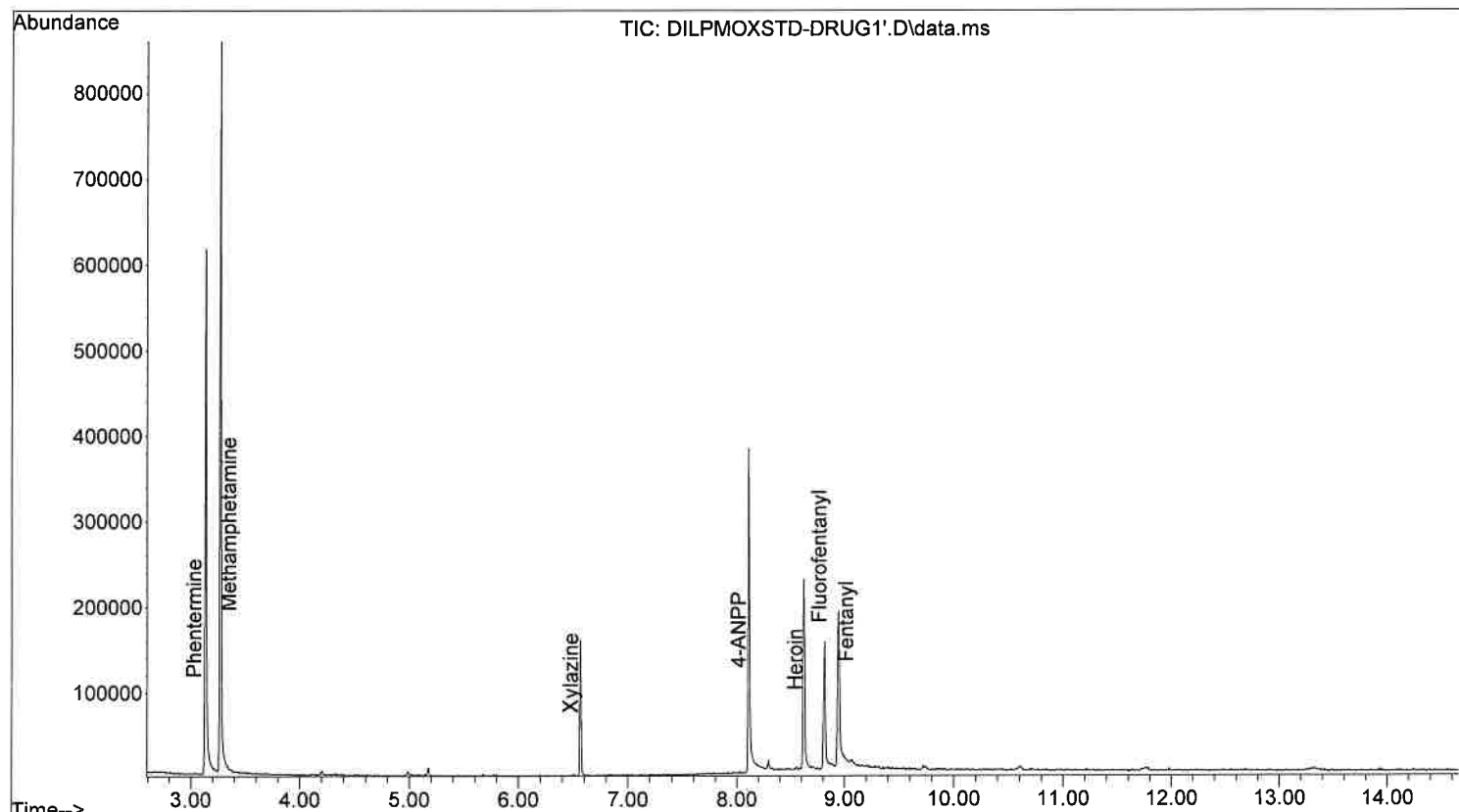
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... LC'.D
Operator : KLAB
Instrument : Buttercup
Acquired : 24 Aug 2023 14:08 using AcqMethod DRUG1LC.M
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3



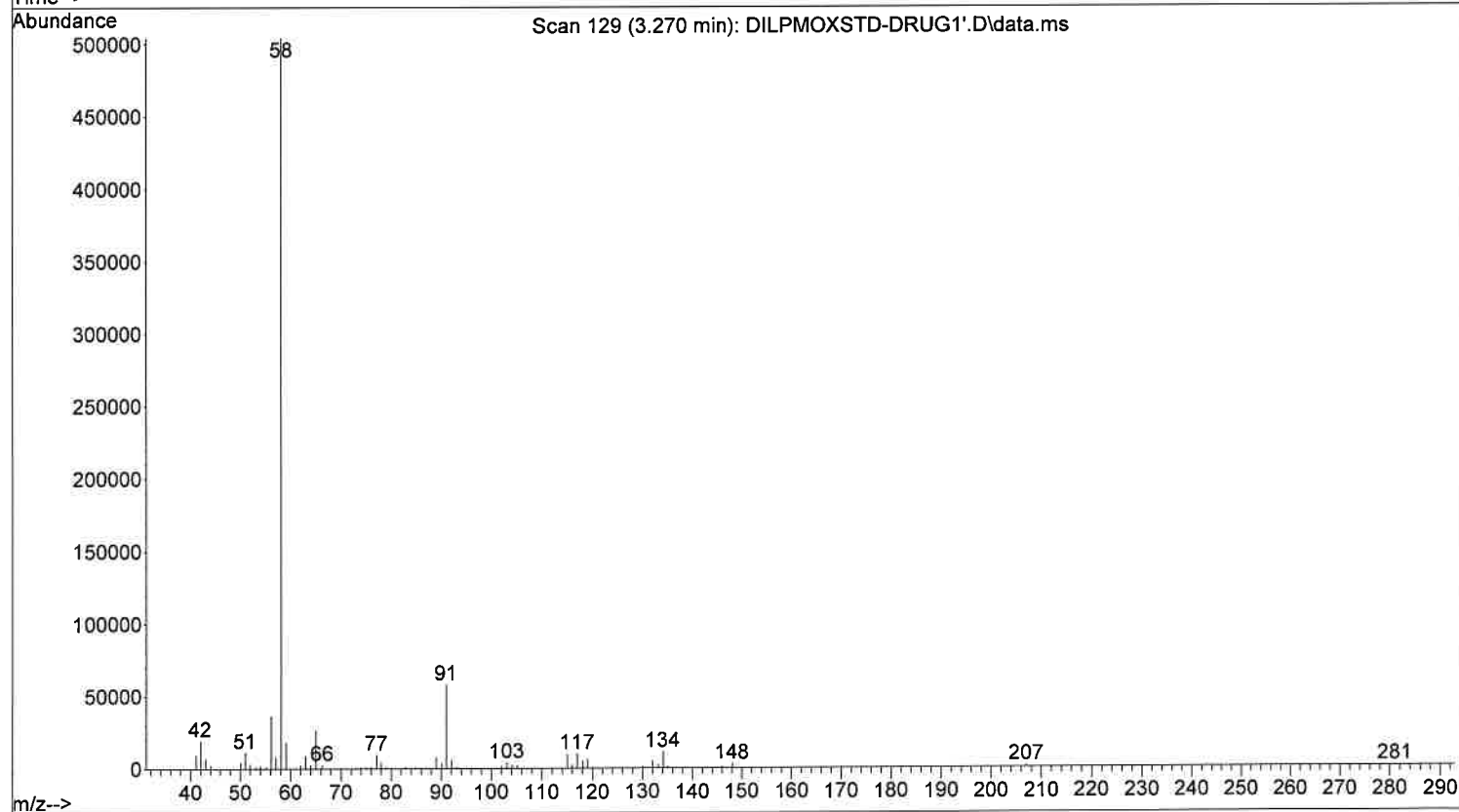
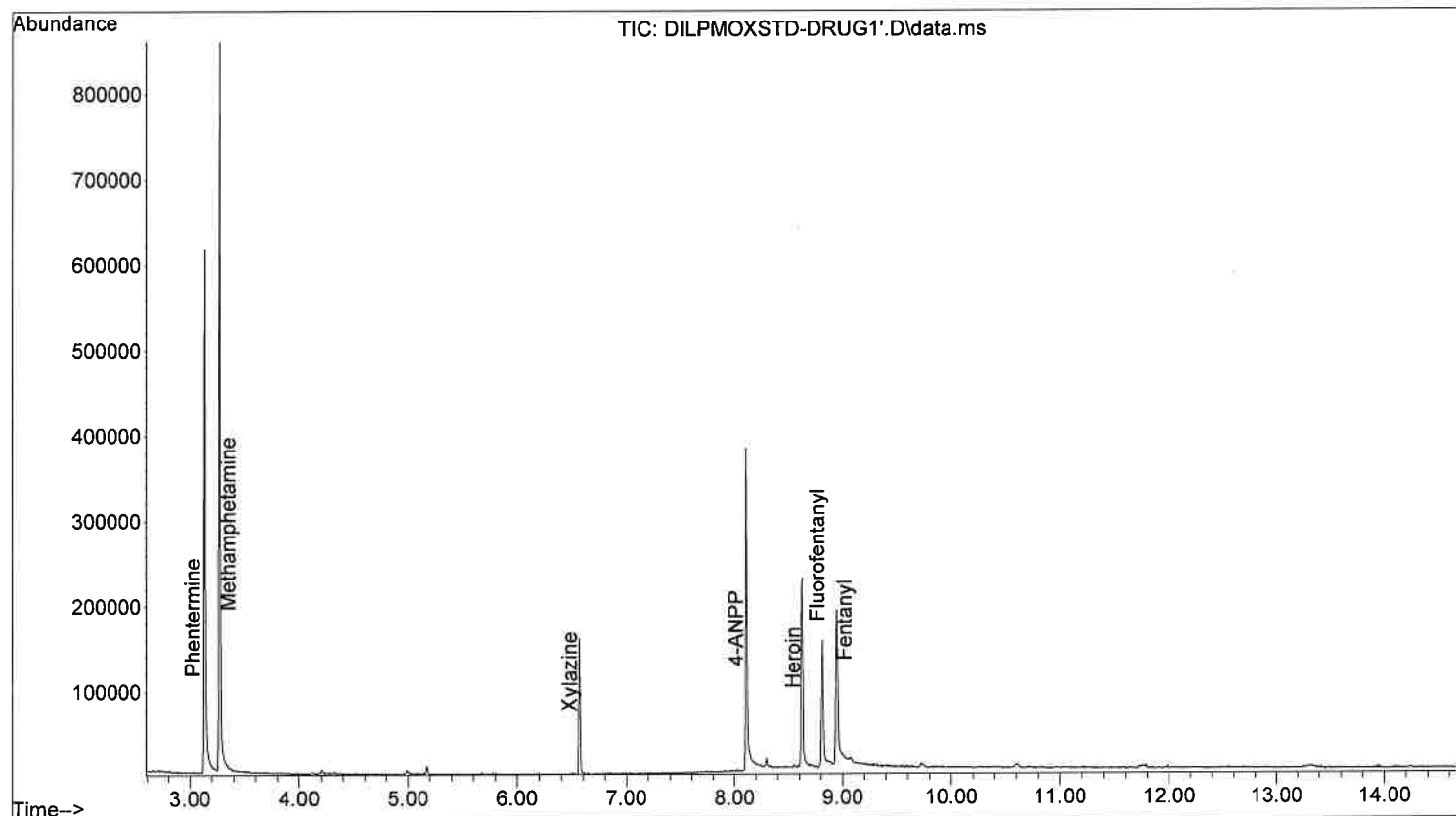
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... LC-B'.D
Operator : KLAB
Acquired : 24 Aug 2023 13:51 using AcqMethod DRUG1LC.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : For Diluted P-MOX
Vial Number: 22



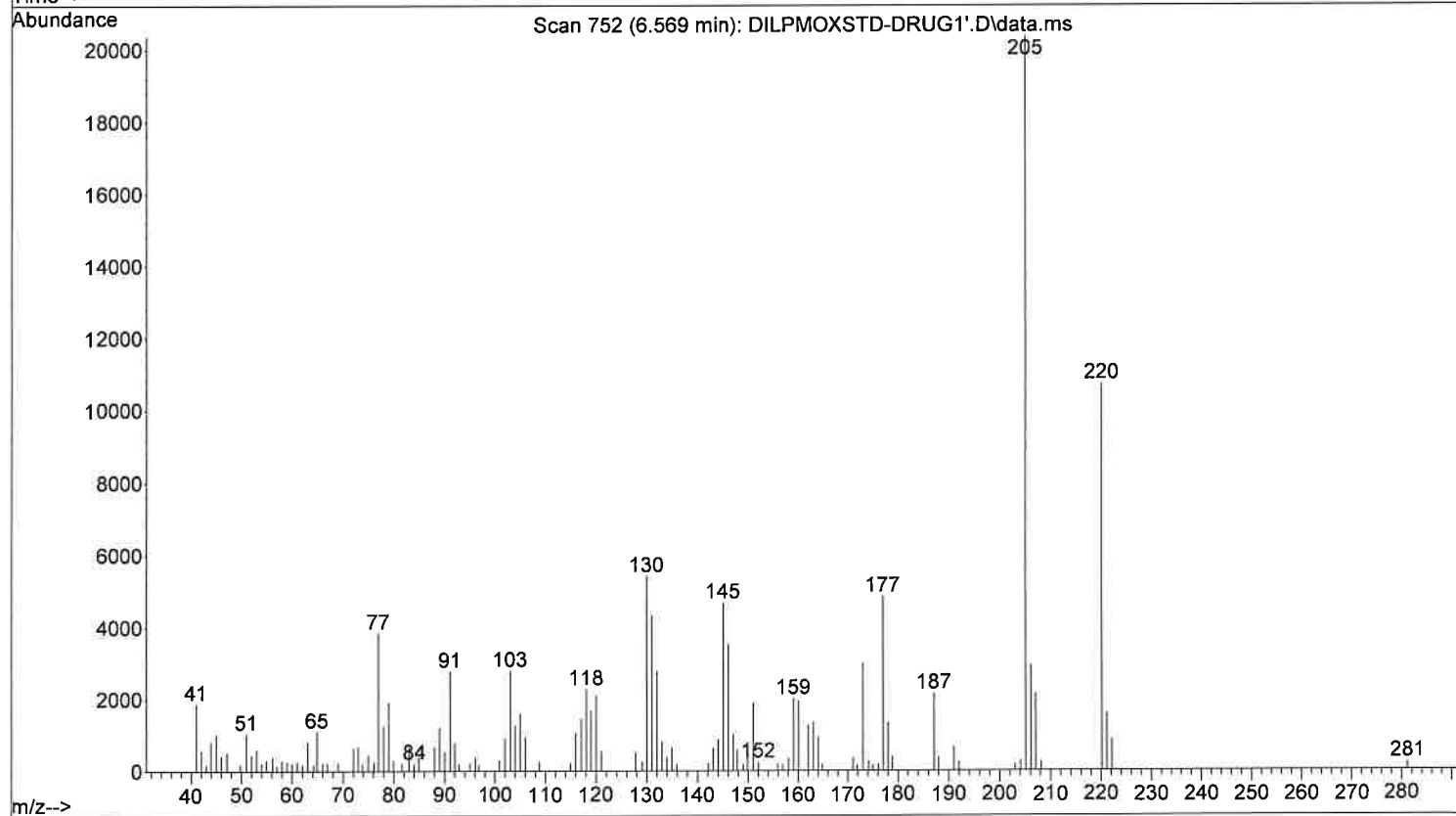
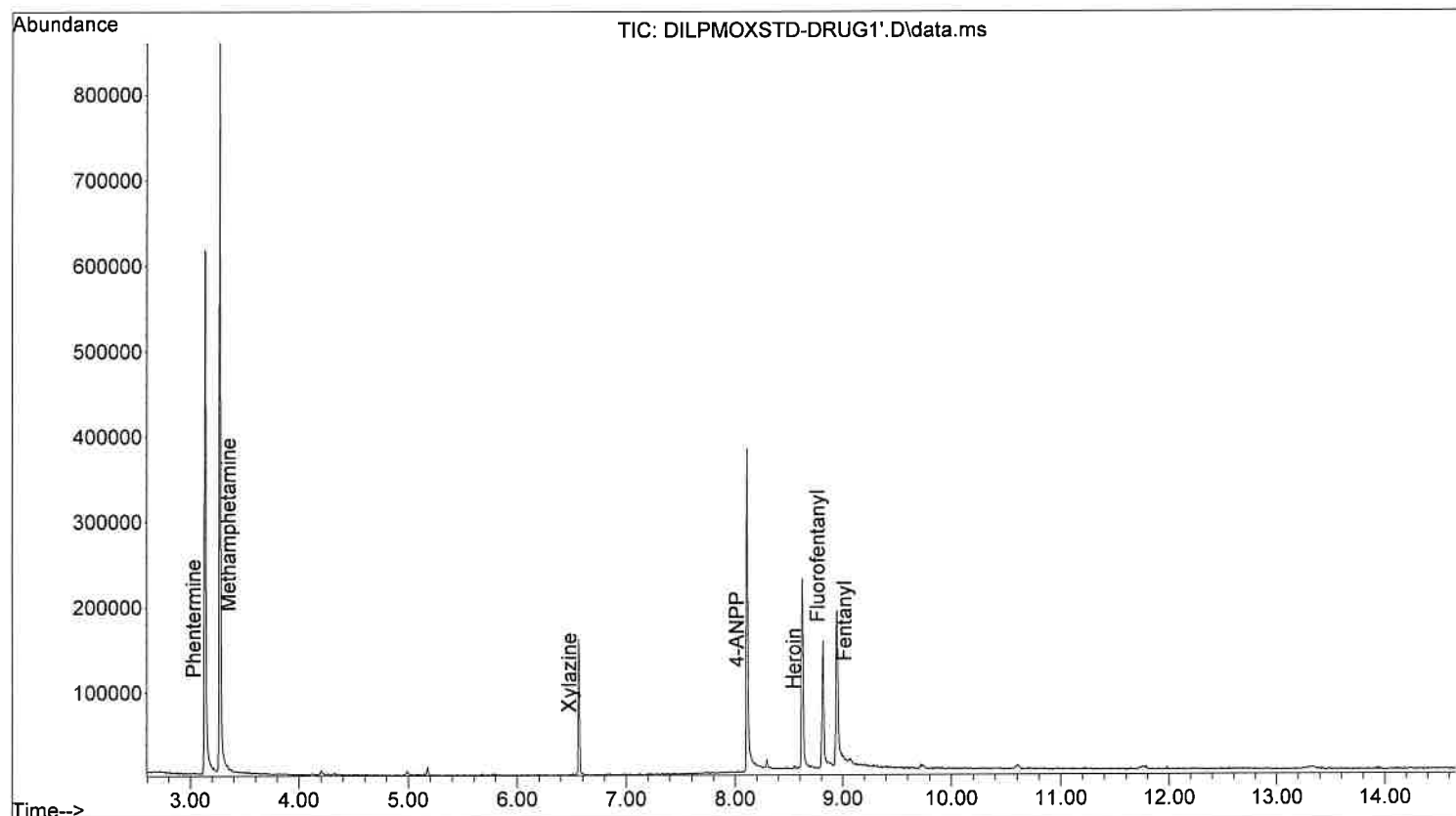
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
...'.D
Operator : KLAB
Acquired : 24 Aug 2023 13:15 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



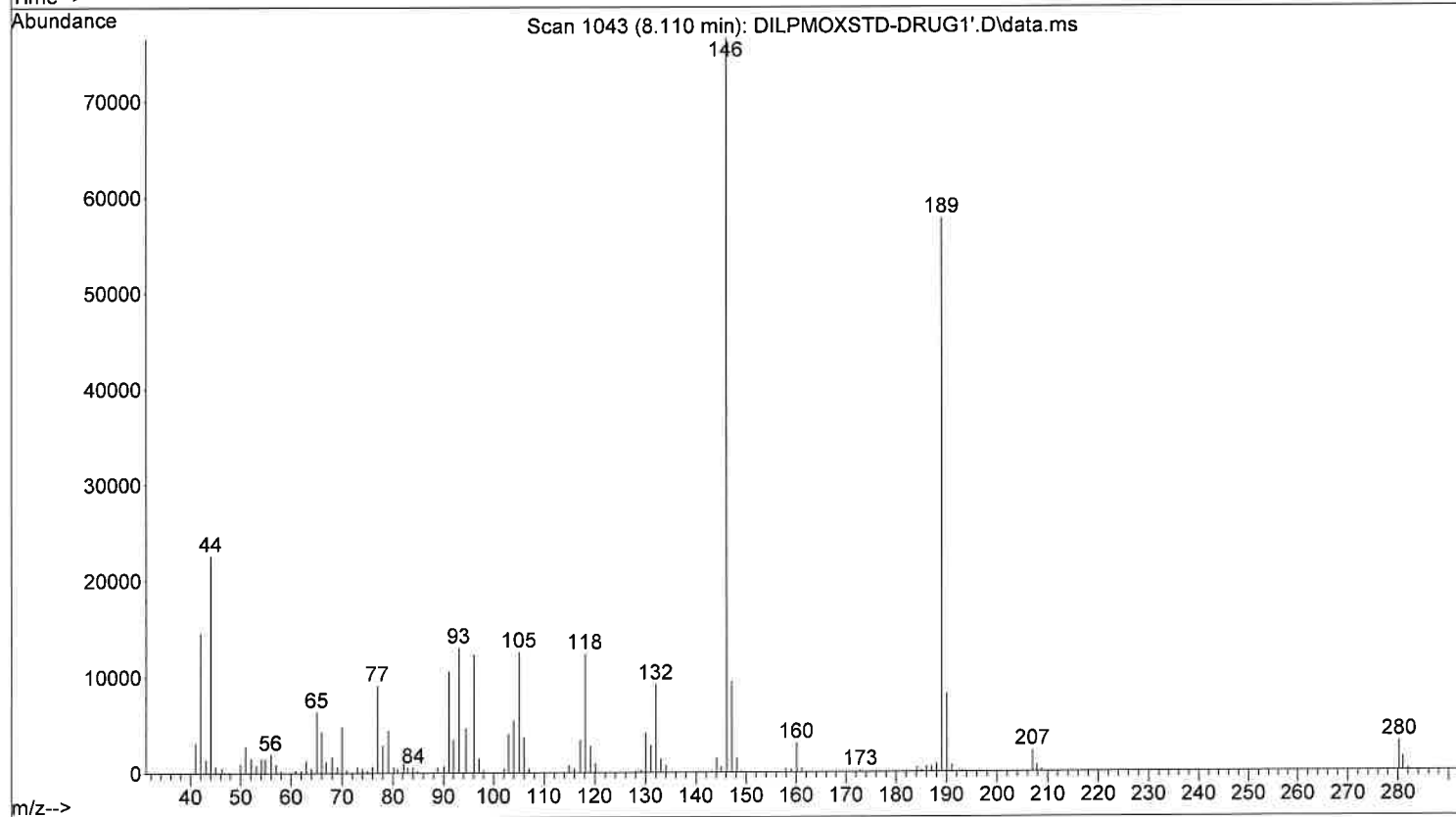
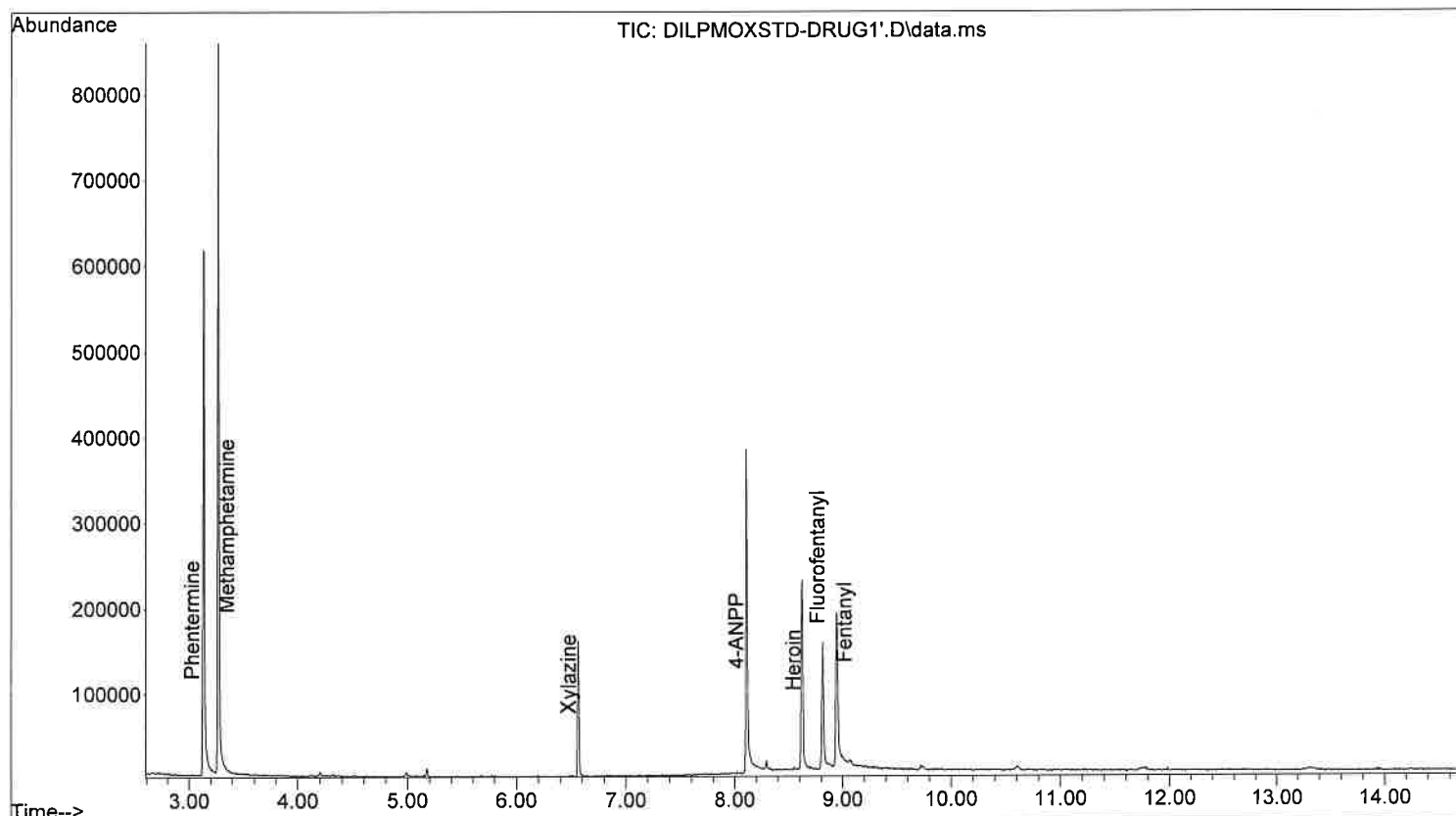
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... '.D
Operator : KLAB
Acquired : 24 Aug 2023 13:15 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



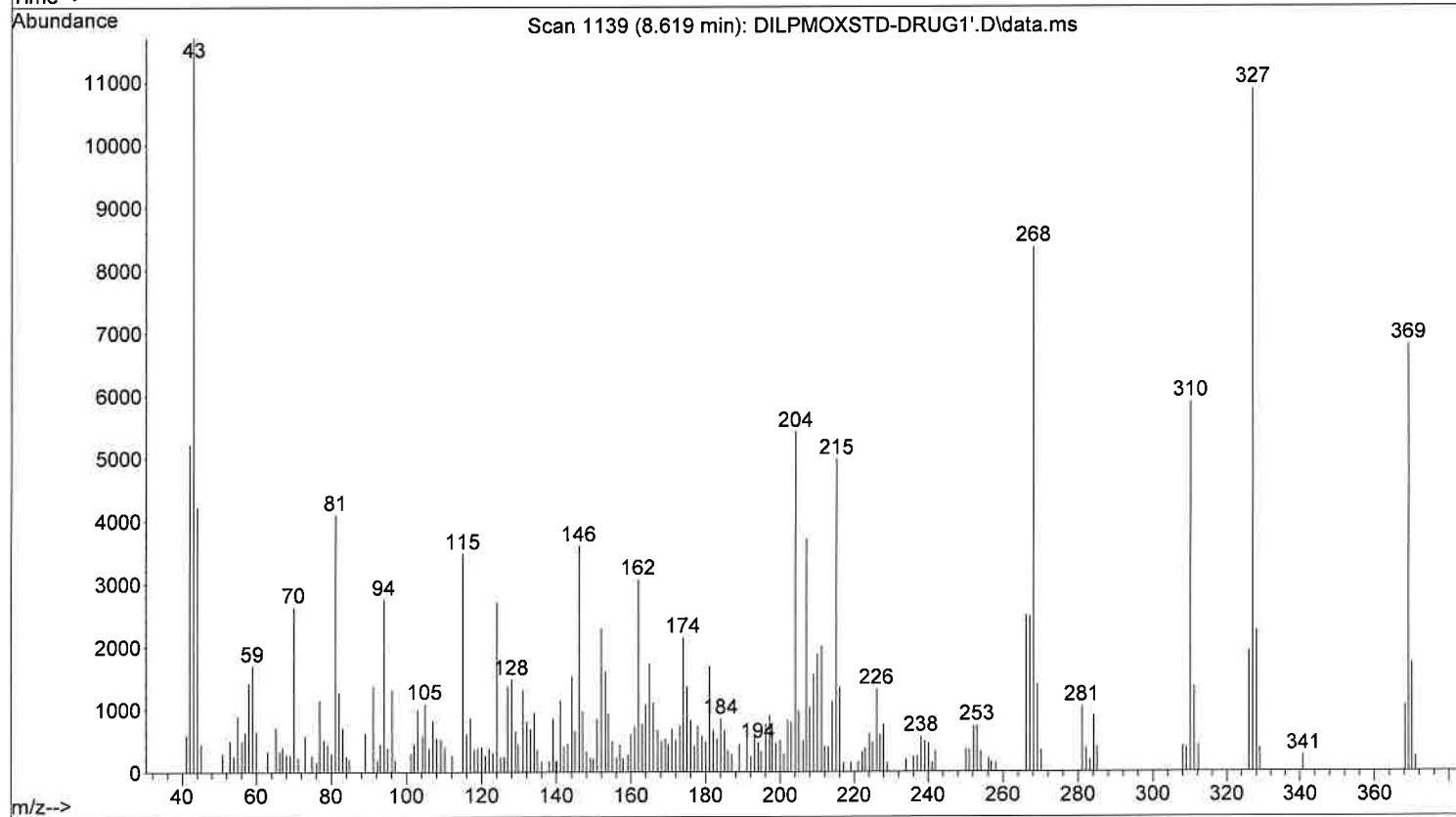
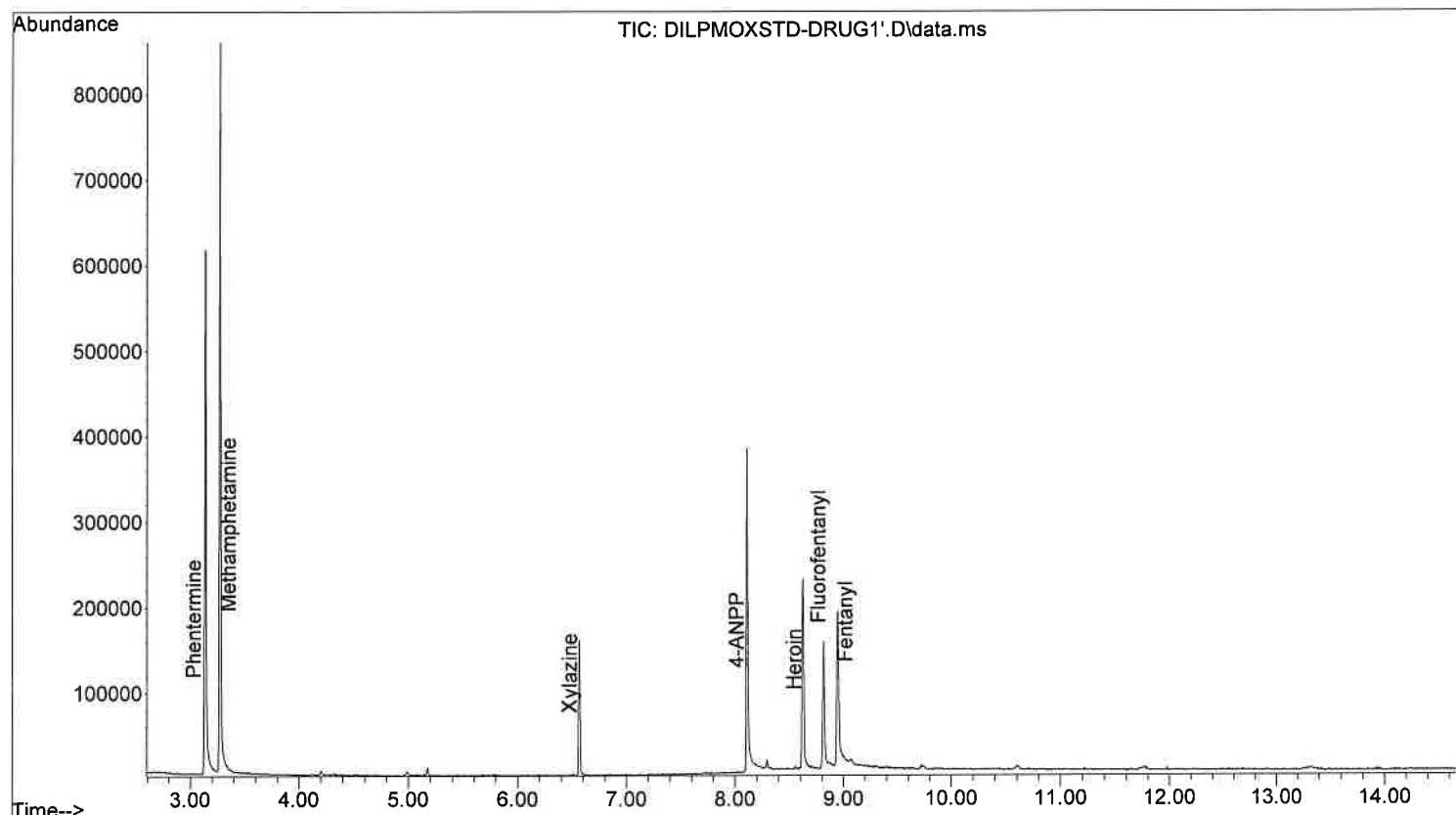
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...'.D
Operator : KLAB
Acquired : 24 Aug 2023 13:15 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



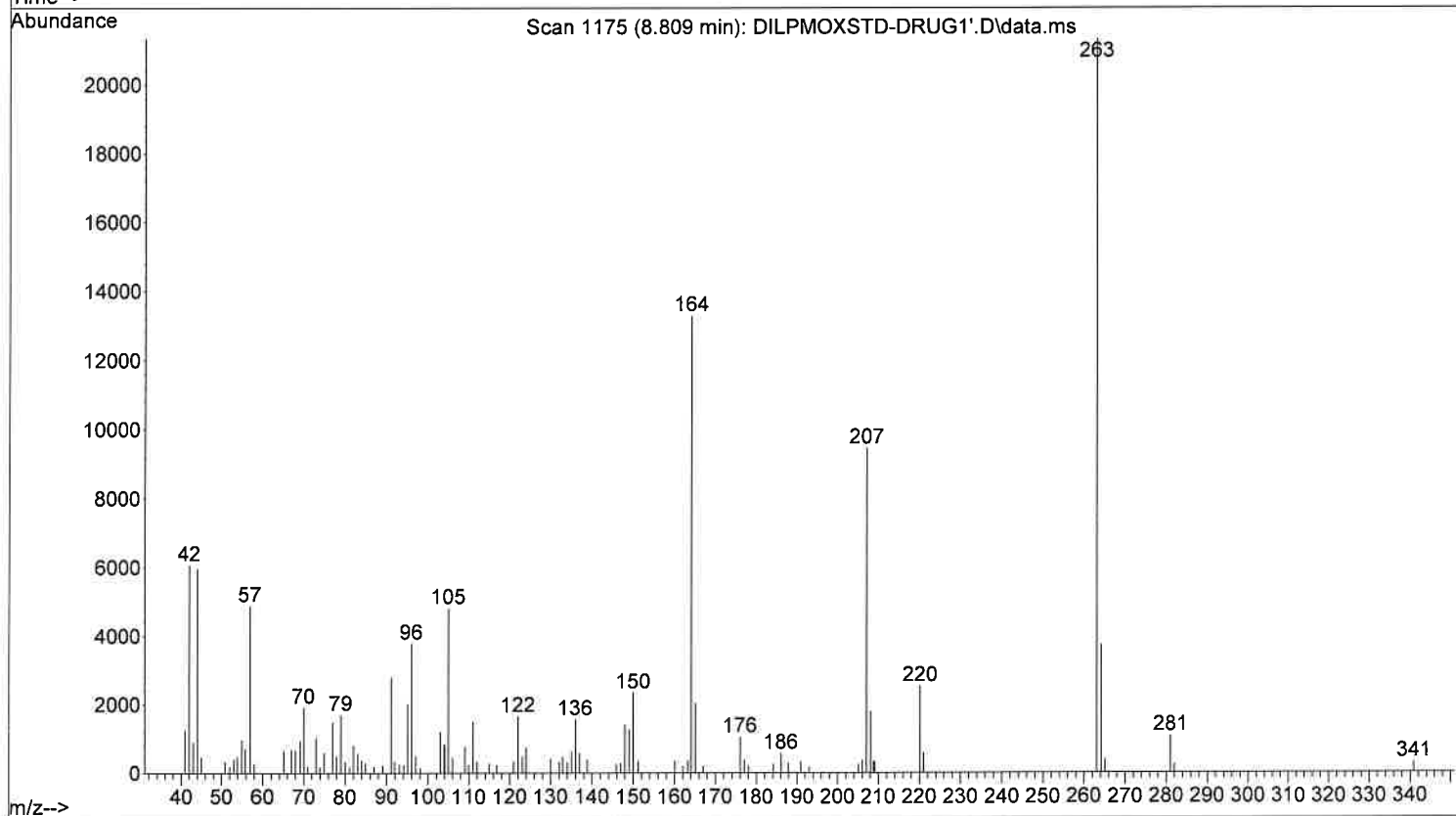
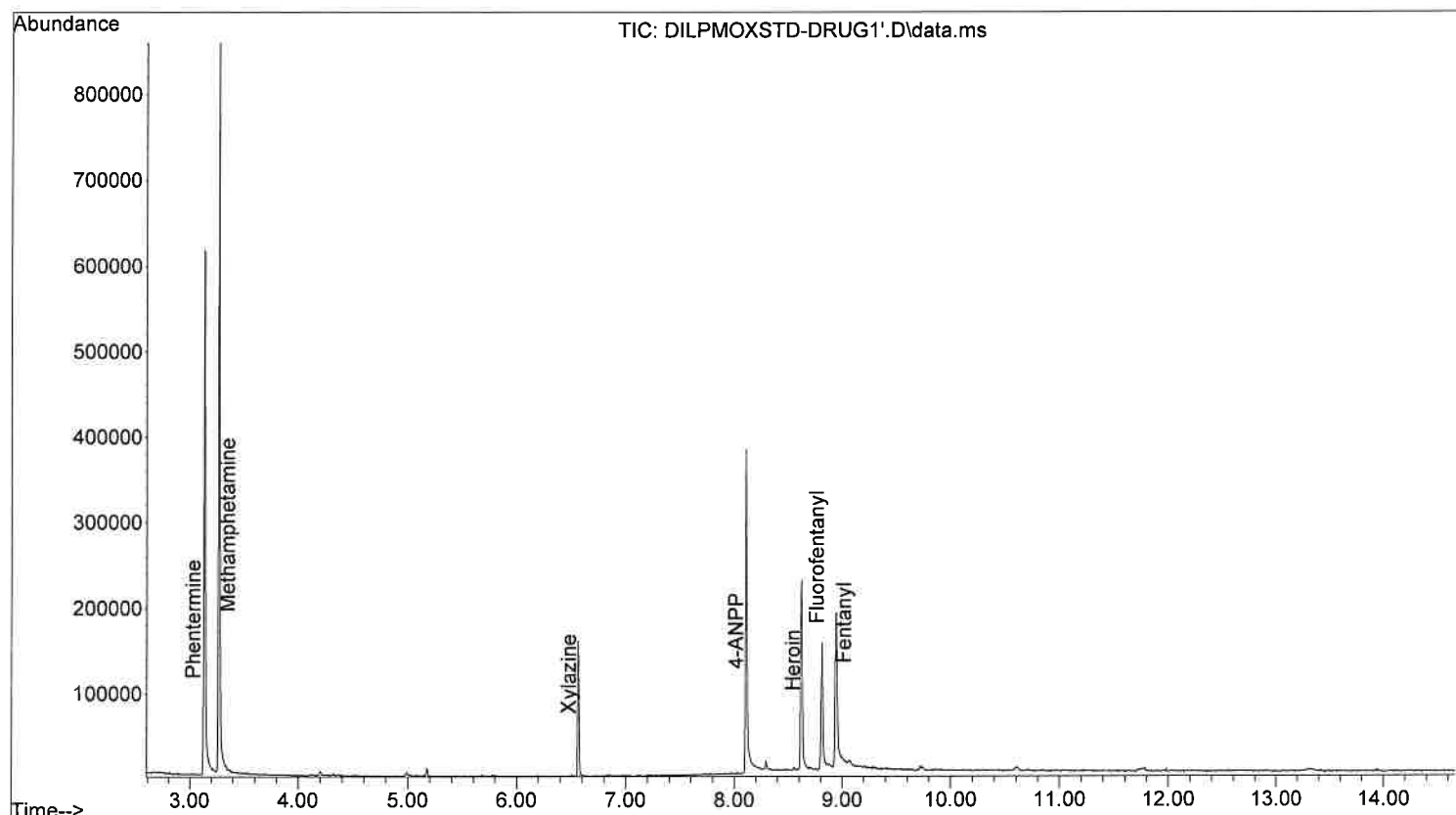
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
...
Operator : KLAB
Acquired : 24 Aug 2023 13:15 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



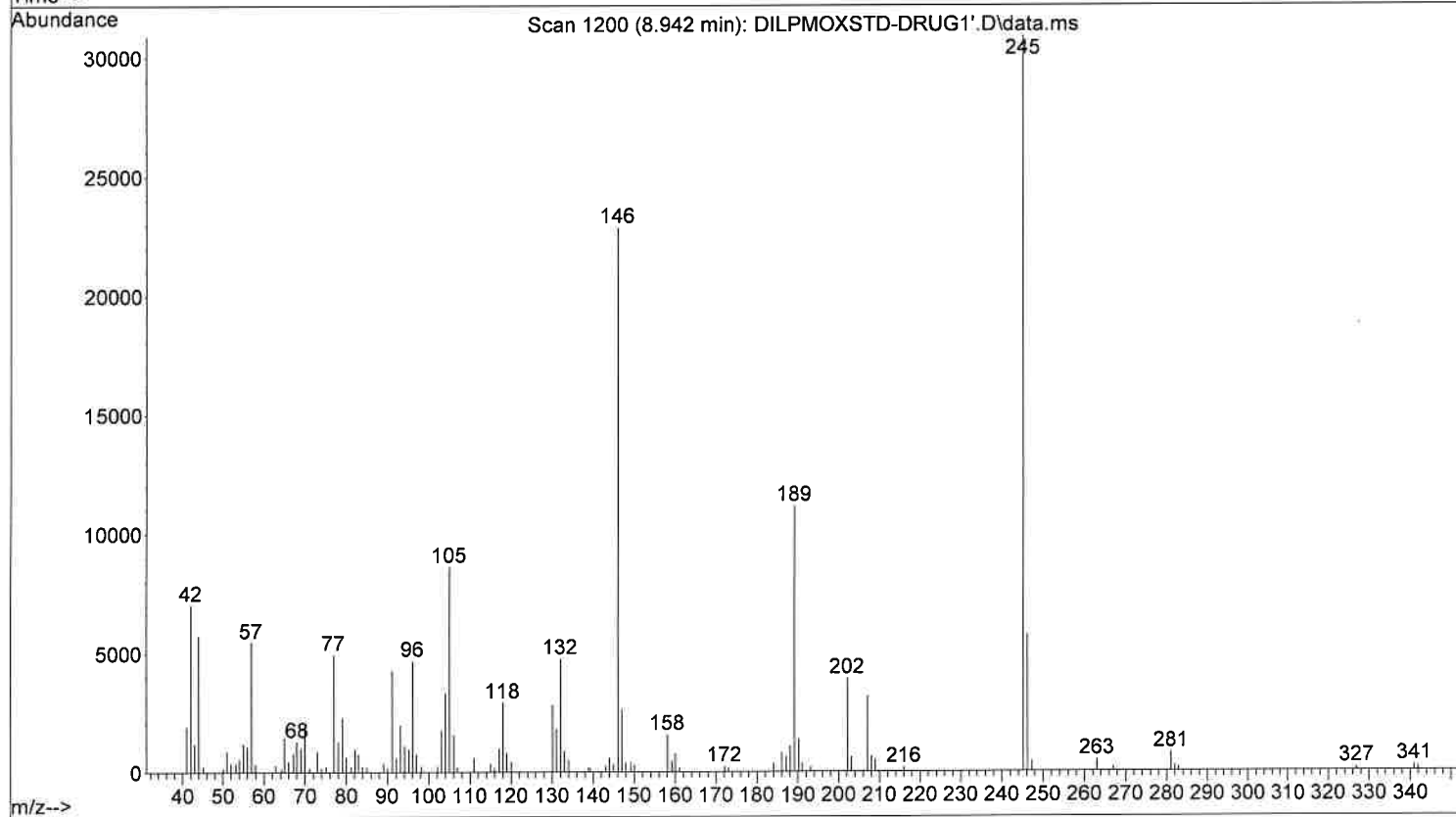
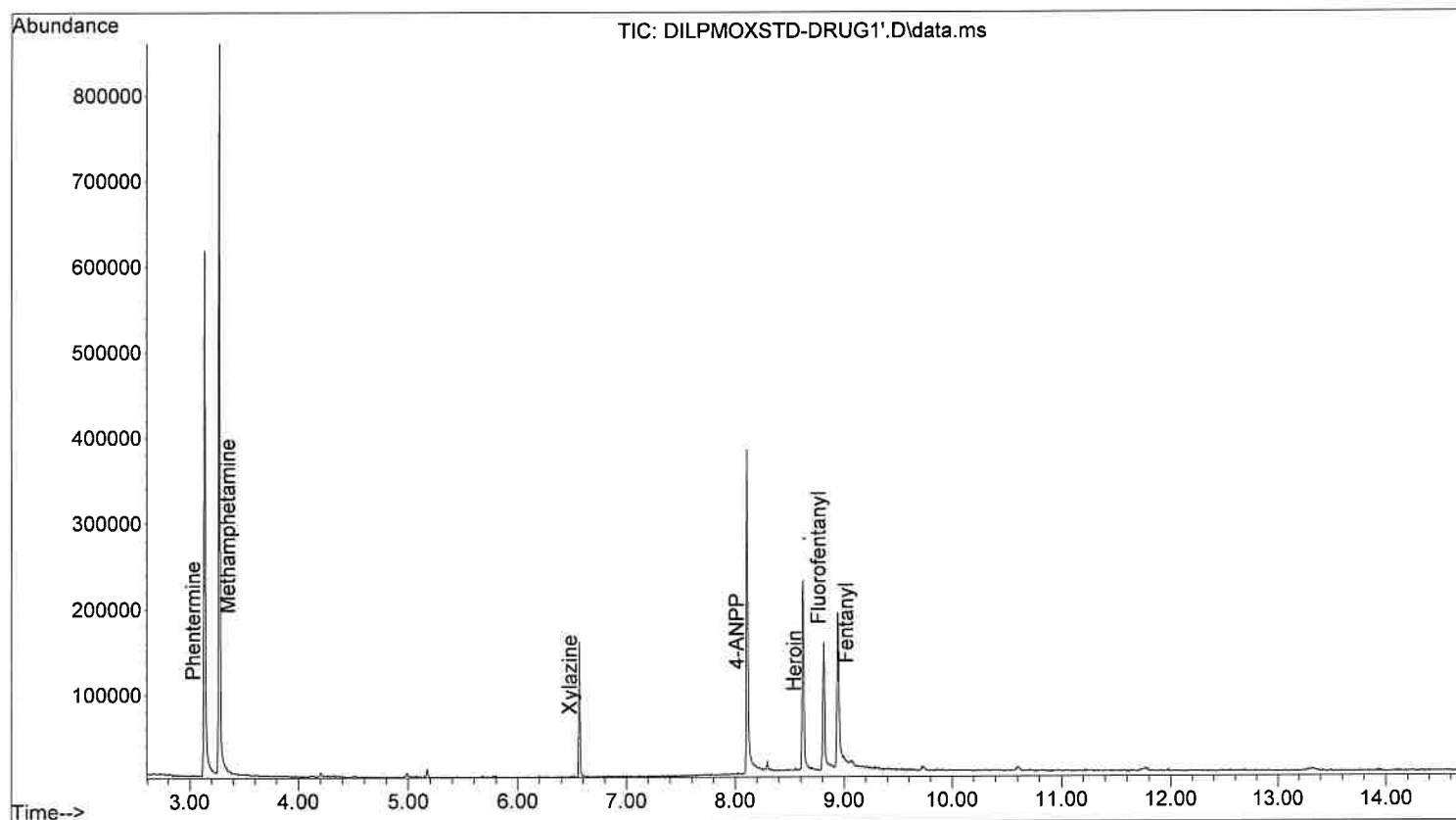
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
...
Operator : KLAB
Acquired : 24 Aug 2023 13:15 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



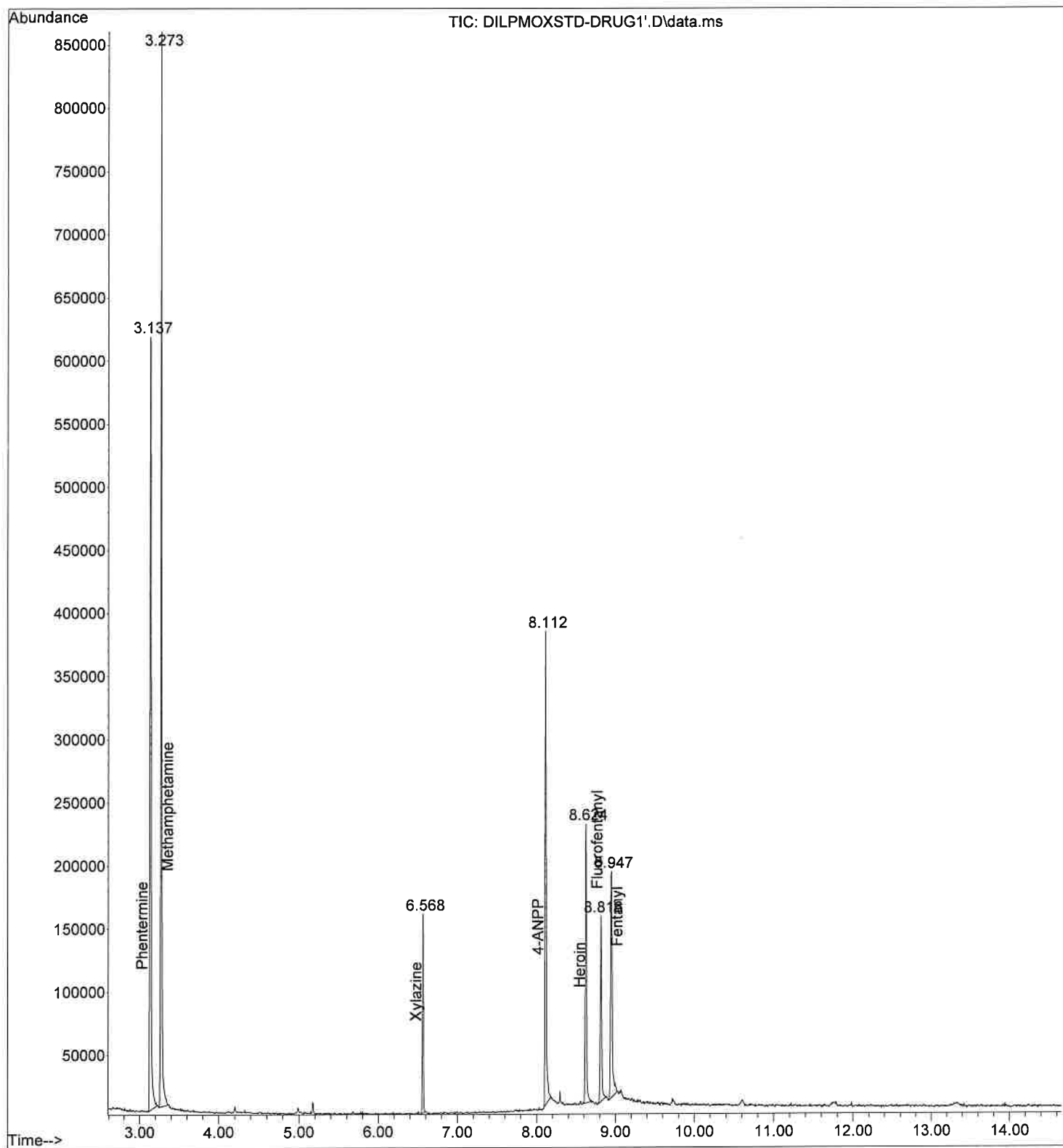
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
...
Operator : KLAB
Acquired : 24 Aug 2023 13:15 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



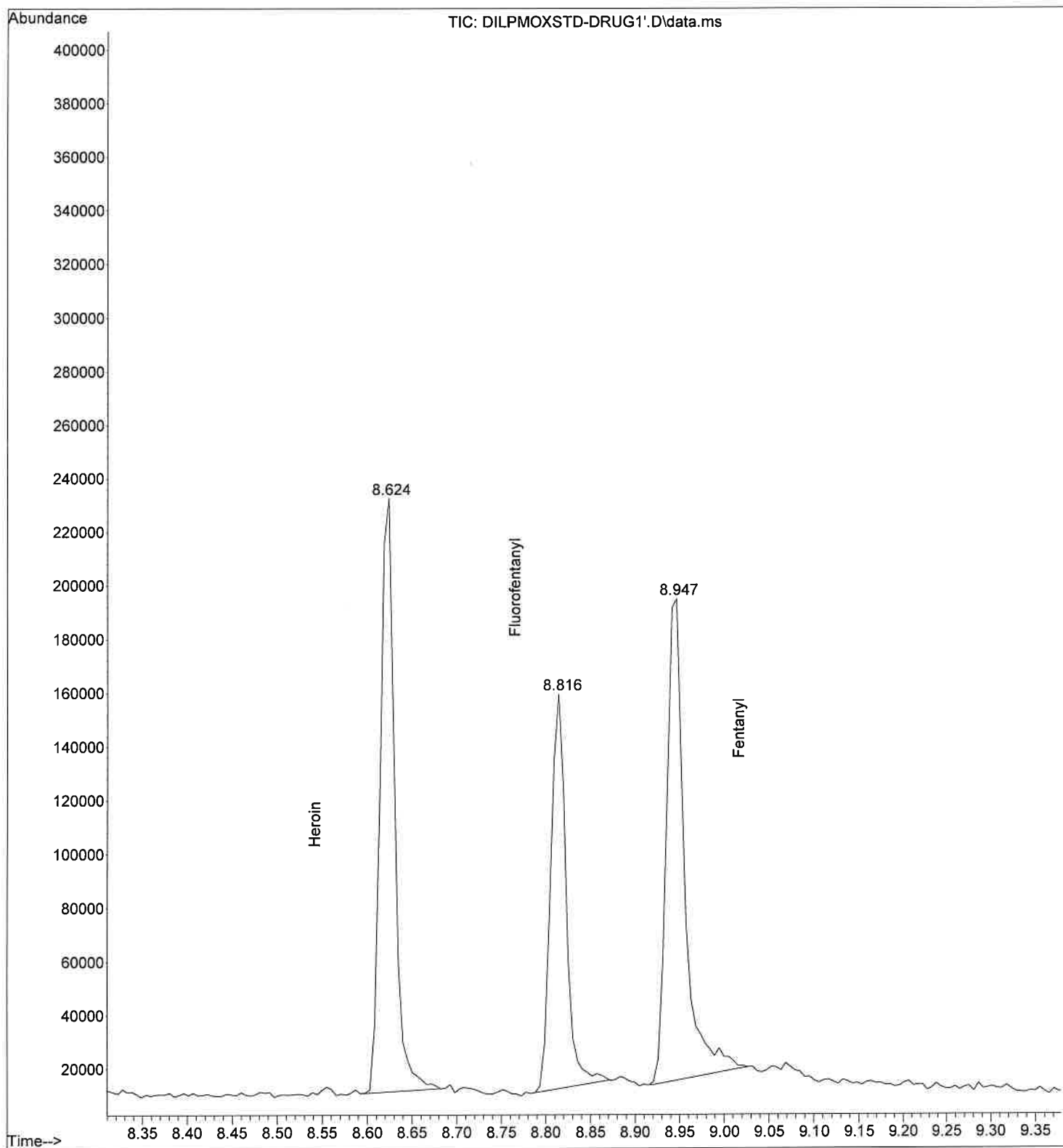
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...'.D
Operator : KLAB
Acquired : 24 Aug 2023 13:15 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3
Vial Number: 23



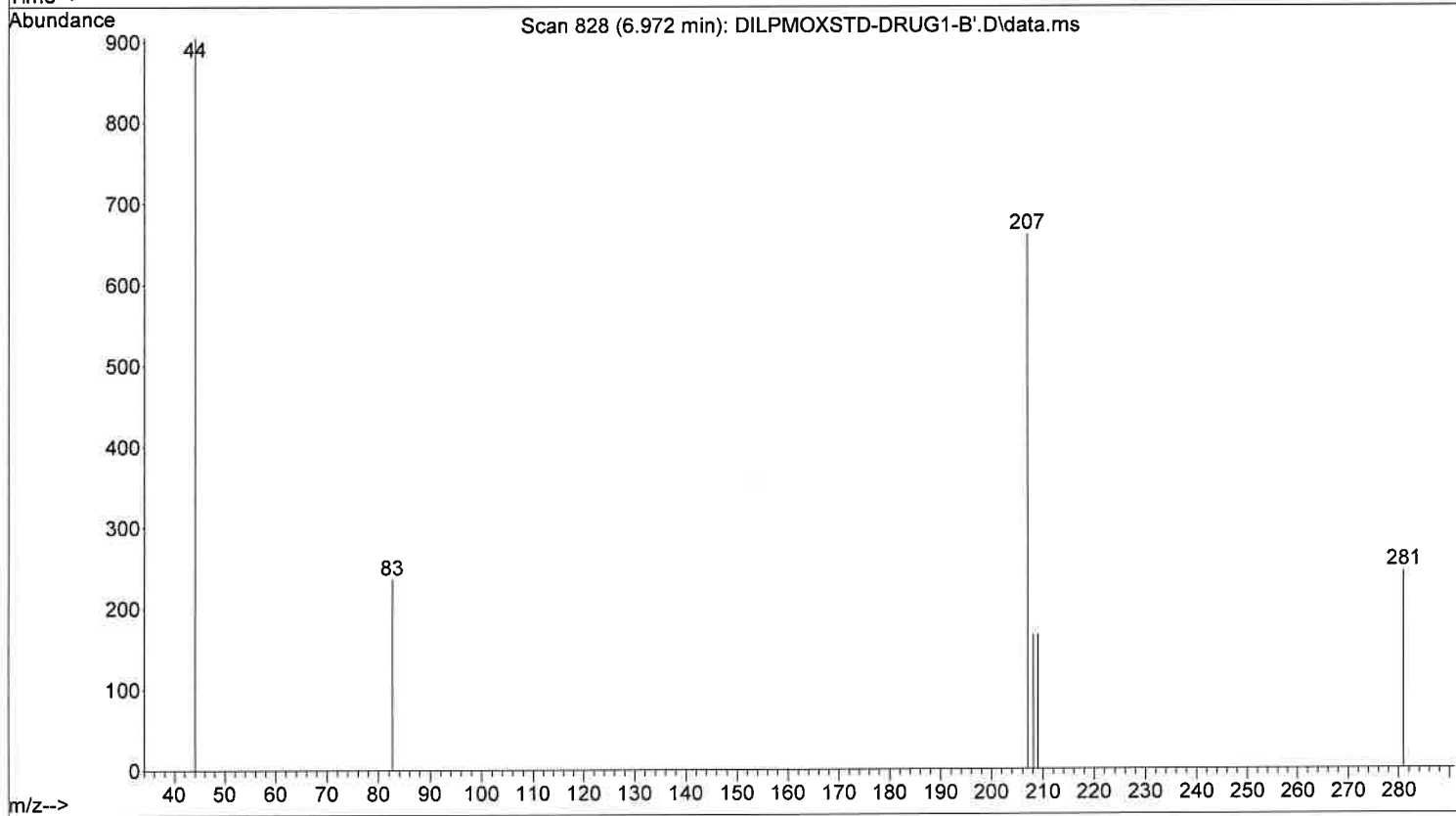
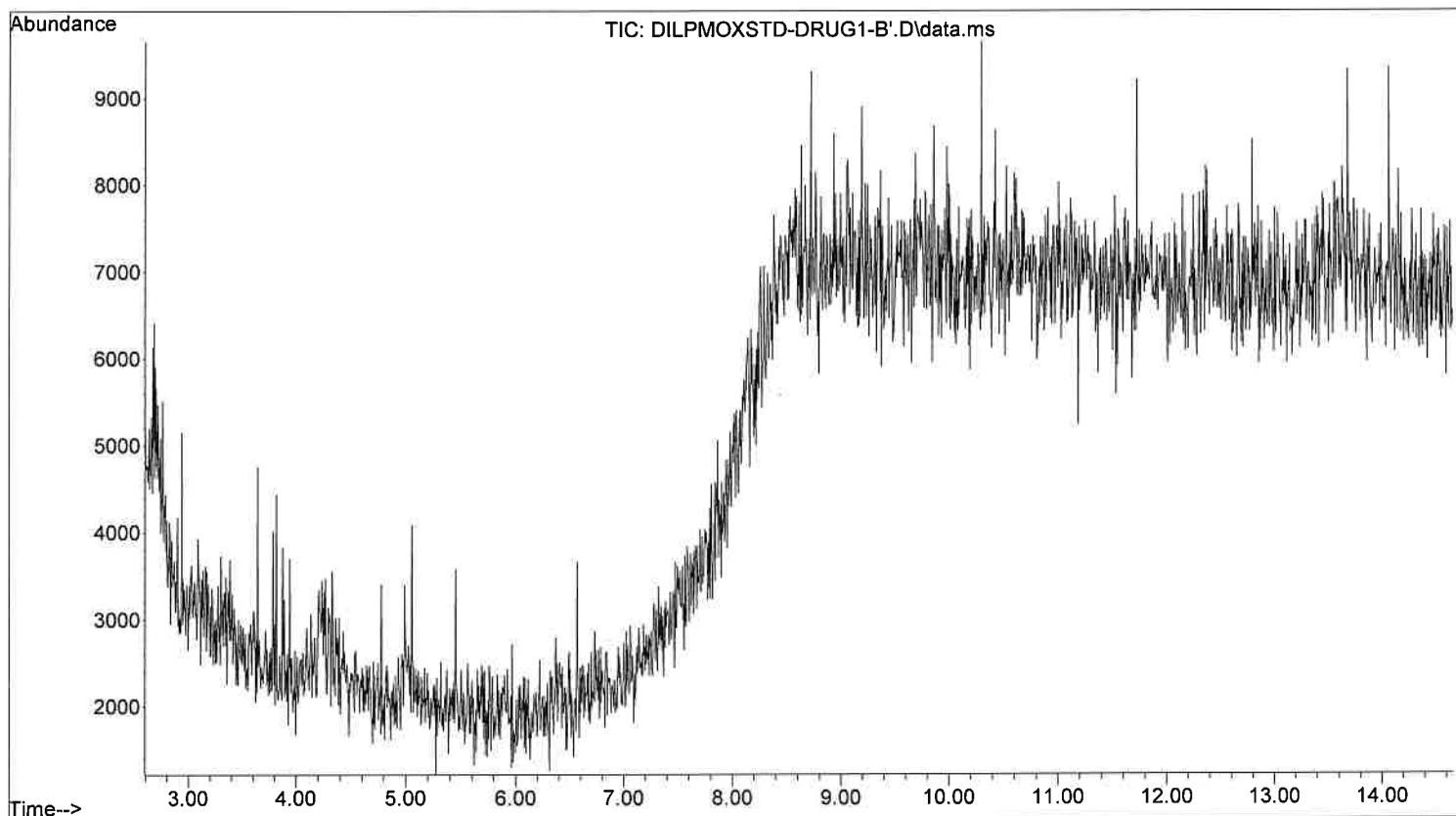
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... '.D
Operator : KLAB
Instrument : Buttercup
Acquired : 24 Aug 2023 13:15 using AcqMethod DRUG1.M
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... '.D
Operator : KLAB
Instrument : Buttercup
Acquired : 24 Aug 2023 13:15 using AcqMethod DRUG1.M
Sample Name: Diluted P-MOX Standard
Misc Info : CHCl3



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\DILPMOXSTD-DRUG1
... -B'.D
Operator : KLAB
Acquired : 24 Aug 2023 12:57 using AcqMethod DRUG1.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : For Diluted P-MOX
Vial Number: 22



METHOD CONTROL PARAMETERS

Method Information for: D:\MassHunter\GCMS\1\methods\GHB.M

Method Sections To Run:

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

Method Comments:

GHB

END OF METHOD CONTROL PARAMETERS

Single Quadrupole Acquisition Method - MS Parameters Report

Method file	D:\MassHunter\GCMS\1\methods\GHB.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)	10.00
Solvent delay (min)	0.00
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
0.00	40	500	150	1,562 [N=2]

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

Self-Cleaning Ion Source Parameters

Mode	No Cleaning
------	-------------

D:\MassHunter\GCMS\1\methods\GHB.M
Thu Aug 24 15:42:59 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 14.167 min
Post Run Time 0 min

Oven
Temperature
Setpoint On
(Initial) 80 °C
Hold Time 1 min
Post Run 0 °C
Program
#1 Rate 30 °C/min
#1 Value 280 °C
#1 Hold Time 6.5 min

Equilibration Time 0 min
Max Temperature 350 °C
Maximum Temperature Override Disabled
Slow Fan Disabled

ALS
Front Injector
Syringe Size 10 µL
Injection Volume 1 µL
Solvent A Washes (PreInj) 1
Solvent A Washes (PostInj) 1
Solvent A Volume 8 µL
Solvent B Washes (PreInj) 1
Solvent B Washes (PostInj) 1
Solvent B Volume 8 µL
Sample Washes 0
Sample Wash Volume 8 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 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
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	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	
Helium Conservation Controlled Mode	Off
Heater	Split
Pressure	On 250 °C
Total Flow	On 12 psi
Septum Purge Flow	On 46.828 mL/min
Pre-Run Flow Test	On 3 mL/min
Gas Saver	Off
Split Ratio	On 20 mL/min after 2 min
Split Flow	34.001 :1
Liner	42.575 mL/min
	Agilent 5190-2271: 900 µL (Splitless, single taper, wool, c
Back SS Inlet He	
Helium Conservation Controlled Mode	Off
Heater	Split
Pressure	Off
Total Flow	Off
Septum Purge Flow	Off
Pre-Run Flow Test	Off
Liner	A Liner has not been selected.
Column	
Column #1	
Flow	
Setpoint	On
(Initial)	1.2522 mL/min
Post Run	1 mL/min
Column Information	Agilent 128-0112: 1
Description	DB-1ms

Temperature Range	-60 °C-340 °C (350 °C)
Dimensions	12 m x 200 µm x 0.33 µm (Calibrated)
Heater	Oven
Column lock	Unlocked
In	Front SS Inlet He
Out	MSD
(Initial)	80 °C
Pressure	12 psi
Flow	1.2522 mL/min
Average Velocity	65.404 cm/sec
Holdup Time	0.30579 min
Control Mode	Constant Flow
Column Outlet Pressure	0 psi
Front Detector FID	
Makeup	He
Heater	Off
H2 Flow	Off
Air Flow	Off
Makeup Flow	Off
Carrier Gas Flow Correction	Constant Makeup and Fuel Flow
Flame	Off
Blank Evaluation Setpoints	
Perform Blank Evaluation Test	Off
Helium Conservation	
Helium Valve	Off
Nitrogen Valve	Off
Detector Evaluation	
Perform Detector Evaluation Test	Off
MSD Transfer Line	
Temperature	
Setpoint	On
(Initial)	280 °C
Signals	
Signal #1:	
Description	None
Signal #2:	
Description	None
Signal #3:	
Description	None
Signal #4:	
Description	None
Signal #5:	
Description	None
Signal #6:	
Description	None
Signal #7:	
Description	None
Signal #8:	
Description	None

TUNE PARAMETERS for SN: US2313MA09

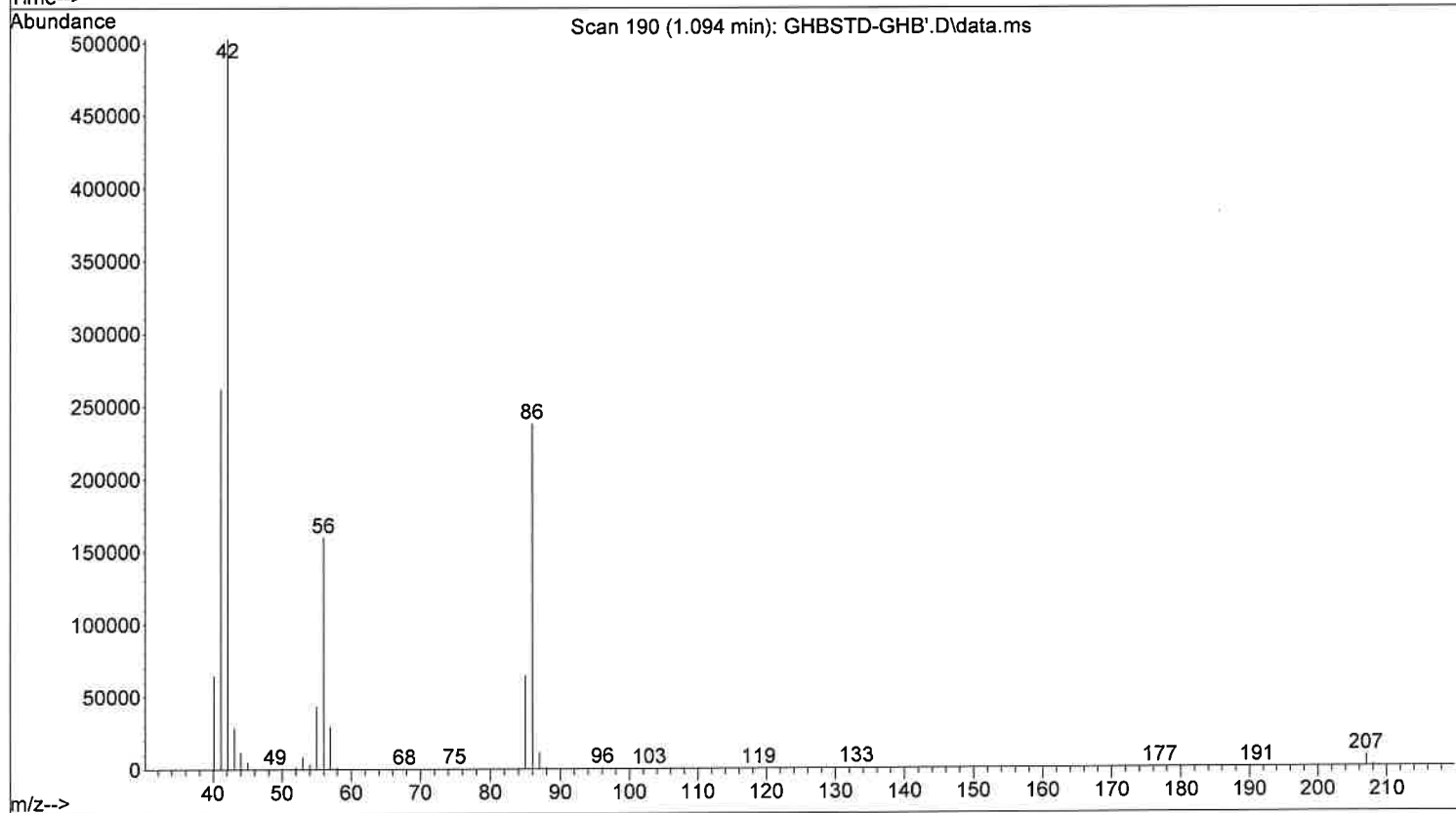
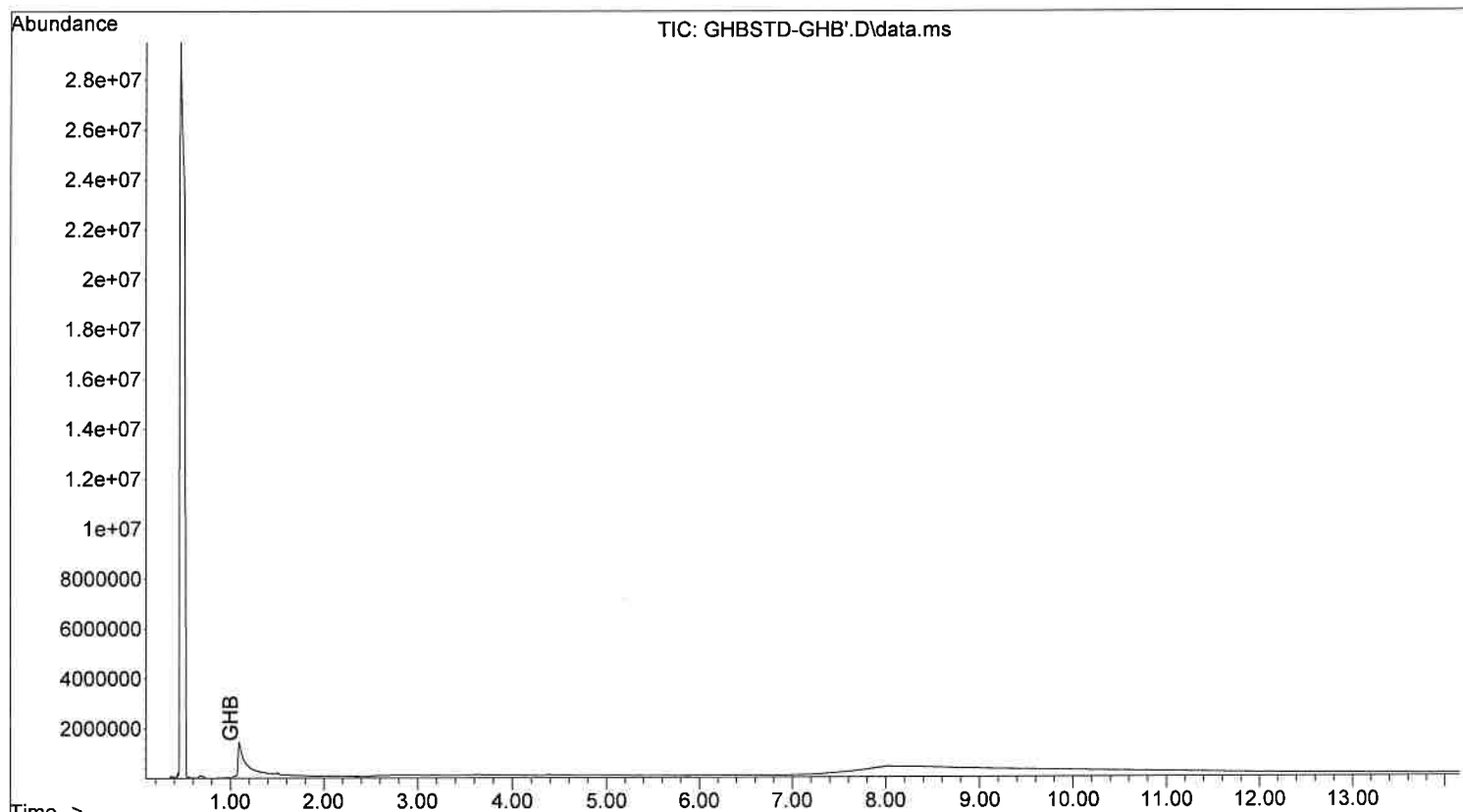
Trace Ion Detection is OFF.

34.593	:	EMISSION	
70.007	:	ENERGY	
29.919	:	REPELLER	
90.331	:	IONFOCUS	
25.226	:	ENTRANCE LENS	
925.472	:	EMVOLTS	
		951.5	: Actual EMV
		1.00	: GAIN FACTOR
2896.000	:	AMUGAIN	
134.625	:	AMUOFFSET	
1.000	:	FILAMENT	
0.000	:	DCPOLARITY	
10.822	:	ENTLENSOFFSET	
0.000	:	Ion_Body	
0.000	:	EXTLENS	
257.000	:	MASSGAIN	
-23.000	:	MASSOFFSET	

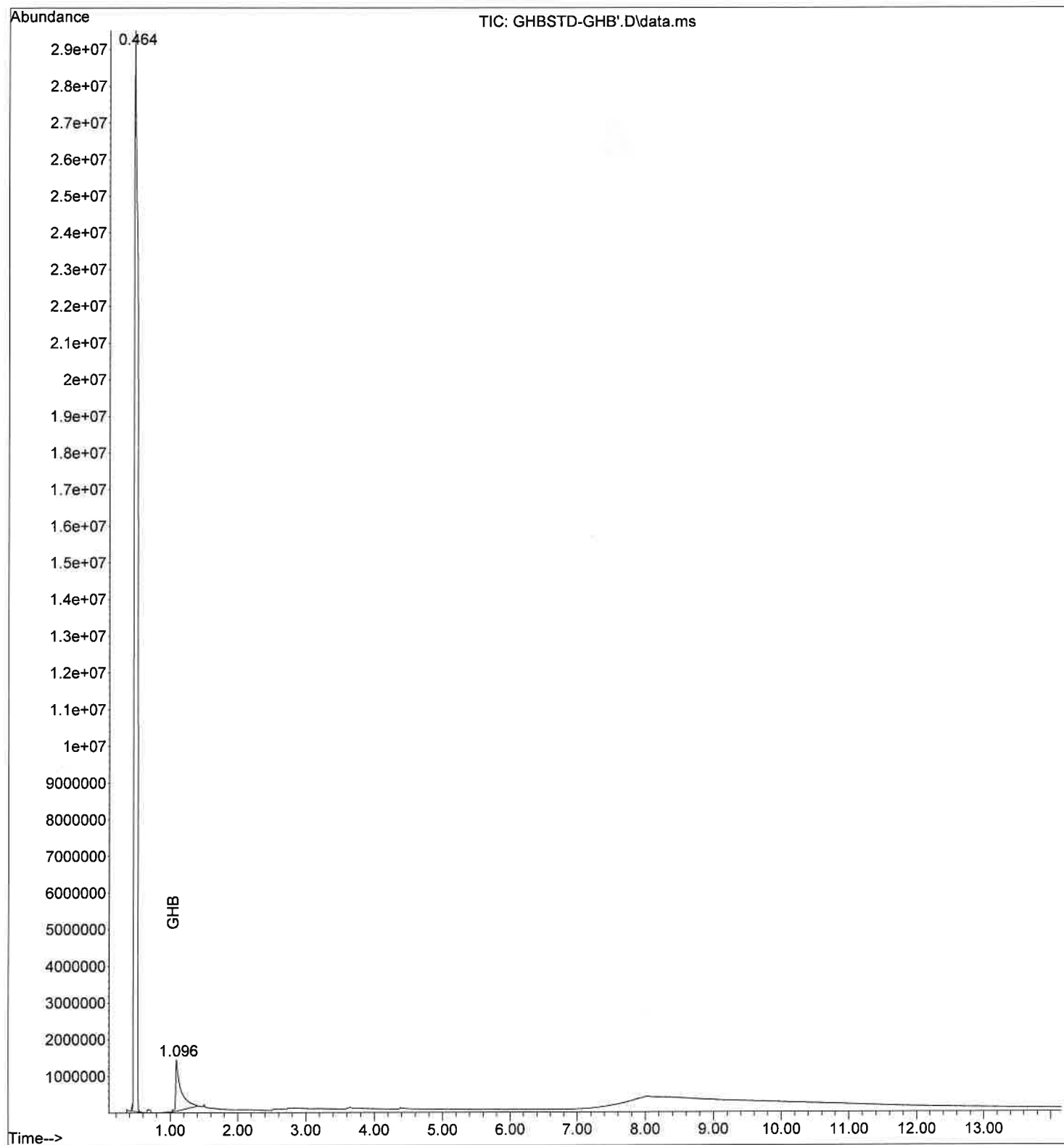
END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

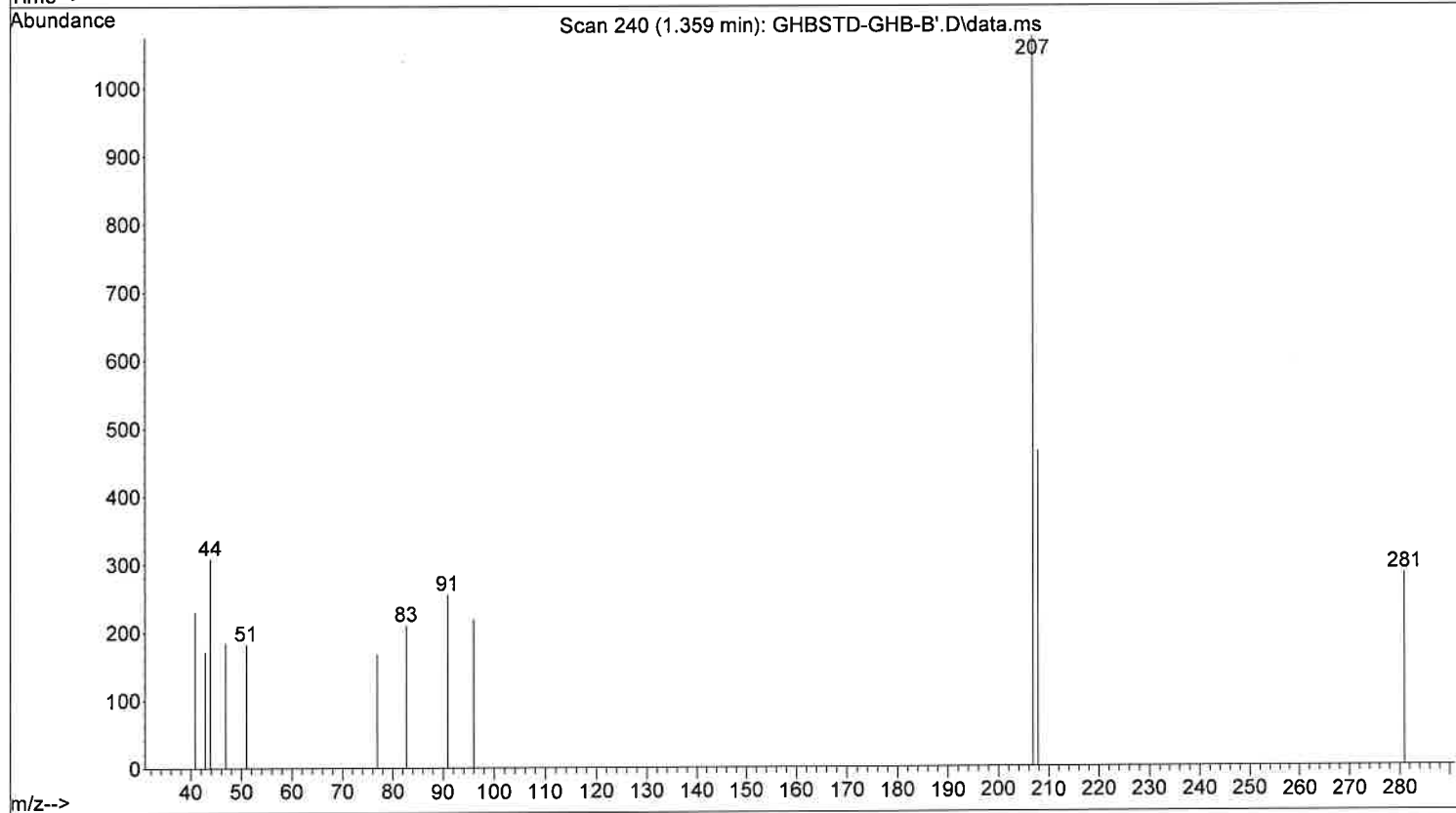
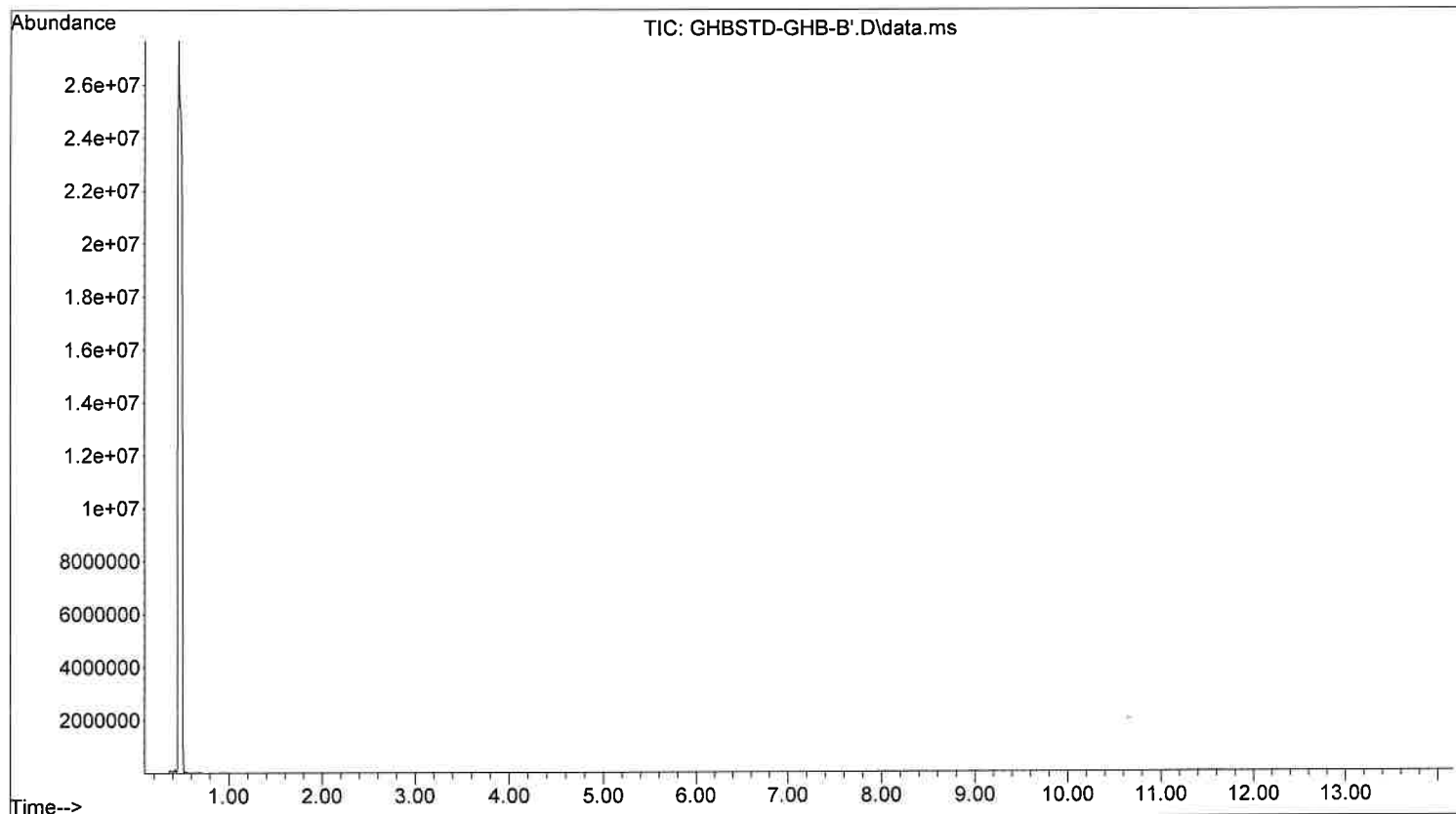
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\GHBSTD-GHB'.D
Operator : KLAB
Acquired : 24 Aug 2023 15:00 using AcqMethod GHB.M
Instrument : Buttercup
Sample Name: GHB Standard
Misc Info : MEOH
Vial Number: 24



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\GHBSTD-GHB'.D
Operator : KLAB
Acquired : 24 Aug 2023 15:00 using AcqMethod GHB.M
Instrument : Buttercup
Sample Name: GHB Standard
Misc Info : MEOH
Vial Number: 24



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\GHBSTD-GHB-B'.D
Operator : KLAB
Acquired : 24 Aug 2023 14:43 using AcqMethod GHB.M
Instrument : Buttercup
Sample Name: Methanol blank
Misc Info : For GHB
Vial Number: 21



METHOD CONTROL PARAMETERS

Method Information for: D:\MassHunter\GCMS\1\methods\XLDRUGS.M

Method Sections To Run:

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

Method Comments:

XLDRUGS

END OF METHOD CONTROL PARAMETERS

Single Quadrupole Acquisition Method - MS Parameters Report

Method file	D:\MassHunter\GCMS\1\methods\XLDRUGS.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)	10.00
Solvent delay (min)	2.50
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
2.50	40	550	150	1,562 [N=2]

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

Self-Cleaning Ion Source Parameters

Mode	No Cleaning
------	-------------

INSTRUMENT CONTROL PARAMETERS: Buttercup

D:\MassHunter\GCMS\1\methods\XLDRUGS.M
Thu Aug 24 15:44:41 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 28.058 min
Post Run Time 0 min

Oven
Temperature
Setpoint On
(Initial) 70 °C
Hold Time 0 min
Post Run 80 °C
Program
#1 Rate 15 °C/min
#1 Value 150 °C
#1 Hold Time 3 min
#2 Rate 40 °C/min
#2 Value 299 °C
#2 Hold Time 16 min

Equilibration Time 0 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) 1
Solvent A Washes (PostInj) 1
Solvent A Volume 8 µL
Solvent B Washes (PreInj) 1
Solvent B Washes (PostInj) 1
Solvent B Volume 8 µL
Sample Washes 0
Sample Wash Volume 8 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 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
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	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	
Helium Conservation Controlled	Off
Mode	Split
Heater	On 250 °C
Pressure	On 9.1 psi
Total Flow	On 45.808 mL/min
Septum Purge Flow	On 3 mL/min
Pre-Run Flow Test	Off
Gas Saver	On 20 mL/min after 2 min
Split Ratio	40 :1
Split Flow	41.764 mL/min
Liner	Agilent 5190-2271: 900 µL (Splitless, single taper, wool, C
Back SS Inlet He	
Helium Conservation Controlled	Off
Mode	Split
Heater	Off
Pressure	Off
Total Flow	Off
Septum Purge Flow	Off
Pre-Run Flow Test	Off
Liner	A Liner has not been selected.
Column	
Column #1	
Flow	
Setpoint	On
(Initial)	1.0441 mL/min
Post Run	1 mL/min

Column Information	Agilent 128-0112: 1
Description	DB-1ms
Temperature Range	-60 °C-340 °C (350 °C)
Dimensions	12 m x 200 µm x 0.33 µm (Calibrated)
Heater	Oven
Column lock	Unlocked
In	Front SS Inlet He
Out	MSD
(Initial)	70 °C
Pressure	9.1 psi
Flow	1.0441 mL/min
Average Velocity	59.449 cm/sec
Holdup Time	0.33642 min
Control Mode	Constant Flow
Column Outlet Pressure	0 psi
Front Detector FID	
Makeup	He
Heater	Off
H2 Flow	Off
Air Flow	Off
Makeup Flow	Off
Carrier Gas Flow Correction	Constant Makeup and Fuel Flow
Flame	Off
Blank Evaluation Setpoints	
Perform Blank Evaluation Test	Off
Helium Conservation	
Helium Valve	Off
Nitrogen Valve	Off
Detector Evaluation	
Perform Detector Evaluation Test	Off
MSD Transfer Line	
Temperature	
Setpoint	On
(Initial)	280 °C
Signals	
Signal #1:	
Description	None
Signal #2:	
Description	None
Signal #3:	
Description	None
Signal #4:	
Description	None
Signal #5:	
Description	None
Signal #6:	
Description	None
Signal #7:	
Description	None

Signal #8:
Description

None

TUNE PARAMETERS for SN: US2313MA09

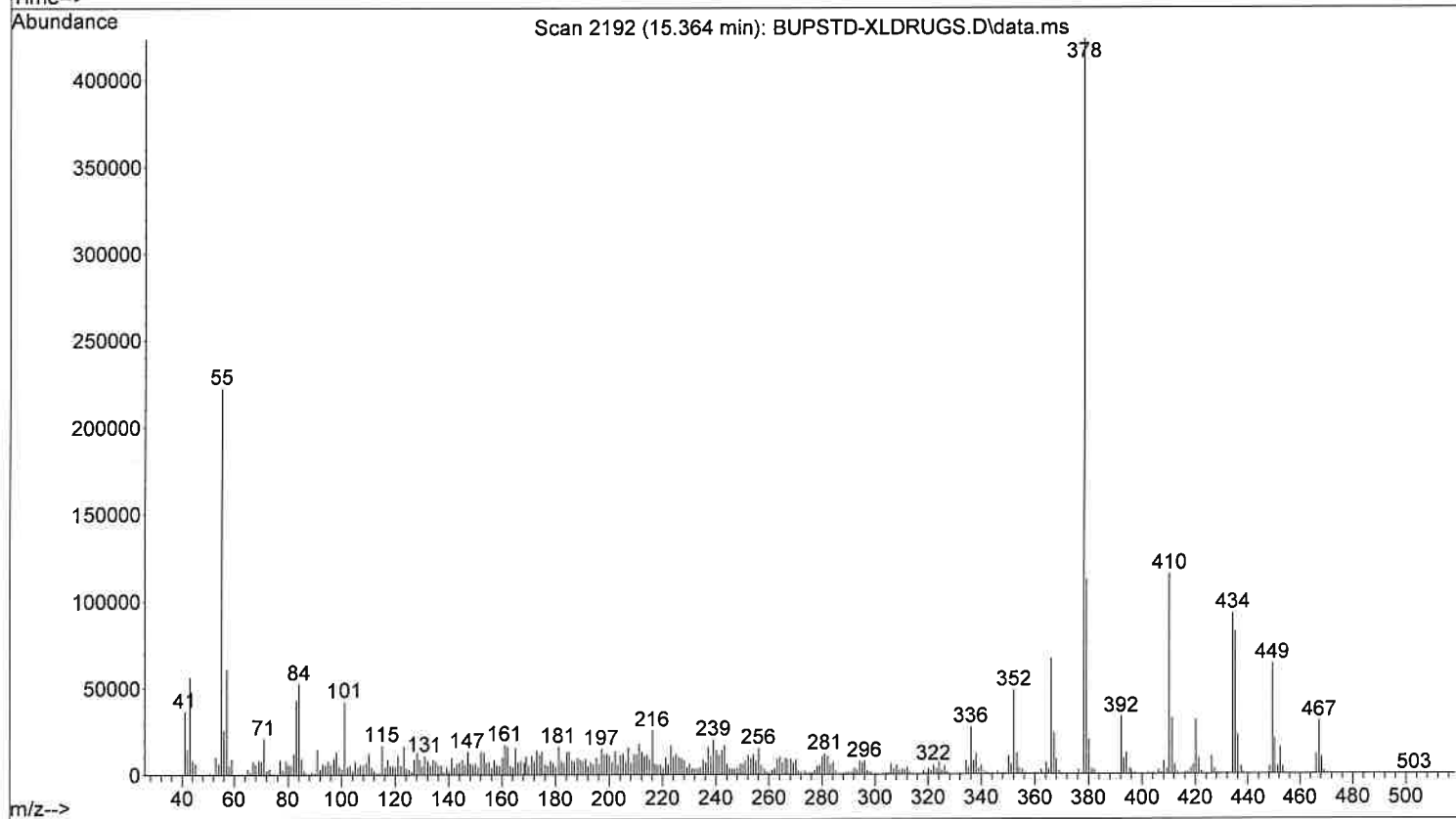
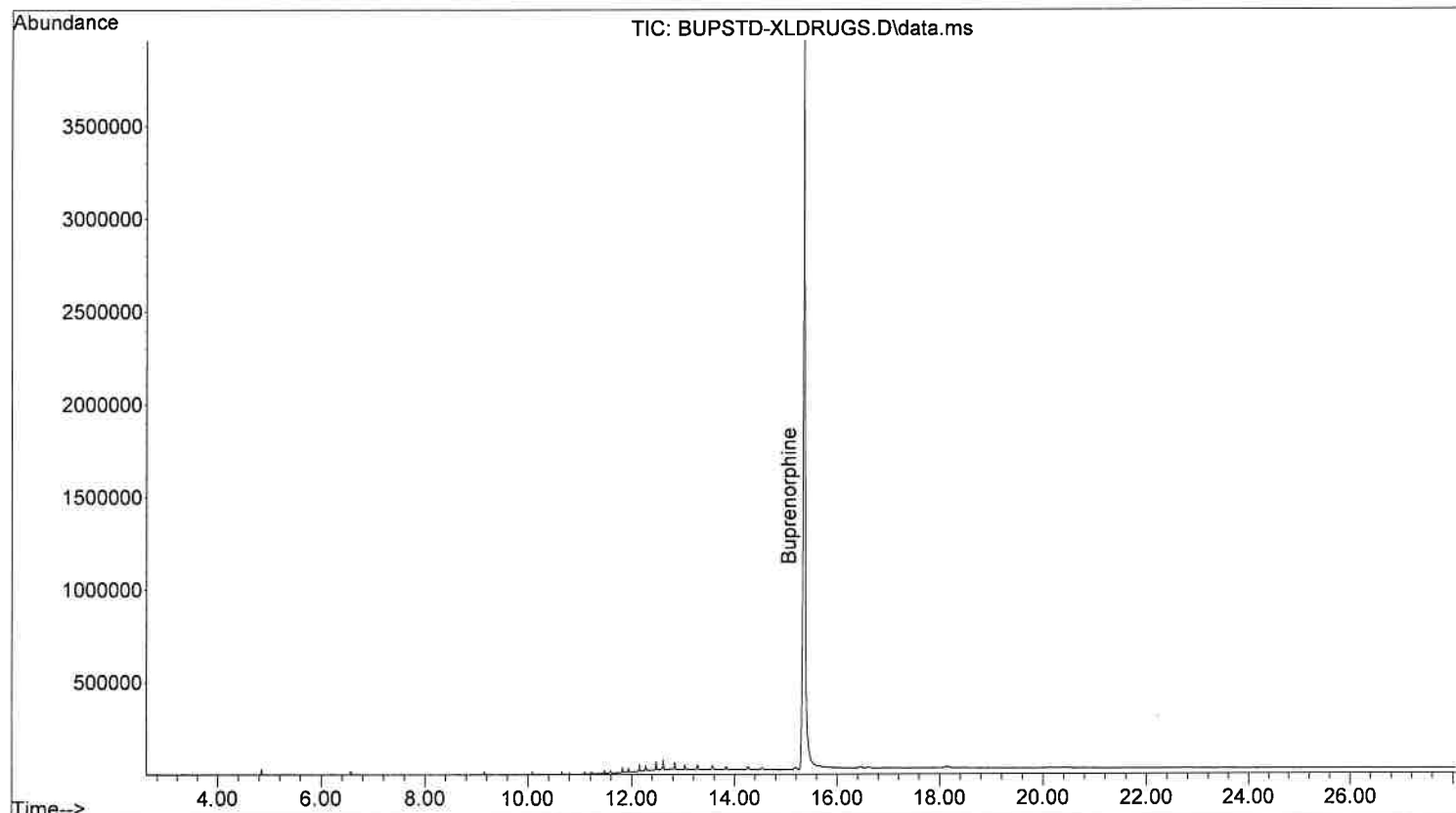
Trace Ion Detection is OFF.

34.593	:	EMISSION	
70.007	:	ENERGY	
29.919	:	REPELLER	
90.331	:	IONFOCUS	
25.226	:	ENTRANCE_LENS	
925.472	:	EMVOLTS	
		951.5	: Actual EMV
		1.00	: GAIN FACTOR
2896.000	:	AMUGAIN	
134.625	:	AMUOFFSET	
1.000	:	FILAMENT	
0.000	:	DCPOLARITY	
10.822	:	ENTLENSOFFSET	
0.000	:	Ion_Body	
0.000	:	EXTLENS	
257.000	:	MASSGAIN	
-23.000	:	MASSOFFSET	

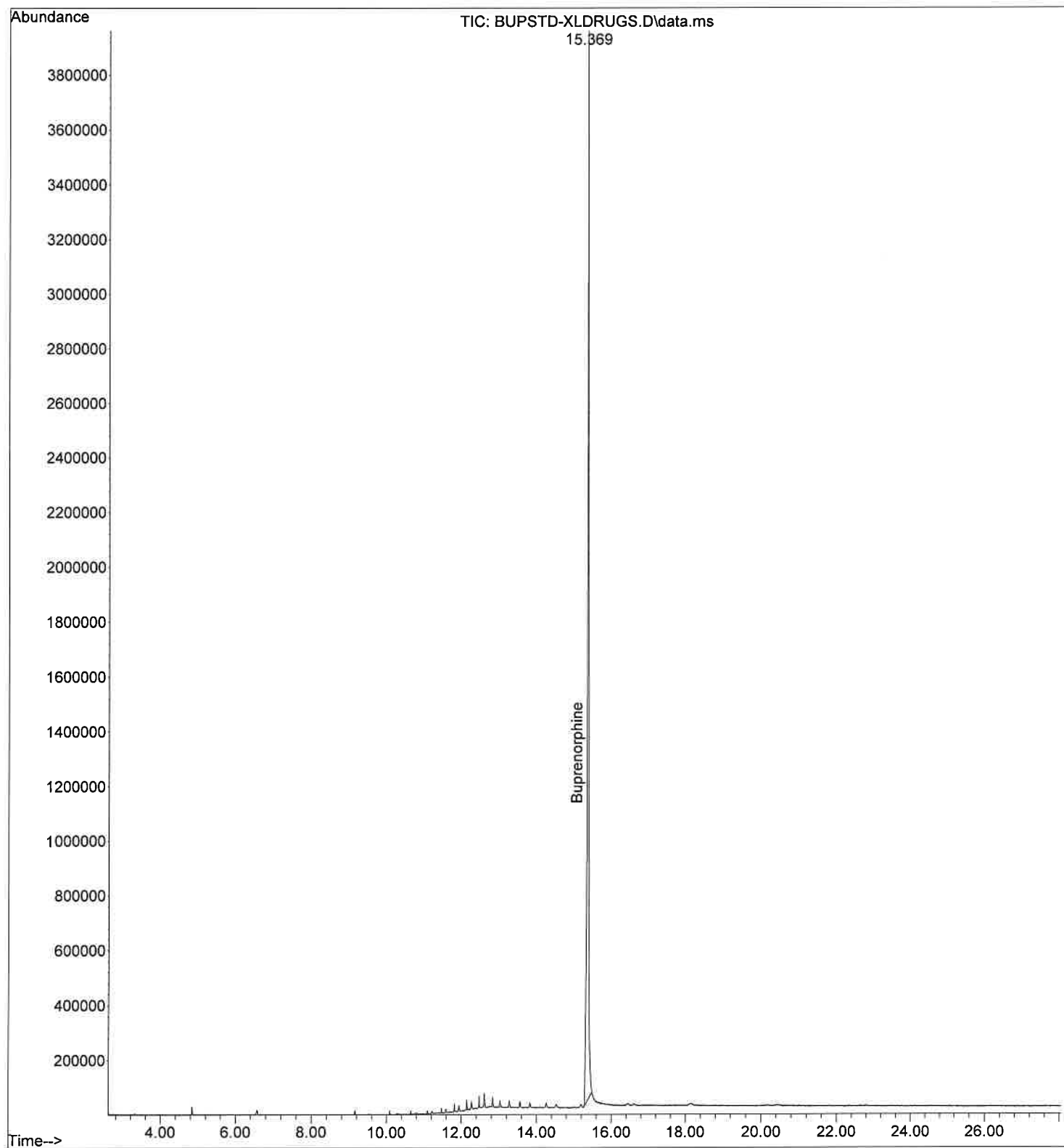
END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

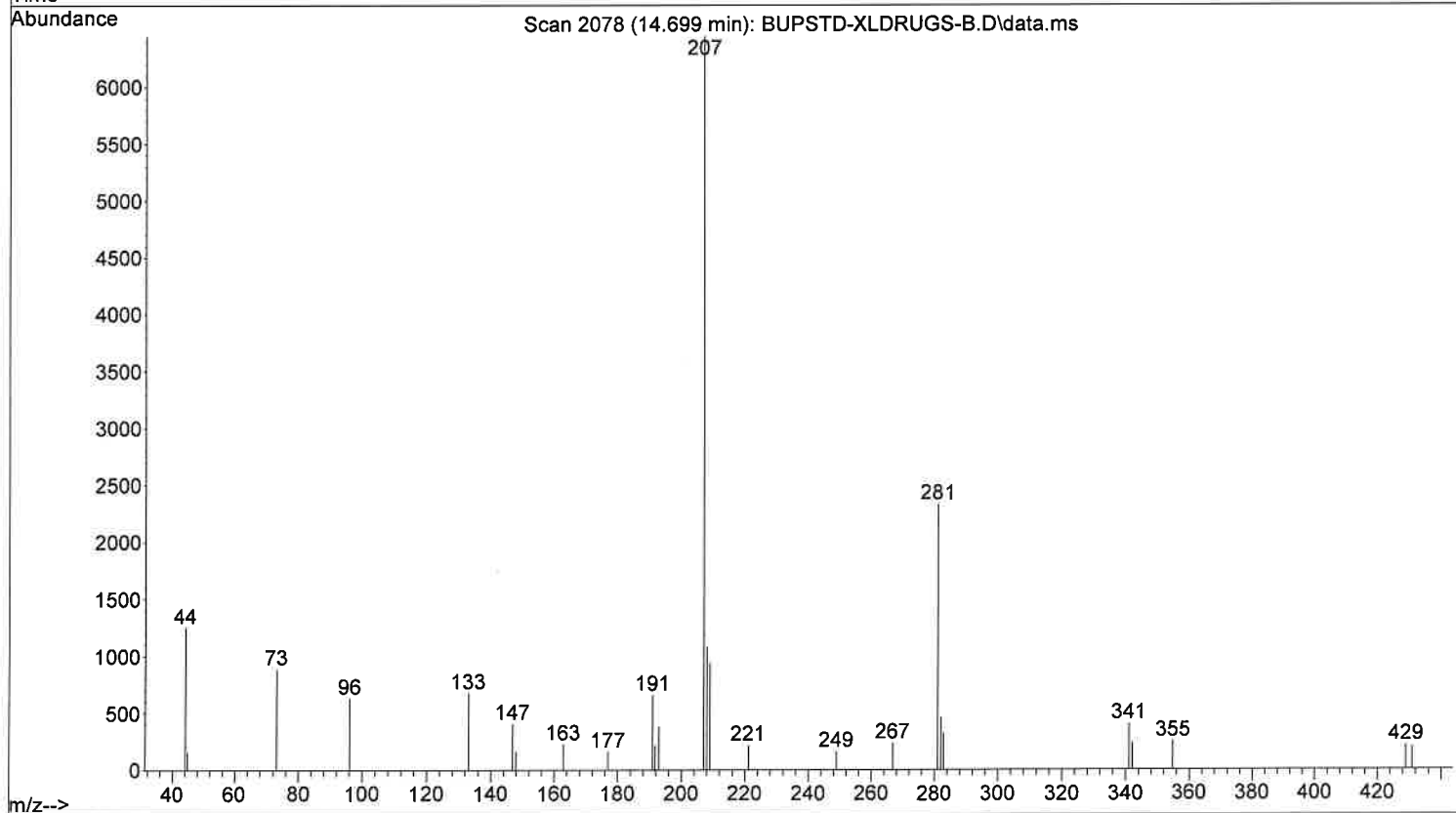
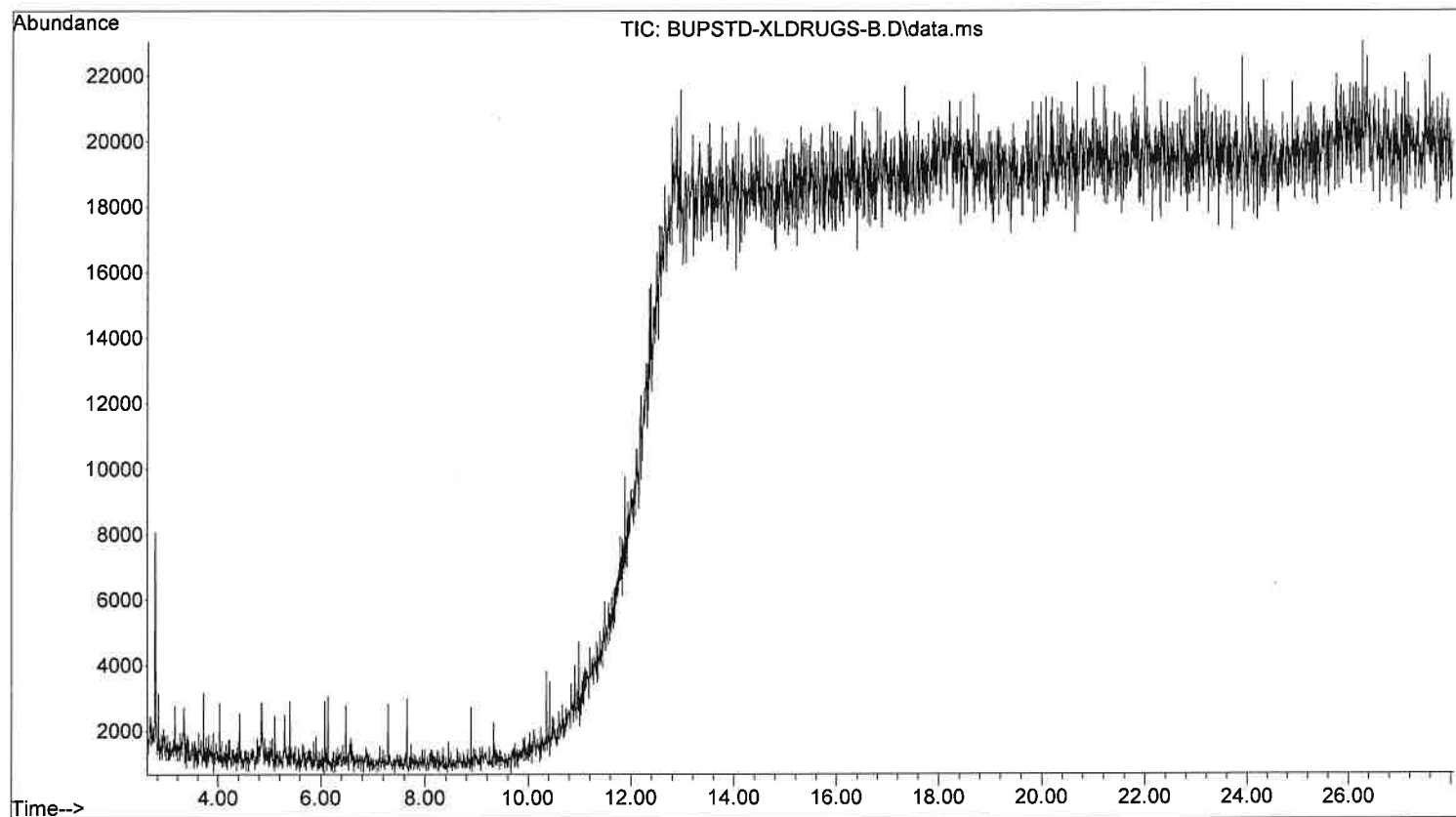
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\BUPSTD-XLDRUGS.D
Operator : KLAB
Acquired : 21 Aug 2023 17:36 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Buprenorphine Standard
Misc Info : MEOH
Vial Number: 55



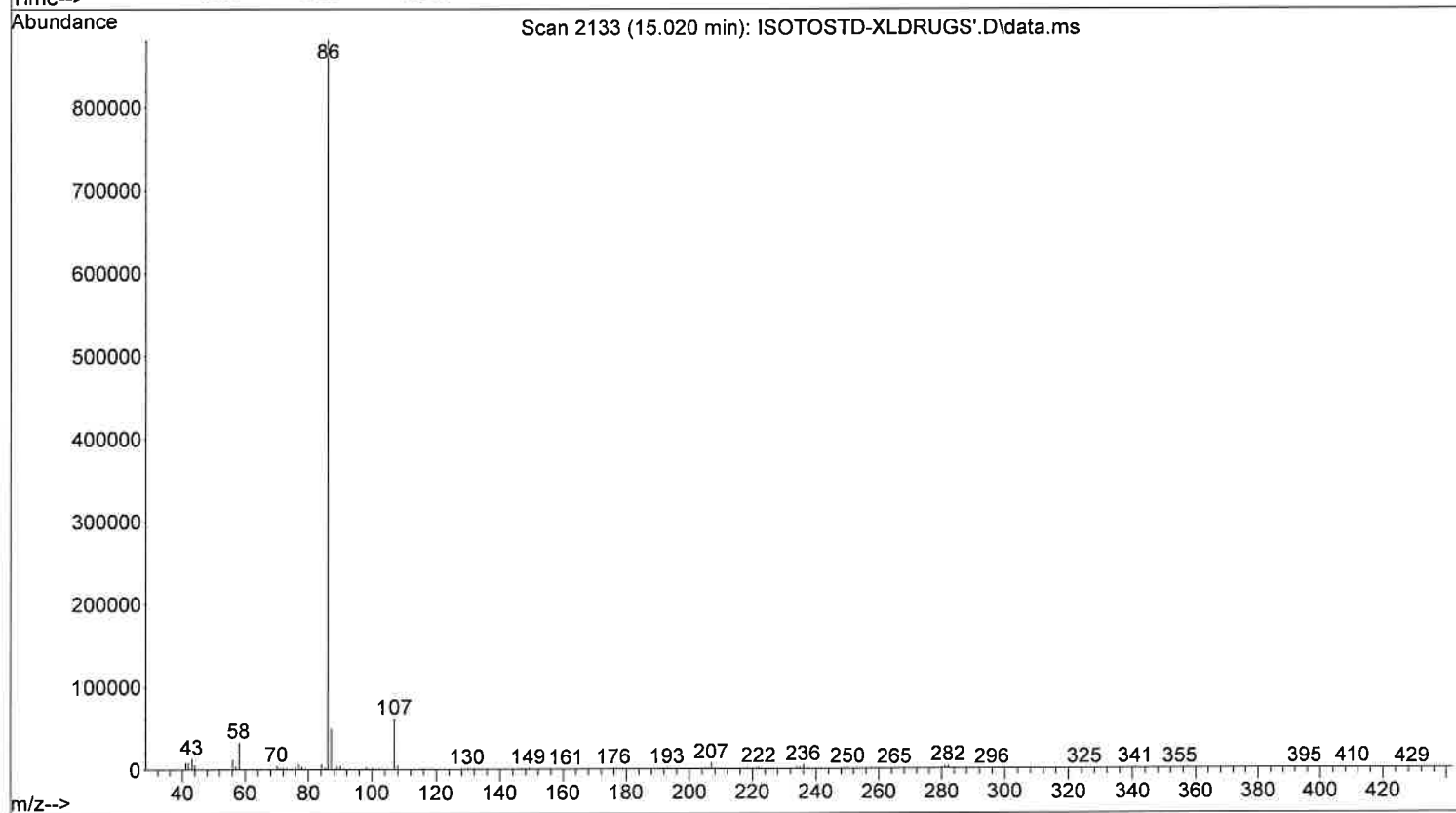
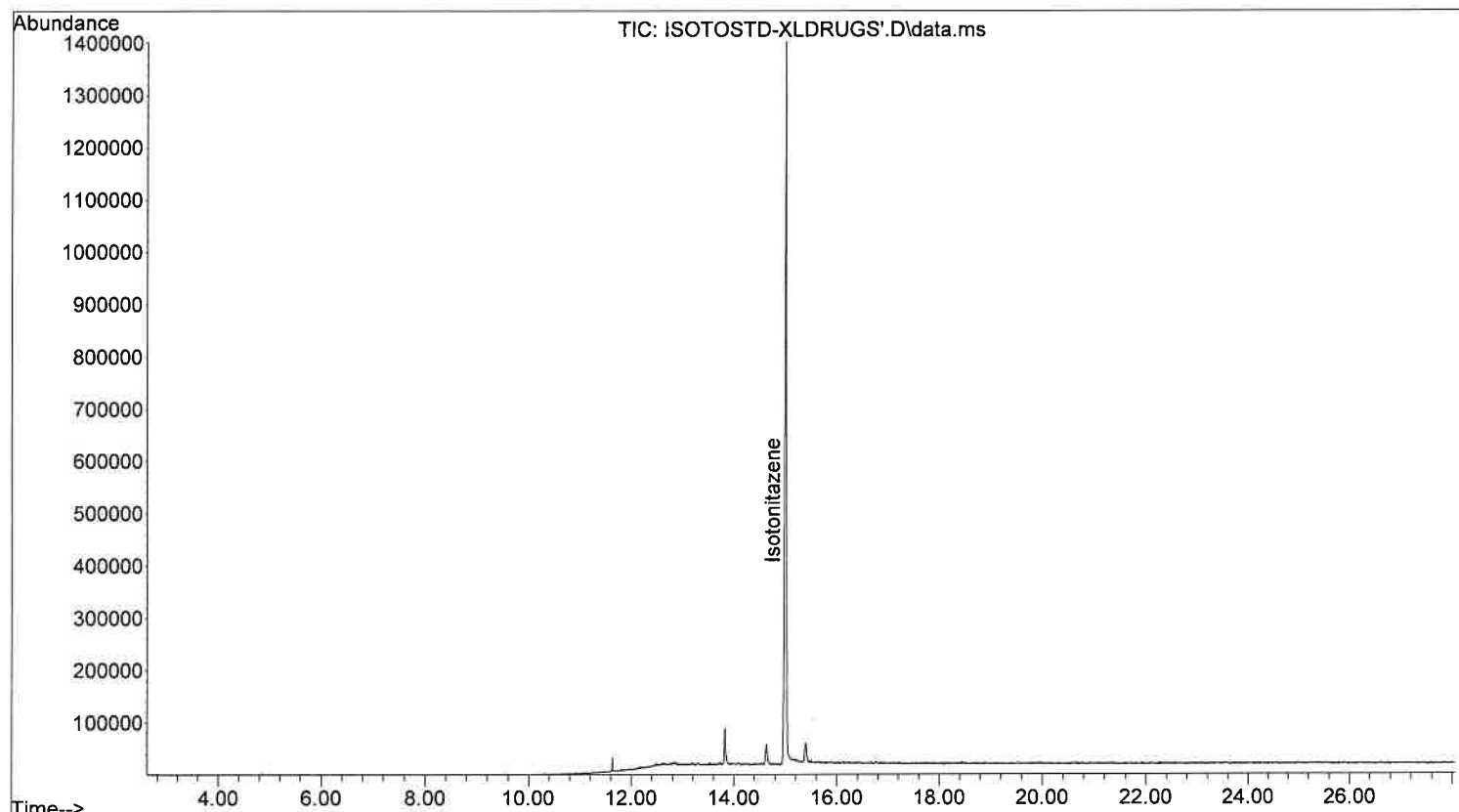
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\BUPSTD-XLDRUGS.D
Operator : KLAB
Acquired : 21 Aug 2023 17:36 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Buprenorphine Standard
Misc Info : MEOH
Vial Number: 55



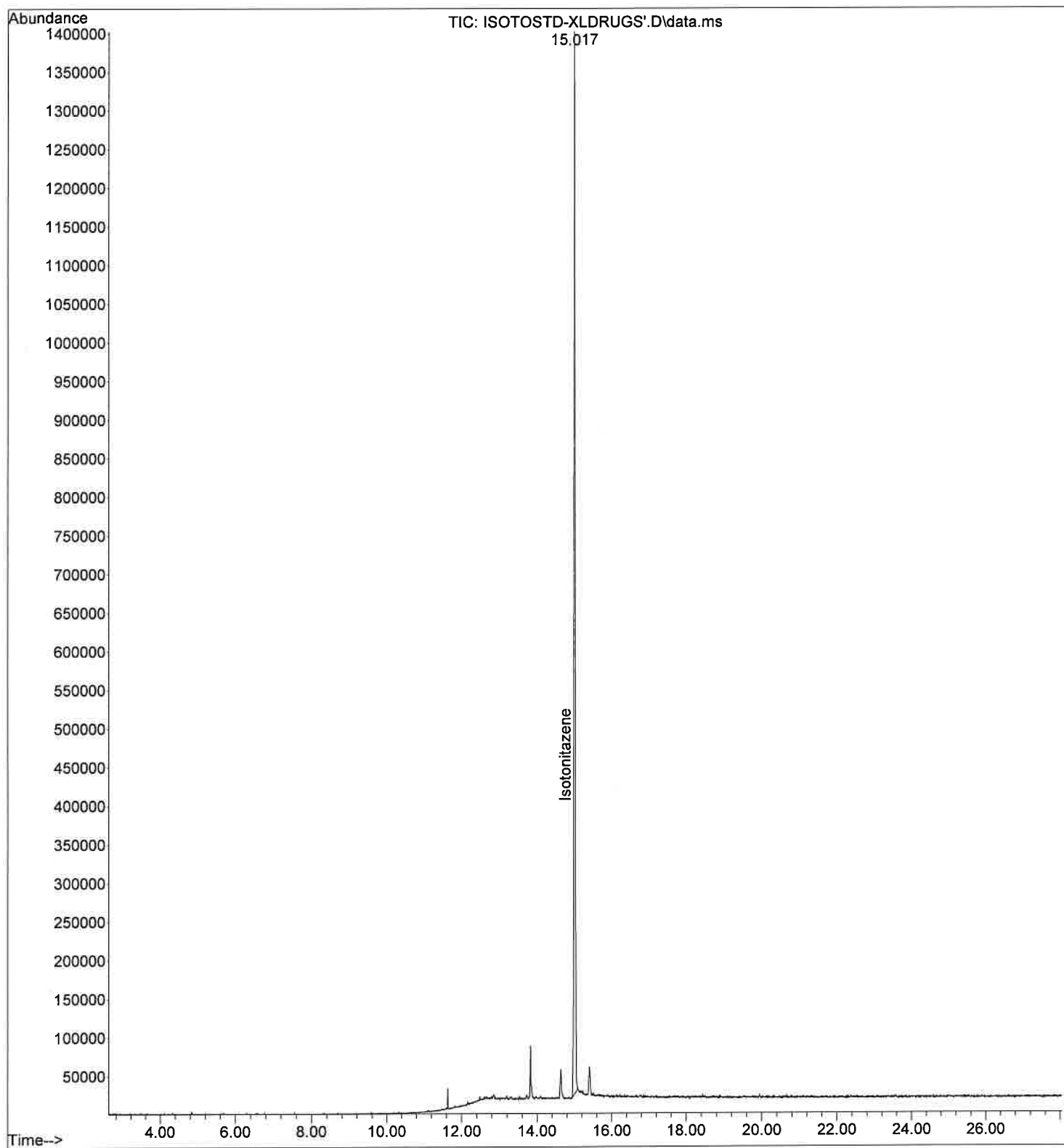
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\BUPSTD-XLDRUGS-B
... .D
Operator : KLAB
Acquired : 21 Aug 2023 17:05 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Methanol blank
Misc Info : For Buprenorphine
Vial Number: 53



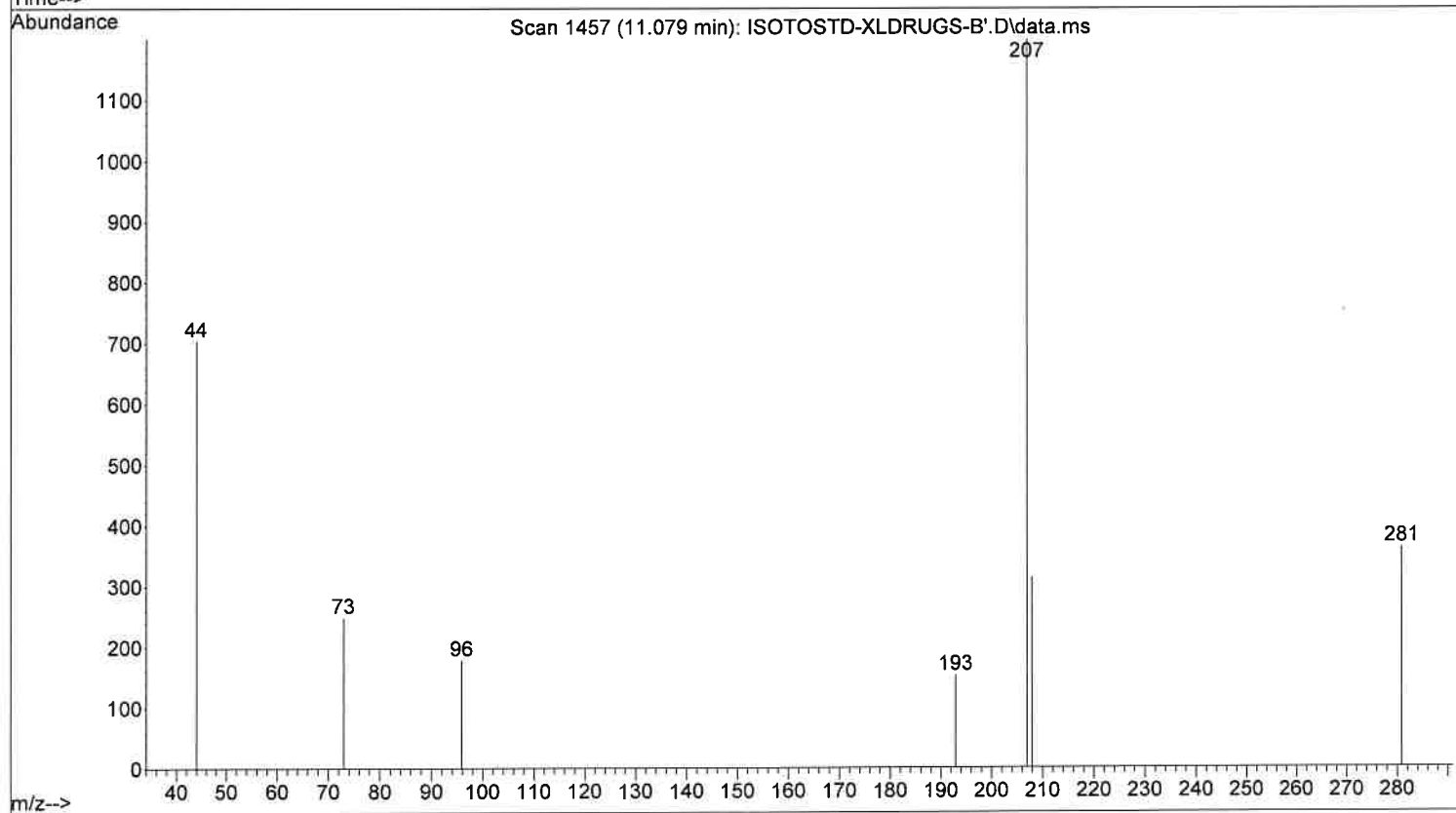
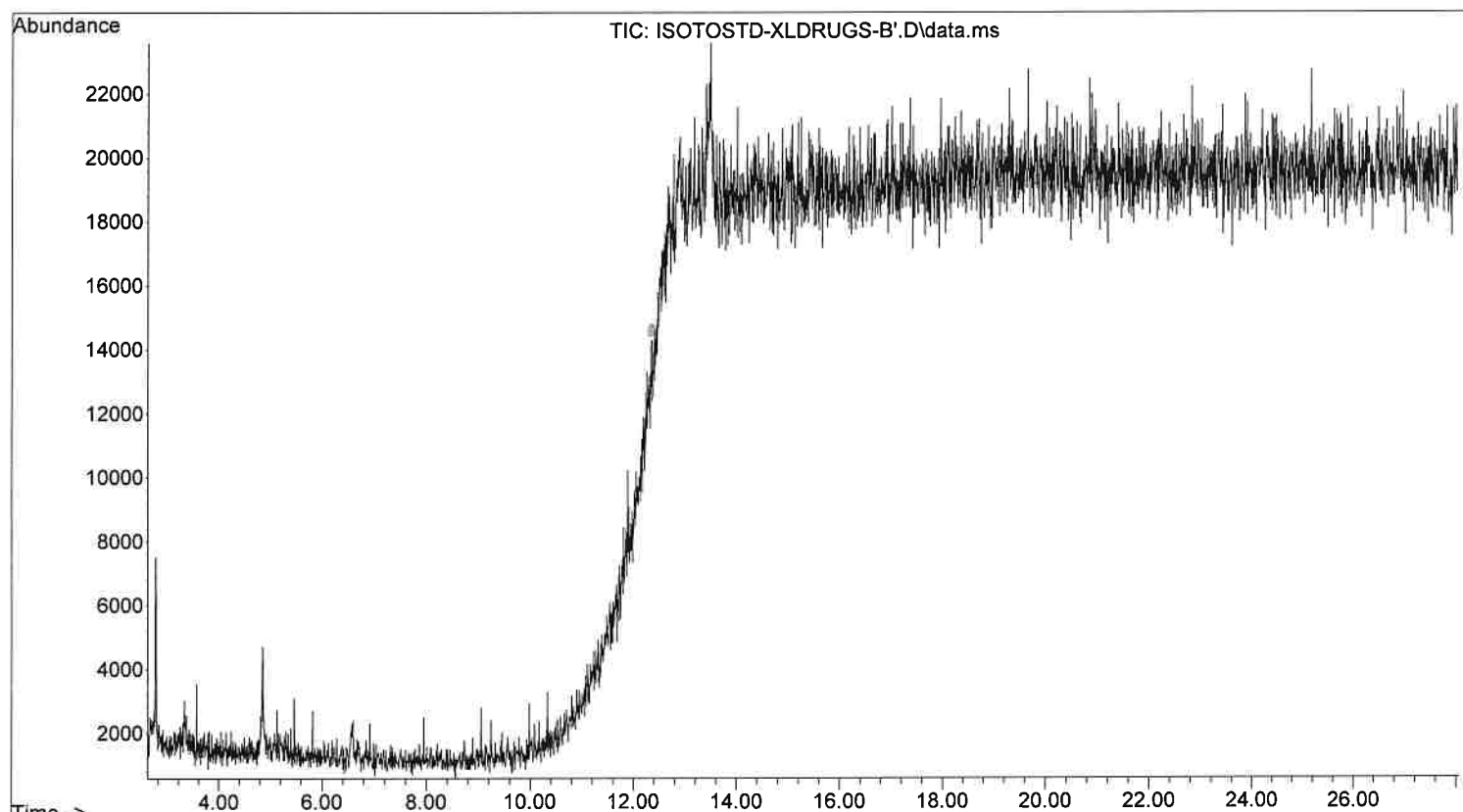
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\ISOTOSTD-XLDRUGS
... '.D
Operator : KLAB
Acquired : 22 Aug 2023 11:25 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Isotonitazene Standard
Misc Info : MEOH
Vial Number: 56



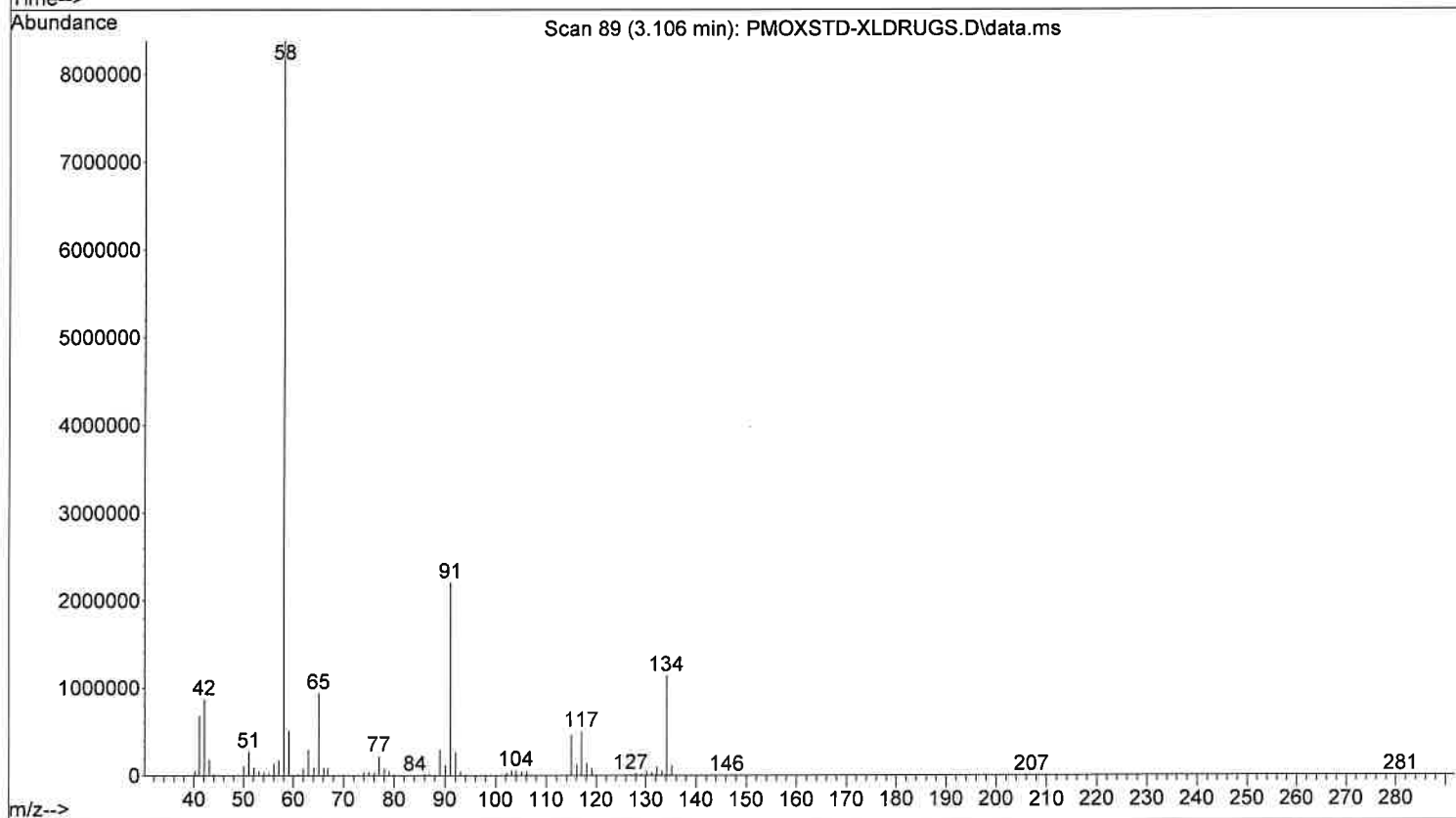
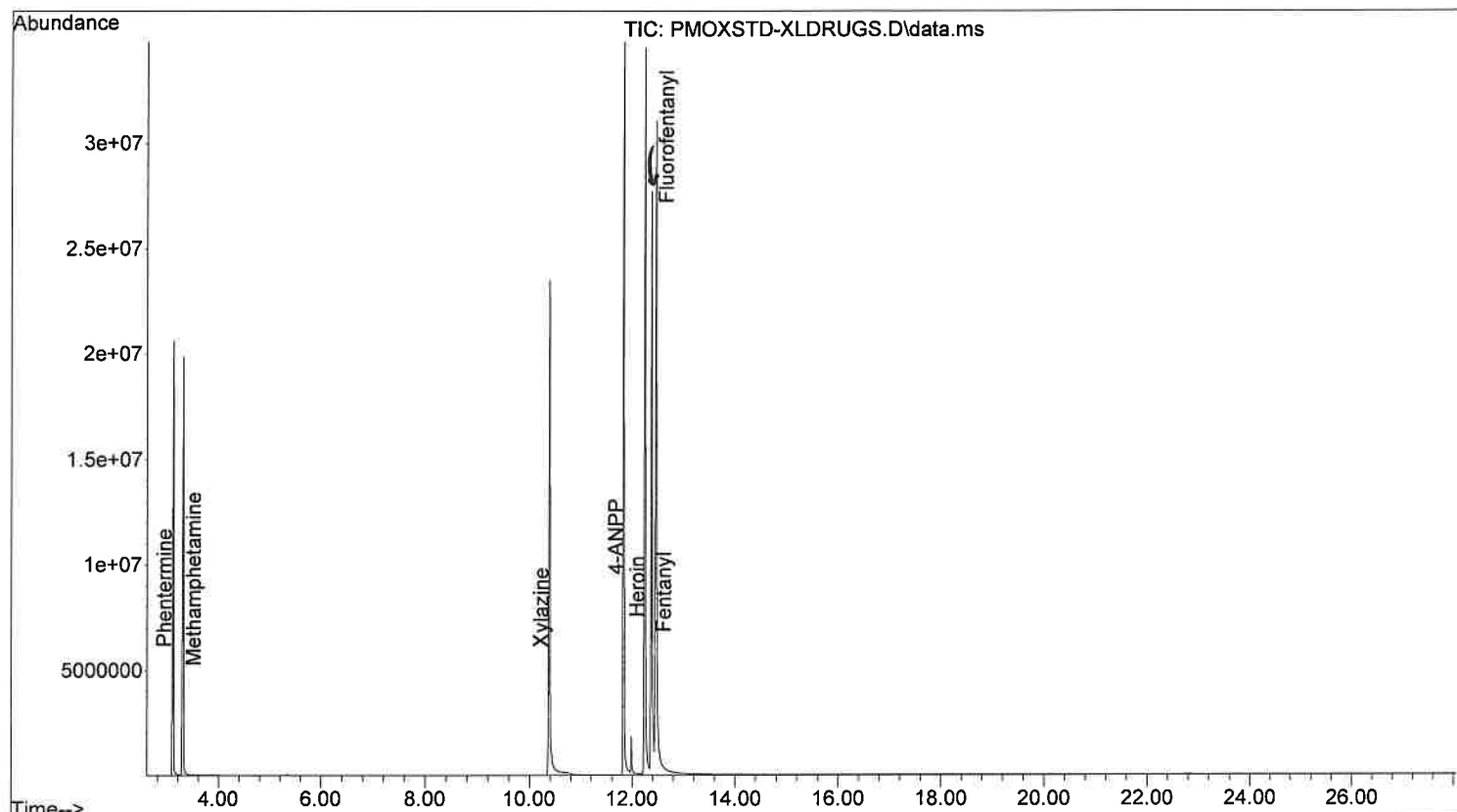
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... '.D
Operator : KLAB
Instrument : Buttercup
Acquired : 22 Aug 2023 11:25 using AcqMethod XLDRUGS.M
Sample Name: Isotonitazene Standard
Misc Info : MEOH



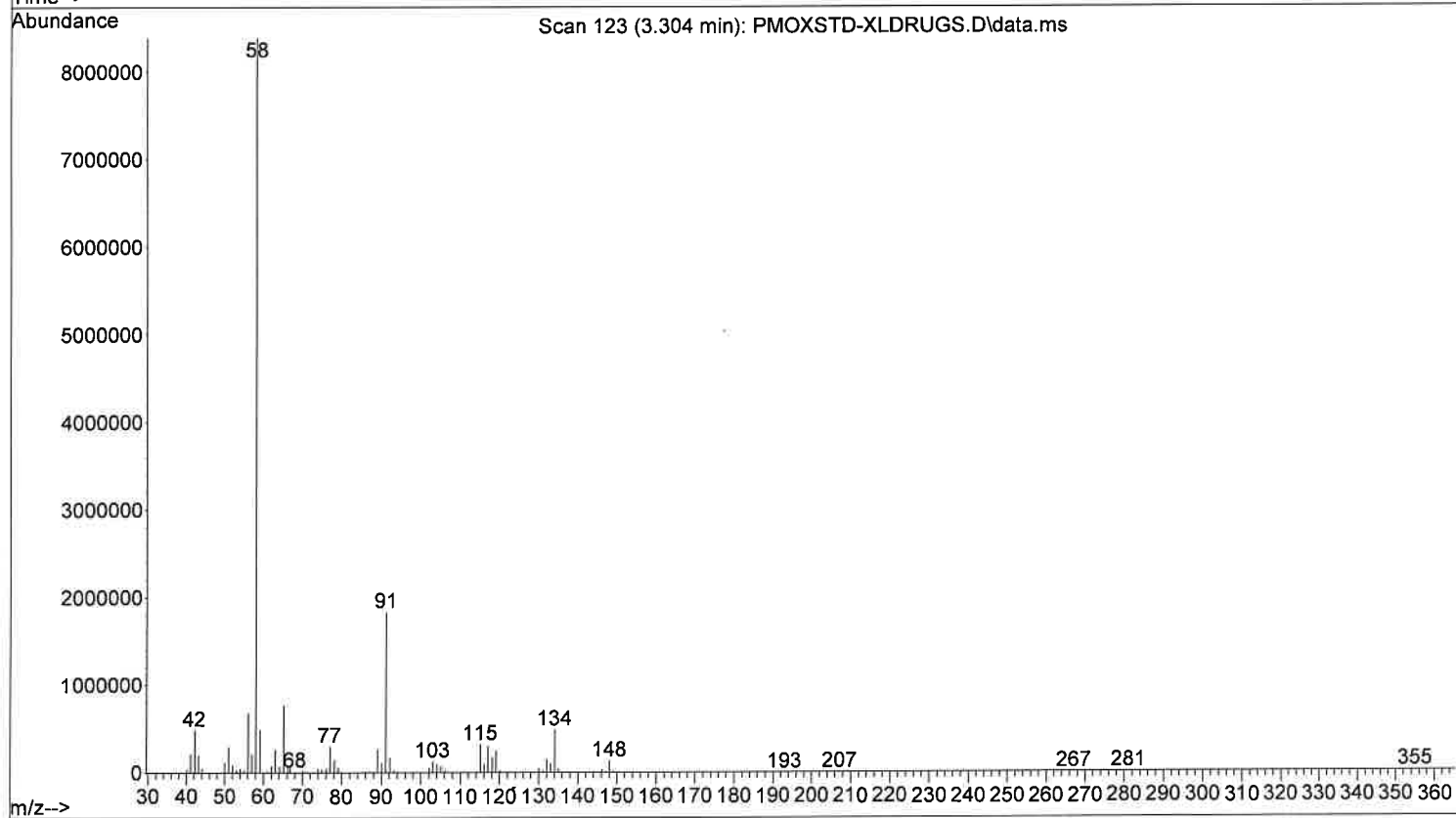
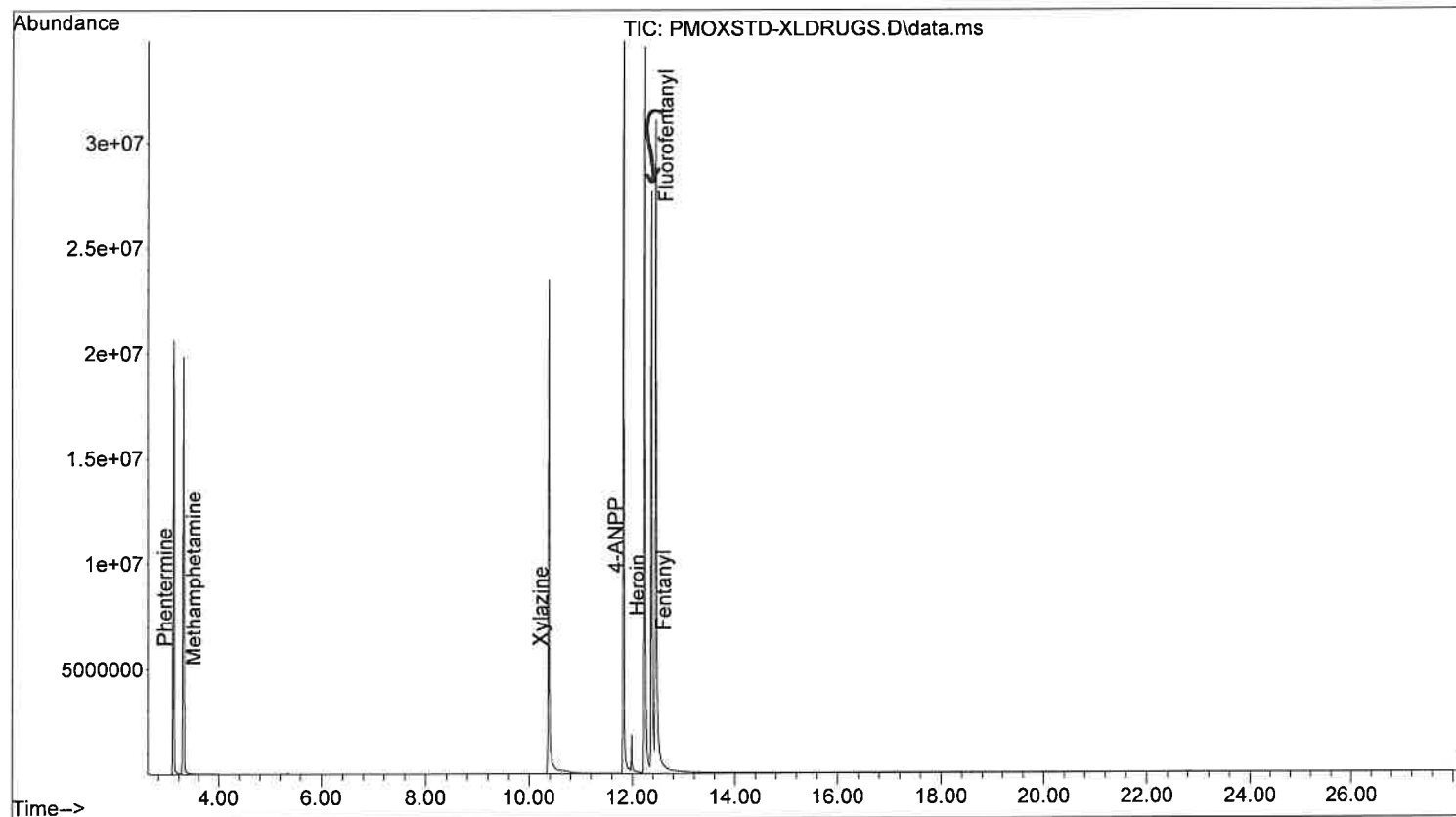
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\ISOTOSTD-XLDRUGS
... -B'.D
Operator : KLAB
Acquired : 22 Aug 2023 10:54 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Methanol blank
Misc Info : For Isotonitazene
Vial Number: 53



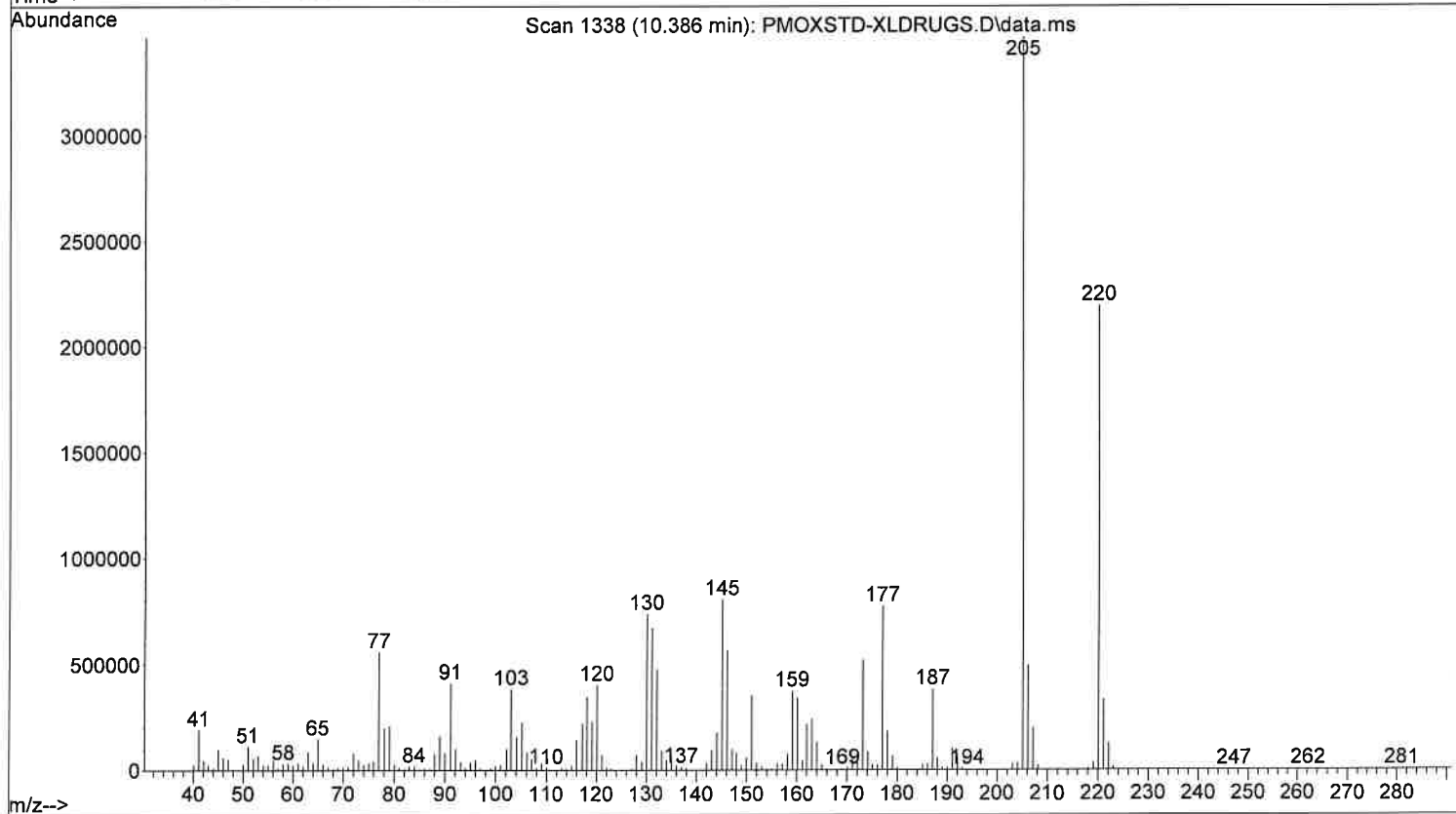
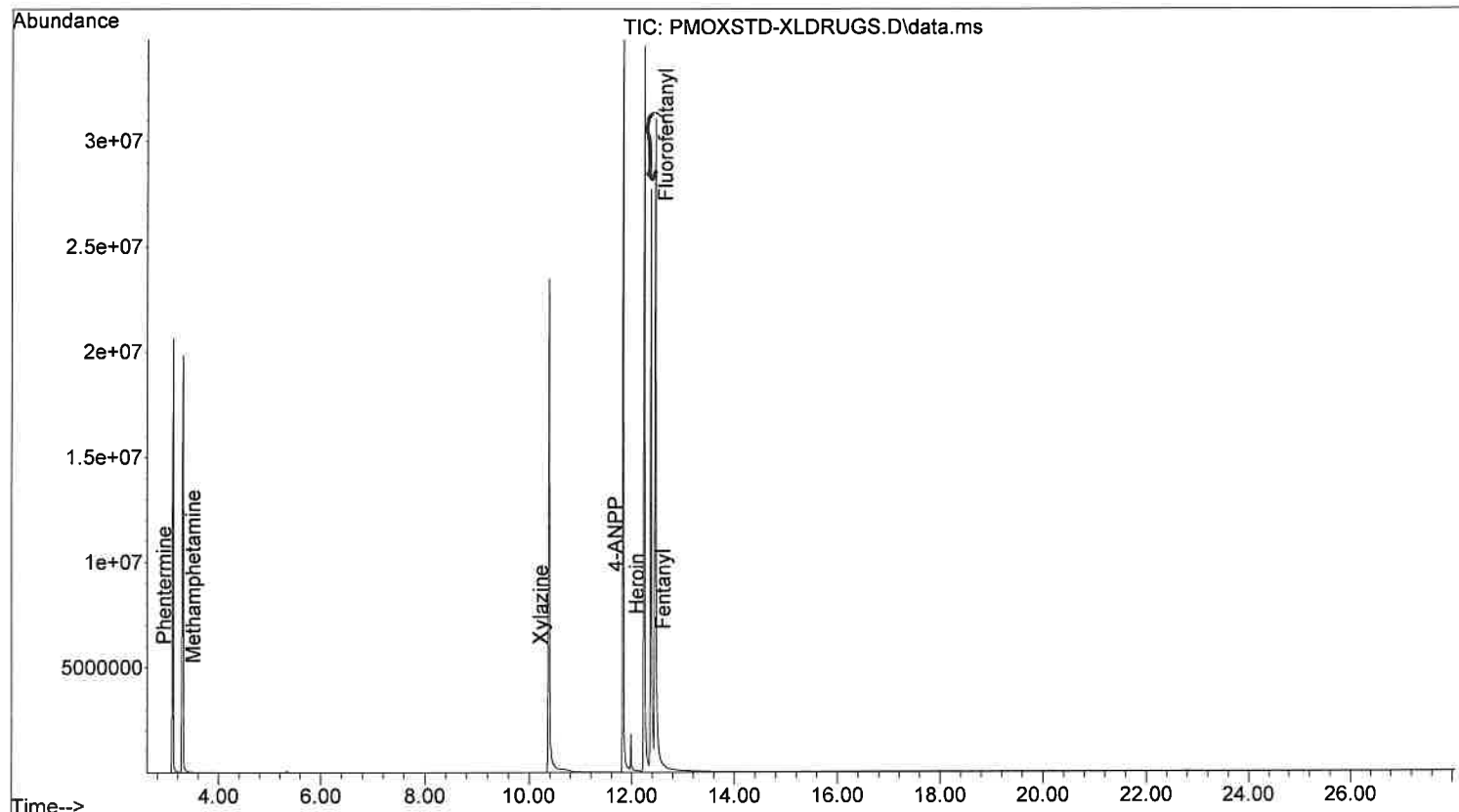
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-XLDRUGS.D
Operator : KLAB
Acquired : 21 Aug 2023 16:16 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



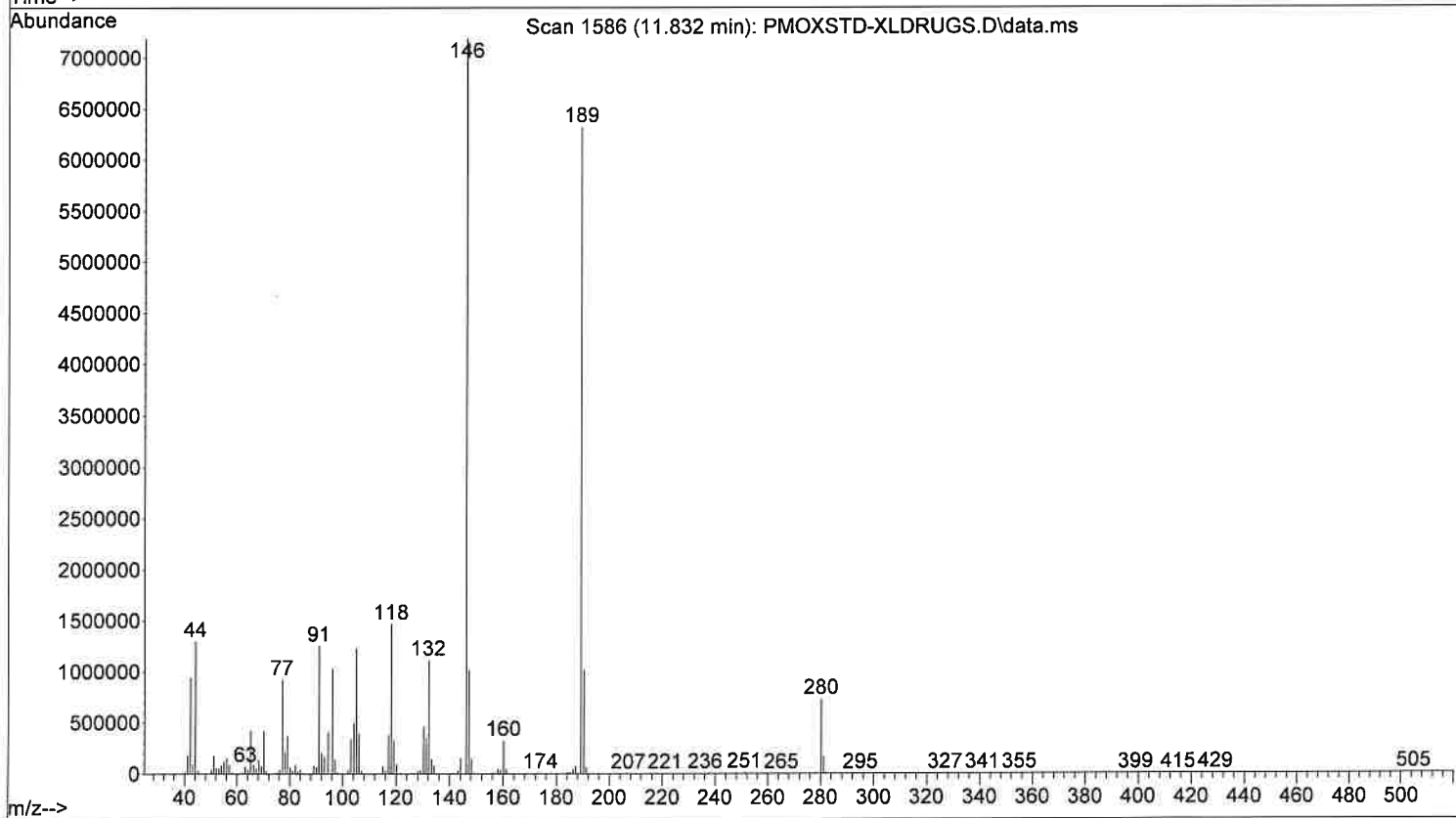
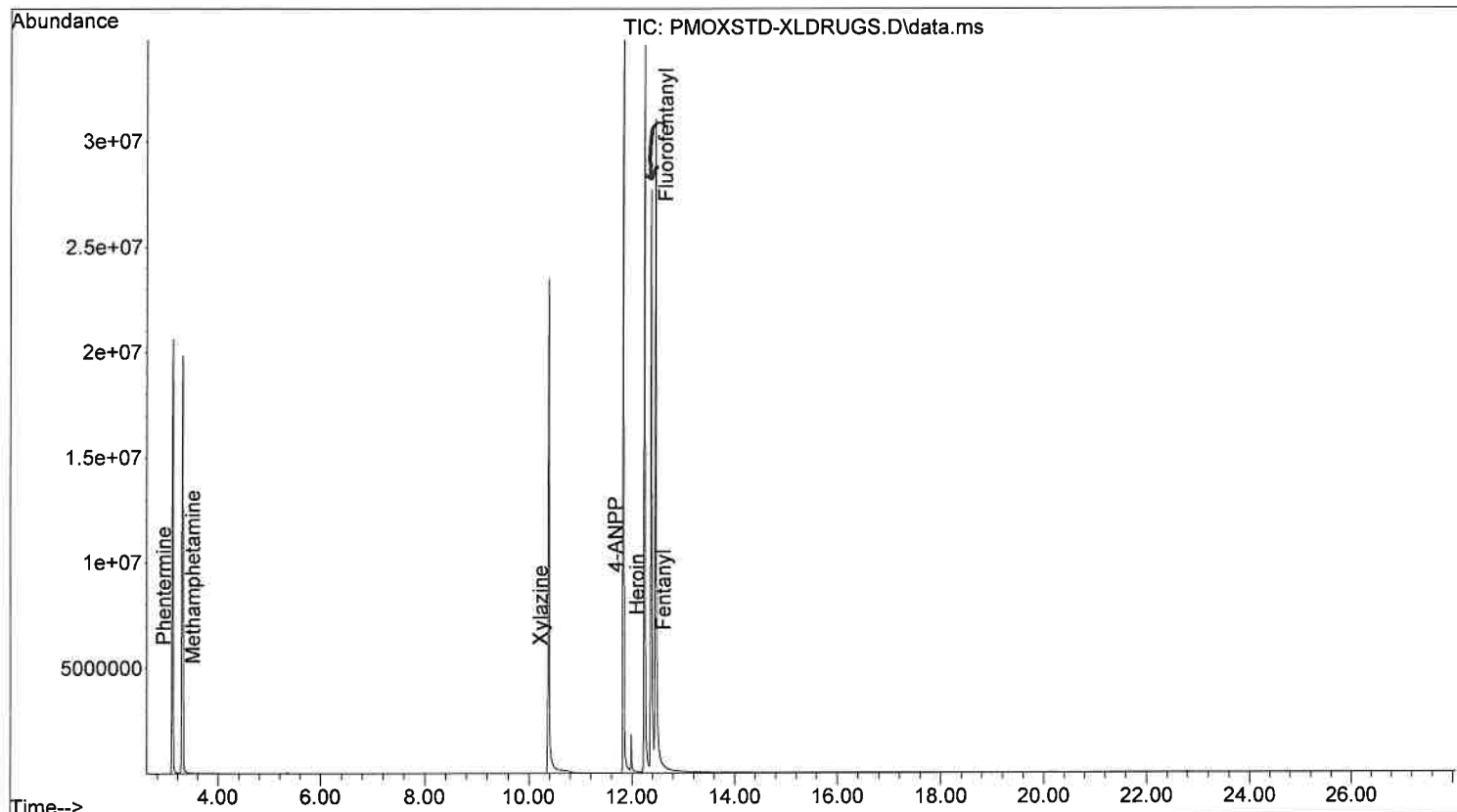
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Operator : KLAB
Acquired : 21 Aug 2023 16:16 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



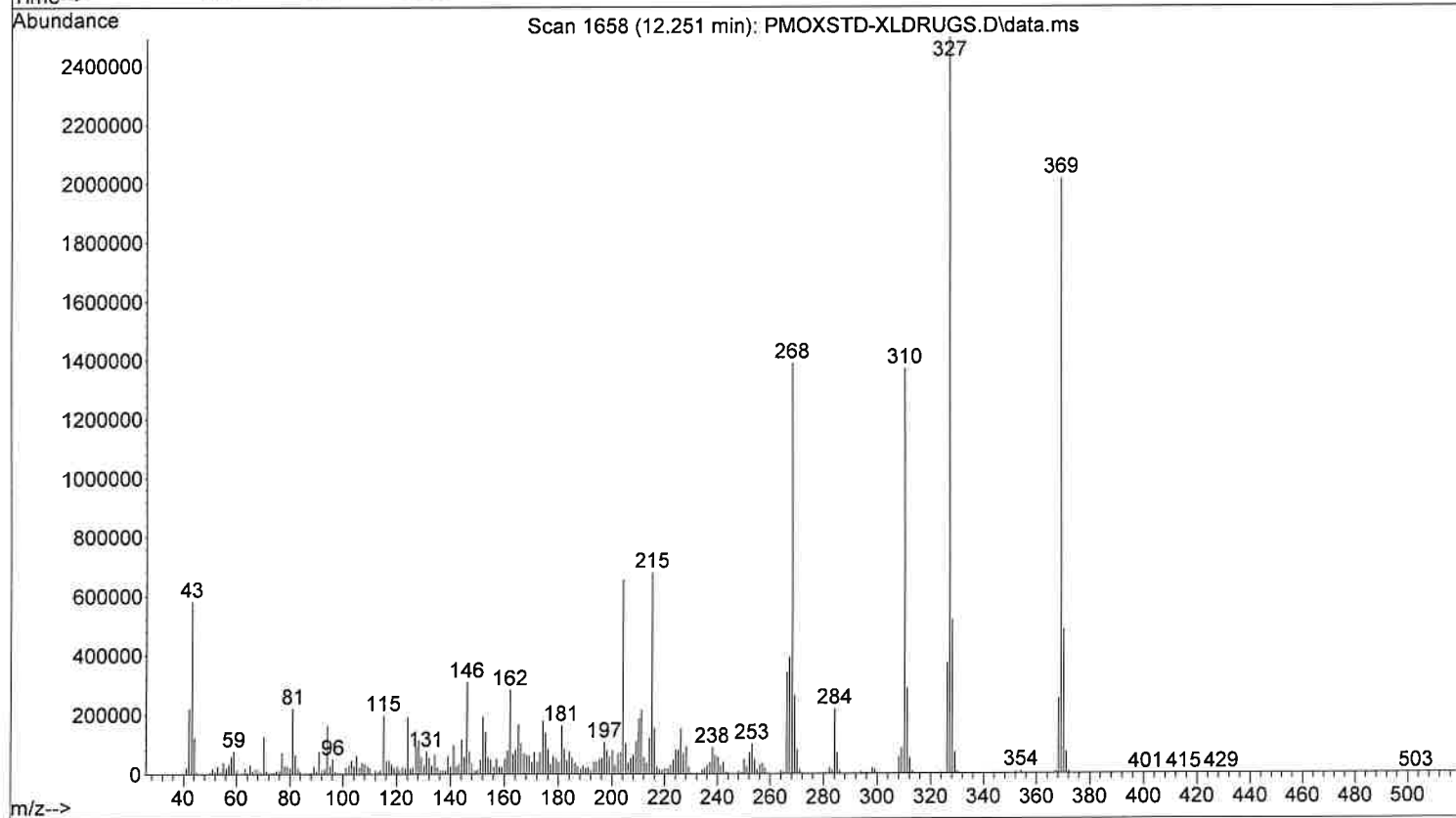
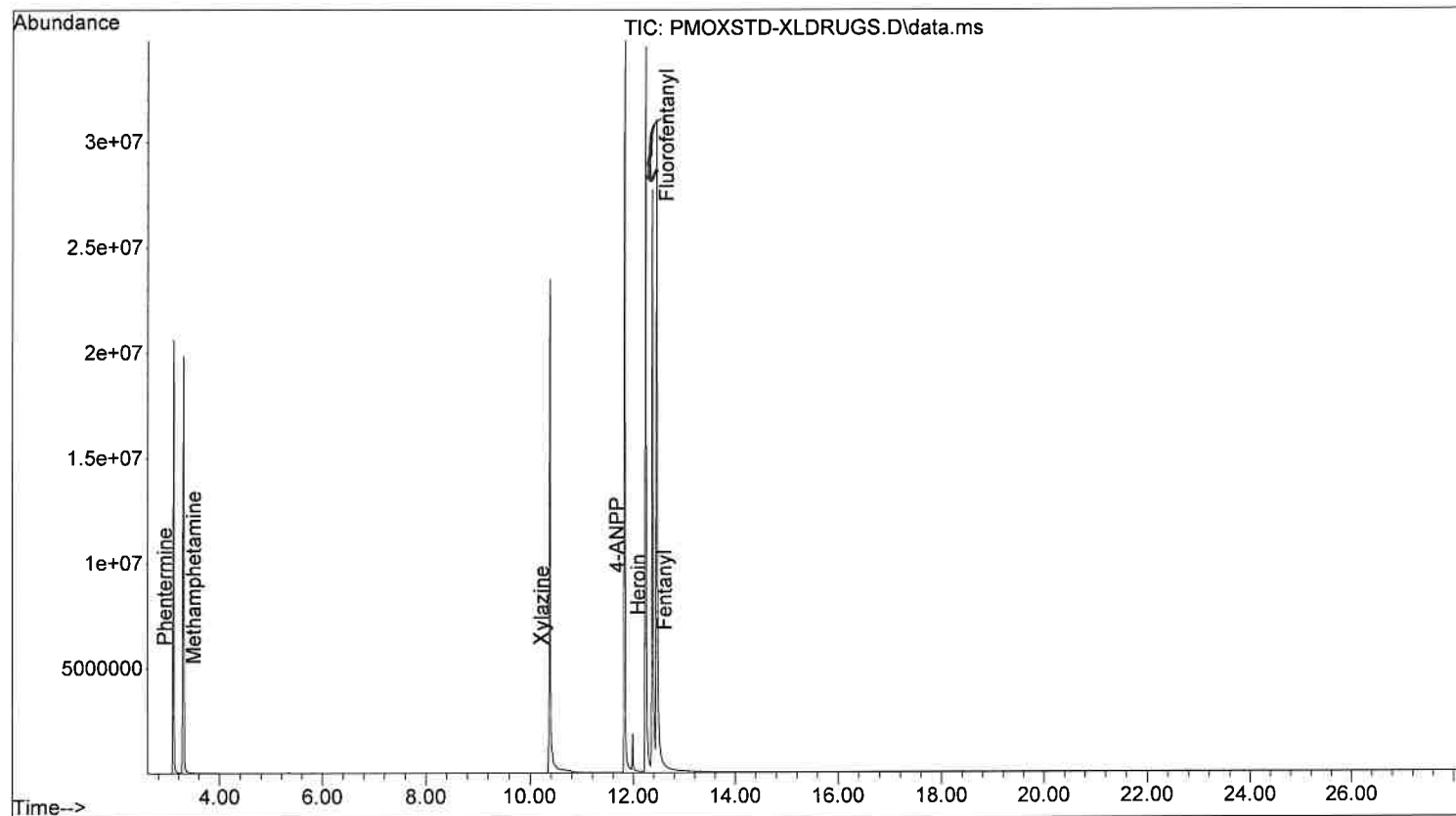
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Operator : KLAB
Acquired : 21 Aug 2023 16:16 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



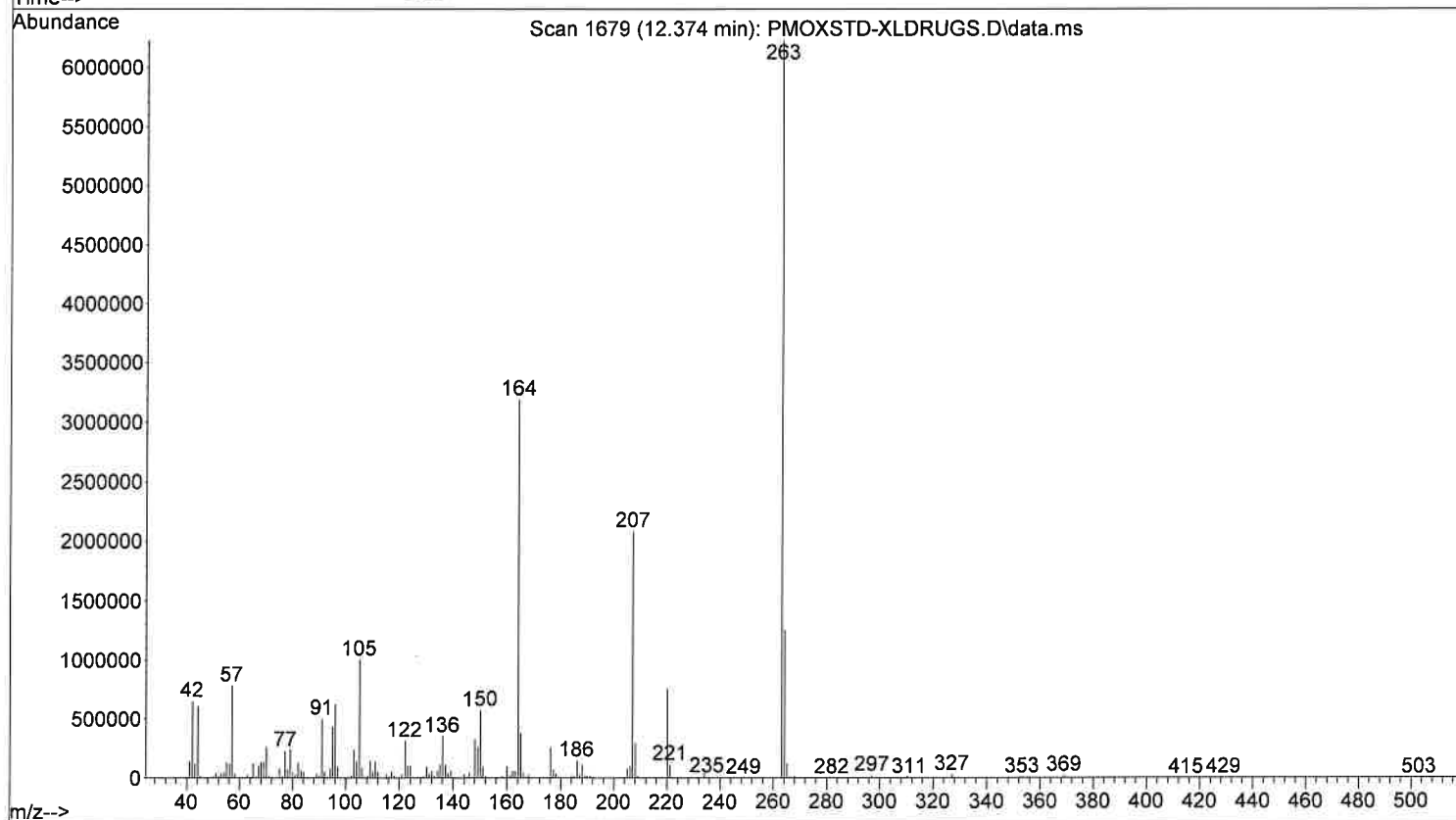
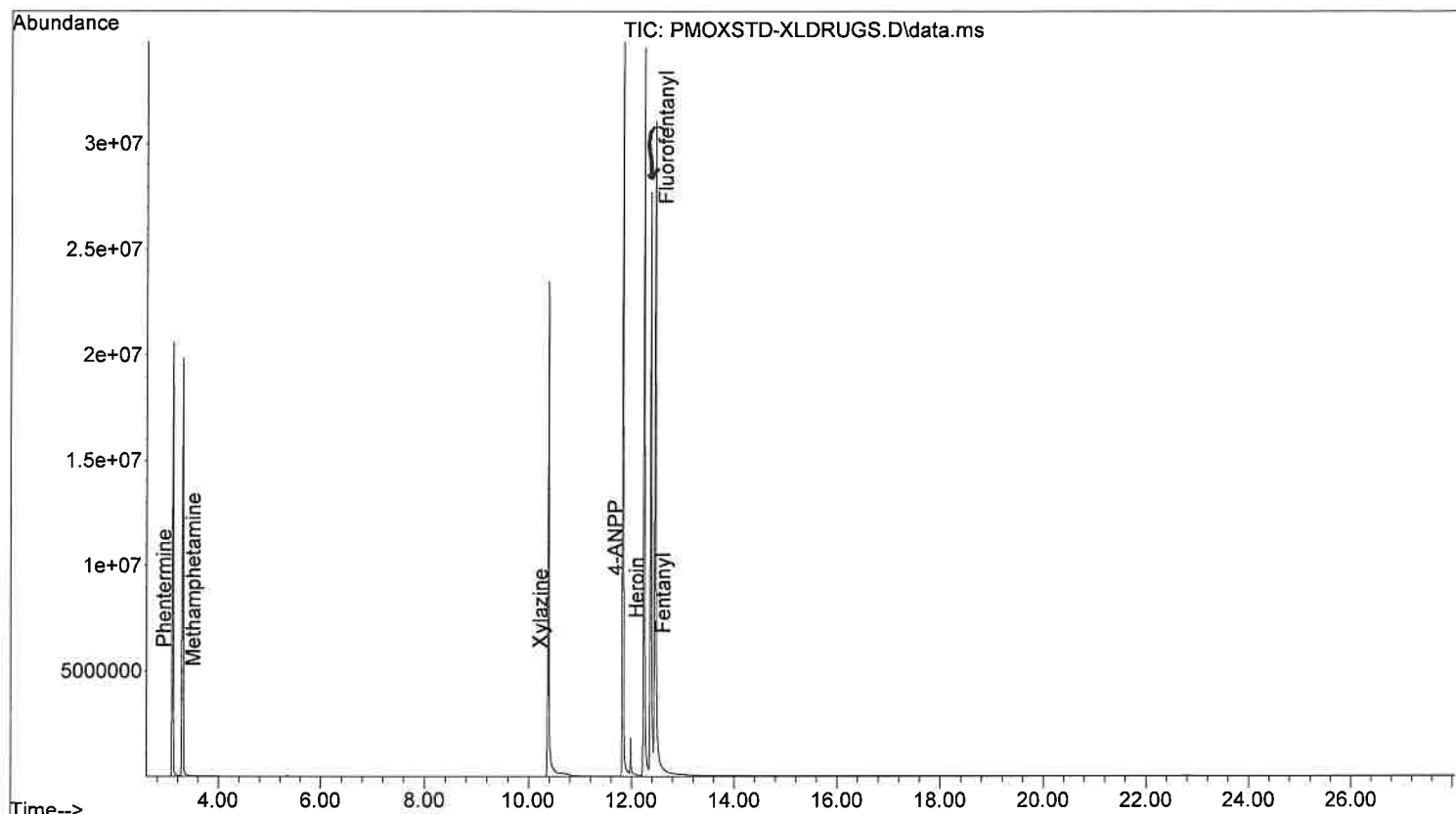
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Operator : KLAB
Acquired : 21 Aug 2023 16:16 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



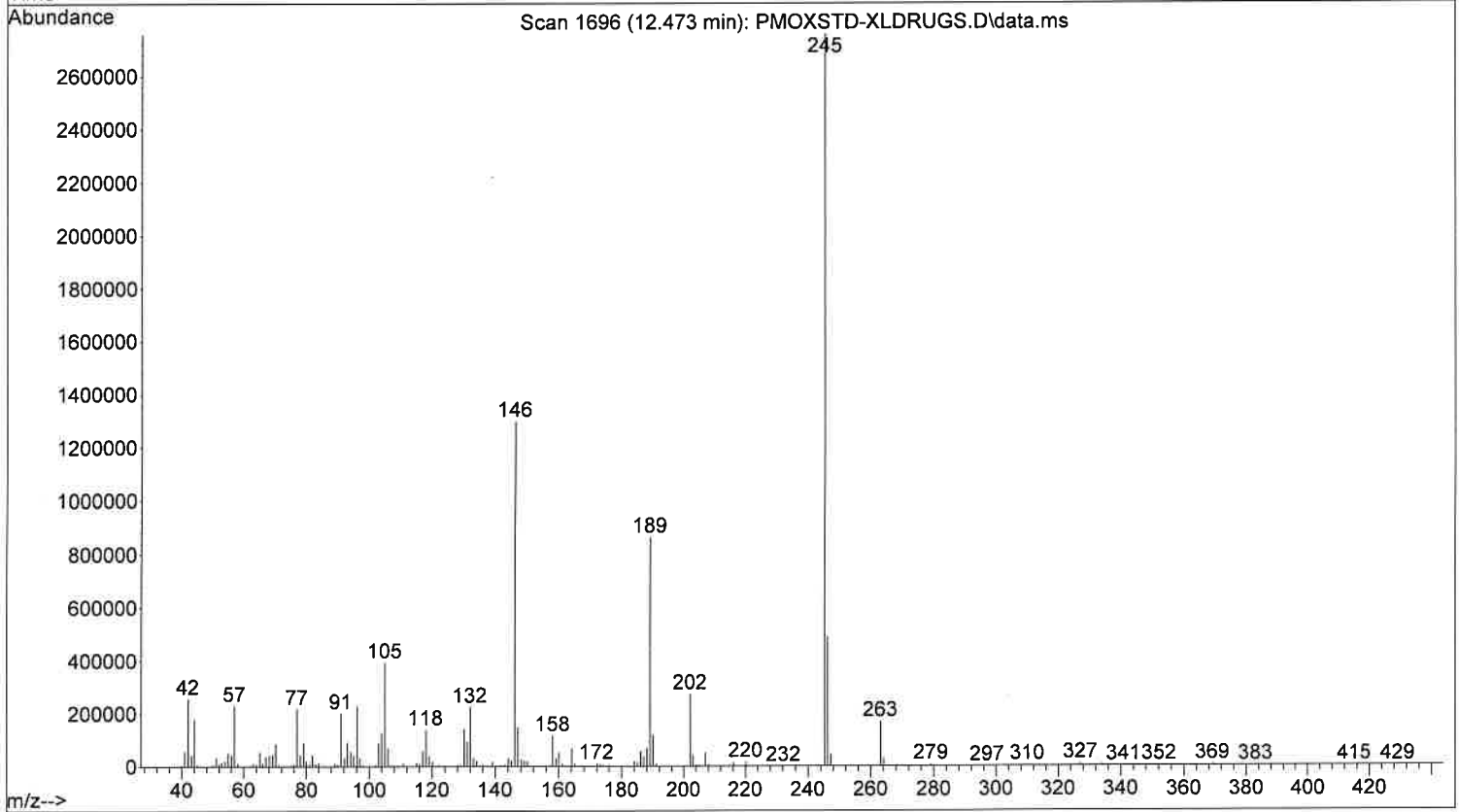
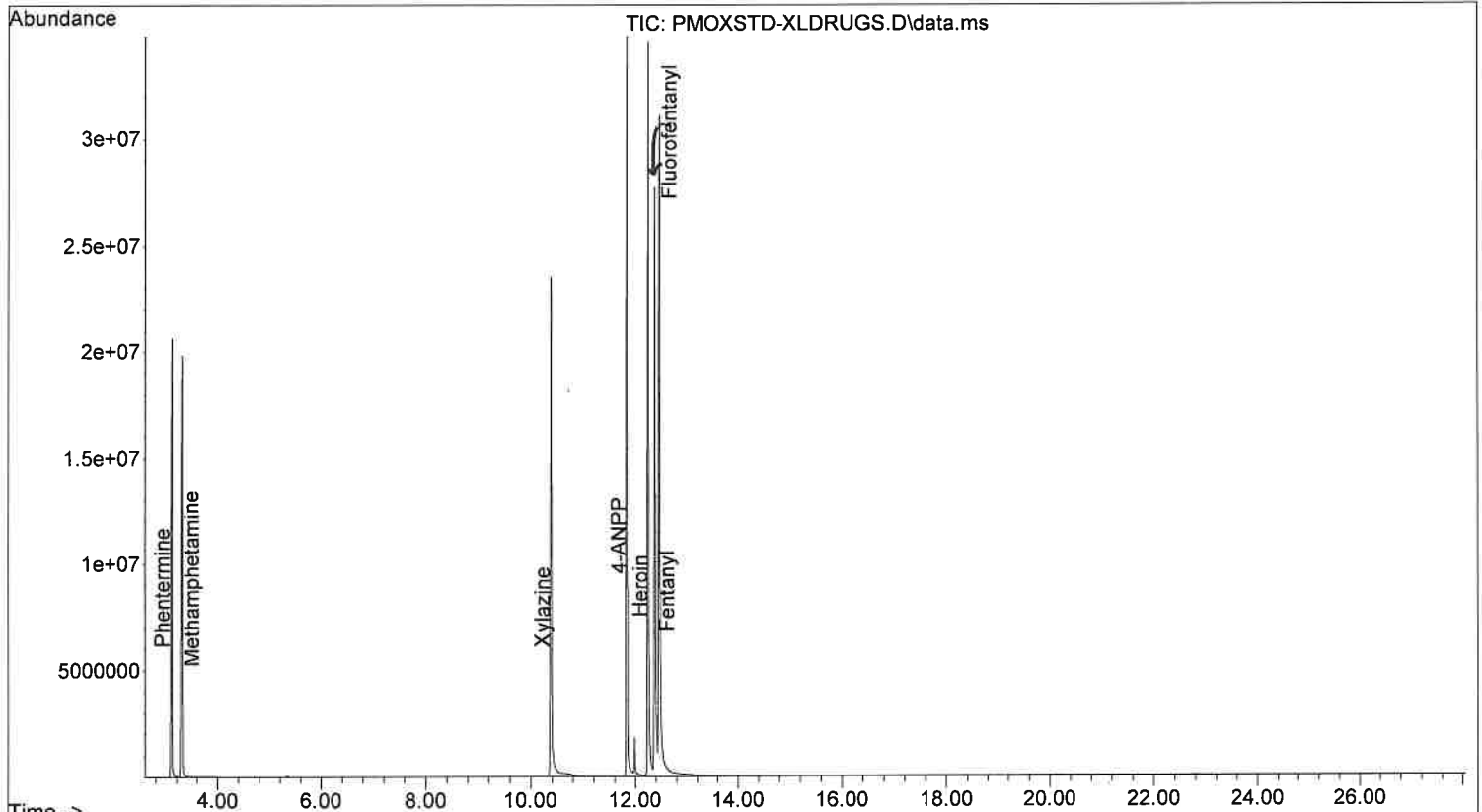
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-XLDRUGS.D
Operator : KLAB
Acquired : 21 Aug 2023 16:16 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



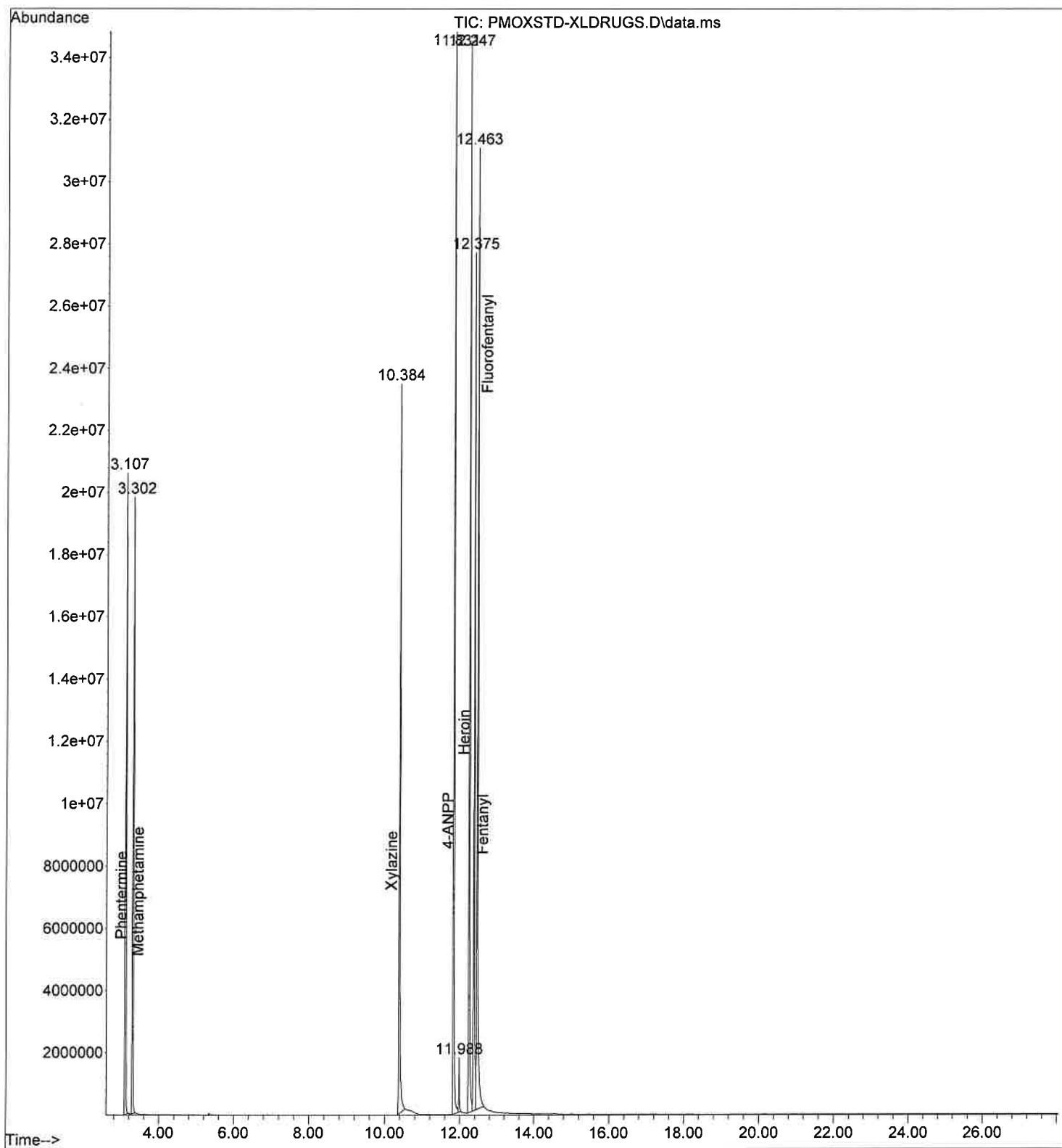
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-XLDRUGS.D
Operator : KLAB
Acquired : 21 Aug 2023 16:16 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



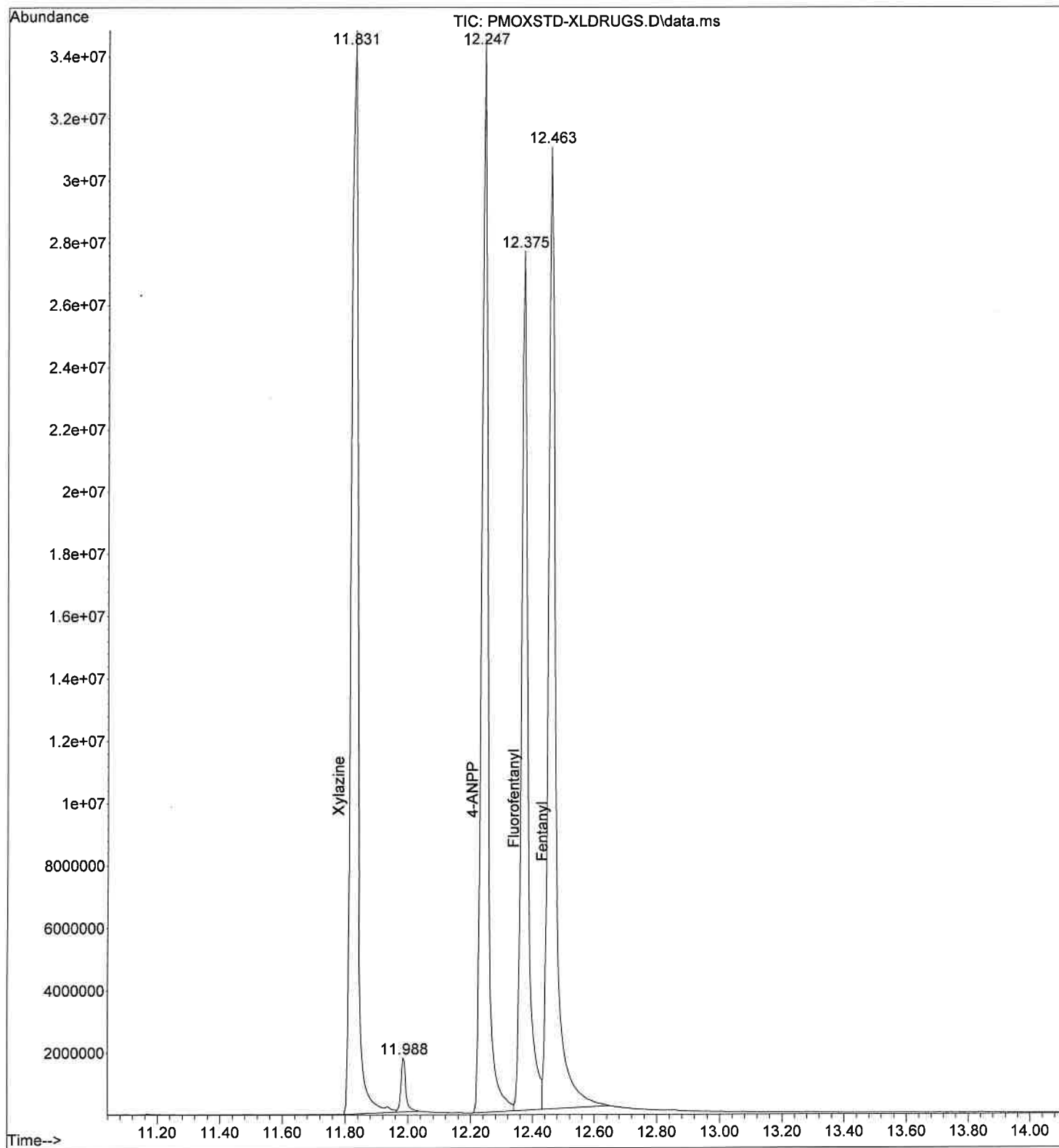
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-XLDRUGS.D
Operator : KLAB
Acquired : 21 Aug 2023 16:16 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



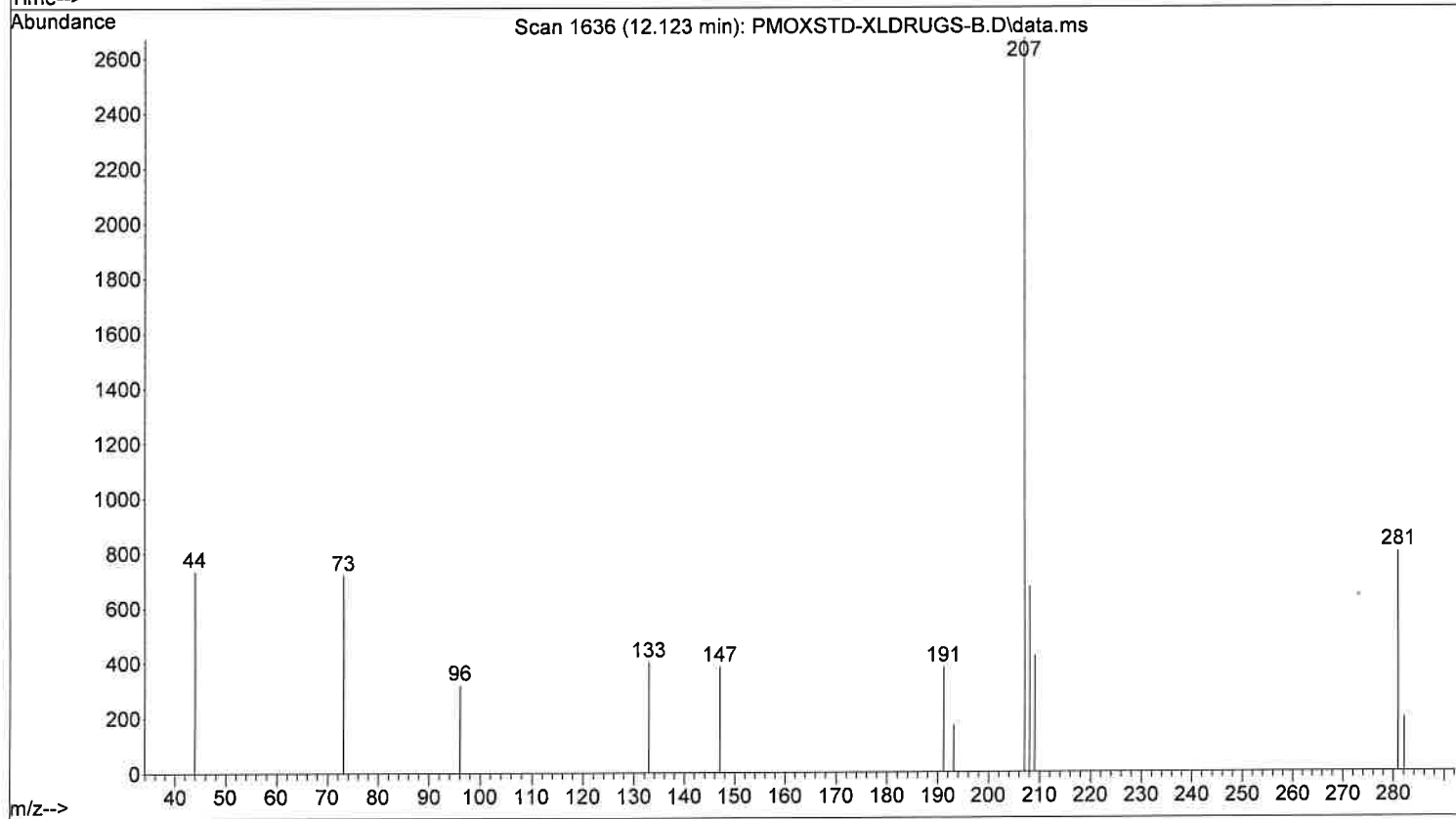
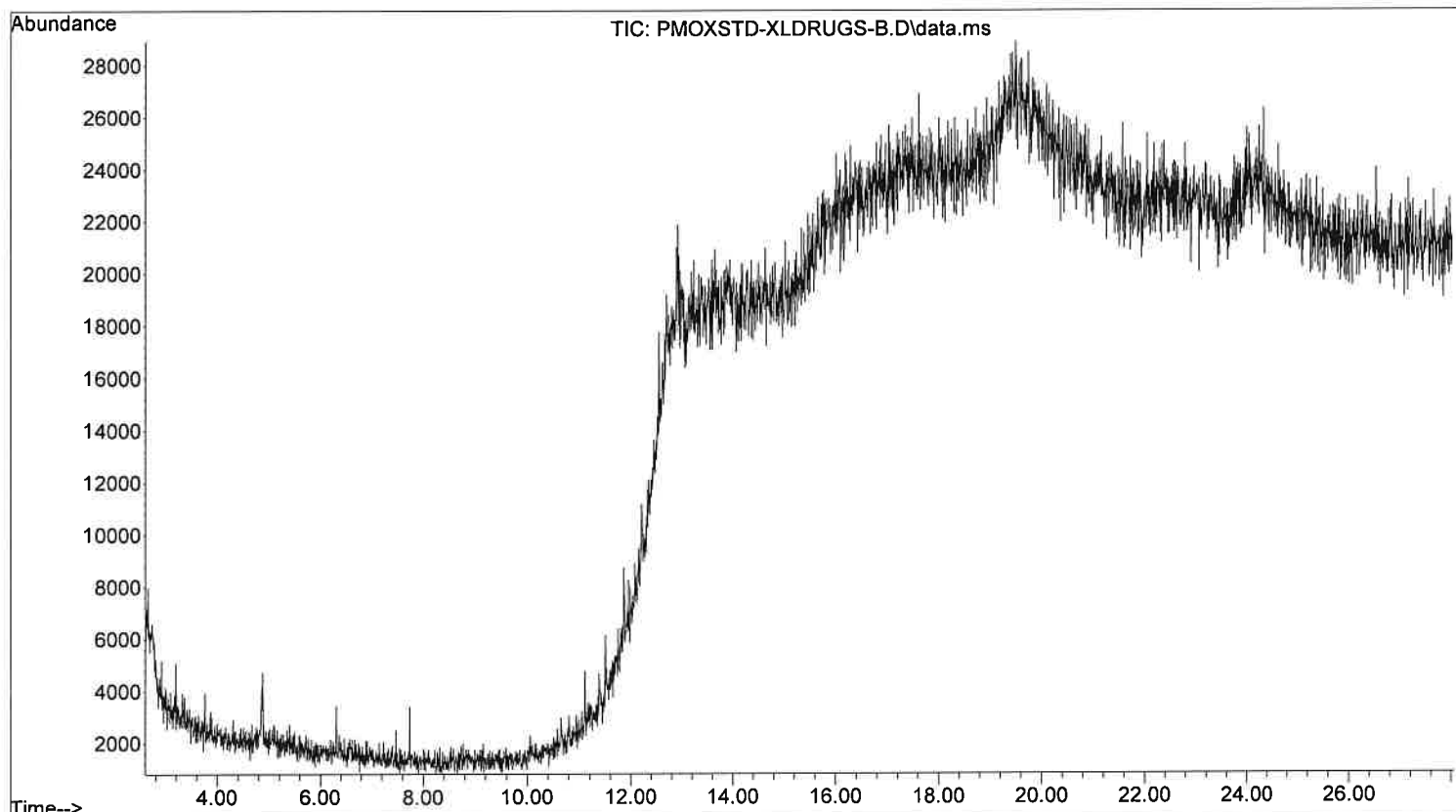
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-XLDRUGS.D
Operator : KLAB
Acquired : 21 Aug 2023 16:16 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



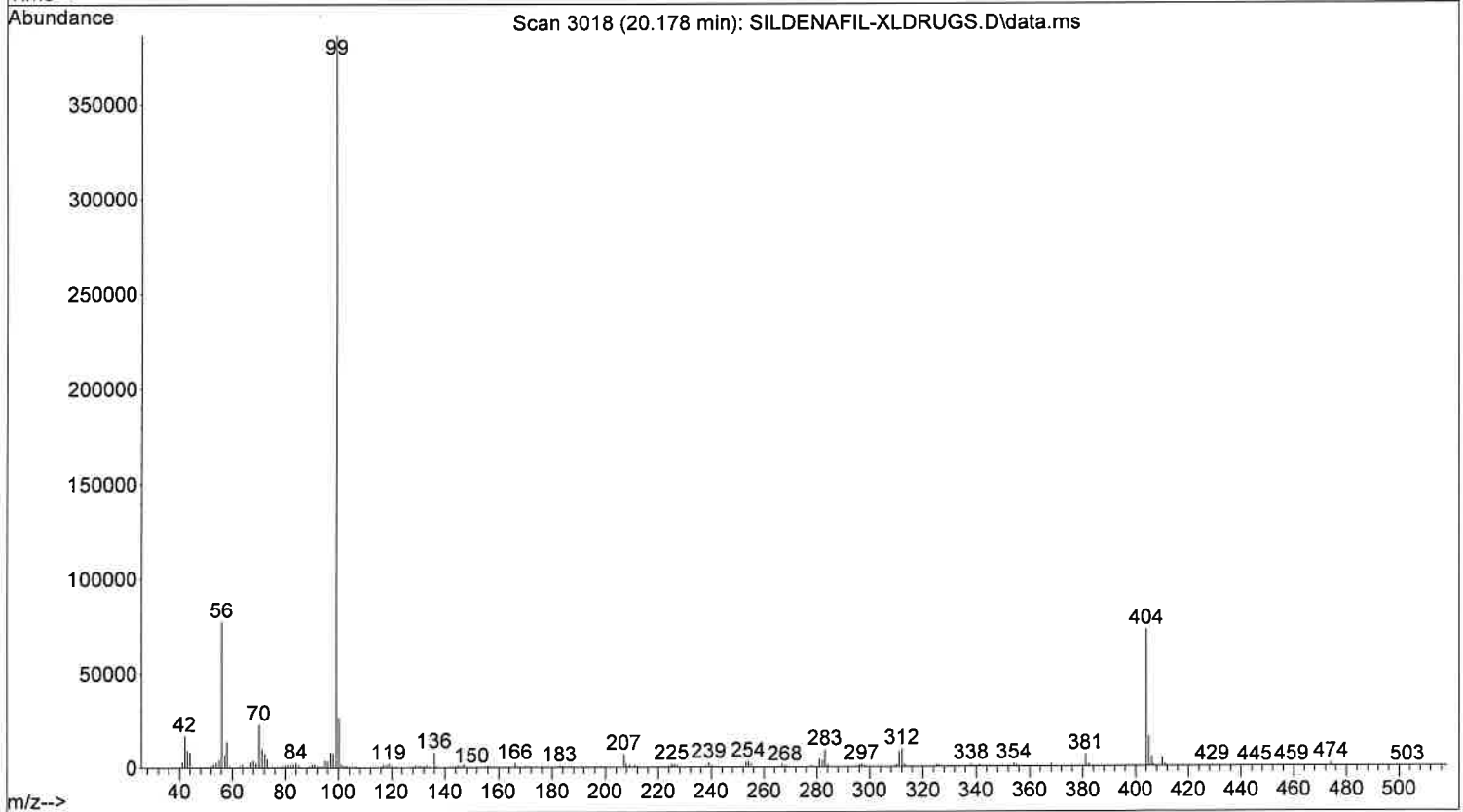
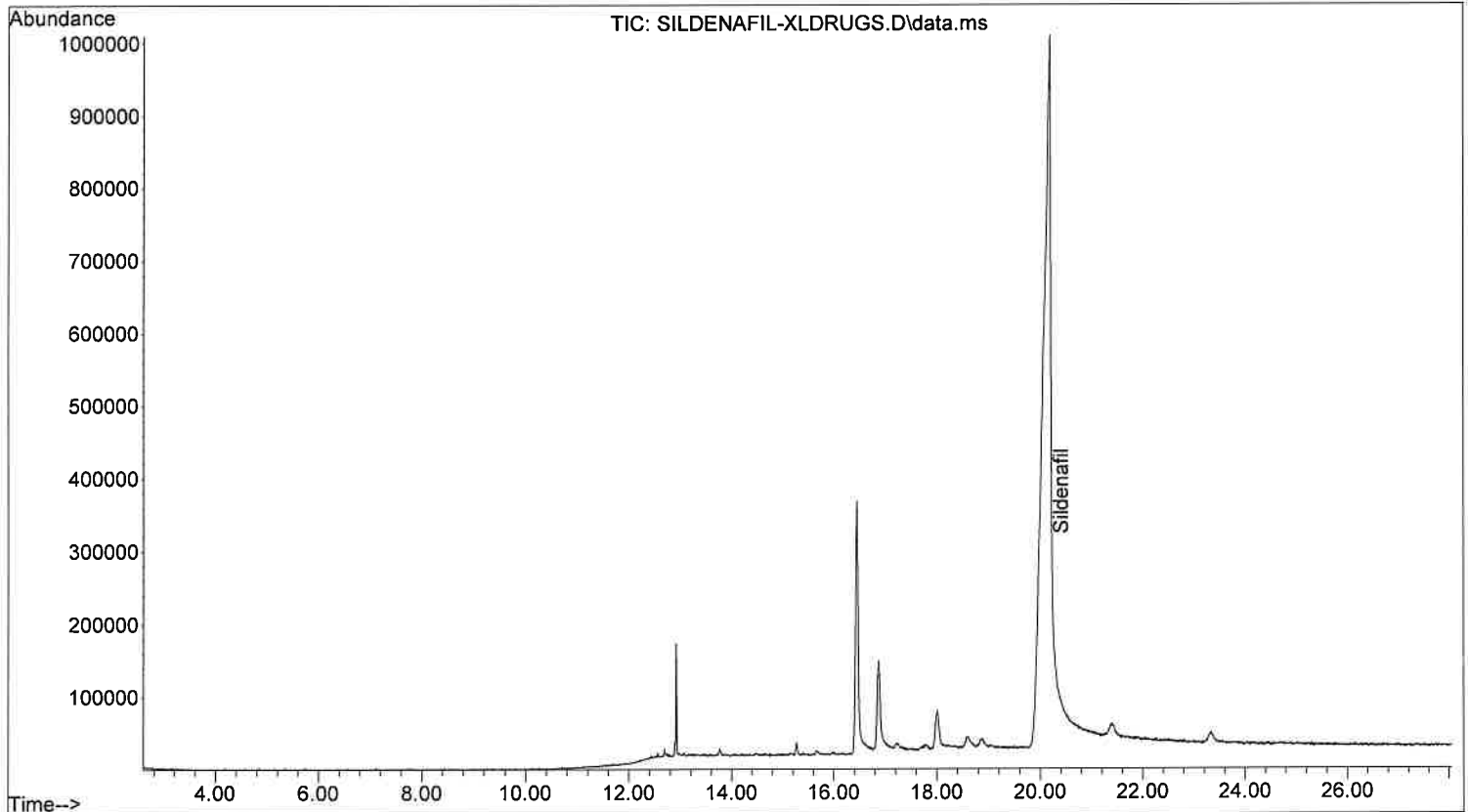
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-XLDRUGS.D
Operator : KLAB
Acquired : 21 Aug 2023 16:16 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 54



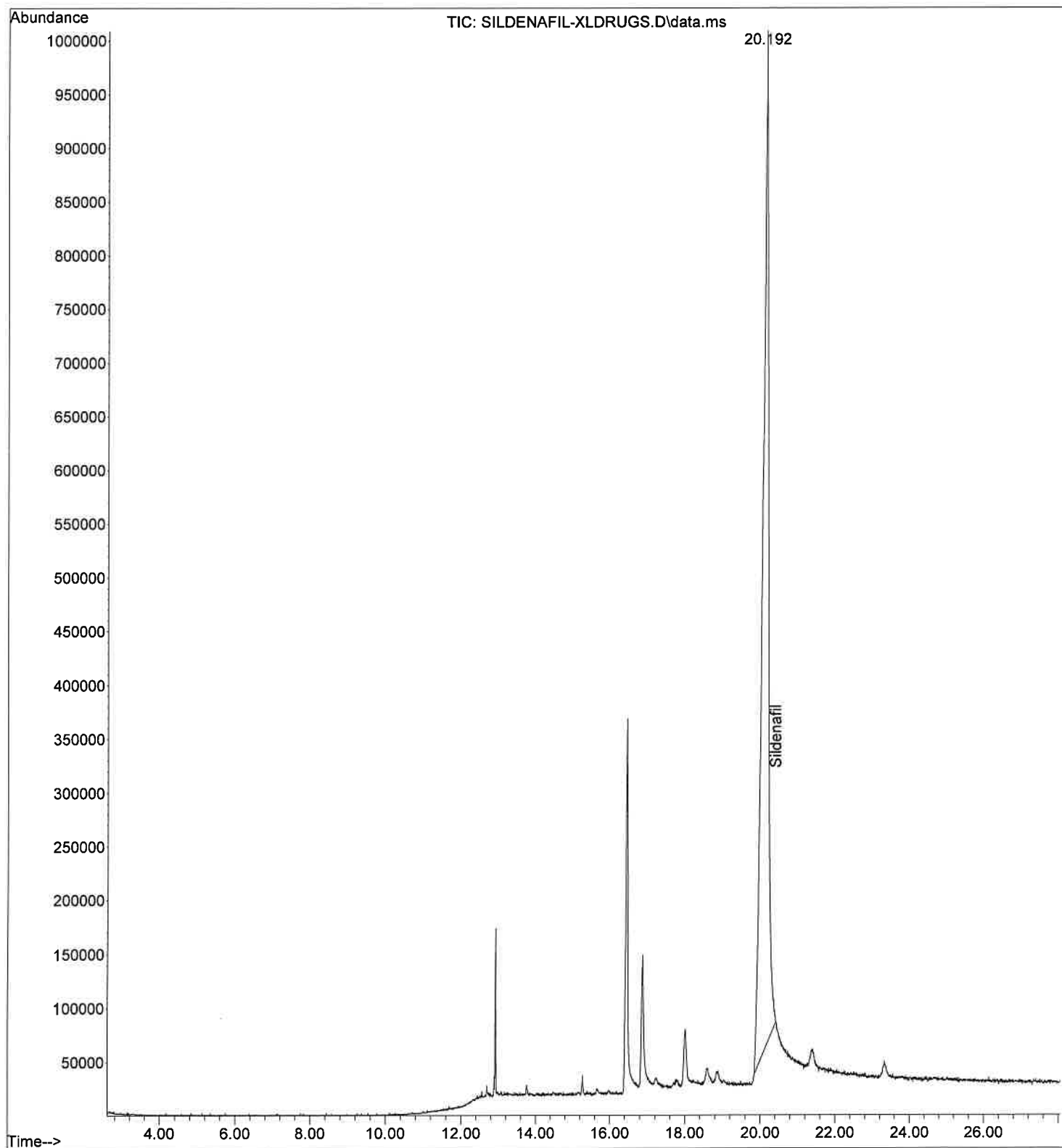
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-XLDRUGS-
... B.D
Operator : KLAB
Acquired : 21 Aug 2023 15:45 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : For P-MOX
Vial Number: 52



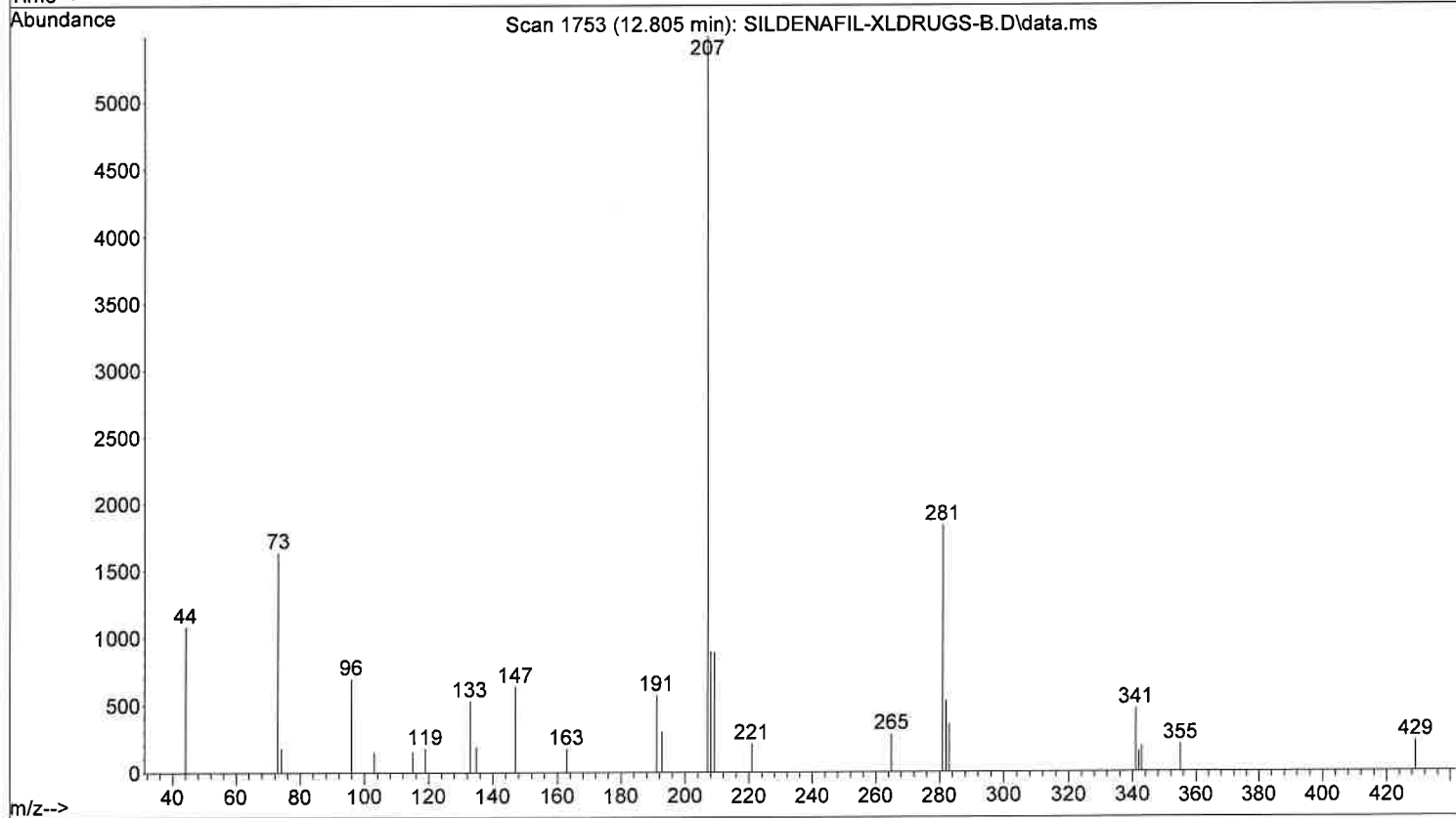
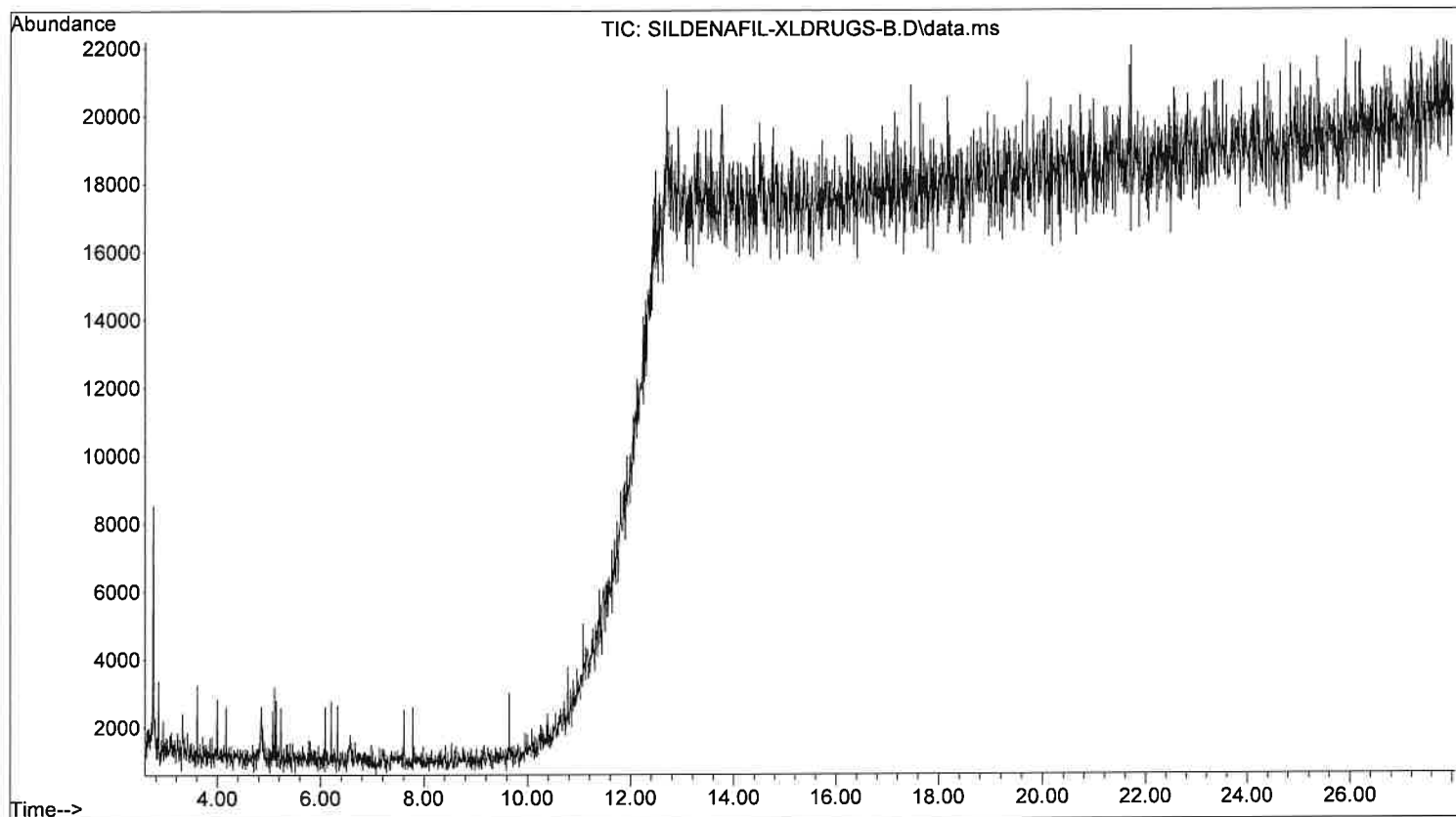
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\SILDENAFIL-XLDRU
... GS.D
Operator : KLAB
Acquired : 21 Aug 2023 20:17 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Sildenafil Standard
Misc Info : MEOH
Vial Number: 58



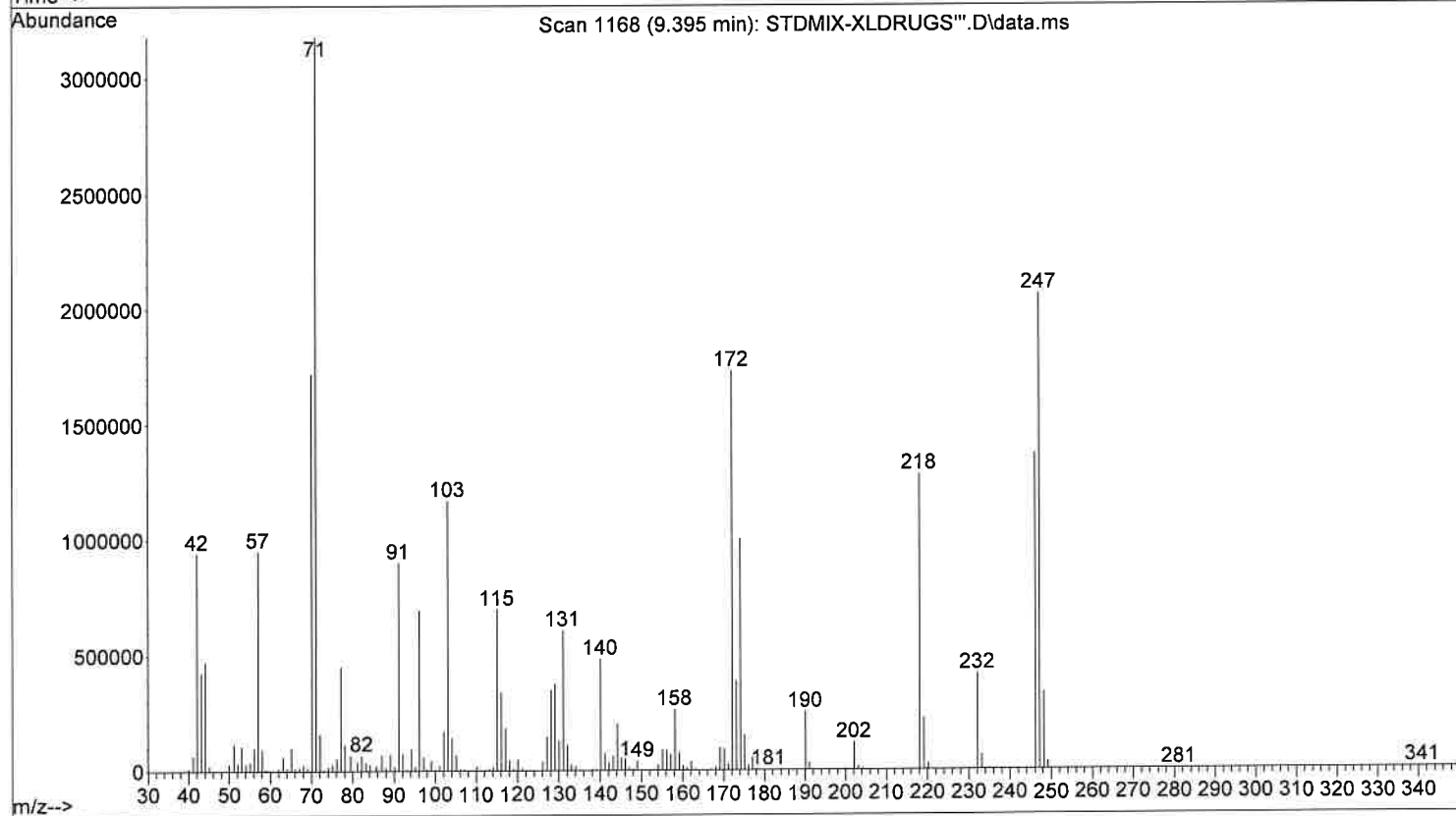
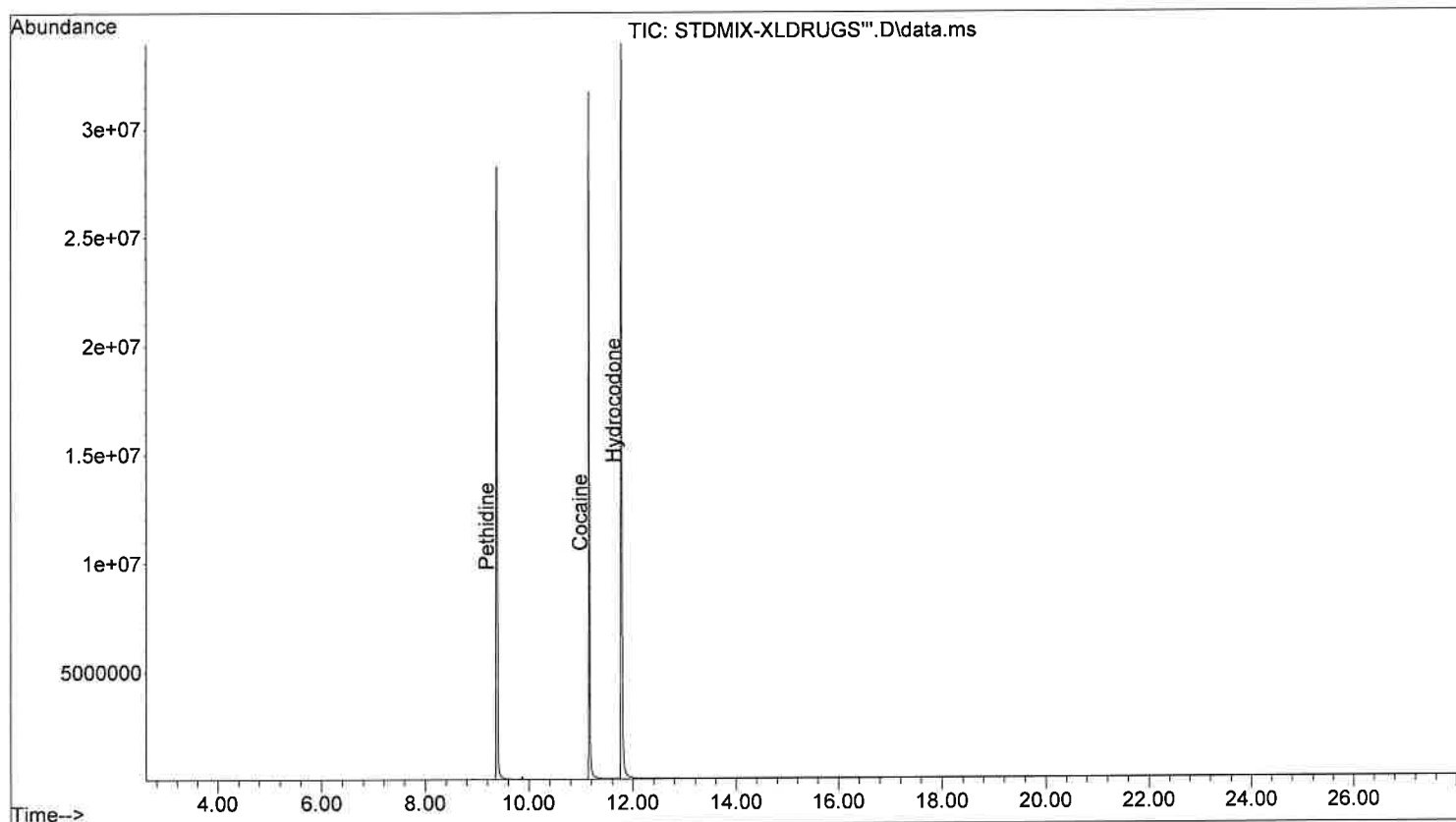
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\SILDENAFIL-XLDRU
... GS.D
Operator : KLAB
Instrument : Buttercup
Acquired : 21 Aug 2023 20:17 using AcqMethod XLDRUGS.M
Sample Name: Sildenafil Standard
Misc Info : MEOH



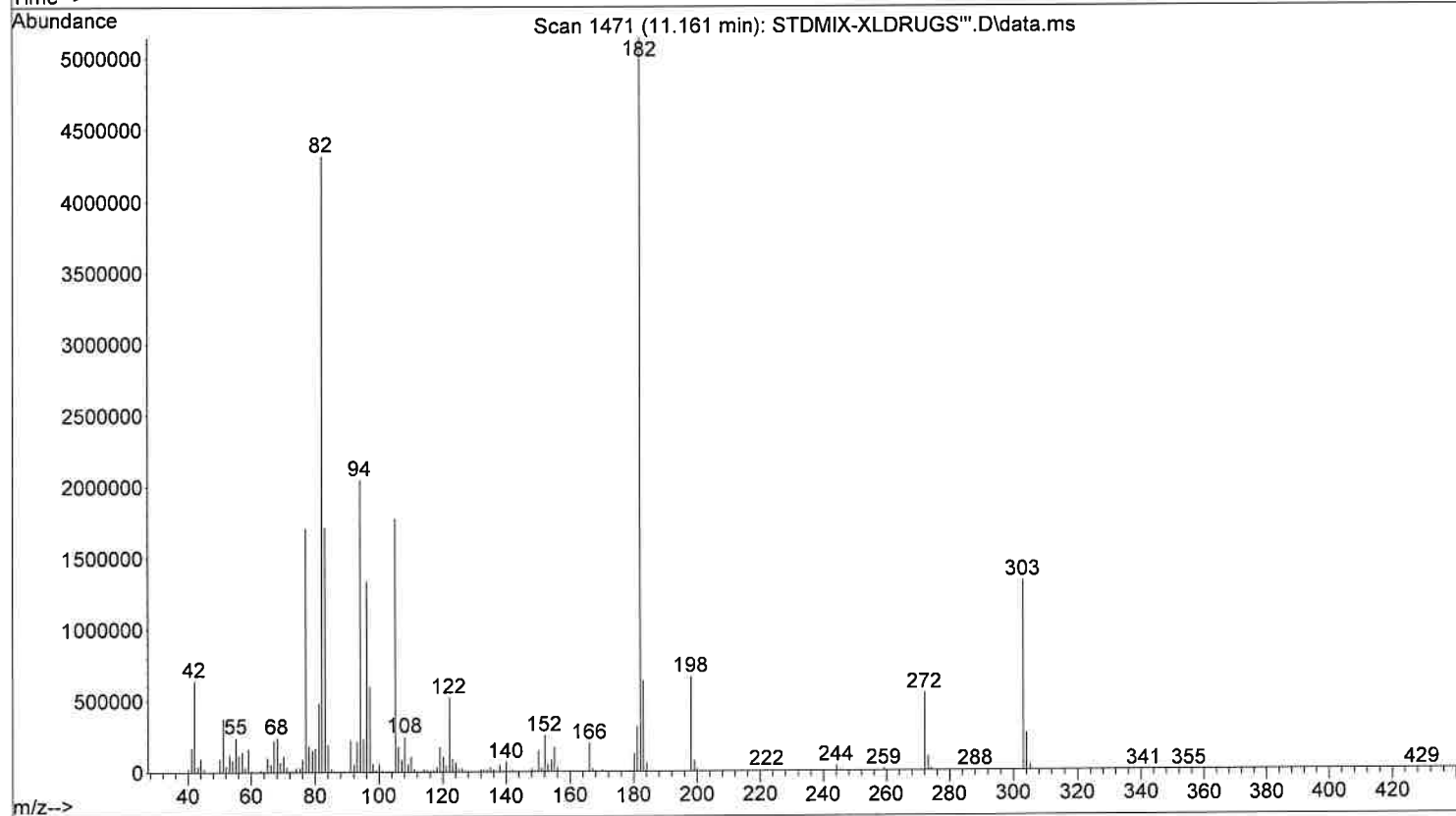
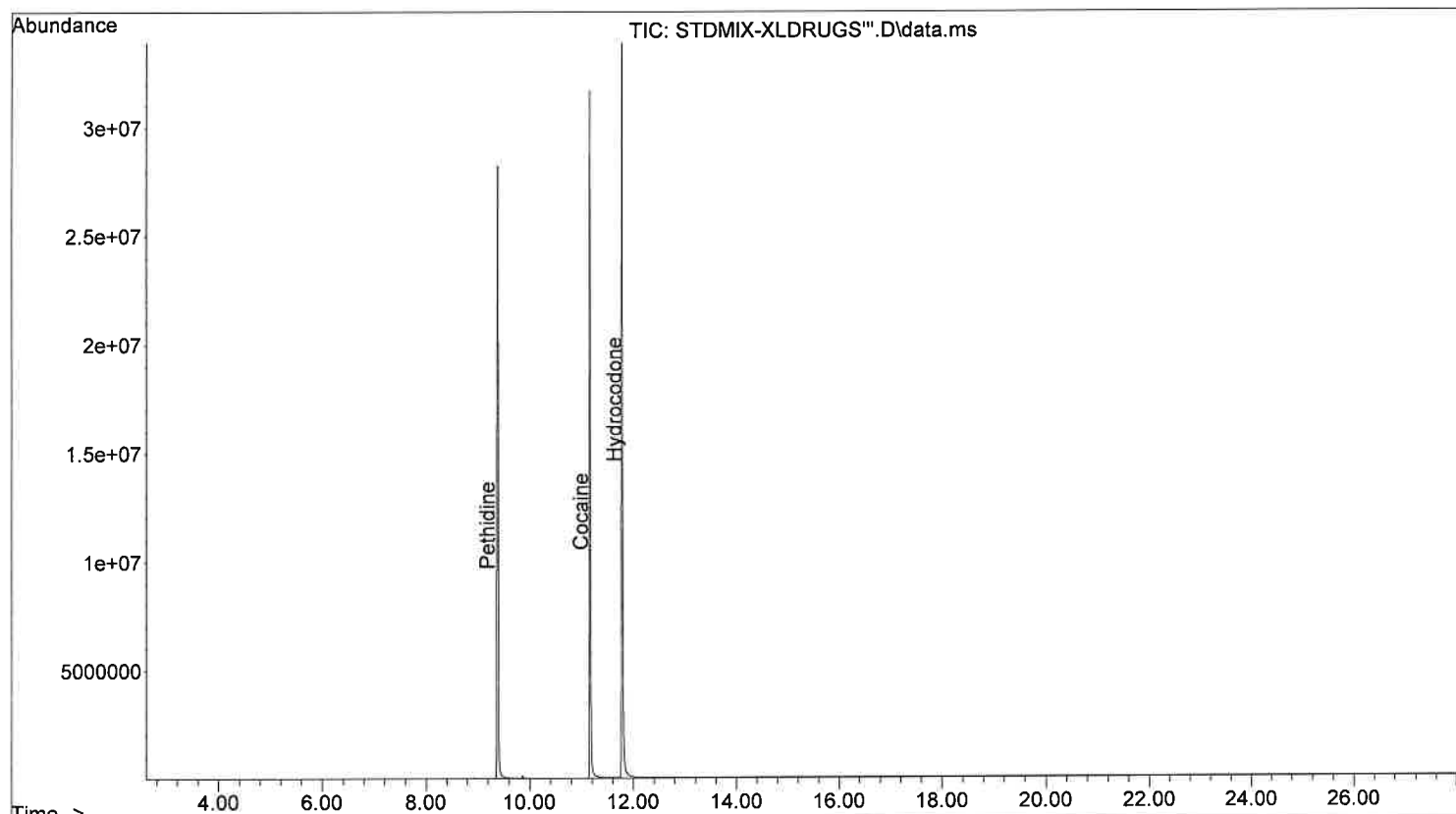
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\SILDENAFIL-XLDRU
... GS-B.D
Operator : KLAB
Acquired : 21 Aug 2023 19:46 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Methanol blank
Misc Info : MEOH
Vial Number: 53



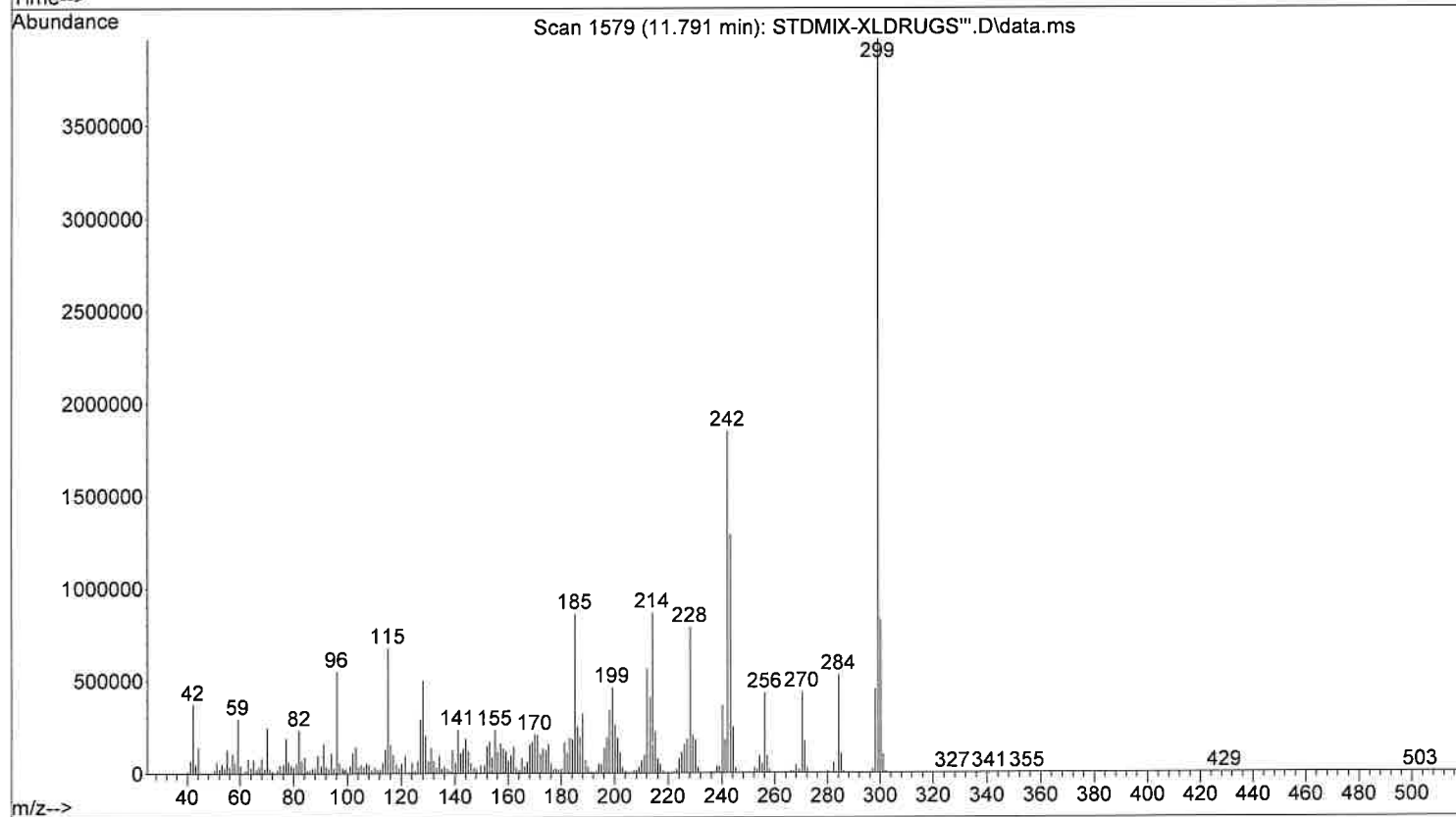
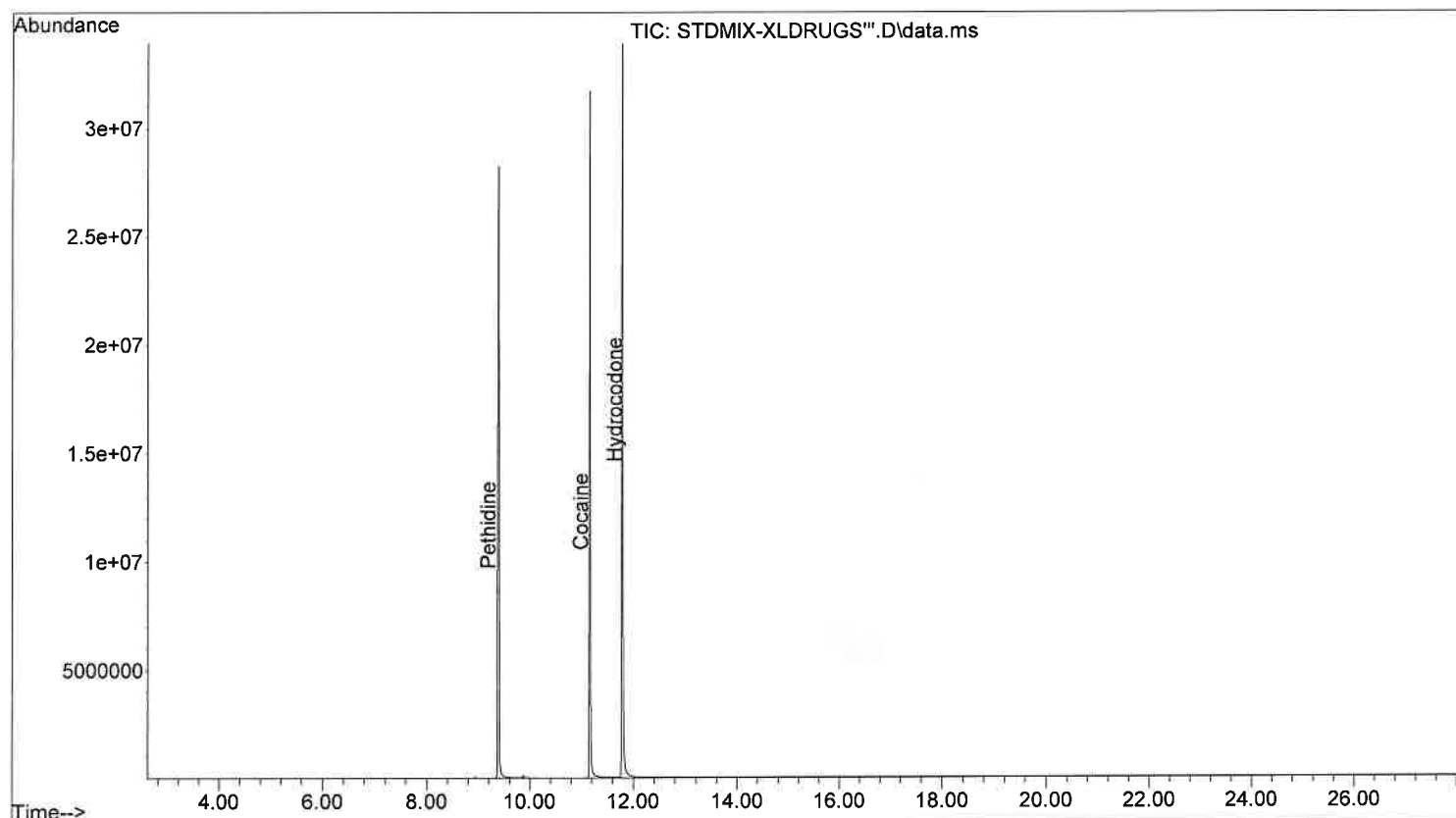
File :D:\MassHunter\GCMS\1\data\2023\SEP23\PC0923\STDMIX-XLDRUGS''
...'.D
Operator : KLAB
Acquired : 01 Sep 2023 14:30 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : CHCl3
Vial Number: 2



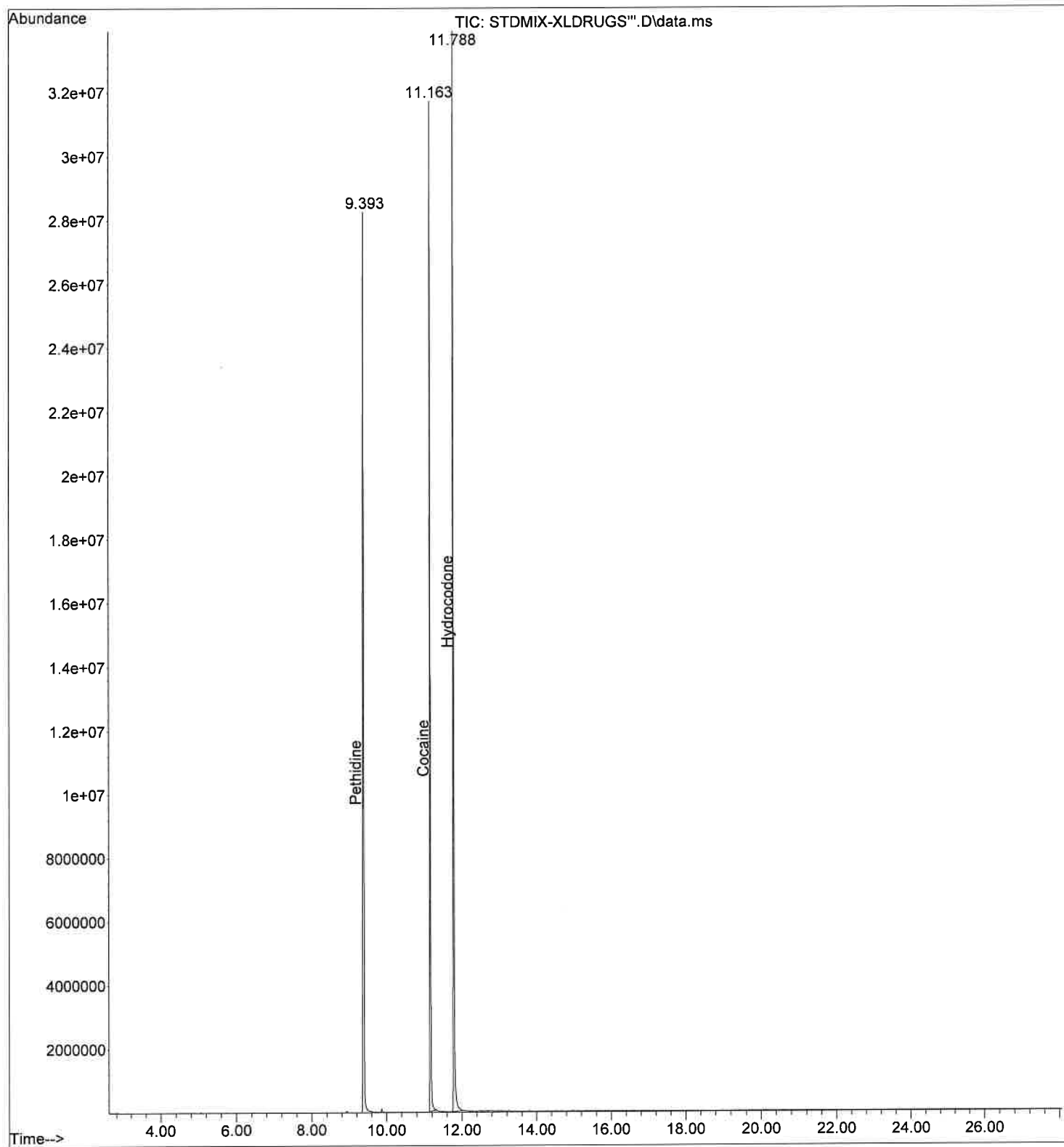
File :D:\MassHunter\GCMS\1\data\2023\SEP23\PC0923\STDMIX-XLDRUGS''
... '.D
Operator : KLAB
Acquired : 01 Sep 2023 14:30 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : CHCl3
Vial Number: 2



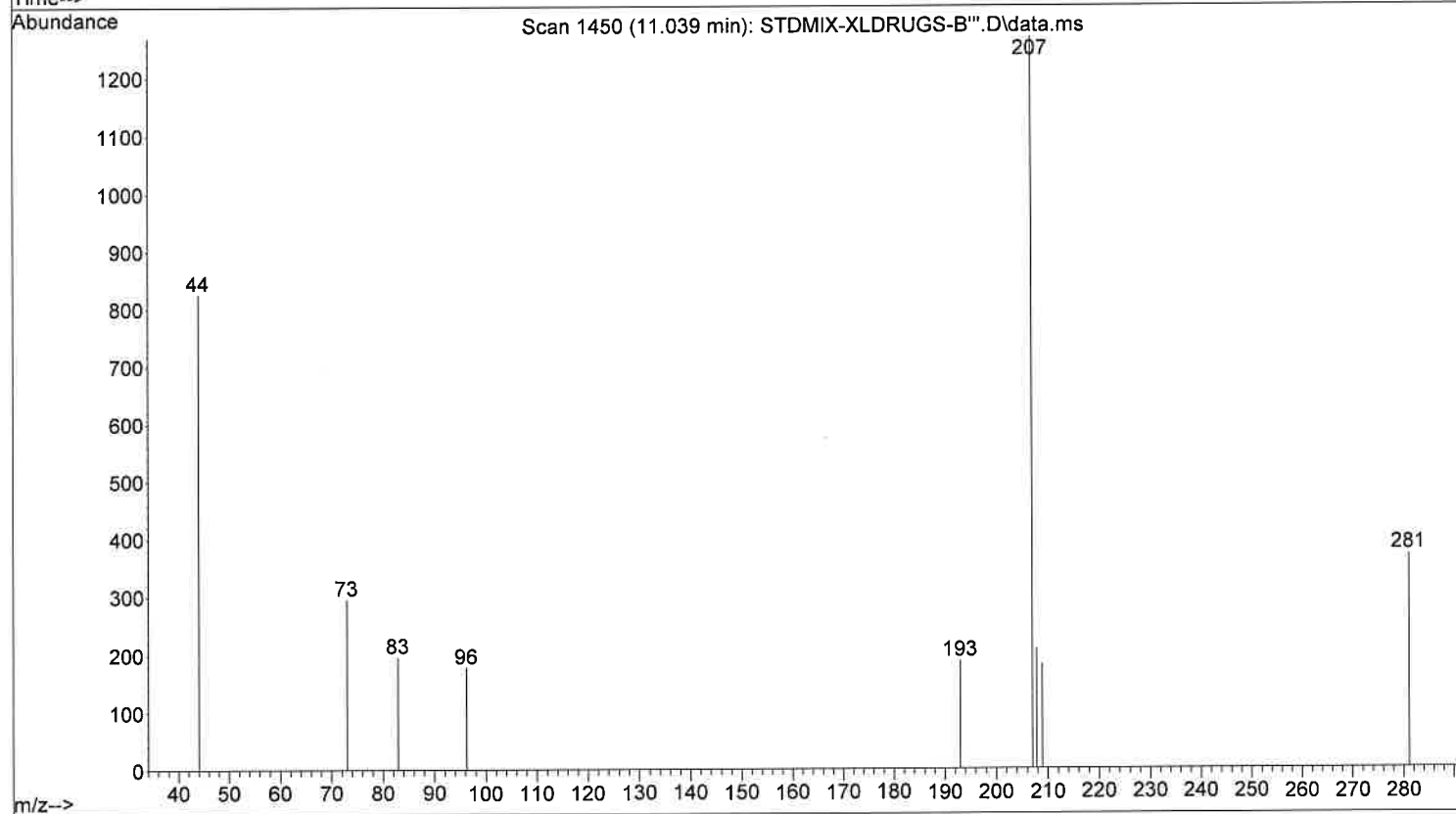
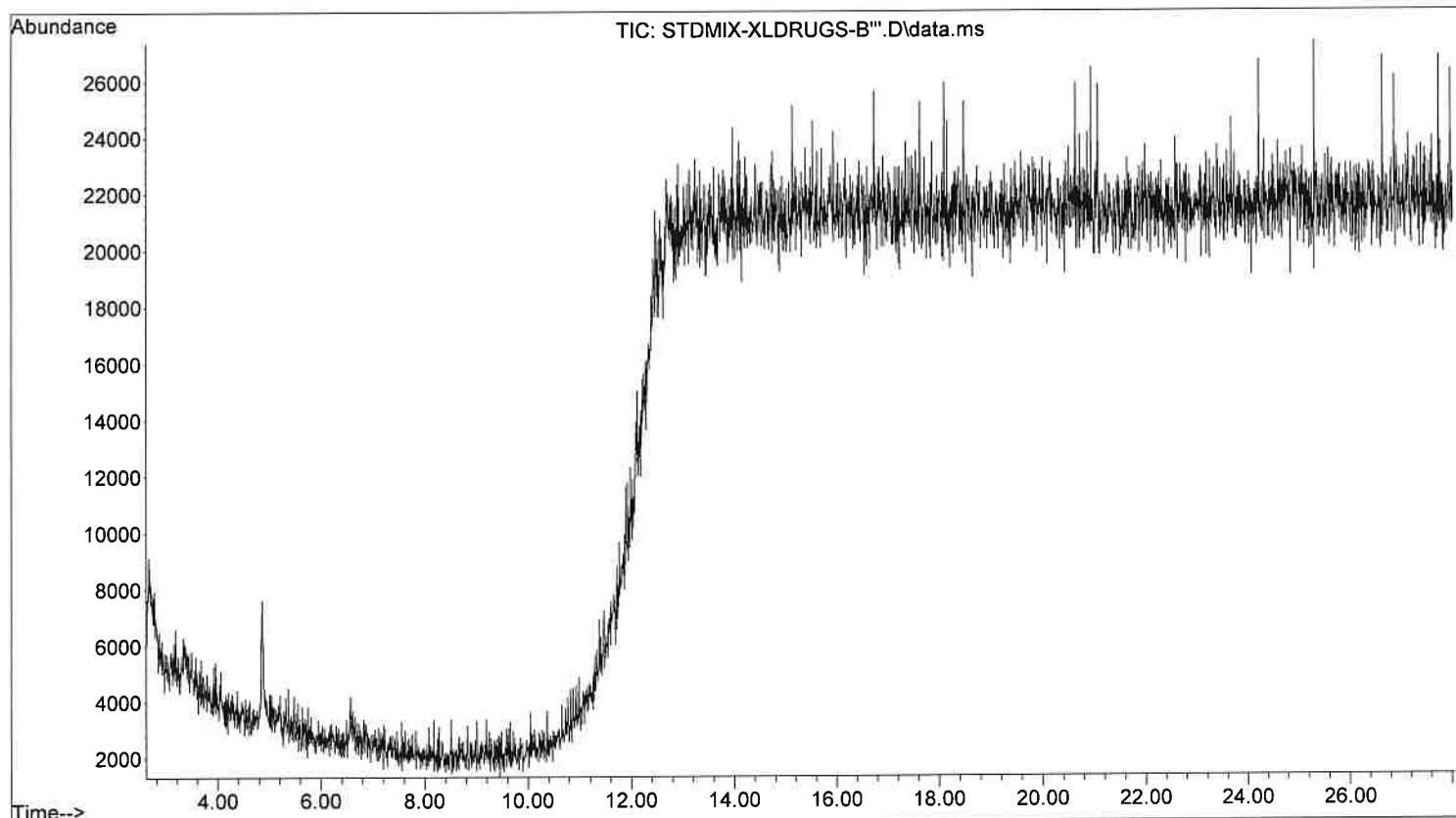
File :D:\MassHunter\GCMS\1\data\2023\SEP23\PC0923\STDMIX-XLDRUGS''
... '.D
Operator : KLAB
Acquired : 01 Sep 2023 14:30 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : CHCl3
Vial Number: 2



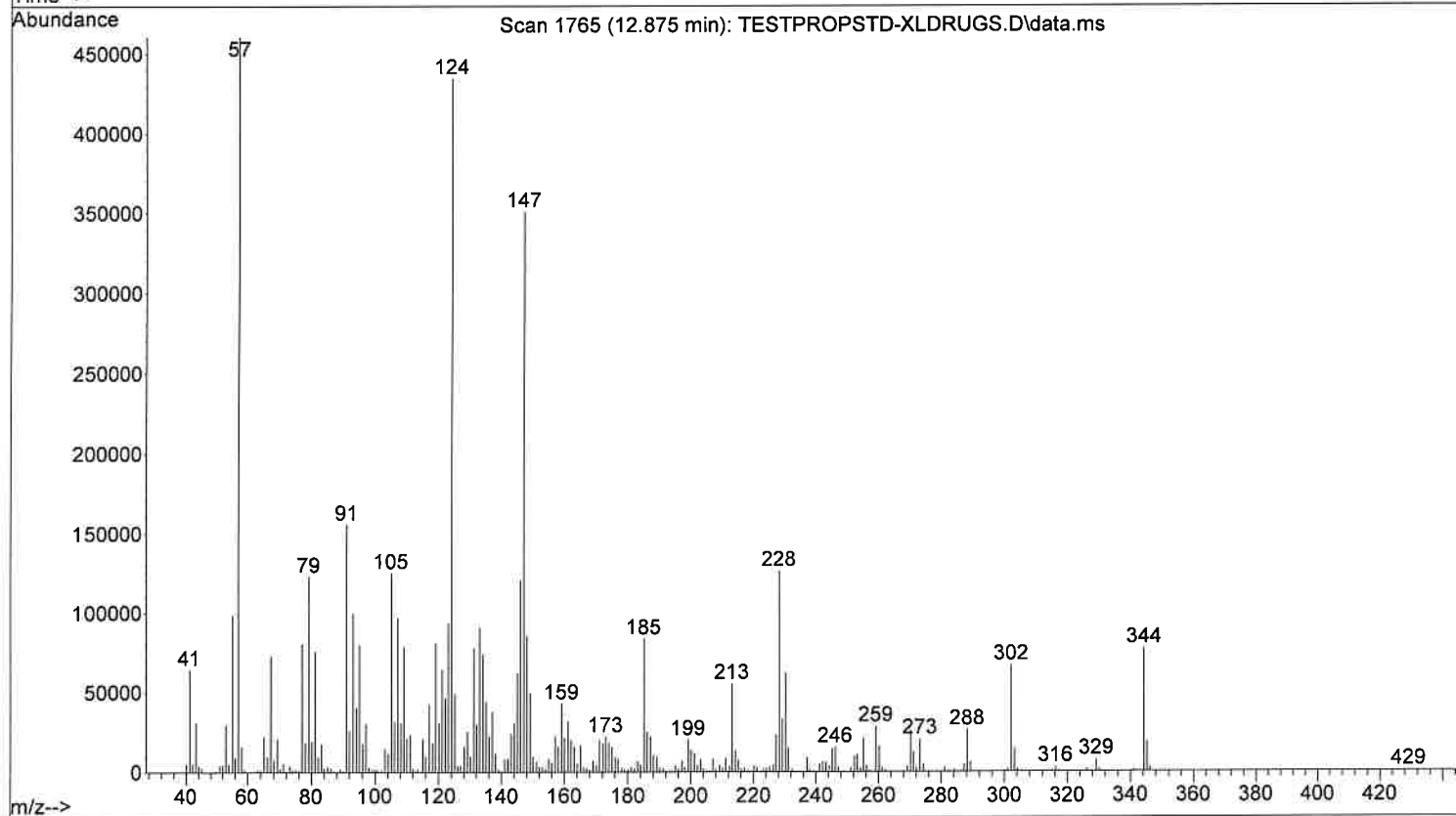
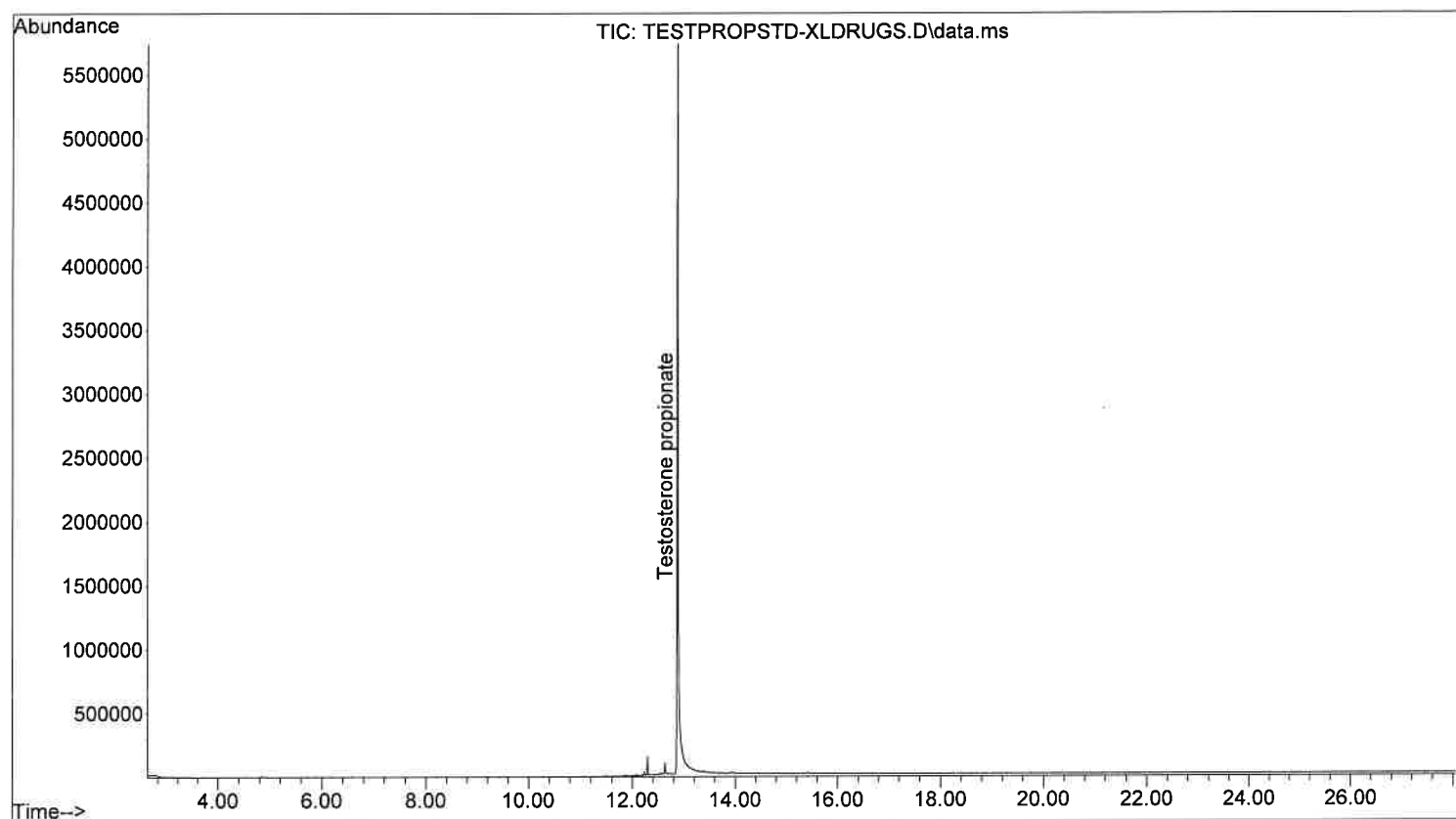
File :D:\MassHunter\GCMS\1\data\2023\SEP23\PC0923\STDMIX-XLDRUGS'
... '.D
Operator : KLAB
Instrument : Buttercup
Acquired : 01 Sep 2023 14:30 using AcqMethod XLDRUGS.M
Sample Name: Standard Mix
Misc Info : CHCl3



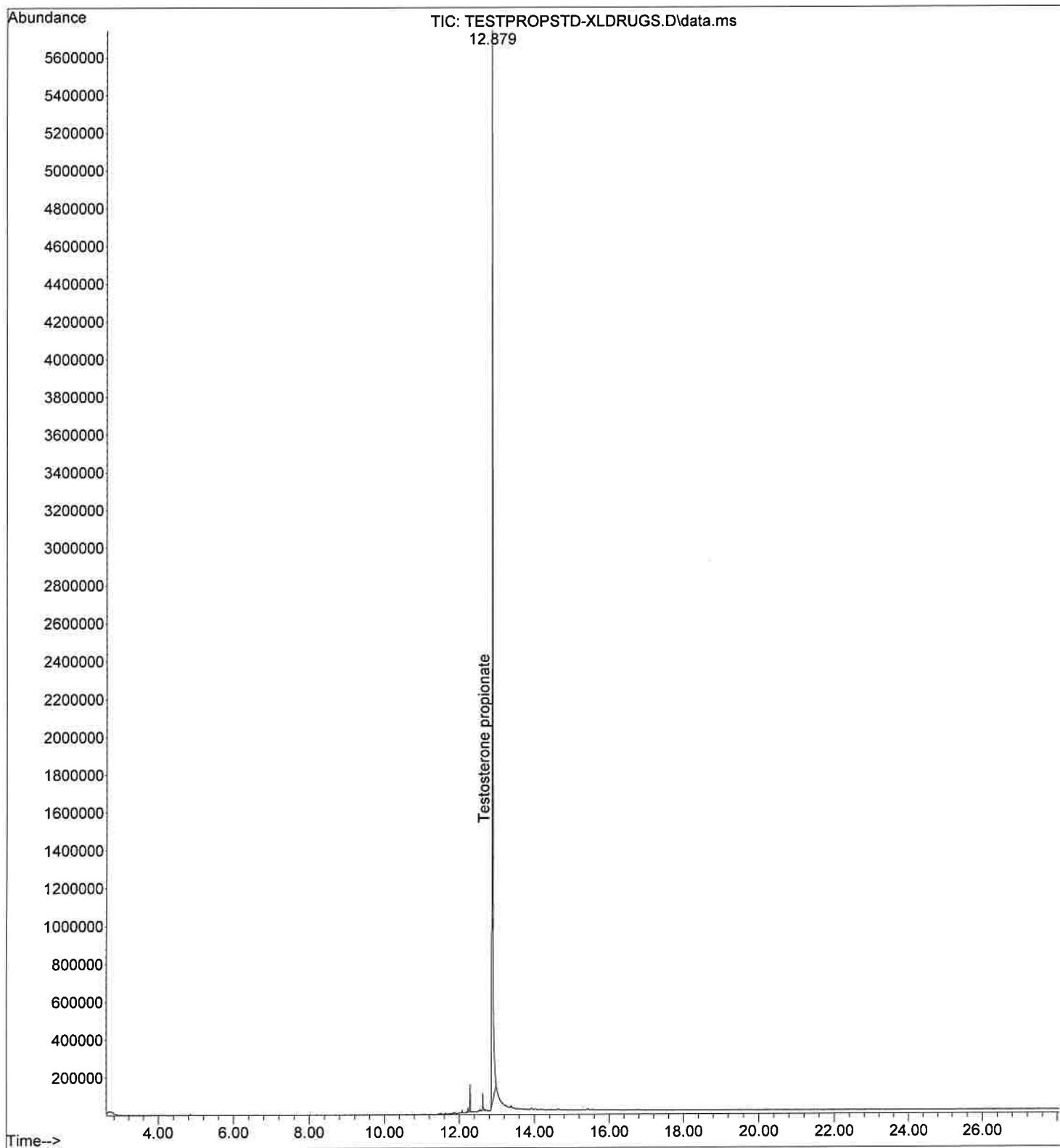
File :D:\MassHunter\GCMS\1\data\2023\SEP23\PC0923\STDMIX-XLDRUGS-B
...'''.D
Operator : KLAB
Acquired : 01 Sep 2023 13:59 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : For Standard Mix
Vial Number: 1



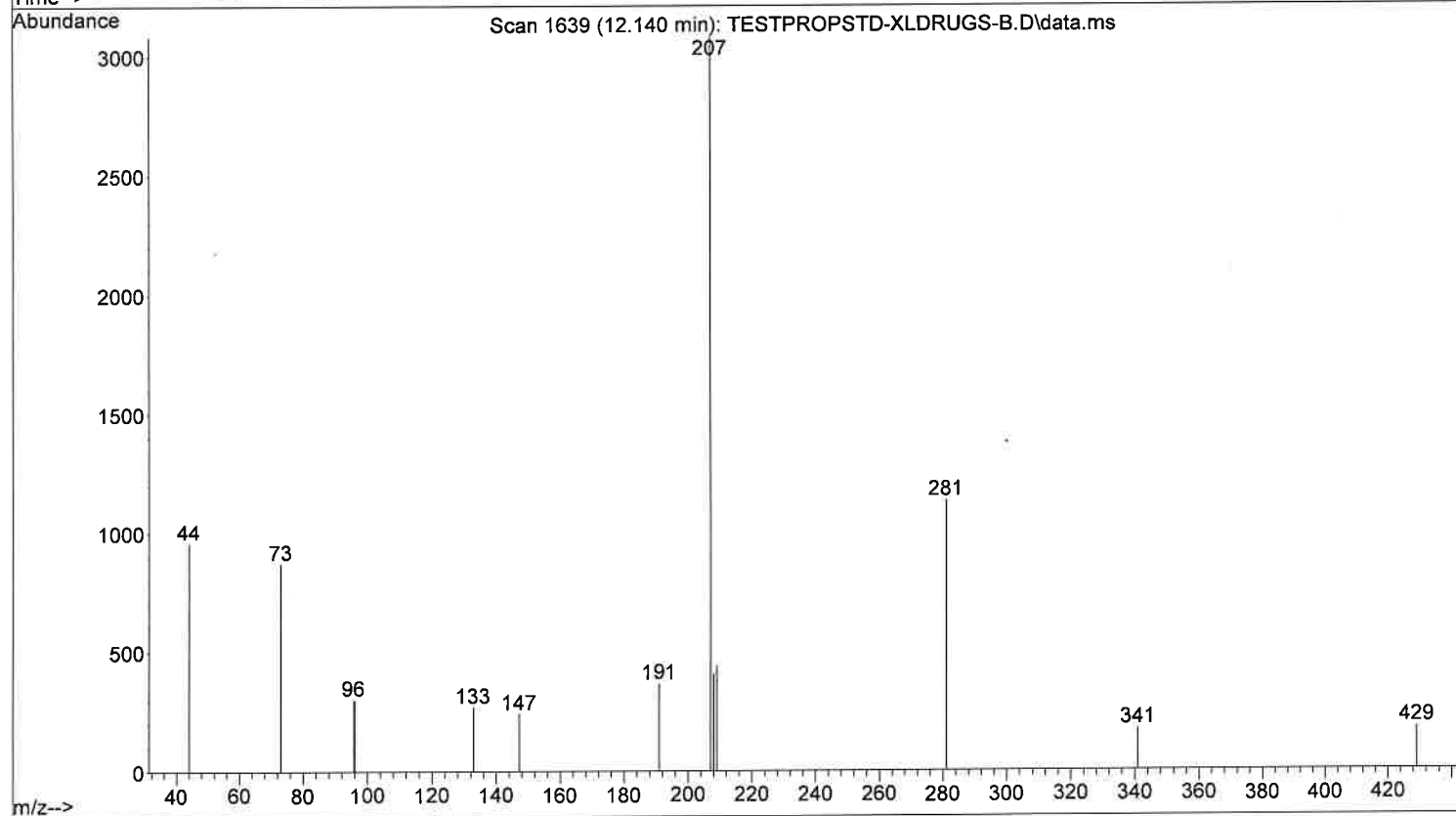
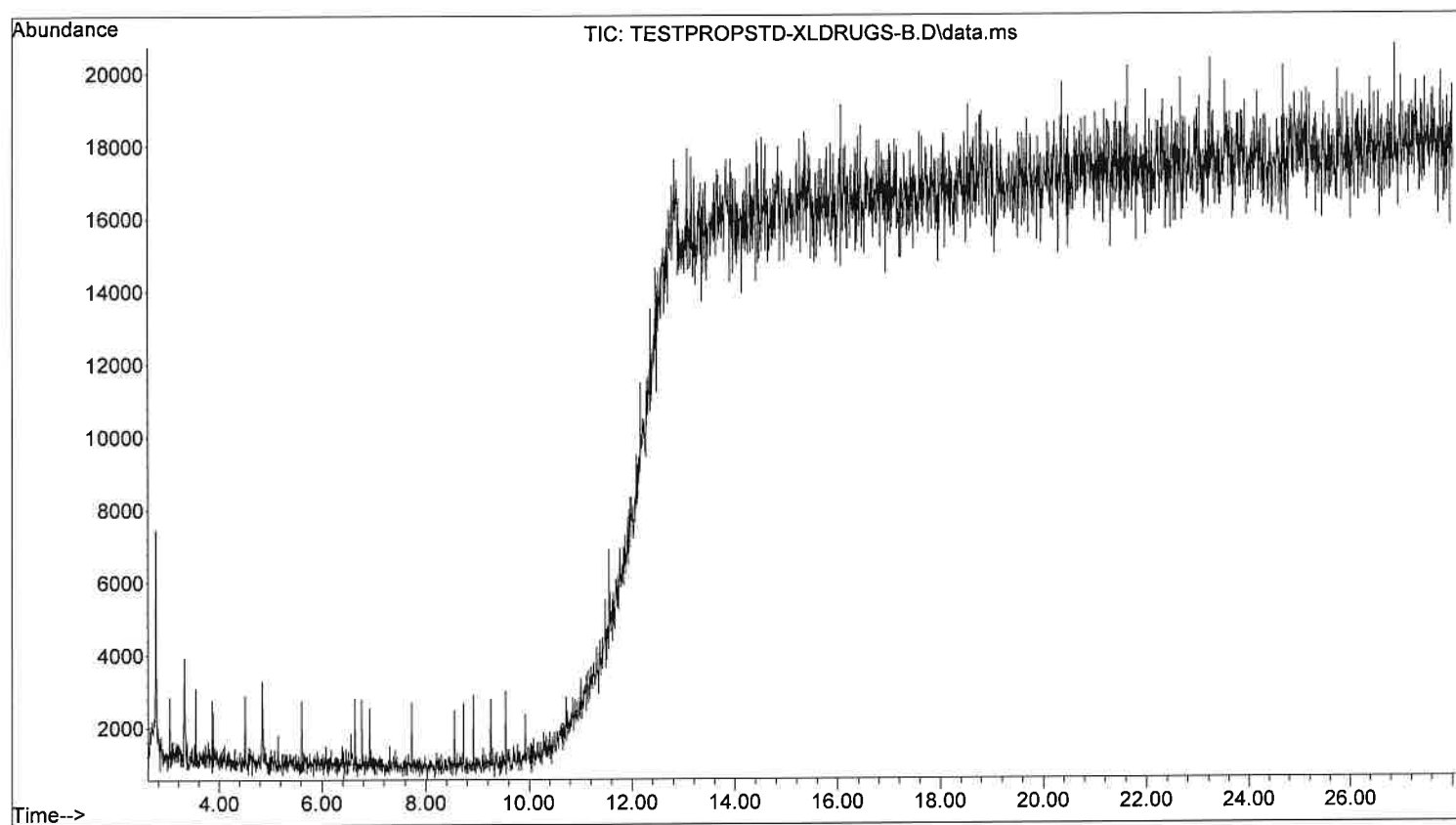
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\TESTPROPSTD-XLDR
... UGS.D
Operator : KLAB
Acquired : 23 Aug 2023 07:24 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Testosterone Propionate Standard
Misc Info : MEOW
Vial Number: 6



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\TESTPROPSTD-XLDR
... UGS.D
Operator : KLAB
Instrument : Buttercup
Acquired : 23 Aug 2023 07:24 using AcqMethod XLDRUGS.M
Sample Name: Testosterone Propionate Standard
Misc Info : MEQH



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\TESTPROPSTD-XLDR
... UGS-B.D
Operator : KLAB
Acquired : 22 Aug 2023 17:01 using AcqMethod XLDRUGS.M
Instrument : Buttercup
Sample Name: Methanol blank
Misc Info : For Testosterone Propionate
Vial Number: 1



METHOD CONTROL PARAMETERS

Method Information for: D:\MassHunter\GCMS\1\methods\STEROID.M

Method Sections To Run:

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

Method Comments:
STEROID

END OF METHOD CONTROL PARAMETERS

Single Quadrupole Acquisition Method - MS Parameters Report

Method file	D:\MassHunter\GCMS\1\methods\STEROID.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)	10.00
Solvent delay (min)	2.50
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
2.50	40	550	150	1,562 [N=2]

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

Self-Cleaning Ion Source Parameters

Mode	No Cleaning
------	-------------

D:\MassHunter\GCMS\1\methods\STEROID.M
Thu Aug 24 15:45:16 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 20 min
Post Run Time 0 min

Oven
Temperature
Setpoint On
(Initial) 70 °C
Hold Time 1 min
Post Run 50 °C
Program
#1 Rate 30 °C/min
#1 Value 280 °C
#1 Hold Time 12 min

Equilibration Time 0.5 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) 1
Solvent A Washes (PostInj) 1
Solvent A Volume 8 µL
Solvent B Washes (PreInj) 1
Solvent B Washes (PostInj) 1
Solvent B Volume 8 µL
Sample Washes 0
Sample Wash Volume 8 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)	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	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	
Helium Conservation Controlled Mode	Off
Heater	Split
Pressure	On 250 °C
Total Flow	On 8.5 psi
Septum Purge Flow	On 48.637 mL/min
Pre-Run Flow Test	On 3 mL/min
Gas Saver	Off
Split Ratio	On 20 mL/min after 2 min
Split Flow	45 :1
Liner	44.645 mL/min
	Agilent 5190-2271: 900 µL (Splitless, single taper, wool, c
Back SS Inlet He	
Helium Conservation Controlled Mode	Off
Heater	Split
Pressure	Off
Total Flow	Off
Septum Purge Flow	Off
Pre-Run Flow Test	Off
Liner	A Liner has not been selected.
Column	
Column #1	
Flow	
Setpoint	On
(Initial)	0.99211 mL/min
Post Run	1 mL/min
Column Information	Agilent 128-0112: 1
Description	DB-lms

Temperature Range	-60 °C-340 °C (350 °C)
Dimensions	12 m x 200 µm x 0.33 µm (Calibrated)
Heater	Oven
Column lock	Unlocked
In	Front SS Inlet He
Out	MSD
(Initial)	70 °C
Pressure	8.5 psi
Flow	0.99211 mL/min
Average Velocity	57.95 cm/sec
Holdup Time	0.34512 min
Control Mode	Constant Flow
Column Outlet Pressure	0 psi
Front Detector FID	
Makeup	He
Heater	Off
H2 Flow	Off
Air Flow	Off
Makeup Flow	Off
Carrier Gas Flow Correction	Constant Makeup and Fuel Flow
Flame	Off
Blank Evaluation Setpoints	
Perform Blank Evaluation Test	Off
Helium Conservation	
Helium Valve	Off
Nitrogen Valve	Off
Detector Evaluation	
Perform Detector Evaluation Test	Off
MSD Transfer Line	
Temperature	
Setpoint	On
(Initial)	280 °C
Signals	
Signal #1:	
Description	None
Signal #2:	
Description	None
Signal #3:	
Description	None
Signal #4:	
Description	None
Signal #5:	
Description	None
Signal #6:	
Description	None
Signal #7:	
Description	None
Signal #8:	
Description	None

TUNE PARAMETERS for SN: US2313MA09

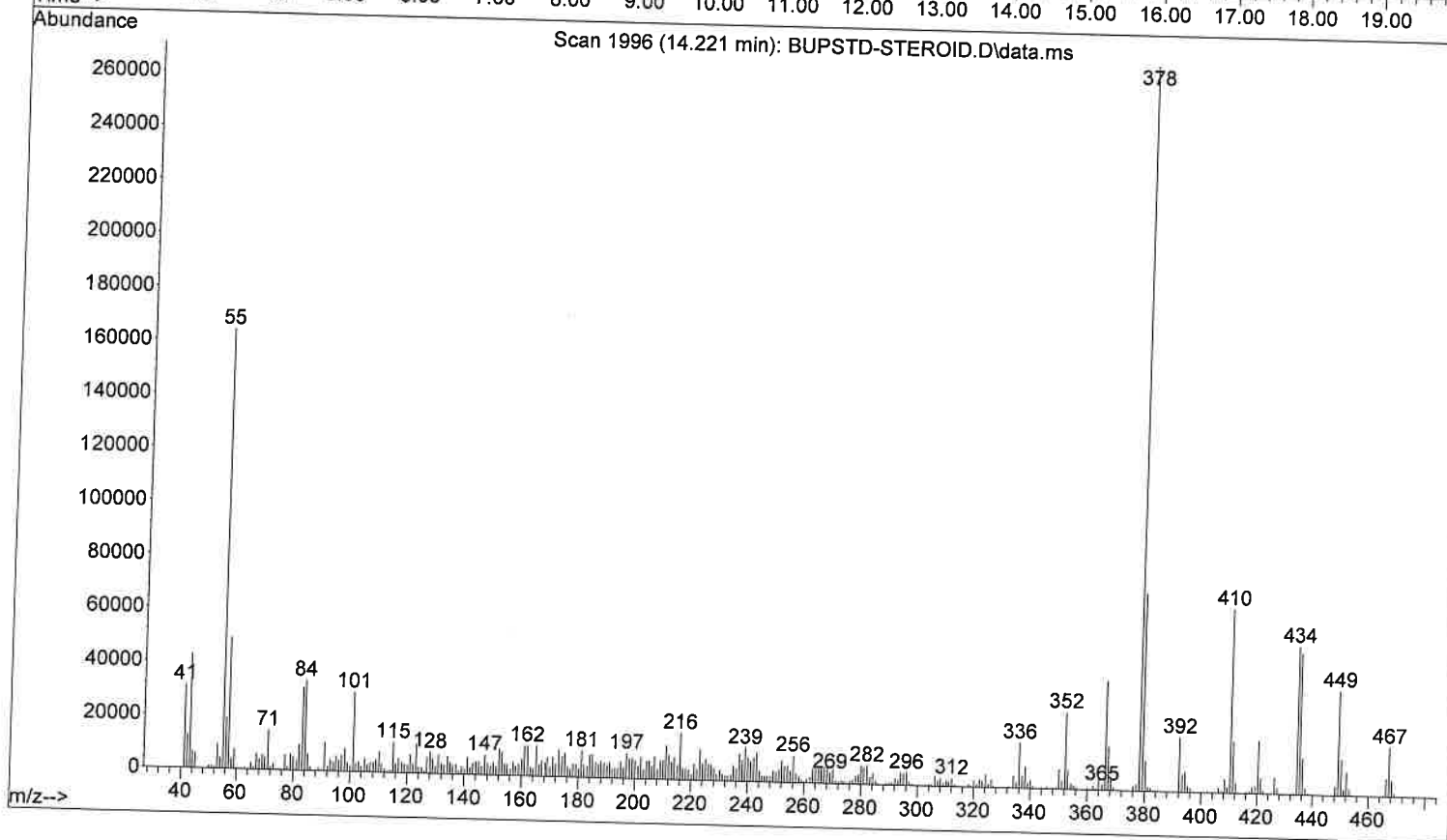
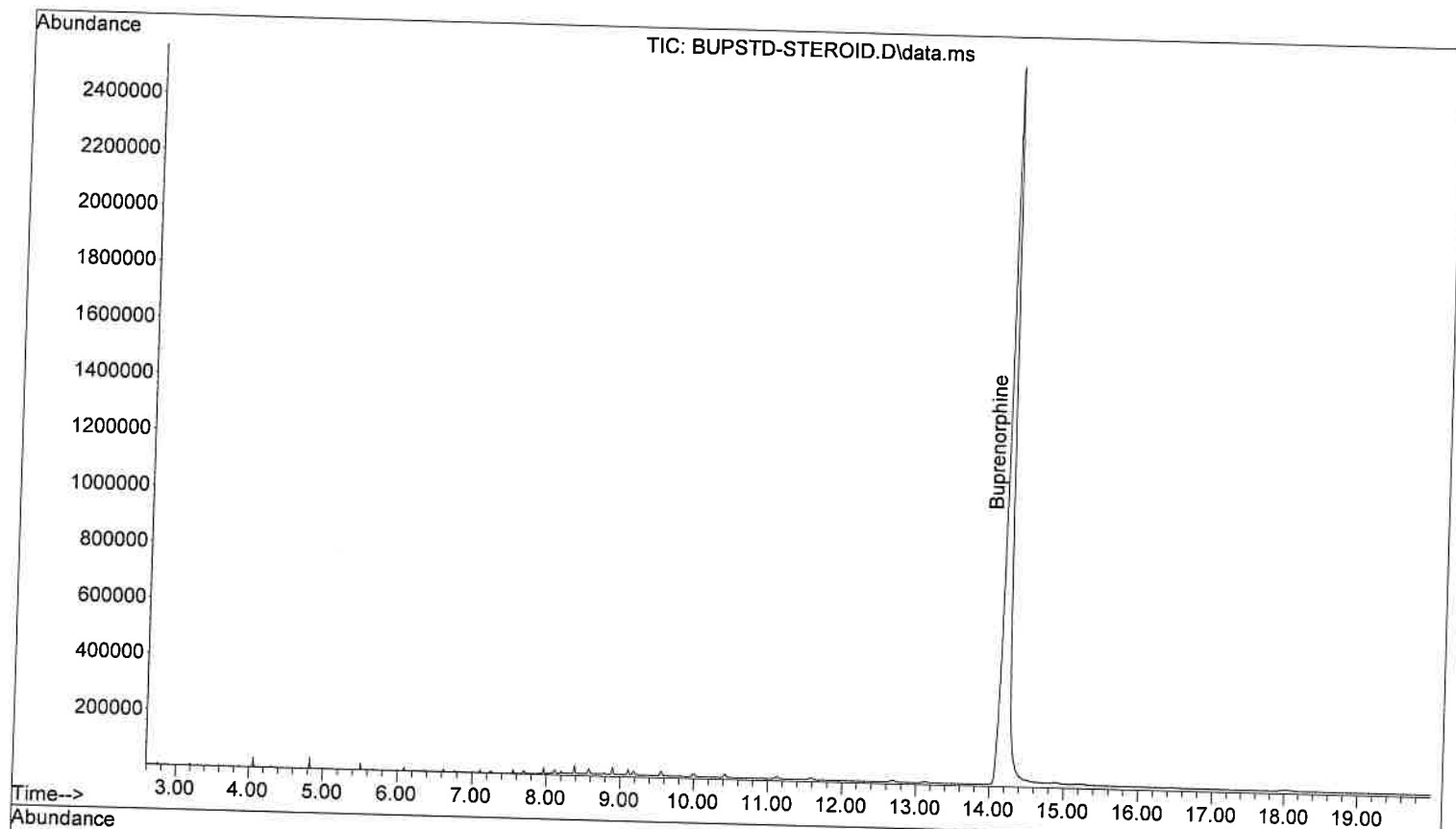
Trace Ion Detection is OFF.

34.593	:	EMISSION	
70.007	:	ENERGY	
29.919	:	REPELLER	
90.331	:	IONFOCUS	
25.226	:	ENTRANCE LENS	
925.472	:	EMVOLTS	
		951.5	: Actual EMV
		1.00	: GAIN FACTOR
2896.000	:	AMUGAIN	
134.625	:	AMUOFFSET	
1.000	:	FILAMENT	
0.000	:	DCPOLARITY	
10.822	:	ENTLENSOFFSET	
0.000	:	Ion_Body	
0.000	:	EXTLENS	
257.000	:	MASSGAIN	
-23.000	:	MASSOFFSET	

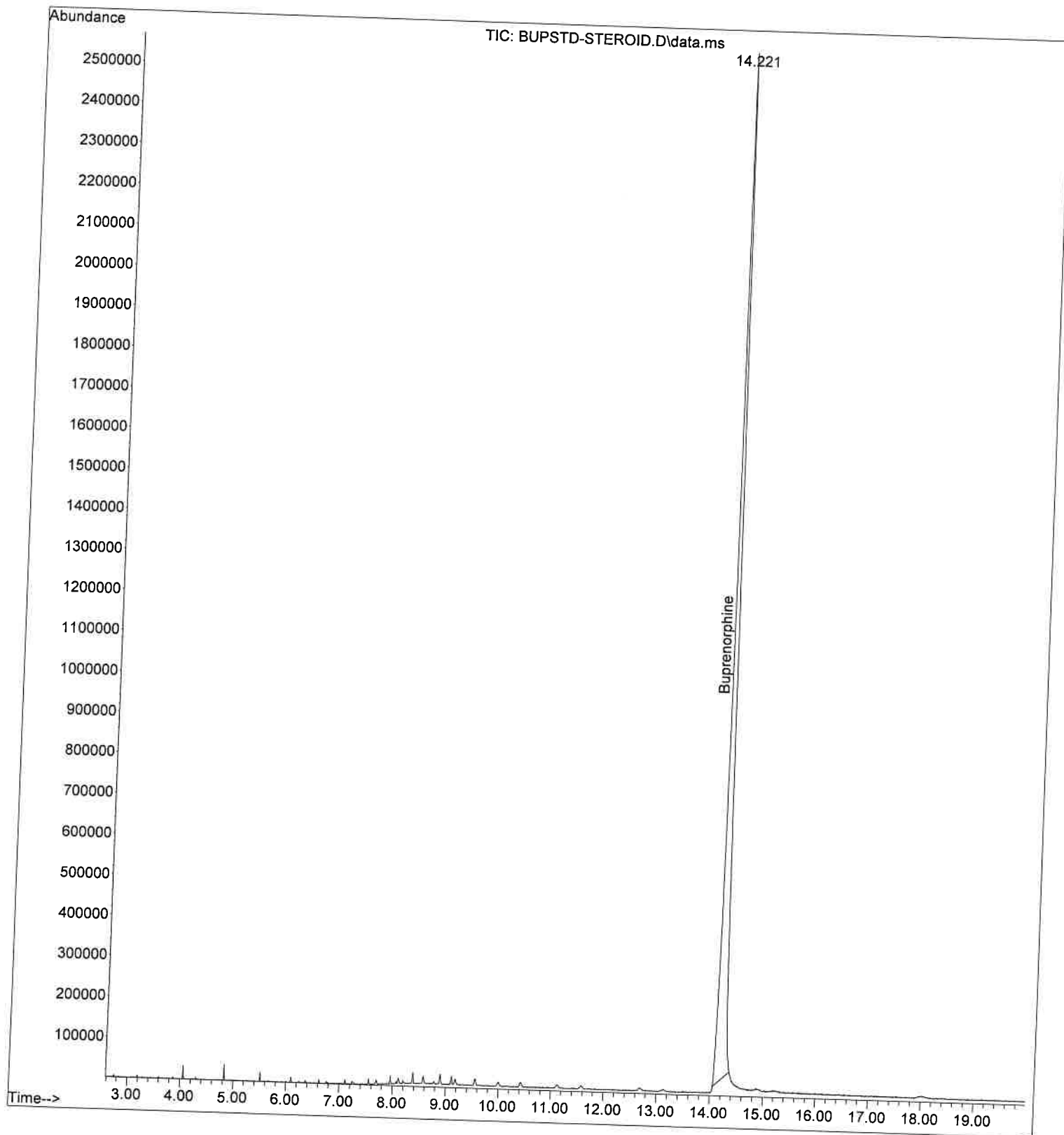
END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

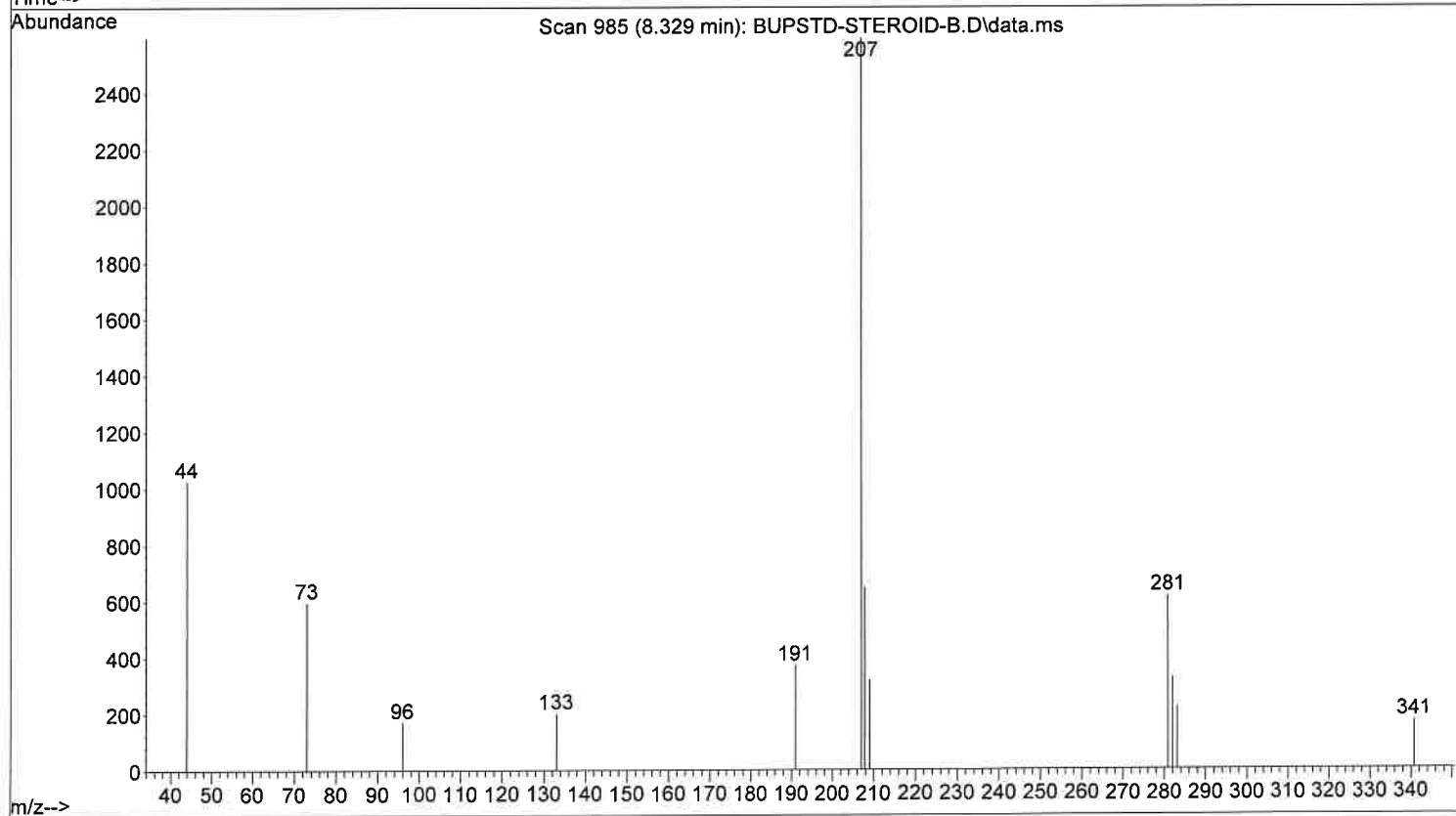
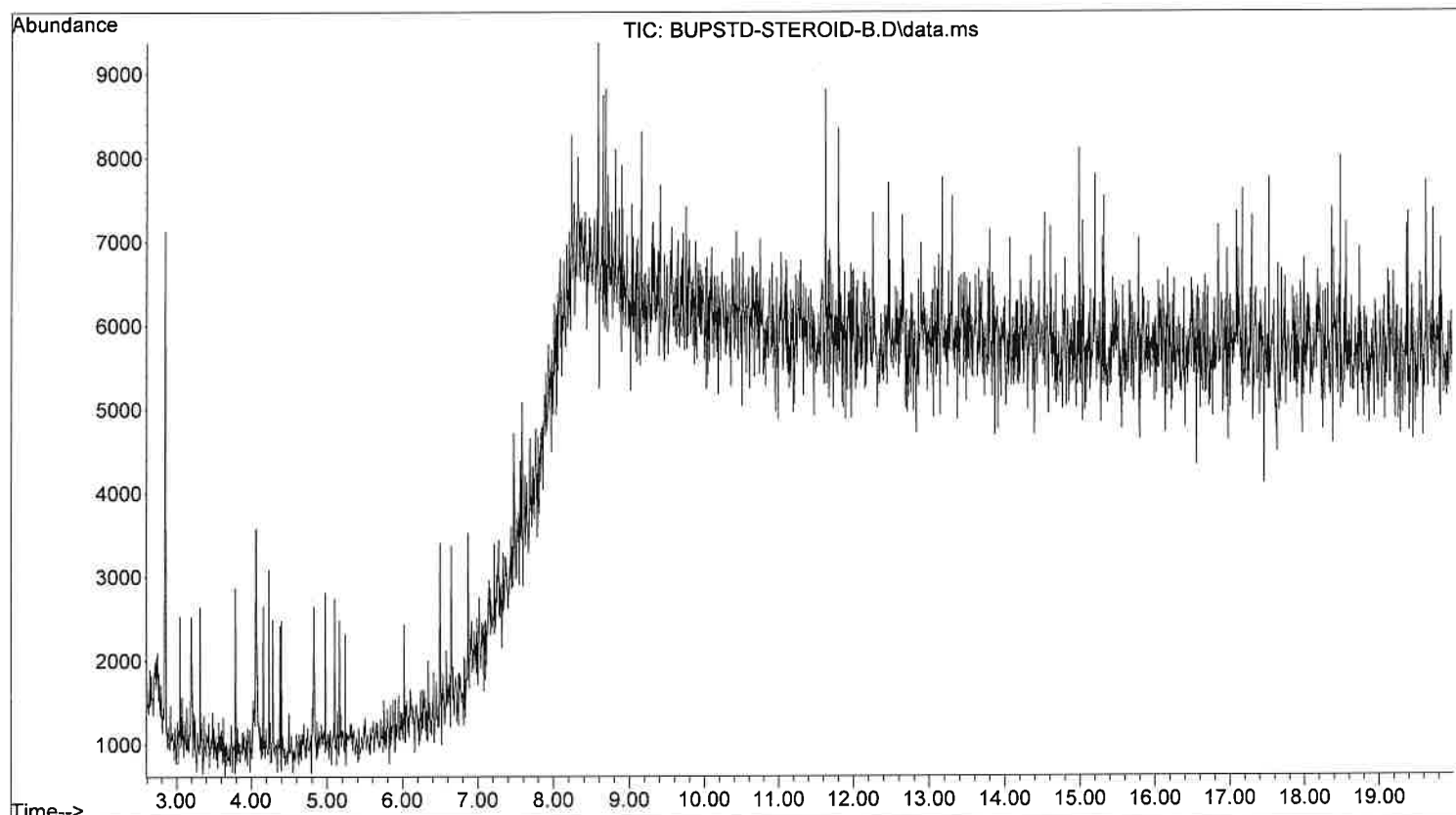
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\BUPSTD-STERIOD.D
Operator : KLAB
Acquired : 22 Aug 2023 15:15 using AcqMethod STERIOD.M
Instrument : Buttercup
Sample Name: Burprenorphine Standard
Misc Info : MEOH
Vial Number: 5



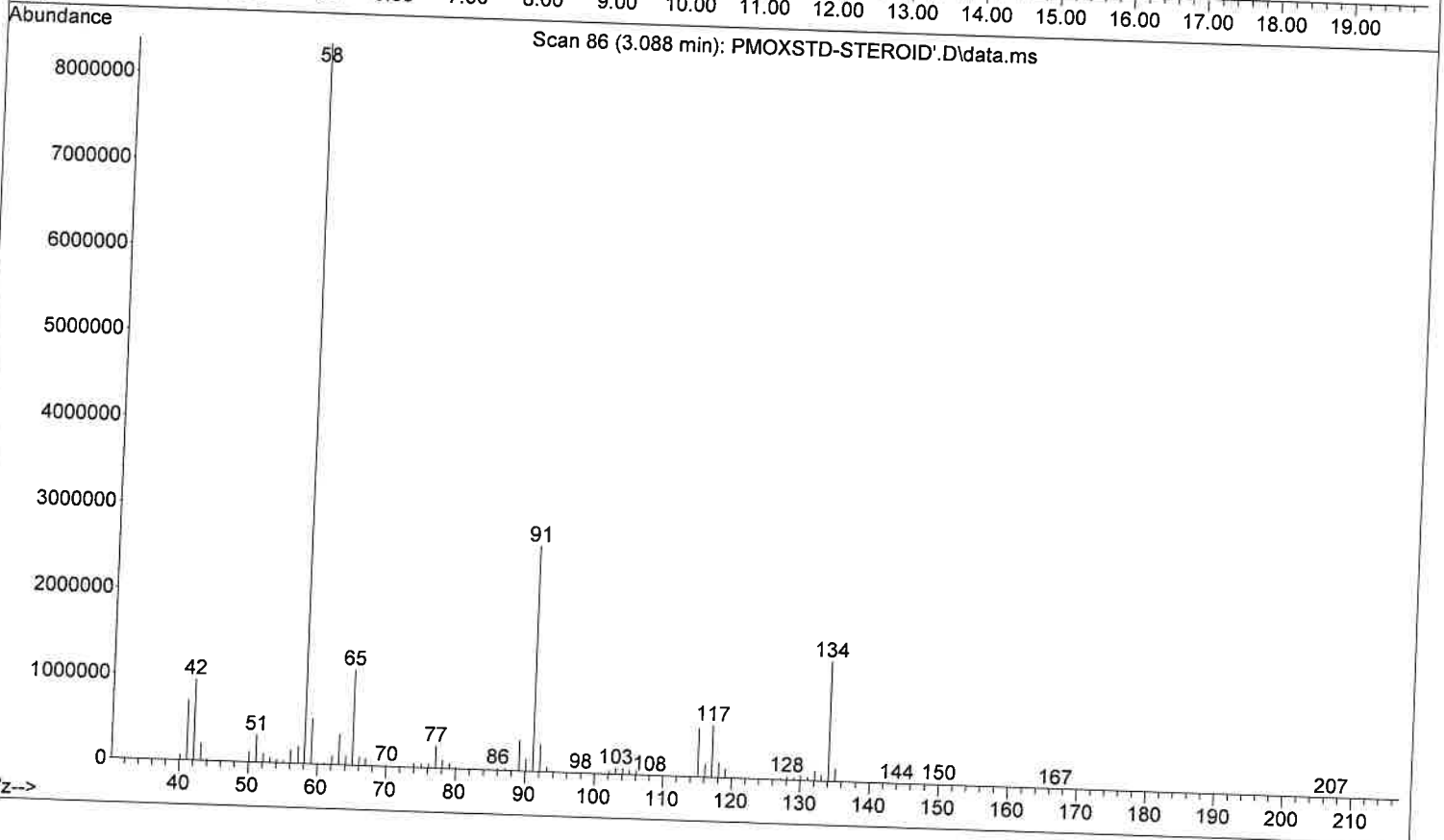
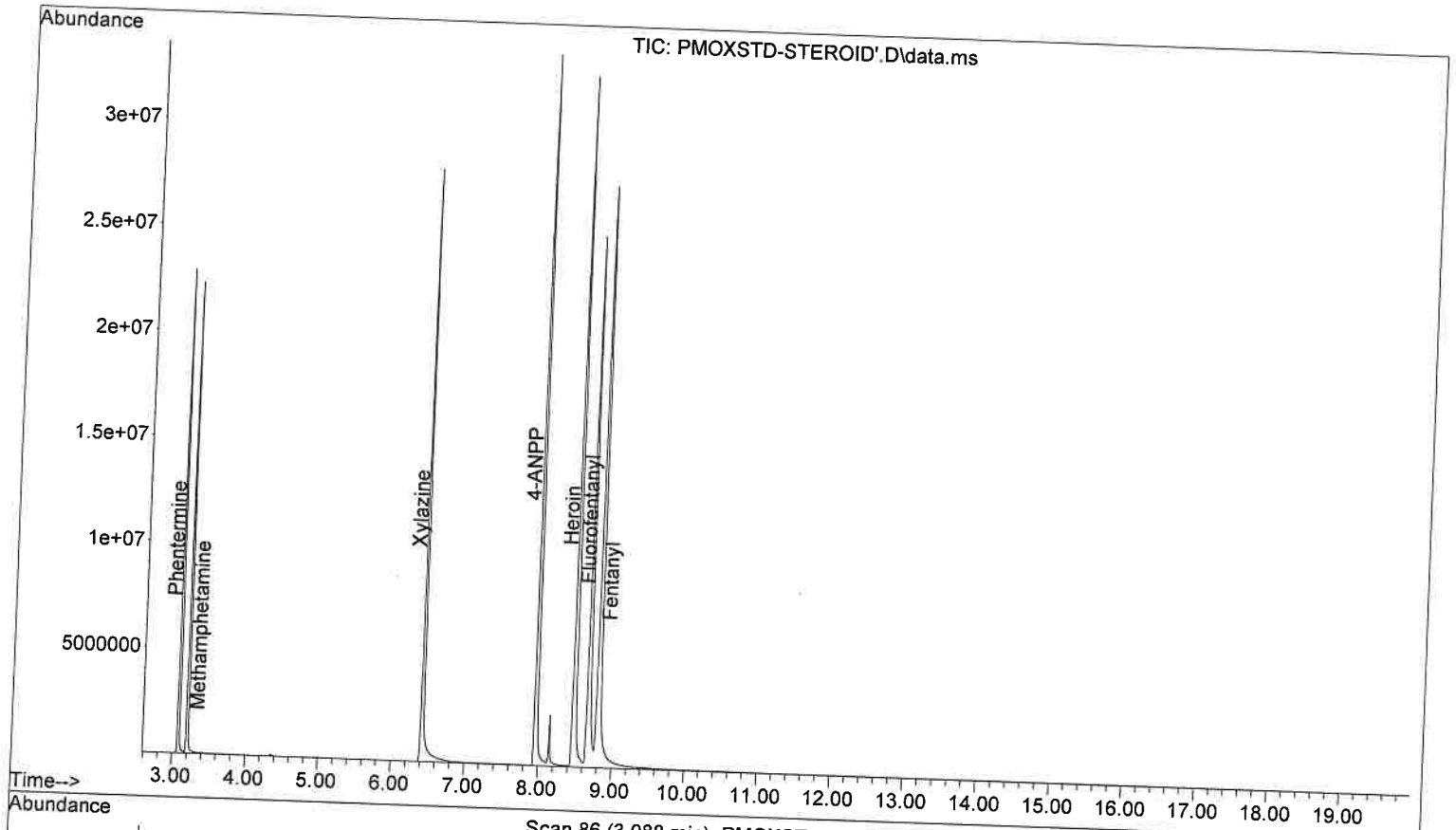
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\BUPSTD-STEROID.D
Operator : KLAB
Acquired : 22 Aug 2023 15:15 using AcqMethod STEROID.M
Instrument : Buttercup
Sample Name: Burprenorphine Standard
Misc Info : MEOH
Vial Number: 5



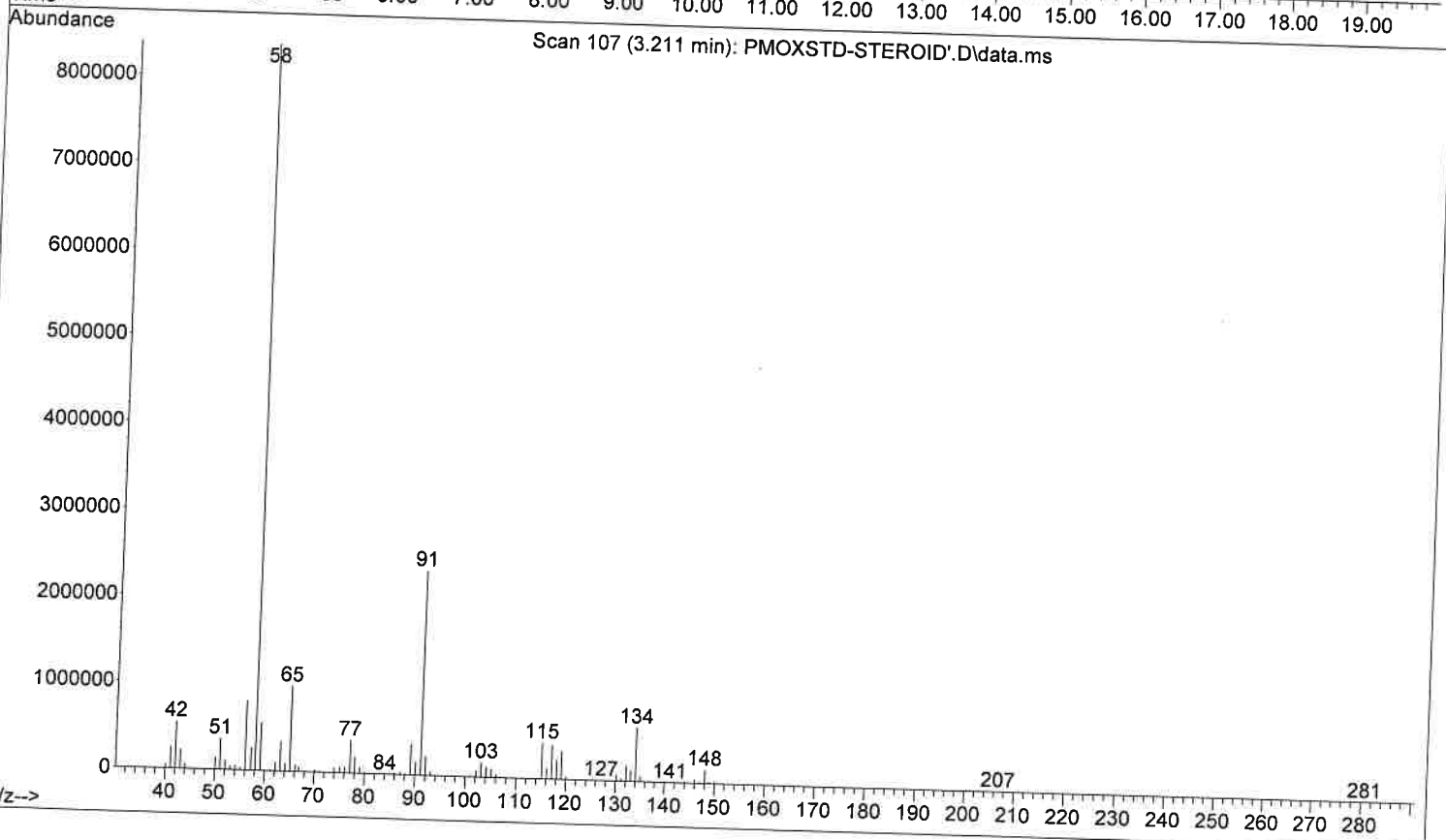
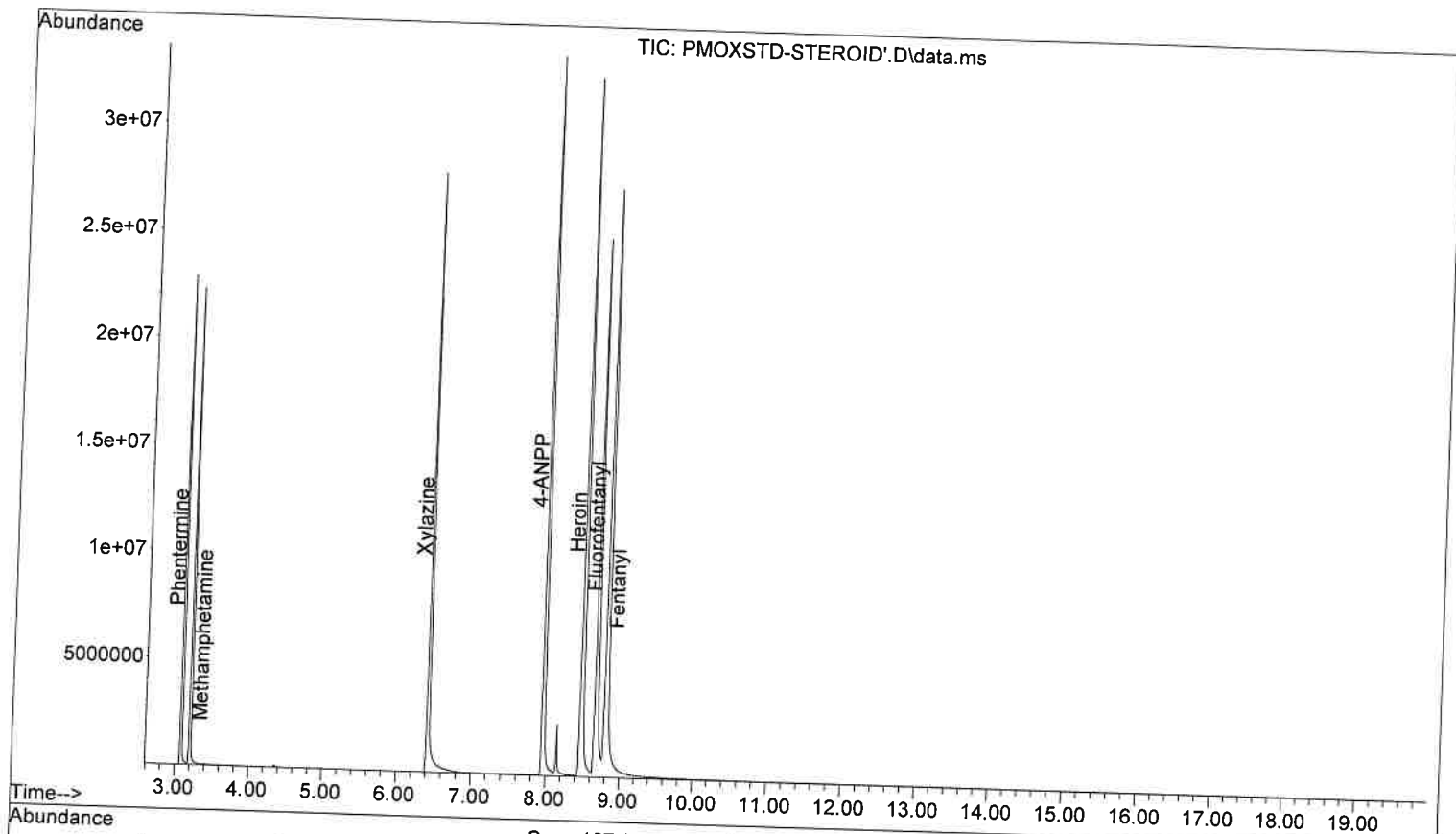
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\BUPSTD-STERIOD-B
... .D
Operator : KLAB
Acquired : 22 Aug 2023 14:52 using AcqMethod STERIOD.M
Instrument : Buttercup
Sample Name: Methanol blank
Misc Info : For Buprenorphine
Vial Number: 1



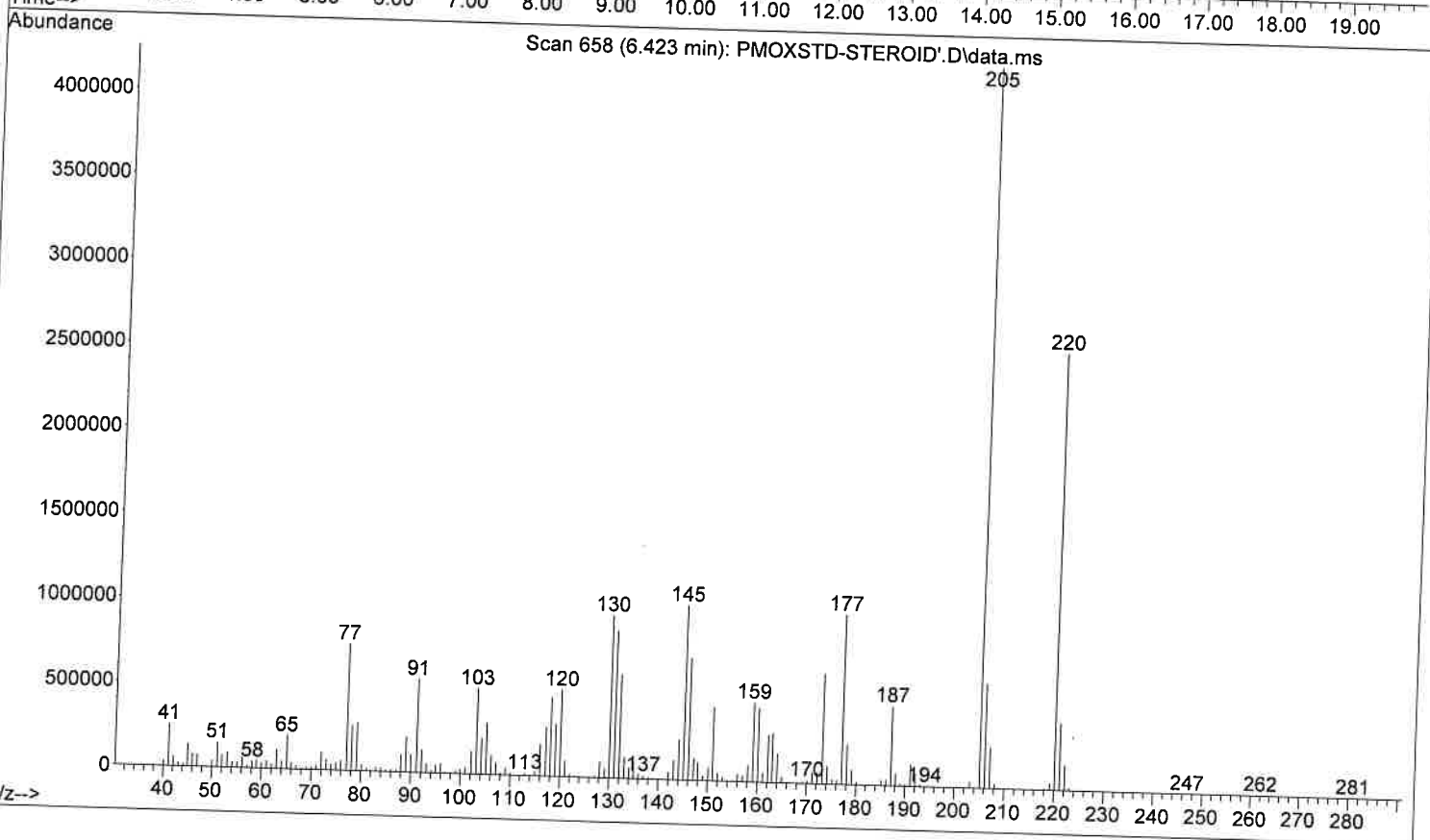
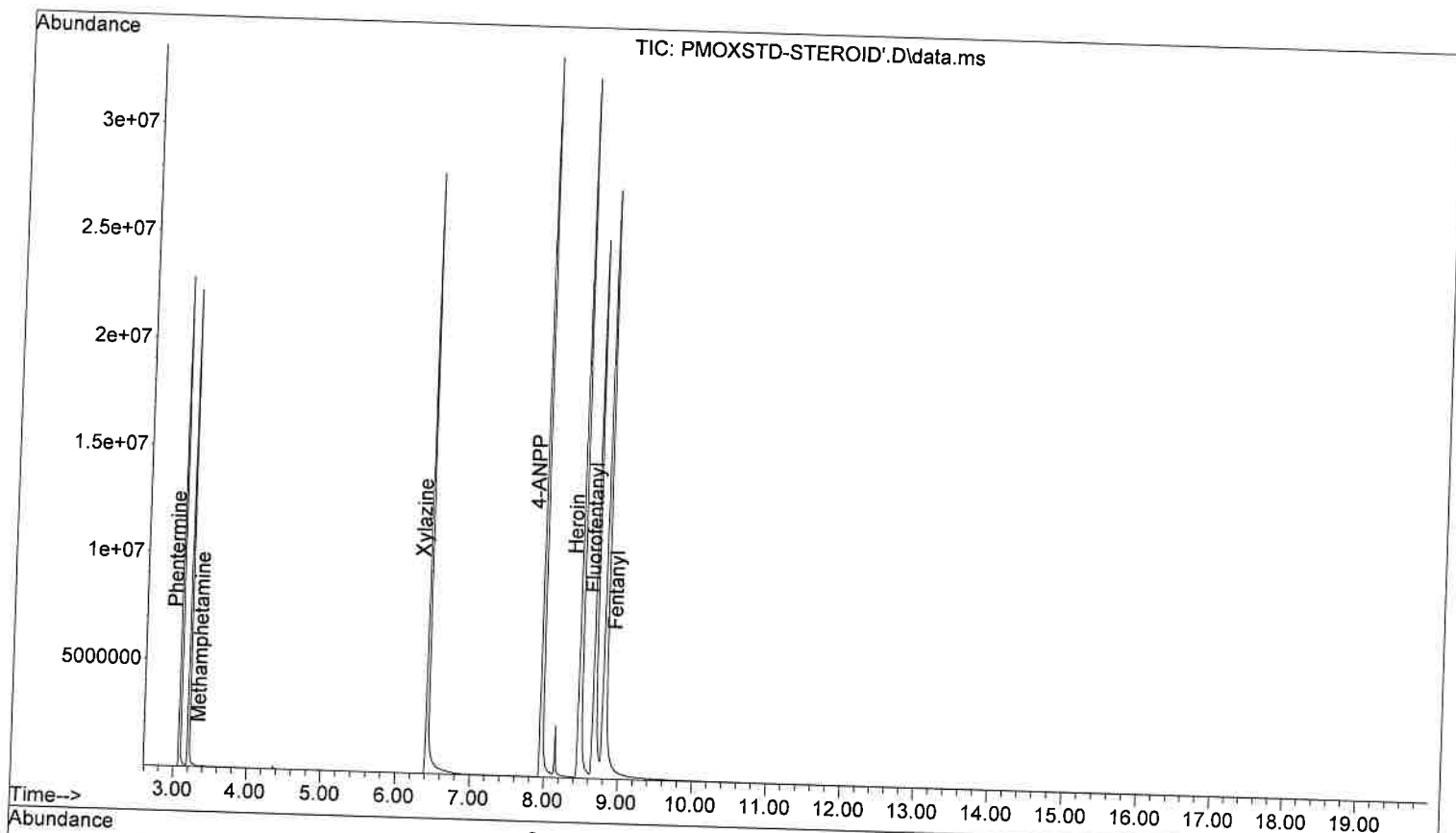
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-STEROID'
... .D
Operator : KLAB
Acquired : 23 Aug 2023 10:24 using AcqMethod STEROID.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 4



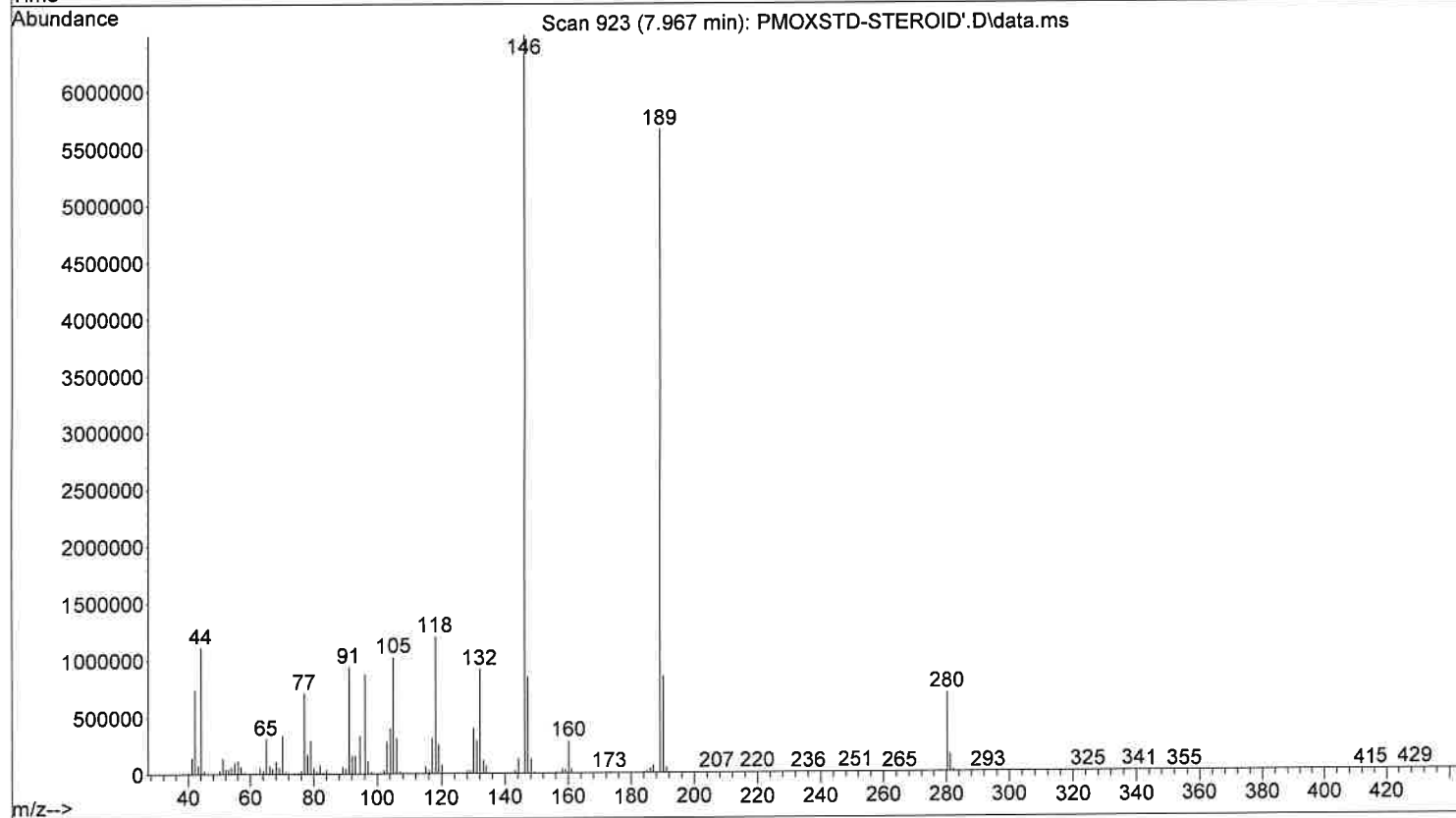
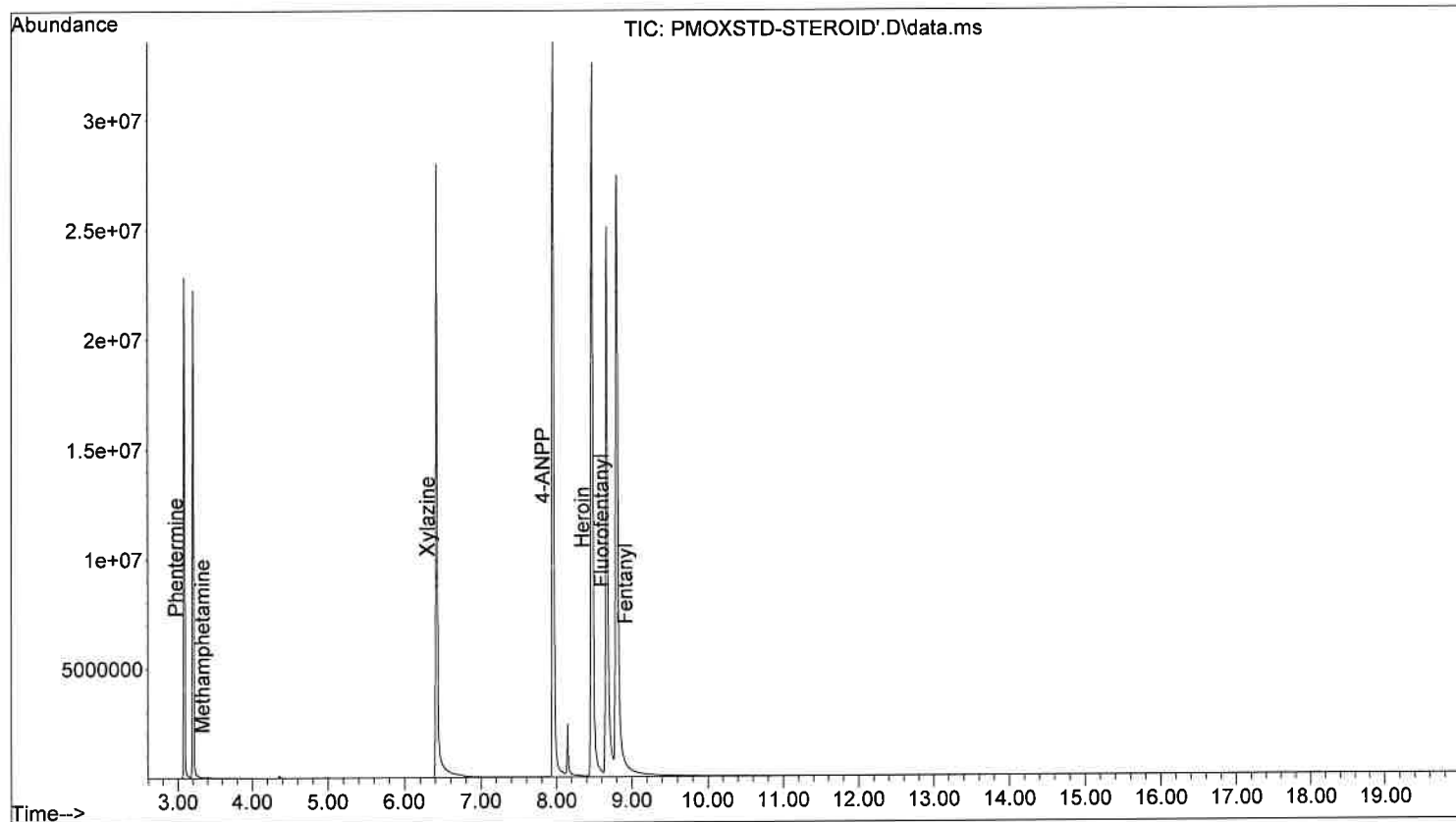
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-STEROID'
... .D
Operator : KLAB
Acquired : 23 Aug 2023 10:24 using AcqMethod STEROID.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHC13
Vial Number: 4



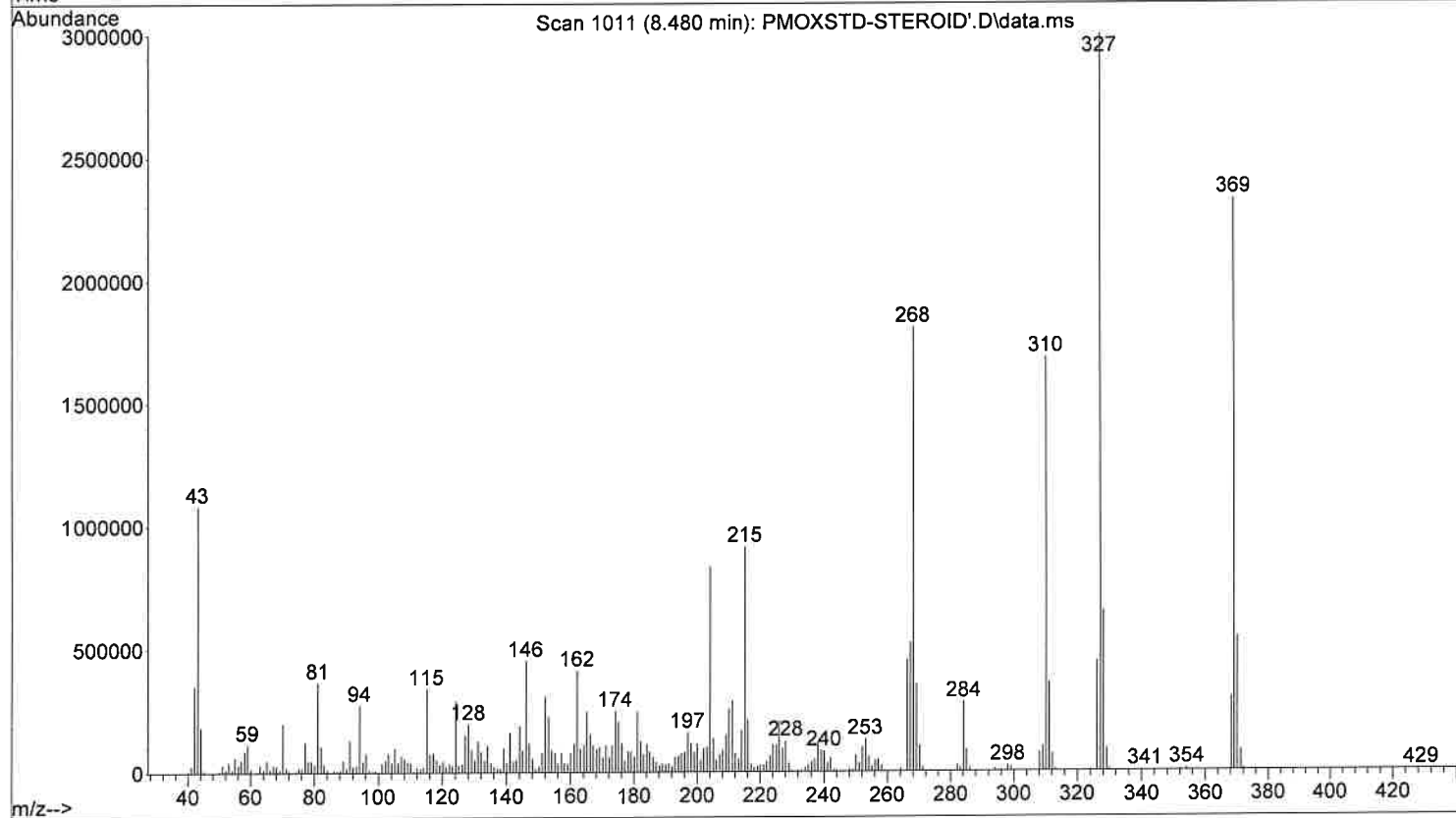
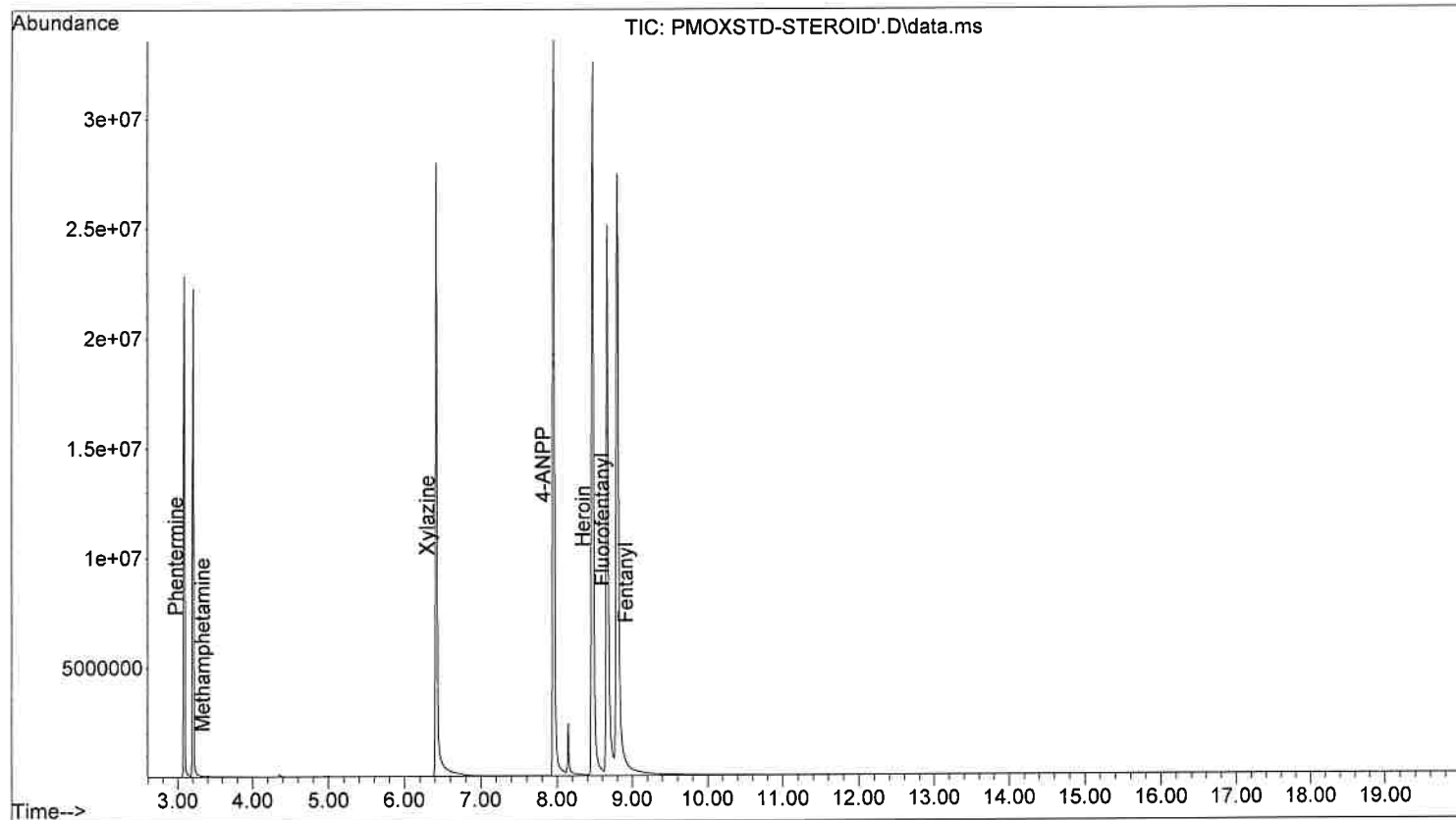
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-STEROID'
... .D
Operator : KLAB
Acquired : 23 Aug 2023 10:24 using AcqMethod STERIOD.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 4



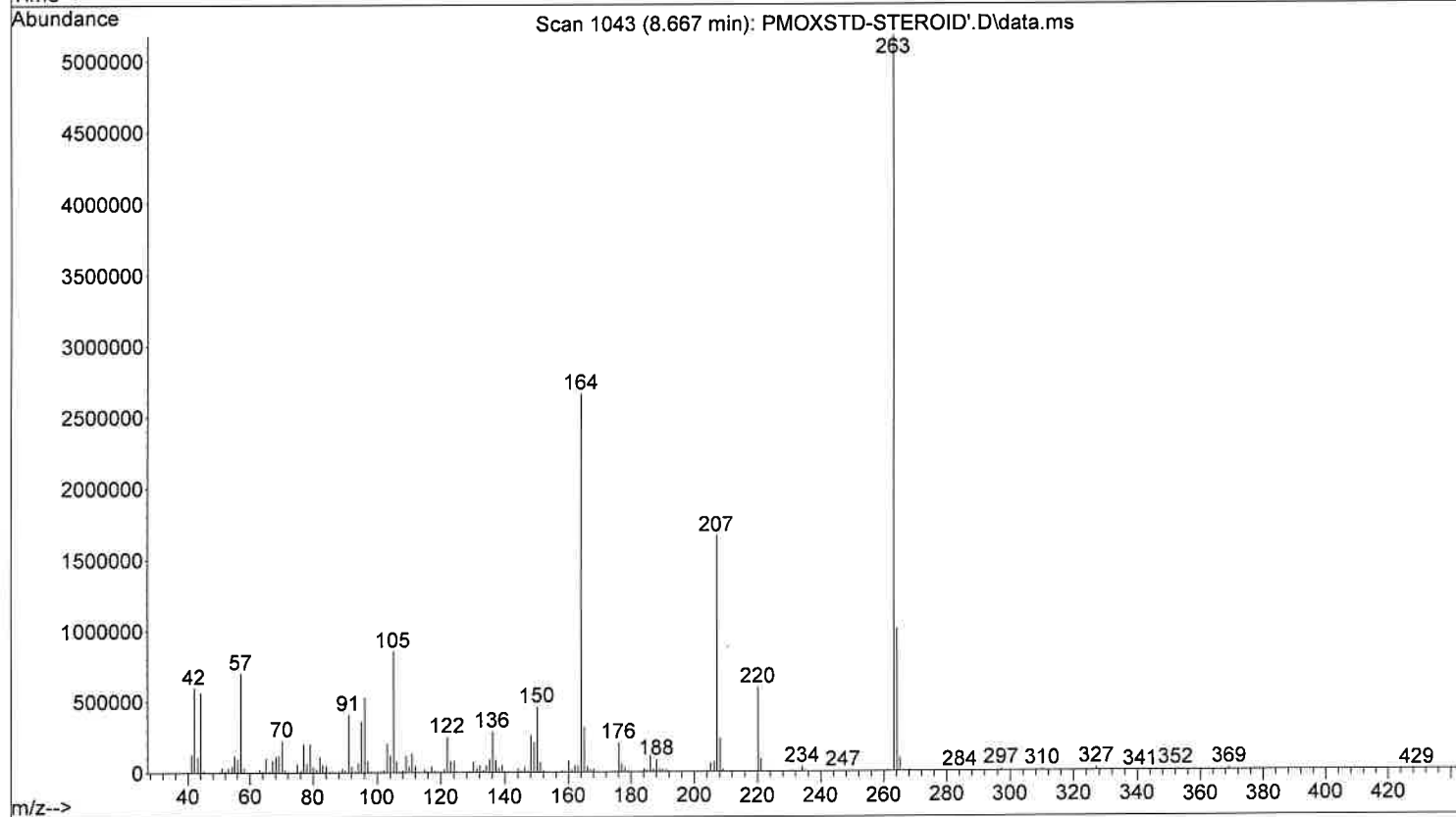
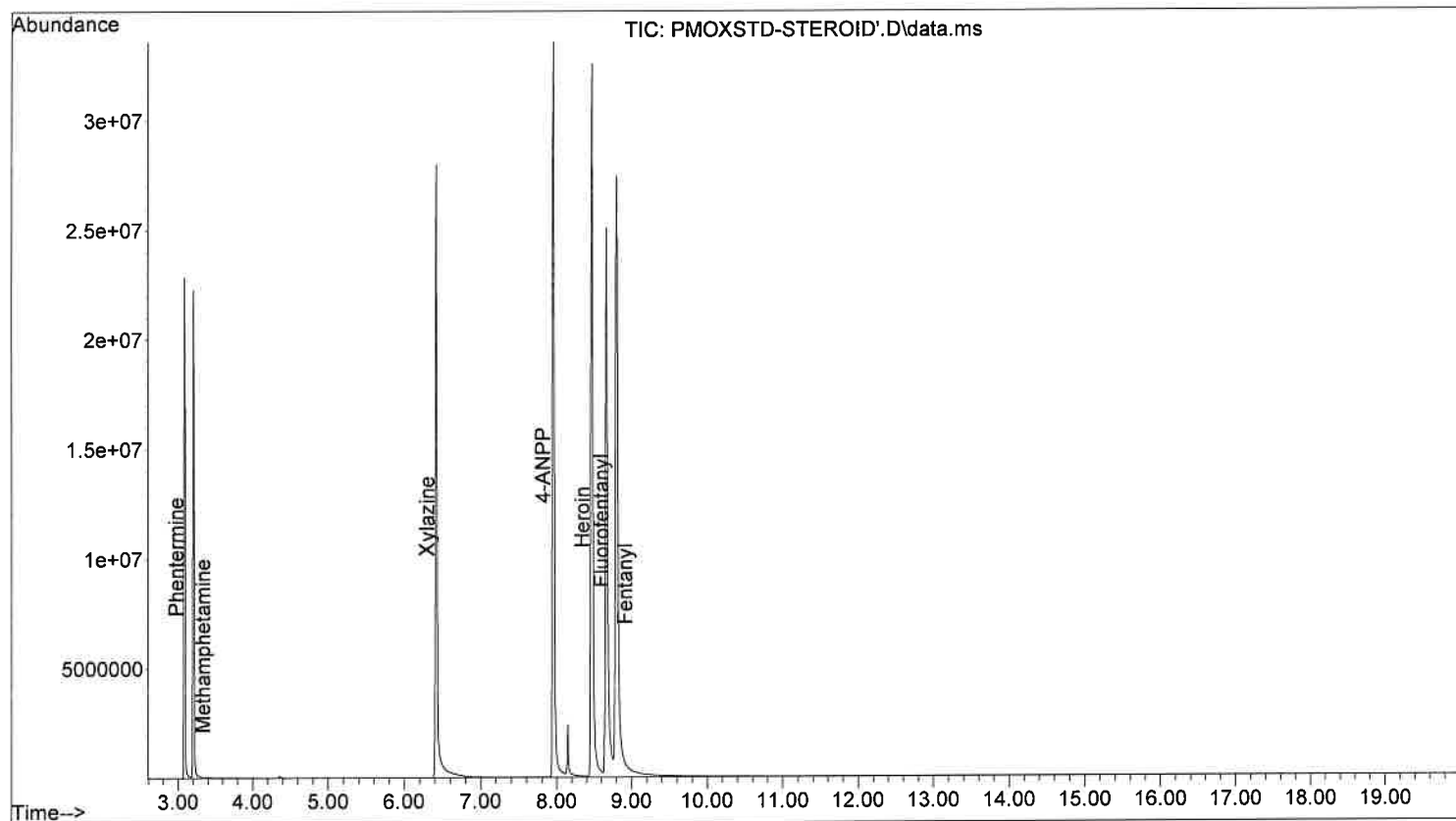
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-STEROID'
... .D
Operator : KLAB
Acquired : 23 Aug 2023 10:24 using AcqMethod STERIOD.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 4



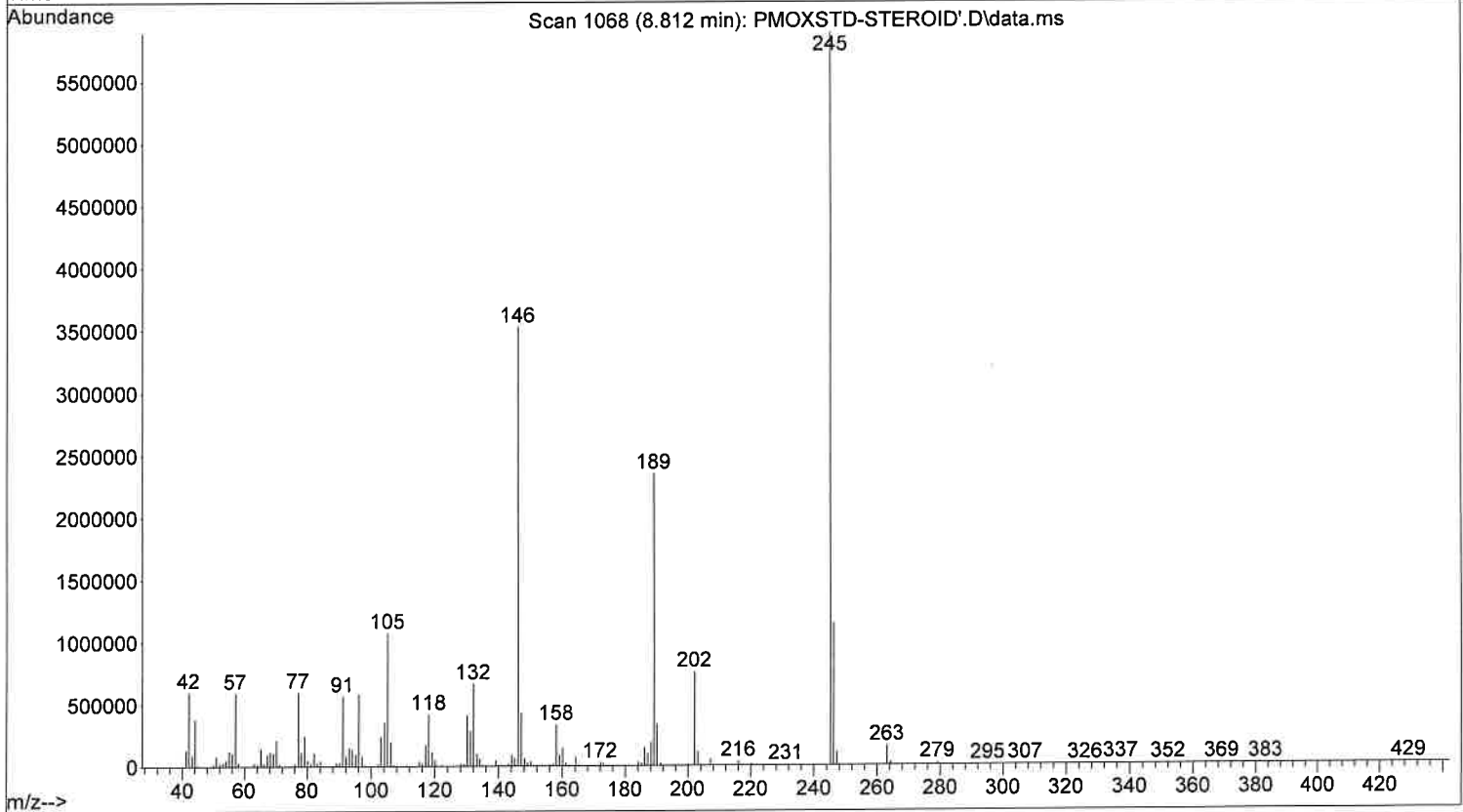
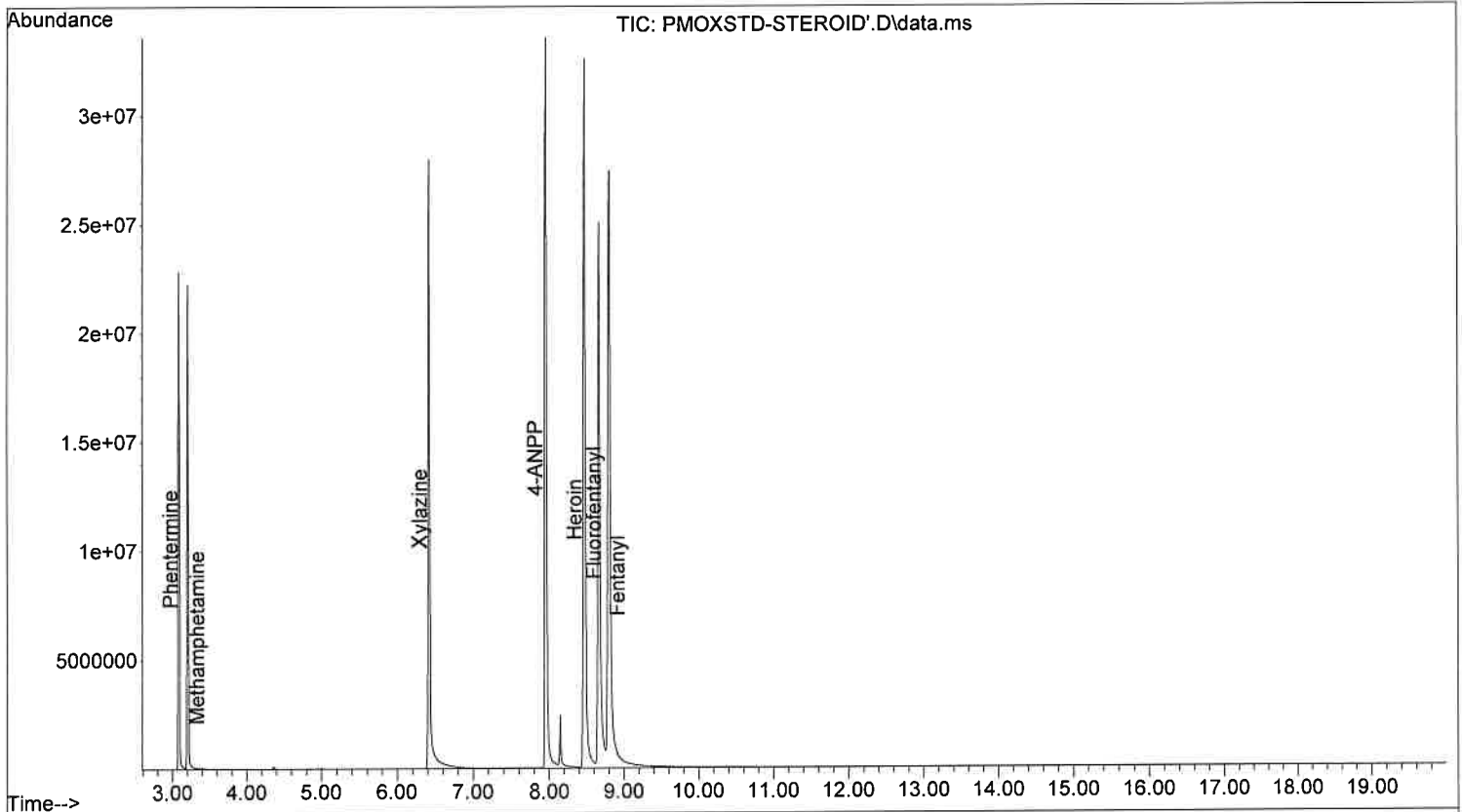
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-STERIOD'
... .D
Operator : KLAB
Acquired : 23 Aug 2023 10:24 using AcqMethod STERIOD.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 4



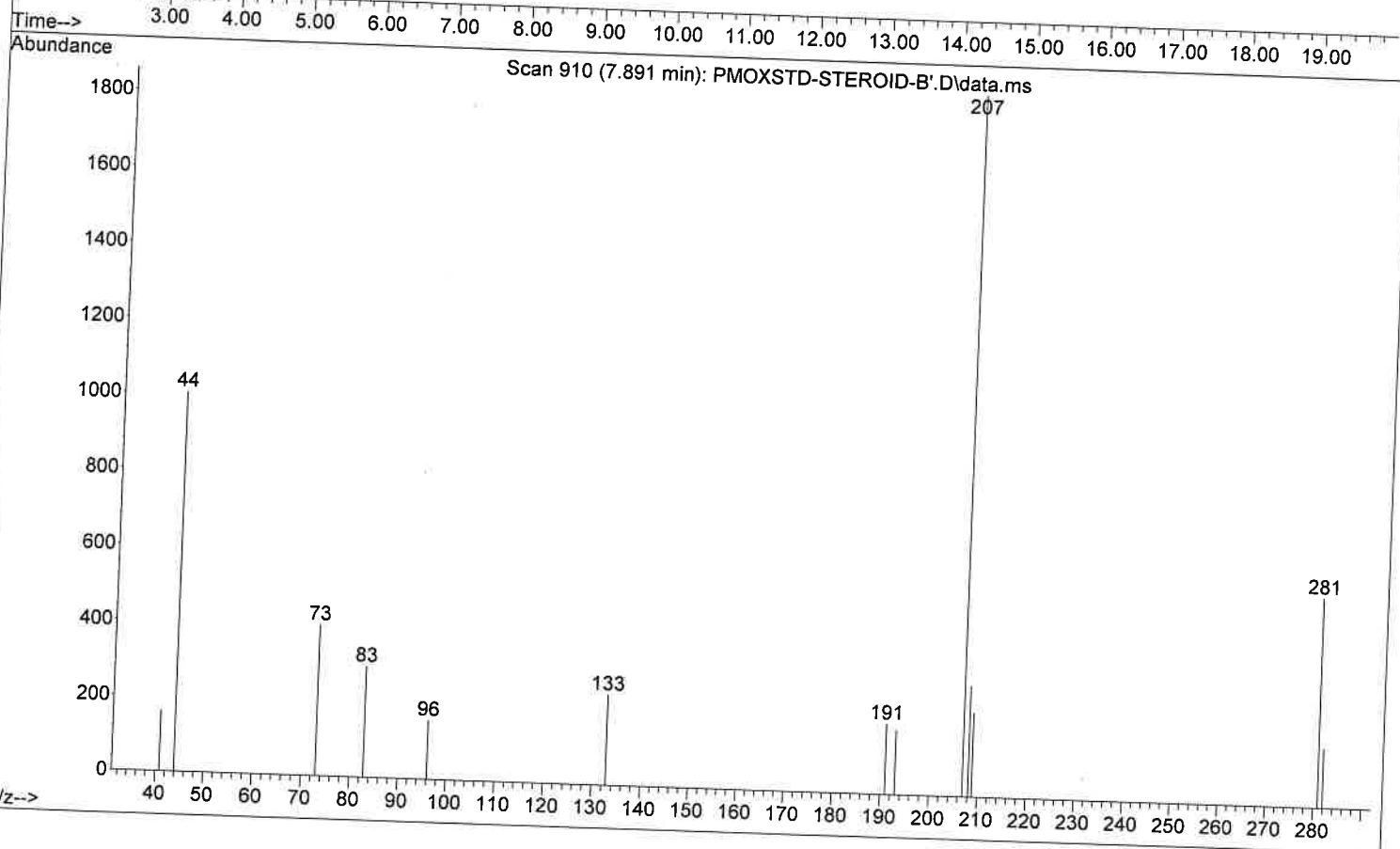
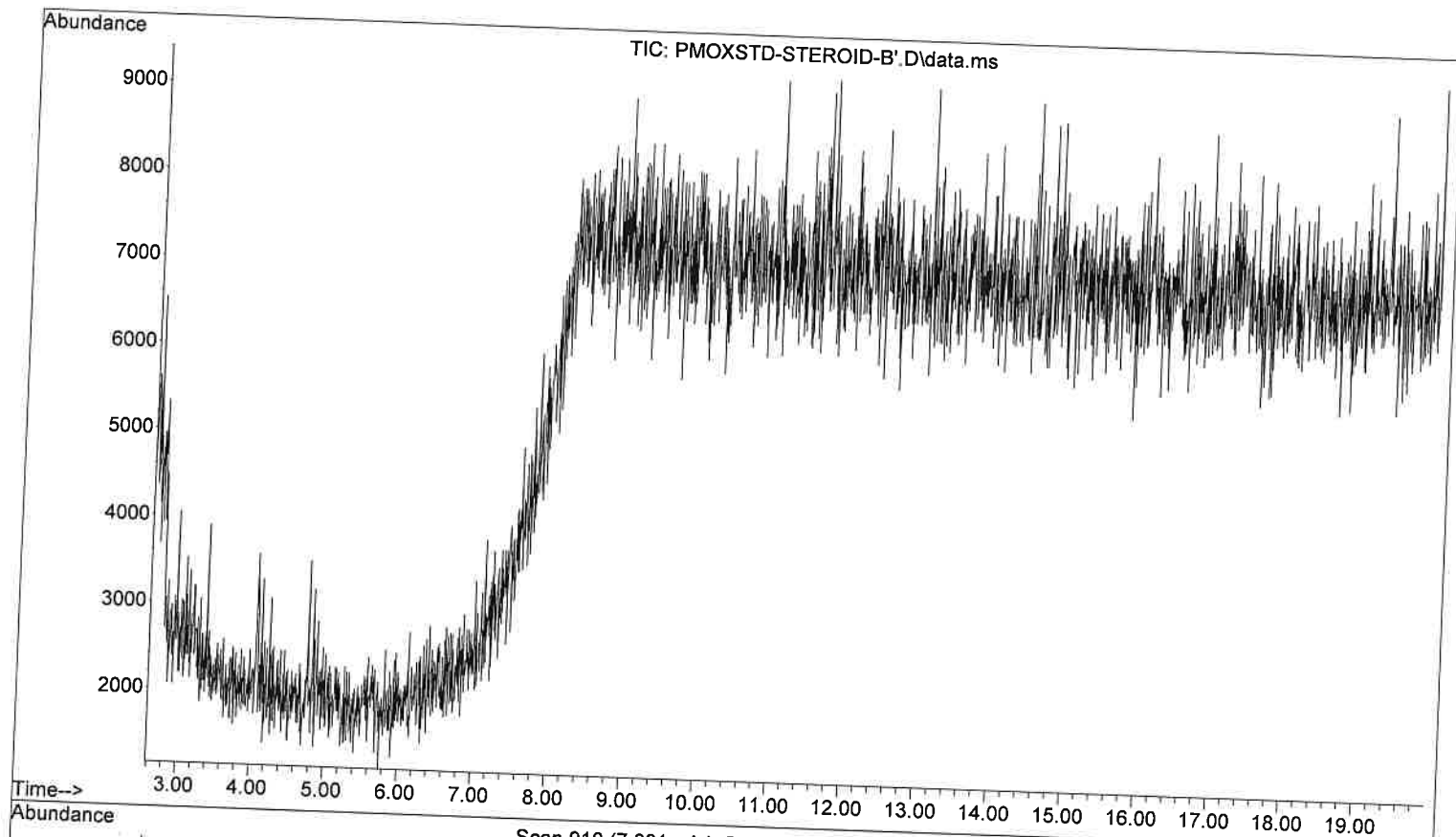
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-STEROID'
... .D
Operator : KLAB
Acquired : 23 Aug 2023 10:24 using AcqMethod STEROID.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 4



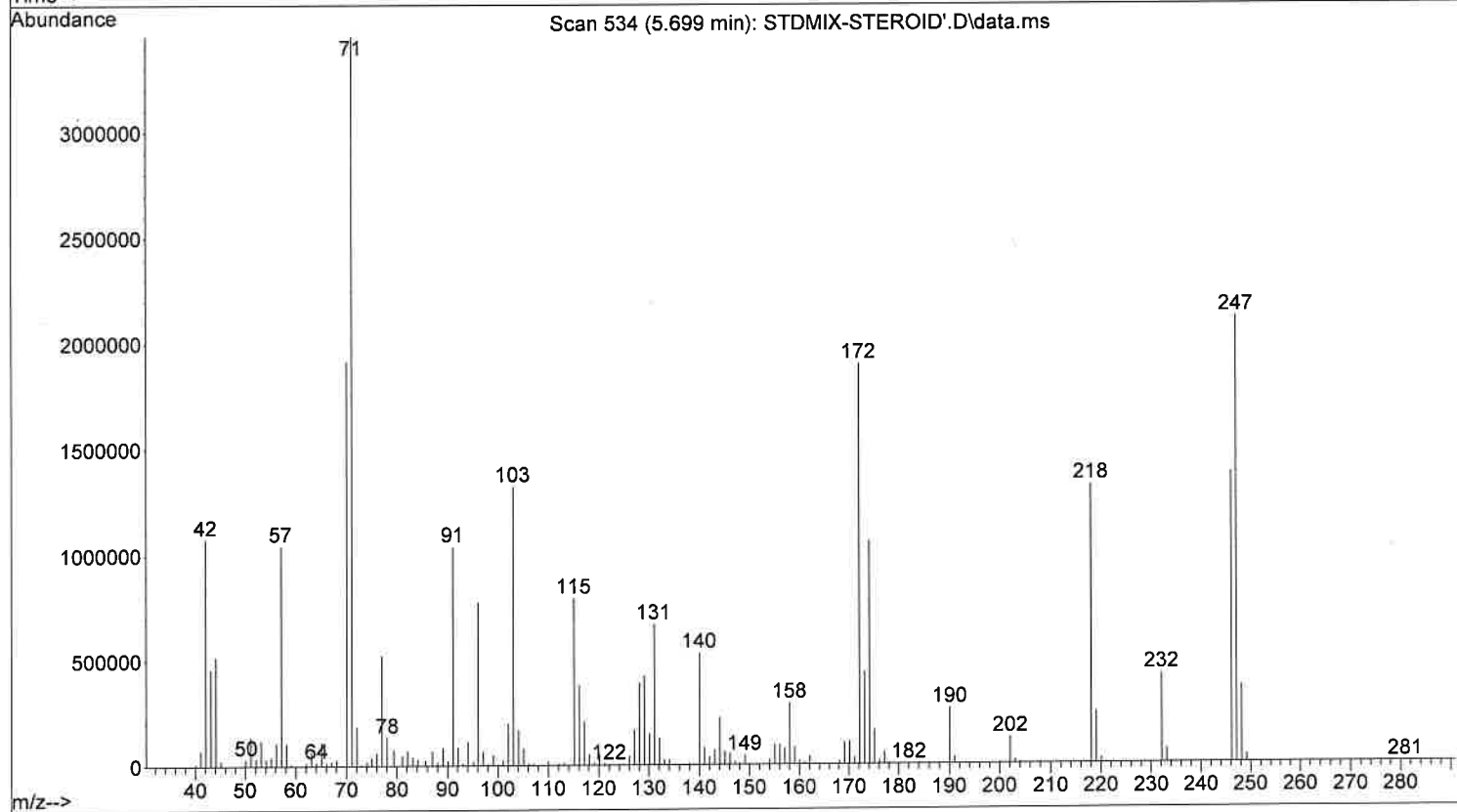
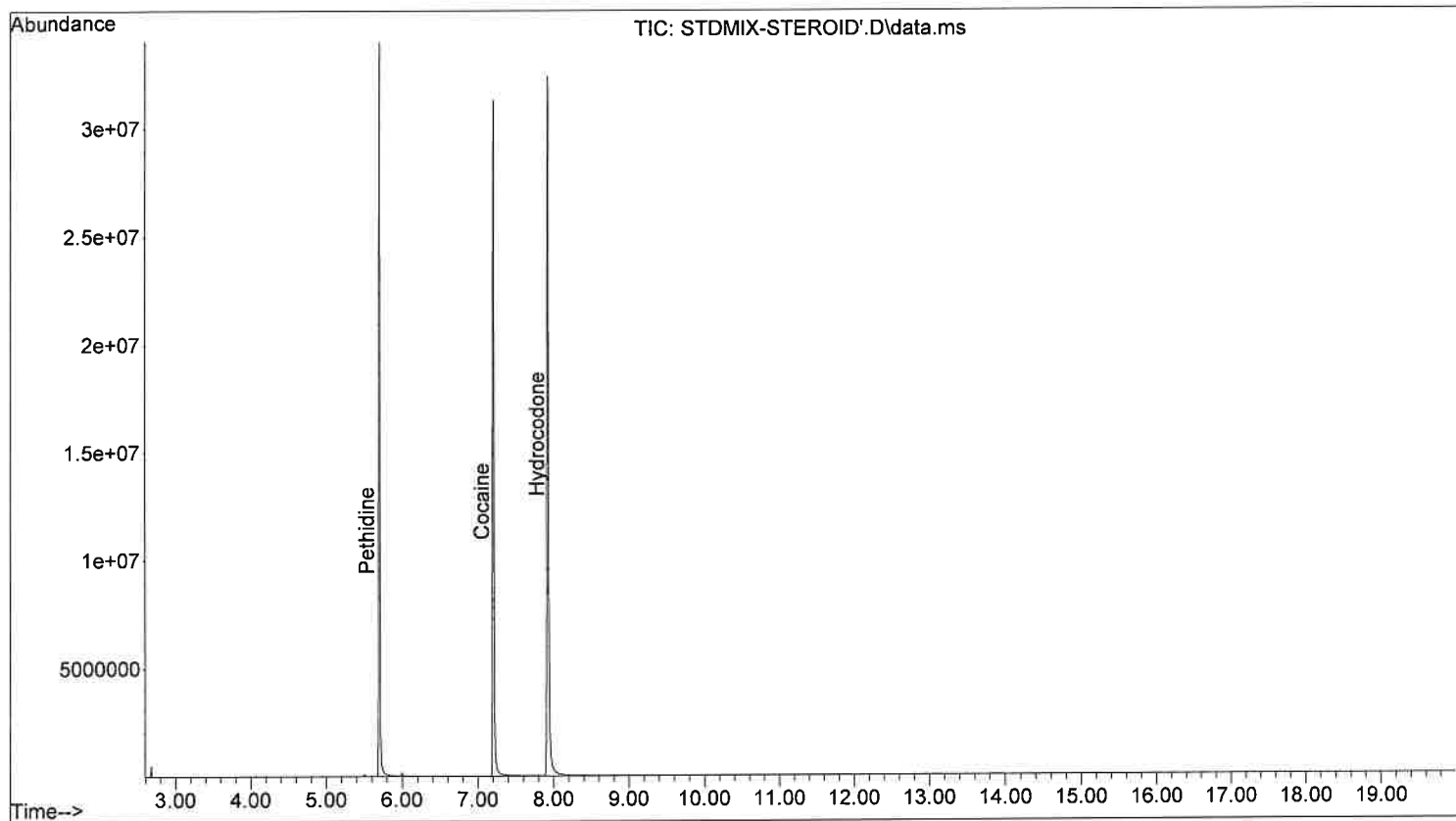
File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\PMOXSTD-STEROID'
... .D
Operator : KLAB
Acquired : 23 Aug 2023 10:24 using AcqMethod STEROID.M
Instrument : Buttercup
Sample Name: P-MOX Standard
Misc Info : CHCl3
Vial Number: 4



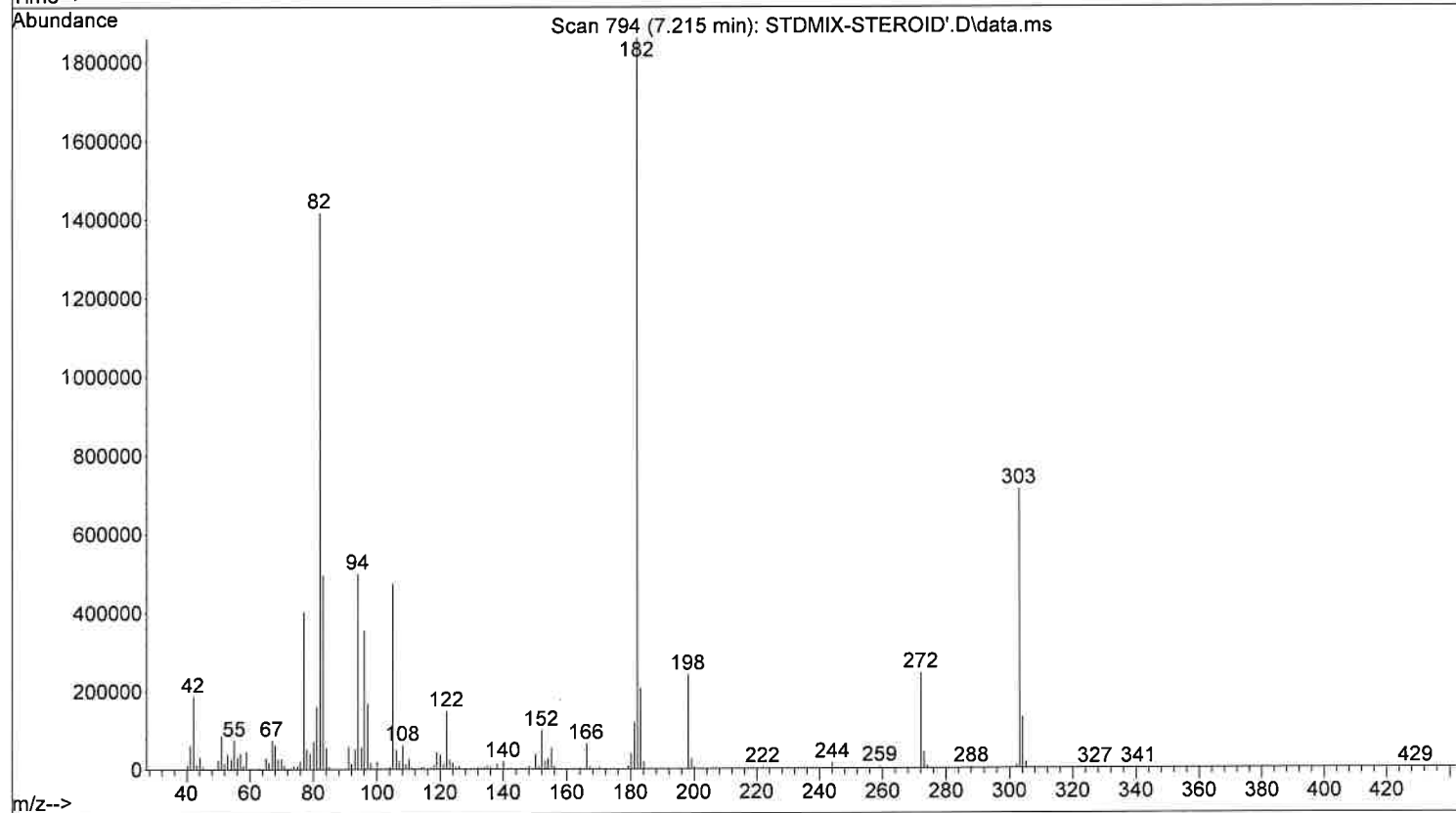
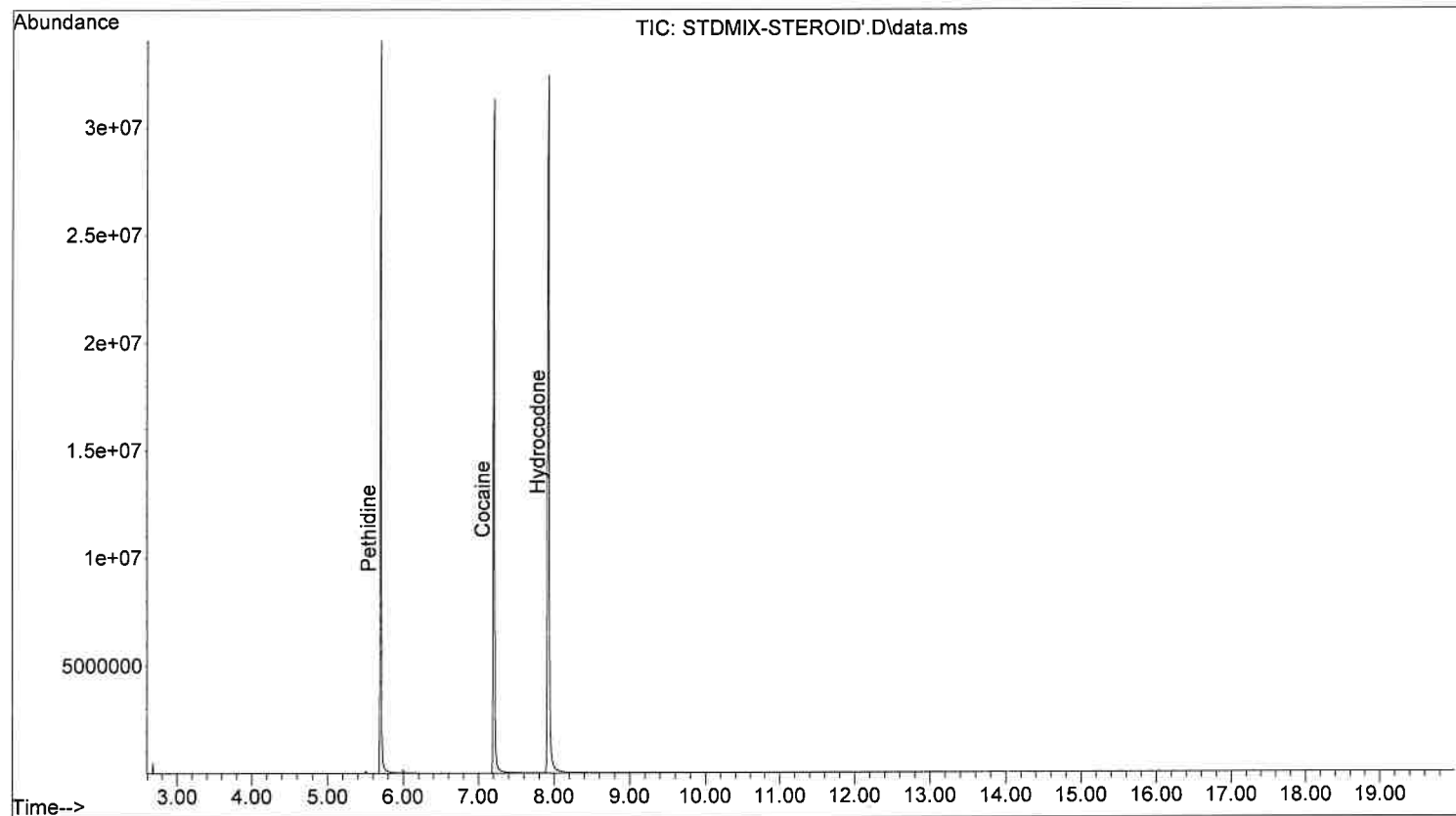
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... B'.D
Operator : KLAB
Acquired : 23 Aug 2023 10:01 using AcqMethod STEROID.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : For P-MOX
Vial Number: 2



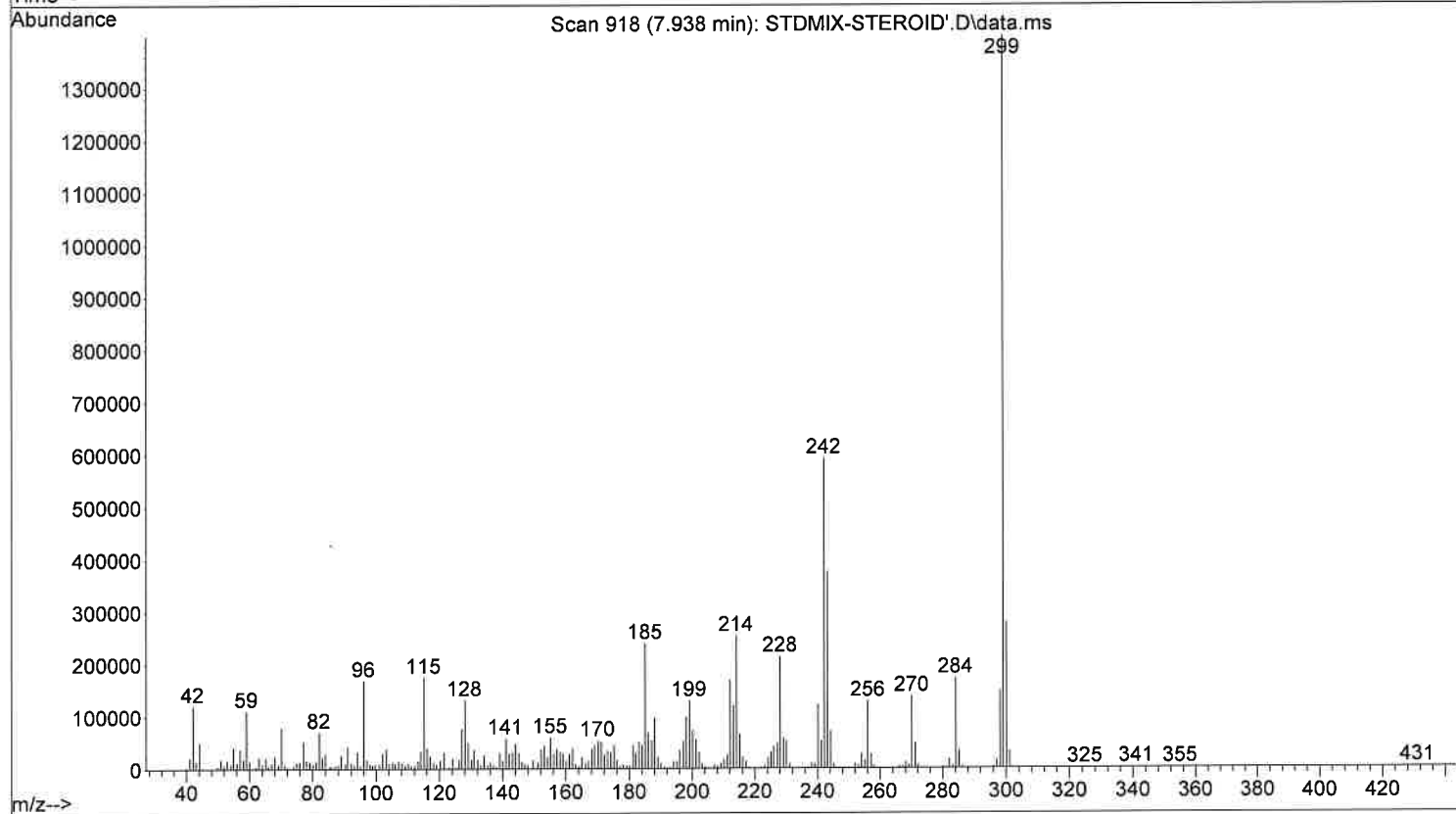
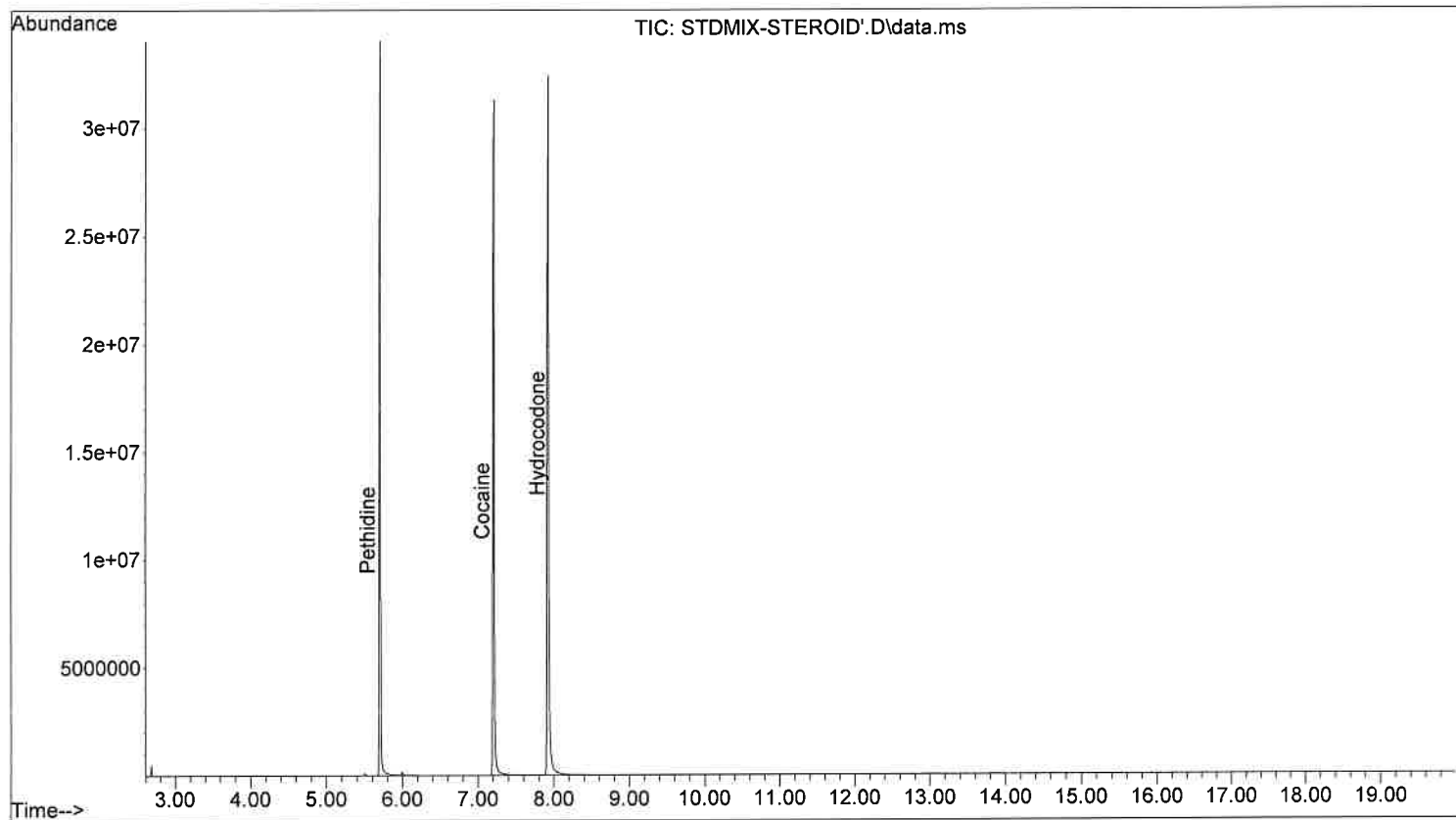
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Operator : KLAB
Acquired : 01 Sep 2023 12:07 using AcqMethod STEROID.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : CHCl3
Vial Number: 2



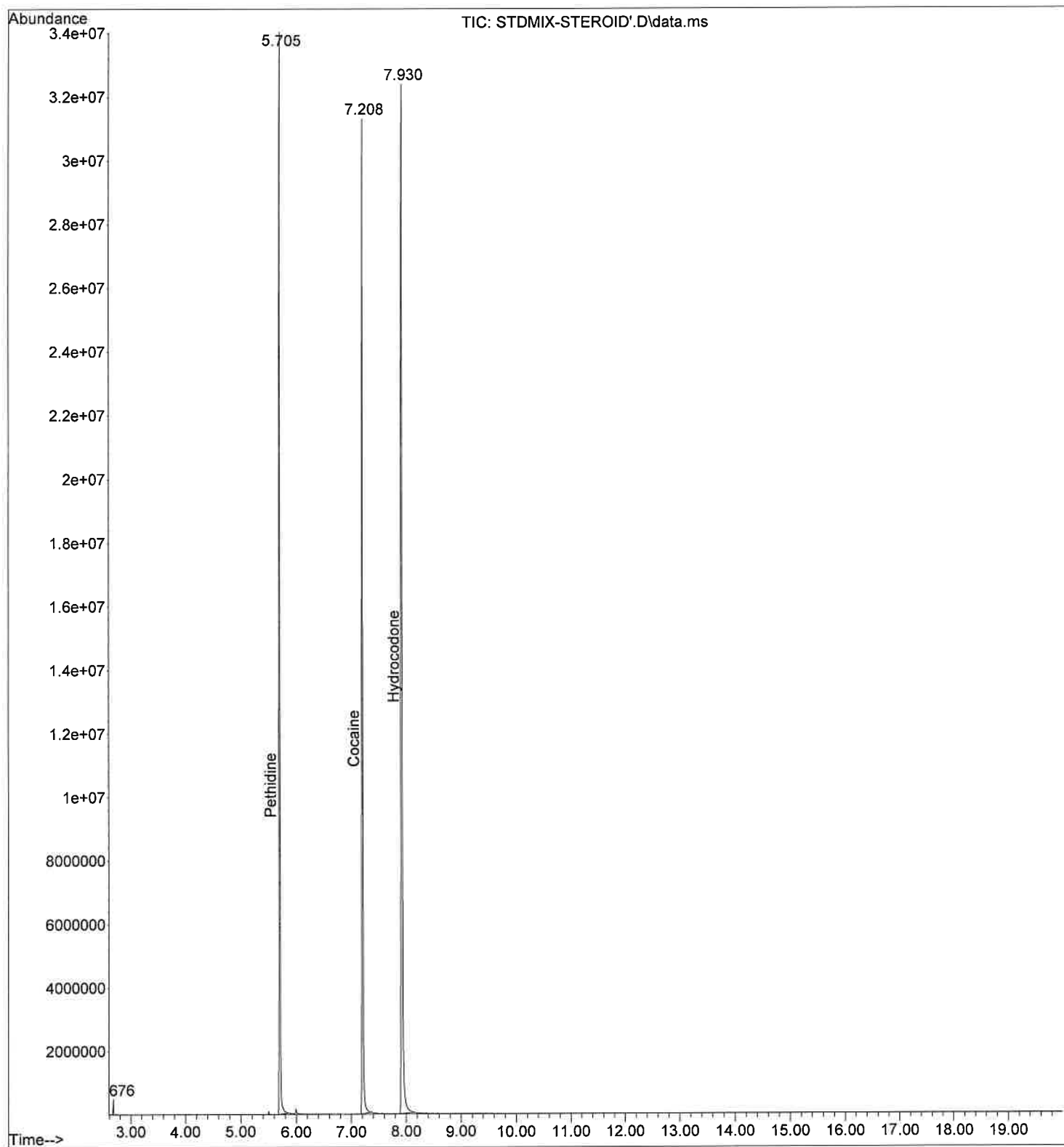
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Operator : KLAB
Acquired : 01 Sep 2023 12:07 using AcqMethod STERIOD.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : CHCl3
Vial Number: 2



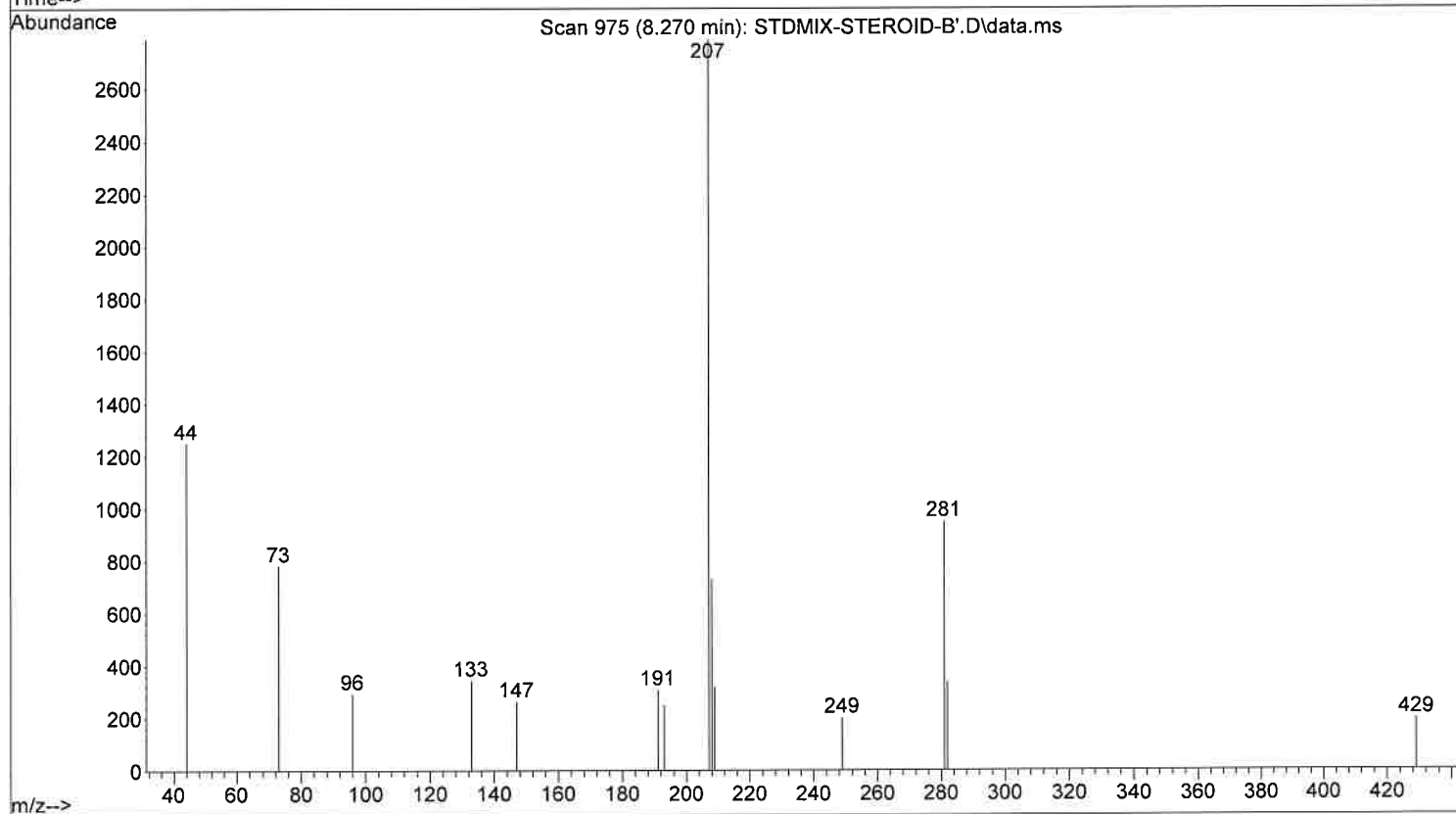
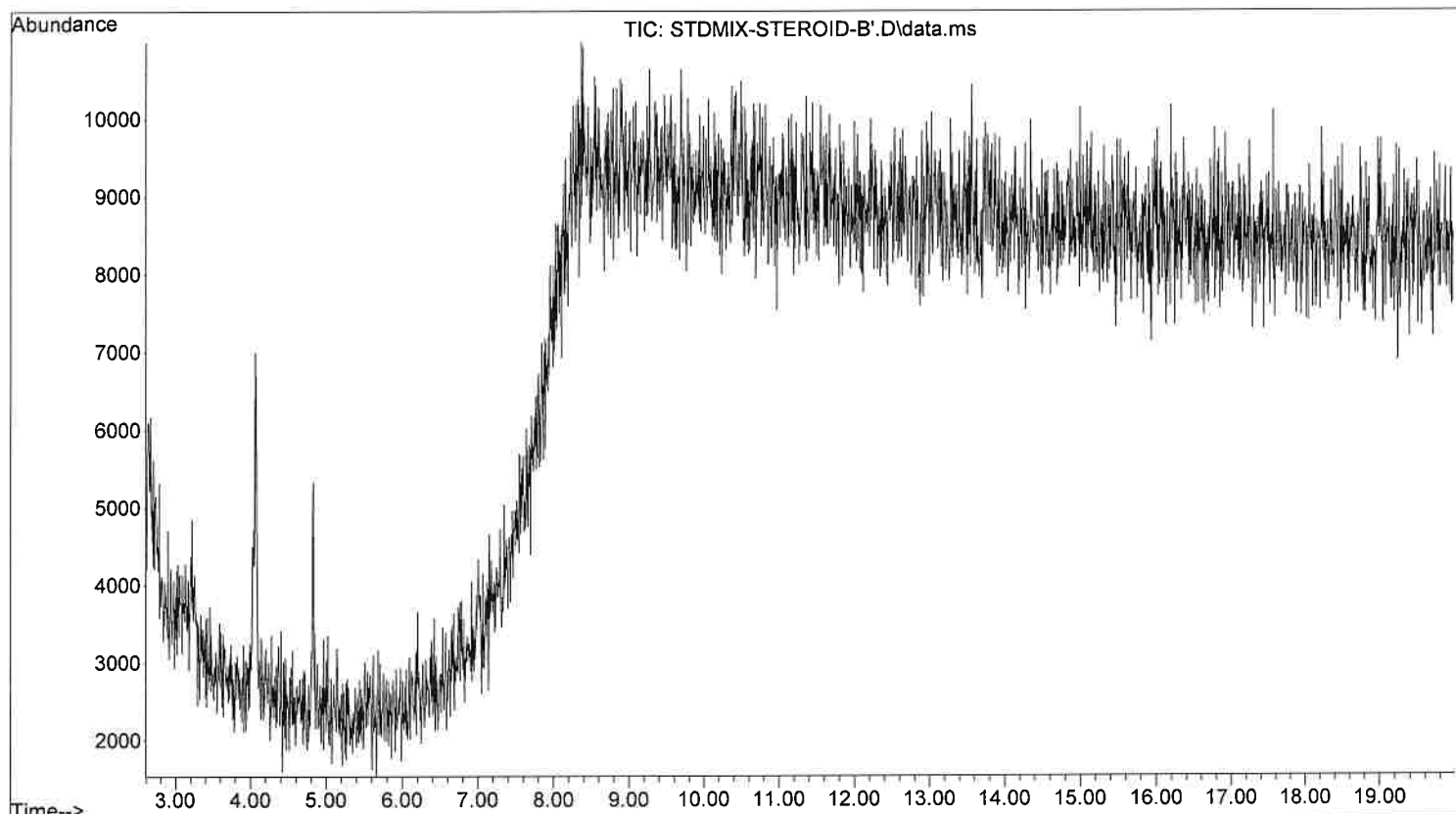
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Operator : KLAB
Acquired : 01 Sep 2023 12:07 using AcqMethod STERIOD.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : CHCl3
Vial Number: 2



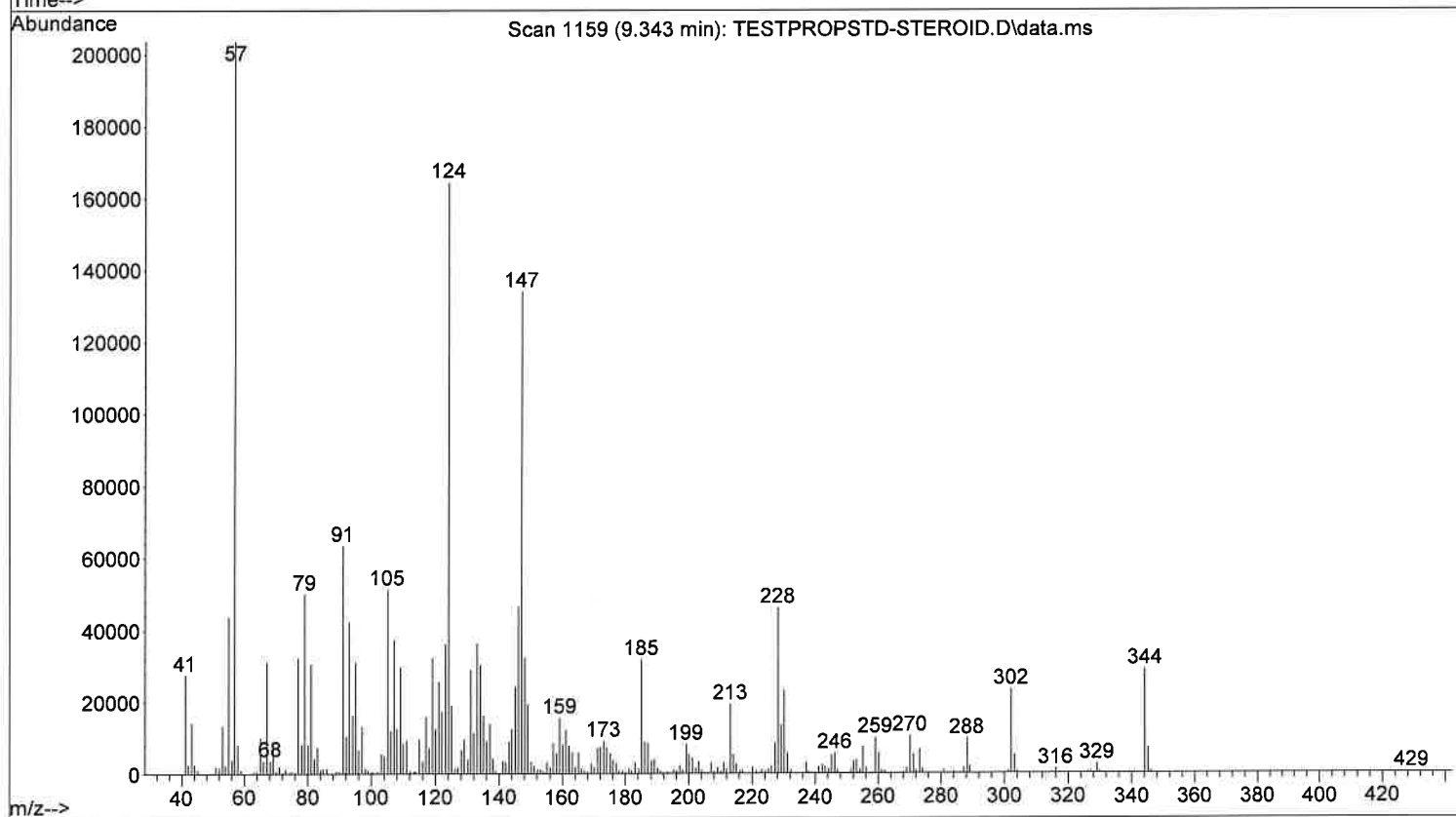
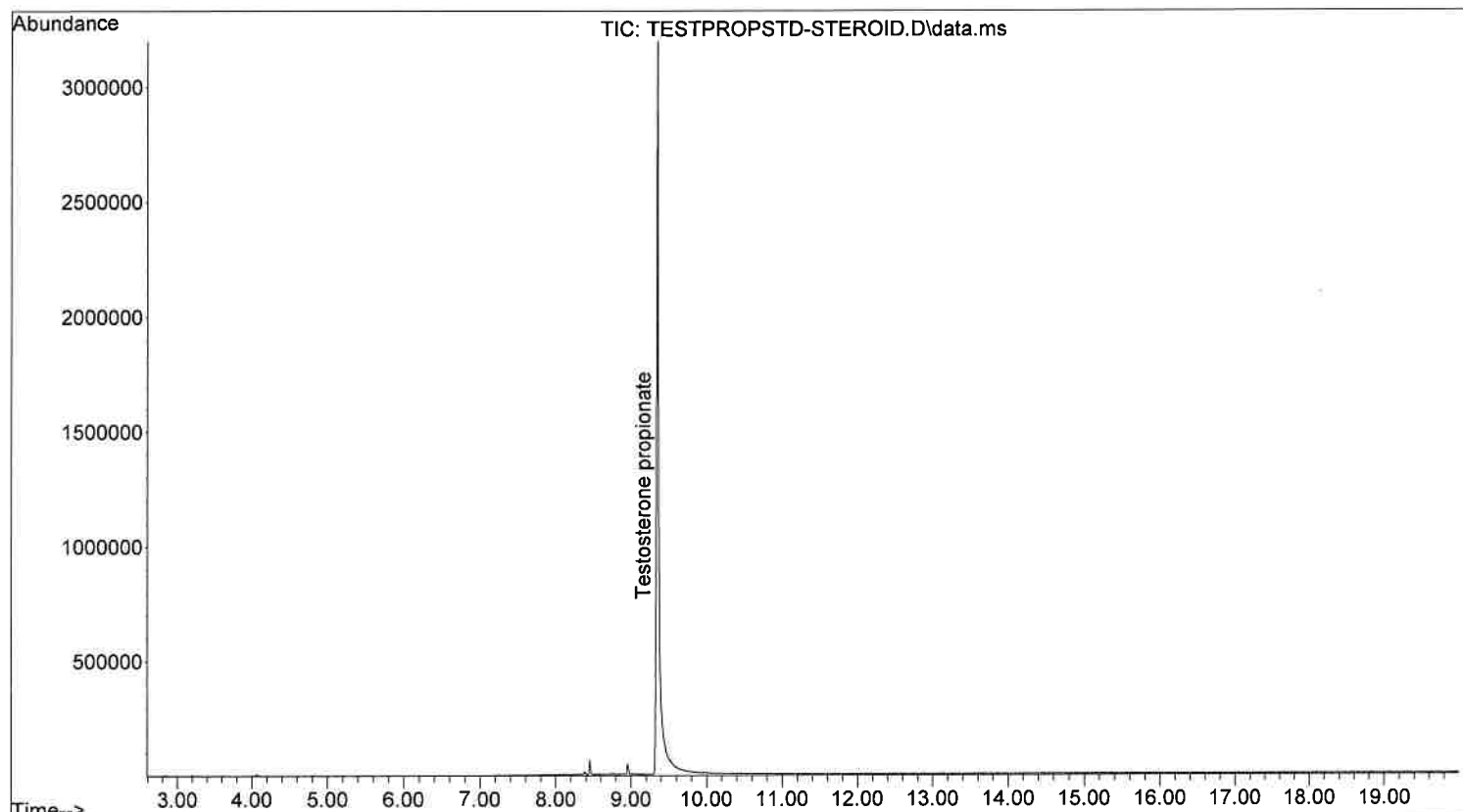
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Operator : KLAB
Acquired : 01 Sep 2023 12:07 using AcqMethod STERIOD.M
Instrument : Buttercup
Sample Name: Standard Mix
Misc Info : CHCl3
Vial Number: 2



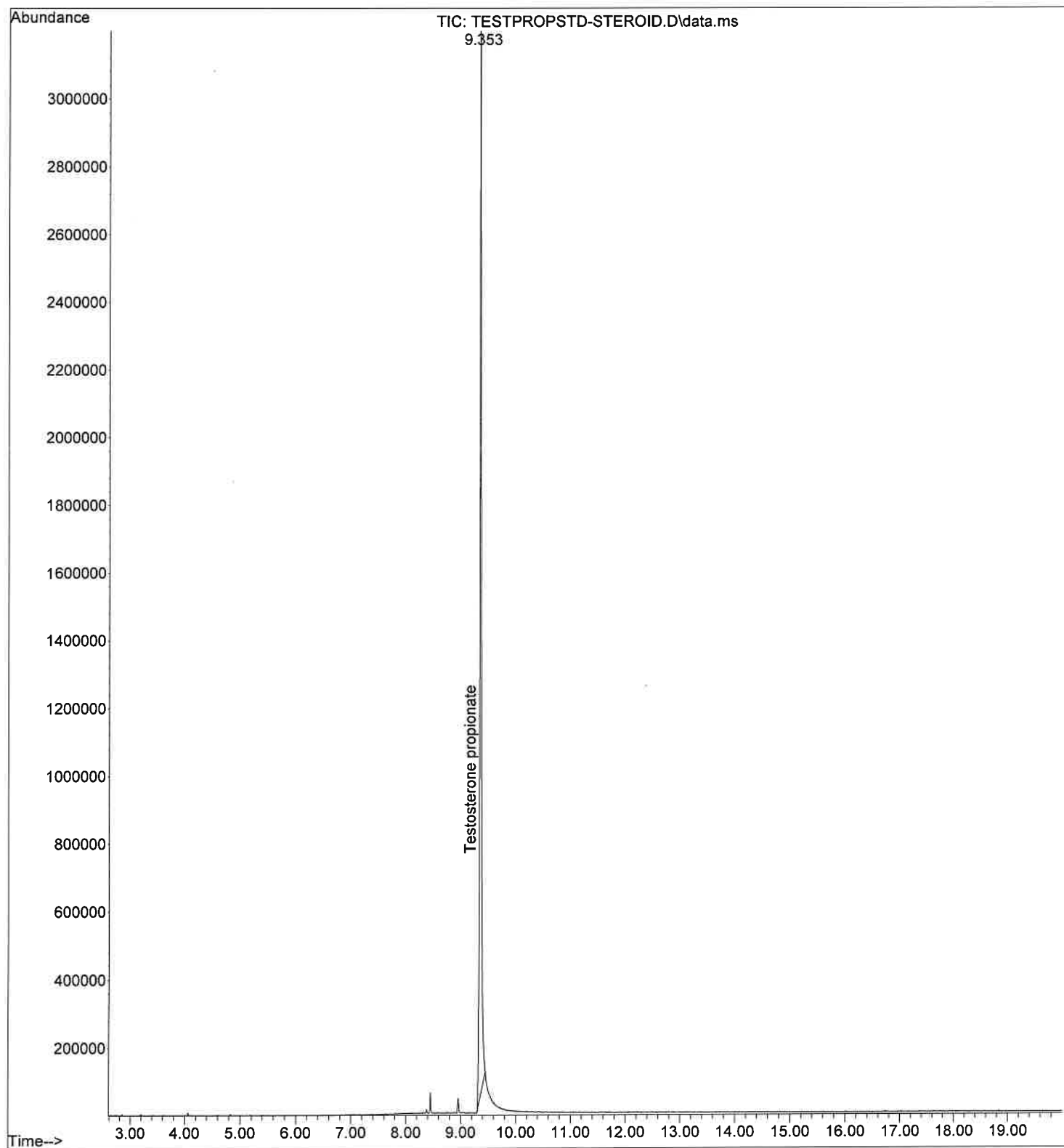
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...
Operator : KLAB
Acquired : 01 Sep 2023 11:44 using AcqMethod STEROID.M
Instrument : Buttercup
Sample Name: Chloroform blank
Misc Info : For Standard Mix
Vial Number: 1



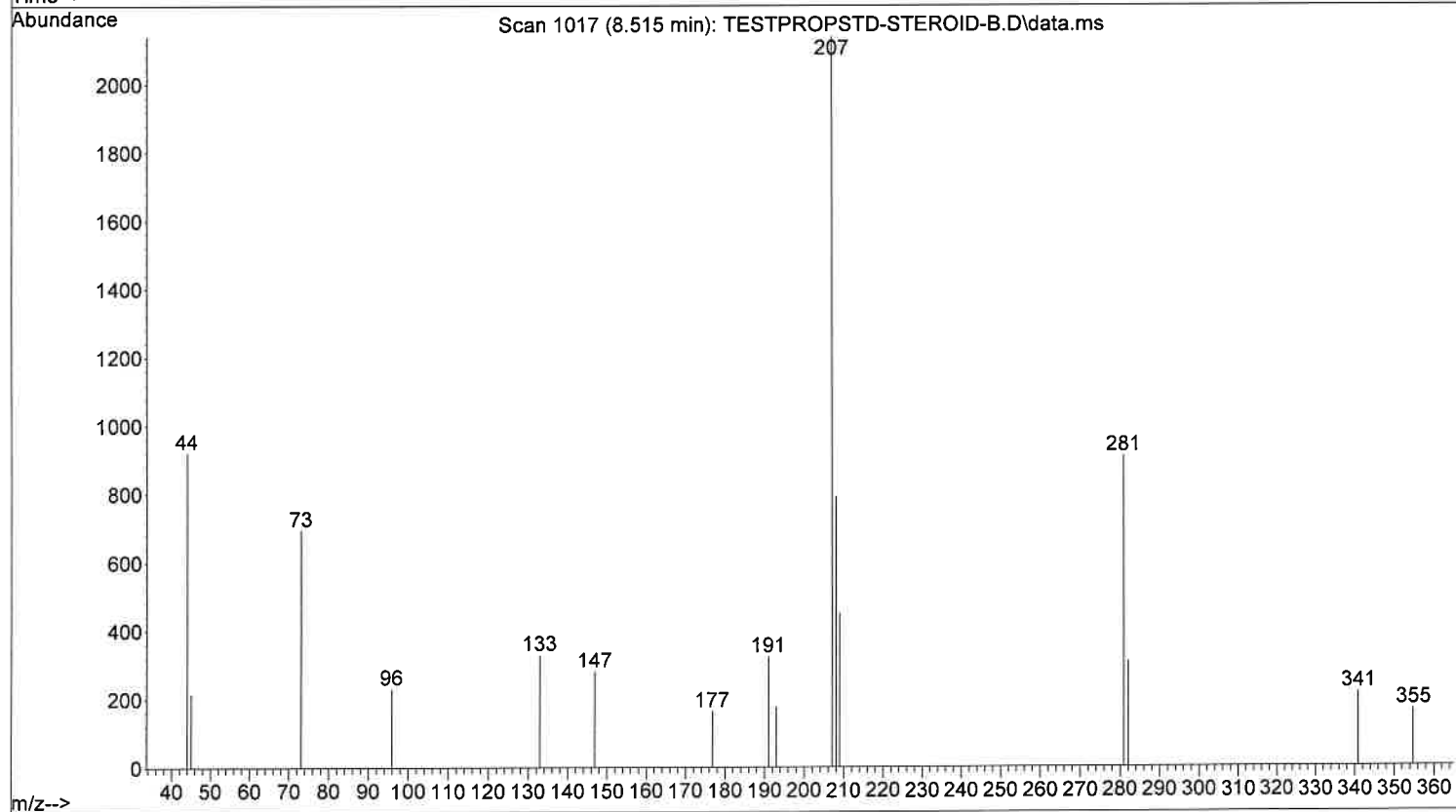
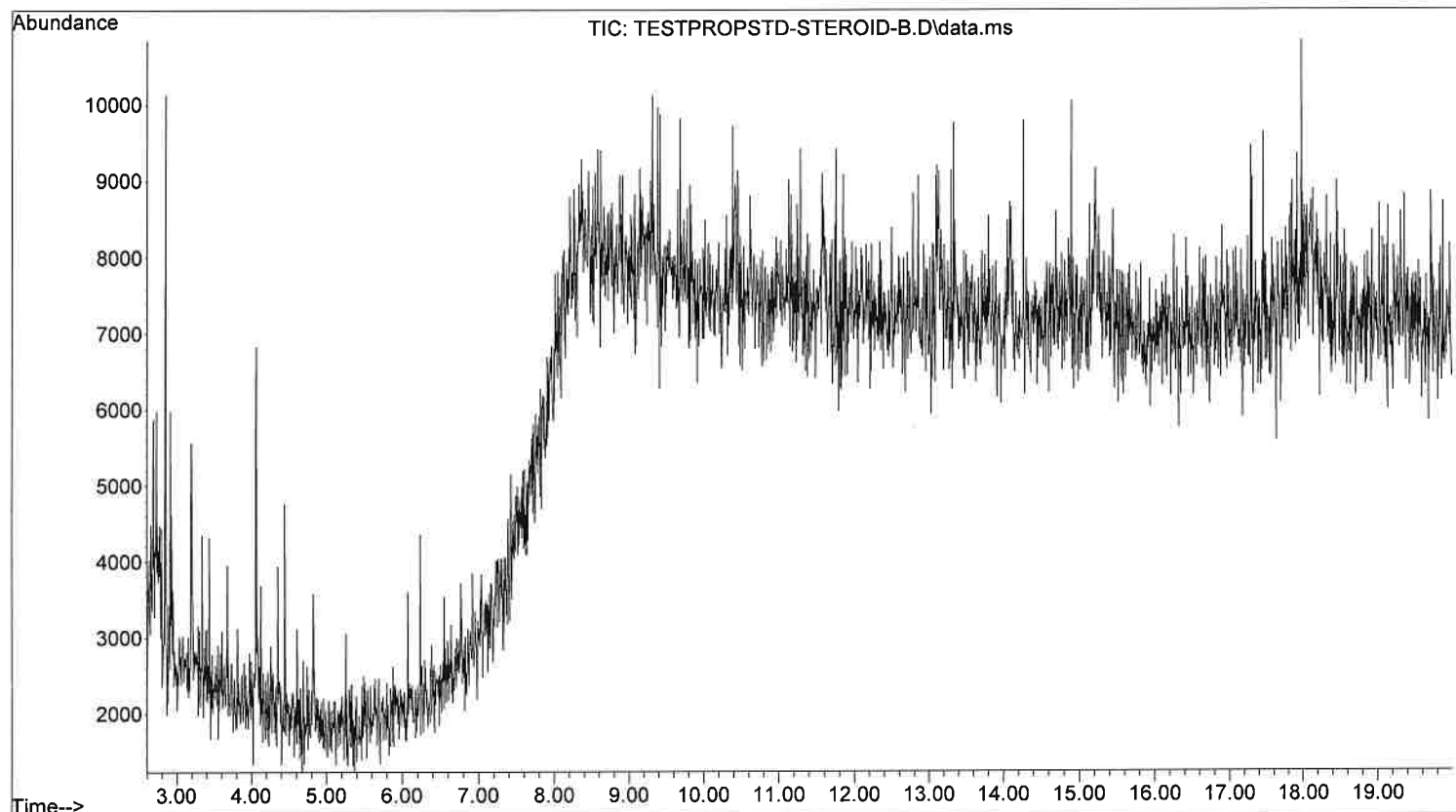
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... 01D.D
Operator : KLAB
Acquired : 22 Aug 2023 16:20 using AcqMethod STERIOD.M
Instrument : Buttercup
Sample Name: Testosterone Propionate Standard
Misc Info : MEOH
Vial Number: 6



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\TESTPROPSTD-STER
... OID.D
Operator : KLAB
Instrument : Buttercup
Acquired : 22 Aug 2023 16:20 using AcqMethod STEROID.M
Sample Name: Testosterone Propionate Standard
Misc Info : MEOH



File :D:\MassHunter\GCMS\1\data\2023\AUG23\PC0823\TESTPROPSTD-STER
... OID-B.D
Operator : KLAB
Acquired : 22 Aug 2023 15:57 using AcqMethod STERIOD.M
Instrument : Buttercup
Sample Name: Methanol blank
Misc Info : For Testosterone Propinoate
Vial Number: 1



restart computer
to adjust time (?)

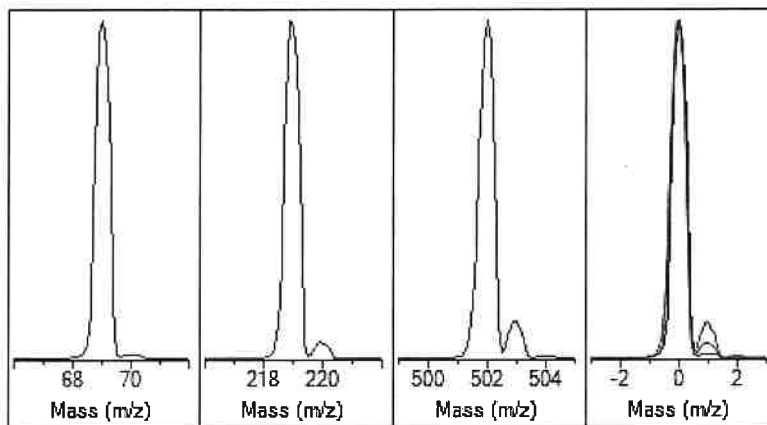
Autotune - 5977C

Tune timestamp: 7/28/2023 7:32 AM (UTC-07:00)

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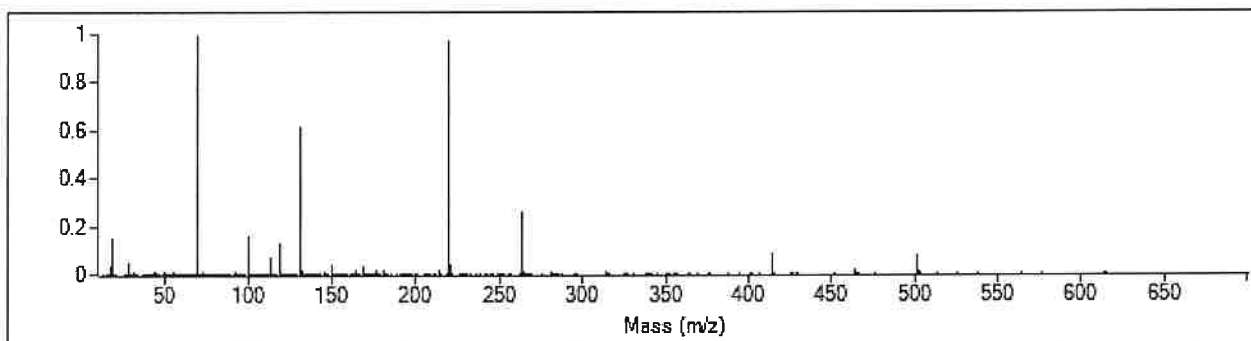


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	255
Electron Energy	70.0	Mass Offset	-23
Filament	1	Amu Gain	2887
Repeller	30.12	Amu Offset	135.56
Ion Focus	90.3	Width219	-0.036
Entrance Lens	20.2	DC Polarity	Pos
Ent Lens Offset	12.19	HED Enable	On
Ion Body	0.00	EM Volts	920.7
Post Extractor 1	0	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	530,663	100.0%	0.60
218.90	513,243	96.7%	0.60
502.00	42,676	8.0%	0.60

Temperatures and Pressures		
MS Source	230 Turbo Speed	100.0
MS Quad	150 Hi Vac	1.20e-05

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	264	69.00	507,392	2,144,887



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio
69.00	69.00	507,392	100.0%	70.00	6,473	1.3%
219.00	219.00	492,736	97.1%	220.00	20,960	4.3%
502.00	502.00	40,240	7.9%	503.00	3,750	9.3%

Air/Water Check: H2O ~15.5% N2 ~4.6% O2 ~0.3% CO2 ~1.2% N2/H2O ~30.0%

Column(1) Flow: 1.20 Column(2): 0.00 ml/min Interface Temp: 250

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 80681.924

Repeller maximum 35 volts using ion 219; Gain Factor 0.8068

Mass Gain Values(Scan Speed): 261(3) 266(2) 279(1) 299(0) 352(FS1) 351(FS2)

TARGET MASS:	50	69	131	219	414	502	1091
Amu Offset	135.6	135.6	135.6	135.6	135.6	135.6	135.6
Entrance Lens Offset	12.2	12.2	12.2	12.2	12.2	12.2	12.2

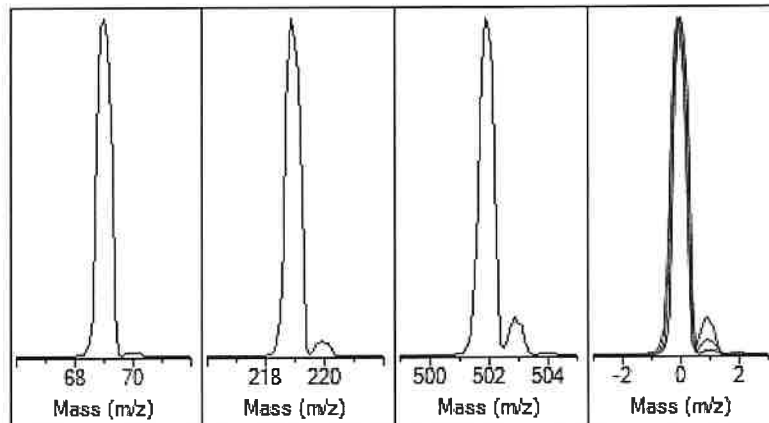
Autotune - 5977C

Tune timestamp: 8/1/2023 10:00 AM (UTC-04:00)

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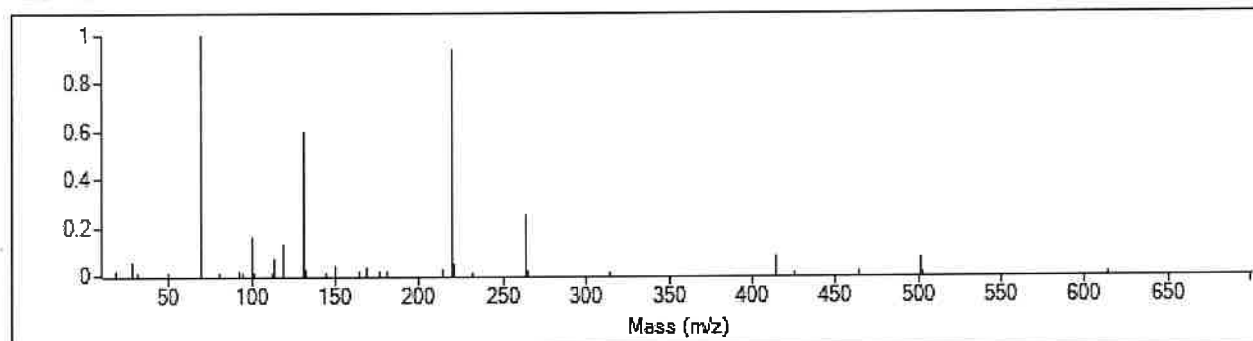


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	248
Electron Energy	70.0	Mass Offset	-23
Filament	1	Amu Gain	2896
Repeller	28.13	Amu Offset	134.50
Ion Focus	90.3	Width219	-0.022
Entrance Lens	22.7	DC Polarity	Pos
Ent Lens Offset	10.98	HED Enable	On
Ion Body	0.00	EM Volts	929.9
Post Extractor 1	0	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	534,564	100.0%	0.60
218.90	504,771	94.4%	0.60
501.90	37,973	7.1%	0.59

Temperatures and Pressures		
MS Source	230 Turbo Speed	100.0
MS Quad	150 Hi Vac	1.07e-05

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	153	69.00	517,696	1,962,952



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio
69.00	69.00	517,696	100.0%	70.00	5,550	1.1%
219.00	219.00	485,184	93.7%	220.00	21,640	4.5%
502.00	502.00	35,584	6.9%	503.00	3,413	9.6%

Air/Water Check: H2O ~1.5% N2 ~5.2% O2 ~0.3% CO2 ~0.3% N2/H2O ~345.2%

Column(1) Flow: 1.25 Column(2): 0.00 ml/min Interface Temp: 280

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 85078.206

Repeller maximum 35 volts using ion 219; Gain Factor 0.8508

Mass Gain Values(Scan Speed): 263(3) 265(2) 282(1) 305(0) 357(FS1) 374(FS2)

TARGET MASS:	50	69	131	219	414	502	1091
Amu Offset		134.5	134.5	134.5	134.5	134.5	134.5
Entrance Lens Offset		11.0	11.0	11.0	11.0	11.0	11.0

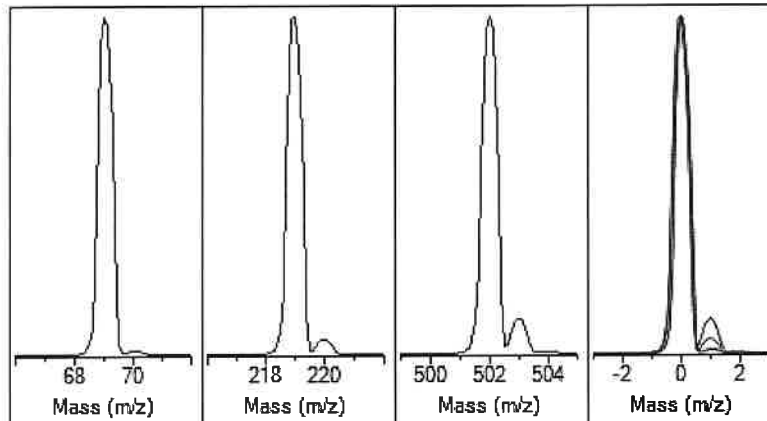
Autotune - 5977C

Tune timestamp: 8/2/2023 3:28 PM (UTC-04:00)

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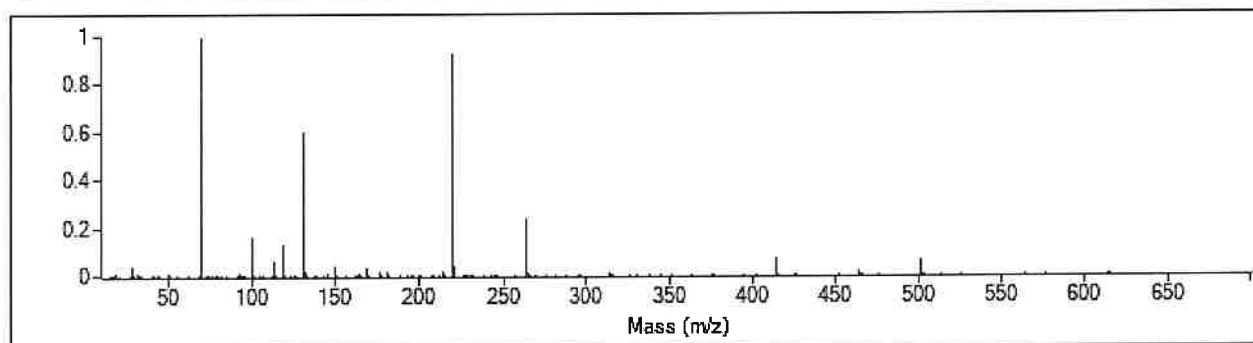


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	256
Electron Energy	70.0	Mass Offset	-21
Filament	1	Amu Gain	2896
Repeller	29.32	Amu Offset	134.56
Ion Focus	90.3	Width219	-0.021
Entrance Lens	25.2	DC Polarity	Pos
Ent Lens Offset	10.82	HED Enable	On
Ion Body	0.00	EM Volts	919.1
Post Extractor 1	0	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	484,833	100.0%	0.60
219.00	438,320	90.4%	0.61
502.00	31,792	6.6%	0.62

Temperatures and Pressures			
MS Source	230	Turbo Speed	100.0
MS Quad	150	Hi Vac	9.37e-06

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	136	69.00	460,736	1,718,671



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio
69.00	69.00	460,736	100.0%	70.00	5,190	1.1%
219.00	219.00	425,920	92.4%	220.00	18,112	4.3%
502.00	502.00	29,632	6.4%	503.00	3,161	10.7%

Air/Water Check: H2O ~1.4% N2 ~4.2% O2 ~0.3% CO2 ~0.2% N2/H2O ~293.6%

Column(1) Flow: 1.07 Column(2): 0.00 ml/min Interface Temp: 280

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 68895.333

Repeller maximum 35 volts using ion 219; Gain Factor 0.6890

Mass Gain Values(Scan Speed): 261(3) 271(2) 282(1) 300(0) 353(FS1) 361(FS2)

TARGET MASS:	50	69	131	219	414	502	1091
Amu Offset	134.6	134.6	134.6	134.6	134.6	134.6	134.6
Entrance Lens Offset	10.8	10.8	10.8	10.8	10.8	10.8	10.8

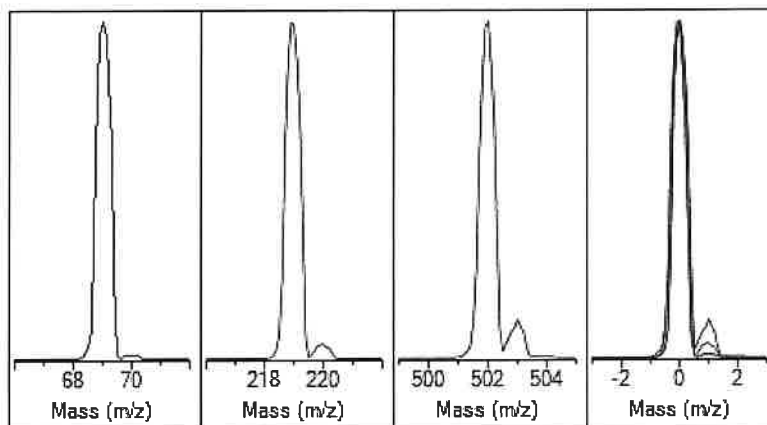
Autotune - 5977C

Tune timestamp: 8/17/2023 9:08 AM (UTC-04:00)

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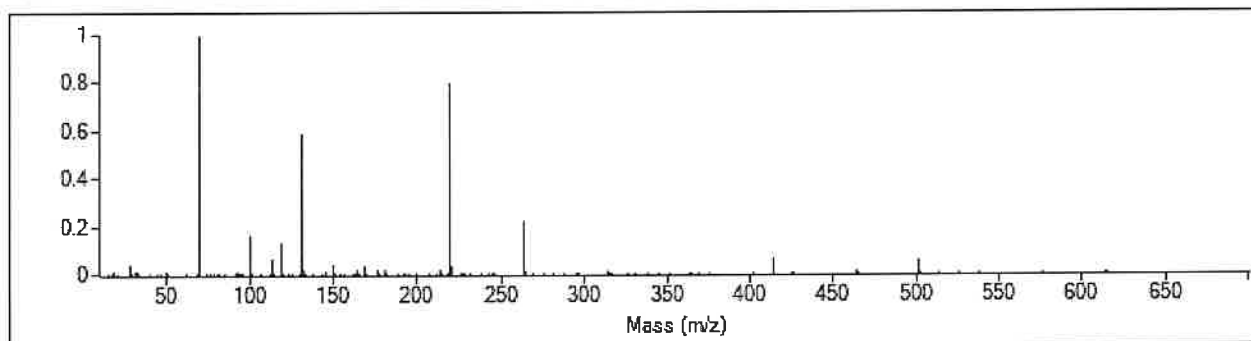


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	255
Electron Energy	70.0	Mass Offset	-22
Filament	1	Amu Gain	2892
Repeller	27.13	Amu Offset	134.56
Ion Focus	90.3	Width219	-0.024
Entrance Lens	22.7	DC Polarity	Pos
Ent Lens Offset	10.98	HED Enable	On
Ion Body	0.00	EM Volts	923.8
Post Extractor 1	0	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	400,672	100.0%	0.61
218.90	325,095	81.1%	0.61
502.00	22,650	5.7%	0.59

Temperatures and Pressures		
MS Source	230 Turbo Speed	100.0
MS Quad	150 Hi Vac	9.59e-06

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	122	69.00	387,008	1,368,487



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio
69.00	69.00	387,008	100.0%	70.00	4,223	1.1%
219.00	219.00	309,632	80.0%	220.00	13,421	4.3%
502.00	502.00	21,496	5.6%	503.00	2,418	11.2%

Air/Water Check: H2O ~1.1% N2 ~3.8% O2 ~0.6% CO2 ~0.1% N2/H2O ~339.9%

Column(1) Flow: 1.25 Column(2): 0.00 ml/min Interface Temp: 280

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 73245.686

Repeller maximum 35 volts using ion 219; Gain Factor 0.7325

Mass Gain Values(Scan Speed): 263(3) 264(2) 284(1) 307(0) 306(FS1) 359(FS2)

TARGET MASS:	50	69	131	219	414	502	1091
Amu Offset	134.6	134.6	134.6	134.6	134.6	134.6	134.6
Entrance Lens Offset	11.0	11.0	11.0	11.0	11.0	11.0	11.0

Report Created: 8/17/2023 9:09 AM (UTC-04:00)

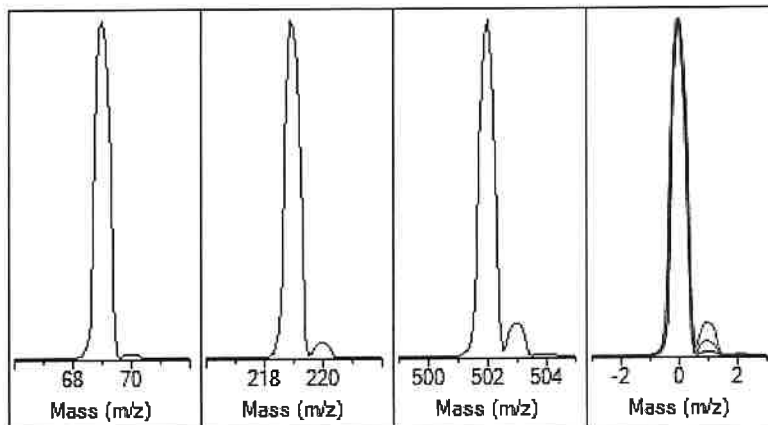
Autotune - 5977C

Tune timestamp: 8/18/2023 8:46 AM (UTC-04:00)

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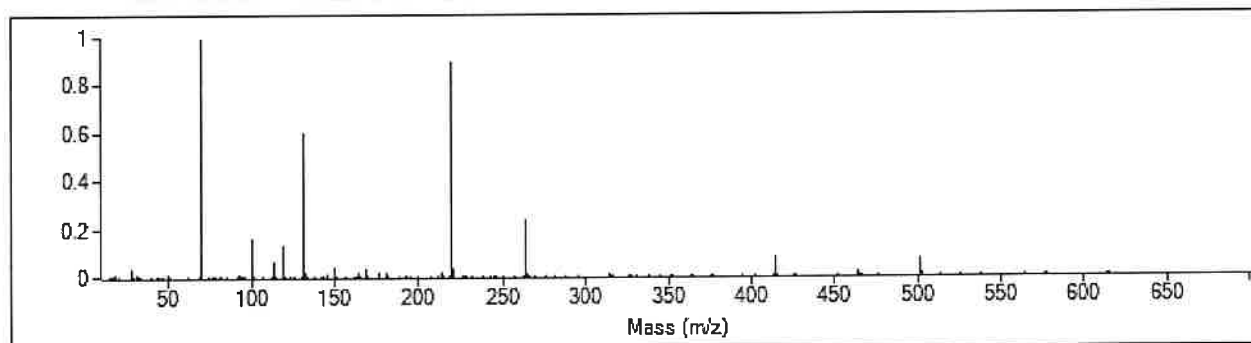


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	259
Electron Energy	70.0	Mass Offset	-23
Filament	1	Amu Gain	2894
Repeller	29.32	Amu Offset	134.06
Ion Focus	90.3	Width219	-0.024
Entrance Lens	25.2	DC Polarity	Pos
Ent Lens Offset	10.82	HED Enable	On
Ion Body	0.00	EM Volts	935.9
Post Extractor 1	0	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	482,254	100.0%	0.60
218.90	439,645	91.2%	0.60
502.00	34,966	7.3%	0.60

Temperatures and Pressures		
MS Source	230 Turbo Speed	100.0
MS Quad	150 Hi Vac	9.53e-06

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	137	69.00	467,200	1,733,595



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio
69.00	69.00	467,200	100.0%	70.00	5,494	1.2%
219.00	219.00	420,352	90.0%	220.00	17,704	4.2%
502.00	502.00	31,992	6.8%	503.00	3,638	11.4%

Air/Water Check: H2O ~1.1% N2 ~3.5% O2 ~0.3% CO2 ~0.1% N2/H2O ~317.7%

Column(1) Flow: 1.25 Column(2): 0.00 ml/min Interface Temp: 280

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 83000.905

Repeller maximum 35 volts using ion 219; Gain Factor 0.8300

Mass Gain Values(Scan Speed): 266(3) 267(2) 280(1) 305(0) 313(FS1) 392(FS2)

TARGET MASS:	50	69	131	219	414	502	1091
Amu Offset	134.1	134.1	134.1	134.1	134.1	134.1	134.1
Entrance Lens Offset	10.8	10.8	10.8	10.8	10.8	10.8	10.8

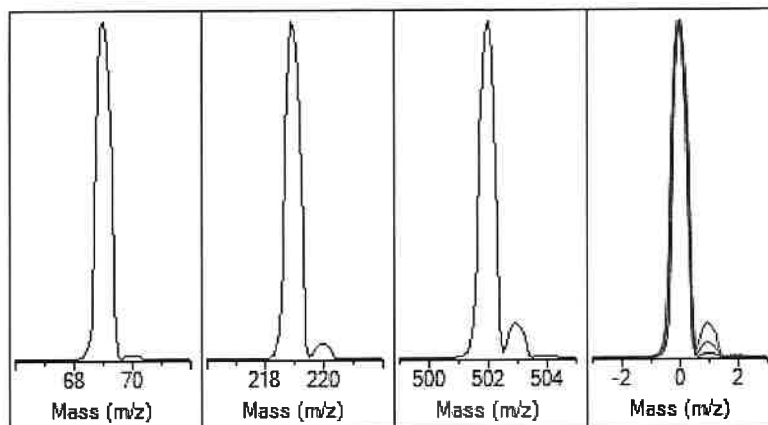
Autotune - 5977C

Tune timestamp: 8/21/2023 11:21 AM (UTC-04:00)

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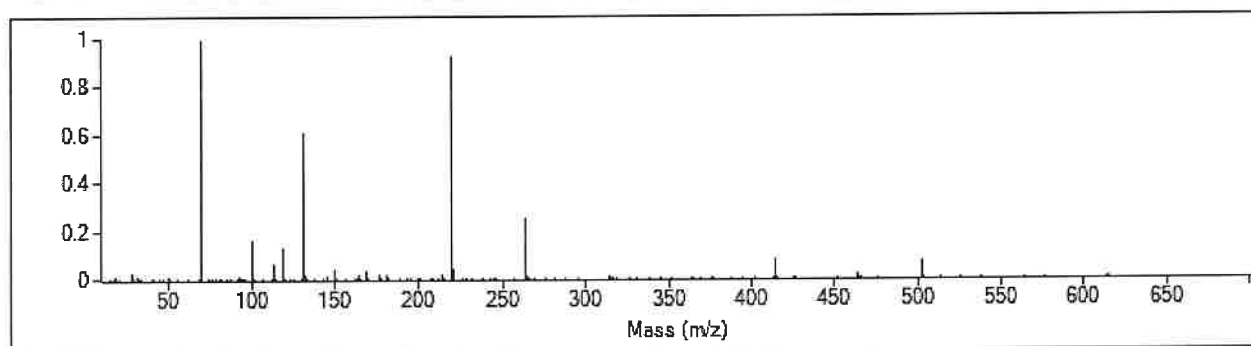


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	257
Electron Energy	70.0	Mass Offset	-23
Filament	1	Amu Gain	2896
Repeller	29.92	Amu Offset	134.63
Ion Focus	90.3	Width219	-0.022
Entrance Lens	25.2	DC Polarity	Pos
Ent Lens Offset	10.82	HED Enable	On
Ion Body	0.00	EM Volts	925.5
Post Extractor 1	0	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	490,041	100.0%	0.60
218.90	463,860	94.7%	0.60
502.00	36,590	7.5%	0.61

Temperatures and Pressures		
MS Source	230 Turbo Speed	100.0
MS Quad	150 Hi Vac	9.86e-06

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	135	69.00	471,808	1,775,705



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio
69.00	69.00	471,808	100.0%	70.00	5,250	1.1%
219.00	219.00	439,104	93.1%	220.00	19,032	4.3%
502.00	502.10	34,040	7.2%	503.10	3,474	10.2%

Air/Water Check: H2O ~1.0% N2 ~2.7% O2 ~0.3% CO2 ~0.1% N2/H2O ~260.2%

Column(1) Flow: 1.25 Column(2): 0.00 ml/min Interface Temp: 280

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 71693.921

Repeller maximum 35 volts using ion 219; Gain Factor 0.7169

Mass Gain Values(Scan Speed): 267(3) 267(2) 280(1) 307(0) 333(FS1) 403(FS2)

TARGET MASS:	50	69	131	219	414	502	1091
Amu Offset	134.6	134.6	134.6	134.6	134.6	134.6	134.6
Entrance Lens Offset	10.8	10.8	10.8	10.8	10.8	10.8	10.8

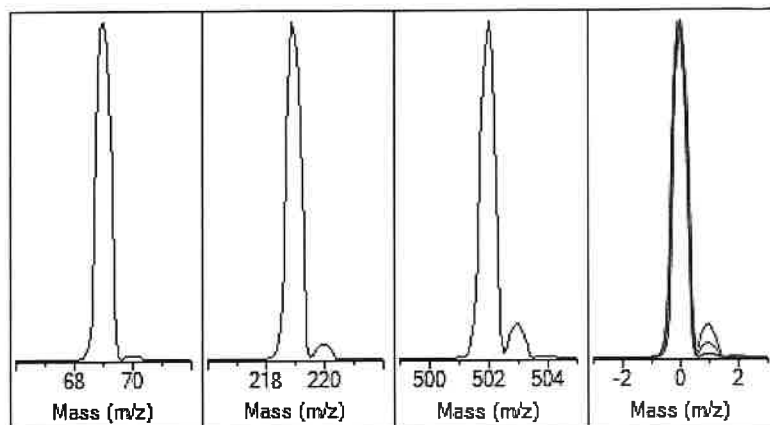
Autotune - 5977C

Tune timestamp: 8/31/2023 11:29 AM (UTC-04:00)

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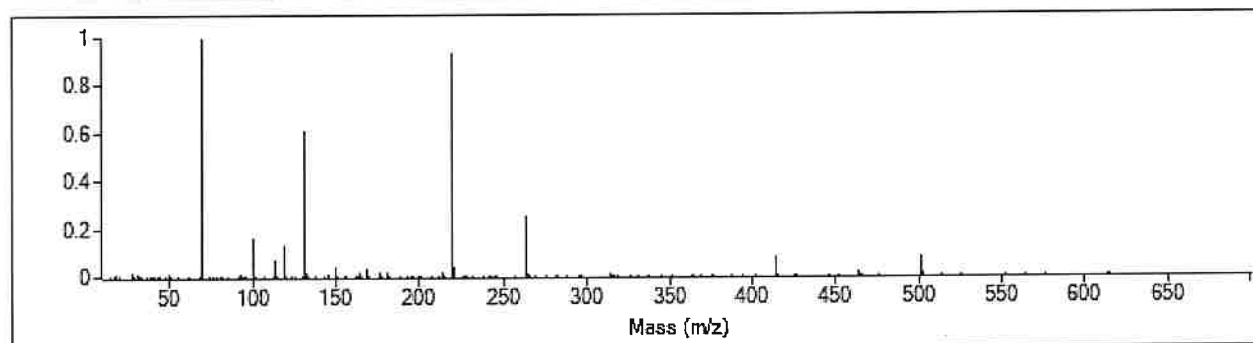


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	256
Electron Energy	70.0	Mass Offset	-23
Filament	1	Amu Gain	2896
Repeller	31.31	Amu Offset	134.56
Ion Focus	90.3	Width219	-0.023
Entrance Lens	25.2	DC Polarity	Pos
Ent Lens Offset	10.82	HED Enable	On
Ion Body	0.00	EM Volts	924.9
Post Extractor 1	0	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	483,595	100.0%	0.60
218.90	462,666	95.7%	0.60
502.00	38,735	8.0%	0.59

Temperatures and Pressures			
MS Source	230	Turbo Speed	100.0
MS Quad	150	Hi Vac	9.86e-06

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	139	69.00	468,032	1,770,386



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio
69.00	69.00	468,032	100.0%	70.00	5,009	1.1%
219.00	219.00	436,096	93.2%	220.00	18,464	4.2%
502.00	502.00	35,584	7.6%	503.00	3,474	9.8%

Air/Water Check: H2O ~1.0% N2 ~2.2% O2 ~0.4% CO2 ~0.1% N2/H2O ~213.6%

Column(1) Flow: 1.25 Column(2): 0.00 ml/min Interface Temp: 280

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 67386.474

Repeller maximum 35 volts using ion 219; Gain Factor 0.6739

Mass Gain Values(Scan Speed): 259(3) 268(2) 282(1) 298(0) 350(FS1) 367(FS2)

TARGET MASS:	50	69	131	219	414	502	1091
Amu Offset	134.6	134.6	134.6	134.6	134.6	134.6	134.6
Entrance Lens Offset	10.8	10.8	10.8	10.8	10.8	10.8	10.8