

Dataset: Untitled
Last Altered: Friday, August 06, 2021 16:06:38 Romance Daylight Time
Printed: Friday, August 06, 2021 16:07:17 Romance Daylight Time

Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51

Calibration: 06 Aug 2021 16:06:38

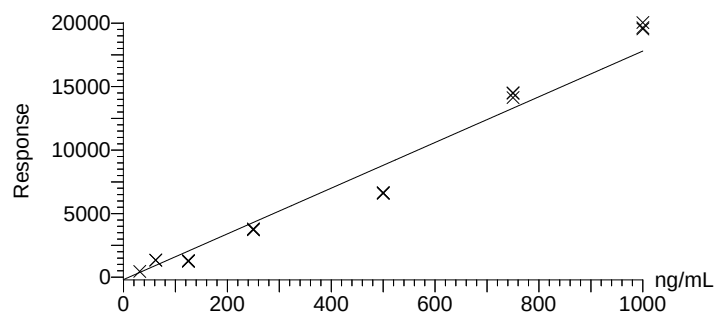
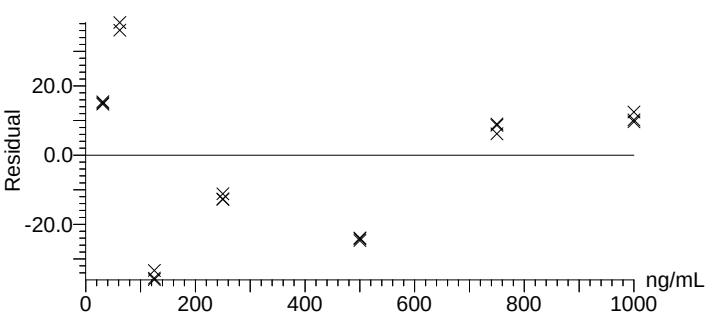
Compound name: A

Correlation coefficient: $r = 0.981517$, $r^2 = 0.963376$

Calibration curve: $17.9926 * x + -191.679$

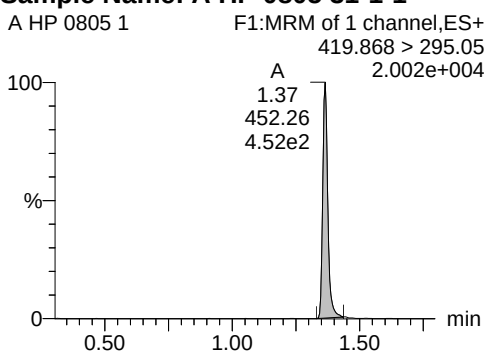
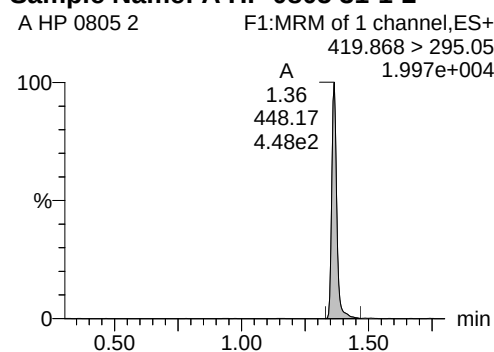
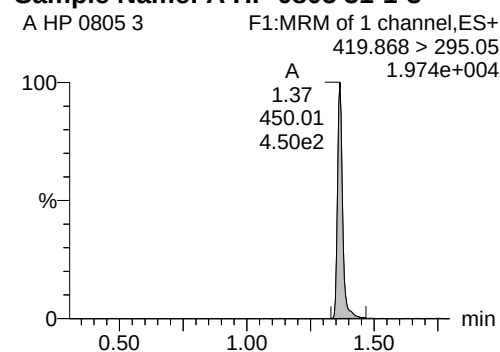
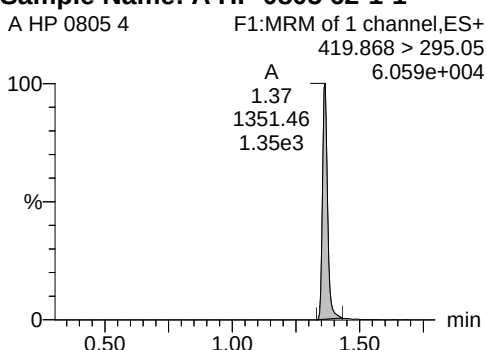
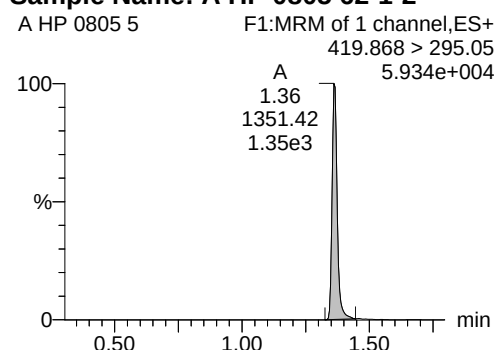
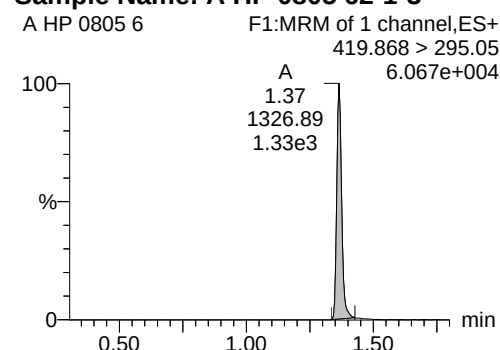
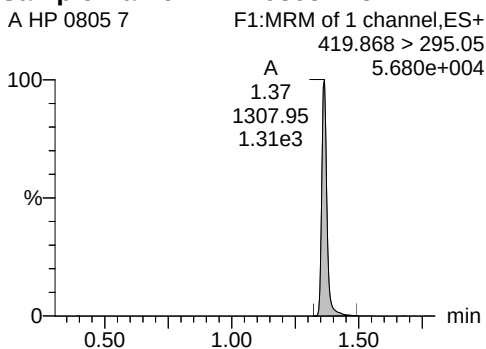
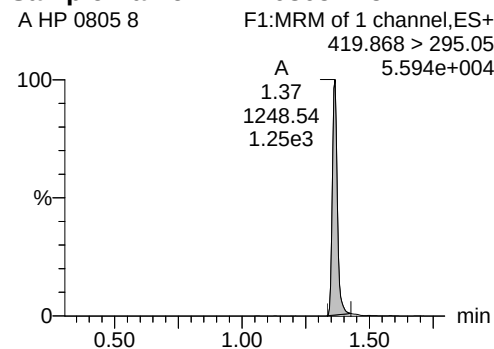
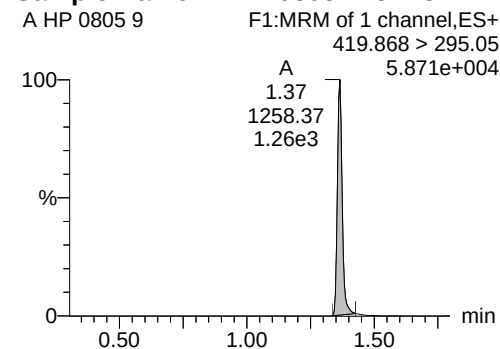
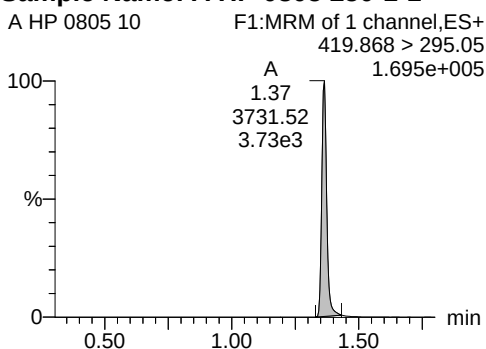
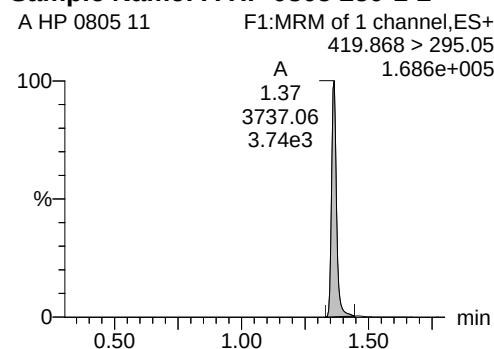
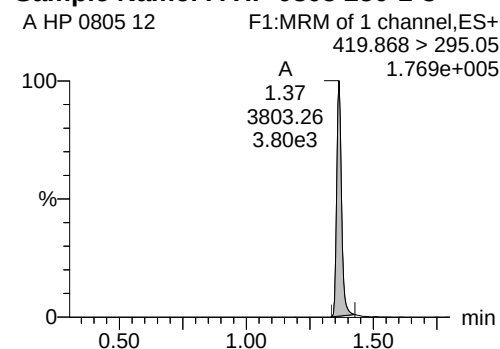
Response type: External Std, Area

Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

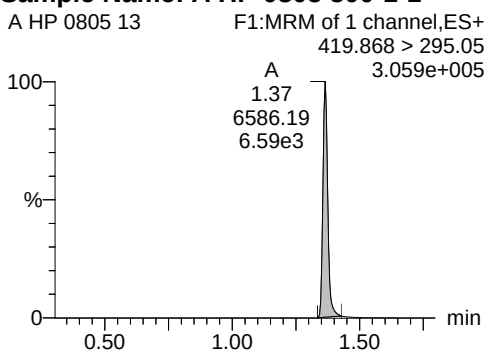
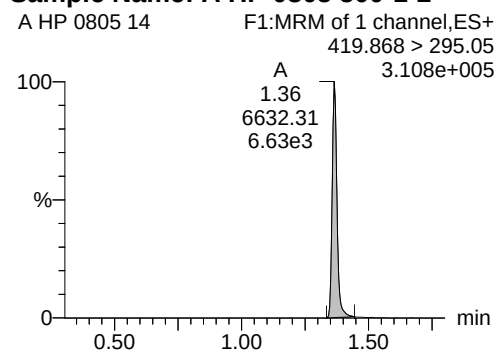
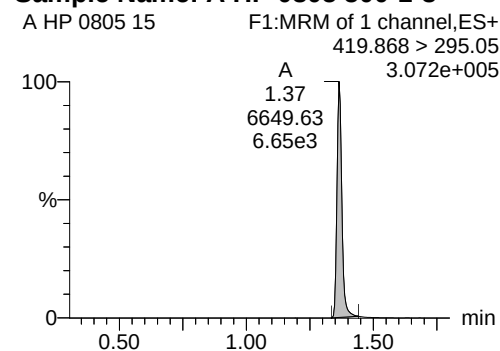
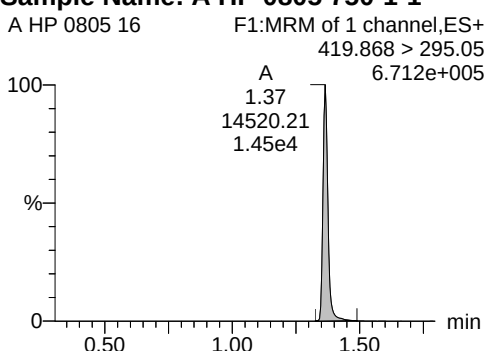
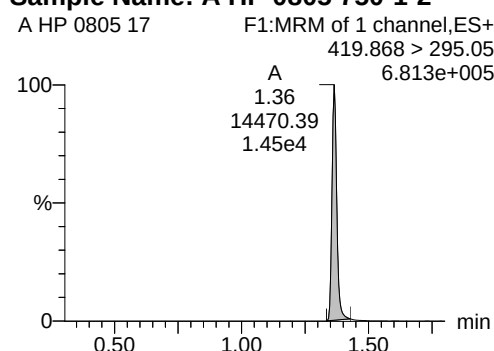
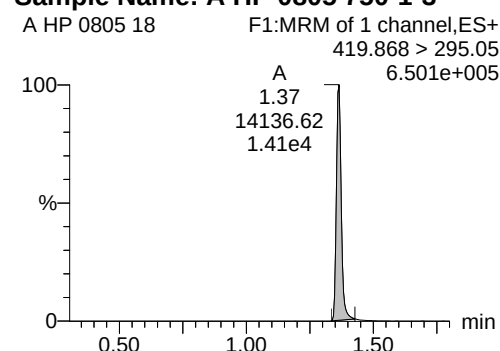
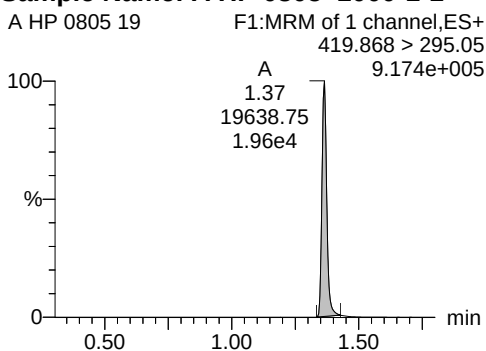
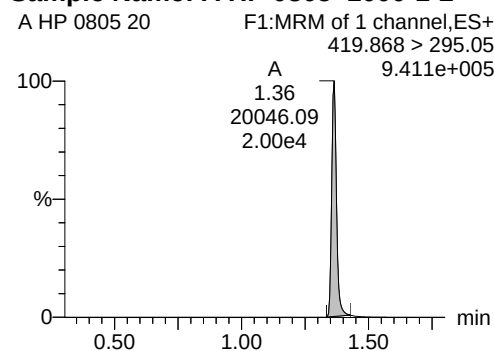
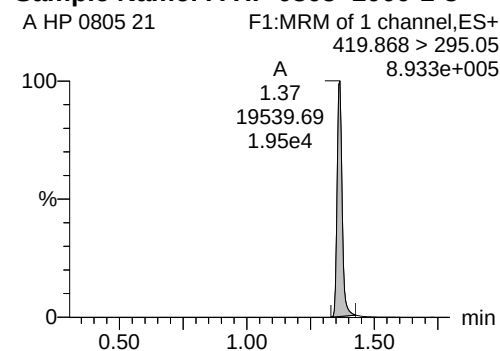
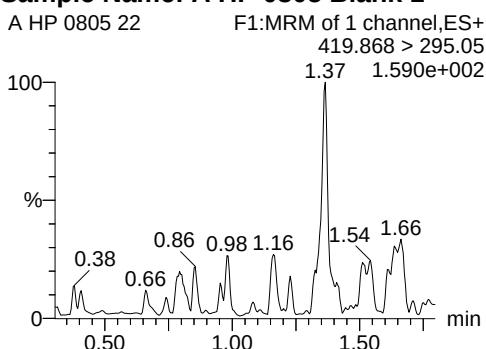
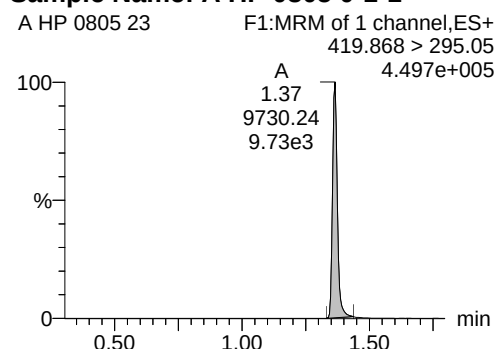
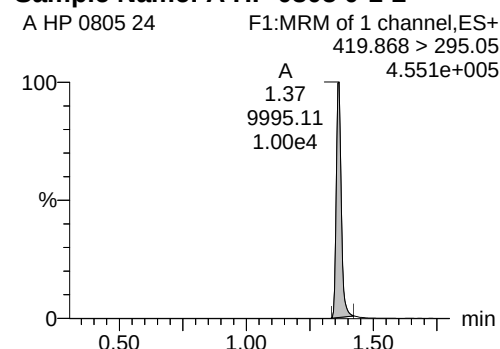
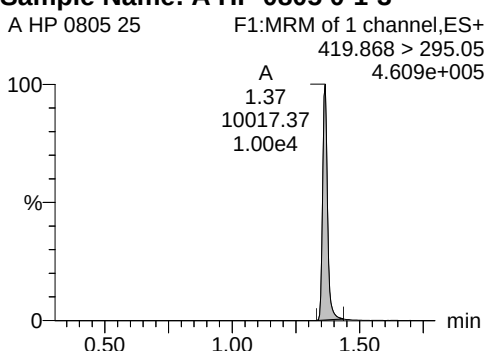
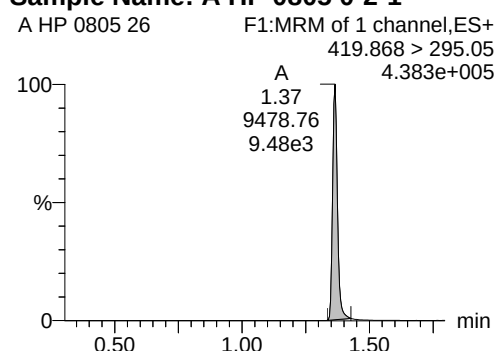
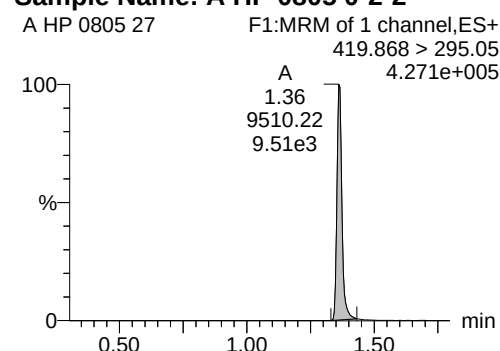


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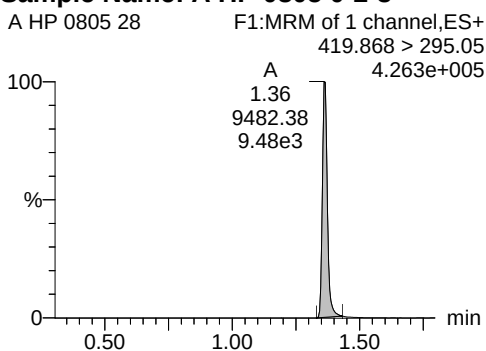
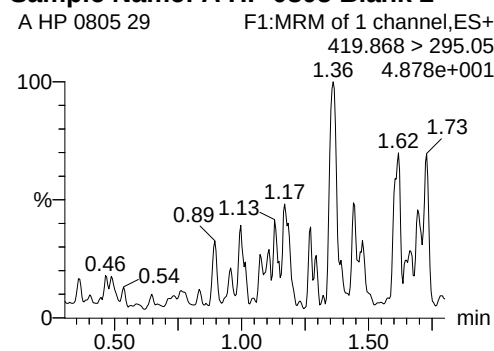
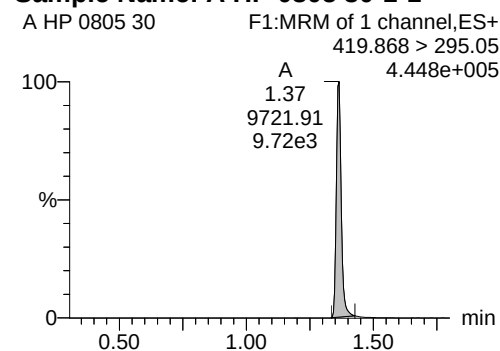
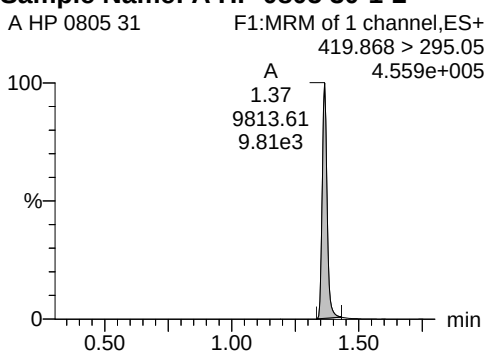
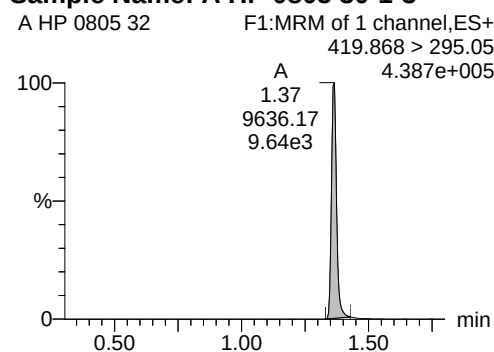
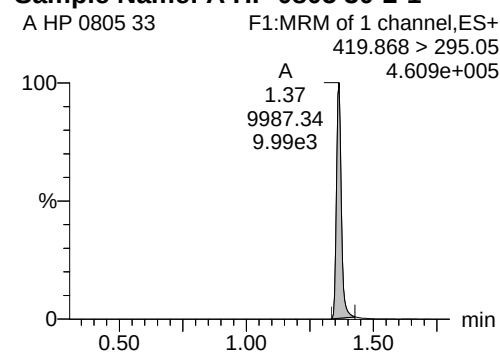
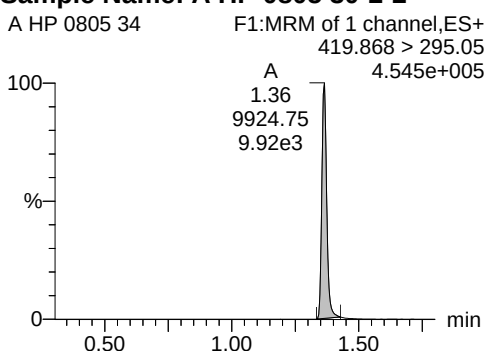
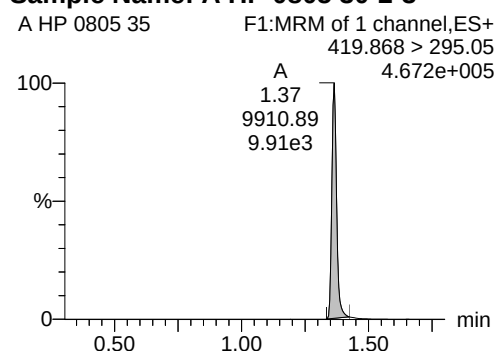
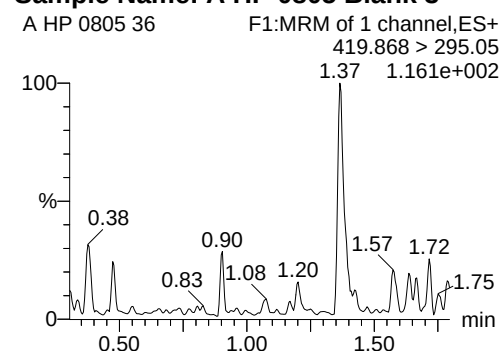
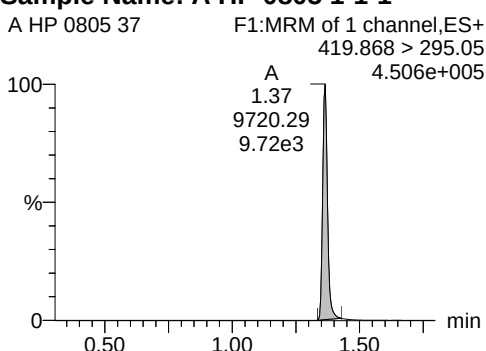
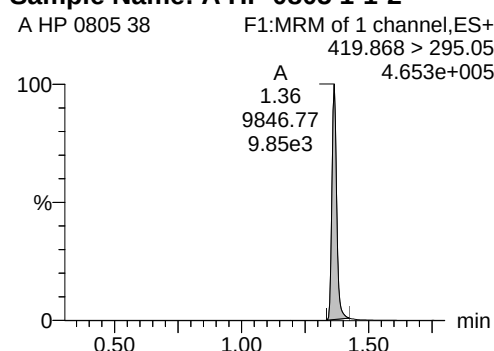
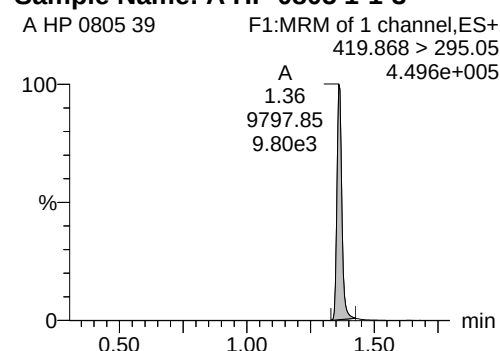
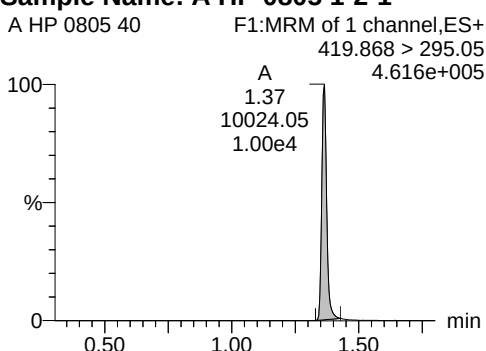
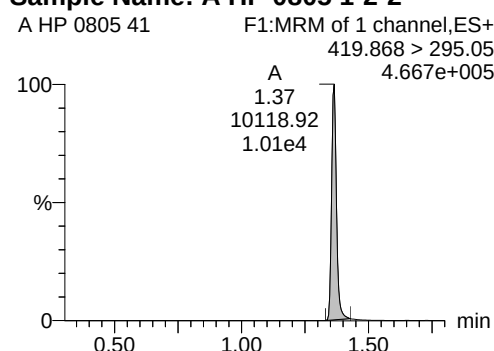
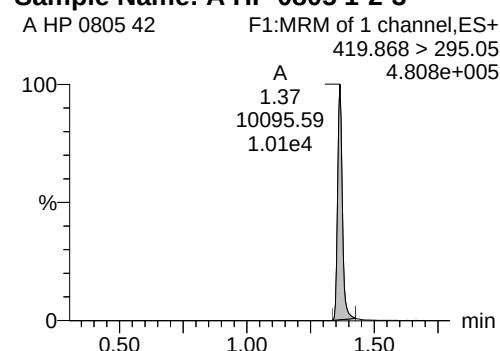
Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51
Calibration: 06 Aug 2021 16:06:38

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Sample Name: A HP 0805 500-1-1**Sample Name: A HP 0805 500-1-2****Sample Name: A HP 0805 500-1-3****Sample Name: A HP 0805 750-1-1****Sample Name: A HP 0805 750-1-2****Sample Name: A HP 0805 750-1-3****Sample Name: A HP 0805 1000-1-1****Sample Name: A HP 0805 1000-1-2****Sample Name: A HP 0805 1000-1-3****Sample Name: A HP 0805 Blank 1****Sample Name: A HP 0805 0-1-1****Sample Name: A HP 0805 0-1-2****Sample Name: A HP 0805 0-1-3****Sample Name: A HP 0805 0-2-1****Sample Name: A HP 0805 0-2-2**

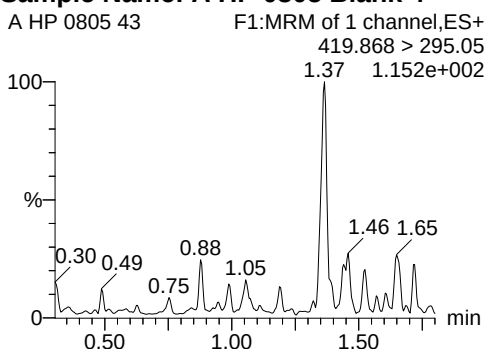
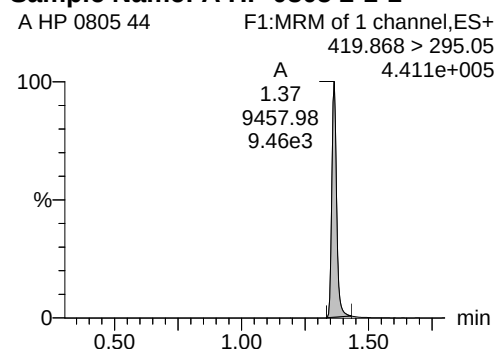
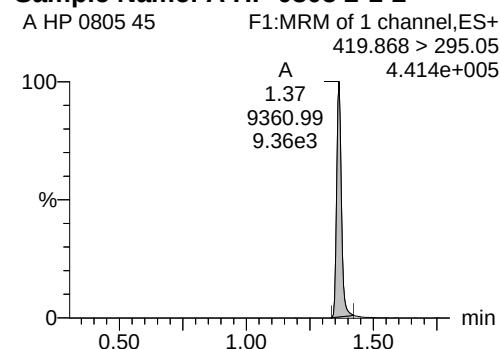
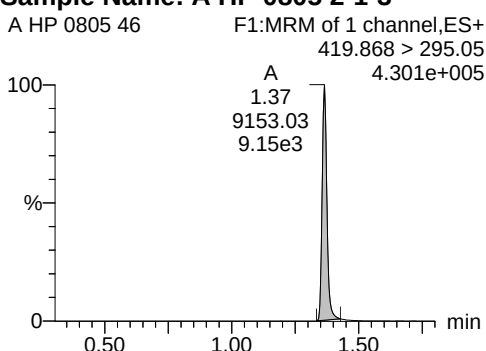
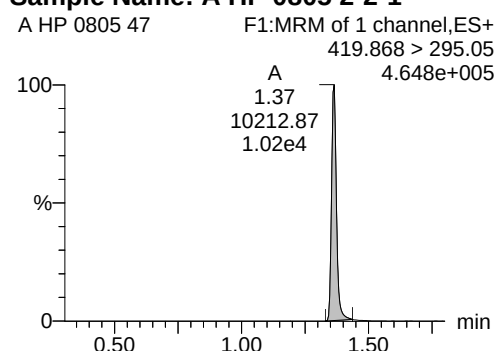
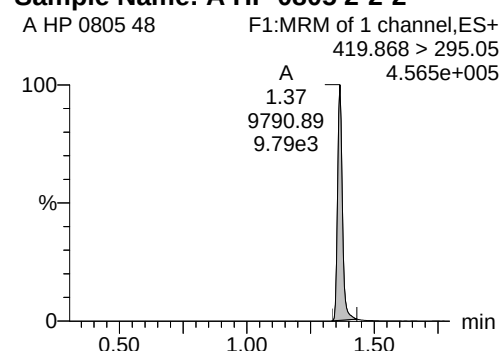
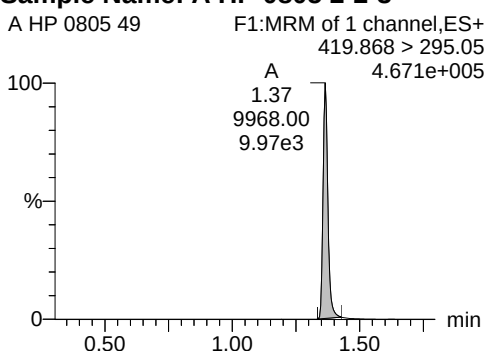
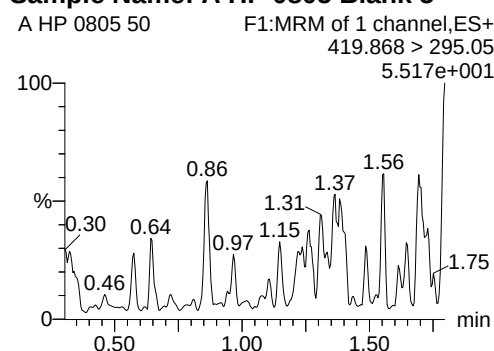
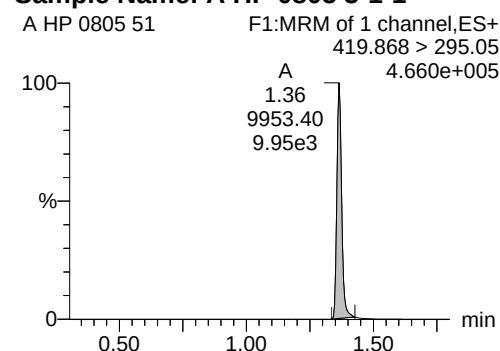
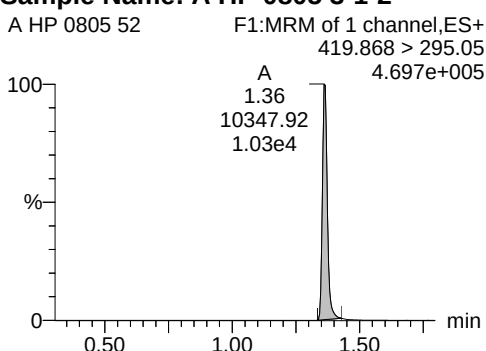
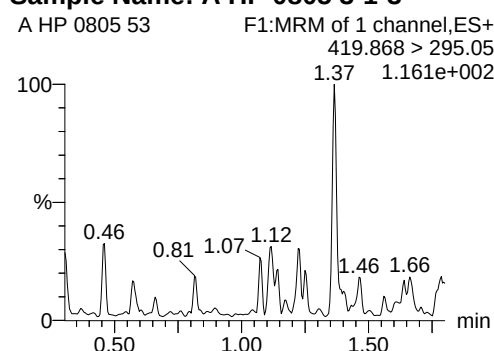
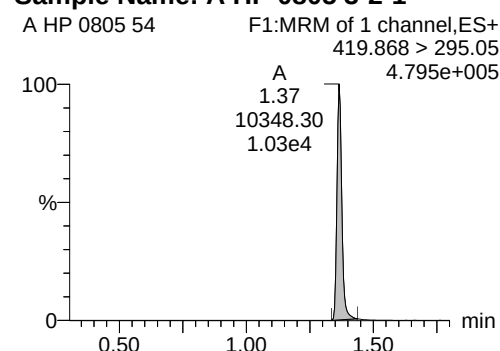
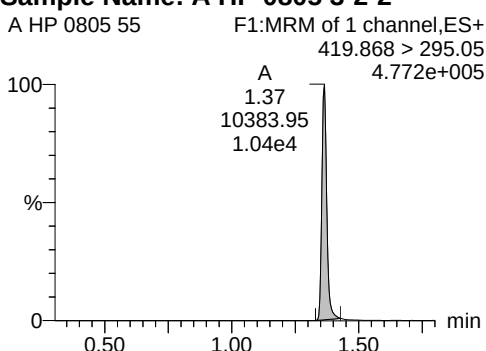
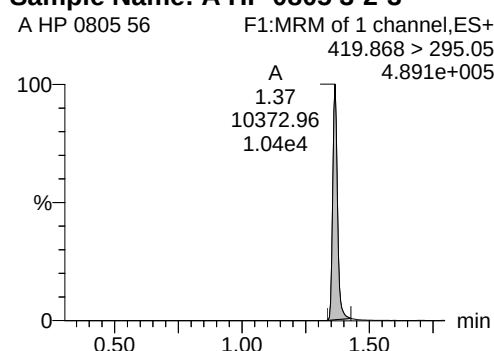
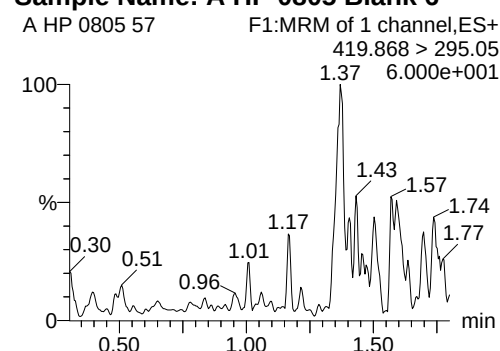
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Sample Name: A HP 0805 0-2-3**Sample Name: A HP 0805 Blank 2****Sample Name: A HP 0805 30-1-1****Sample Name: A HP 0805 30-1-2****Sample Name: A HP 0805 30-1-3****Sample Name: A HP 0805 30-2-1****Sample Name: A HP 0805 30-2-2****Sample Name: A HP 0805 30-2-3****Sample Name: A HP 0805 Blank 3****Sample Name: A HP 0805 1-1-1****Sample Name: A HP 0805 1-1-2****Sample Name: A HP 0805 1-1-3****Sample Name: A HP 0805 1-2-1****Sample Name: A HP 0805 1-2-2****Sample Name: A HP 0805 1-2-3**

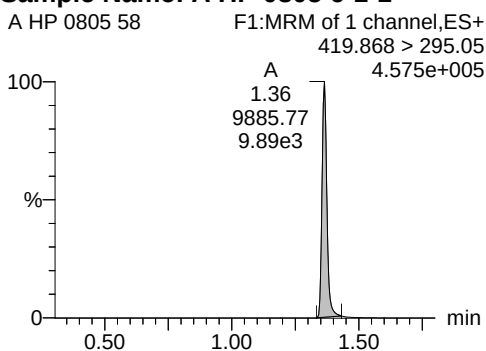
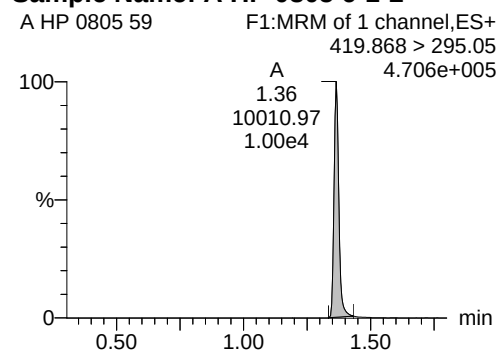
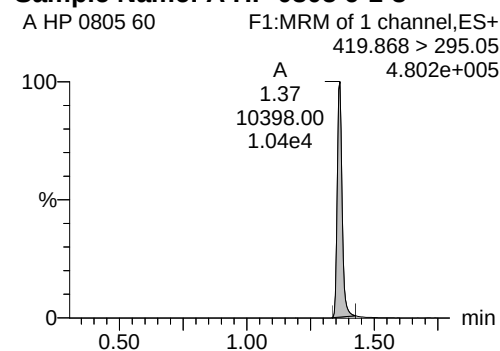
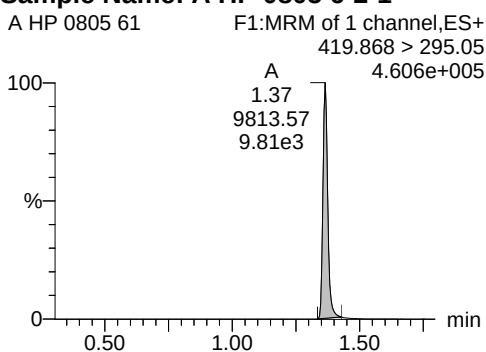
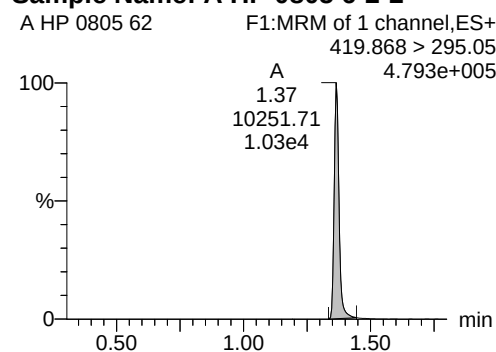
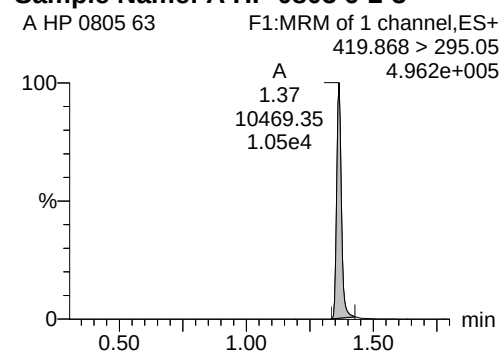
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Sample Name: A HP 0805 Blank 4**Sample Name: A HP 0805 2-1-1****Sample Name: A HP 0805 2-1-2****Sample Name: A HP 0805 2-1-3****Sample Name: A HP 0805 2-2-1****Sample Name: A HP 0805 2-2-2****Sample Name: A HP 0805 2-2-3****Sample Name: A HP 0805 Blank 5****Sample Name: A HP 0805 3-1-1****Sample Name: A HP 0805 3-1-2****Sample Name: A HP 0805 3-1-3****Sample Name: A HP 0805 3-2-1****Sample Name: A HP 0805 3-2-2****Sample Name: A HP 0805 3-2-3****Sample Name: A HP 0805 Blank 6**

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Sample Name: A HP 0805 6-1-1**Sample Name: A HP 0805 6-1-2****Sample Name: A HP 0805 6-1-3****Sample Name: A HP 0805 6-2-1****Sample Name: A HP 0805 6-2-2****Sample Name: A HP 0805 6-2-3**

	# Name	Type	Std. Conc	RT	Area	IS Area	Response	Detecti...	ng/mL	%Dev
1	1 A HP 0805 31-1-1	Stan...	31.000	1.37	452.262		452.262	bb	35.8	15.4
2	2 A HP 0805 31-1-2	Stan...	31.000	1.36	448.172		448.172	bb	35.6	14.7
3	3 A HP 0805 31-1-3	Stan...	31.000	1.37	450.010		450.010	bb	35.7	15.0
4	4 A HP 0805 62-1-1	Stan...	62.000	1.37	1351.462		1351.462	bb	85.8	38.3
5	5 A HP 0805 62-1-2	Stan...	62.000	1.36	1351.417		1351.417	bb	85.8	38.3
6	6 A HP 0805 62-1-3	Stan...	62.000	1.37	1326.890		1326.890	bb	84.4	36.1
7	7 A HP 0805 125-1-1	Stan...	125.000	1.37	1307.955		1307.955	bb	83.3	-33.3
8	8 A HP 0805 125-1-2	Stan...	125.000	1.37	1248.538		1248.538	bb	80.0	-36.0
9	9 A HP 0805 125-1-3	Stan...	125.000	1.37	1258.365		1258.365	bb	80.6	-35.5
10	10 A HP 0805 250-1-1	Stan...	250.000	1.37	3731.521		3731.521	bb	218.0	-12.8
11	11 A HP 0805 250-1-2	Stan...	250.000	1.37	3737.057		3737.057	bb	218.4	-12.7
12	12 A HP 0805 250-1-3	Stan...	250.000	1.37	3803.258		3803.258	bb	222.0	-11.2
13	13 A HP 0805 500-1-1	Stan...	500.000	1.37	6586.194		6586.194	bb	376.7	-24.7
14	14 A HP 0805 500-1-2	Stan...	500.000	1.36	6632.315		6632.315	bb	379.3	-24.1
15	15 A HP 0805 500-1-3	Stan...	500.000	1.37	6649.627		6649.627	bb	380.2	-24.0
16	16 A HP 0805 750-1-1	Stan...	750.000	1.37	14520.214		14520.214	bb	817.7	9.0
17	17 A HP 0805 750-1-2	Stan...	750.000	1.36	14470.389		14470.389	bb	814.9	8.7
18	18 A HP 0805 750-1-3	Stan...	750.000	1.37	14136.617		14136.617	bb	796.3	6.2
19	19 A HP 0805 1000-1-1	Stan...	1000.000	1.37	19638.746		19638.746	bb	1102.1	10.2
20	20 A HP 0805 1000-1-2	Stan...	1000.000	1.36	20046.088		20046.088	bb	1124.8	12.5
21	21 A HP 0805 1000-1-3	Stan...	1000.000	1.37	19539.691		19539.691	bb	1096.6	9.7
22	22 A HP 0805 Blank 1	Blank								
23	23 A HP 0805 0-1-1	Anal...		1.37	9730.243		9730.243	bb	551.4	
24	24 A HP 0805 0-1-2	Anal...		1.37	9995.113		9995.113	bb	566.2	
25	25 A HP 0805 0-1-3	Anal...		1.37	10017.368		10017.368	bb	567.4	
26	26 A HP 0805 0-2-1	Anal...		1.37	9478.764		9478.764	bb	537.5	
27	27 A HP 0805 0-2-2	Anal...		1.36	9510.215		9510.215	bb	539.2	
28	28 A HP 0805 0-2-3	Anal...		1.36	9482.383		9482.383	bb	537.7	
29	29 A HP 0805 Blank 2	Blank								
30	30 A HP 0805 30-1-1	Anal...		1.37	9721.905		9721.905	bb	551.0	
31	31 A HP 0805 30-1-2	Anal...		1.37	9813.613		9813.613	bb	556.1	
32	32 A HP 0805 30-1-3	Anal...		1.37	9636.169		9636.169	bb	546.2	
33	33 A HP 0805 30-2-1	Anal...		1.37	9987.337		9987.337	bb	565.7	
34	34 A HP 0805 30-2-2	Anal...		1.36	9924.747		9924.747	bb	562.3	
35	35 A HP 0805 30-2-3	Anal...		1.37	9910.893		9910.893	bb	561.5	
36	36 A HP 0805 Blank 3	Blank								
37	37 A HP 0805 1-1-1	Anal...		1.37	9720.288		9720.288	bb	550.9	
38	38 A HP 0805 1-1-2	Anal...		1.36	9846.772		9846.772	bb	557.9	
39	39 A HP 0805 1-1-3	Anal...		1.36	9797.854		9797.854	bb	555.2	
40	40 A HP 0805 1-2-1	Anal...		1.37	10024.047		10024.047	bb	567.8	
41	41 A HP 0805 1-2-2	Anal...		1.37	10118.918		10118.918	bb	573.0	
42	42 A HP 0805 1-2-3	Anal...		1.37	10095.590		10095.590	bb	571.7	
43	43 A HP 0805 Blank 4	Blank								
44	44 A HP 0805 2-1-1	Anal...		1.37	9457.978		9457.978	bb	536.3	
45	45 A HP 0805 2-1-2	Anal...		1.37	9360.990		9360.990	bb	530.9	
46	46 A HP 0805 2-1-3	Anal...		1.37	9153.032		9153.032	bb	519.4	
47	47 A HP 0805 2-2-1	Anal...		1.37	10212.867		10212.867	bb	578.3	
48	48 A HP 0805 2-2-2	Anal...		1.37	9790.886		9790.886	bb	554.8	
49	49 A HP 0805 2-2-3	Anal...		1.37	9968.002		9968.002	bb	564.7	
50	50 A HP 0805 Blank 5	Blank								
51	51 A HP 0805 3-1-1	Anal...		1.36	9953.403		9953.403	bb	563.8	
52	52 A HP 0805 3-1-2	Anal...		1.36	10347.916		10347.916	bb	585.8	
53	53 A HP 0805 3-1-3	Anal...								
54	54 A HP 0805 3-2-1	Anal...		1.37	10348.301		10348.301	bb	585.8	
55	55 A HP 0805 3-2-2	Anal...		1.37	10383.954		10383.954	bb	587.8	
56	56 A HP 0805 3-2-3	Anal...		1.37	10372.957		10372.957	bb	587.2	
57	57 A HP 0805 Blank 6	Blank								
58	58 A HP 0805 6-1-1	Anal...		1.36	9885.768		9885.768	bb	560.1	

Dataset: Untitled
Last Altered: Friday, August 06, 2021 16:06:38 Romance Daylight Time
Printed: Friday, August 06, 2021 16:07:17 Romance Daylight Time

	# Name	Type	Std. Conc	RT	Area	IS Area	Response Detecti...	ng/mL	%Dev
59	59 A HP 0805 6-1-2	Anal...		1.36	10010.969		10010.969	bb	567.0
60	60 A HP 0805 6-1-3	Anal...		1.37	10398.004		10398.004	bb	588.6
61	61 A HP 0805 6-2-1	Anal...		1.37	9813.566		9813.566	bb	556.1
62	62 A HP 0805 6-2-2	Anal...		1.37	10251.705		10251.705	bb	580.4
63	63 A HP 0805 6-2-3	Anal...		1.37	10469.347		10469.347	bb	592.5

Dataset: Untitled
Last Altered: Friday, August 06, 2021 16:06:38 Romance Daylight Time
Printed: Friday, August 06, 2021 16:07:17 Romance Daylight Time

Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51
Calibration: 06 Aug 2021 16:06:38

Header

Acquired File Name: A HP 0805 31-1-1
Acquired Date: 06-Aug-2021
Acquired Time: 03:42:00
Job Code: PSHP - 20210805 - N - 216 - 075 - A
Task Code:
User Name:
Laboratory Name:
Instrument: ACQ-TQD#QBA320
Conditions:
Submitter:
SampleID: A HP 0805 1
Bottle Number: 2:79
Description:
Instrument Calibration:
Calibration File: C:\MassLynx\IntelliStart\Results\Unit Mass Resolution\Calib 20161209.cal

Parameters

MS1 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS1

MS1 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS1
MS1 Scan Speed Compensation:
Scan: 339 to 2000 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS1

MS2 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS2

MS2 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS2
MS2 Scan Speed Compensation:
Scan: 339 to 10165 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS2
Calibration Time: 10:33
Calibration Date: 12/09/16

Coefficients

MS1 Static: $-0.000000000000 \cdot x^4 + 0.000000000843 \cdot x^3 + -0.000001360559 \cdot x^2 + 1.000940122634 \cdot x + -0.253266439024$
MS2 Static: $-0.000000000000 \cdot x^4 + 0.000000000573 \cdot x^3 + -0.000001239648 \cdot x^2 + 1.000902600483 \cdot x + -0.192715155436$

Function 1: None

Function 2: None

Parameters for C:\Documents and Settings\Administrator\Desktop\old desktop\log D\EA.EXP

Data Processing:

SIR / MRM Chromatogram Spike Removal ON

Dataset: Untitled
Last Altered: Friday, August 06, 2021 16:06:38 Romance Daylight Time
Printed: Friday, August 06, 2021 16:07:17 Romance Daylight Time

SIR / MRM Smoothing OFF
Smoothing window size (scans) 3
Number of smooths 2
Prescan Statistics:
Initial Average Intensity 21.9169
Initial Average Std Dev 1.7908
Bunch Zero Level 0.0027
Bunch Std Dev 0.0088
Bunch Threshold 0.0702
Spike Removal Std Dev 1.7757

Method Events:

Initial Stop Flow: No Change
Initial Switch 2: No Change
Initial Switch 3: No Change
Initial Switch 4: No Change
Initial Infusion: No Change
Initial Flow State: LC
Initial Flow Rate: 5
Initial Reservoir: No Action
API Probe Delay Temp: 20
Initial Refill: No Action

Timed Events Enabled

Event Time	Name	Action
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Instrument Parameters - Function 1:

Parameter File - C:\Documents and Settings\Administrator\Desktop\old desktop\log D\log D tune file.

IPR

Polarity ES+
Calibration Static 2
Capillary (kV) 3.50 3.48
Cone (V) 38.00 33.46
Extractor (V) 3.00 2.69
RF (V) 0.10
Source Temperature (°C) 140 139
Desolvation Temperature (°C) 450 444
Cone Gas Flow (L/Hr) 90 90
Desolvation Gas Flow (L/Hr) 900 900
Collision Gas Flow (mL/Min) 0.20 0.20
LM 1 Resolution 15.50
HM 1 Resolution 14.84
Ion Energy 1 0.30
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance -2.00
MSMS Mode Collision Energy 2.00
MSMS Mode Exit 2.00
LM 2 Resolution 15.00
HM 2 Resolution 15.50
Ion Energy 2 1.22
Gain 1.00
Multiplier -493.56

Active Reservoir B

Engineers Settings:

MS1 Low Mass Position	518
MS1 High Mass Position	284
MS1 Low Mass Resolution	513
MS1 High Mass Resolution	1732
MS1 Resolution Linearity	834
MS1 High Mass DC Balance	0
MS1 DC Polarity	Positive
MS2 Low Mass Position	519
MS2 High Mass Position	238
MS2 Low Mass Resolution	518
MS2 High Mass Resolution	644
MS2 Resolution Linearity	756
MS2 High Mass DC Balance	-0
MS2 DC Polarity	Positive
HM RF Lens Correction +	0

Dataset: Untitled
Last Altered: Friday, August 06, 2021 16:06:38 Romance Daylight Time
Printed: Friday, August 06, 2021 16:07:17 Romance Daylight Time

HM RF Lens Correction - 0

Inter-scan delays:

Automatic Mode

MS 1 Delay Table:

	R	delay
<=	0.500	0.005
<=	1.200	0.010
<=	2.400	0.015
<=	6.000	0.020
<=	15.000	0.025
<=	25.000	0.028
>	25.000	0.030

MS 2 Delay Table:

	R	delay
<=	2.000	0.005
<=	4.000	0.008
<=	7.000	0.010
<=	10.000	0.012
<=	20.000	0.014
>	20.000	0.016

ACE Experimental Record

Inlet Method File: c:\masslynx_projects\medchem su.pro\acqudb\adme sophie

----- Prerun method parameters -----

Waters ACQUITY QSM

Waters Acquity TUV

Run Time: 0.20 min

Wavelength Mode: Single Wavelength

Lamp On: On

Channel A...

Comment:

Wavelength: 254 nm

Sampling Rate: 20 points/sec

Data Mode: Absorbance

Time Constant: 0.1000 sec

Auto Zero On Wavelength Change: Maintain Baseline

Auto Zero On Inject Start: Yes

Analog 1...

Sensitivity: 2.000 AUFS

Chart Polarity: Positive (+)

Voltage Offset: 0 mV

Enable Chart Mark: Yes

Run Events: Yes

Pulse Width: 1.0 sec

Rect Wave Period: 0.2 sec

----- o0o -----

----- Run method parameters -----

Waters ACQUITY QSM

Solvent A Name: Water

Solvent B Name: Acetonitrile

Solvent C Name: water 1 % FA

Solvent D Name:

Low Pressure Limit: 0 psi

High Pressure Limit: 15000 psi

Seal Wash Period: 5.00 min

[Gradient Table]

	Time(min)	Flow Rate(mL/min)	%A	%B	%C	%D	Curve
--	-----------	-------------------	----	----	----	----	-------

1.	Initial	0.700	90.0	5.0	5.0	0.0	Initial
----	---------	-------	------	-----	-----	-----	---------

2.	0.15	0.700	45.0	50.0	5.0	0.0	6
----	------	-------	------	------	-----	-----	---

3.	1.50	0.700	0.0	95.0	5.0	0.0	6
----	------	-------	-----	------	-----	-----	---

4.	1.80	0.700	90.0	5.0	5.0	0.0	1
----	------	-------	------	-----	-----	-----	---

Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm

Flow Ramp Rate: 0.45 min

D Solvent Selection (if supported): No Change

System Pressure Data Channel: No

Flow Rate Data Channel: No

%A Data Channel: No

%B Data Channel: No

%C Data Channel: No

Dataset: Untitled
Last Altered: Friday, August 06, 2021 16:06:38 Romance Daylight Time
Printed: Friday, August 06, 2021 16:07:17 Romance Daylight Time

%D Data Channel: No
Primary Data Channel: No
Accumulator Data Channel: No
Degasser Data Channel: No
Gradient Start: At Injection
Gradient Start Volume: 0 uL
Gradient Start Time: 0.00 min
Participate in pre-analysis: No
Waters Acquity TUV
Run Time: 1.80 min
Wavelength Mode: Single Wavelength
Lamp On: On
Channel A...
Comment:
Wavelength: 214 nm
Sampling Rate: 20 points/sec
Data Mode: Absorbance
Time Constant: 0.1000 sec
Auto Zero On Wavelength Change: Maintain Baseline
Auto Zero On Inject Start: Yes

Analog 1...
Sensitivity: 2.000 AUFS
Chart Polarity: Positive (+)
Voltage Offset: 0 mV
Enable Chart Mark: Yes
Run Events: Yes
Pulse Width: 1.0 sec
Rect Wave Period: 0.2 sec
Waters ACQUITY FTN AutoSampler
Run Time: 1.80 min
Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm
Load Ahead: Disabled
Loop Offline: Automatic min
Wash Solvent Name: Acetonitrile
Pre-Inject Wash Time: 0.0 sec
Post-Inject Wash Time: 6.0 sec
Purge Solvent Name: Water
Dilution: Disabled
Dilution Volume: 0 uL
Delay Time: 0 min
Dilution Needle Placement: 4.0 mm
Target Column Temperature: 40.0 C
Column Temperature Alarm Band: Disabled
Target Sample Temperature: 15.0 C
Sample Temperature Alarm Band: Disabled
Syringe Draw Rate: Automatic
Needle Placement: Automatic
Pre-Aspirate Air Gap: Automatic
Post-Aspirate Air Gap: Automatic
Column Temperature Data Channel: No
Room Temperature Data Channel: No
Sample Temperature Data Channel: No
Sample Organizer Temperature Data Channel: No
Sample Pressure Data Channel: No
Preheater Temperature Data Channel: No
Seal Force Data Channel: No
No Injection Mode Enabled: No
Run Events: No

Sample Run Injection Parameter

Injection Volume (ul) - 3.00

----- o0o -----

End of experimental record.

----- Waters ACQUITY QSM Postrun Report -----

Firmware Version: 1.50.237 (May 18 2011)

Software Version: 1.50.1621

Checksum: 0xae400516

Serial Number: M09QSM056N

Minimum System Pressure: 0.0 psi

Dataset: Untitled
Last Altered: Friday, August 06, 2021 16:06:38 Romance Daylight Time
Printed: Friday, August 06, 2021 16:07:17 Romance Daylight Time

Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi

-----o0o-----

-----Waters ACQUITY FTN Postrun Report-----

Software Version: 1.50.1481
Firmware Version: 1.50.317 (Jul 11 2011)
Checksum: 0x3e83519d
Serial Number: M09SDI055N
Sample Syringe Size: 100.0
Extension Loop Size: 0.0
Needle Size: 15.0

Column Type: ACQUITY UPLC® BEH C18 1.7µm
Column Serial Number: 02343407715781
Total Injections on Column: 6319
Minimum Sample Temperature: 0.0
Maximum Sample Temperature: 0.0
Average Sample Temperature: 0.0
Minimum Column Temperature: 40.0
Maximum Column Temperature: 40.1
Average Column Temperature: 0.0

-----o0o-----

-----Generic Instrument Postrun Report-----

Software Version: 1.50.2530
Firmware Version: 1.50.2182 (May 11 2011)
Checksum: 0xc09b9cb2
Serial Number: J08UPT460M
Lamp On/Off Event: No
Lamp Life: 798.00
Lamp Serial Number: 000296721
Flow Cell Type: Other
Flow Cell Path Length: 0.00 mm
Flow Cell Volume: 0.00 microliters
Flow Cell Serial Number: 1
Flow Cell Part Number: 1
Optics Temperature Stabilization Setting: unknown

-----o0o-----

-----Waters ACQUITY QSM Postrun Report-----

Firmware Version: 1.50.237 (May 18 2011)
Software Version: 1.50.1621
Checksum: 0xae400516
Serial Number: M09QSM056N
Minimum System Pressure: 0.0 psi
Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi

-----o0o-----

Function 1

Scans in function: 337
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.500
Start and End Time(mins): 0.300 to 1.800
Ionization mode: ES+

Data type: SIR or MRM data
Function type: MRM of 1 channel

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula	Mass Comm
---------------	-------------	------------	------------	-------------	----------	---------	-----------

1 : 419.87 > 295.05	0.260	30.0	18.0	Auto	EA	418.9	Inte
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llicStart Generated

Function 2

Scans in function: 2161
Function type: Diode Array
Wavelength range (nm): 214 to 214

Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
Printed: Tuesday, August 10, 2021 16:07:40 Romance Daylight Time

Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51

Calibration: 10 Aug 2021 16:06:43

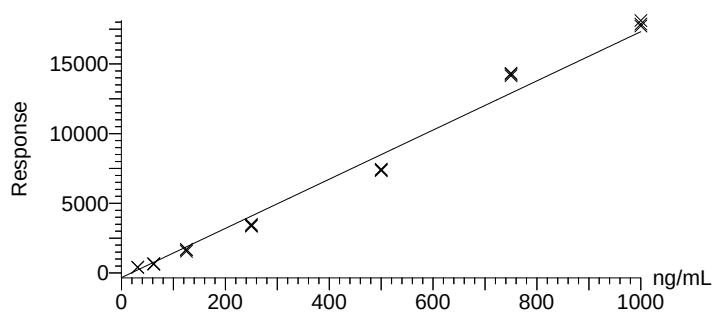
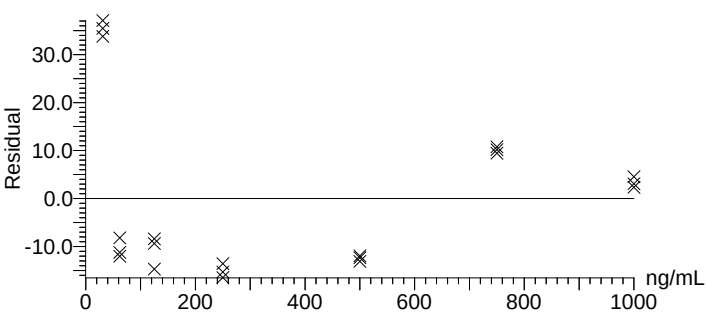
Compound name: A

Correlation coefficient: $r = 0.992787$, $r^2 = 0.985626$

Calibration curve: $17.6488 * x + -329.92$

Response type: External Std, Area

Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

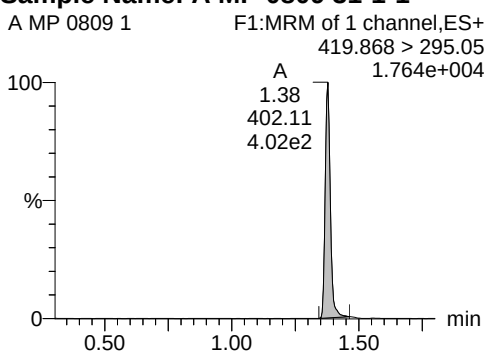


Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
Printed: Tuesday, August 10, 2021 16:07:40 Romance Daylight Time

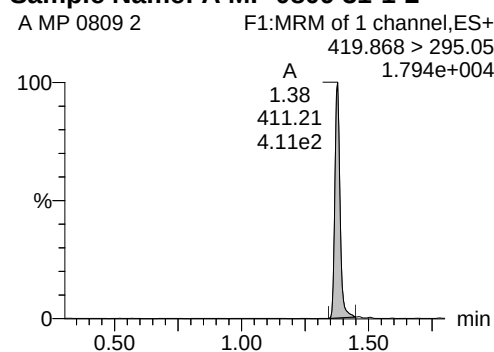
Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51

Calibration: 10 Aug 2021 16:06:43

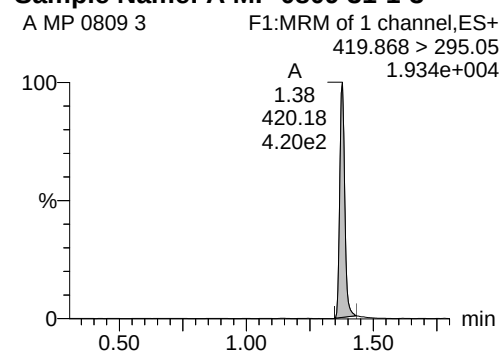
Sample Name: A MP 0809 31-1-1



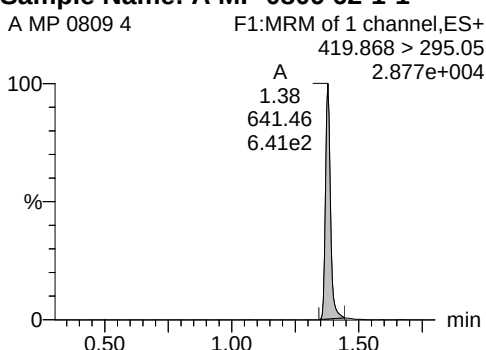
Sample Name: A MP 0809 31-1-2



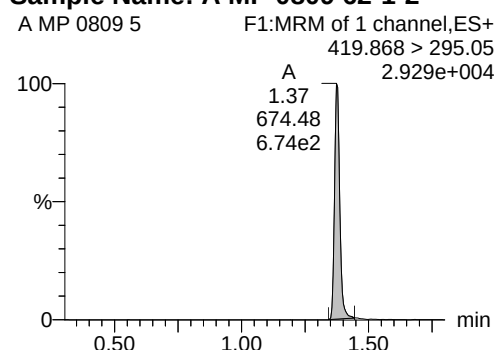
Sample Name: A MP 0809 31-1-3



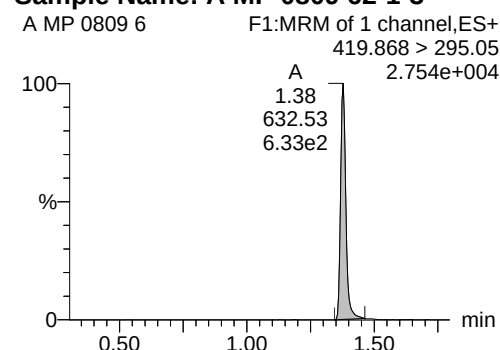
Sample Name: A MP 0809 62-1-1



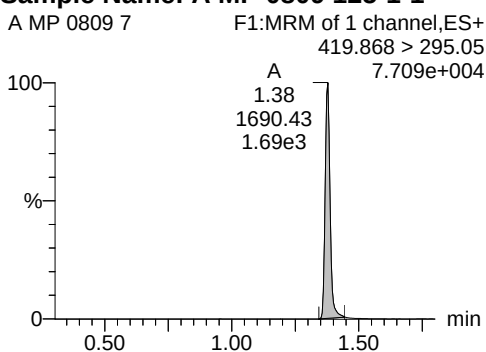
Sample Name: A MP 0809 62-1-2



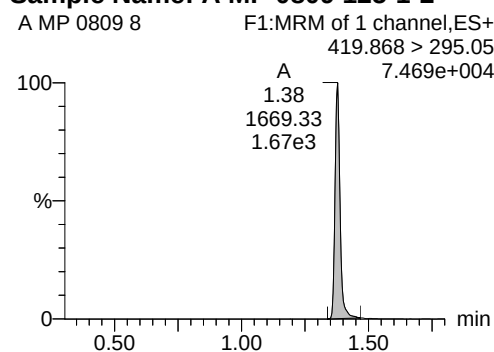
Sample Name: A MP 0809 62-1-3



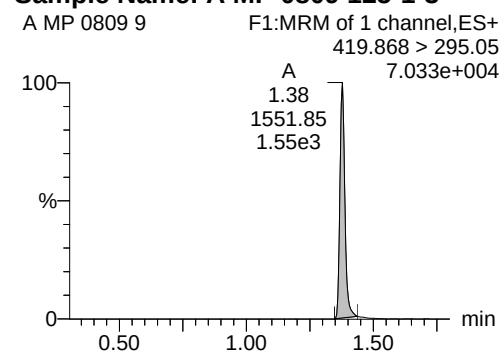
Sample Name: A MP 0809 125-1-1



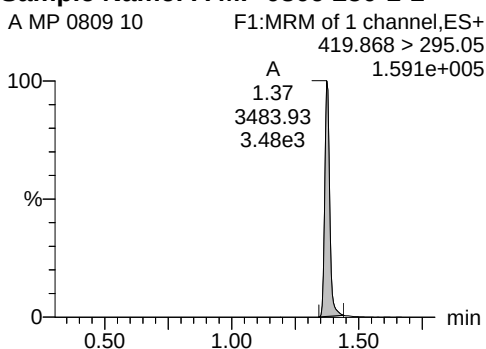
Sample Name: A MP 0809 125-1-2



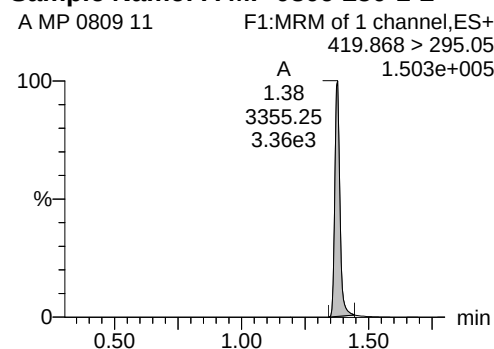
Sample Name: A MP 0809 125-1-3



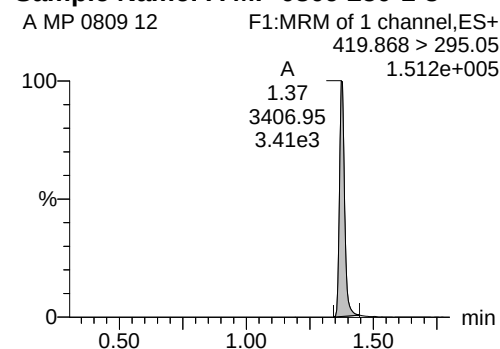
Sample Name: A MP 0809 250-1-1



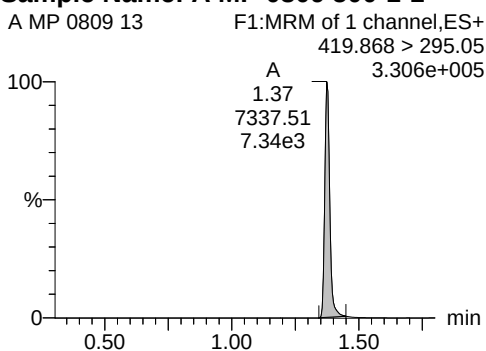
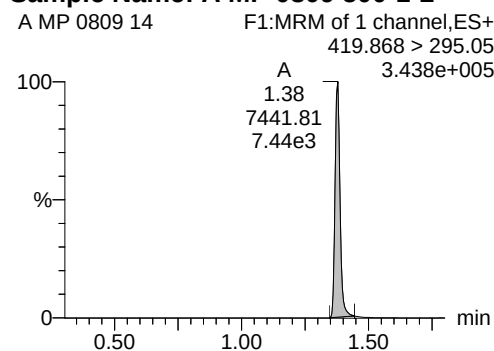
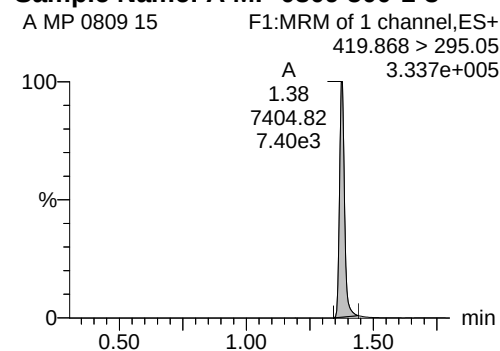
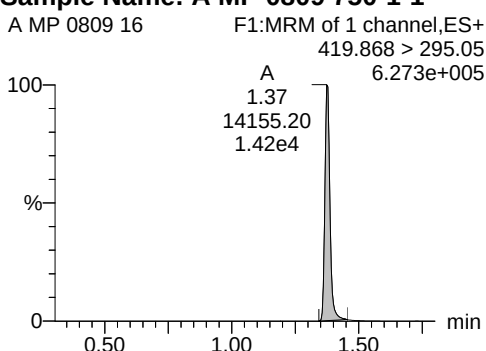
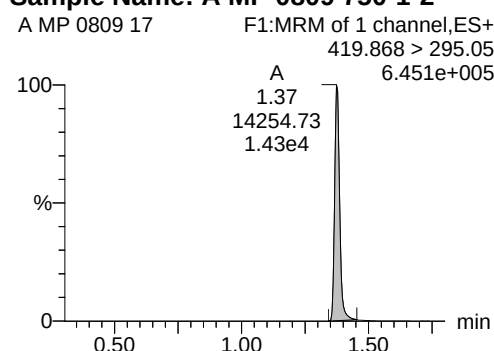
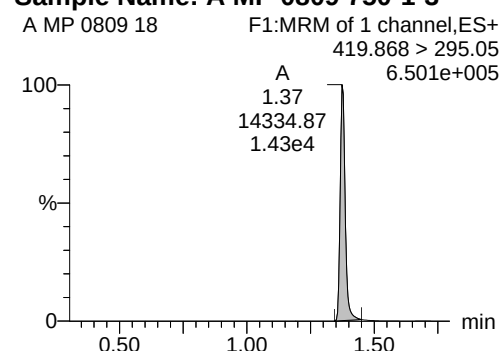
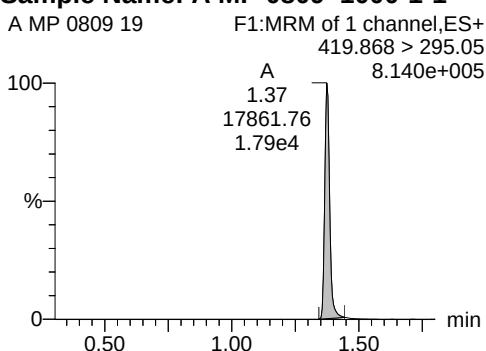
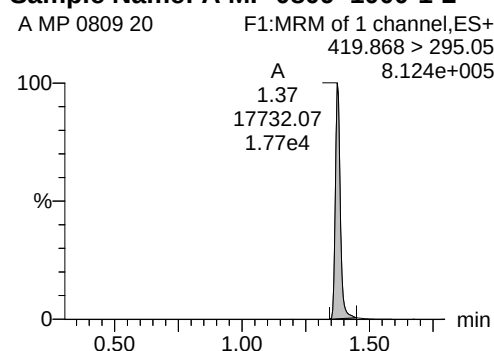
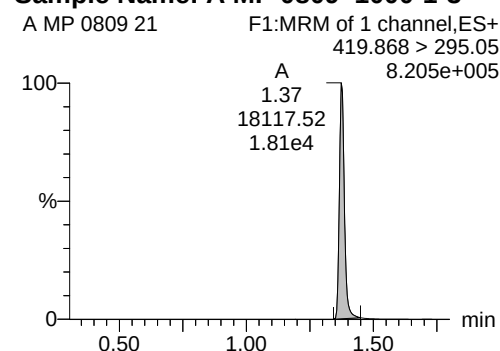
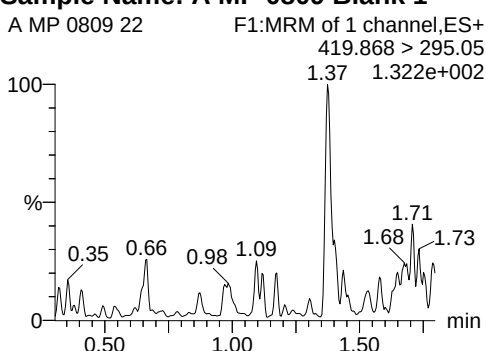
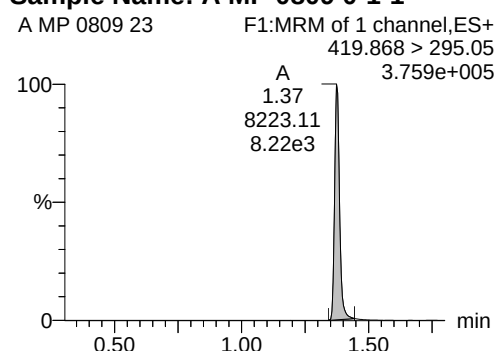
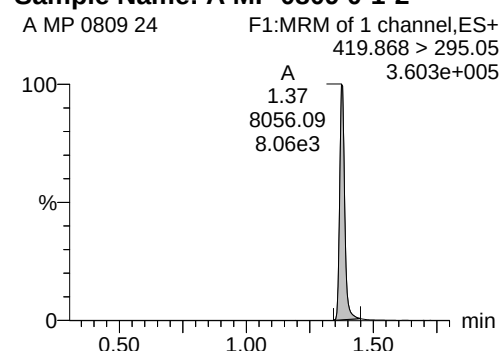
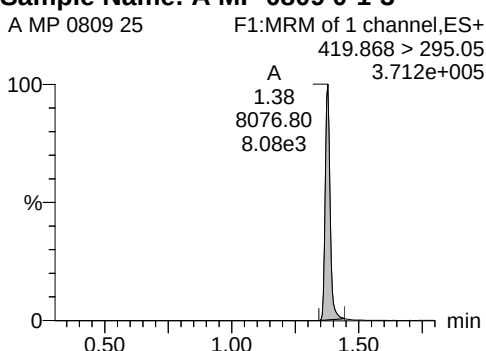
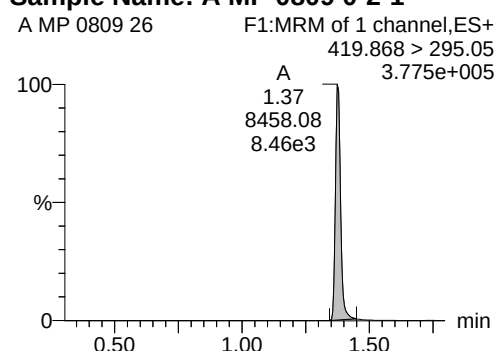
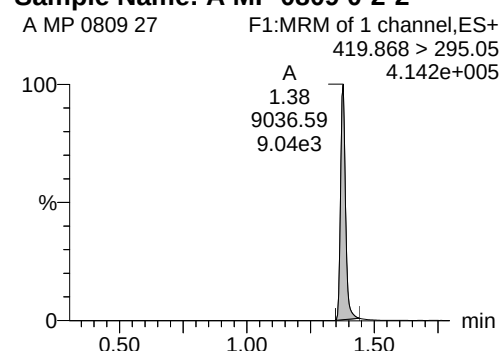
Sample Name: A MP 0809 250-1-2



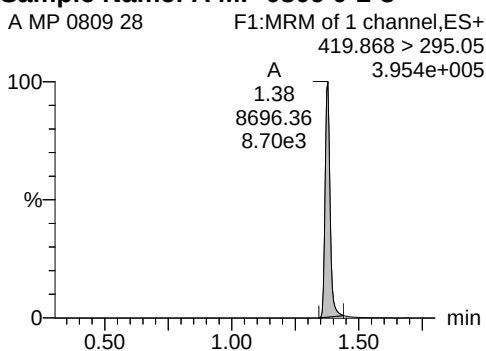
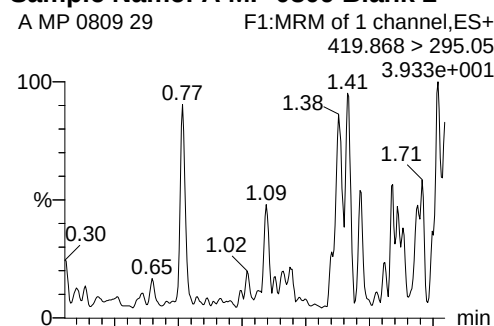
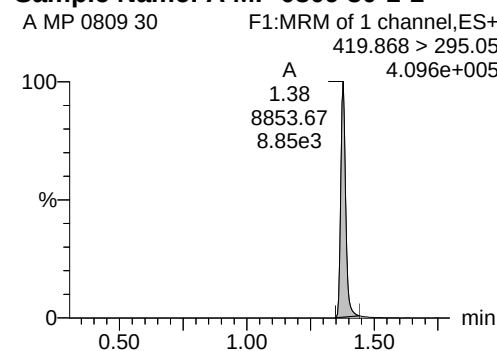
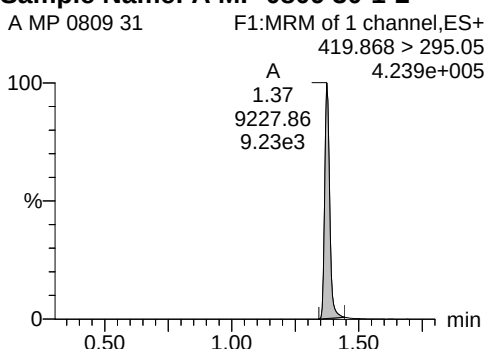
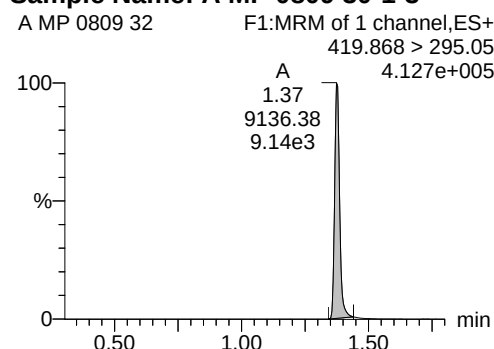
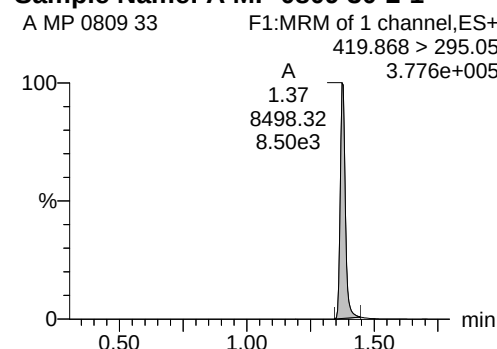
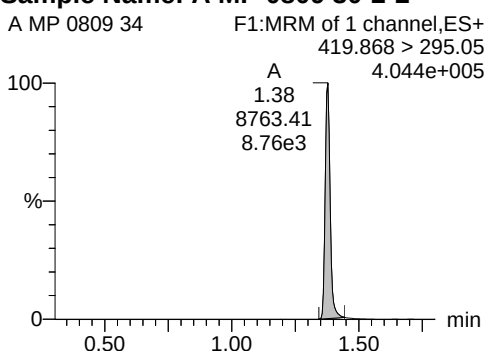
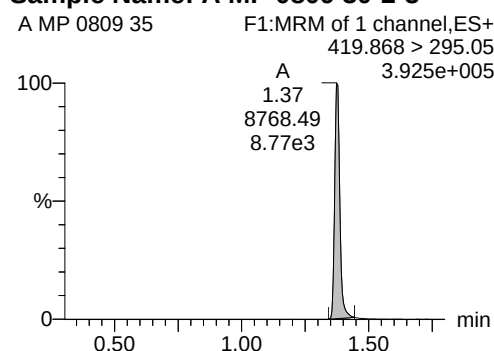
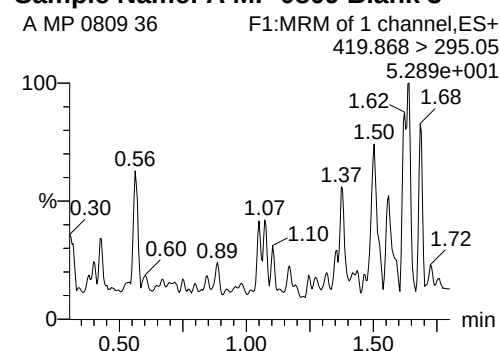
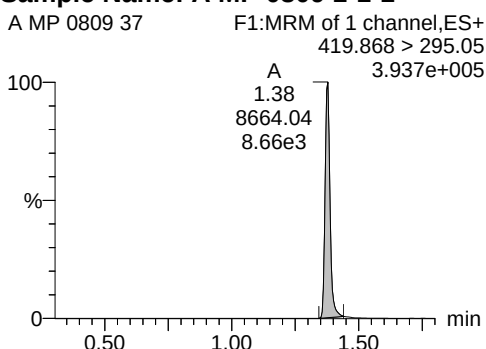
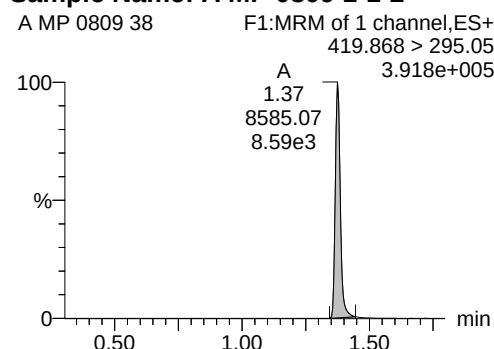
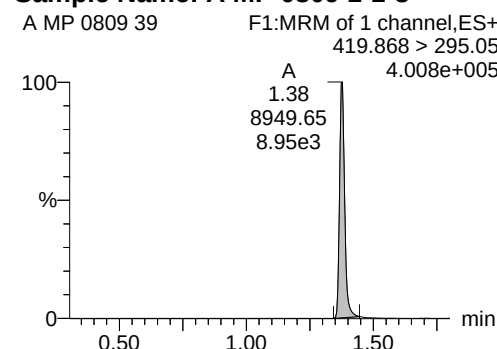
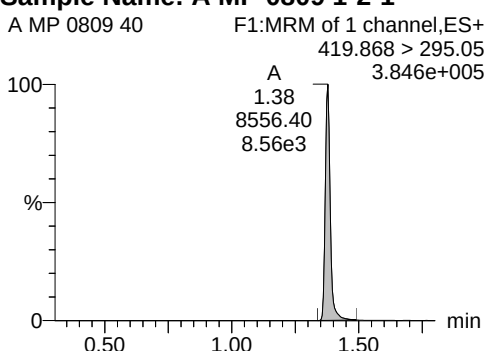
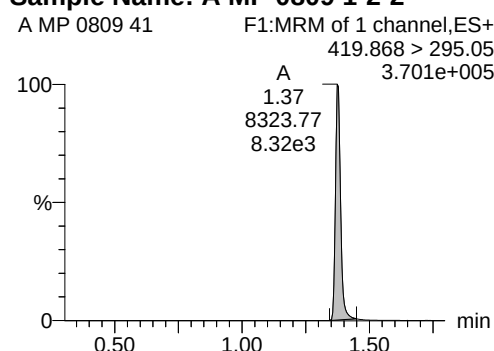
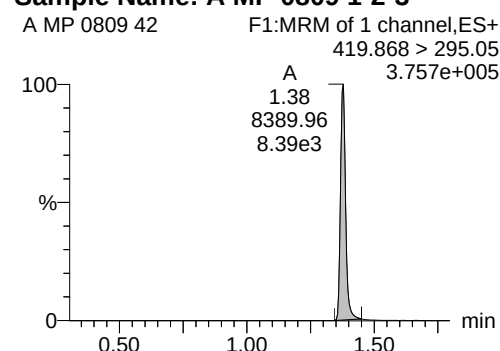
Sample Name: A MP 0809 250-1-3



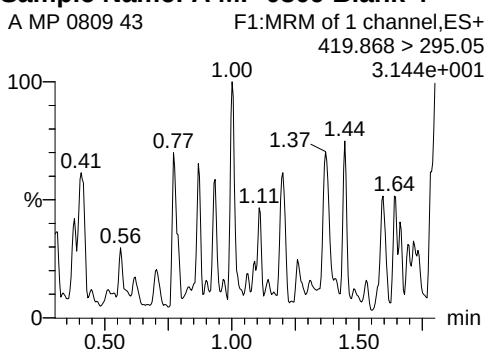
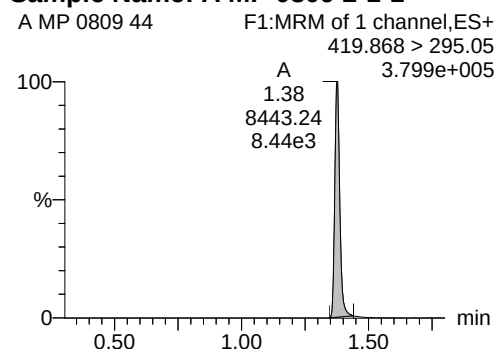
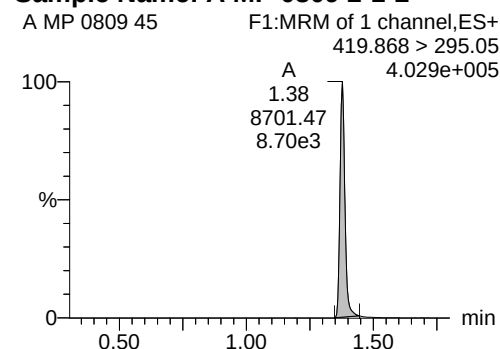
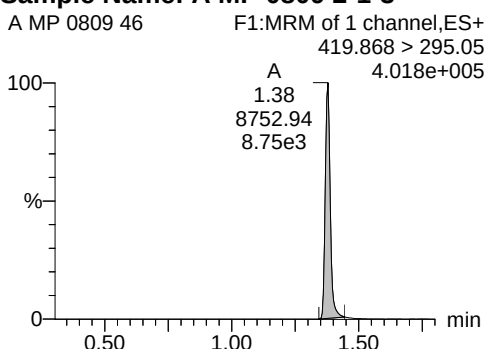
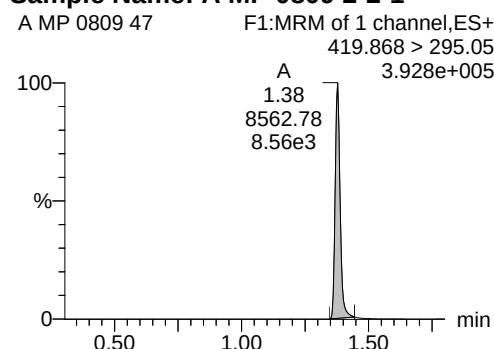
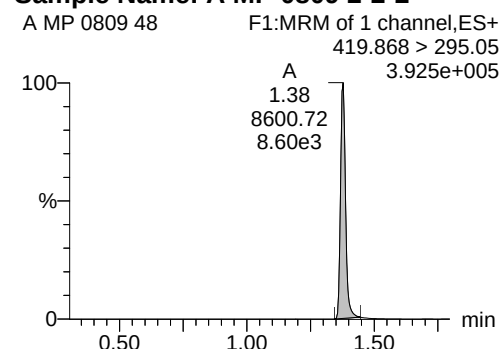
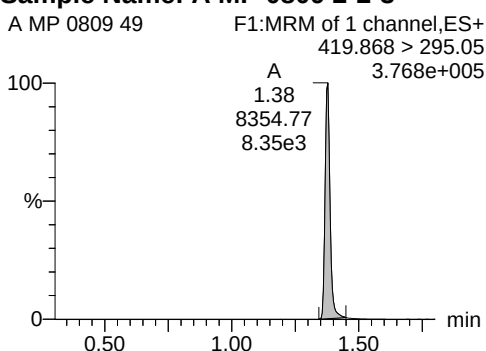
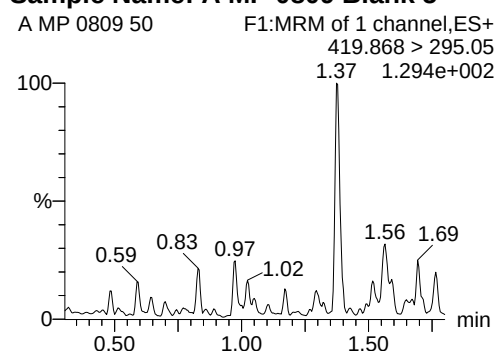
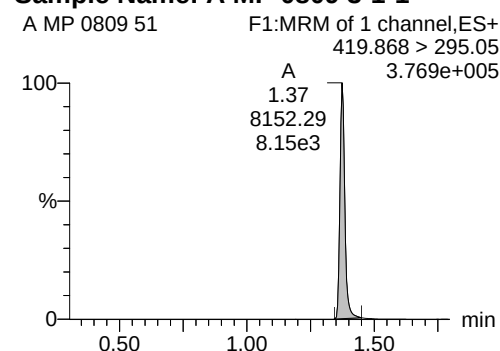
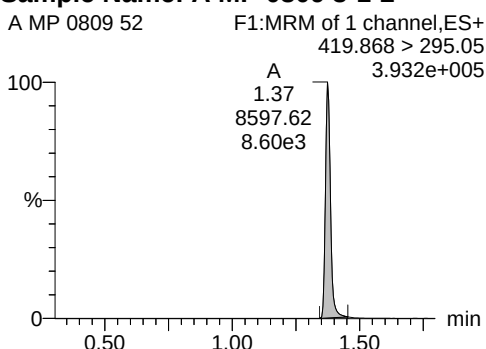
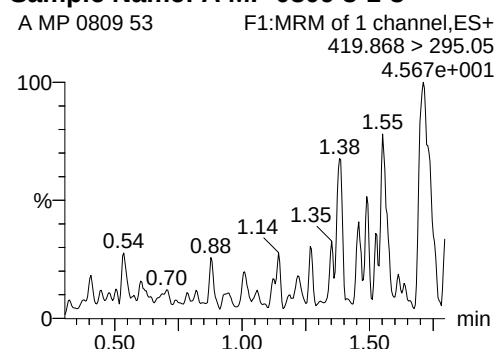
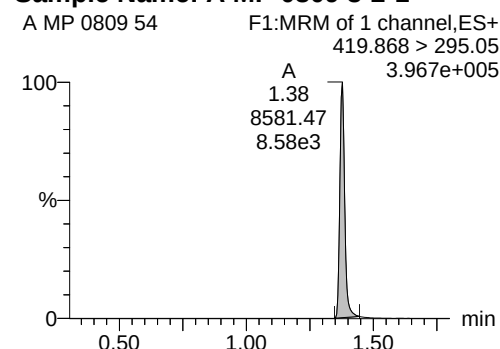
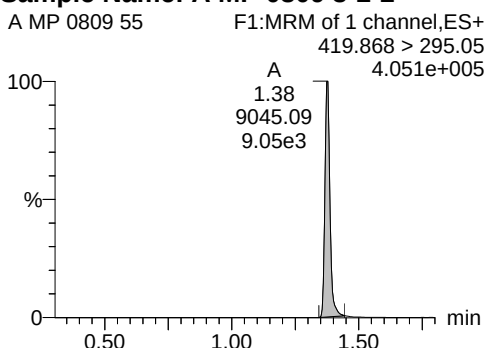
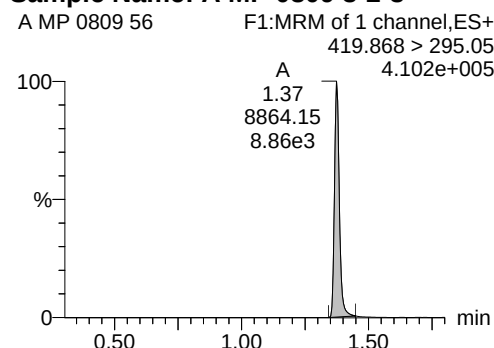
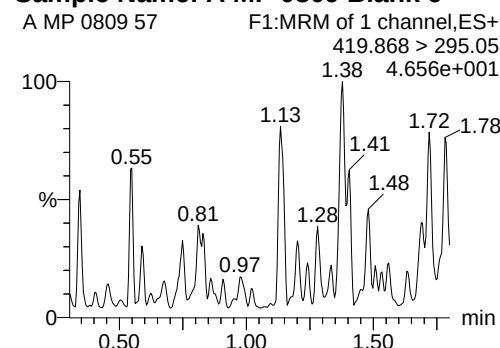
Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
Printed: Tuesday, August 10, 2021 16:07:40 Romance Daylight Time

Sample Name: A MP 0809 500-1-1**Sample Name: A MP 0809 500-1-2****Sample Name: A MP 0809 500-1-3****Sample Name: A MP 0809 750-1-1****Sample Name: A MP 0809 750-1-2****Sample Name: A MP 0809 750-1-3****Sample Name: A MP 0809 1000-1-1****Sample Name: A MP 0809 1000-1-2****Sample Name: A MP 0809 1000-1-3****Sample Name: A MP 0809 Blank 1****Sample Name: A MP 0809 0-1-1****Sample Name: A MP 0809 0-1-2****Sample Name: A MP 0809 0-1-3****Sample Name: A MP 0809 0-2-1****Sample Name: A MP 0809 0-2-2**

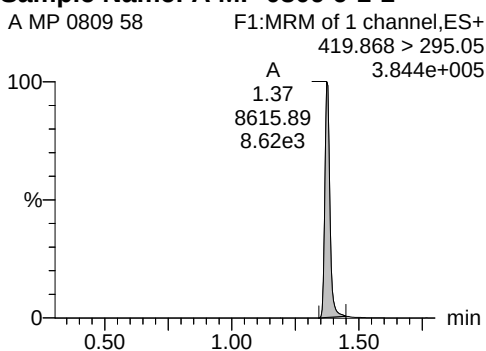
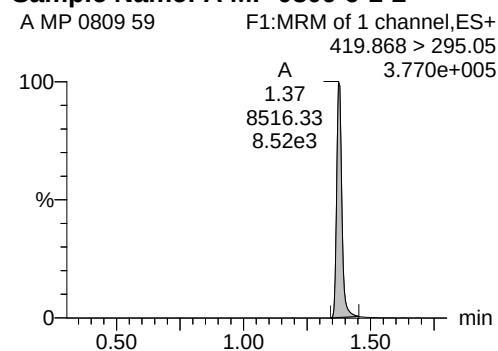
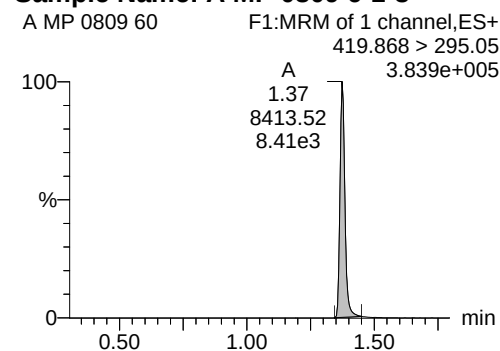
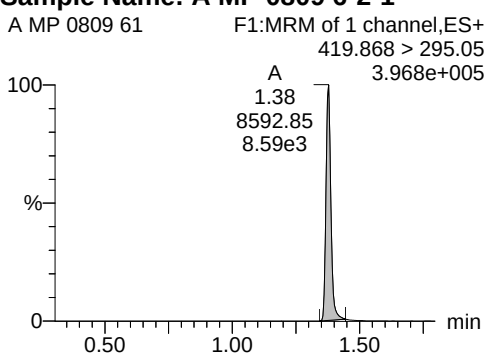
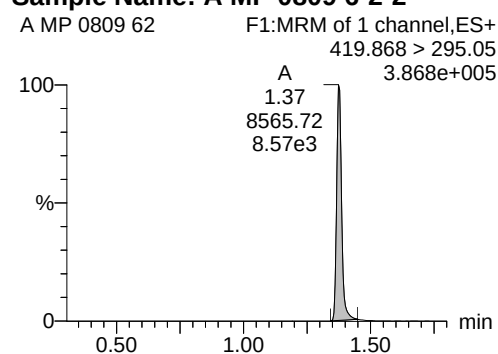
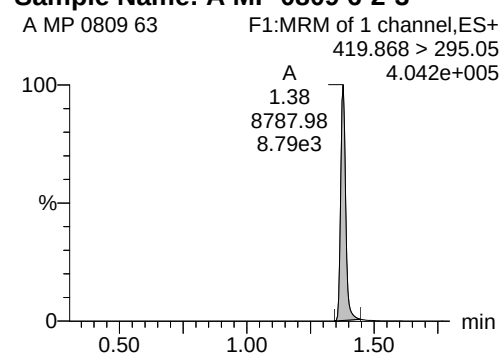
Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
Printed: Tuesday, August 10, 2021 16:07:40 Romance Daylight Time

Sample Name: A MP 0809 0-2-3**Sample Name: A MP 0809 Blank 2****Sample Name: A MP 0809 30-1-1****Sample Name: A MP 0809 30-1-2****Sample Name: A MP 0809 30-1-3****Sample Name: A MP 0809 30-2-1****Sample Name: A MP 0809 30-2-2****Sample Name: A MP 0809 30-2-3****Sample Name: A MP 0809 Blank 3****Sample Name: A MP 0809 1-1-1****Sample Name: A MP 0809 1-1-2****Sample Name: A MP 0809 1-1-3****Sample Name: A MP 0809 1-2-1****Sample Name: A MP 0809 1-2-2****Sample Name: A MP 0809 1-2-3**

Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
Printed: Tuesday, August 10, 2021 16:07:40 Romance Daylight Time

Sample Name: A MP 0809 Blank 4**Sample Name: A MP 0809 2-1-1****Sample Name: A MP 0809 2-1-2****Sample Name: A MP 0809 2-1-3****Sample Name: A MP 0809 2-2-1****Sample Name: A MP 0809 2-2-2****Sample Name: A MP 0809 2-2-3****Sample Name: A MP 0809 Blank 5****Sample Name: A MP 0809 3-1-1****Sample Name: A MP 0809 3-1-2****Sample Name: A MP 0809 3-1-3****Sample Name: A MP 0809 3-2-1****Sample Name: A MP 0809 3-2-2****Sample Name: A MP 0809 3-2-3****Sample Name: A MP 0809 Blank 6**

Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
Printed: Tuesday, August 10, 2021 16:07:40 Romance Daylight Time

Sample Name: A MP 0809 6-1-1**Sample Name: A MP 0809 6-1-2****Sample Name: A MP 0809 6-1-3****Sample Name: A MP 0809 6-2-1****Sample Name: A MP 0809 6-2-2****Sample Name: A MP 0809 6-2-3**

	# Name	Type	Std. Conc	RT	Area	IS Area	Response	Detecti...	ng/mL	%Dev
1	1 A MP 0809 31-1-1	Stan...	31.000	1.38	402.107		402.107	bb	41.5	33.8
2	2 A MP 0809 31-1-2	Stan...	31.000	1.38	411.210		411.210	bb	42.0	35.5
3	3 A MP 0809 31-1-3	Stan...	31.000	1.38	420.178		420.178	bb	42.5	37.1
4	4 A MP 0809 62-1-1	Stan...	62.000	1.38	641.458		641.458	bb	55.0	-11.2
5	5 A MP 0809 62-1-2	Stan...	62.000	1.37	674.476		674.476	bb	56.9	-8.2
6	6 A MP 0809 62-1-3	Stan...	62.000	1.38	632.529		632.529	bb	54.5	-12.0
7	7 A MP 0809 125-1-1	Stan...	125.000	1.38	1690.431		1690.431	bb	114.5	-8.4
8	8 A MP 0809 125-1-2	Stan...	125.000	1.38	1669.333		1669.333	bb	113.3	-9.4
9	9 A MP 0809 125-1-3	Stan...	125.000	1.38	1551.851		1551.851	bb	106.6	-14.7
10	10 A MP 0809 250-1-1	Stan...	250.000	1.37	3483.929		3483.929	bb	216.1	-13.6
11	11 A MP 0809 250-1-2	Stan...	250.000	1.38	3355.248		3355.248	bb	208.8	-16.5
12	12 A MP 0809 250-1-3	Stan...	250.000	1.37	3406.949		3406.949	bb	211.7	-15.3
13	13 A MP 0809 500-1-1	Stan...	500.000	1.37	7337.505		7337.505	bb	434.4	-13.1
14	14 A MP 0809 500-1-2	Stan...	500.000	1.38	7441.806		7441.806	bb	440.4	-11.9
15	15 A MP 0809 500-1-3	Stan...	500.000	1.38	7404.821		7404.821	bb	438.3	-12.3
16	16 A MP 0809 750-1-1	Stan...	750.000	1.37	14155.195		14155.195	bb	820.7	9.4
17	17 A MP 0809 750-1-2	Stan...	750.000	1.37	14254.726		14254.726	bb	826.4	10.2
18	18 A MP 0809 750-1-3	Stan...	750.000	1.37	14334.868		14334.868	bb	830.9	10.8
19	19 A MP 0809 1000-1-1	Stan...	1000.000	1.37	17861.760		17861.760	bb	1030.8	3.1
20	20 A MP 0809 1000-1-2	Stan...	1000.000	1.37	17732.070		17732.070	bb	1023.4	2.3
21	21 A MP 0809 1000-1-3	Stan...	1000.000	1.37	18117.516		18117.516	bb	1045.3	4.5
22	22 A MP 0809 Blank 1	Blank								
23	23 A MP 0809 0-1-1	Anal...		1.37	8223.114		8223.114	bb	484.6	
24	24 A MP 0809 0-1-2	Anal...		1.37	8056.094		8056.094	bb	475.2	
25	25 A MP 0809 0-1-3	Anal...		1.38	8076.796		8076.796	bb	476.3	
26	26 A MP 0809 0-2-1	Anal...		1.37	8458.085		8458.085	bb	497.9	
27	27 A MP 0809 0-2-2	Anal...		1.38	9036.594		9036.594	bb	530.7	
28	28 A MP 0809 0-2-3	Anal...		1.38	8696.356		8696.356	bb	511.4	
29	29 A MP 0809 Blank 2	Blank								
30	30 A MP 0809 30-1-1	Anal...		1.38	8853.674		8853.674	bb	520.4	
31	31 A MP 0809 30-1-2	Anal...		1.37	9227.857		9227.857	bb	541.6	
32	32 A MP 0809 30-1-3	Anal...		1.37	9136.378		9136.378	bb	536.4	
33	33 A MP 0809 30-2-1	Anal...		1.37	8498.318		8498.318	bb	500.2	
34	34 A MP 0809 30-2-2	Anal...		1.38	8763.412		8763.412	bb	515.2	
35	35 A MP 0809 30-2-3	Anal...		1.37	8768.485		8768.485	bb	515.5	
36	36 A MP 0809 Blank 3	Blank								
37	37 A MP 0809 1-1-1	Anal...		1.38	8664.037		8664.037	bb	509.6	
38	38 A MP 0809 1-1-2	Anal...		1.37	8585.073		8585.073	bb	505.1	
39	39 A MP 0809 1-1-3	Anal...		1.38	8949.646		8949.646	bb	525.8	
40	40 A MP 0809 1-2-1	Anal...		1.38	8556.404		8556.404	bb	503.5	
41	41 A MP 0809 1-2-2	Anal...		1.37	8323.767		8323.767	bb	490.3	
42	42 A MP 0809 1-2-3	Anal...		1.38	8389.962		8389.962	bb	494.1	
43	43 A MP 0809 Blank 4	Blank								
44	44 A MP 0809 2-1-1	Anal...		1.38	8443.240		8443.240	bb	497.1	
45	45 A MP 0809 2-1-2	Anal...		1.38	8701.473		8701.473	bb	511.7	
46	46 A MP 0809 2-1-3	Anal...		1.38	8752.936		8752.936	bb	514.6	
47	47 A MP 0809 2-2-1	Anal...		1.38	8562.783		8562.783	bb	503.9	
48	48 A MP 0809 2-2-2	Anal...		1.38	8600.715		8600.715	bb	506.0	
49	49 A MP 0809 2-2-3	Anal...		1.38	8354.774		8354.774	bb	492.1	
50	50 A MP 0809 Blank 5	Blank								
51	51 A MP 0809 3-1-1	Anal...		1.37	8152.294		8152.294	bb	480.6	
52	52 A MP 0809 3-1-2	Anal...		1.37	8597.622		8597.622	bb	505.8	
53	53 A MP 0809 3-1-3	Anal...								
54	54 A MP 0809 3-2-1	Anal...		1.38	8581.473		8581.473	bb	504.9	
55	55 A MP 0809 3-2-2	Anal...		1.38	9045.090		9045.090	bb	531.2	
56	56 A MP 0809 3-2-3	Anal...		1.37	8864.148		8864.148	bb	520.9	
57	57 A MP 0809 Blank 6	Blank								
58	58 A MP 0809 6-1-1	Anal...		1.37	8615.894		8615.894	bb	506.9	

Dataset: Untitled
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	# Name	Type	Std. Conc	RT	Area	IS Area	Response Detecti...	ng/mL	%Dev
59	59 A MP 0809 6-1-2	Anal...		1.37	8516.327		8516.327 bb	501.2	
60	60 A MP 0809 6-1-3	Anal...		1.37	8413.519		8413.519 bb	495.4	
61	61 A MP 0809 6-2-1	Anal...		1.38	8592.851		8592.851 bb	505.6	
62	62 A MP 0809 6-2-2	Anal...		1.37	8565.722		8565.722 bb	504.0	
63	63 A MP 0809 6-2-3	Anal...		1.38	8787.980		8787.980 bb	516.6	

Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
Printed: Tuesday, August 10, 2021 16:07:40 Romance Daylight Time

Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51
Calibration: 10 Aug 2021 16:06:43

Header

Acquired File Name: A MP 0809 31-1-1
Acquired Date: 10-Aug-2021
Acquired Time: 02:07:30
Job Code: PSMP - 20210809 - N - 216 - 075 - A
Task Code:
User Name:
Laboratory Name:
Instrument: ACQ-TQD#QBA320
Conditions:
Submitter:
SampleID: A MP 0809 1
Bottle Number: 2:79
Description:
Instrument Calibration:
Calibration File: C:\MassLynx\IntelliStart\Results\Unit Mass Resolution\Calib 20161209.cal

Parameters

MS1 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS1

MS1 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS1
MS1 Scan Speed Compensation:
Scan: 339 to 2000 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS1

MS2 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS2

MS2 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS2
MS2 Scan Speed Compensation:
Scan: 339 to 10165 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS2
Calibration Time: 10:33
Calibration Date: 12/09/16

Coefficients

MS1 Static: $-0.000000000000 \times x^4 + 0.000000000843 \times x^3 + -0.000001360559 \times x^2 + 1.000940122634 \times x + -0.253266439024$
MS2 Static: $-0.000000000000 \times x^4 + 0.000000000573 \times x^3 + -0.000001239648 \times x^2 + 1.000902600483 \times x + -0.192715155436$

Function 1: None

Function 2: None

Parameters for C:\Documents and Settings\Administrator\Desktop\old desktop\log D\EA.EXP

Data Processing:

SIR / MRM Chromatogram Spike Removal ON

Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
Printed: Tuesday, August 10, 2021 16:07:40 Romance Daylight Time

SIR / MRM Smoothing OFF

Smoothing window size (scans) 3

Number of smooths 2

Prescan Statistics:

Initial Average Intensity 21.8092

Initial Average Std Dev 1.7357

Bunch Zero Level 0.0135

Bunch Std Dev 0.0170

Bunch Threshold 0.1363

Spike Removal Std Dev 1.7258

Method Events:

Initial Stop Flow: No Change

Initial Switch 2: No Change

Initial Switch 3: No Change

Initial Switch 4: No Change

Initial Infusion: No Change

Initial Flow State: LC

Initial Flow Rate: 5

Initial Reservoir: No Action

API Probe Delay Temp: 20

Initial Refill: No Action

Timed Events Enabled

Event Time Name Action

Instrument Parameters - Function 1:

Parameter File - C:\Documents and Settings\Administrator\Desktop\old desktop\log D\log D tune file.

IPR

Polarity ES+

Calibration Static 2

Capillary (kV) 3.50 3.48

Cone (V) 38.00 28.57

Extractor (V) 3.00 2.20

RF (V) 0.10

Source Temperature (°C) 140 139

Desolvation Temperature (°C) 450 450

Cone Gas Flow (L/Hr) 90 90

Desolvation Gas Flow (L/Hr) 900 901

Collision Gas Flow (mL/Min) 0.20 0.20

LM 1 Resolution 15.50

HM 1 Resolution 14.84

Ion Energy 1 0.30

MS Mode Entrance 50.00

MS Mode Collision Energy 3.00

MS Mode Exit 50.00

MSMS Mode Entrance -2.00

MSMS Mode Collision Energy 2.00

MSMS Mode Exit 2.00

LM 2 Resolution 15.00

HM 2 Resolution 15.50

Ion Energy 2 1.22

Gain 1.00

Multiplier -493.82

Active Reservoir B

Engineers Settings:

MS1 Low Mass Position 518

MS1 High Mass Position 284

MS1 Low Mass Resolution 513

MS1 High Mass Resolution 1732

MS1 Resolution Linearity 834

MS1 High Mass DC Balance 0

MS1 DC Polarity Positive

MS2 Low Mass Position 519

MS2 High Mass Position 238

MS2 Low Mass Resolution 518

MS2 High Mass Resolution 644

MS2 Resolution Linearity 756

MS2 High Mass DC Balance -0

MS2 DC Polarity Positive

HM RF Lens Correction + 0

Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
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HM RF Lens Correction - 0

Inter-scan delays:

Automatic Mode

MS 1 Delay Table:

	R	delay
<=	0.500	0.005
<=	1.200	0.010
<=	2.400	0.015
<=	6.000	0.020
<=	15.000	0.025
<=	25.000	0.028
>	25.000	0.030

MS 2 Delay Table:

	R	delay
<=	2.000	0.005
<=	4.000	0.008
<=	7.000	0.010
<=	10.000	0.012
<=	20.000	0.014
>	20.000	0.016

ACE Experimental Record

Inlet Method File: c:\masslynx_projects\medchem su.pro\acqudb\adme sophie

----- Prerun method parameters -----

Waters ACQUITY QSM

Waters Acquity TUV

Run Time: 0.20 min

Wavelength Mode: Single Wavelength

Lamp On: On

Channel A...

Comment:

Wavelength: 254 nm

Sampling Rate: 20 points/sec

Data Mode: Absorbance

Time Constant: 0.1000 sec

Auto Zero On Wavelength Change: Maintain Baseline

Auto Zero On Inject Start: Yes

Analog 1...

Sensitivity: 2.000 AUFS

Chart Polarity: Positive (+)

Voltage Offset: 0 mV

Enable Chart Mark: Yes

Run Events: Yes

Pulse Width: 1.0 sec

Rect Wave Period: 0.2 sec

----- o0o -----

----- Run method parameters -----

Waters ACQUITY QSM

Solvent A Name: Water

Solvent B Name: Acetonitrile

Solvent C Name: water 1 % FA

Solvent D Name:

Low Pressure Limit: 0 psi

High Pressure Limit: 15000 psi

Seal Wash Period: 5.00 min

[Gradient Table]

	Time(min)	Flow Rate(mL/min)	%A	%B	%C	%D	Curve
--	-----------	-------------------	----	----	----	----	-------

1.	Initial	0.700	90.0	5.0	5.0	0.0	Initial
----	---------	-------	------	-----	-----	-----	---------

2.	0.15	0.700	45.0	50.0	5.0	0.0	6
----	------	-------	------	------	-----	-----	---

3.	1.50	0.700	0.0	95.0	5.0	0.0	6
----	------	-------	-----	------	-----	-----	---

4.	1.80	0.700	90.0	5.0	5.0	0.0	1
----	------	-------	------	-----	-----	-----	---

Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm

Flow Ramp Rate: 0.45 min

D Solvent Selection (if supported): No Change

System Pressure Data Channel: No

Flow Rate Data Channel: No

%A Data Channel: No

%B Data Channel: No

%C Data Channel: No

Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
Printed: Tuesday, August 10, 2021 16:07:40 Romance Daylight Time

%D Data Channel: No
Primary Data Channel: No
Accumulator Data Channel: No
Degasser Data Channel: No
Gradient Start: At Injection
Gradient Start Volume: 0 uL
Gradient Start Time: 0.00 min
Participate in pre-analysis: No
Waters Acquity TUV
Run Time: 1.80 min
Wavelength Mode: Single Wavelength
Lamp On: On
Channel A...
Comment:
Wavelength: 214 nm
Sampling Rate: 20 points/sec
Data Mode: Absorbance
Time Constant: 0.1000 sec
Auto Zero On Wavelength Change: Maintain Baseline
Auto Zero On Inject Start: Yes

Analog 1...
Sensitivity: 2.000 AUFS
Chart Polarity: Positive (+)
Voltage Offset: 0 mV
Enable Chart Mark: Yes
Run Events: Yes
Pulse Width: 1.0 sec
Rect Wave Period: 0.2 sec
Waters ACQUITY FTN AutoSampler
Run Time: 1.80 min
Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm
Load Ahead: Disabled
Loop Offline: Automatic min
Wash Solvent Name: Acetonitrile
Pre-Inject Wash Time: 0.0 sec
Post-Inject Wash Time: 6.0 sec
Purge Solvent Name: Water
Dilution: Disabled
Dilution Volume: 0 uL
Delay Time: 0 min
Dilution Needle Placement: 4.0 mm
Target Column Temperature: 40.0 C
Column Temperature Alarm Band: Disabled
Target Sample Temperature: 15.0 C
Sample Temperature Alarm Band: Disabled
Syringe Draw Rate: Automatic
Needle Placement: Automatic
Pre-Aspirate Air Gap: Automatic
Post-Aspirate Air Gap: Automatic
Column Temperature Data Channel: No
Room Temperature Data Channel: No
Sample Temperature Data Channel: No
Sample Organizer Temperature Data Channel: No
Sample Pressure Data Channel: No
Preheater Temperature Data Channel: No
Seal Force Data Channel: No
No Injection Mode Enabled: No
Run Events: No

Sample Run Injection Parameter

Injection Volume (ul) - 3.00

----- o0o -----

End of experimental record.

----- Waters ACQUITY QSM Postrun Report -----

Firmware Version: 1.50.237 (May 18 2011)

Software Version: 1.50.1621

Checksum: 0xae400516

Serial Number: M09QSM056N

Minimum System Pressure: 0.0 psi

Dataset: Untitled
Last Altered: Tuesday, August 10, 2021 16:06:43 Romance Daylight Time
Printed: Tuesday, August 10, 2021 16:07:40 Romance Daylight Time

Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi

-----o0o-----

-----Waters ACQUITY FTN Postrun Report-----

Software Version: 1.50.1481
Firmware Version: 1.50.317 (Jul 11 2011)
Checksum: 0x3e83519d
Serial Number: M09SDI055N
Sample Syringe Size: 100.0
Extension Loop Size: 0.0
Needle Size: 15.0
Column Type: ACQUITY UPLC® BEH C18 1.7µm
Column Serial Number: 02343407715781
Total Injections on Column: 6739
Minimum Sample Temperature: 0.0
Maximum Sample Temperature: 0.0
Average Sample Temperature: 0.0
Minimum Column Temperature: 40.0
Maximum Column Temperature: 40.1
Average Column Temperature: 0.0

-----o0o-----

-----Generic Instrument Postrun Report-----

Software Version: 1.50.2530
Firmware Version: 1.50.2182 (May 11 2011)
Checksum: 0xc09b9cb2
Serial Number: J08UPT460M
Lamp On/Off Event: No
Lamp Life: 823.00
Lamp Serial Number: 000296721
Flow Cell Type: Other
Flow Cell Path Length: 0.00 mm
Flow Cell Volume: 0.00 microliters
Flow Cell Serial Number: 1
Flow Cell Part Number: 1
Optics Temperature Stabilization Setting: unknown

-----o0o-----

-----Waters ACQUITY QSM Postrun Report-----

Firmware Version: 1.50.237 (May 18 2011)
Software Version: 1.50.1621
Checksum: 0xae400516
Serial Number: M09QSM056N
Minimum System Pressure: 0.0 psi
Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi

-----o0o-----

Function 1

Scans in function: 338
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.500
Start and End Time(mins): 0.300 to 1.800
Ionization mode: ES+

Data type: SIR or MRM data
Function type: MRM of 1 channel

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula	Mass Comm
---------------	-------------	------------	------------	-------------	----------	---------	-----------

1 : 419.87 > 295.05	0.260	30.0	18.0	Auto	EA	418.9	Inte
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Function 2

Scans in function: 2161
Function type: Diode Array
Wavelength range (nm): 214 to 214

Dataset: Untitled
Last Altered: Monday, January 18, 2021 11:54:53 Romance Standard Time
Printed: Monday, January 18, 2021 11:55:44 Romance Standard Time

Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 10:59:51

Calibration: 18 Jan 2021 11:54:53

Compound name: A

No Calibration

Response type: External Std, Area

Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

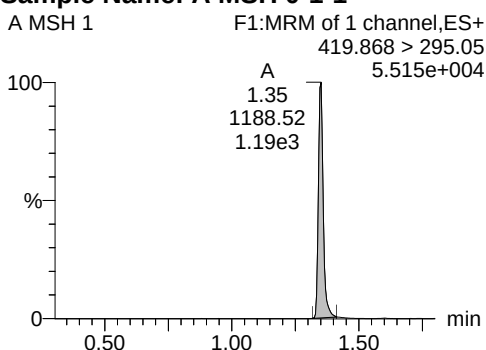


Dataset: Untitled
Last Altered: Monday, January 18, 2021 11:54:53 Romance Standard Time
Printed: Monday, January 18, 2021 11:55:44 Romance Standard Time

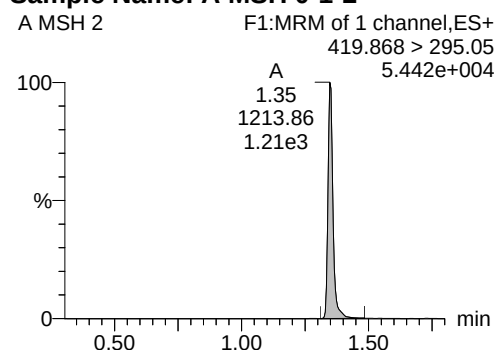
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Calibration: 18 Jan 2021 11:54:53

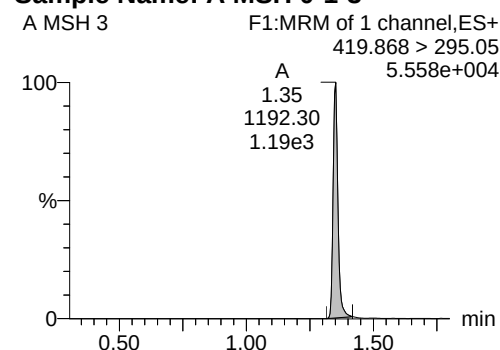
Sample Name: A MSH 0-1-1



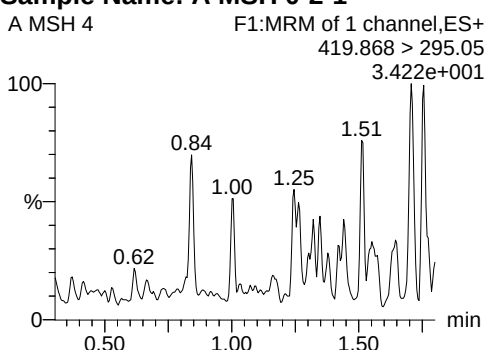
Sample Name: A MSH 0-1-2



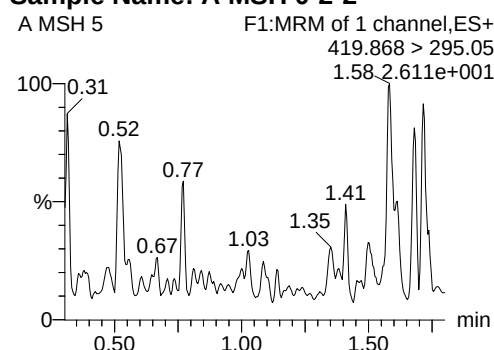
Sample Name: A MSH 0-1-3



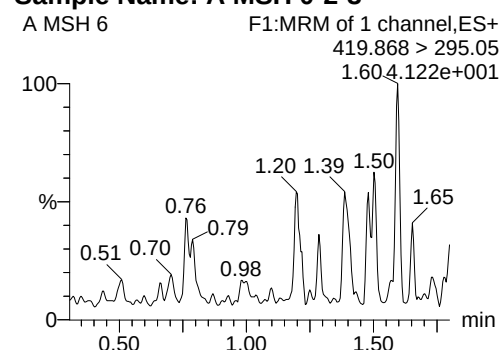
Sample Name: A MSH 0-2-1



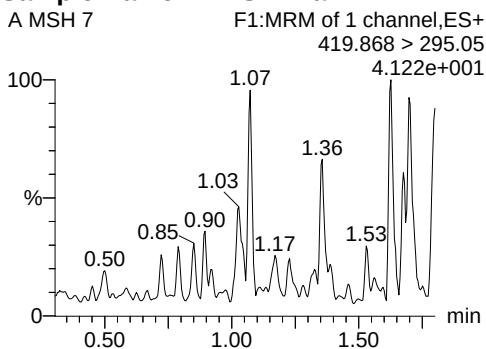
Sample Name: A MSH 0-2-2



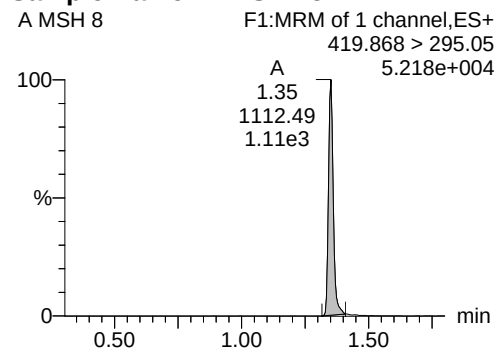
Sample Name: A MSH 0-2-3



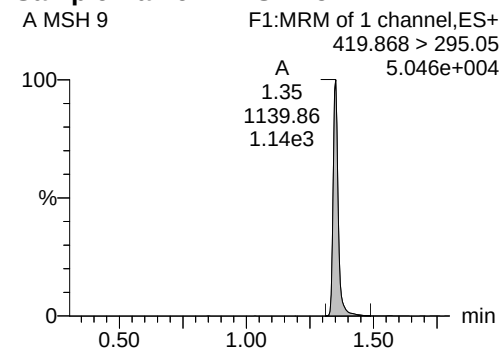
Sample Name: A MSH Blank 1



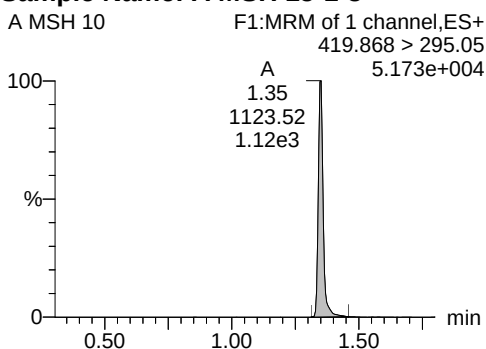
Sample Name: A MSH 15-1-1



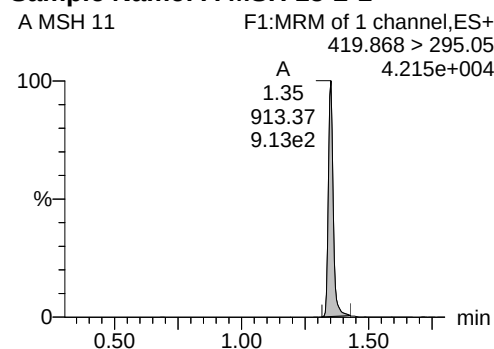
Sample Name: A MSH 15-1-2



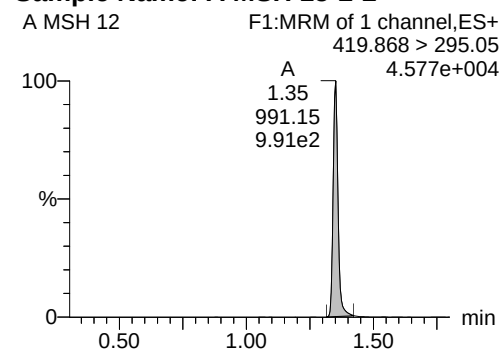
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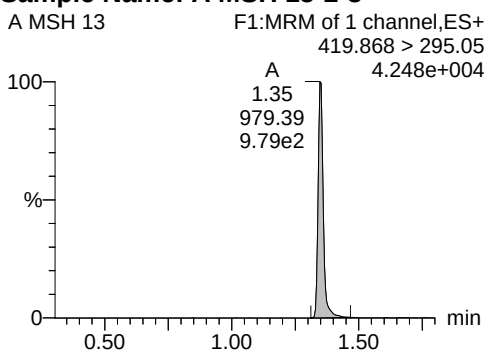
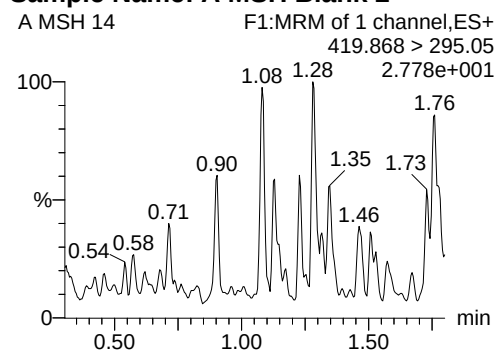
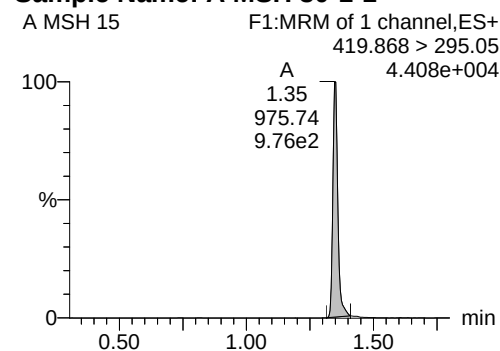
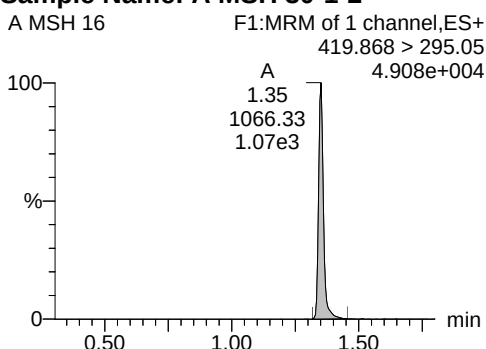
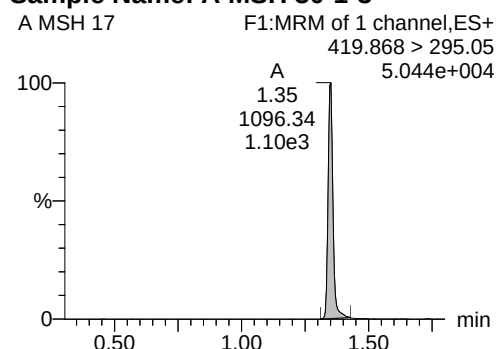
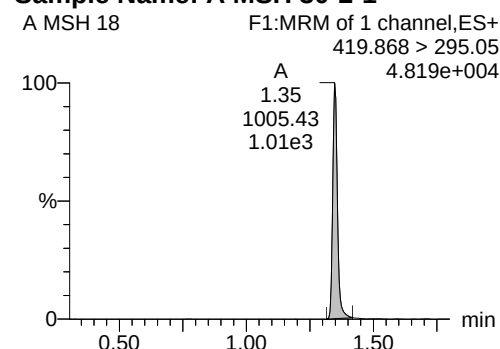
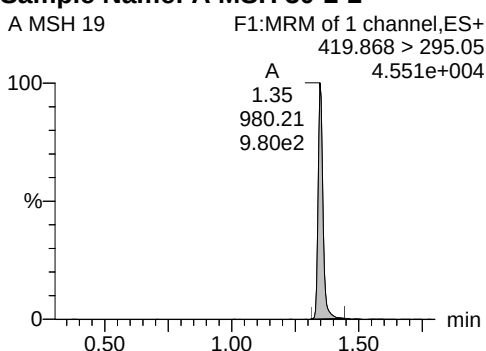
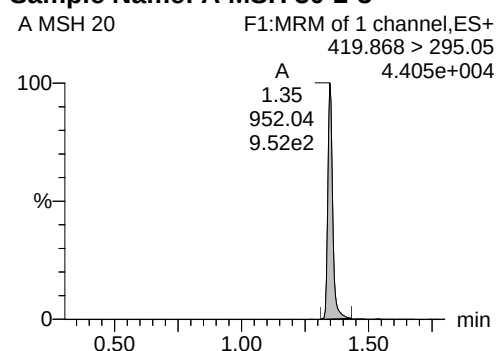
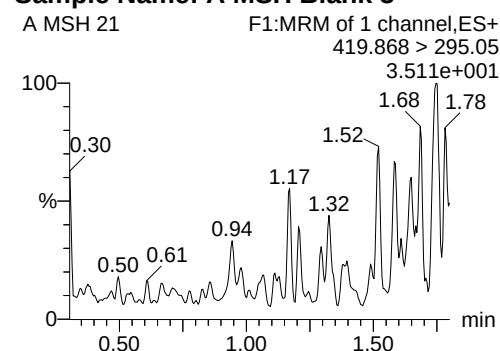
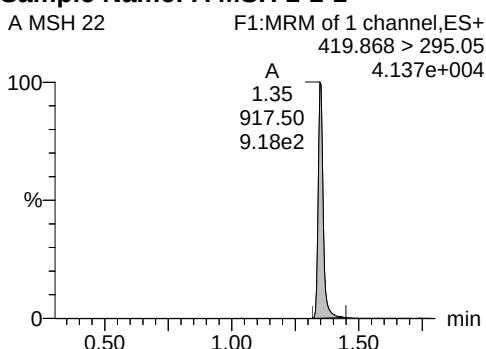
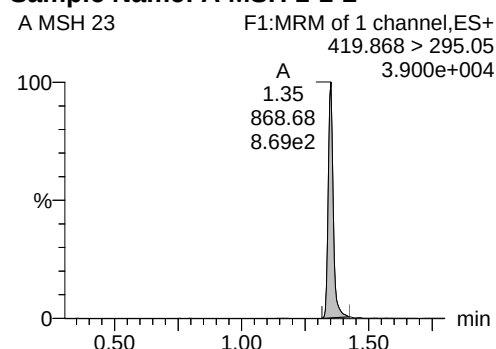
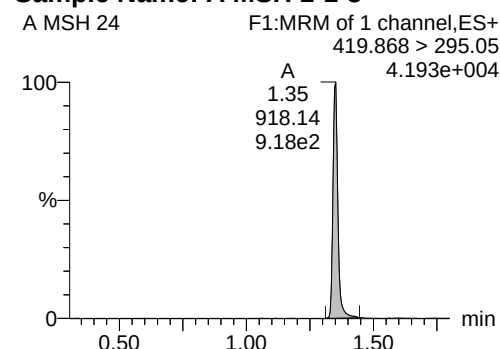
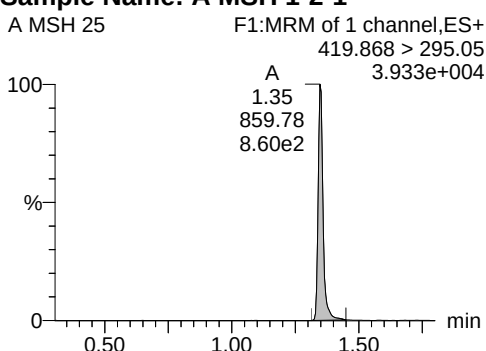
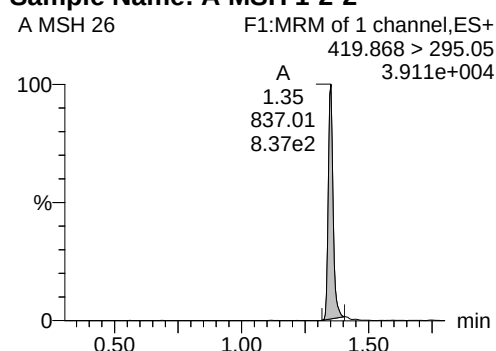
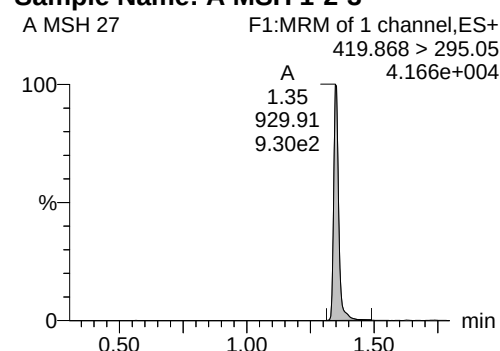
Sample Name: A MSH 15-2-1



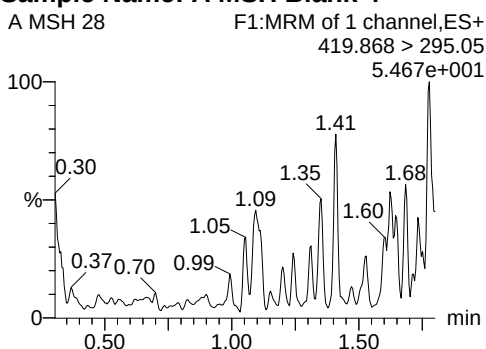
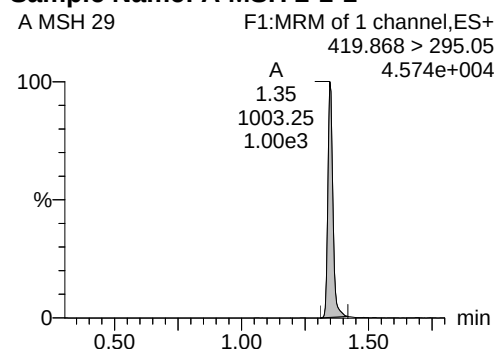
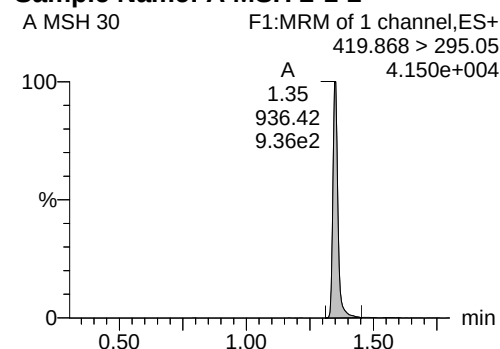
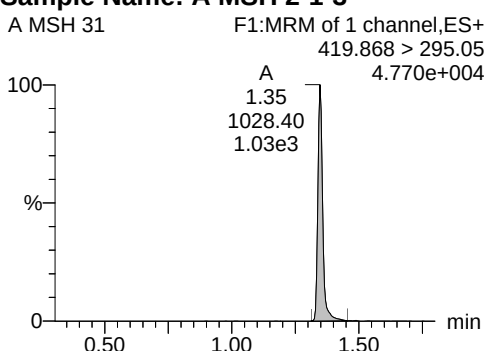
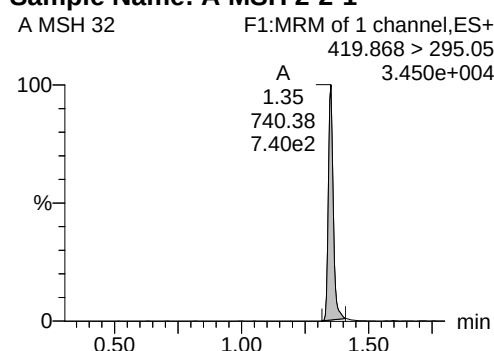
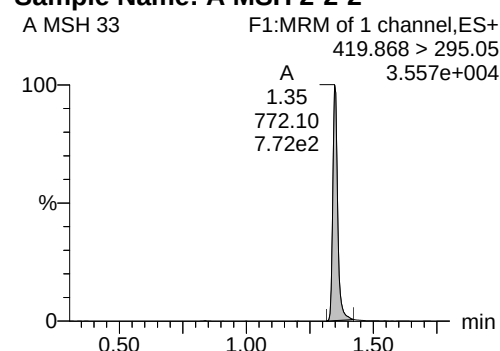
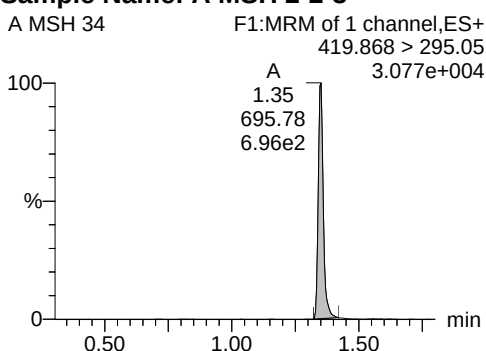
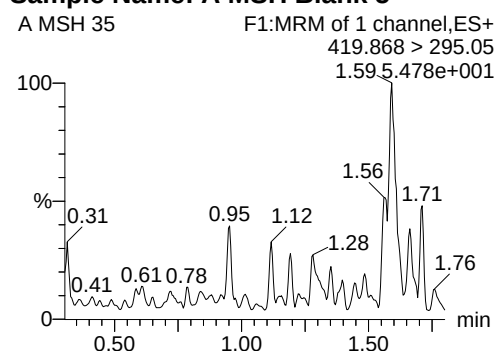
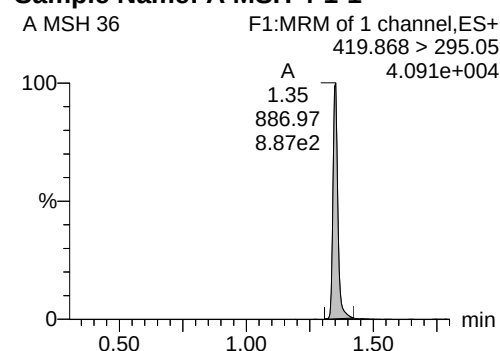
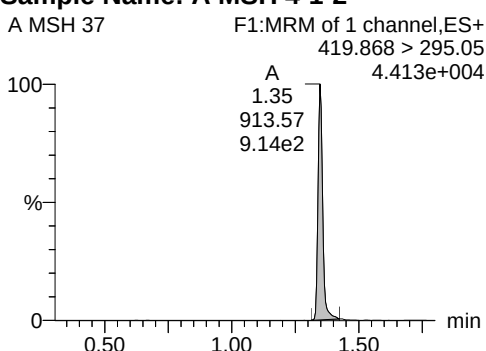
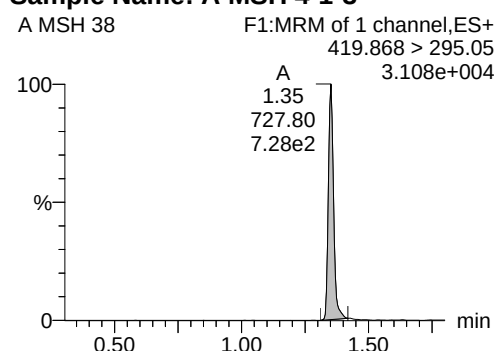
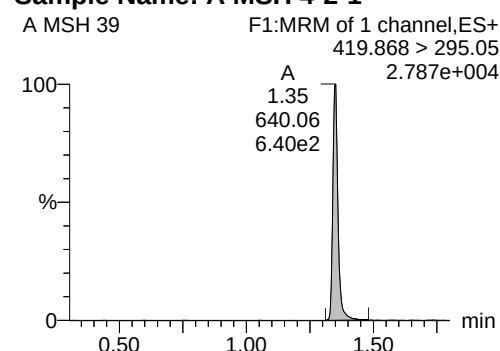
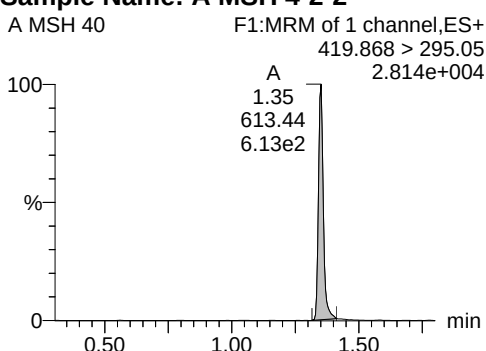
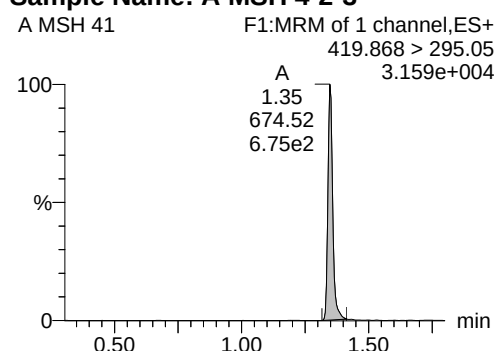
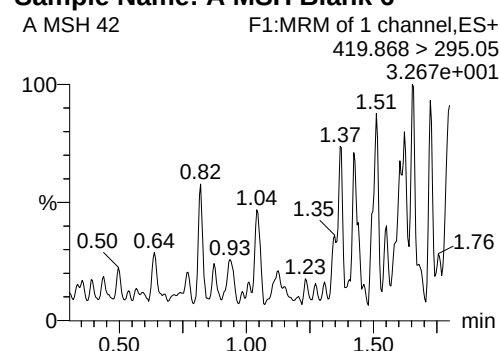
Sample Name: A MSH 15-2-2



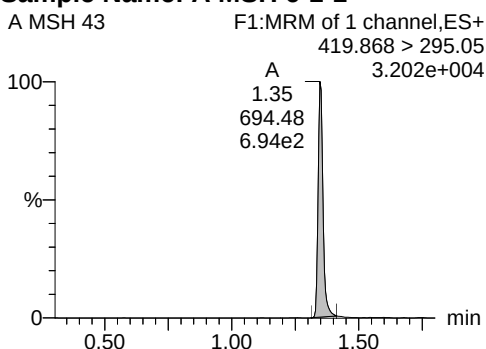
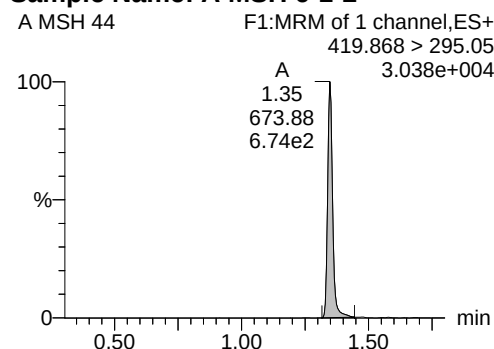
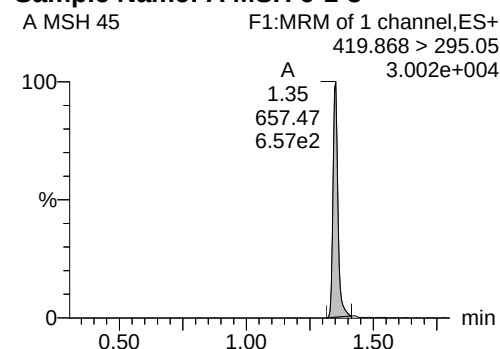
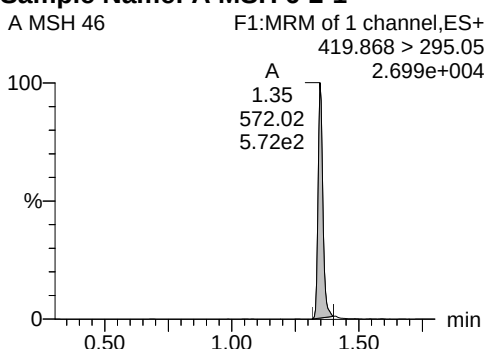
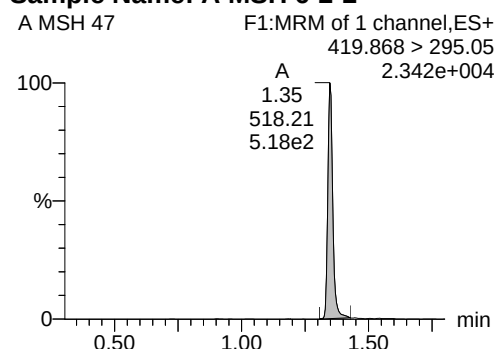
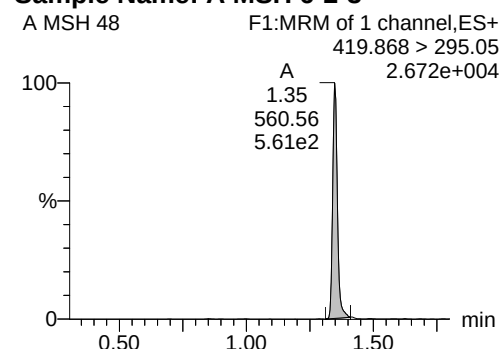
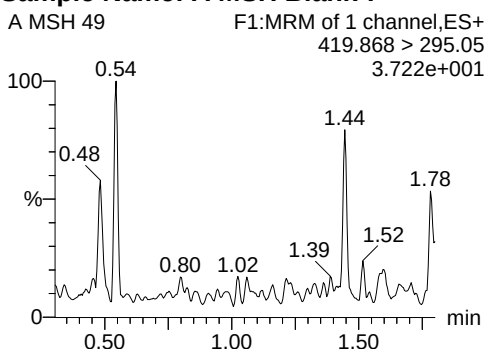
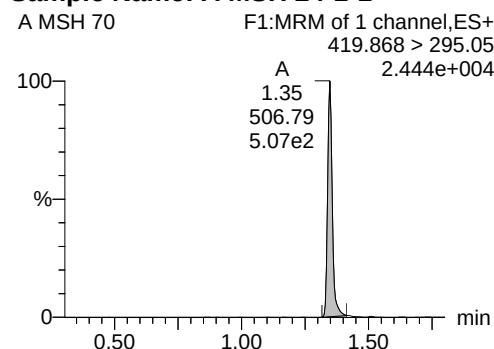
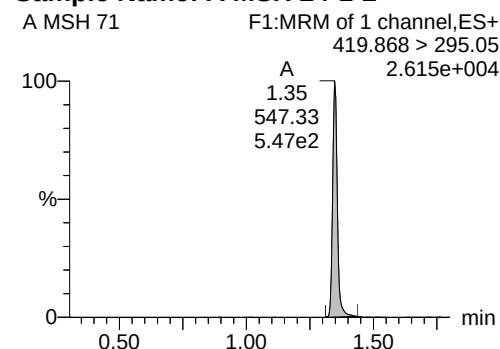
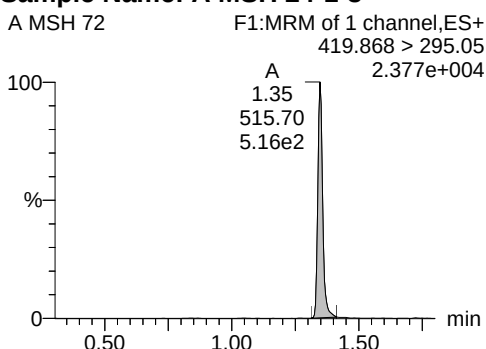
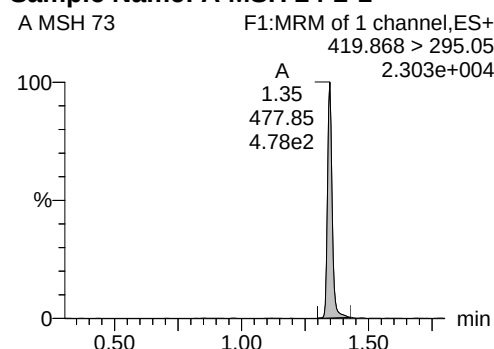
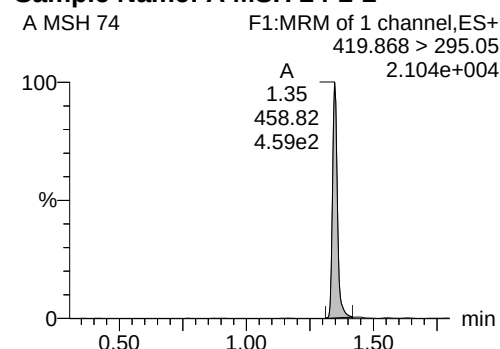
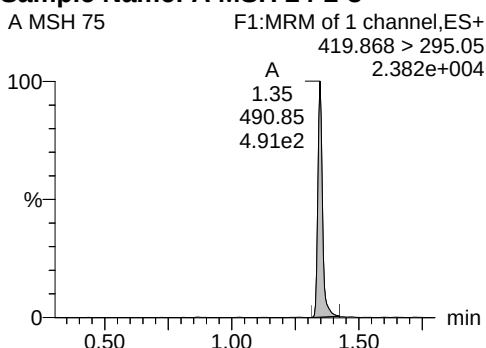
Dataset: Untitled
Last Altered: Monday, January 18, 2021 11:54:53 Romance Standard Time
Printed: Monday, January 18, 2021 11:55:44 Romance Standard Time

Sample Name: A MSH 15-2-3**Sample Name: A MSH Blank 2****Sample Name: A MSH 30-1-1****Sample Name: A MSH 30-1-2****Sample Name: A MSH 30-1-3****Sample Name: A MSH 30-2-1****Sample Name: A MSH 30-2-2****Sample Name: A MSH 30-2-3****Sample Name: A MSH Blank 3****Sample Name: A MSH 1-1-1****Sample Name: A MSH 1-1-2****Sample Name: A MSH 1-1-3****Sample Name: A MSH 1-2-1****Sample Name: A MSH 1-2-2****Sample Name: A MSH 1-2-3**

Dataset: Untitled
Last Altered: Monday, January 18, 2021 11:54:53 Romance Standard Time
Printed: Monday, January 18, 2021 11:55:44 Romance Standard Time

Sample Name: A MSH Blank 4**Sample Name: A MSH 2-1-1****Sample Name: A MSH 2-1-2****Sample Name: A MSH 2-1-3****Sample Name: A MSH 2-2-1****Sample Name: A MSH 2-2-2****Sample Name: A MSH 2-2-3****Sample Name: A MSH Blank 5****Sample Name: A MSH 4-1-1****Sample Name: A MSH 4-1-2****Sample Name: A MSH 4-1-3****Sample Name: A MSH 4-2-1****Sample Name: A MSH 4-2-2****Sample Name: A MSH 4-2-3****Sample Name: A MSH Blank 6**

Dataset: Untitled
Last Altered: Monday, January 18, 2021 11:54:53 Romance Standard Time
Printed: Monday, January 18, 2021 11:55:44 Romance Standard Time

Sample Name: A MSH 6-1-1**Sample Name: A MSH 6-1-2****Sample Name: A MSH 6-1-3****Sample Name: A MSH 6-2-1****Sample Name: A MSH 6-2-2****Sample Name: A MSH 6-2-3****Sample Name: A MSH Blank 7****Sample Name: A MSH 24-1-1****Sample Name: A MSH 24-1-2****Sample Name: A MSH 24-1-3****Sample Name: A MSH 24-2-1****Sample Name: A MSH 24-2-2****Sample Name: A MSH 24-2-3**

	# Name	Type	Std. Conc	RT	Area	IS Area	Response	Detecti...	ng/mL	%Dev
1	1 A MSH 0-1-1	Anal...		1.35	1188.518		1188.518	bb		
2	2 A MSH 0-1-2	Anal...		1.35	1213.861		1213.861	bb		
3	3 A MSH 0-1-3	Anal...		1.35	1192.295		1192.295	bb		
4	4 A MSH 0-2-1	Anal...								
5	5 A MSH 0-2-2	Anal...								
6	6 A MSH 0-2-3	Anal...								
7	7 A MSH Blank 1	Blank								
8	8 A MSH 15-1-1	Anal...		1.35	1112.486		1112.486	bb		
9	9 A MSH 15-1-2	Anal...		1.35	1139.862		1139.862	bb		
10	10 A MSH 15-1-3	Anal...		1.35	1123.516		1123.516	bb		
11	11 A MSH 15-2-1	Anal...		1.35	913.365		913.365	bb		
12	12 A MSH 15-2-2	Anal...		1.35	991.147		991.147	bb		
13	13 A MSH 15-2-3	Anal...		1.35	979.387		979.387	bb		
14	14 A MSH Blank 2	Blank								
15	15 A MSH 30-1-1	Anal...		1.35	975.743		975.743	bb		
16	16 A MSH 30-1-2	Anal...		1.35	1066.325		1066.325	bb		
17	17 A MSH 30-1-3	Anal...		1.35	1096.340		1096.340	bb		
18	18 A MSH 30-2-1	Anal...		1.35	1005.427		1005.427	bb		
19	19 A MSH 30-2-2	Anal...		1.35	980.210		980.210	bb		
20	20 A MSH 30-2-3	Anal...		1.35	952.038		952.038	bb		
21	21 A MSH Blank 3	Blank								
22	22 A MSH 1-1-1	Anal...		1.35	917.503		917.503	bb		
23	23 A MSH 1-1-2	Anal...		1.35	868.685		868.685	bb		
24	24 A MSH 1-1-3	Anal...		1.35	918.138		918.138	bb		
25	25 A MSH 1-2-1	Anal...		1.35	859.782		859.782	bb		
26	26 A MSH 1-2-2	Anal...		1.35	837.005		837.005	bb		
27	27 A MSH 1-2-3	Anal...		1.35	929.915		929.915	bb		
28	28 A MSH Blank 4	Blank								
29	29 A MSH 2-1-1	Anal...		1.35	1003.246		1003.246	bb		
30	30 A MSH 2-1-2	Anal...		1.35	936.425		936.425	bb		
31	31 A MSH 2-1-3	Anal...		1.35	1028.403		1028.403	bb		
32	32 A MSH 2-2-1	Anal...		1.35	740.377		740.377	bb		
33	33 A MSH 2-2-2	Anal...		1.35	772.104		772.104	bb		
34	34 A MSH 2-2-3	Anal...		1.35	695.778		695.778	bb		
35	35 A MSH Blank 5	Blank								
36	36 A MSH 4-1-1	Anal...		1.35	886.971		886.971	bb		
37	37 A MSH 4-1-2	Anal...		1.35	913.571		913.571	bb		
38	38 A MSH 4-1-3	Anal...		1.35	727.796		727.796	bb		
39	39 A MSH 4-2-1	Anal...		1.35	640.058		640.058	bb		
40	40 A MSH 4-2-2	Anal...		1.35	613.442		613.442	bb		
41	41 A MSH 4-2-3	Anal...		1.35	674.522		674.522	bb		
42	42 A MSH Blank 6	Blank								
43	43 A MSH 6-1-1	Anal...		1.35	694.484		694.484	bb		
44	44 A MSH 6-1-2	Anal...		1.35	673.878		673.878	bb		
45	45 A MSH 6-1-3	Anal...		1.35	657.468		657.468	bb		
46	46 A MSH 6-2-1	Anal...		1.35	572.024		572.024	bb		
47	47 A MSH 6-2-2	Anal...		1.35	518.209		518.209	bb		
48	48 A MSH 6-2-3	Anal...		1.35	560.557		560.557	bb		
49	49 A MSH Blank 7	Blank								
50	50 A MSH 24-1-1	Anal...		1.35	506.786		506.786	bb		
51	51 A MSH 24-1-2	Anal...		1.35	547.331		547.331	bb		
52	52 A MSH 24-1-3	Anal...		1.35	515.698		515.698	bb		
53	53 A MSH 24-2-1	Anal...		1.35	477.848		477.848	bb		
54	54 A MSH 24-2-2	Anal...		1.35	458.824		458.824	bb		
55	55 A MSH 24-2-3	Anal...		1.35	490.852		490.852	bb		

Dataset: Untitled
Last Altered: Monday, January 18, 2021 11:54:53 Romance Standard Time
Printed: Monday, January 18, 2021 11:55:44 Romance Standard Time

Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 10:59:51

Calibration: 18 Jan 2021 11:54:53

Header

Acquired File Name: A MSH 0-1-1
Acquired Date: 12-Jan-2021
Acquired Time: 20:53:33
Job Code: MSH 20210112 - 002 - 026 - 75 - A
Task Code:
User Name:
Laboratory Name:
Instrument: ACQ-TQD#QBA320
Conditions:
Submitter:
SampleID: A MSH 1
Bottle Number: 2:64
Description:
Instrument Calibration:
Calibration File: C:\MassLynx\IntelliStart\Results\Unit Mass Resolution\Calib 20161209.cal

Parameters

MS1 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS1

MS1 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS1
MS1 Scan Speed Compensation:
Scan: 339 to 2000 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS1

MS2 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS2

MS2 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS2
MS2 Scan Speed Compensation:
Scan: 339 to 10165 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS2

Calibration Time: 10:33

Calibration Date: 12/09/16

Coefficients

MS1 Static: $-0.000000000000 \times x^4 + 0.000000000843 \times x^3 + -0.000001360559 \times x^2 + 1.000940122634 \times x + -0.253266439024$
MS2 Static: $-0.000000000000 \times x^4 + 0.000000000573 \times x^3 + -0.000001239648 \times x^2 + 1.000902600483 \times x + -0.192715155436$

Function 1: None

Function 2: None

Parameters for C:\Documents and Settings\Administrator\Desktop\old desktop\log D\EA.EXP

Data Processing:

SIR / MRM Chromatogram Spike Removal ON

Dataset: Untitled
Last Altered: Monday, January 18, 2021 11:54:53 Romance Standard Time
Printed: Monday, January 18, 2021 11:55:44 Romance Standard Time

SIR / MRM Smoothing OFF
Smoothing window size (scans) 3
Number of smooths 2
Prescan Statistics:
Initial Average Intensity 22.0947
Initial Average Std Dev 1.7772
Bunch Zero Level 0.0032
Bunch Std Dev 0.0089
Bunch Threshold 0.0716
Spike Removal Std Dev 1.7691

Method Events:

Initial Stop Flow: No Change
Initial Switch 2: No Change
Initial Switch 3: No Change
Initial Switch 4: No Change
Initial Infusion: No Change
Initial Flow State: LC
Initial Flow Rate: 5
Initial Reservoir: No Action
API Probe Delay Temp: 20
Initial Refill: No Action

Timed Events Enabled

Event Time	Name	Action
------------	------	--------

Instrument Parameters - Function 1:

Parameter File - C:\Documents and Settings\Administrator\Desktop\old desktop\log D\log D tune file.

IPR

Polarity ES+
Calibration Static 2
Capillary (kV) 3.50 3.48
Cone (V) 38.00 33.46
Extractor (V) 3.00 2.20
RF (V) 0.10
Source Temperature (°C) 140 138
Desolvation Temperature (°C) 450 450
Cone Gas Flow (L/Hr) 90 90
Desolvation Gas Flow (L/Hr) 900 900
Collision Gas Flow (mL/Min) 0.20 0.20
LM 1 Resolution 15.50
HM 1 Resolution 14.84
Ion Energy 1 0.30
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance -2.00
MSMS Mode Collision Energy 2.00
MSMS Mode Exit 2.00
LM 2 Resolution 15.00
HM 2 Resolution 15.50
Ion Energy 2 1.22
Gain 1.00
Multiplier -495.12

Active Reservoir B

Engineers Settings:

MS1 Low Mass Position	518
MS1 High Mass Position	284
MS1 Low Mass Resolution	513
MS1 High Mass Resolution	1732
MS1 Resolution Linearity	834
MS1 High Mass DC Balance	0
MS1 DC Polarity	Positive
MS2 Low Mass Position	519
MS2 High Mass Position	238
MS2 Low Mass Resolution	518
MS2 High Mass Resolution	644
MS2 Resolution Linearity	756
MS2 High Mass DC Balance	-0
MS2 DC Polarity	Positive
HM RF Lens Correction +	0

Dataset: Untitled
Last Altered: Monday, January 18, 2021 11:54:53 Romance Standard Time
Printed: Monday, January 18, 2021 11:55:44 Romance Standard Time

HM RF Lens Correction - 0

Inter-scan delays:

Automatic Mode

MS 1 Delay Table:

	R	delay
<=	0.500	0.005
<=	1.200	0.010
<=	2.400	0.015
<=	6.000	0.020
<=	15.000	0.025
<=	25.000	0.028
>	25.000	0.030

MS 2 Delay Table:

	R	delay
<=	2.000	0.005
<=	4.000	0.008
<=	7.000	0.010
<=	10.000	0.012
<=	20.000	0.014
>	20.000	0.016

ACE Experimental Record

Inlet Method File: c:\masslynx_projects\medchem su.pro\acqudb\adme sophie

----- Prerun method parameters -----

Waters ACQUITY QSM

Waters Acquity TUV

Run Time: 0.20 min

Wavelength Mode: Single Wavelength

Lamp On: On

Channel A...

Comment:

Wavelength: 254 nm

Sampling Rate: 20 points/sec

Data Mode: Absorbance

Time Constant: 0.1000 sec

Auto Zero On Wavelength Change: Maintain Baseline

Auto Zero On Inject Start: Yes

Analog 1...

Sensitivity: 2.000 AUFS

Chart Polarity: Positive (+)

Voltage Offset: 0 mV

Enable Chart Mark: Yes

Run Events: Yes

Pulse Width: 1.0 sec

Rect Wave Period: 0.2 sec

----- oOo -----

----- Run method parameters -----

Waters ACQUITY QSM

Solvent A Name: Water

Solvent B Name: Acetonitrile

Solvent C Name: water 1 % FA

Solvent D Name:

Low Pressure Limit: 0 psi

High Pressure Limit: 15000 psi

Seal Wash Period: 5.00 min

[Gradient Table]

	Time(min)	Flow Rate(mL/min)	%A	%B	%C	%D	Curve
--	-----------	-------------------	----	----	----	----	-------

1.	Initial	0.700	90.0	5.0	5.0	0.0	Initial
----	---------	-------	------	-----	-----	-----	---------

2.	0.15	0.700	45.0	50.0	5.0	0.0	6
----	------	-------	------	------	-----	-----	---

3.	1.50	0.700	0.0	95.0	5.0	0.0	6
----	------	-------	-----	------	-----	-----	---

4.	1.80	0.700	90.0	5.0	5.0	0.0	1
----	------	-------	------	-----	-----	-----	---

Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm

Flow Ramp Rate: 0.45 min

D Solvent Selection (if supported): No Change

System Pressure Data Channel: No

Flow Rate Data Channel: No

%A Data Channel: No

%B Data Channel: No

%C Data Channel: No

Dataset: Untitled
Last Altered: Monday, January 18, 2021 11:54:53 Romance Standard Time
Printed: Monday, January 18, 2021 11:55:44 Romance Standard Time

%D Data Channel: No
Primary Data Channel: No
Accumulator Data Channel: No
Degasser Data Channel: No
Gradient Start: At Injection
Gradient Start Volume: 0 uL
Gradient Start Time: 0.00 min
Participate in pre-analysis: No
Waters Acquity TUV
Run Time: 1.80 min
Wavelength Mode: Single Wavelength
Lamp On: On
Channel A...
Comment:
Wavelength: 214 nm
Sampling Rate: 20 points/sec
Data Mode: Absorbance
Time Constant: 0.1000 sec
Auto Zero On Wavelength Change: Maintain Baseline
Auto Zero On Inject Start: Yes

Analog 1...
Sensitivity: 2.000 AUFS
Chart Polarity: Positive (+)
Voltage Offset: 0 mV
Enable Chart Mark: Yes
Run Events: Yes
Pulse Width: 1.0 sec
Rect Wave Period: 0.2 sec
Waters ACQUITY FTN AutoSampler
Run Time: 1.80 min
Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm
Load Ahead: Disabled
Loop Offline: Automatic min
Wash Solvent Name: Acetonitrile
Pre-Inject Wash Time: 0.0 sec
Post-Inject Wash Time: 6.0 sec
Purge Solvent Name: Water
Dilution: Disabled
Dilution Volume: 0 uL
Delay Time: 0 min
Dilution Needle Placement: 4.0 mm
Target Column Temperature: 40.0 C
Column Temperature Alarm Band: Disabled
Target Sample Temperature: 15.0 C
Sample Temperature Alarm Band: Disabled
Syringe Draw Rate: Automatic
Needle Placement: Automatic
Pre-Aspirate Air Gap: Automatic
Post-Aspirate Air Gap: Automatic
Column Temperature Data Channel: No
Room Temperature Data Channel: No
Sample Temperature Data Channel: No
Sample Organizer Temperature Data Channel: No
Sample Pressure Data Channel: No
Preheater Temperature Data Channel: No
Seal Force Data Channel: No
No Injection Mode Enabled: No
Run Events: No

Sample Run Injection Parameter

Injection Volume (ul) - 3.00

-----o0o-----

End of experimental record.

-----Waters ACQUITY QSM Postrun Report-----

Firmware Version: 1.50.237 (May 18 2011)

Software Version: 1.50.1621

Checksum: 0xae400516

Serial Number: M09QSM056N

Minimum System Pressure: 0.0 psi

Dataset: Untitled
Last Altered: Monday, January 18, 2021 11:54:53 Romance Standard Time
Printed: Monday, January 18, 2021 11:55:44 Romance Standard Time

Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi
-----o0o-----

-----Waters ACQUITY FTN Postrun Report-----

Software Version: 1.50.1481
Firmware Version: 1.50.317 (Jul 11 2011)
Checksum: 0x3e83519d
Serial Number: M09SDI055N
Sample Syringe Size: 100.0
Extension Loop Size: 0.0
Needle Size: 15.0
Column Type: ACQUITY UPLC® BEH C18 1.7µm
Column Serial Number: 02343407715781
Total Injections on Column: 1145
Minimum Sample Temperature: 0.0
Maximum Sample Temperature: 0.0
Average Sample Temperature: 0.0
Minimum Column Temperature: 30.0
Maximum Column Temperature: 41.4
Average Column Temperature: 0.0
-----o0o-----

-----Generic Instrument Postrun Report-----

Software Version: 1.50.2530
Firmware Version: 1.50.2182 (May 11 2011)
Checksum: 0xc09b9cb2
Serial Number: J08UPT460M
Lamp On/Off Event: No
Lamp Life: 100.00
Lamp Serial Number: 000296721
Flow Cell Type: Other
Flow Cell Path Length: 0.00 mm
Flow Cell Volume: 0.00 microliters
Flow Cell Serial Number: 1
Flow Cell Part Number: 1
Optics Temperature Stabilization Setting: unknown
-----o0o-----

-----Waters ACQUITY QSM Postrun Report-----

Firmware Version: 1.50.237 (May 18 2011)
Software Version: 1.50.1621
Checksum: 0xae400516
Serial Number: M09QSM056N
Minimum System Pressure: 0.0 psi
Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi
-----o0o-----

Function 1

Scans in function:	338							
Cycle time (secs):	Automatic							
Inter Scan Delay (secs):	Automatic							
Inter Channel Delay (secs):	Automatic							
Span (Da):	2.000							
Start and End Time(mins):	0.300 to 1.800							
Ionization mode:	ES+							
Data type:	SIR or MRM data							
Function type:	MRM of 1 channel							
Chan Reaction	Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound Formula Mass Comm							
ents								
1 : 419.87 > 295.05	0.260	30.0	18.0	Auto	EA	418.9		Inte
lliStart Generated								

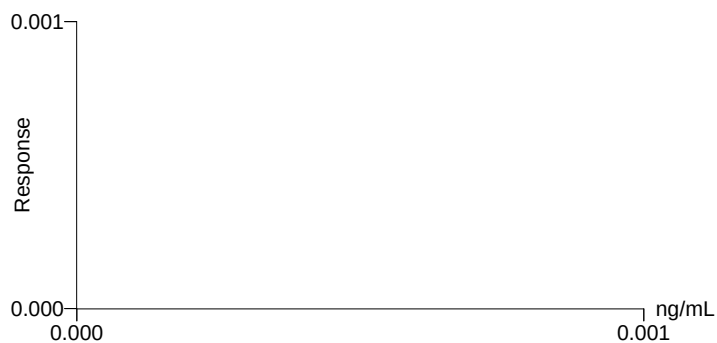
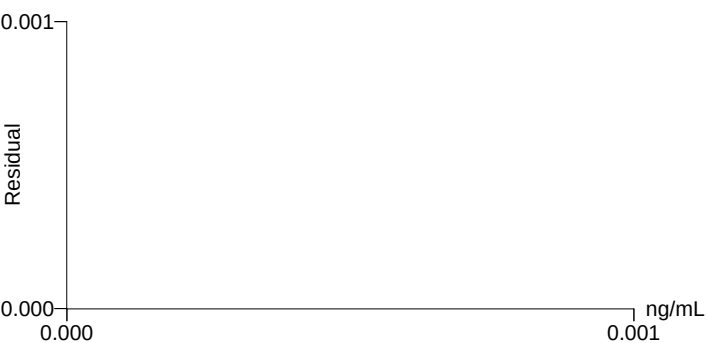
Function 2

Scans in function: 2161
Function type: Diode Array
Wavelength range (nm): 214 to 214

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 15:58:43 Romance Daylight Time
Printed: Wednesday, August 18, 2021 15:59:15 Romance Daylight Time

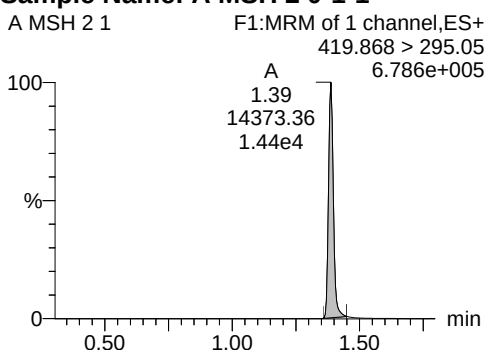
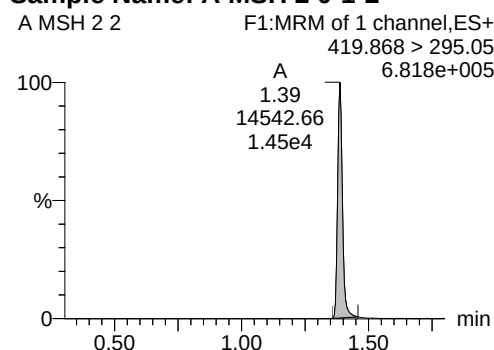
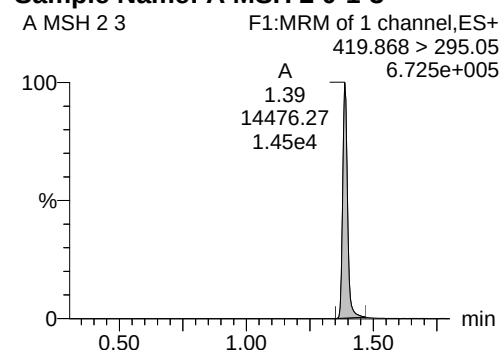
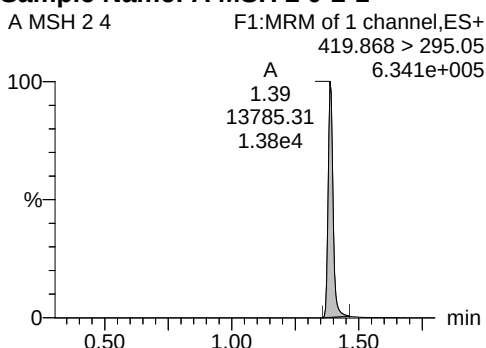
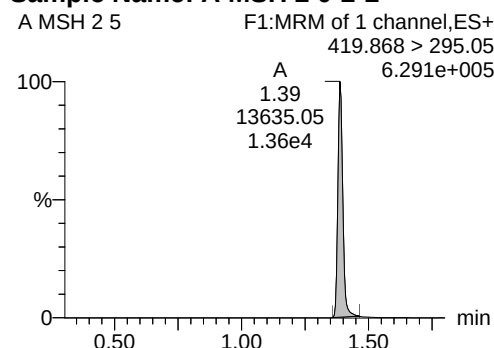
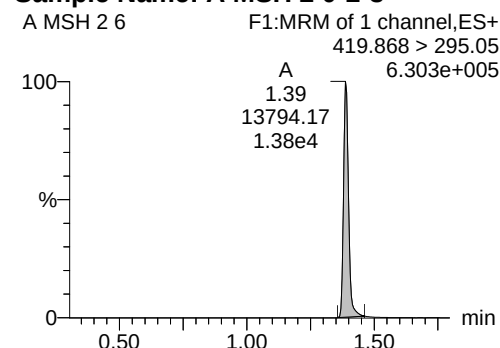
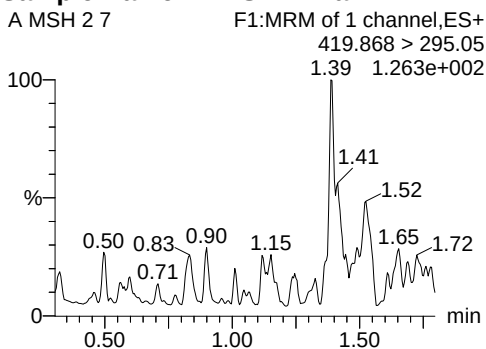
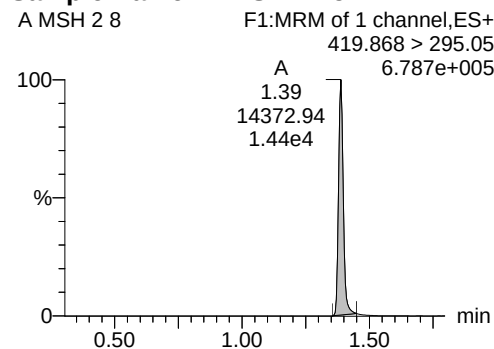
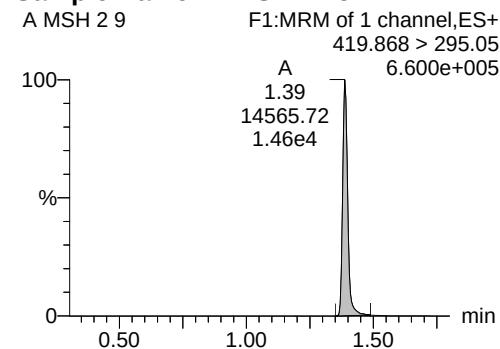
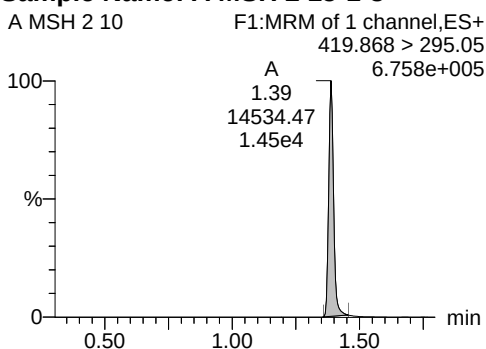
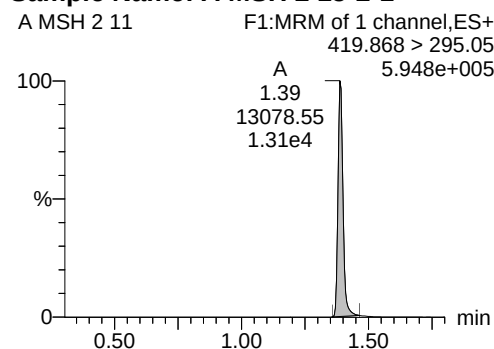
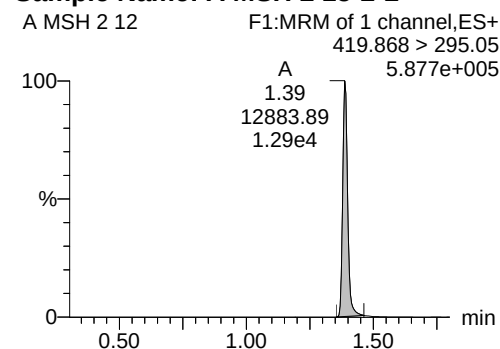
Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51
Calibration: 18 Aug 2021 15:58:43

Compound name: A
No Calibration
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

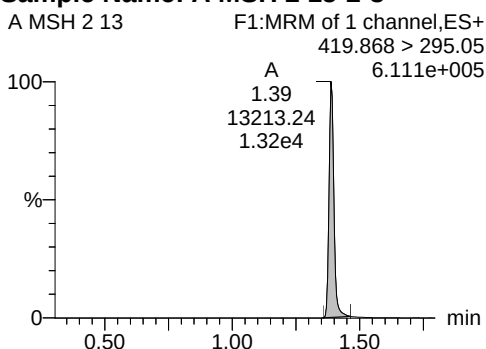
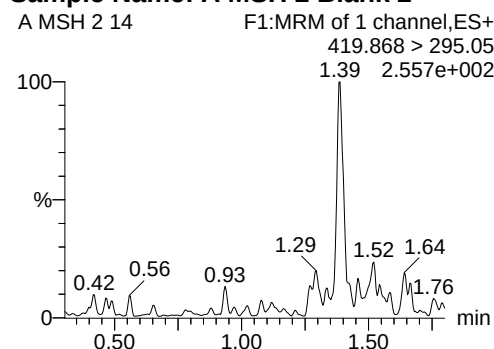
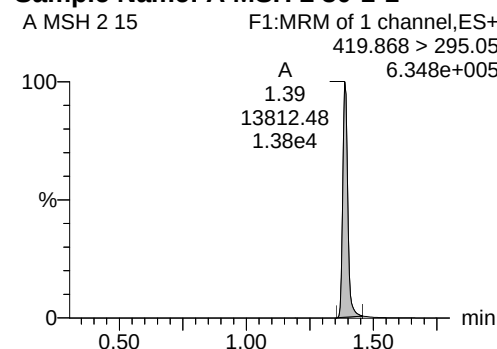
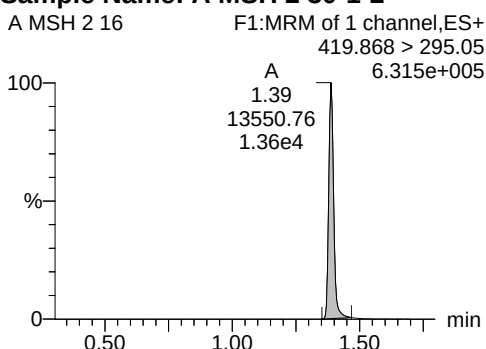
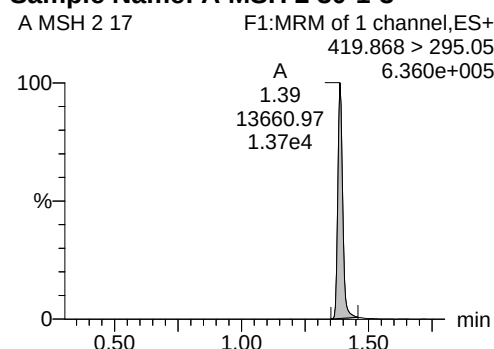
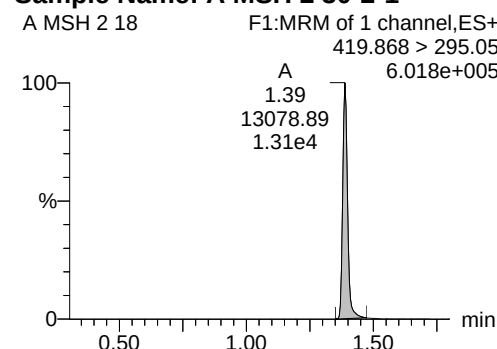
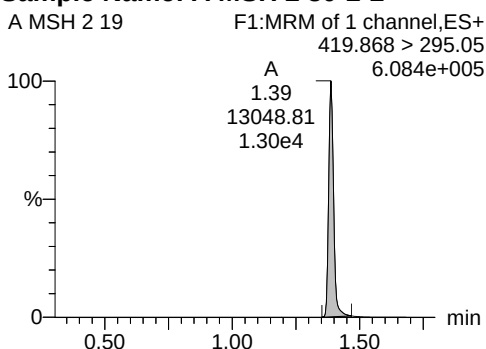
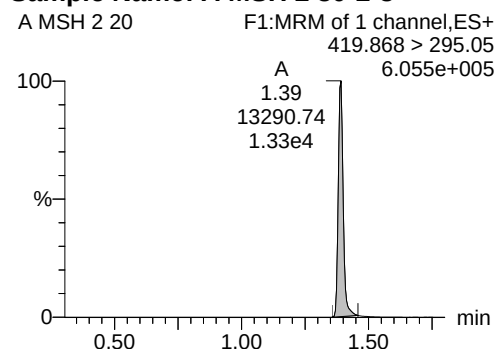
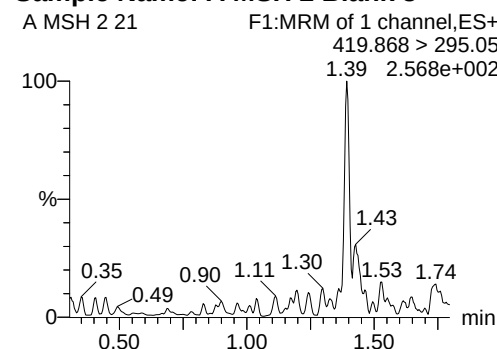
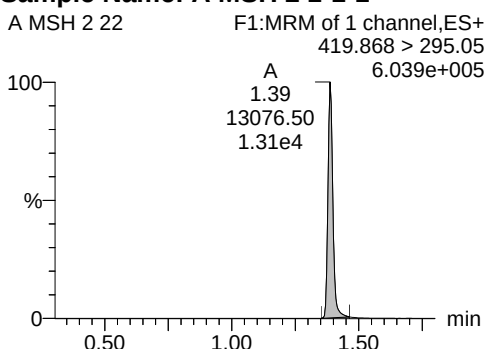
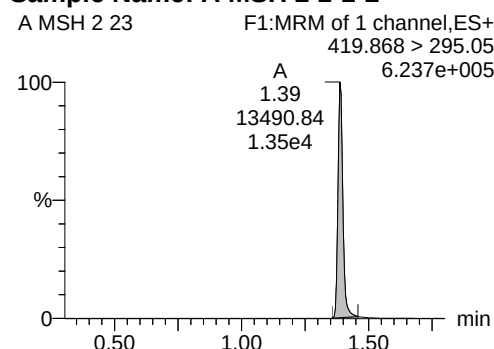
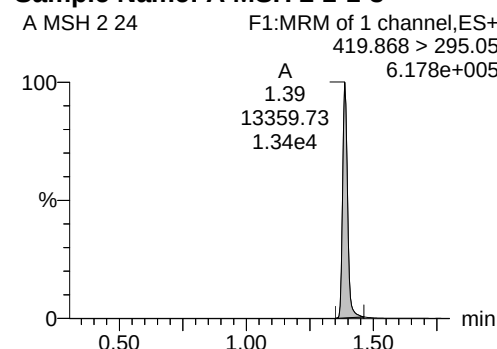
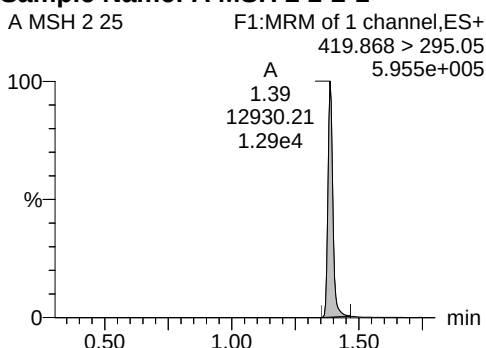
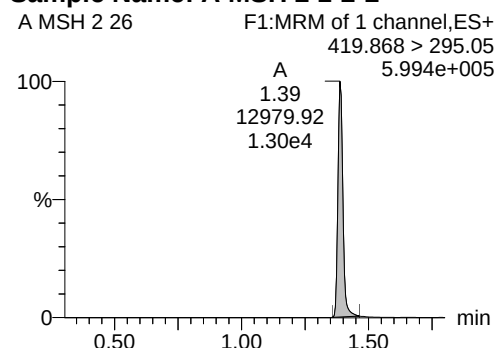
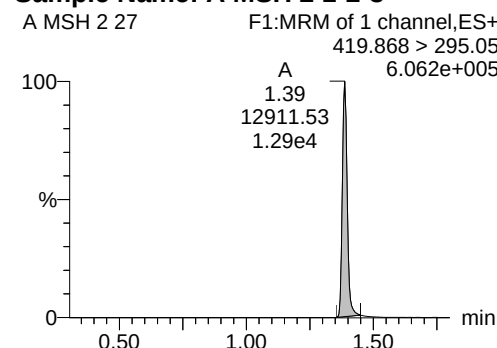


Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 15:58:43 Romance Daylight Time
Printed: Wednesday, August 18, 2021 15:59:15 Romance Daylight Time

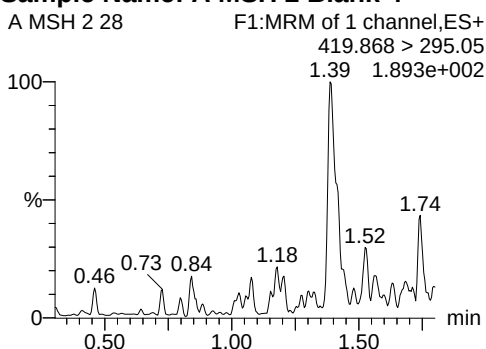
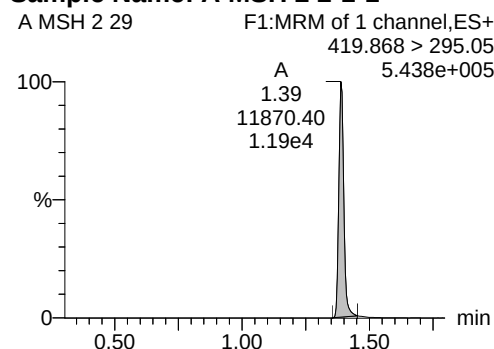
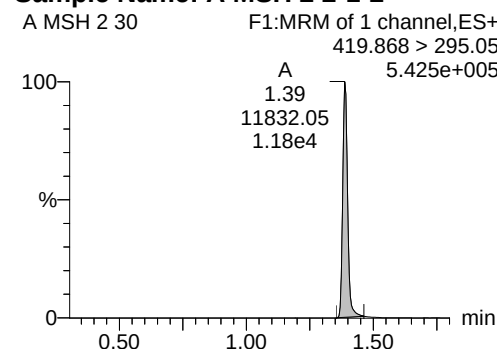
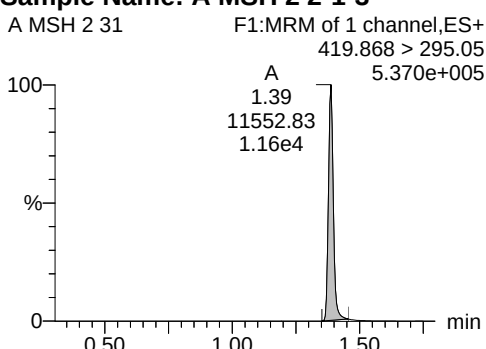
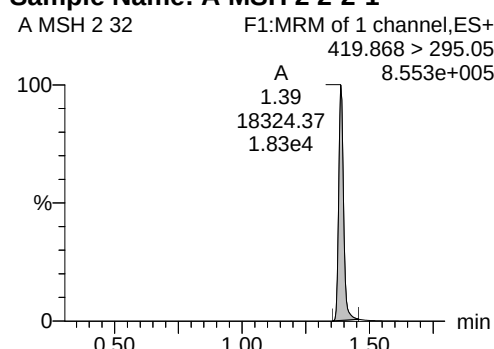
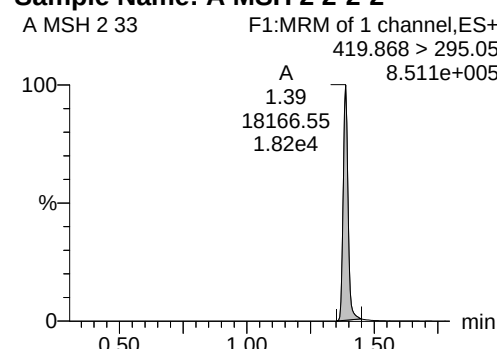
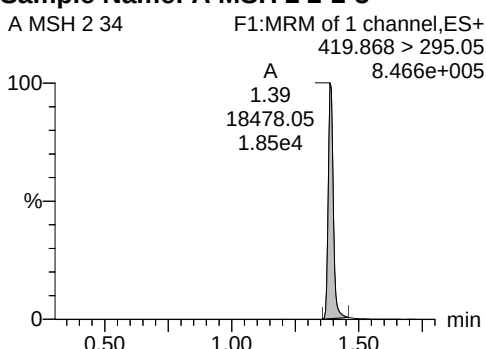
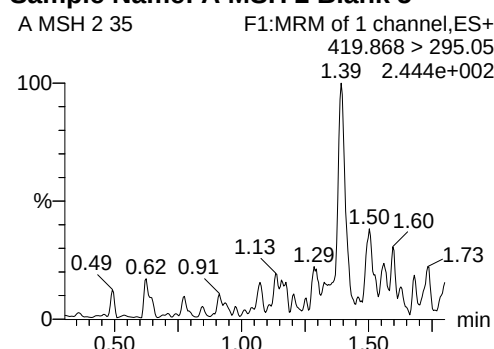
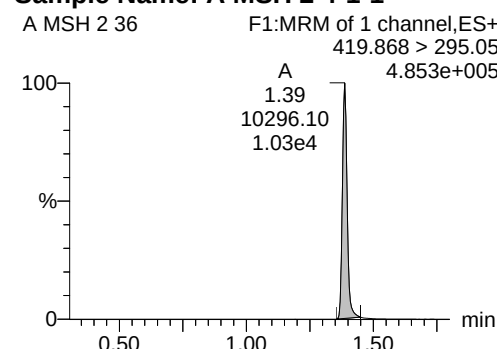
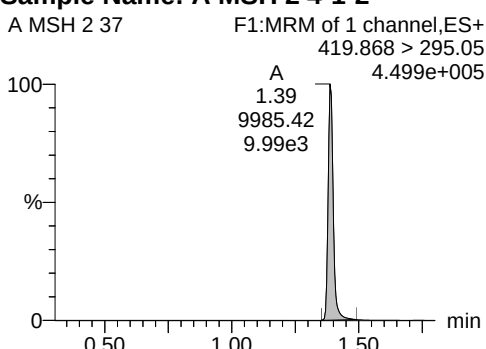
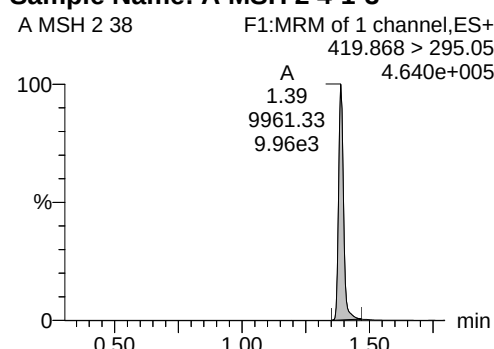
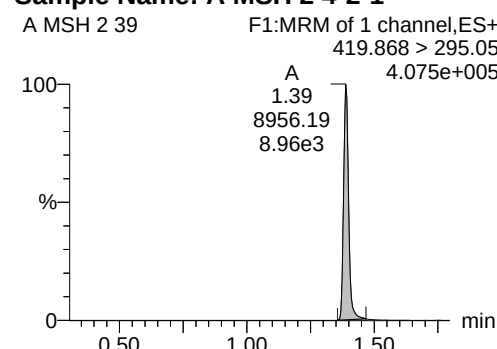
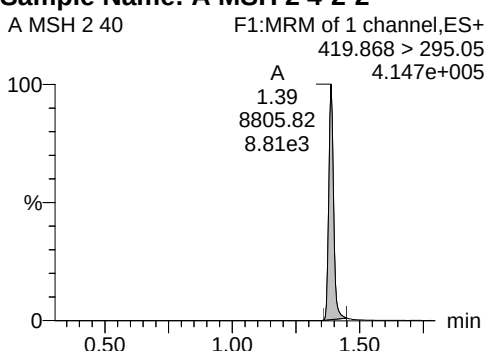
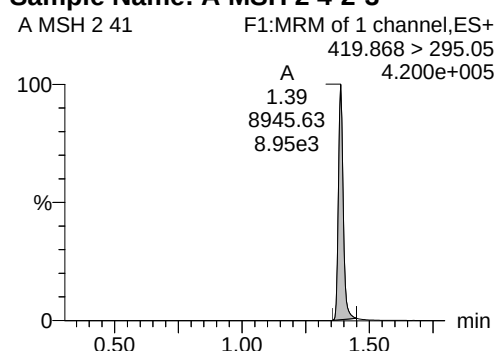
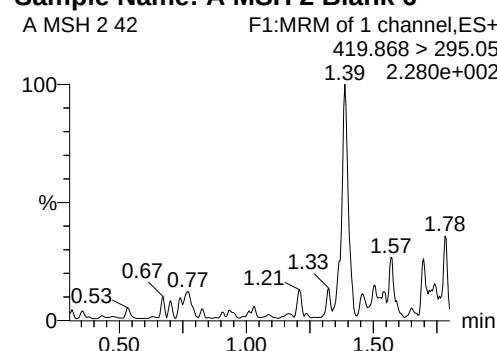
Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51
Calibration: 18 Aug 2021 15:58:43

Sample Name: A MSH 2 0-1-1**Sample Name: A MSH 2 0-1-2****Sample Name: A MSH 2 0-1-3****Sample Name: A MSH 2 0-2-1****Sample Name: A MSH 2 0-2-2****Sample Name: A MSH 2 0-2-3****Sample Name: A MSH 2 Blank 1****Sample Name: A MSH 2 15-1-1****Sample Name: A MSH 2 15-1-2****Sample Name: A MSH 2 15-1-3****Sample Name: A MSH 2 15-2-1****Sample Name: A MSH 2 15-2-2**

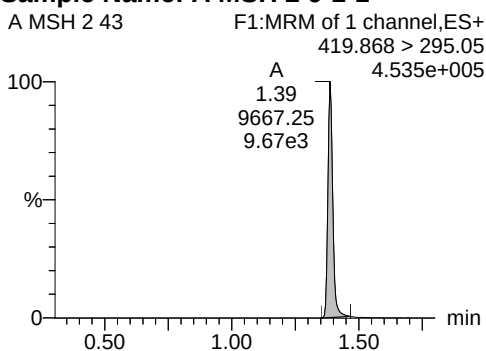
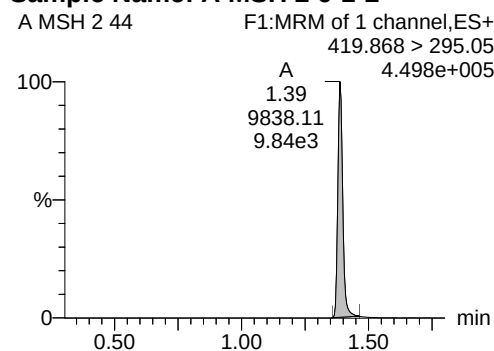
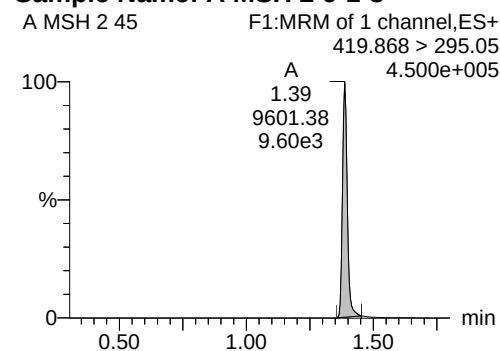
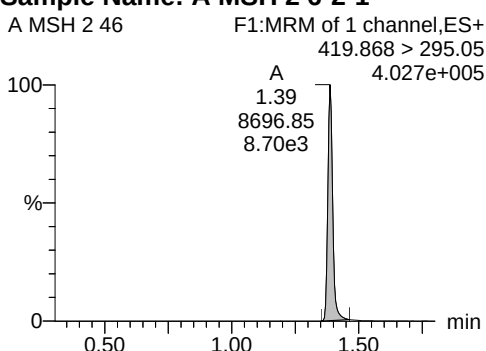
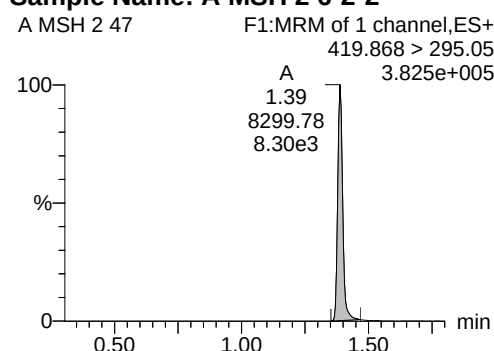
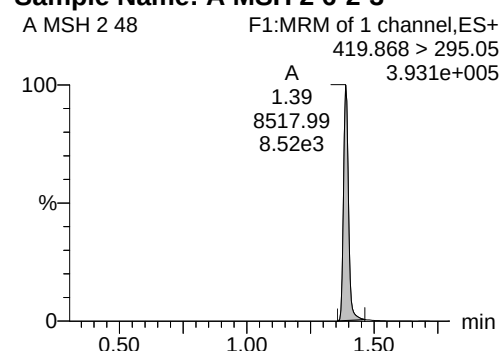
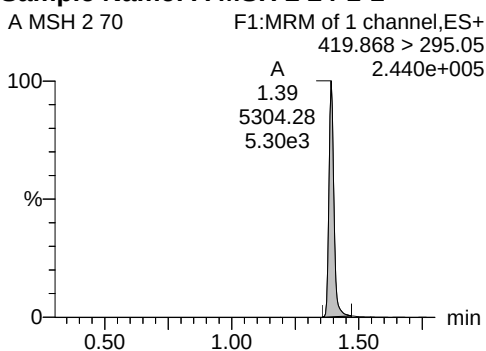
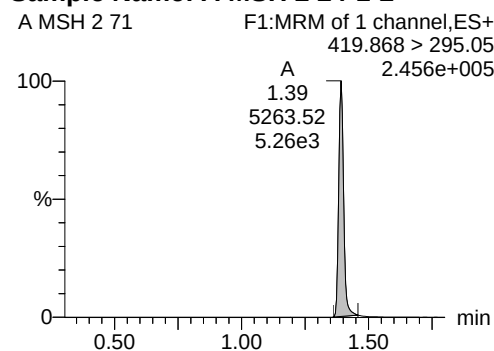
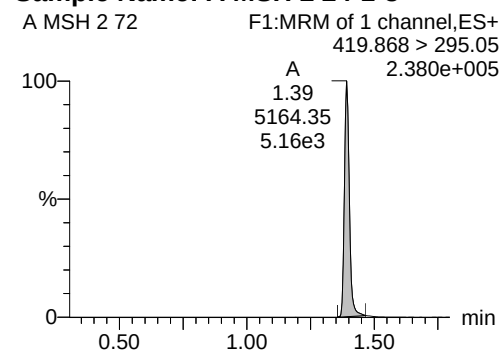
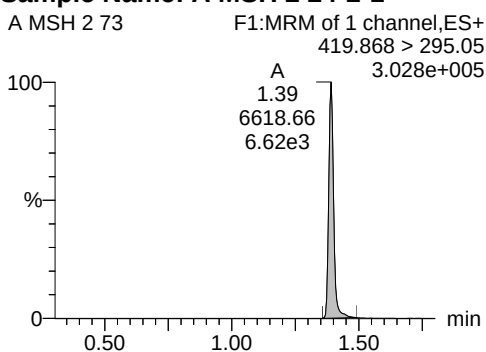
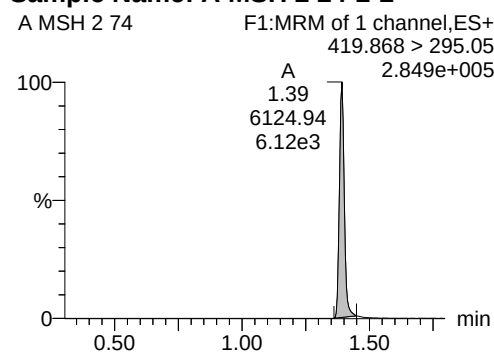
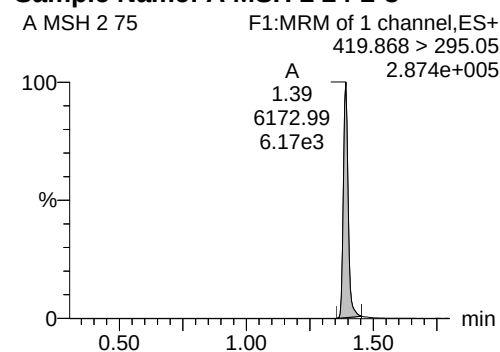
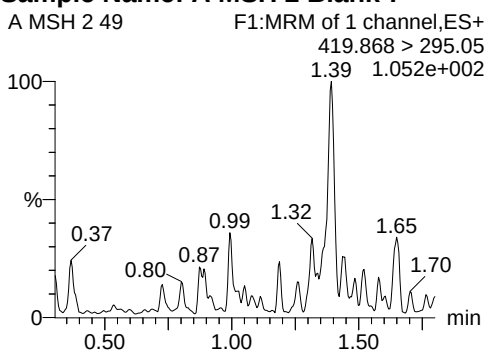
Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 15:58:43 Romance Daylight Time
Printed: Wednesday, August 18, 2021 15:59:15 Romance Daylight Time

Sample Name: A MSH 2 15-2-3**Sample Name: A MSH 2 Blank 2****Sample Name: A MSH 2 30-1-1****Sample Name: A MSH 2 30-1-2****Sample Name: A MSH 2 30-1-3****Sample Name: A MSH 2 30-2-1****Sample Name: A MSH 2 30-2-2****Sample Name: A MSH 2 30-2-3****Sample Name: A MSH 2 Blank 3****Sample Name: A MSH 2 1-1-1****Sample Name: A MSH 2 1-1-2****Sample Name: A MSH 2 1-1-3****Sample Name: A MSH 2 1-2-1****Sample Name: A MSH 2 1-2-2****Sample Name: A MSH 2 1-2-3**

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 15:58:43 Romance Daylight Time
Printed: Wednesday, August 18, 2021 15:59:15 Romance Daylight Time

Sample Name: A MSH 2 Blank 4**Sample Name: A MSH 2 2-1-1****Sample Name: A MSH 2 2-1-2****Sample Name: A MSH 2 2-1-3****Sample Name: A MSH 2 2-2-1****Sample Name: A MSH 2 2-2-2****Sample Name: A MSH 2 2-2-3****Sample Name: A MSH 2 Blank 5****Sample Name: A MSH 2 4-1-1****Sample Name: A MSH 2 4-1-2****Sample Name: A MSH 2 4-1-3****Sample Name: A MSH 2 4-2-1****Sample Name: A MSH 2 4-2-2****Sample Name: A MSH 2 4-2-3****Sample Name: A MSH 2 Blank 6**

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 15:58:43 Romance Daylight Time
Printed: Wednesday, August 18, 2021 15:59:15 Romance Daylight Time

Sample Name: A MSH 2 6-1-1**Sample Name: A MSH 2 6-1-2****Sample Name: A MSH 2 6-1-3****Sample Name: A MSH 2 6-2-1****Sample Name: A MSH 2 6-2-2****Sample Name: A MSH 2 6-2-3****Sample Name: A MSH 2 24-1-1****Sample Name: A MSH 2 24-1-2****Sample Name: A MSH 2 24-1-3****Sample Name: A MSH 2 24-2-1****Sample Name: A MSH 2 24-2-2****Sample Name: A MSH 2 24-2-3****Sample Name: A MSH 2 Blank 7**

	# Name	Type	Std. Conc	RT	Area	IS Area	Response	Detecti...	ng/mL	%Dev
1	1 A MSH 2 0-1-1	Anal...		1.39	14373.364		14373.364	bb		
2	2 A MSH 2 0-1-2	Anal...		1.39	14542.664		14542.664	bb		
3	3 A MSH 2 0-1-3	Anal...		1.39	14476.271		14476.271	bb		
4	4 A MSH 2 0-2-1	Anal...		1.39	13785.313		13785.313	bb		
5	5 A MSH 2 0-2-2	Anal...		1.39	13635.054		13635.054	bb		
6	6 A MSH 2 0-2-3	Anal...		1.39	13794.165		13794.165	bb		
7	7 A MSH 2 Blank 1	Blank								
8	8 A MSH 2 15-1-1	Anal...		1.39	14372.942		14372.942	bb		
9	9 A MSH 2 15-1-2	Anal...		1.39	14565.716		14565.716	bb		
10	10 A MSH 2 15-1-3	Anal...		1.39	14534.468		14534.468	bb		
11	11 A MSH 2 15-2-1	Anal...		1.39	13078.553		13078.553	bb		
12	12 A MSH 2 15-2-2	Anal...		1.39	12883.891		12883.891	bb		
13	13 A MSH 2 15-2-3	Anal...		1.39	13213.239		13213.239	bb		
14	14 A MSH 2 Blank 2	Blank								
15	15 A MSH 2 30-1-1	Anal...		1.39	13812.484		13812.484	bb		
16	16 A MSH 2 30-1-2	Anal...		1.39	13550.757		13550.757	bb		
17	17 A MSH 2 30-1-3	Anal...		1.39	13660.965		13660.965	bb		
18	18 A MSH 2 30-2-1	Anal...		1.39	13078.886		13078.886	bb		
19	19 A MSH 2 30-2-2	Anal...		1.39	13048.814		13048.814	bb		
20	20 A MSH 2 30-2-3	Anal...		1.39	13290.737		13290.737	bb		
21	21 A MSH 2 Blank 3	Blank								
22	22 A MSH 2 1-1-1	Anal...		1.39	13076.497		13076.497	bb		
23	23 A MSH 2 1-1-2	Anal...		1.39	13490.843		13490.843	bb		
24	24 A MSH 2 1-1-3	Anal...		1.39	13359.727		13359.727	bb		
25	25 A MSH 2 1-2-1	Anal...		1.39	12930.208		12930.208	bb		
26	26 A MSH 2 1-2-2	Anal...		1.39	12979.922		12979.922	bb		
27	27 A MSH 2 1-2-3	Anal...		1.39	12911.531		12911.531	bb		
28	28 A MSH 2 Blank 4	Blank								
29	29 A MSH 2 2-1-1	Anal...		1.39	11870.403		11870.403	bb		
30	30 A MSH 2 2-1-2	Anal...		1.39	11832.053		11832.053	bb		
31	31 A MSH 2 2-1-3	Anal...		1.39	11552.827		11552.827	bb		
32	32 A MSH 2 2-2-1	Anal...		1.39	18324.371		18324.371	bb		
33	33 A MSH 2 2-2-2	Anal...		1.39	18166.551		18166.551	bb		
34	34 A MSH 2 2-2-3	Anal...		1.39	18478.051		18478.051	bb		
35	35 A MSH 2 Blank 5	Blank								
36	36 A MSH 2 4-1-1	Anal...		1.39	10296.097		10296.097	bb		
37	37 A MSH 2 4-1-2	Anal...		1.39	9985.418		9985.418	bb		
38	38 A MSH 2 4-1-3	Anal...		1.39	9961.325		9961.325	bb		
39	39 A MSH 2 4-2-1	Anal...		1.39	8956.191		8956.191	bb		
40	40 A MSH 2 4-2-2	Anal...		1.39	8805.820		8805.820	bb		
41	41 A MSH 2 4-2-3	Anal...		1.39	8945.634		8945.634	bb		
42	42 A MSH 2 Blank 6	Blank								
43	43 A MSH 2 6-1-1	Anal...		1.39	9667.248		9667.248	bb		
44	44 A MSH 2 6-1-2	Anal...		1.39	9838.114		9838.114	bb		
45	45 A MSH 2 6-1-3	Anal...		1.39	9601.378		9601.378	bb		
46	46 A MSH 2 6-2-1	Anal...		1.39	8696.854		8696.854	bb		
47	47 A MSH 2 6-2-2	Anal...		1.39	8299.785		8299.785	bb		
48	48 A MSH 2 6-2-3	Anal...		1.39	8517.988		8517.988	bb		
49	49 A MSH 2 24-1-1	Anal...		1.39	5304.283		5304.283	bb		
50	50 A MSH 2 24-1-2	Anal...		1.39	5263.518		5263.518	bb		
51	51 A MSH 2 24-1-3	Anal...		1.39	5164.347		5164.347	bb		
52	52 A MSH 2 24-2-1	Anal...		1.39	6618.657		6618.657	bb		
53	53 A MSH 2 24-2-2	Anal...		1.39	6124.943		6124.943	bb		
54	54 A MSH 2 24-2-3	Anal...		1.39	6172.987		6172.987	bb		
55	55 A MSH 2 Blank 7	Blank								

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 15:58:43 Romance Daylight Time
Printed: Wednesday, August 18, 2021 15:59:15 Romance Daylight Time

Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51
Calibration: 18 Aug 2021 15:58:43

Header

Acquired File Name: A MSH 2 0-1-1
Acquired Date: 17-Aug-2021
Acquired Time: 21:01:17
Job Code: MSH 20210817 - N - 216 - 75 - A
Task Code:
User Name:
Laboratory Name:
Instrument: ACQ-TQD#QBA320
Conditions:
Submitter:
SampleID: A MSH 2 1
Bottle Number: 2:64
Description:
Instrument Calibration:
Calibration File: C:\MassLynx\IntelliStart\Results\Unit Mass Resolution\Calib 20161209.cal

Parameters

MS1 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS1

MS1 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS1
MS1 Scan Speed Compensation:
Scan: 339 to 2000 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS1

MS2 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS2

MS2 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS2
MS2 Scan Speed Compensation:
Scan: 339 to 10165 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS2
Calibration Time: 10:33
Calibration Date: 12/09/16

Coefficients

MS1 Static: $-0.000000000000 \times x^4 + 0.000000000843 \times x^3 + -0.000001360559 \times x^2 + 1.000940122634 \times x + -0.253266439024$
MS2 Static: $-0.000000000000 \times x^4 + 0.000000000573 \times x^3 + -0.000001239648 \times x^2 + 1.000902600483 \times x + -0.192715155436$

Function 1: None

Function 2: None

Parameters for C:\Documents and Settings\Administrator\Desktop\old desktop\log D\EA.EXP

Data Processing:

SIR / MRM Chromatogram Spike Removal ON

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 15:58:43 Romance Daylight Time
Printed: Wednesday, August 18, 2021 15:59:15 Romance Daylight Time

SIR / MRM Smoothing OFF
Smoothing window size (scans) 3
Number of smooths 2
Prescan Statistics:
Initial Average Intensity 21.8547
Initial Average Std Dev 2.0631
Bunch Zero Level 0.0016
Bunch Std Dev 0.0064
Bunch Threshold 0.0511
Spike Removal Std Dev 1.7324

Method Events:
Initial Stop Flow: No Change
Initial Switch 2: No Change
Initial Switch 3: No Change
Initial Switch 4: No Change
Initial Infusion: No Change
Initial Flow State: LC
Initial Flow Rate: 5
Initial Reservoir: No Action
API Probe Delay Temp: 20
Initial Refill: No Action

Timed Events Enabled

Event Time	Name	Action
------------	------	--------

Instrument Parameters - Function 1:

Parameter File - C:\Documents and Settings\Administrator\Desktop\old desktop\log D\log D tune file.

IPR
Polarity ES+
Calibration Static 2
Capillary (kV) 3.50 3.48
Cone (V) 38.00 32.48
Extractor (V) 3.00 2.20
RF (V) 0.10
Source Temperature (°C) 140 139
Desolvation Temperature (°C) 450 450
Cone Gas Flow (L/Hr) 90 90
Desolvation Gas Flow (L/Hr) 900 901
Collision Gas Flow (mL/Min) 0.20 0.20
LM 1 Resolution 15.50
HM 1 Resolution 14.84
Ion Energy 1 0.30
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance -2.00
MSMS Mode Collision Energy 2.00
MSMS Mode Exit 2.00
LM 2 Resolution 15.00
HM 2 Resolution 15.50
Ion Energy 2 1.22
Gain 1.00
Multiplier -494.34

Active Reservoir B

Engineers Settings:

MS1 Low Mass Position	518
MS1 High Mass Position	284
MS1 Low Mass Resolution	513
MS1 High Mass Resolution	1732
MS1 Resolution Linearity	834
MS1 High Mass DC Balance	0
MS1 DC Polarity	Positive
MS2 Low Mass Position	519
MS2 High Mass Position	238
MS2 Low Mass Resolution	518
MS2 High Mass Resolution	644
MS2 Resolution Linearity	756
MS2 High Mass DC Balance	-0
MS2 DC Polarity	Positive
HM RF Lens Correction +	0

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 15:58:43 Romance Daylight Time
Printed: Wednesday, August 18, 2021 15:59:15 Romance Daylight Time

HM RF Lens Correction - 0

Inter-scan delays:

Automatic Mode

MS 1 Delay Table:

	R	delay
<=	0.500	0.005
<=	1.200	0.010
<=	2.400	0.015
<=	6.000	0.020
<=	15.000	0.025
<=	25.000	0.028
>	25.000	0.030

MS 2 Delay Table:

	R	delay
<=	2.000	0.005
<=	4.000	0.008
<=	7.000	0.010
<=	10.000	0.012
<=	20.000	0.014
>	20.000	0.016

ACE Experimental Record

Inlet Method File: c:\masslynx_projects\medchem su.pro\acqudb\adme sophie

----- Prerun method parameters -----

Waters ACQUITY QSM

Waters Acquity TUV

Run Time: 0.20 min

Wavelength Mode: Single Wavelength

Lamp On: On

Channel A...

Comment:

Wavelength: 254 nm

Sampling Rate: 20 points/sec

Data Mode: Absorbance

Time Constant: 0.1000 sec

Auto Zero On Wavelength Change: Maintain Baseline

Auto Zero On Inject Start: Yes

Analog 1...

Sensitivity: 2.000 AUFS

Chart Polarity: Positive (+)

Voltage Offset: 0 mV

Enable Chart Mark: Yes

Run Events: Yes

Pulse Width: 1.0 sec

Rect Wave Period: 0.2 sec

----- oOo -----

----- Run method parameters -----

Waters ACQUITY QSM

Solvent A Name: Water

Solvent B Name: Acetonitrile

Solvent C Name: water 1 % FA

Solvent D Name:

Low Pressure Limit: 0 psi

High Pressure Limit: 15000 psi

Seal Wash Period: 5.00 min

[Gradient Table]

	Time(min)	Flow Rate(mL/min)	%A	%B	%C	%D	Curve
--	-----------	-------------------	----	----	----	----	-------

1.	Initial	0.700	90.0	5.0	5.0	0.0	Initial
----	---------	-------	------	-----	-----	-----	---------

2.	0.15	0.700	45.0	50.0	5.0	0.0	6
----	------	-------	------	------	-----	-----	---

3.	1.50	0.700	0.0	95.0	5.0	0.0	6
----	------	-------	-----	------	-----	-----	---

4.	1.80	0.700	90.0	5.0	5.0	0.0	1
----	------	-------	------	-----	-----	-----	---

Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm

Flow Ramp Rate: 0.45 min

D Solvent Selection (if supported): No Change

System Pressure Data Channel: No

Flow Rate Data Channel: No

%A Data Channel: No

%B Data Channel: No

%C Data Channel: No

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 15:58:43 Romance Daylight Time
Printed: Wednesday, August 18, 2021 15:59:15 Romance Daylight Time

%D Data Channel: No
Primary Data Channel: No
Accumulator Data Channel: No
Degasser Data Channel: No
Gradient Start: At Injection
Gradient Start Volume: 0 uL
Gradient Start Time: 0.00 min
Participate in pre-analysis: No
Waters Acquity TUV
Run Time: 1.80 min
Wavelength Mode: Single Wavelength
Lamp On: On
Channel A...
Comment:
Wavelength: 214 nm
Sampling Rate: 20 points/sec
Data Mode: Absorbance
Time Constant: 0.1000 sec
Auto Zero On Wavelength Change: Maintain Baseline
Auto Zero On Inject Start: Yes

Analog 1...
Sensitivity: 2.000 AUFS
Chart Polarity: Positive (+)
Voltage Offset: 0 mV
Enable Chart Mark: Yes
Run Events: Yes
Pulse Width: 1.0 sec
Rect Wave Period: 0.2 sec
Waters ACQUITY FTN AutoSampler
Run Time: 1.80 min
Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm
Load Ahead: Disabled
Loop Offline: Automatic min
Wash Solvent Name: Acetonitrile
Pre-Inject Wash Time: 0.0 sec
Post-Inject Wash Time: 6.0 sec
Purge Solvent Name: Water
Dilution: Disabled
Dilution Volume: 0 uL
Delay Time: 0 min
Dilution Needle Placement: 4.0 mm
Target Column Temperature: 40.0 C
Column Temperature Alarm Band: Disabled
Target Sample Temperature: 15.0 C
Sample Temperature Alarm Band: Disabled
Syringe Draw Rate: Automatic
Needle Placement: Automatic
Pre-Aspirate Air Gap: Automatic
Post-Aspirate Air Gap: Automatic
Column Temperature Data Channel: No
Room Temperature Data Channel: No
Sample Temperature Data Channel: No
Sample Organizer Temperature Data Channel: No
Sample Pressure Data Channel: No
Preheater Temperature Data Channel: No
Seal Force Data Channel: No
No Injection Mode Enabled: No
Run Events: No

Sample Run Injection Parameter

Injection Volume (ul) - 3.00

----- o0o -----

End of experimental record.

----- Waters ACQUITY QSM Postrun Report -----

Firmware Version: 1.50.237 (May 18 2011)

Software Version: 1.50.1621

Checksum: 0xae400516

Serial Number: M09QSM056N

Minimum System Pressure: 0.0 psi

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 15:58:43 Romance Daylight Time
Printed: Wednesday, August 18, 2021 15:59:15 Romance Daylight Time

Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi
-----o0o-----

-----Waters ACQUITY FTN Postrun Report-----

Software Version: 1.50.1481
Firmware Version: 1.50.317 (Jul 11 2011)
Checksum: 0x3e83519d
Serial Number: M09SDI055N
Sample Syringe Size: 100.0
Extension Loop Size: 0.0
Needle Size: 15.0
Column Type: ACQUITY UPLC® BEH C18 1.7µm
Column Serial Number: 02343407715781
Total Injections on Column: 7742
Minimum Sample Temperature: 0.0
Maximum Sample Temperature: 0.0
Average Sample Temperature: 0.0
Minimum Column Temperature: 40.0
Maximum Column Temperature: 40.2
Average Column Temperature: 0.0
-----o0o-----

-----Generic Instrument Postrun Report-----

Software Version: 1.50.2530
Firmware Version: 1.50.2182 (May 11 2011)
Checksum: 0xc09b9cb2
Serial Number: J08UPT460M
Lamp On/Off Event: No
Lamp Life: 903.00
Lamp Serial Number: 000296721
Flow Cell Type: Other
Flow Cell Path Length: 0.00 mm
Flow Cell Volume: 0.00 microliters
Flow Cell Serial Number: 1
Flow Cell Part Number: 1
Optics Temperature Stabilization Setting: unknown
-----o0o-----

-----Waters ACQUITY QSM Postrun Report-----

Firmware Version: 1.50.237 (May 18 2011)
Software Version: 1.50.1621
Checksum: 0xae400516
Serial Number: M09QSM056N
Minimum System Pressure: 0.0 psi
Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi
-----o0o-----

Function 1

Scans in function:	337							
Cycle time (secs):	Automatic							
Inter Scan Delay (secs):	Automatic							
Inter Channel Delay (secs):	Automatic							
Span (Da):	0.500							
Start and End Time(mins):	0.300 to 1.800							
Ionization mode:	ES+							
Data type:	SIR or MRM data							
Function type:	MRM of 1 channel							
Chan Reaction	Dwell(secs) Cone Volt. Col.Energy Delay(secs)	Compound	Formula	Mass	Comm			
ents								
1 : 419.87 > 295.05	0.260	30.0	18.0	Auto	EA	418.9		Inte
lliStart Generated								

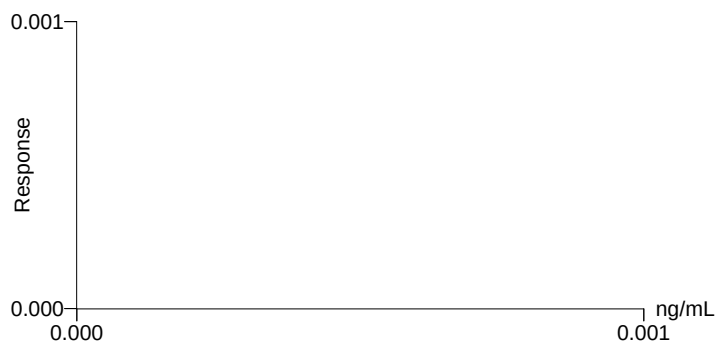
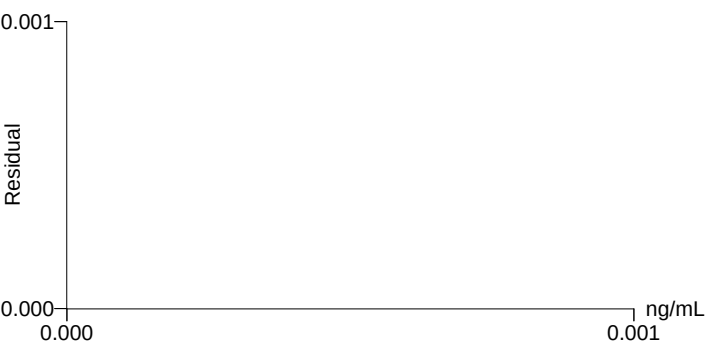
Function 2

Scans in function: 2161
Function type: Diode Array
Wavelength range (nm): 214 to 214

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 16:17:53 Romance Daylight Time
Printed: Wednesday, August 18, 2021 16:18:18 Romance Daylight Time

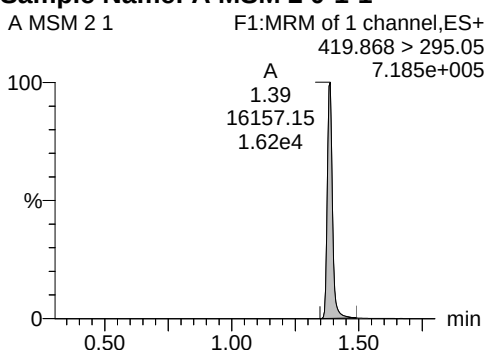
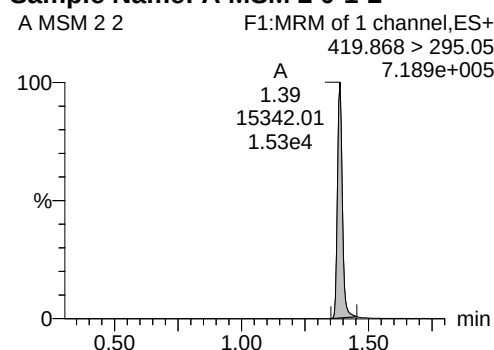
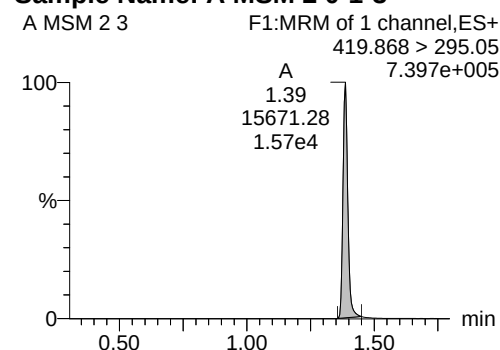
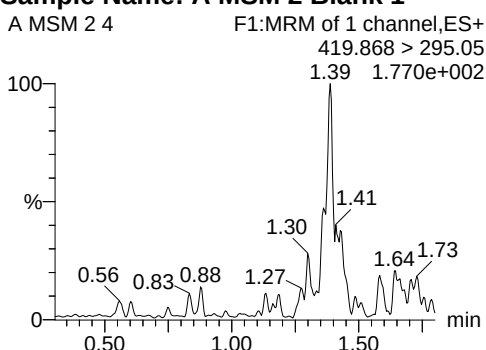
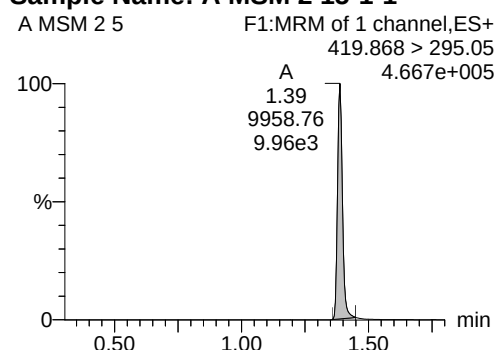
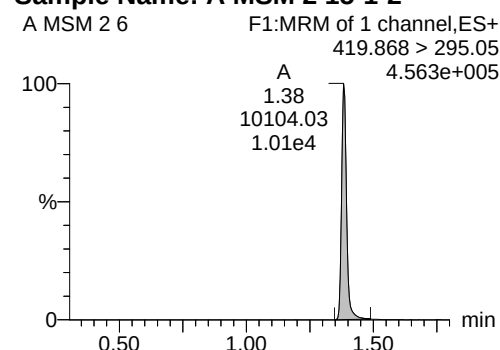
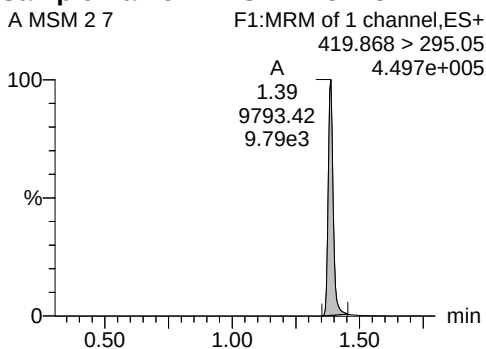
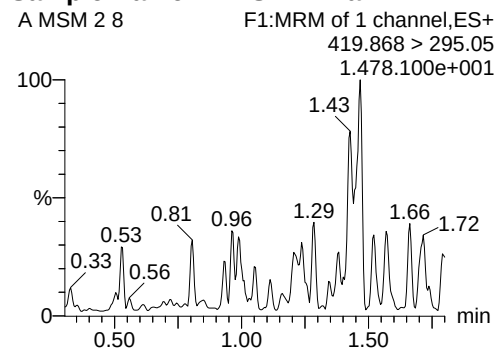
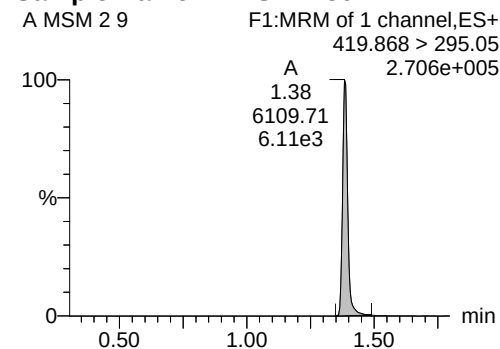
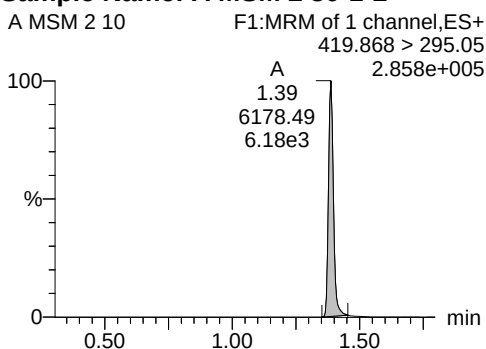
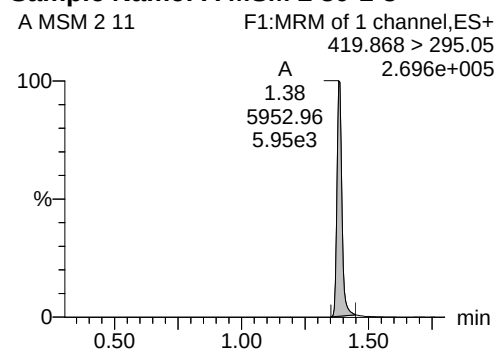
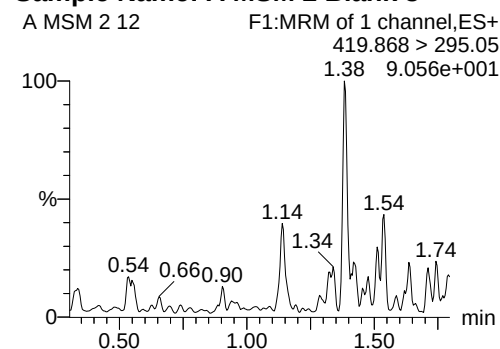
Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51
Calibration: 18 Aug 2021 16:17:53

Compound name: A
No Calibration
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

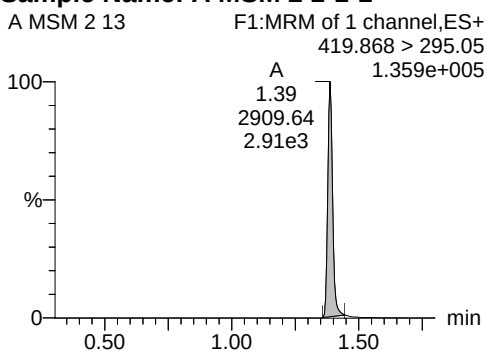
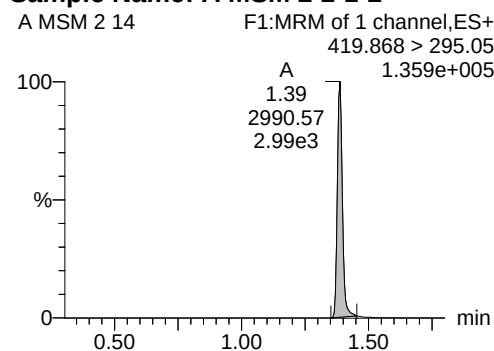
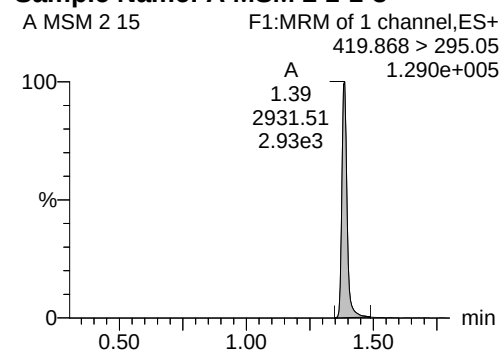
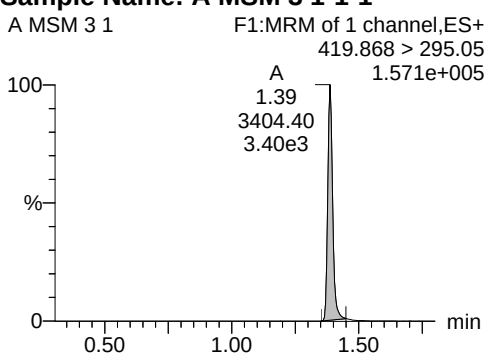
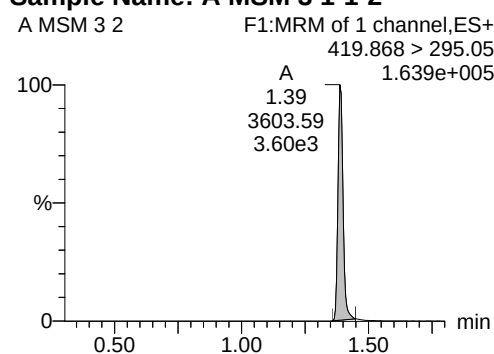
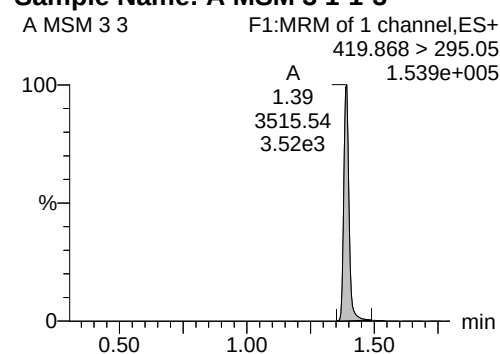
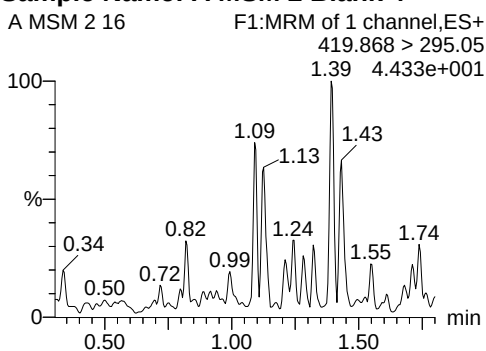
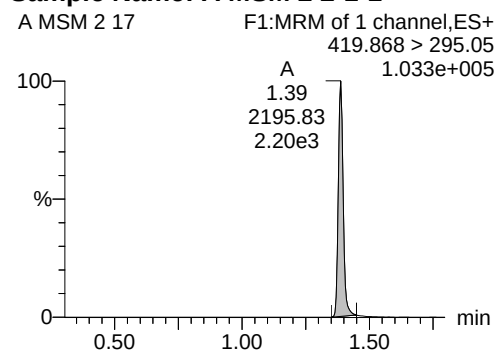
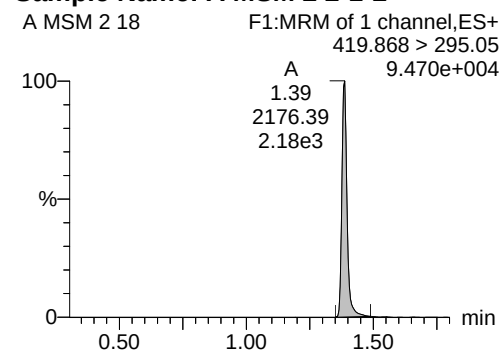
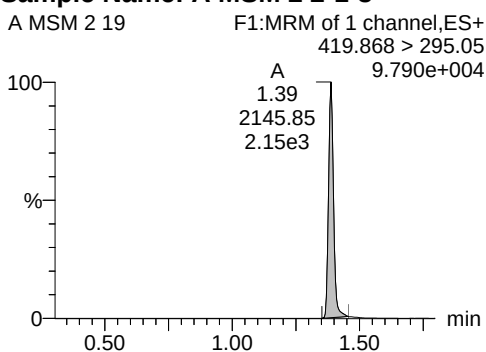
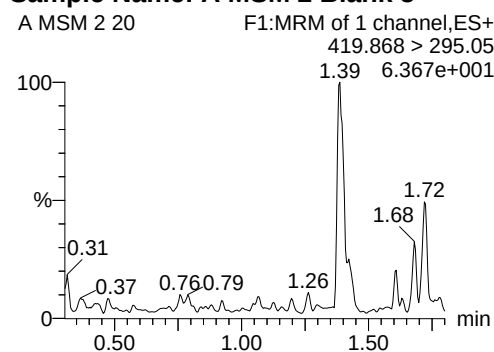
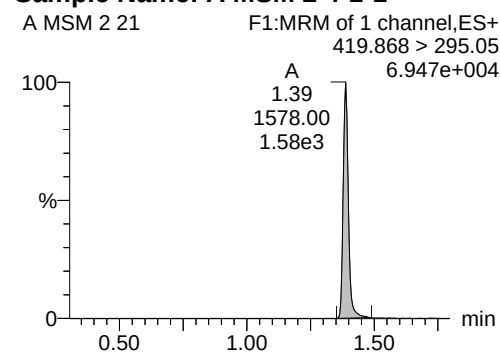
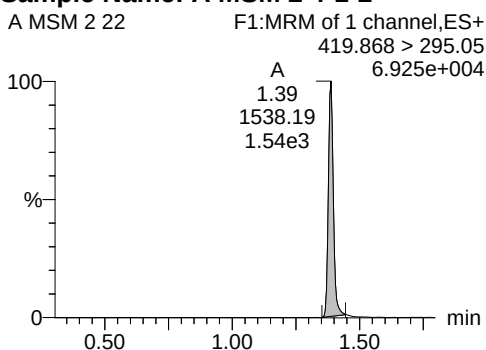
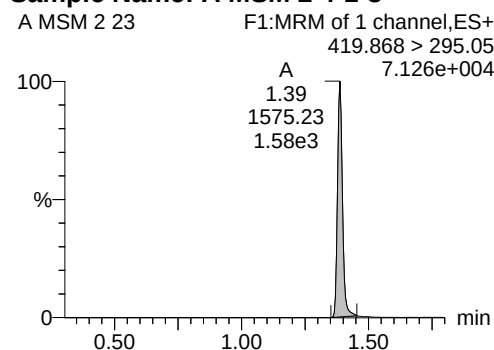
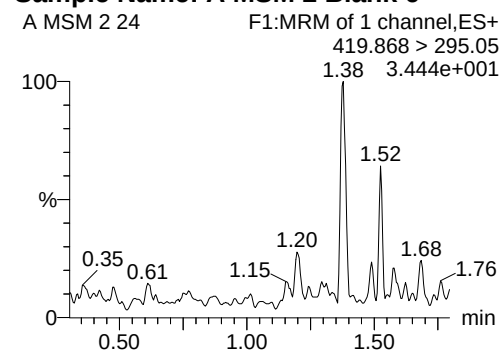


Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 16:17:53 Romance Daylight Time
Printed: Wednesday, August 18, 2021 16:18:18 Romance Daylight Time

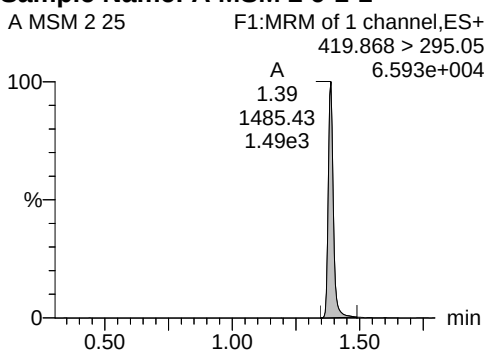
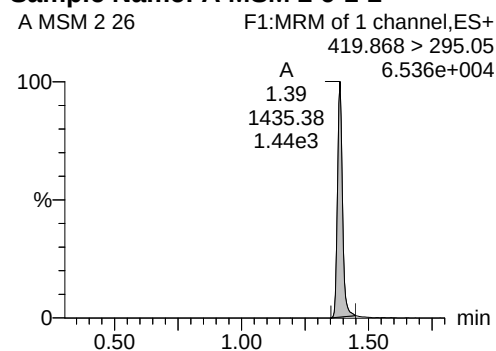
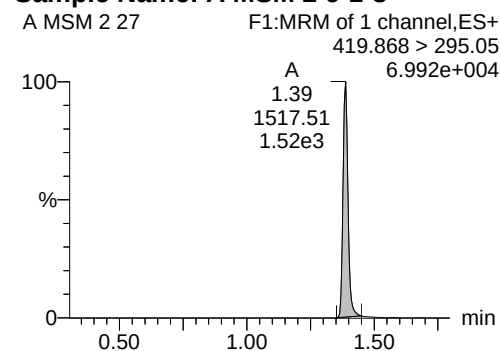
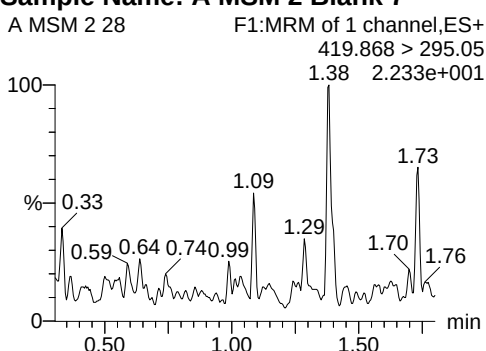
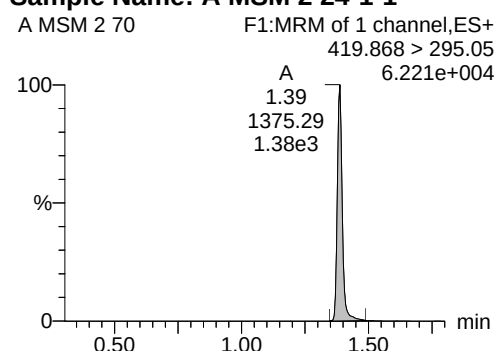
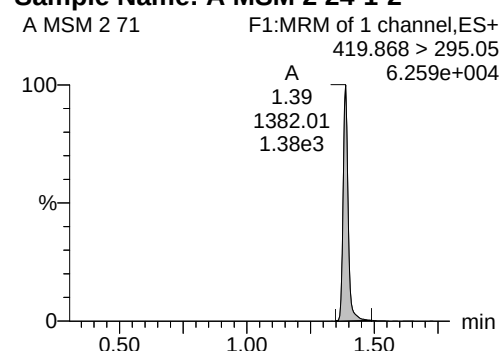
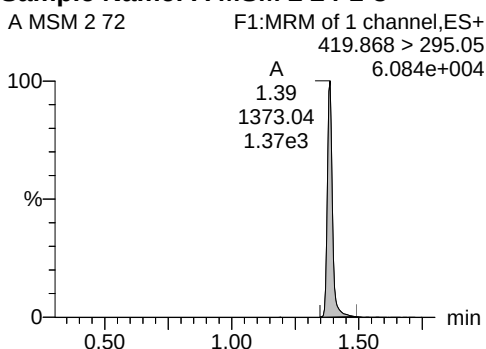
Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51
Calibration: 18 Aug 2021 16:17:53

Sample Name: A MSM 2 0-1-1**Sample Name: A MSM 2 0-1-2****Sample Name: A MSM 2 0-1-3****Sample Name: A MSM 2 Blank 1****Sample Name: A MSM 2 15-1-1****Sample Name: A MSM 2 15-1-2****Sample Name: A MSM 2 15-1-3****Sample Name: A MSM 2 Blank 2****Sample Name: A MSM 2 30-1-1****Sample Name: A MSM 2 30-1-2****Sample Name: A MSM 2 30-1-3****Sample Name: A MSM 2 Blank 3**

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 16:17:53 Romance Daylight Time
Printed: Wednesday, August 18, 2021 16:18:18 Romance Daylight Time

Sample Name: A MSM 2 1-1-1**Sample Name: A MSM 2 1-1-2****Sample Name: A MSM 2 1-1-3****Sample Name: A MSM 3 1-1-1****Sample Name: A MSM 3 1-1-2****Sample Name: A MSM 3 1-1-3****Sample Name: A MSM 2 Blank 4****Sample Name: A MSM 2 2-1-1****Sample Name: A MSM 2 2-1-2****Sample Name: A MSM 2 2-1-3****Sample Name: A MSM 2 Blank 5****Sample Name: A MSM 2 4-1-1****Sample Name: A MSM 2 4-1-2****Sample Name: A MSM 2 4-1-3****Sample Name: A MSM 2 Blank 6**

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 16:17:53 Romance Daylight Time
Printed: Wednesday, August 18, 2021 16:18:18 Romance Daylight Time

Sample Name: A MSM 2 6-1-1**Sample Name: A MSM 2 6-1-2****Sample Name: A MSM 2 6-1-3****Sample Name: A MSM 2 Blank 7****Sample Name: A MSM 2 24-1-1****Sample Name: A MSM 2 24-1-2****Sample Name: A MSM 2 24-1-3**

	# Name	Type	Std. Conc	RT	Area	IS Area	Response Detecti...	ng/mL	%Dev
1	1 A MSM 2 0-1-1	Anal...		1.39	16157.149		16157.149	bb	
2	2 A MSM 2 0-1-2	Anal...		1.39	15342.006		15342.006	bb	
3	3 A MSM 2 0-1-3	Anal...		1.39	15671.279		15671.279	bb	
4	4 A MSM 2 Blank 1	Blank							
5	5 A MSM 2 15-1-1	Anal...		1.39	9958.758		9958.758	bb	
6	6 A MSM 2 15-1-2	Anal...		1.38	10104.032		10104.032	bb	
7	7 A MSM 2 15-1-3	Anal...		1.39	9793.418		9793.418	bb	
8	8 A MSM 2 Blank 2	Blank							
9	9 A MSM 2 30-1-1	Anal...		1.38	6109.706		6109.706	bb	
10	10 A MSM 2 30-1-2	Anal...		1.39	6178.494		6178.494	bb	
11	11 A MSM 2 30-1-3	Anal...		1.38	5952.958		5952.958	bb	
12	12 A MSM 2 Blank 3	Blank							
13	13 A MSM 2 1-1-1	Anal...		1.39	2909.640		2909.640	bb	
14	14 A MSM 2 1-1-2	Anal...		1.39	2990.573		2990.573	bb	
15	15 A MSM 2 1-1-3	Anal...		1.39	2931.514		2931.514	bb	
16	16 A MSM 3 1-1-1	Anal...		1.39	3404.404		3404.404	bb	
17	17 A MSM 3 1-1-2	Anal...		1.39	3603.594		3603.594	bb	
18	18 A MSM 3 1-1-3	Anal...		1.39	3515.543		3515.543	bb	
19	19 A MSM 2 Blank 4	Blank							
20	20 A MSM 2 2-1-1	Anal...		1.39	2195.831		2195.831	bb	
21	21 A MSM 2 2-1-2	Anal...		1.39	2176.388		2176.388	bb	
22	22 A MSM 2 2-1-3	Anal...		1.39	2145.854		2145.854	bb	
23	23 A MSM 2 Blank 5	Blank							
24	24 A MSM 2 4-1-1	Anal...		1.39	1577.997		1577.997	bb	
25	25 A MSM 2 4-1-2	Anal...		1.39	1538.186		1538.186	bb	
26	26 A MSM 2 4-1-3	Anal...		1.39	1575.230		1575.230	bb	
27	27 A MSM 2 Blank 6	Blank							
28	28 A MSM 2 6-1-1	Anal...		1.39	1485.430		1485.430	bb	
29	29 A MSM 2 6-1-2	Anal...		1.39	1435.381		1435.381	bb	
30	30 A MSM 2 6-1-3	Anal...		1.39	1517.512		1517.512	bb	
31	31 A MSM 2 Blank 7	Blank							
32	32 A MSM 2 24-1-1	Anal...		1.39	1375.290		1375.290	bb	
33	33 A MSM 2 24-1-2	Anal...		1.39	1382.014		1382.014	bb	
34	34 A MSM 2 24-1-3	Anal...		1.39	1373.035		1373.035	bb	

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 16:17:53 Romance Daylight Time
Printed: Wednesday, August 18, 2021 16:18:18 Romance Daylight Time

Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 11:59:51
Calibration: 18 Aug 2021 16:17:53

Header

Acquired File Name: A MSM 2 0-1-1
Acquired Date: 16-Aug-2021
Acquired Time: 21:04:16
Job Code: MSM 20210816 - N - 216 - 75 - A
Task Code:
User Name:
Laboratory Name:
Instrument: ACQ-TQD#QBA320
Conditions:
Submitter:
SampleID: A MSM 2 1
Bottle Number: 2:64
Description:
Instrument Calibration:
Calibration File: C:\MassLynx\IntelliStart\Results\Unit Mass Resolution\Calib 20161209.cal

Parameters

MS1 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS1

MS1 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS1
MS1 Scan Speed Compensation:
Scan: 339 to 2000 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS1

MS2 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS2

MS2 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS2
MS2 Scan Speed Compensation:
Scan: 339 to 10165 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS2
Calibration Time: 10:33
Calibration Date: 12/09/16

Coefficients

MS1 Static: $-0.000000000000 \times x^4 + 0.000000000843 \times x^3 + -0.000001360559 \times x^2 + 1.000940122634 \times x + -0.253266439024$
MS2 Static: $-0.000000000000 \times x^4 + 0.000000000573 \times x^3 + -0.000001239648 \times x^2 + 1.000902600483 \times x + -0.192715155436$

Function 1: None

Function 2: None

Parameters for C:\Documents and Settings\Administrator\Desktop\old desktop\log D\EA.EXP

Data Processing:

SIR / MRM Chromatogram Spike Removal ON

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 16:17:53 Romance Daylight Time
Printed: Wednesday, August 18, 2021 16:18:18 Romance Daylight Time

SIR / MRM Smoothing OFF

Smoothing window size (scans) 3

Number of smooths 2

Prescan Statistics:

Initial Average Intensity 21.8777

Initial Average Std Dev 1.7606

Bunch Zero Level 0.0018

Bunch Std Dev 0.0066

Bunch Threshold 0.0526

Spike Removal Std Dev 1.7559

Method Events:

Initial Stop Flow: No Change

Initial Switch 2: No Change

Initial Switch 3: No Change

Initial Switch 4: No Change

Initial Infusion: No Change

Initial Flow State: LC

Initial Flow Rate: 5

Initial Reservoir: No Action

API Probe Delay Temp: 20

Initial Refill: No Action

Timed Events Enabled

Event Time	Name	Action
------------	------	--------

Instrument Parameters - Function 1:

Parameter File - C:\Documents and Settings\Administrator\Desktop\old desktop\log D\log D tune file.

IPR

Polarity ES+

Calibration Static 2

Capillary (kV)	3.50	3.48
----------------	------	------

Cone (V)	38.00	31.01
----------	-------	-------

Extractor (V)	3.00	2.20
---------------	------	------

RF (V)	0.10
--------	------

Source Temperature (°C)	140	138
-------------------------	-----	-----

Desolvation Temperature (°C)	450	440
------------------------------	-----	-----

Cone Gas Flow (L/Hr)	90	90
----------------------	----	----

Desolvation Gas Flow (L/Hr)	900	900
-----------------------------	-----	-----

Collision Gas Flow (mL/Min)	0.20	0.20
-----------------------------	------	------

LM 1 Resolution	15.50
-----------------	-------

HM 1 Resolution	14.84
-----------------	-------

Ion Energy 1	0.30
--------------	------

MS Mode Entrance	50.00
------------------	-------

MS Mode Collision Energy	3.00
--------------------------	------

MS Mode Exit	50.00
--------------	-------

MSMS Mode Entrance	-2.00
--------------------	-------

MSMS Mode Collision Energy	2.00
----------------------------	------

MSMS Mode Exit	2.00
----------------	------

LM 2 Resolution	15.00
-----------------	-------

HM 2 Resolution	15.50
-----------------	-------

Ion Energy 2	1.22
--------------	------

Gain 1.00

Multiplier -493.56

Active Reservoir B

Engineers Settings:

MS1 Low Mass Position	518
-----------------------	-----

MS1 High Mass Position	284
------------------------	-----

MS1 Low Mass Resolution	513
-------------------------	-----

MS1 High Mass Resolution	1732
--------------------------	------

MS1 Resolution Linearity	834
--------------------------	-----

MS1 High Mass DC Balance	0
--------------------------	---

MS1 DC Polarity	Positive
-----------------	----------

MS2 Low Mass Position	519
-----------------------	-----

MS2 High Mass Position	238
------------------------	-----

MS2 Low Mass Resolution	518
-------------------------	-----

MS2 High Mass Resolution	644
--------------------------	-----

MS2 Resolution Linearity	756
--------------------------	-----

MS2 High Mass DC Balance	-0
--------------------------	----

MS2 DC Polarity	Positive
-----------------	----------

HM RF Lens Correction +	0
-------------------------	---

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 16:17:53 Romance Daylight Time
Printed: Wednesday, August 18, 2021 16:18:18 Romance Daylight Time

HM RF Lens Correction - 0

Inter-scan delays:

Automatic Mode

MS 1 Delay Table:

	R	delay
<=	0.500	0.005
<=	1.200	0.010
<=	2.400	0.015
<=	6.000	0.020
<=	15.000	0.025
<=	25.000	0.028
>	25.000	0.030

MS 2 Delay Table:

	R	delay
<=	2.000	0.005
<=	4.000	0.008
<=	7.000	0.010
<=	10.000	0.012
<=	20.000	0.014
>	20.000	0.016

ACE Experimental Record

Inlet Method File: c:\masslynx_projects\medchem su.pro\acqudb\adme sophie

----- Prerun method parameters -----

Waters ACQUITY QSM

Waters Acquity TUV

Run Time: 0.20 min

Wavelength Mode: Single Wavelength

Lamp On: On

Channel A...

Comment:

Wavelength: 254 nm

Sampling Rate: 20 points/sec

Data Mode: Absorbance

Time Constant: 0.1000 sec

Auto Zero On Wavelength Change: Maintain Baseline

Auto Zero On Inject Start: Yes

Analog 1...

Sensitivity: 2.000 AUFS

Chart Polarity: Positive (+)

Voltage Offset: 0 mV

Enable Chart Mark: Yes

Run Events: Yes

Pulse Width: 1.0 sec

Rect Wave Period: 0.2 sec

----- oOo -----

----- Run method parameters -----

Waters ACQUITY QSM

Solvent A Name: Water

Solvent B Name: Acetonitrile

Solvent C Name: water 1 % FA

Solvent D Name:

Low Pressure Limit: 0 psi

High Pressure Limit: 15000 psi

Seal Wash Period: 5.00 min

[Gradient Table]

	Time(min)	Flow Rate(mL/min)	%A	%B	%C	%D	Curve
--	-----------	-------------------	----	----	----	----	-------

1.	Initial	0.700	90.0	5.0	5.0	0.0	Initial
----	---------	-------	------	-----	-----	-----	---------

2.	0.15	0.700	45.0	50.0	5.0	0.0	6
----	------	-------	------	------	-----	-----	---

3.	1.50	0.700	0.0	95.0	5.0	0.0	6
----	------	-------	-----	------	-----	-----	---

4.	1.80	0.700	90.0	5.0	5.0	0.0	1
----	------	-------	------	-----	-----	-----	---

Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm

Flow Ramp Rate: 0.45 min

D Solvent Selection (if supported): No Change

System Pressure Data Channel: No

Flow Rate Data Channel: No

%A Data Channel: No

%B Data Channel: No

%C Data Channel: No

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 16:17:53 Romance Daylight Time
Printed: Wednesday, August 18, 2021 16:18:18 Romance Daylight Time

%D Data Channel: No
Primary Data Channel: No
Accumulator Data Channel: No
Degasser Data Channel: No
Gradient Start: At Injection
Gradient Start Volume: 0 uL
Gradient Start Time: 0.00 min
Participate in pre-analysis: No
Waters Acquity TUV
Run Time: 1.80 min
Wavelength Mode: Single Wavelength
Lamp On: On
Channel A...
Comment:
Wavelength: 214 nm
Sampling Rate: 20 points/sec
Data Mode: Absorbance
Time Constant: 0.1000 sec
Auto Zero On Wavelength Change: Maintain Baseline
Auto Zero On Inject Start: Yes

Analog 1...
Sensitivity: 2.000 AUFS
Chart Polarity: Positive (+)
Voltage Offset: 0 mV
Enable Chart Mark: Yes
Run Events: Yes
Pulse Width: 1.0 sec
Rect Wave Period: 0.2 sec
Waters ACQUITY FTN AutoSampler
Run Time: 1.80 min
Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm
Load Ahead: Disabled
Loop Offline: Automatic min
Wash Solvent Name: Acetonitrile
Pre-Inject Wash Time: 0.0 sec
Post-Inject Wash Time: 6.0 sec
Purge Solvent Name: Water
Dilution: Disabled
Dilution Volume: 0 uL
Delay Time: 0 min
Dilution Needle Placement: 4.0 mm
Target Column Temperature: 40.0 C
Column Temperature Alarm Band: Disabled
Target Sample Temperature: 15.0 C
Sample Temperature Alarm Band: Disabled
Syringe Draw Rate: Automatic
Needle Placement: Automatic
Pre-Aspirate Air Gap: Automatic
Post-Aspirate Air Gap: Automatic
Column Temperature Data Channel: No
Room Temperature Data Channel: No
Sample Temperature Data Channel: No
Sample Organizer Temperature Data Channel: No
Sample Pressure Data Channel: No
Preheater Temperature Data Channel: No
Seal Force Data Channel: No
No Injection Mode Enabled: No
Run Events: No

Sample Run Injection Parameter

Injection Volume (ul) - 3.00

----- o0o -----

End of experimental record.

----- Waters ACQUITY QSM Postrun Report -----

Firmware Version: 1.50.237 (May 18 2011)

Software Version: 1.50.1621

Checksum: 0xae400516

Serial Number: M09QSM056N

Minimum System Pressure: 0.0 psi

Dataset: Untitled
Last Altered: Wednesday, August 18, 2021 16:17:53 Romance Daylight Time
Printed: Wednesday, August 18, 2021 16:18:18 Romance Daylight Time

Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi
----- o0o -----

----- Waters ACQUITY FTN Postrun Report -----

Software Version: 1.50.1481
Firmware Version: 1.50.317 (Jul 11 2011)
Checksum: 0x3e83519d
Serial Number: M09SDI055N
Sample Syringe Size: 100.0
Extension Loop Size: 0.0
Needle Size: 15.0
Column Type: ACQUITY UPLC® BEH C18 1.7µm
Column Serial Number: 02343407715781
Total Injections on Column: 7503
Minimum Sample Temperature: 0.0
Maximum Sample Temperature: 0.0
Average Sample Temperature: 0.0
Minimum Column Temperature: 40.0
Maximum Column Temperature: 40.1
Average Column Temperature: 0.0
----- o0o -----

----- Generic Instrument Postrun Report -----

Software Version: 1.50.2530
Firmware Version: 1.50.2182 (May 11 2011)
Checksum: 0xc09b9cb2
Serial Number: J08UPT460M
Lamp On/Off Event: No
Lamp Life: 879.00
Lamp Serial Number: 000296721
Flow Cell Type: Other
Flow Cell Path Length: 0.00 mm
Flow Cell Volume: 0.00 microliters
Flow Cell Serial Number: 1
Flow Cell Part Number: 1
Optics Temperature Stabilization Setting: unknown
----- o0o -----

----- Waters ACQUITY QSM Postrun Report -----

Firmware Version: 1.50.237 (May 18 2011)
Software Version: 1.50.1621
Checksum: 0xae400516
Serial Number: M09QSM056N
Minimum System Pressure: 0.0 psi
Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi
----- o0o -----

Function 1

Scans in function:	338								
Cycle time (secs):	Automatic								
Inter Scan Delay (secs):	Automatic								
Inter Channel Delay (secs):	Automatic								
Span (Da):	0.500								
Start and End Time(mins):	0.300 to 1.800								
Ionization mode:	ES+								
Data type:	SIR or MRM data								
Function type:	MRM of 1 channel								
Chan Reaction	Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound Formula Mass Comm								
ents									
1 : 419.87 > 295.05	0.260	30.0	18.0	Auto	EA	418.9			Inte
lliStart Generated									

Function 2

Scans in function: 2161
Function type: Diode Array
Wavelength range (nm): 214 to 214

Dataset: Untitled
Last Altered: Monday, January 11, 2021 11:02:27 Romance Standard Time
Printed: Monday, January 11, 2021 11:02:34 Romance Standard Time

Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 10:59:51

Calibration: 11 Jan 2021 11:00:12

Compound name: A

No Calibration

Response type: External Std, Area

Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

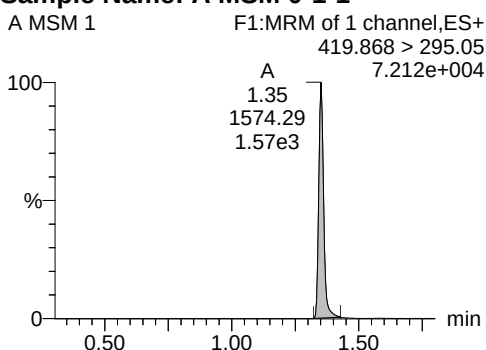


Dataset: Untitled
Last Altered: Monday, January 11, 2021 11:02:27 Romance Standard Time
Printed: Monday, January 11, 2021 11:02:34 Romance Standard Time

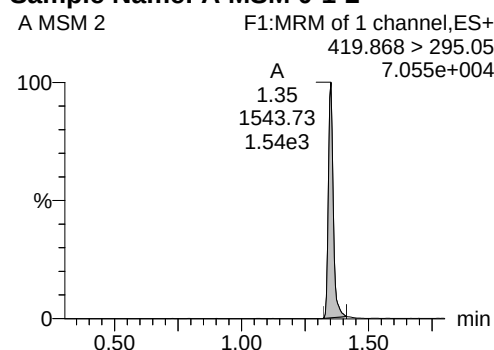
Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 10:59:51

Calibration: 11 Jan 2021 11:00:12

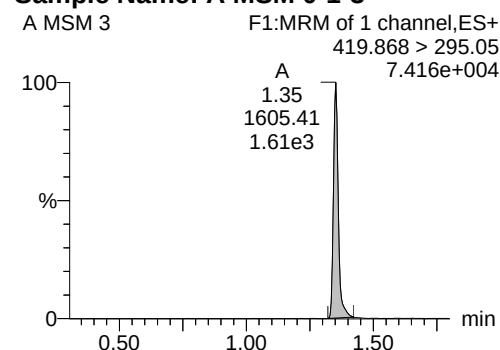
Sample Name: A MSM 0-1-1



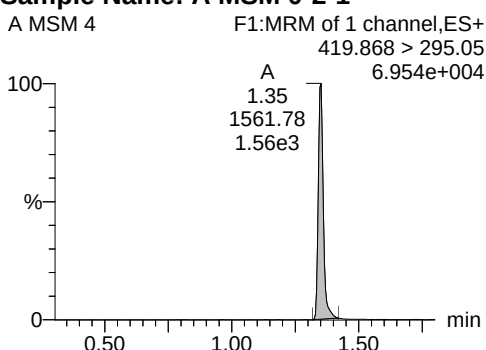
Sample Name: A MSM 0-1-2



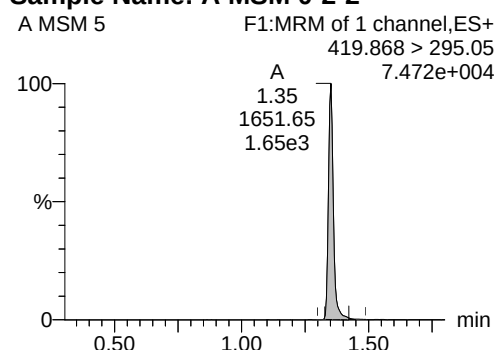
Sample Name: A MSM 0-1-3



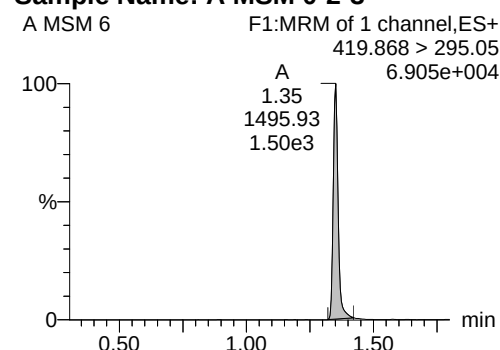
Sample Name: A MSM 0-2-1



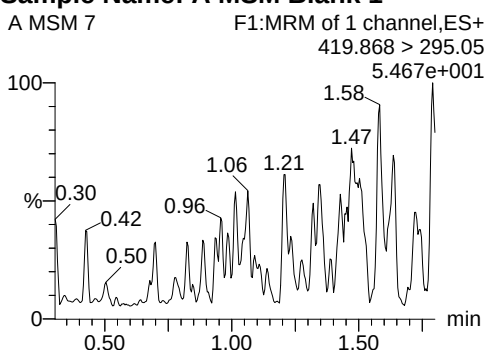
Sample Name: A MSM 0-2-2



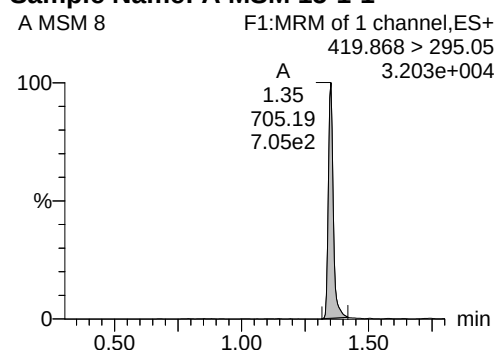
Sample Name: A MSM 0-2-3



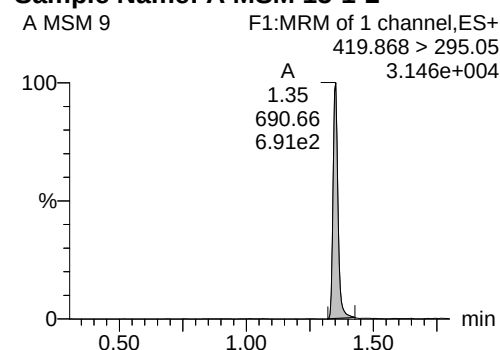
Sample Name: A MSM Blank 1



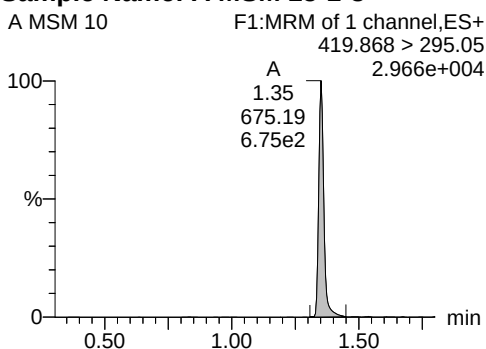
Sample Name: A MSM 15-1-1



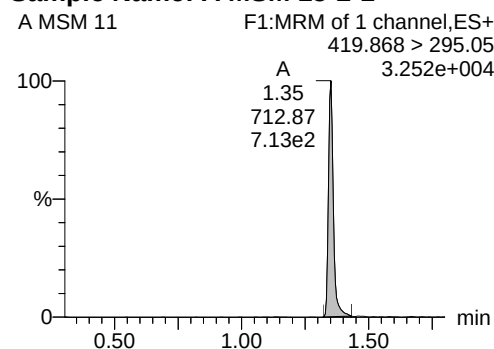
Sample Name: A MSM 15-1-2



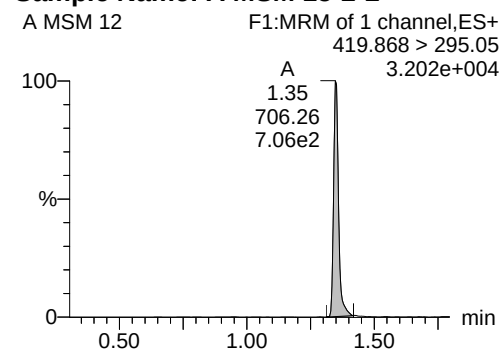
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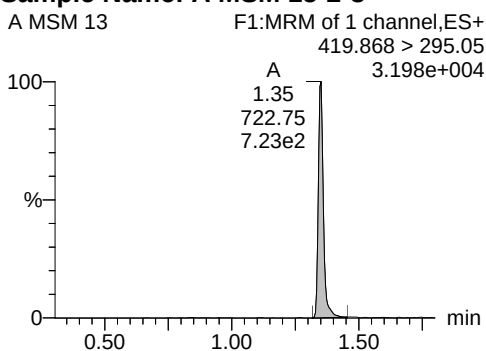
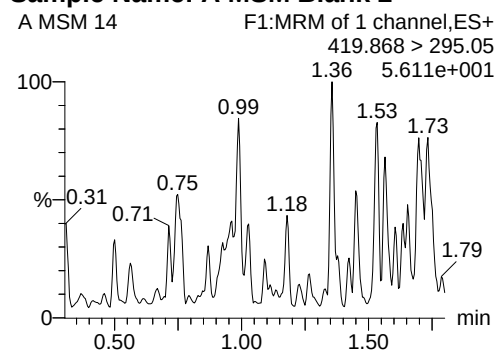
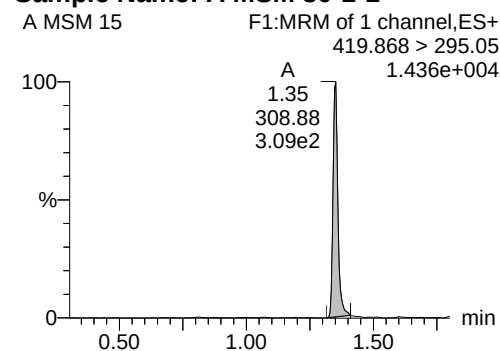
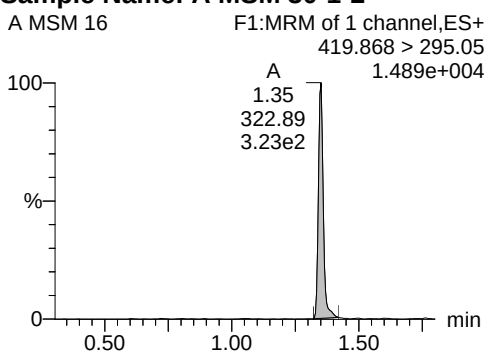
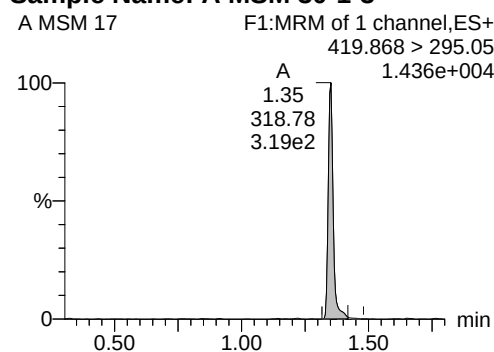
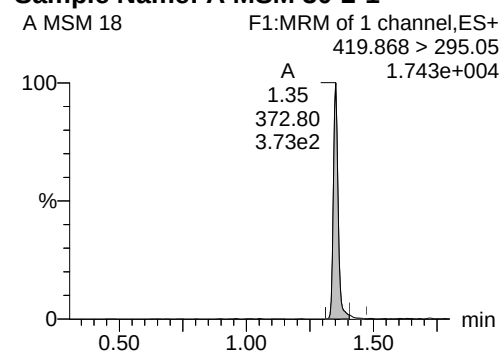
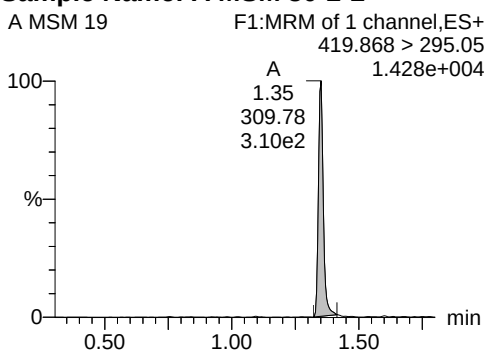
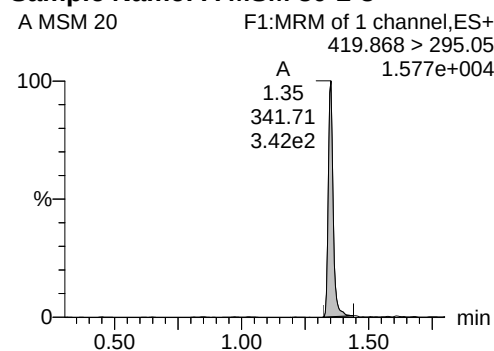
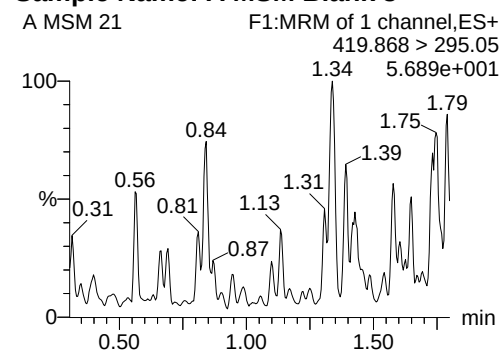
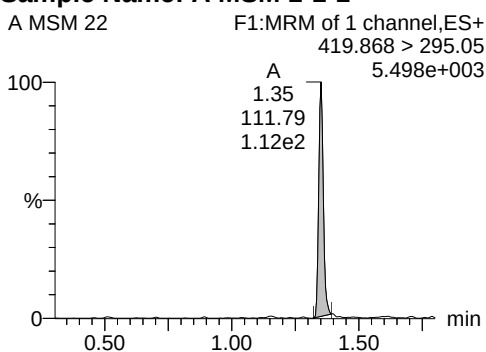
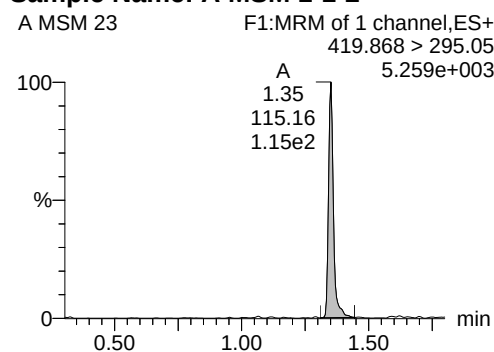
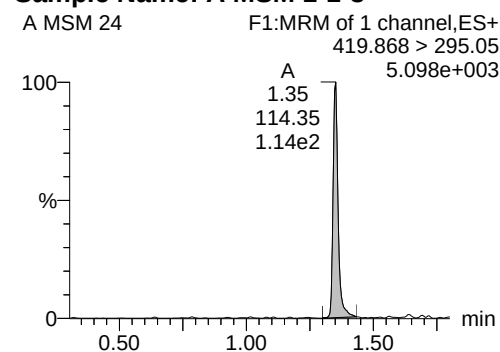
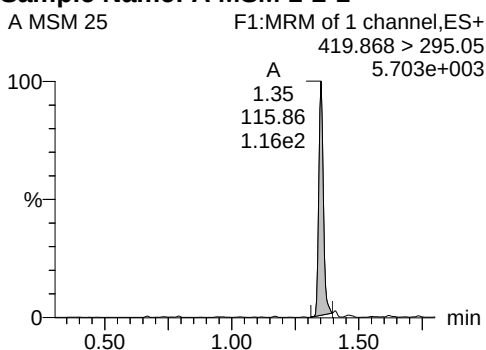
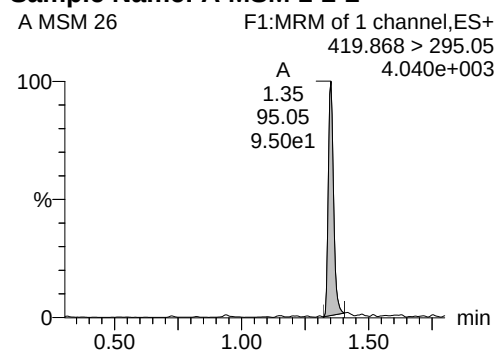
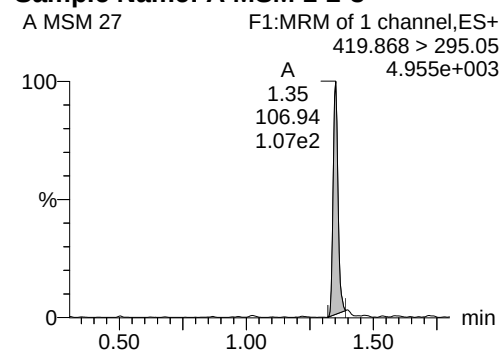
Sample Name: A MSM 15-2-1



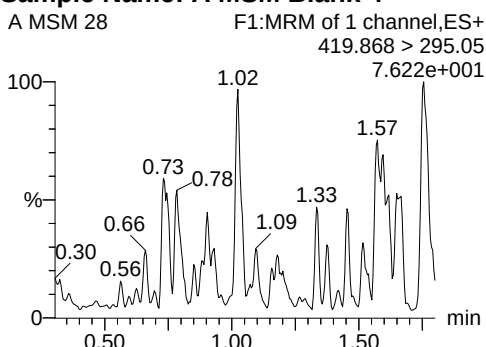
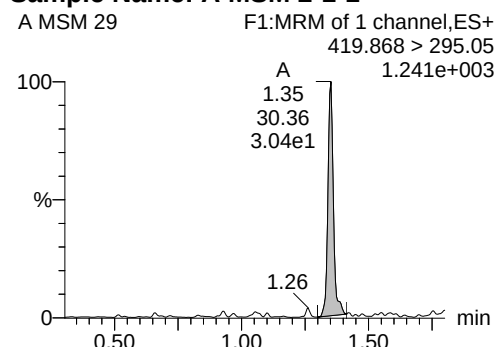
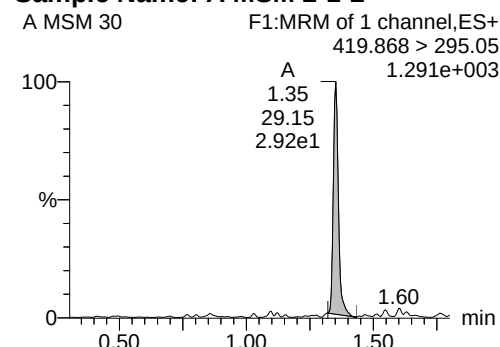
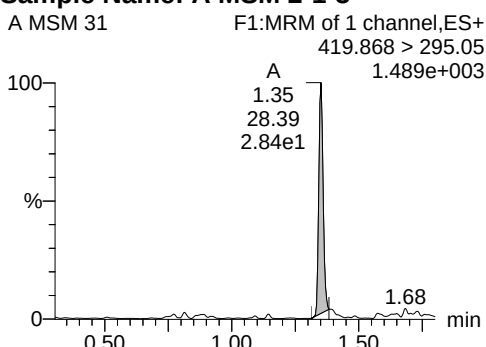
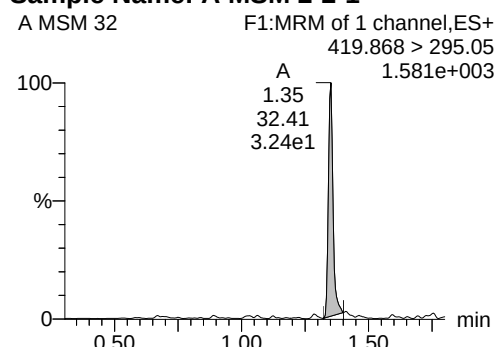
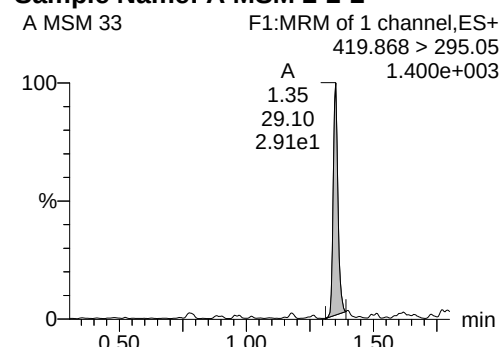
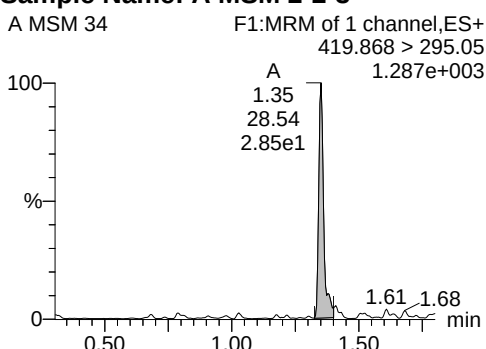
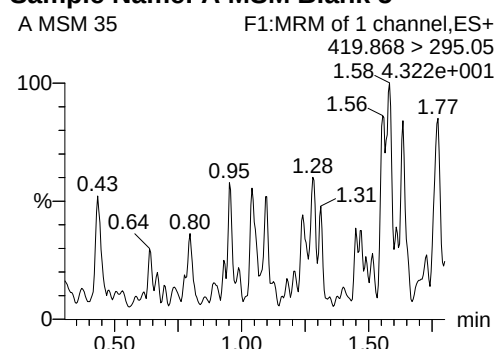
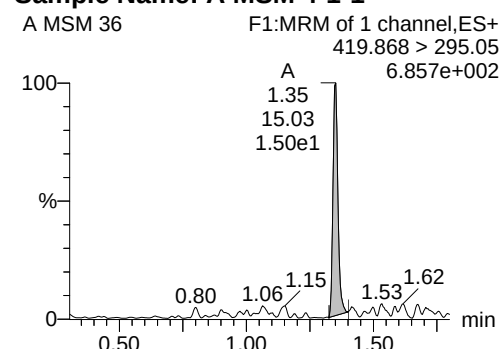
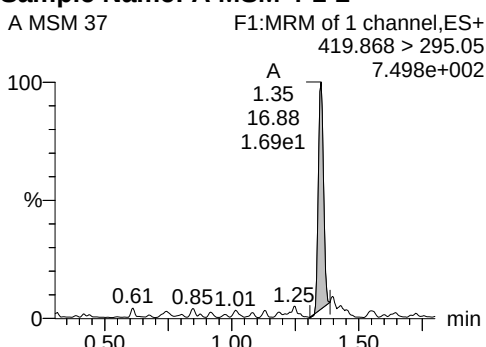
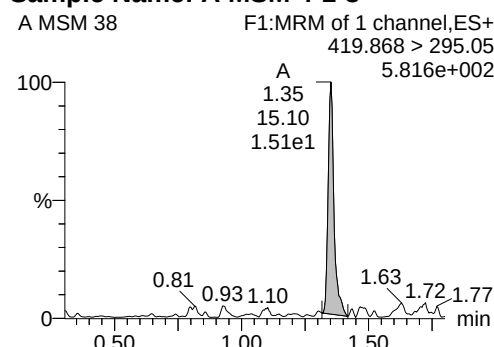
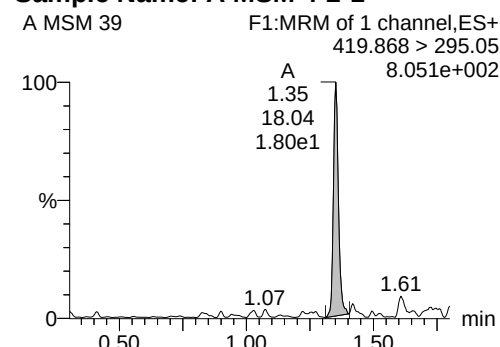
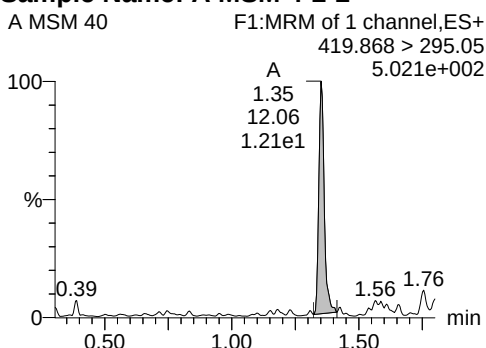
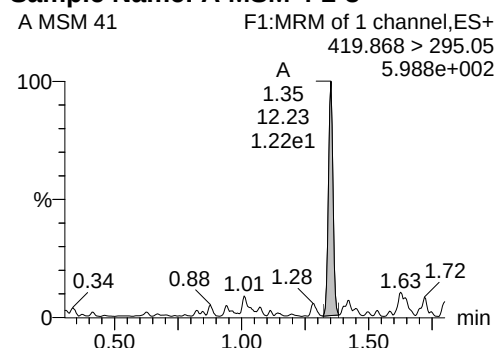
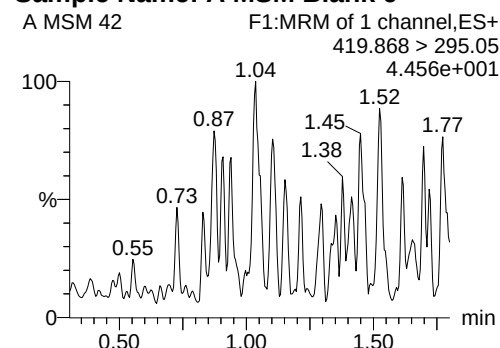
Sample Name: A MSM 15-2-2



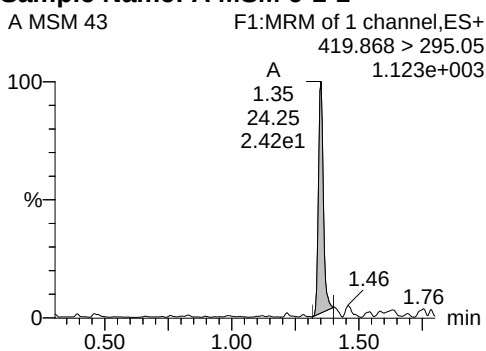
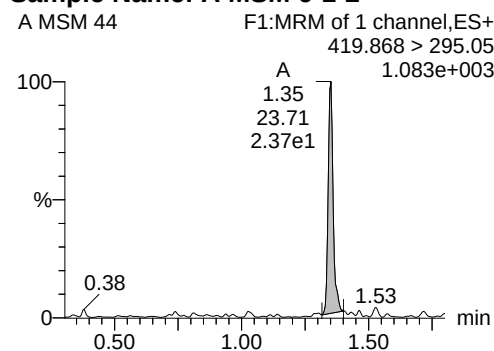
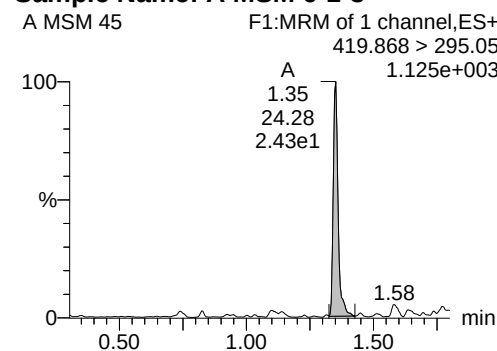
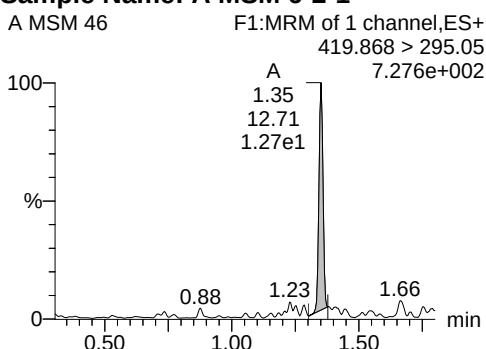
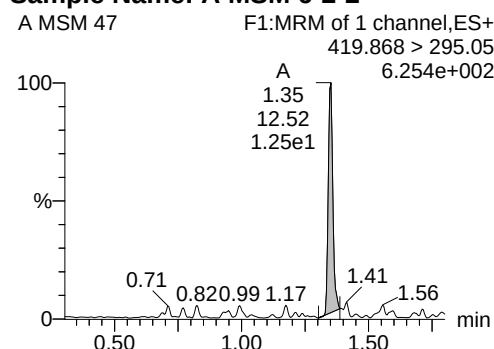
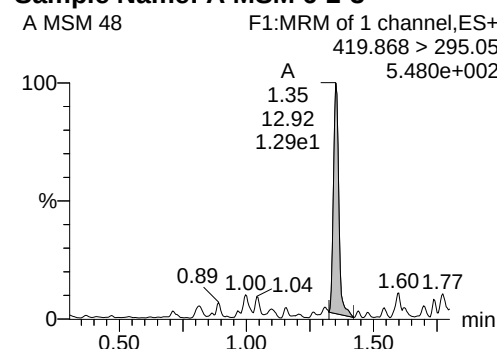
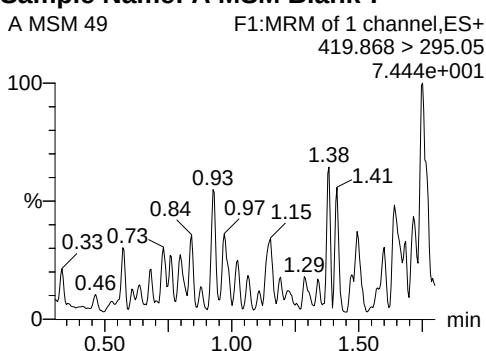
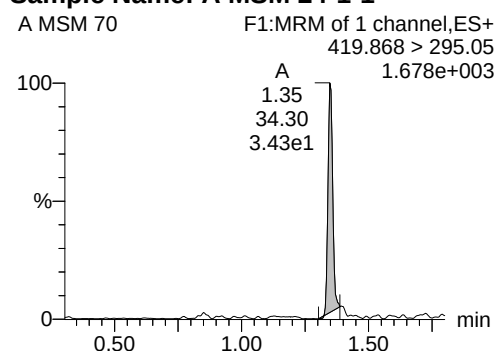
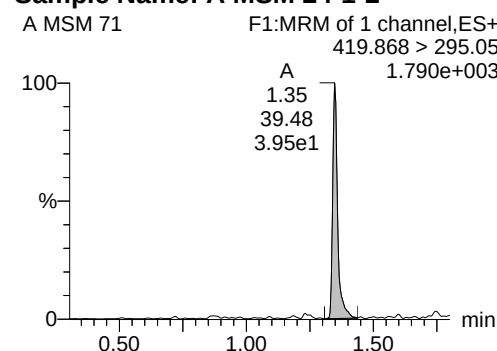
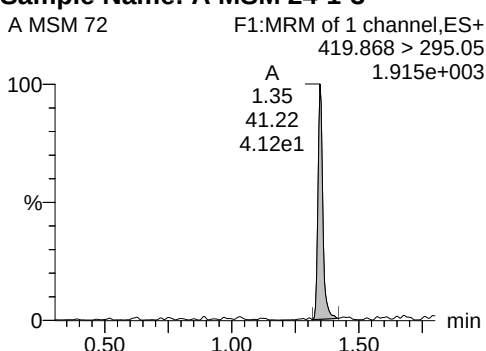
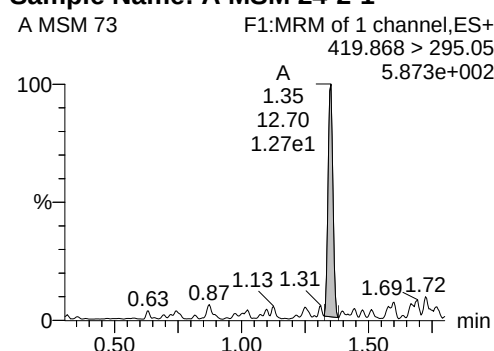
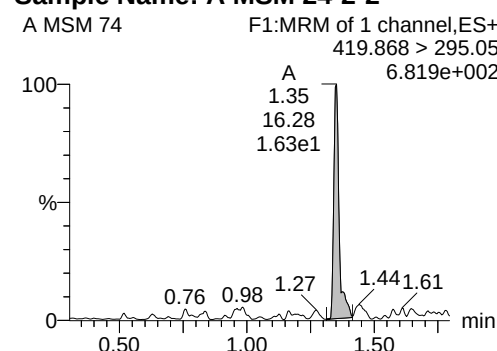
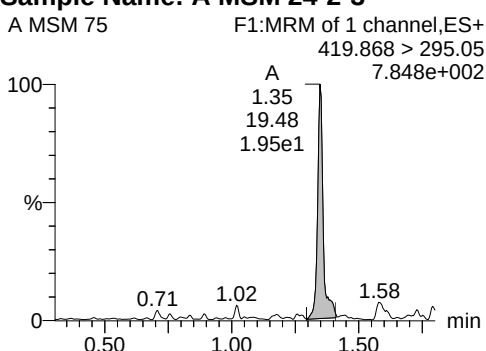
Dataset: Untitled
Last Altered: Monday, January 11, 2021 11:02:27 Romance Standard Time
Printed: Monday, January 11, 2021 11:02:34 Romance Standard Time

Sample Name: A MSM 15-2-3**Sample Name: A MSM Blank 2****Sample Name: A MSM 30-1-1****Sample Name: A MSM 30-1-2****Sample Name: A MSM 30-1-3****Sample Name: A MSM 30-2-1****Sample Name: A MSM 30-2-2****Sample Name: A MSM 30-2-3****Sample Name: A MSM Blank 3****Sample Name: A MSM 1-1-1****Sample Name: A MSM 1-1-2****Sample Name: A MSM 1-1-3****Sample Name: A MSM 1-2-1****Sample Name: A MSM 1-2-2****Sample Name: A MSM 1-2-3**

Dataset: Untitled
Last Altered: Monday, January 11, 2021 11:02:27 Romance Standard Time
Printed: Monday, January 11, 2021 11:02:34 Romance Standard Time

Sample Name: A MSM Blank 4**Sample Name: A MSM 2-1-1****Sample Name: A MSM 2-1-2****Sample Name: A MSM 2-1-3****Sample Name: A MSM 2-2-1****Sample Name: A MSM 2-2-2****Sample Name: A MSM 2-2-3****Sample Name: A MSM Blank 5****Sample Name: A MSM 4-1-1****Sample Name: A MSM 4-1-2****Sample Name: A MSM 4-1-3****Sample Name: A MSM 4-2-1****Sample Name: A MSM 4-2-2****Sample Name: A MSM 4-2-3****Sample Name: A MSM Blank 6**

Dataset: Untitled
Last Altered: Monday, January 11, 2021 11:02:27 Romance Standard Time
Printed: Monday, January 11, 2021 11:02:34 Romance Standard Time

Sample Name: A MSM 6-1-1**Sample Name: A MSM 6-1-2****Sample Name: A MSM 6-1-3****Sample Name: A MSM 6-2-1****Sample Name: A MSM 6-2-2****Sample Name: A MSM 6-2-3****Sample Name: A MSM Blank 7****Sample Name: A MSM 24-1-1****Sample Name: A MSM 24-1-2****Sample Name: A MSM 24-1-3****Sample Name: A MSM 24-2-1****Sample Name: A MSM 24-2-2****Sample Name: A MSM 24-2-3**

	# Name	Type	Std. Conc	RT	Area	IS Area	Response	Detecti...	ng/mL	%Dev
1	1 A MSM 0-1-1	Anal...		1.35	1574.286		1574.286	bb		
2	2 A MSM 0-1-2	Anal...		1.35	1543.731		1543.731	bb		
3	3 A MSM 0-1-3	Anal...		1.35	1605.405		1605.405	bb		
4	4 A MSM 0-2-1	Anal...		1.35	1561.776		1561.776	bb		
5	5 A MSM 0-2-2	Anal...		1.35	1651.649		1651.649	MM		
6	6 A MSM 0-2-3	Anal...		1.35	1495.935		1495.935	bb		
7	7 A MSM Blank 1	Blank								
8	8 A MSM 15-1-1	Anal...		1.35	705.189		705.189	bb		
9	9 A MSM 15-1-2	Anal...		1.35	690.656		690.656	bb		
10	10 A MSM 15-1-3	Anal...		1.35	675.189		675.189	bb		
11	11 A MSM 15-2-1	Anal...		1.35	712.874		712.874	bb		
12	12 A MSM 15-2-2	Anal...		1.35	706.255		706.255	bb		
13	13 A MSM 15-2-3	Anal...		1.35	722.751		722.751	bb		
14	14 A MSM Blank 2	Blank								
15	15 A MSM 30-1-1	Anal...		1.35	308.876		308.876	bb		
16	16 A MSM 30-1-2	Anal...		1.35	322.889		322.889	bb		
17	17 A MSM 30-1-3	Anal...		1.35	318.783		318.783	MM		
18	18 A MSM 30-2-1	Anal...		1.35	372.798		372.798	MM		
19	19 A MSM 30-2-2	Anal...		1.35	309.781		309.781	bb		
20	20 A MSM 30-2-3	Anal...		1.35	341.714		341.714	bb		
21	21 A MSM Blank 3	Blank								
22	22 A MSM 1-1-1	Anal...		1.35	111.793		111.793	bb		
23	23 A MSM 1-1-2	Anal...		1.35	115.160		115.160	bb		
24	24 A MSM 1-1-3	Anal...		1.35	114.349		114.349	bb		
25	25 A MSM 1-2-1	Anal...		1.35	115.862		115.862	bb		
26	26 A MSM 1-2-2	Anal...		1.35	95.047		95.047	MM		
27	27 A MSM 1-2-3	Anal...		1.35	106.940		106.940	bb		
28	28 A MSM Blank 4	Blank								
29	29 A MSM 2-1-1	Anal...		1.35	30.357		30.357	MM		
30	30 A MSM 2-1-2	Anal...		1.35	29.151		29.151	MM		
31	31 A MSM 2-1-3	Anal...		1.35	28.388		28.388	MM		
32	32 A MSM 2-2-1	Anal...		1.35	32.411		32.411	MM		
33	33 A MSM 2-2-2	Anal...		1.35	29.102		29.102	MM		
34	34 A MSM 2-2-3	Anal...		1.35	28.537		28.537	MM		
35	35 A MSM Blank 5	Blank								
36	36 A MSM 4-1-1	Anal...		1.35	15.026		15.026	MM		
37	37 A MSM 4-1-2	Anal...		1.35	16.883		16.883	MM		
38	38 A MSM 4-1-3	Anal...		1.35	15.103		15.103	MM		
39	39 A MSM 4-2-1	Anal...		1.35	18.040		18.040	MM		
40	40 A MSM 4-2-2	Anal...		1.35	12.064		12.064	MM		
41	41 A MSM 4-2-3	Anal...		1.35	12.229		12.229	MM		
42	42 A MSM Blank 6	Blank								
43	43 A MSM 6-1-1	Anal...		1.35	24.249		24.249	MM		
44	44 A MSM 6-1-2	Anal...		1.35	23.711		23.711	MM		
45	45 A MSM 6-1-3	Anal...		1.35	24.281		24.281	MM		
46	46 A MSM 6-2-1	Anal...		1.35	12.707		12.707	MM		
47	47 A MSM 6-2-2	Anal...		1.35	12.524		12.524	MM		
48	48 A MSM 6-2-3	Anal...		1.35	12.917		12.917	MM		
49	49 A MSM Blank 7	Blank								
50	50 A MSM 24-1-1	Anal...		1.35	34.303		34.303	MM		
51	51 A MSM 24-1-2	Anal...		1.35	39.484		39.484	MM		
52	52 A MSM 24-1-3	Anal...		1.35	41.216		41.216	MM		
53	53 A MSM 24-2-1	Anal...		1.35	12.700		12.700	MM		
54	54 A MSM 24-2-2	Anal...		1.35	16.283		16.283	MM		
55	55 A MSM 24-2-3	Anal...		1.35	19.478		19.478	MM		

Dataset: Untitled
Last Altered: Monday, January 11, 2021 11:02:27 Romance Standard Time
Printed: Monday, January 11, 2021 11:02:34 Romance Standard Time

Method: C:\MassLynx_Projects\Medchem SU.PRO\MethDB\A.mdb 11 Jan 2021 10:59:51
Calibration: 11 Jan 2021 11:00:12

Header

Acquired File Name: A MSM 0-1-1
Acquired Date: 07-Jan-2021
Acquired Time: 20:49:57
Job Code: MSM 20210107 - 002 - 026 - 75 - A
Task Code:
User Name:
Laboratory Name:
Instrument: ACQ-TQD#QBA320
Conditions:
Submitter:
SampleID: A MSM 1
Bottle Number: 2:64
Description:
Instrument Calibration:
Calibration File: C:\MassLynx\IntelliStart\Results\Unit Mass Resolution\Calib 20161209.cal
Parameters

MS1 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS1

MS1 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS1
MS1 Scan Speed Compensation:
Scan: 339 to 2000 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS1

MS2 Static:

Mass: 20 Da to 1974 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: STATMS2

MS2 Scanning:

Mass: 15 Da to 2048 Da.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: SCNMS2
MS2 Scan Speed Compensation:
Scan: 339 to 10165 amu/sec.
Resolution: 15.0/15.0
Ion Energy: 0.5
Reference File: Naics2
Acquisition File: FASTMS2
Calibration Time: 10:33
Calibration Date: 12/09/16

Coefficients

MS1 Static: $-0.000000000000 \times x^4 + 0.000000000843 \times x^3 + -0.000001360559 \times x^2 + 1.000940122634 \times x + -0.253266439024$
MS2 Static: $-0.000000000000 \times x^4 + 0.000000000573 \times x^3 + -0.000001239648 \times x^2 + 1.000902600483 \times x + -0.192715155436$

Function 1: None

Function 2: None

Parameters for C:\Documents and Settings\Administrator\Desktop\old desktop\log D\EA.EXP

Data Processing:

SIR / MRM Chromatogram Spike Removal ON

Dataset: Untitled
Last Altered: Monday, January 11, 2021 11:02:27 Romance Standard Time
Printed: Monday, January 11, 2021 11:02:34 Romance Standard Time

SIR / MRM Smoothing OFF
Smoothing window size (scans) 3
Number of smooths 2
Prescan Statistics:
Initial Average Intensity 22.1158
Initial Average Std Dev 1.8762
Bunch Zero Level 0.0036
Bunch Std Dev 0.0096
Bunch Threshold 0.0768
Spike Removal Std Dev 1.7801

Method Events:

Initial Stop Flow: No Change
Initial Switch 2: No Change
Initial Switch 3: No Change
Initial Switch 4: No Change
Initial Infusion: No Change
Initial Flow State: LC
Initial Flow Rate: 5
Initial Reservoir: No Action
API Probe Delay Temp: 20
Initial Refill: No Action

Timed Events Enabled

Event Time	Name	Action
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Instrument Parameters - Function 1:

Parameter File - C:\Documents and Settings\Administrator\Desktop\old desktop\log D\log D tune file.

IPR

Polarity ES+
Calibration Static 2
Capillary (kV) 3.50 3.48
Cone (V) 38.00 35.41
Extractor (V) 3.00 2.20
RF (V) 0.10
Source Temperature (°C) 140 139
Desolvation Temperature (°C) 450 450
Cone Gas Flow (L/Hr) 90 90
Desolvation Gas Flow (L/Hr) 900 900
Collision Gas Flow (mL/Min) 0.20 0.20
LM 1 Resolution 15.50
HM 1 Resolution 14.84
Ion Energy 1 0.30
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance -2.00
MSMS Mode Collision Energy 2.00
MSMS Mode Exit 2.00
LM 2 Resolution 15.00
HM 2 Resolution 15.50
Ion Energy 2 1.22
Gain 1.00
Multiplier -493.30

Active Reservoir B

Engineers Settings:

MS1 Low Mass Position	518
MS1 High Mass Position	284
MS1 Low Mass Resolution	513
MS1 High Mass Resolution	1732
MS1 Resolution Linearity	834
MS1 High Mass DC Balance	0
MS1 DC Polarity	Positive
MS2 Low Mass Position	519
MS2 High Mass Position	238
MS2 Low Mass Resolution	518
MS2 High Mass Resolution	644
MS2 Resolution Linearity	756
MS2 High Mass DC Balance	-0
MS2 DC Polarity	Positive
HM RF Lens Correction +	0

Dataset: Untitled
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HM RF Lens Correction - 0

Inter-scan delays:

Automatic Mode

MS 1 Delay Table:

	R	delay
<=	0.500	0.005
<=	1.200	0.010
<=	2.400	0.015
<=	6.000	0.020
<=	15.000	0.025
<=	25.000	0.028
>	25.000	0.030

MS 2 Delay Table:

	R	delay
<=	2.000	0.005
<=	4.000	0.008
<=	7.000	0.010
<=	10.000	0.012
<=	20.000	0.014
>	20.000	0.016

ACE Experimental Record

Inlet Method File: c:\masslynx_projects\medchem su.pro\acqudb\adme sophie

----- Prerun method parameters -----

Waters ACQUITY QSM

Waters Acquity TUV

Run Time: 0.20 min

Wavelength Mode: Single Wavelength

Lamp On: On

Channel A...

Comment:

Wavelength: 254 nm

Sampling Rate: 20 points/sec

Data Mode: Absorbance

Time Constant: 0.1000 sec

Auto Zero On Wavelength Change: Maintain Baseline

Auto Zero On Inject Start: Yes

Analog 1...

Sensitivity: 2.000 AUFS

Chart Polarity: Positive (+)

Voltage Offset: 0 mV

Enable Chart Mark: Yes

Run Events: Yes

Pulse Width: 1.0 sec

Rect Wave Period: 0.2 sec

----- oOo -----

----- Run method parameters -----

Waters ACQUITY QSM

Solvent A Name: Water

Solvent B Name: Acetonitrile

Solvent C Name: water 1 % FA

Solvent D Name:

Low Pressure Limit: 0 psi

High Pressure Limit: 15000 psi

Seal Wash Period: 5.00 min

[Gradient Table]

	Time(min)	Flow Rate(mL/min)	%A	%B	%C	%D	Curve
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1.	Initial	0.700	90.0	5.0	5.0	0.0	Initial
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2.	0.15	0.700	45.0	50.0	5.0	0.0	6
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3.	1.50	0.700	0.0	95.0	5.0	0.0	6
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4.	1.80	0.700	90.0	5.0	5.0	0.0	1
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Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm

Flow Ramp Rate: 0.45 min

D Solvent Selection (if supported): No Change

System Pressure Data Channel: No

Flow Rate Data Channel: No

%A Data Channel: No

%B Data Channel: No

%C Data Channel: No

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%D Data Channel: No
Primary Data Channel: No
Accumulator Data Channel: No
Degasser Data Channel: No
Gradient Start: At Injection
Gradient Start Volume: 0 uL
Gradient Start Time: 0.00 min
Participate in pre-analysis: No
Waters Acquity TUV
Run Time: 1.80 min
Wavelength Mode: Single Wavelength
Lamp On: On
Channel A...
Comment:
Wavelength: 214 nm
Sampling Rate: 20 points/sec
Data Mode: Absorbance
Time Constant: 0.1000 sec
Auto Zero On Wavelength Change: Maintain Baseline
Auto Zero On Inject Start: Yes

Analog 1...
Sensitivity: 2.000 AUFS
Chart Polarity: Positive (+)
Voltage Offset: 0 mV
Enable Chart Mark: Yes
Run Events: Yes
Pulse Width: 1.0 sec
Rect Wave Period: 0.2 sec
Waters ACQUITY FTN AutoSampler
Run Time: 1.80 min
Comment: ACQUITY UPLC BEH C18 2.1 x 50 mm
Load Ahead: Disabled
Loop Offline: Automatic min
Wash Solvent Name: Acetonitrile
Pre-Inject Wash Time: 0.0 sec
Post-Inject Wash Time: 6.0 sec
Purge Solvent Name: Water
Dilution: Disabled
Dilution Volume: 0 uL
Delay Time: 0 min
Dilution Needle Placement: 4.0 mm
Target Column Temperature: 40.0 C
Column Temperature Alarm Band: Disabled
Target Sample Temperature: 15.0 C
Sample Temperature Alarm Band: Disabled
Syringe Draw Rate: Automatic
Needle Placement: Automatic
Pre-Aspirate Air Gap: Automatic
Post-Aspirate Air Gap: Automatic
Column Temperature Data Channel: No
Room Temperature Data Channel: No
Sample Temperature Data Channel: No
Sample Organizer Temperature Data Channel: No
Sample Pressure Data Channel: No
Preheater Temperature Data Channel: No
Seal Force Data Channel: No
No Injection Mode Enabled: No
Run Events: No

Sample Run Injection Parameter

Injection Volume (ul) - 3.00

-----o0o-----

End of experimental record.

-----Waters ACQUITY QSM Postrun Report-----

Firmware Version: 1.50.237 (May 18 2011)

Software Version: 1.50.1621

Checksum: 0xae400516

Serial Number: M09QSM056N

Minimum System Pressure: 0.0 psi

Dataset: Untitled
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Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi
-----o0o-----

-----Waters ACQUITY FTN Postrun Report-----

Software Version: 1.50.1481
Firmware Version: 1.50.317 (Jul 11 2011)
Checksum: 0x3e83519d
Serial Number: M09SDI055N
Sample Syringe Size: 100.0
Extension Loop Size: 0.0
Needle Size: 15.0
Column Type: ACQUITY UPLC® BEH C18 1.7µm
Column Serial Number: 02343407715781
Total Injections on Column: 456
Minimum Sample Temperature: 0.0
Maximum Sample Temperature: 0.0
Average Sample Temperature: 0.0
Minimum Column Temperature: 30.0
Maximum Column Temperature: 41.4
Average Column Temperature: 0.0
-----o0o-----

-----Generic Instrument Postrun Report-----

Software Version: 1.50.2530
Firmware Version: 1.50.2182 (May 11 2011)
Checksum: 0xc09b9cb2
Serial Number: J08UPT460M
Lamp On/Off Event: No
Lamp Life: 39.00
Lamp Serial Number: 000296721
Flow Cell Type: Other
Flow Cell Path Length: 0.00 mm
Flow Cell Volume: 0.00 microliters
Flow Cell Serial Number: 1
Flow Cell Part Number: 1
Optics Temperature Stabilization Setting: unknown
-----o0o-----

-----Waters ACQUITY QSM Postrun Report-----

Firmware Version: 1.50.237 (May 18 2011)
Software Version: 1.50.1621
Checksum: 0xae400516
Serial Number: M09QSM056N
Minimum System Pressure: 0.0 psi
Maximum System Pressure: 0.0 psi
Average System Pressure: 0.0 psi
-----o0o-----

Function 1

Scans in function: 338
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 2.000
Start and End Time(mins): 0.300 to 1.800
Ionization mode: ES+
Data type: SIR or MRM data
Function type: MRM of 1 channel

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula	Mass Comm
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1 : 419.87 > 295.05	0.260	30.0	18.0	Auto	EA	418.9	Inte
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lliStart Generated

Function 2

Scans in function: 2161
Function type: Diode Array
Wavelength range (nm): 214 to 214