

7.762
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7.755
7.742
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7.629
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7.591
7.527
7.524
7.509
7.506
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7.433
7.421
7.401
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7.309
7.260
7.239
7.237
7.202
7.199
7.183
7.181
5.270
5.261
5.228
5.219
4.422
4.415
4.379
4.158
4.141
4.089
4.054
4.050
3.926
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3.114
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1.757
1.745
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1.200



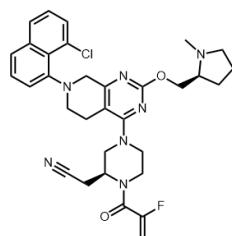
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

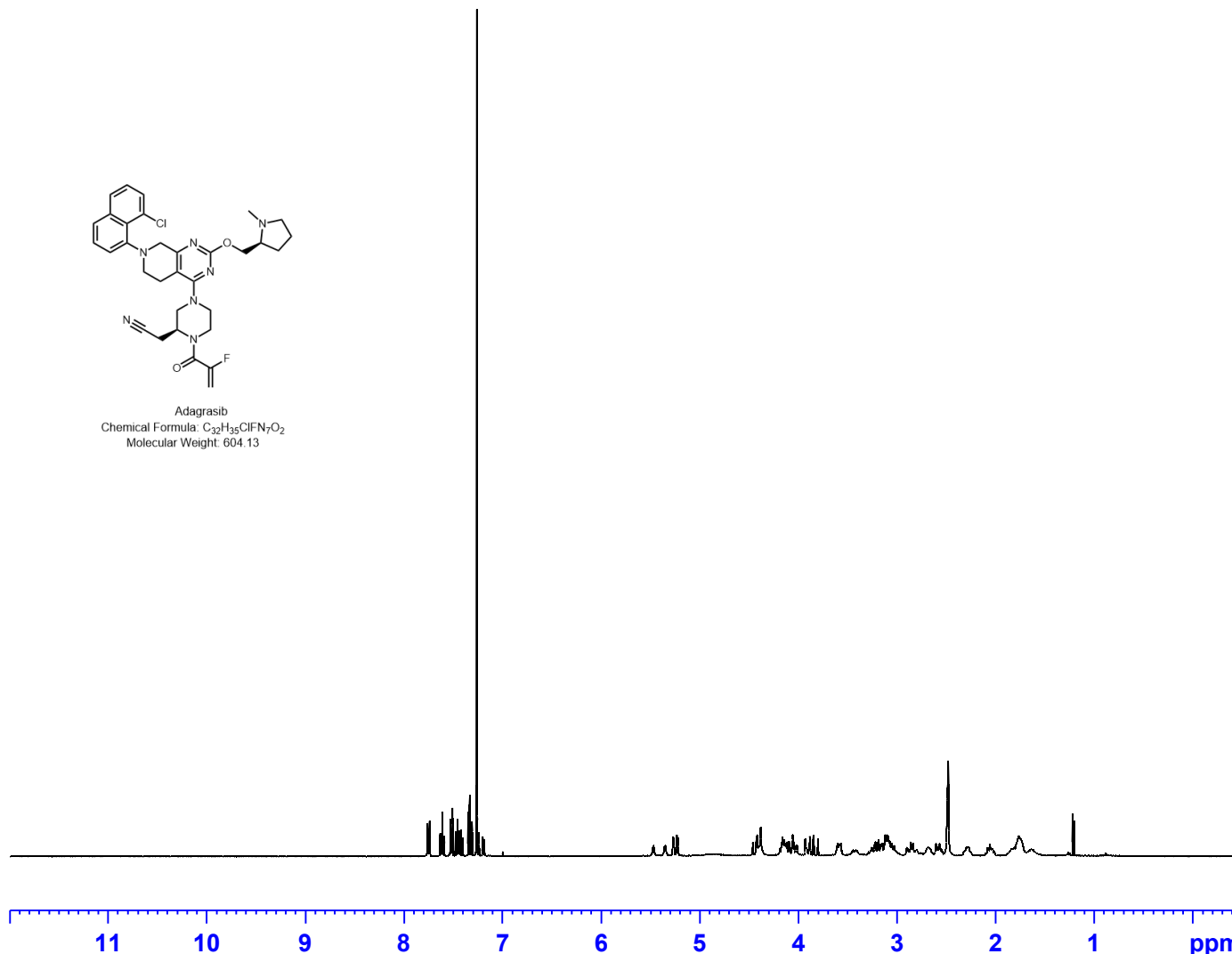
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Time 10.50 h
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PULPROG zg30
TD 65536
SOLVENT CDC13
NS 128
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 3.9845889 sec
RG 80.6
DW 60.800 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324710 MHz
NUC1 1H
P0 4.95 usec
P1 14.86 usec
PLW1 9.92000008 W

F2 - Processing parameters

SI 32768
SF 400.1300097 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



Adagrasib
Chemical Formula: C₃₂H₃₅ClF₇N₇O₂
Molecular Weight: 604.13



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1.0183
1.0221
1.0160
0.6873

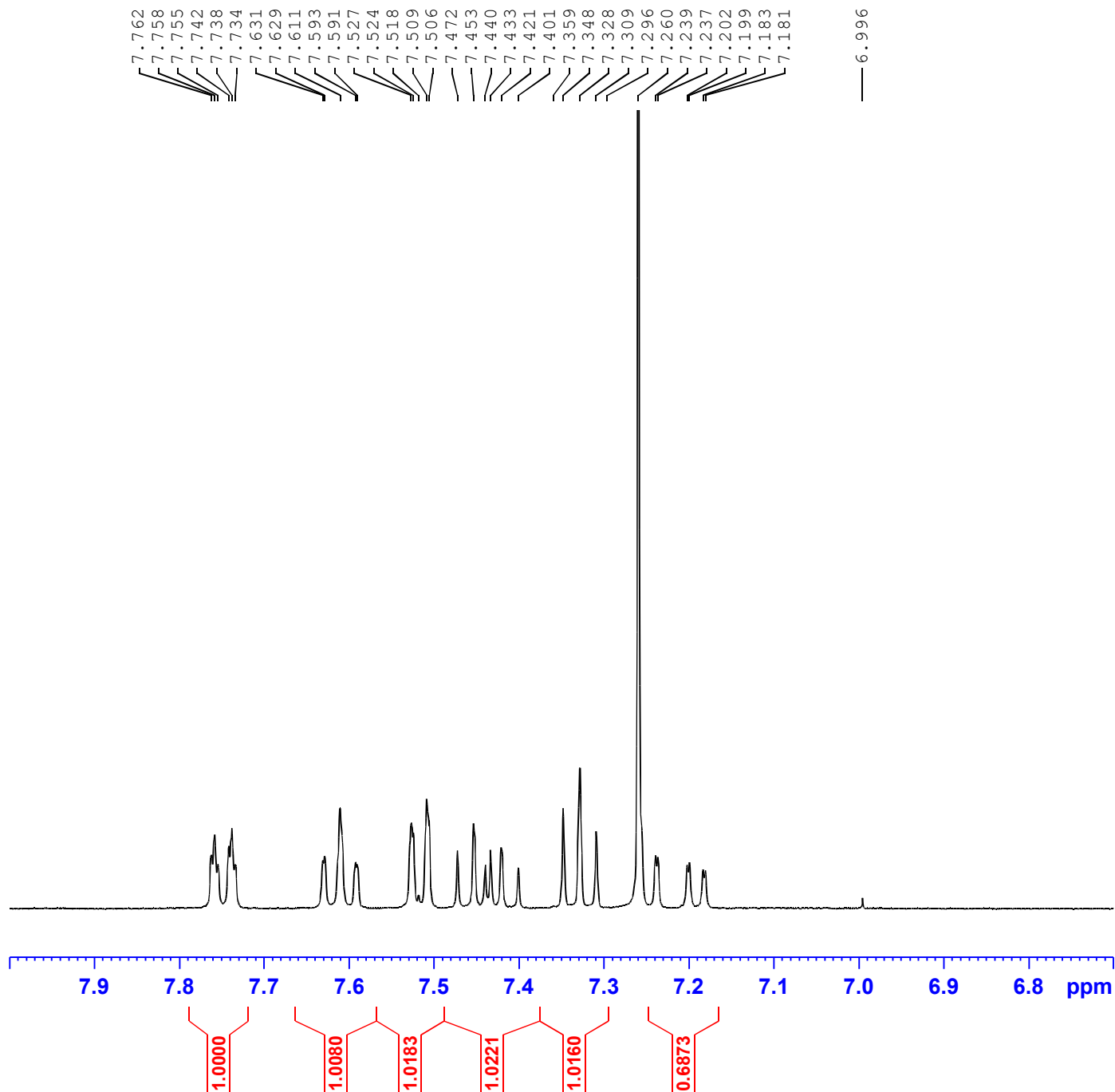
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6.1257
3.5856
5.1695
6.8289
1.1147
1.1053
3.2829



Current Data Parameters
NAME NSC-831453-M1_repeat
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210720
Time 10.50 h
INSTRUM spect
PROBHD Z104450_0348 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 128
DS 2
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PLW1 9.92000008 W

F2 - Processing parameters
SI 32768
SF 400.1300097 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



5.465
5.346
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5.261
5.228
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4.422
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4.379
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4.158
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3.155
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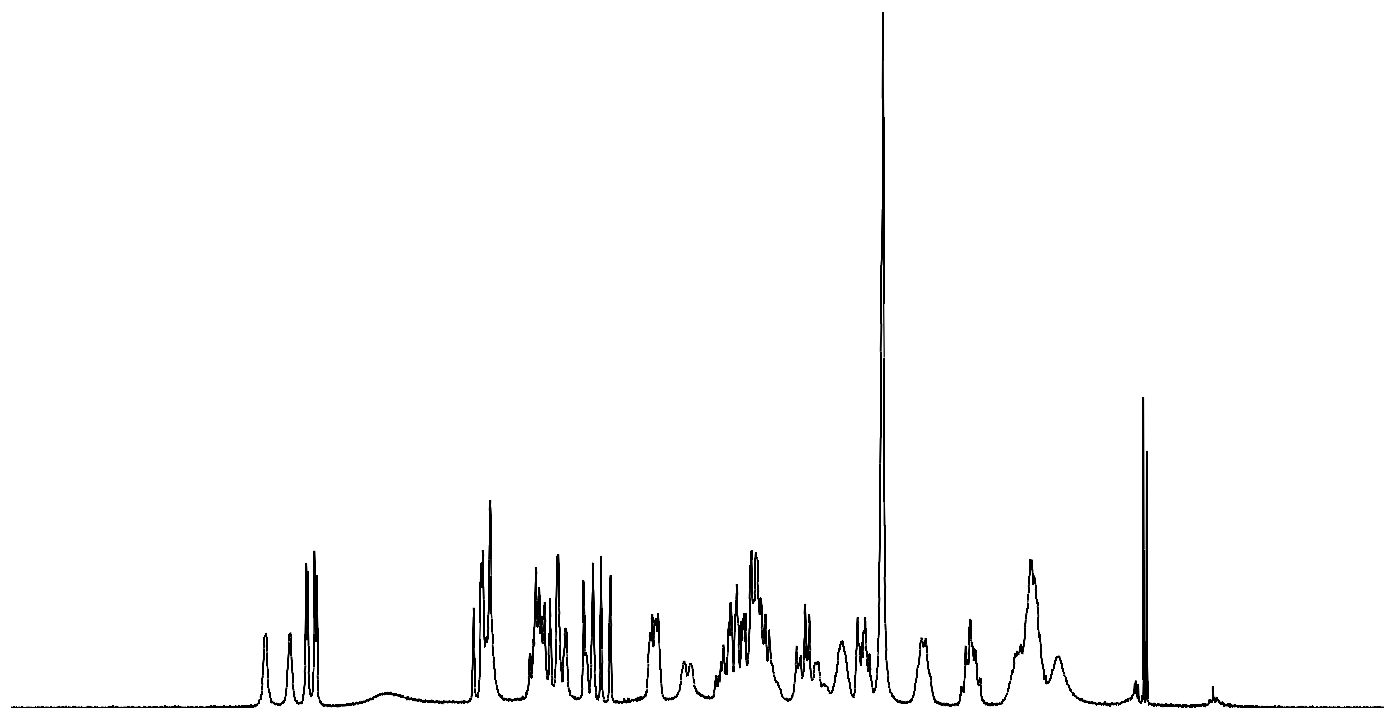
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20210720
Time_ 10.50 h
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PROBHD Z104450_0348 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 128
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 3.9845889 sec
RG 80.6
DW 60.800 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324710 MHz
NUC1 1H
P0 4.95 usec
P1 14.86 usec
PLW1 9.92000008 W

F2 - Processing parameters

SI 32768
SF 400.1300097 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

1.0229
1.0554
0.9950
6.1257
3.5856
5.1695
6.8289
1.1147
1.1053
3.2829

Qualitative Analysis Report

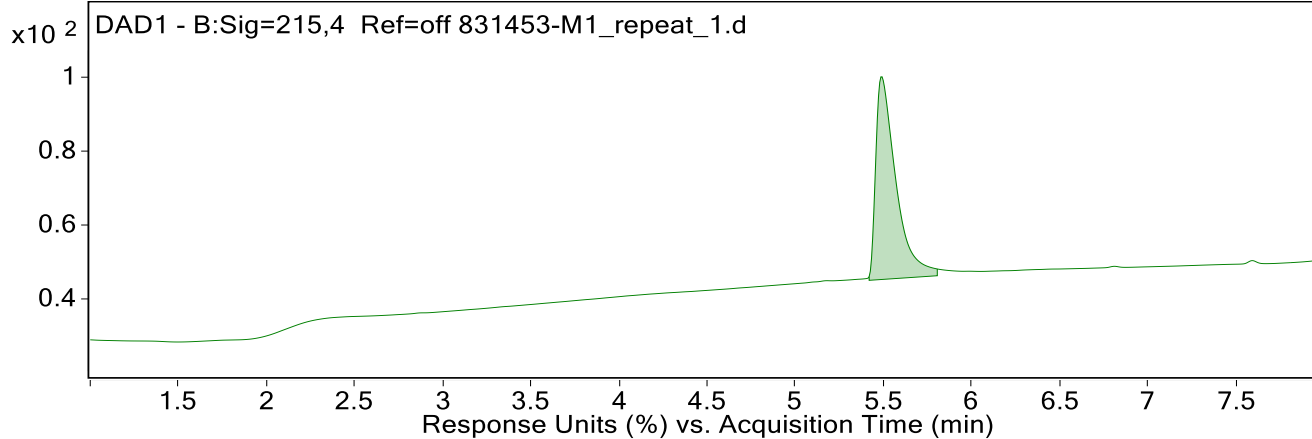
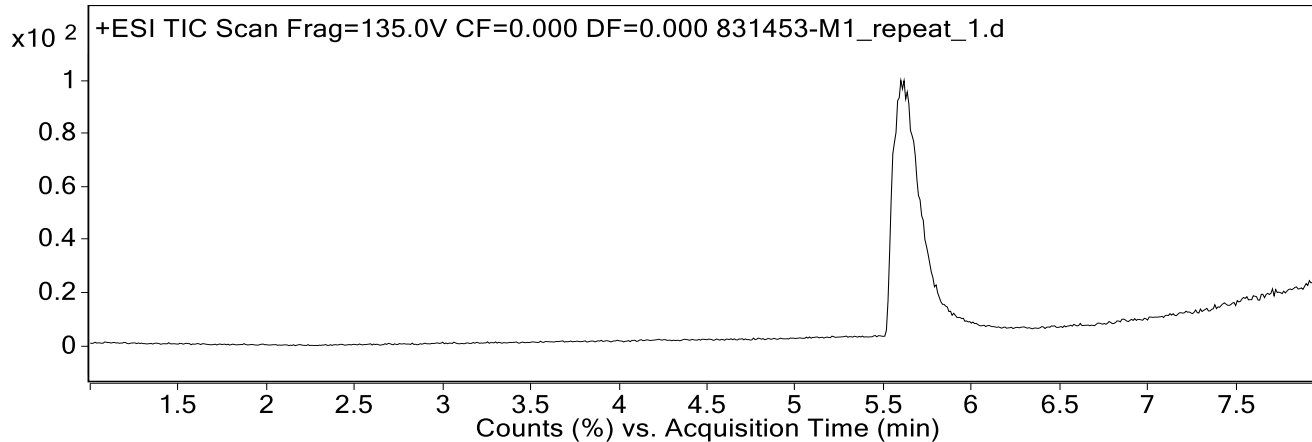
Data Filename 831453-M1_repeat_1.d **Sample Name** 831453-M1_repeat
Sample Type Sample **Position** P1-A2
Instrument Name Instrument 1 **User Name**
Acq Method Leidos_10min_pos.m **Acquired Time** 7/20/2021 10:22:11 AM
IRM Calibration Status Not Applicable **DA Method** uv integration test.m
Comment

Sample Group
Stream Name LC 1

Info.
Acquisition SW 6400 Series Triple
Version Quadrupole B.08.00 (B8023.0)

User Chromatograms

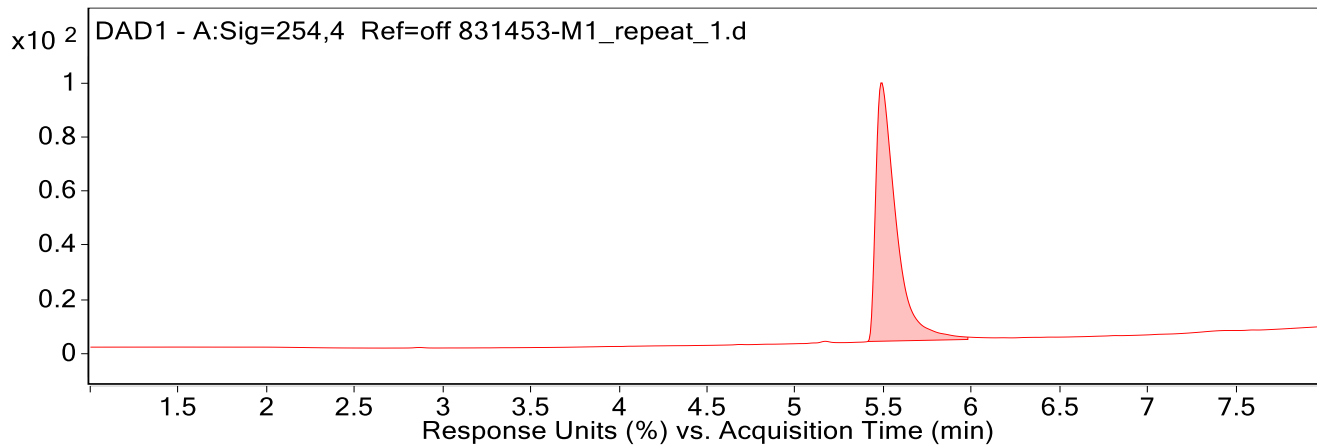
Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area Sum %
1	5.420	5.493	5.807	478.6	3816.9	100.0

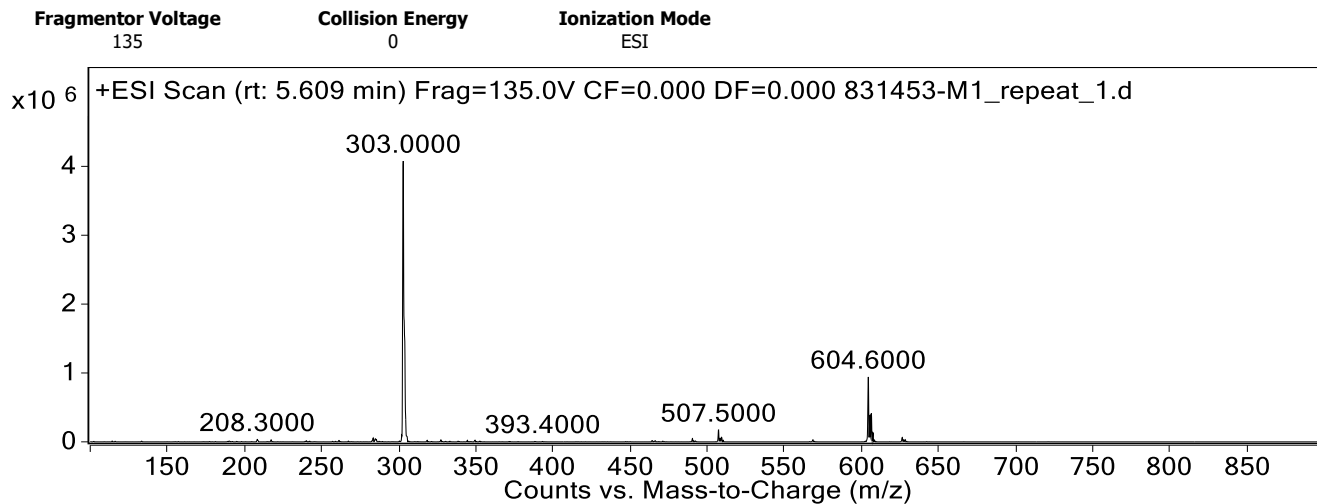
Qualitative Analysis Report



Integration Peak List

Peak	Start	RT	End	Height	Area	Area Sum %
1	5.412	5.493	5.980	158.6	1269.6	100.0

User Spectra



Peak List

m/z	z	Abund
283.5	2	56650
303.0		4066701
507.5		172290
508.6		53168
509.5	1	62958
604.6		939958
605.7		381100
606.6	1	410869
607.6	1	133200
626.6	1	62768

--- End Of Report ---