

NAME NSC-804520-M1
 EXPNO 1
 PROCNO 1
 Date_ 20180320
 Time 14.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 203
 DW 60.800 usec
 DE 6.50 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.30 usec
 PL1 0.00 dB
 PL1W 9.92195129 W
 SFO1 400.1324710 MHz
 SI 32768
 SF 400.1300031 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

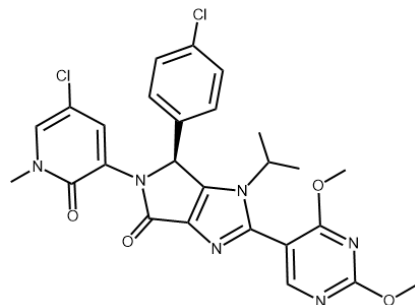
8.493
 7.933
 7.926
 7.514
 7.507
 7.439
 7.436
 7.418
 7.337
 7.316
 6.717

3.981
 3.935
 3.436
 3.329

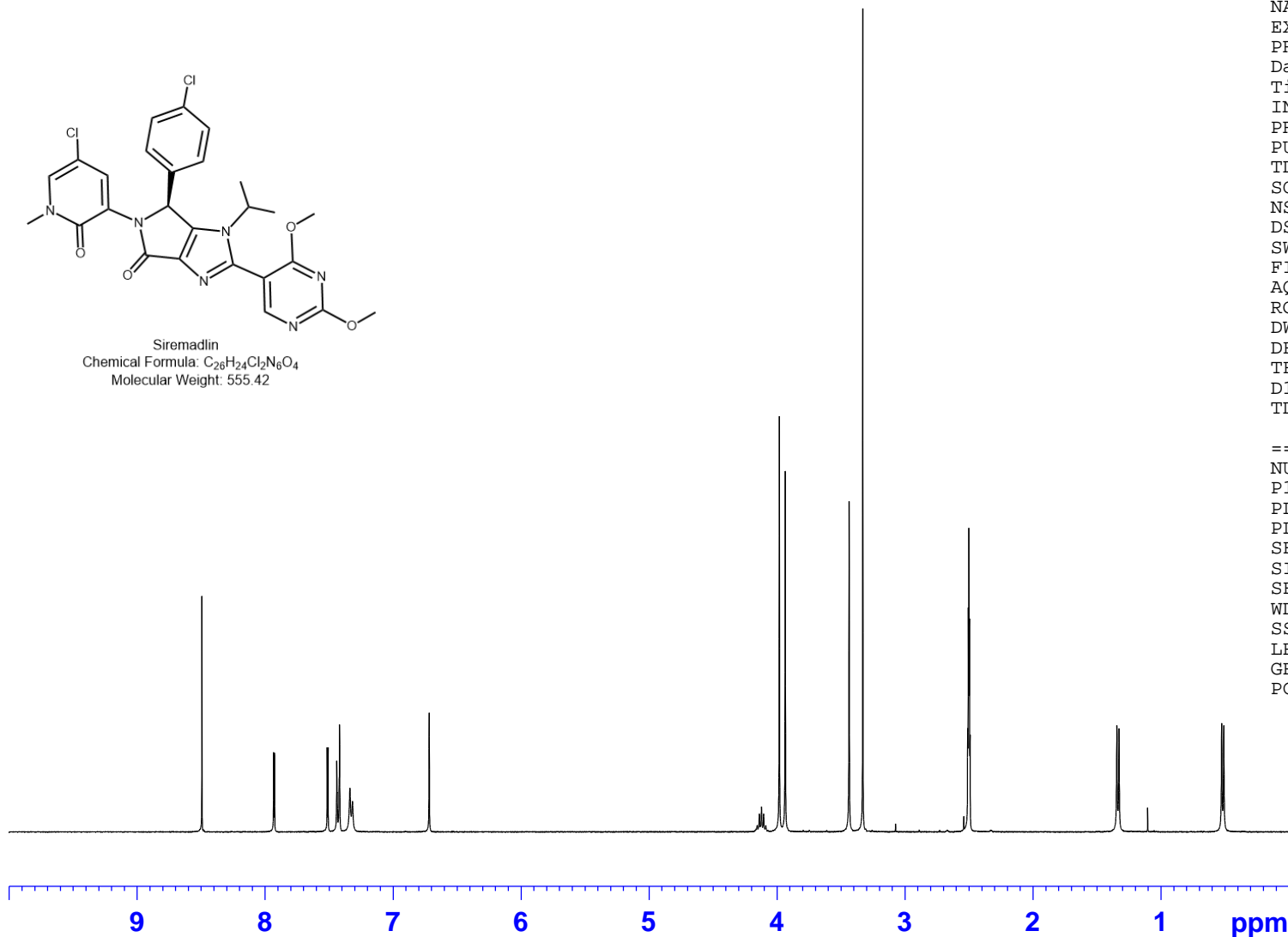
2.509
 2.505
 2.500
 2.495
 2.491

1.344
 1.327

0.525
 0.508



Siremadlin
 Chemical Formula: C₂₈H₂₄Cl₂N₆O₄
 Molecular Weight: 555.42



1.04

1.00

1.12

2.05

2.01

1.08

1.11

2.98

2.91

3.02

3.00

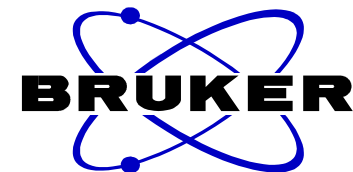
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— 8.493

< 7.933
< 7.926

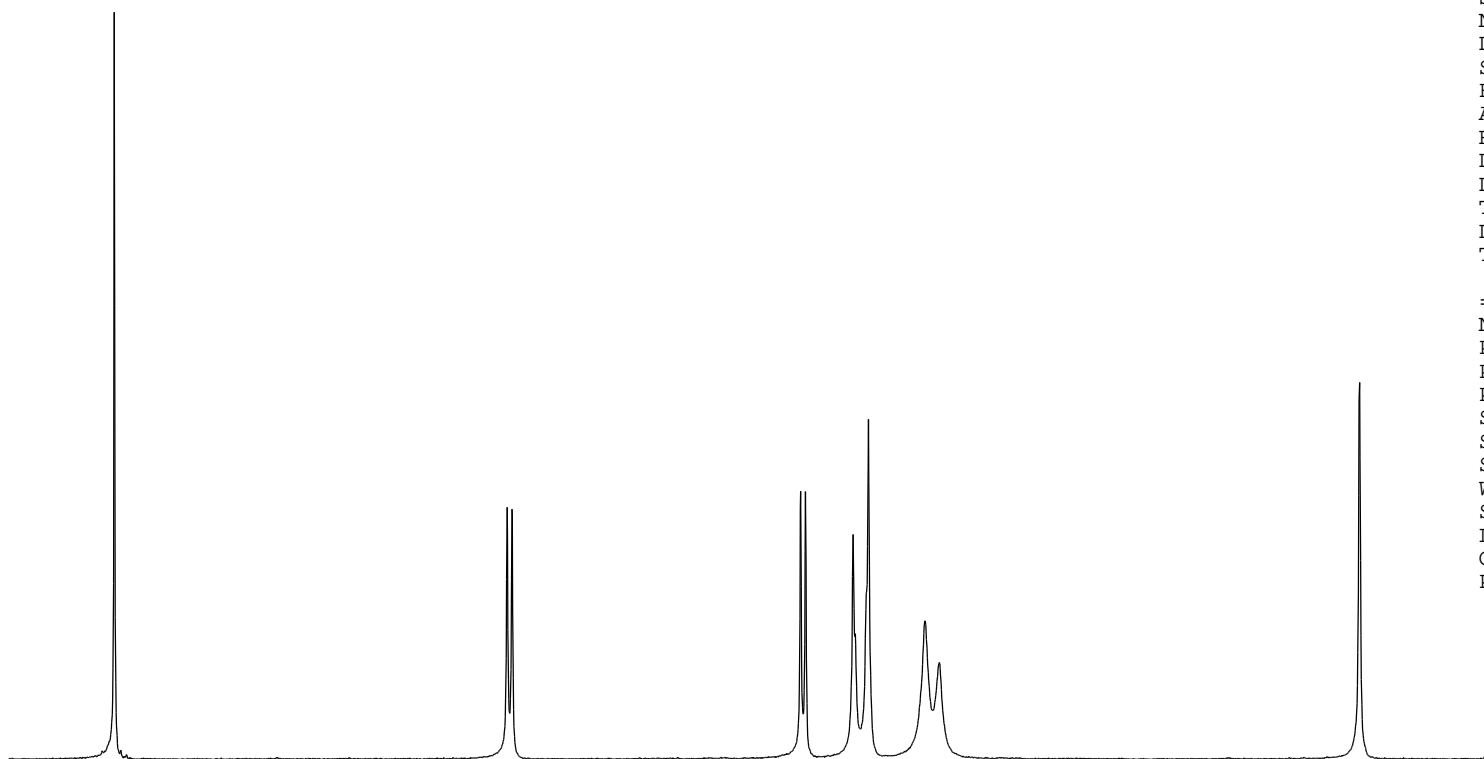
< 7.514
< 7.507
< 7.439
< 7.436
< 7.418
< 7.337
< 7.316

— 6.717



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8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm

1.04

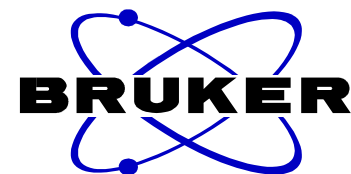
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1.12

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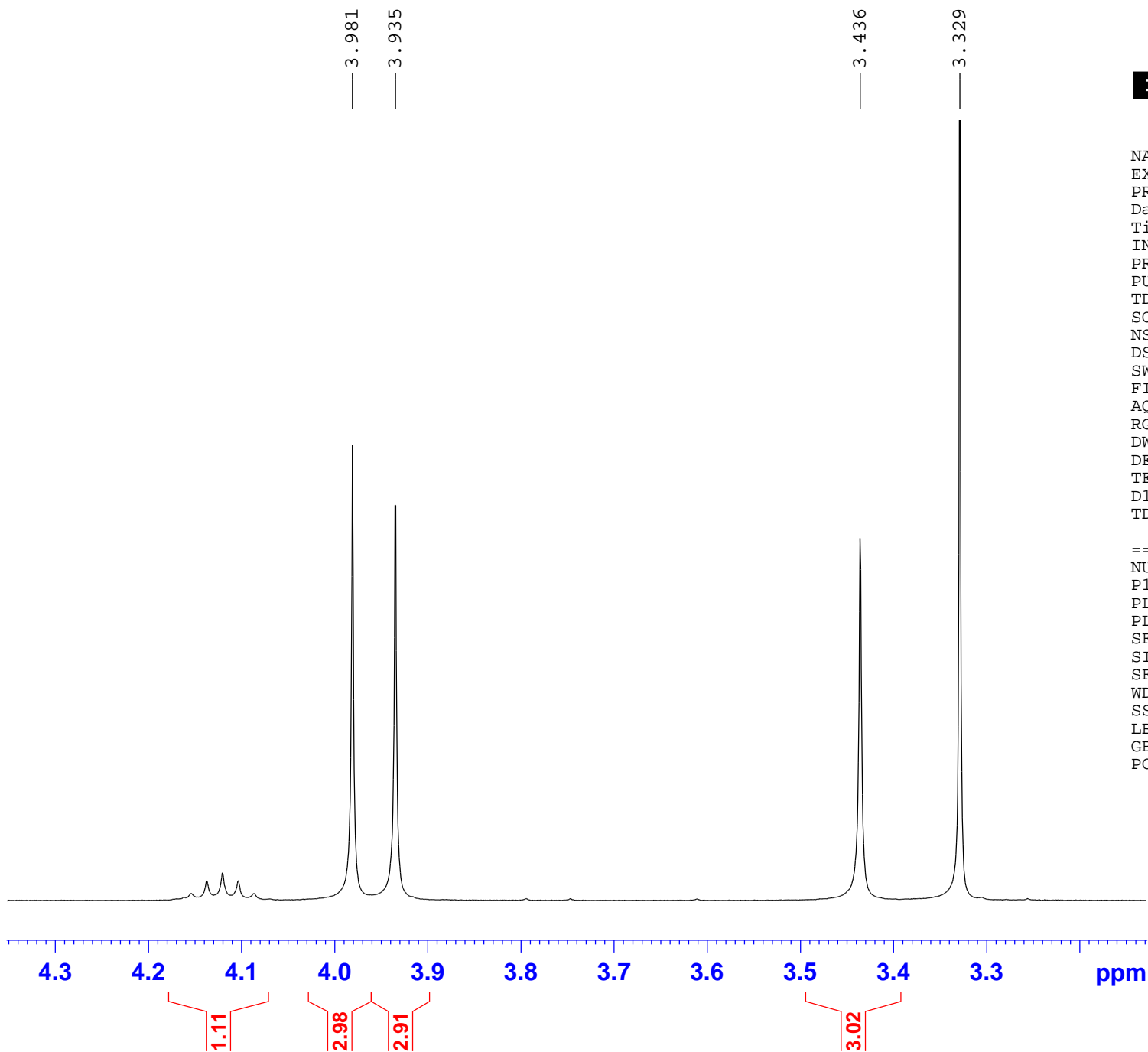
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1.08



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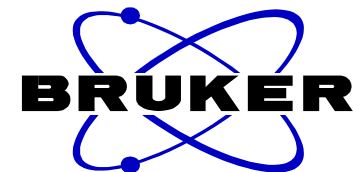
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2.509
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2.500
2.495
2.491

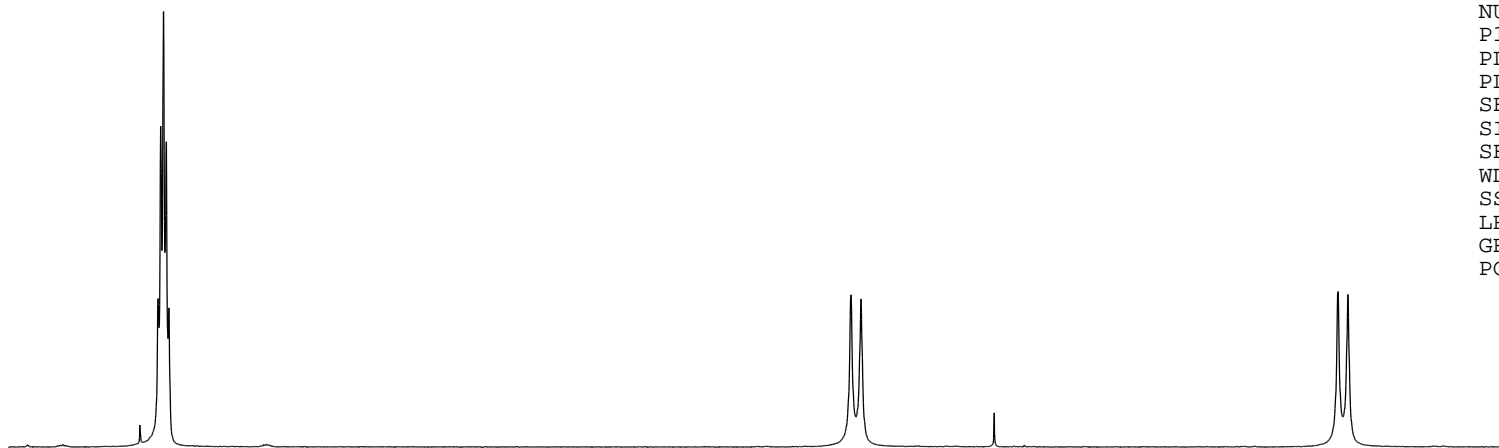
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1.327

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LB 0.00 Hz
GB 0
PC 1.00



2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 ppm

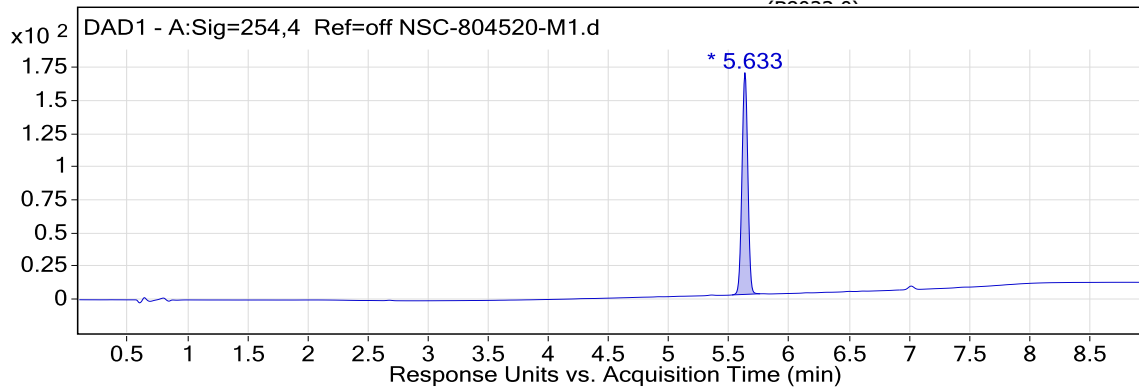
3.00

3.07

Qualitative Analysis Report

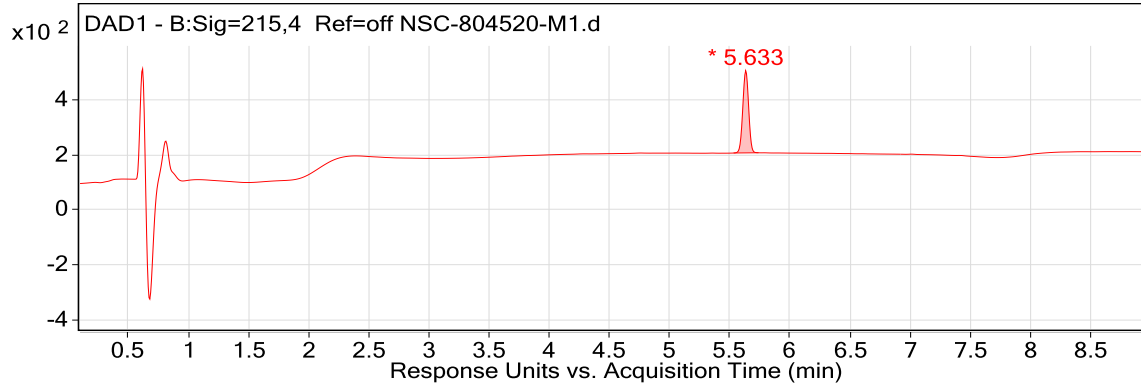
Data Filename	NSC-804520-M1.d	Sample Name	NSC-804520-M1
Sample Type	Sample	Position	P1-F5
Instrument Name	Instrument 1	User Name	
Acq Method	Leidos_10min_pos.m	Acquired Time	3/20/2018 11:36:44 AM
IRM Calibration Status	Not Applicable	DA Method	Default.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6400 Series Triple
		Version	Quadrupole B.08.00



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	5.527	5.633	5.76	167.7	567.18	100



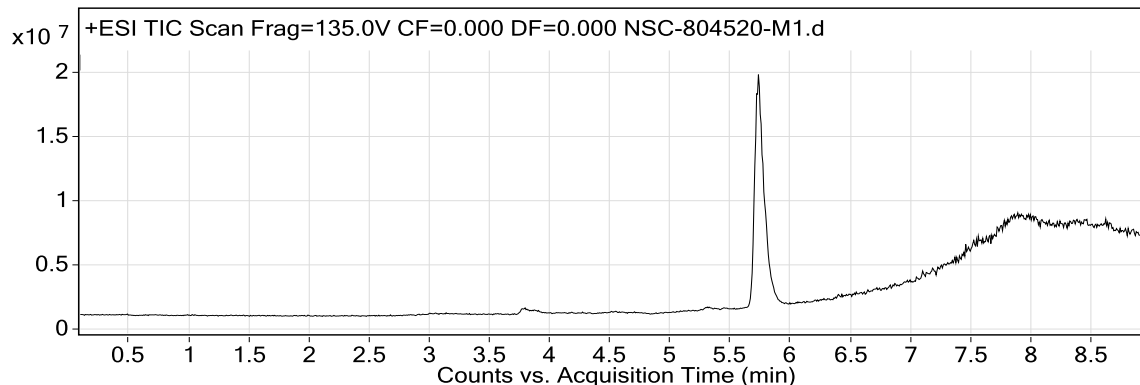
Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	5.533	5.633	5.74	300.2	1013.84	100

Qualitative Analysis Report

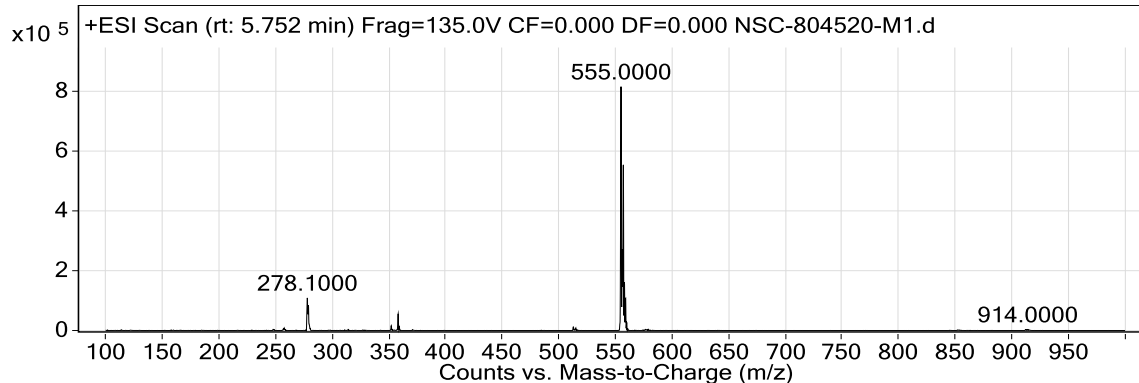
User Chromatograms

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



User Spectra

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



Peak List

m/z	z	Abund
278.1		108815.59
279.1		84803.16
352.2		15913.32
358.3	1	55501.14
555		814331.31
556.1		272078.63
557.1		553192.19
558		161596.53
559.1		107029.25
560	1	26779.38

--- End Of Report ---