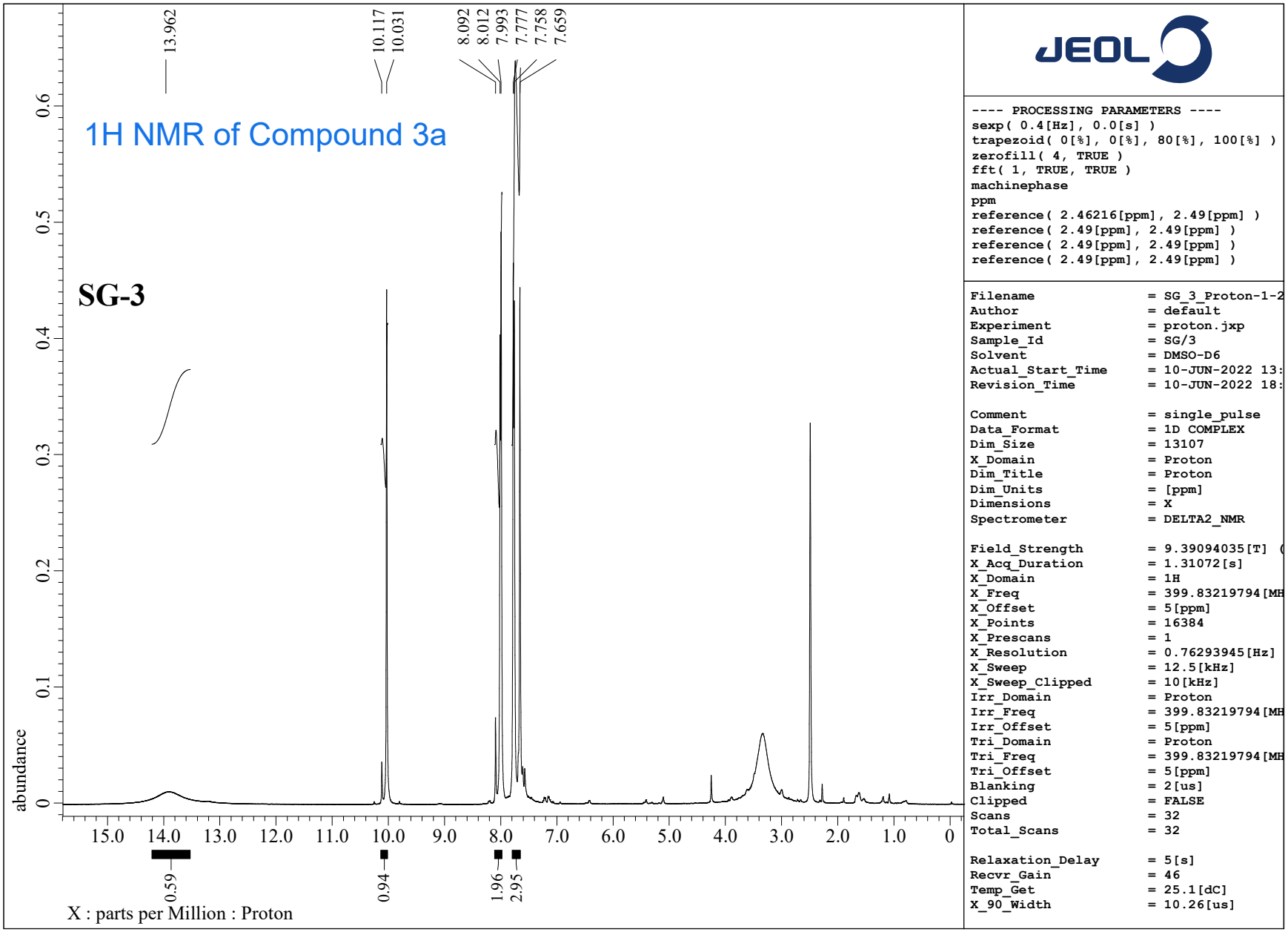
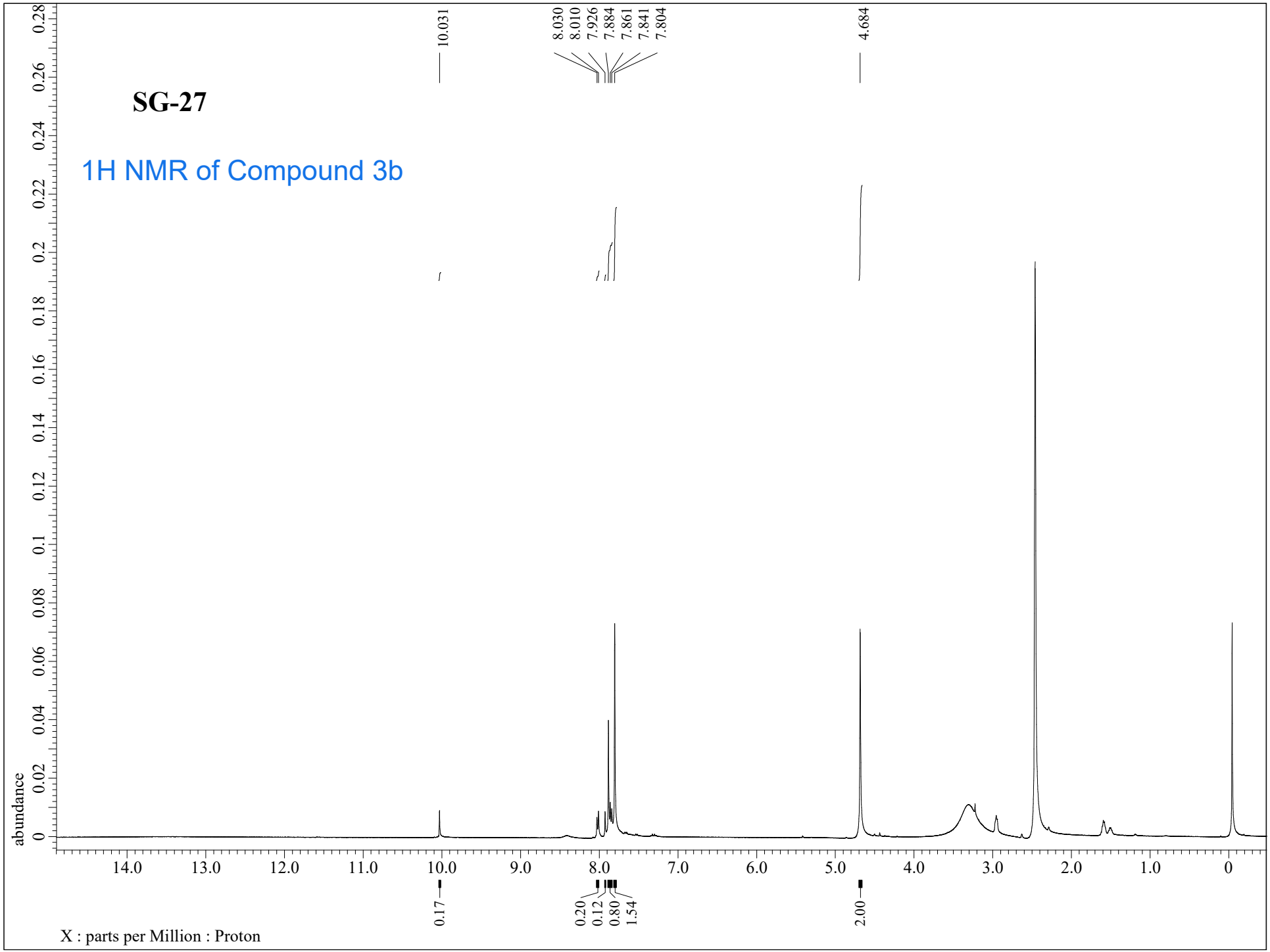
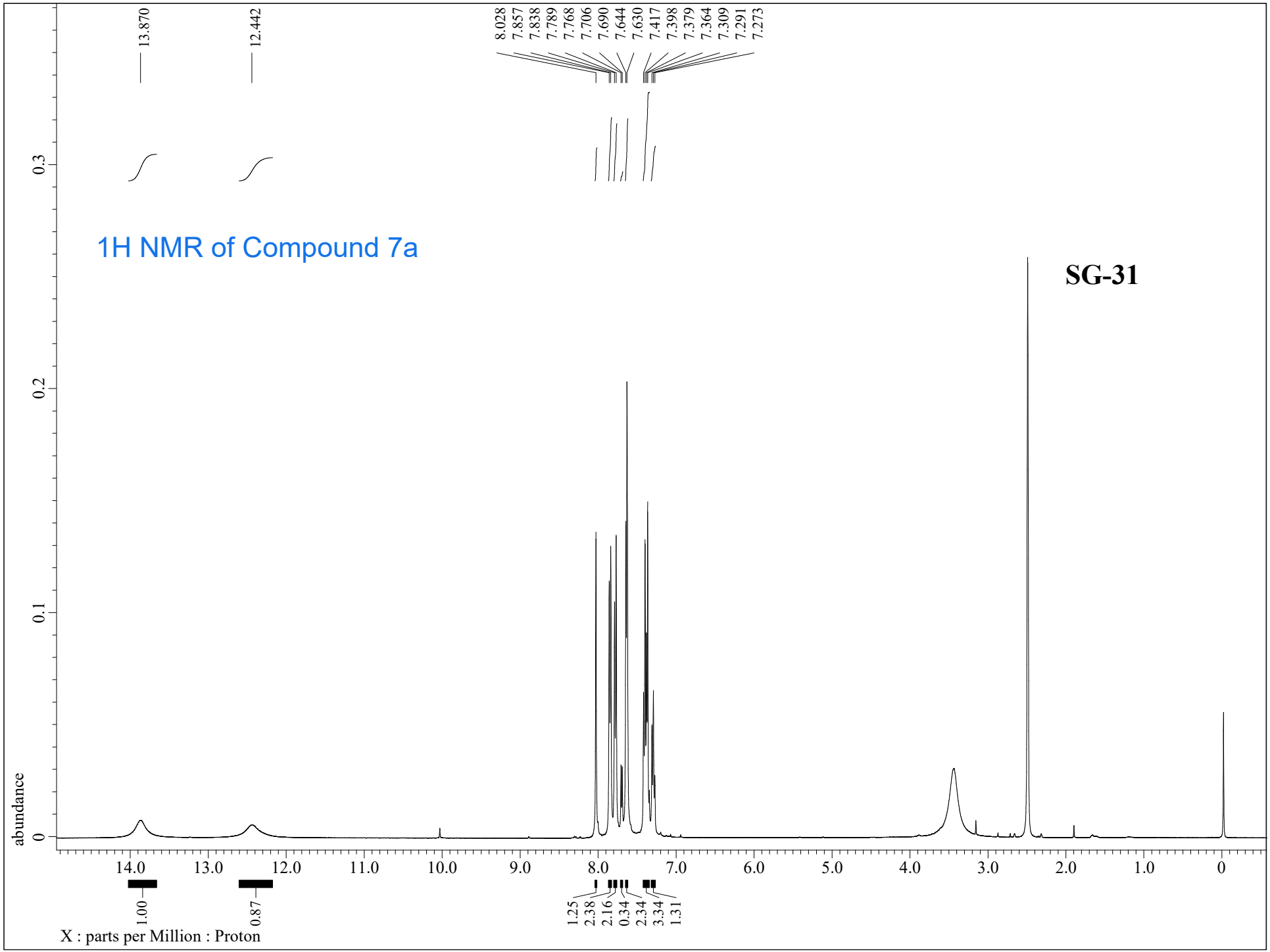
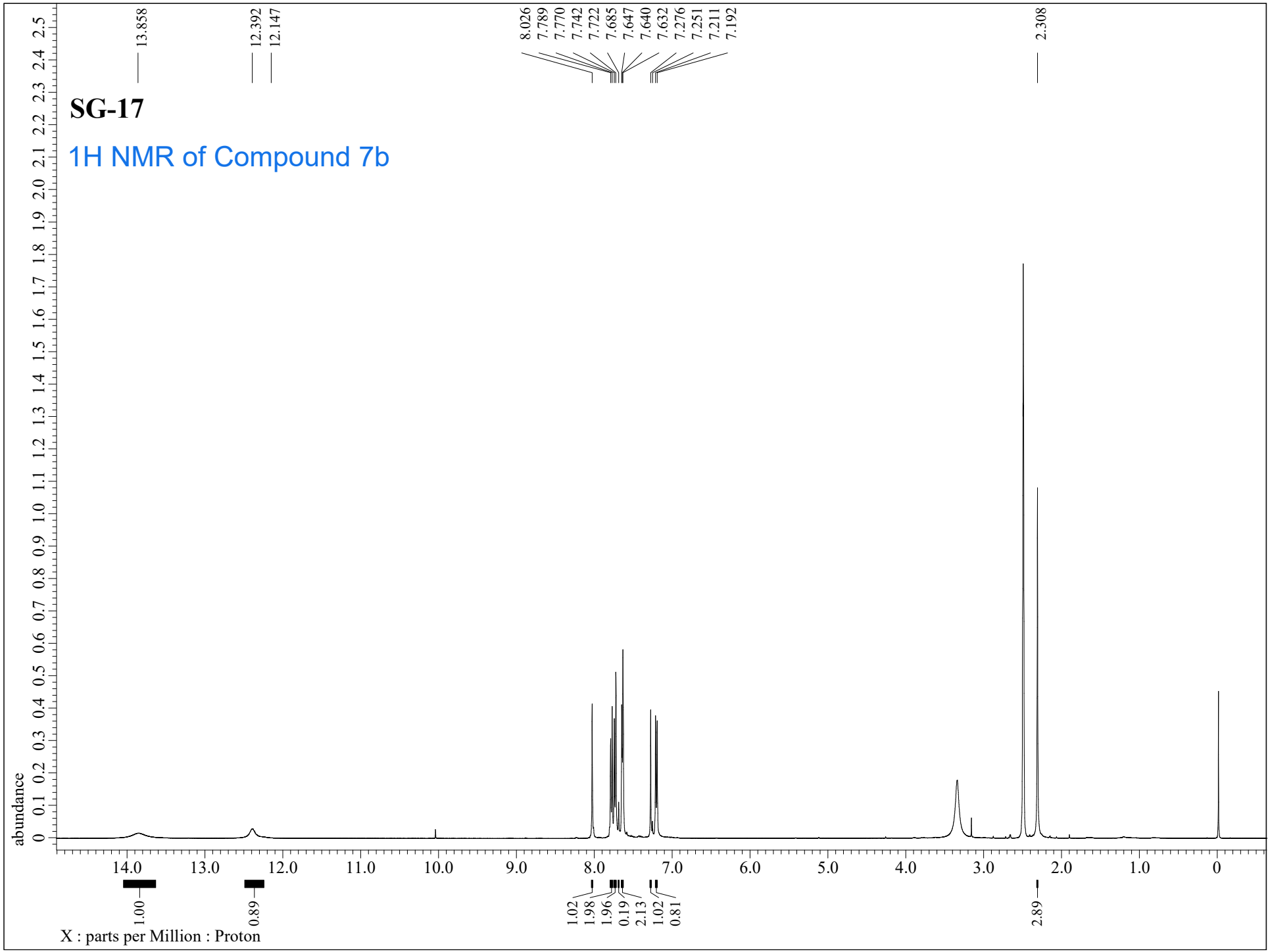


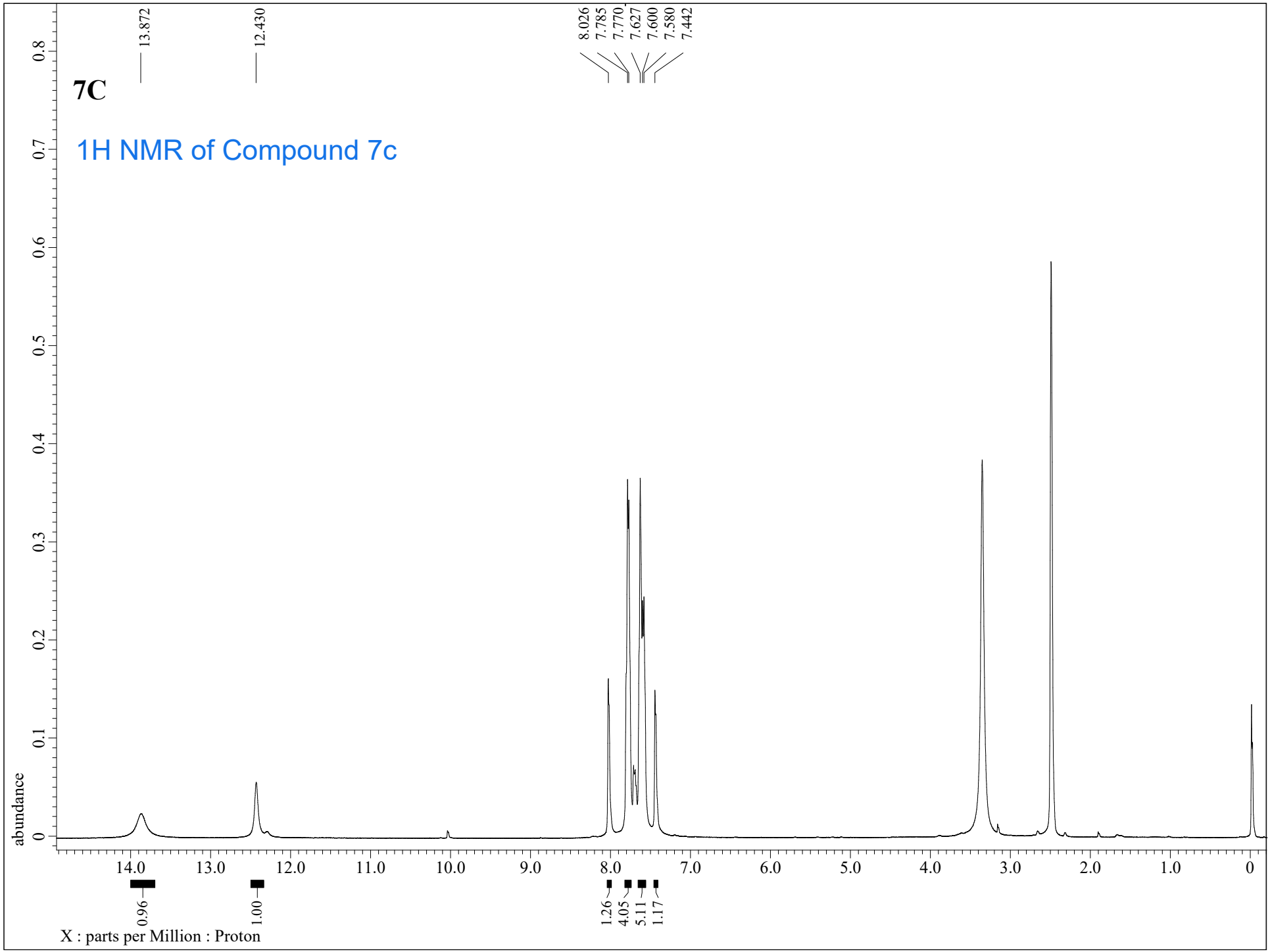
SG-27

1H NMR of Compound 3b




13.870
12.442
8.028
7.857
7.838
7.789
7.768
7.706
7.690
7.644
7.630
7.417
7.398
7.379
7.364
7.309
7.291
7.273
1H NMR of Compound 7a
SG-31
abundance
0
0.1
0.2
0.3
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
0.87
1.25
2.38
2.16
0.34
2.34
3.34
1.31
X : parts per Million : Proton


SG-17
1H NMR of Compound 7b
13.858
12.392
12.147
8.026
7.789
7.770
7.742
7.722
7.685
7.647
7.640
7.632
7.276
7.251
7.211
7.192
2.308
abundance
X : parts per Million : Proton
1.00
0.89
1.02
1.98
1.96
0.19
2.13
1.02
0.81
2.89

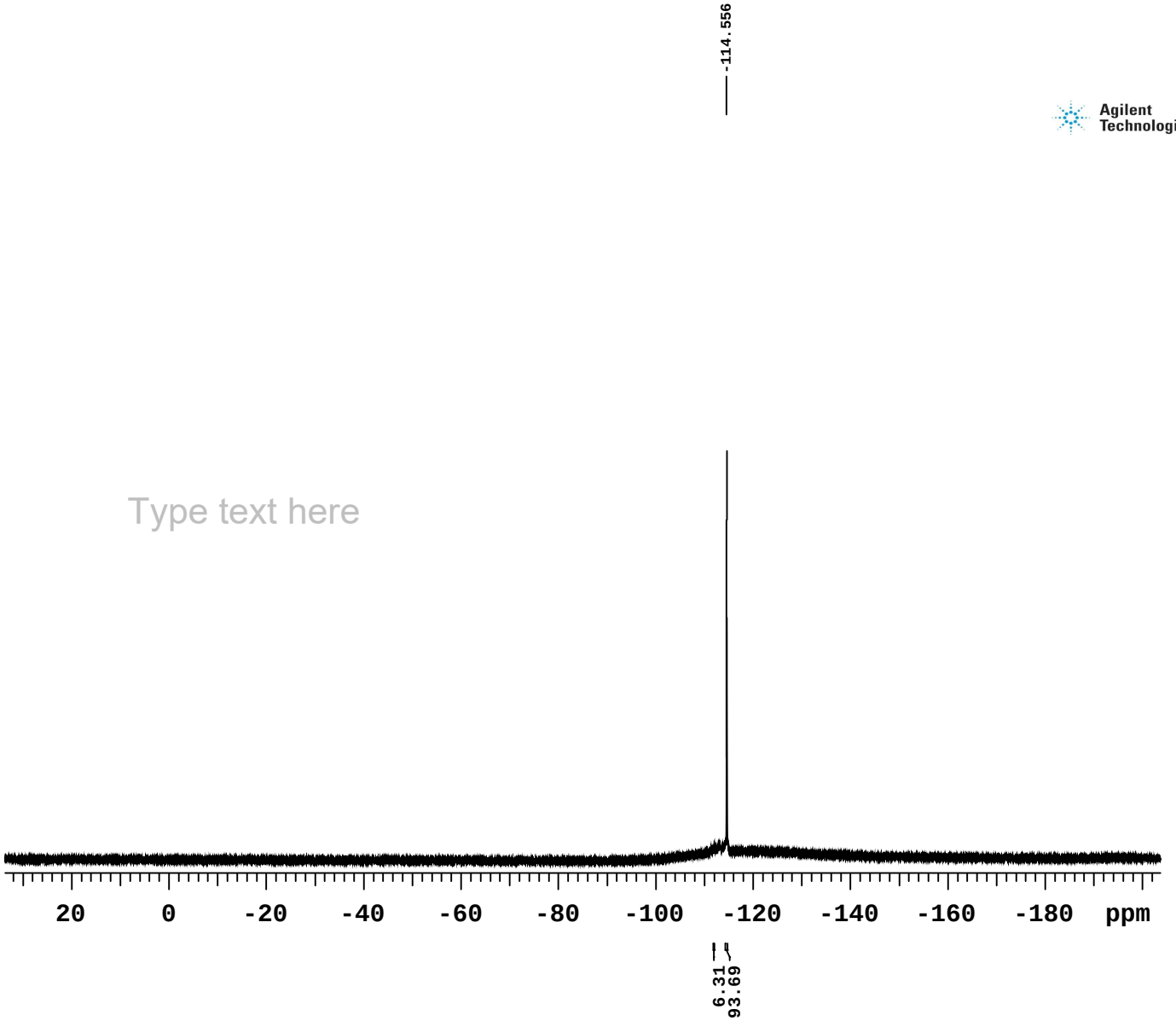

7C
1H NMR of Compound 7c
13.872
12.430
8.026
7.785
7.770
7.627
7.600
7.580
7.442
abundance
0.96
1.00
1.26
4.05
5.11
1.17
X : parts per Million : Proton

19F NMR of Compound 7c

SG-60

Sample Name:
SG-60
Data Collected on:
localhost.localdomain-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2024/Oct/20241023
Sample directory:
SG-60_20241023_01
FidFile: SG-60-FLUORINE_01

Pulse Sequence: FLUORINE (s2pul)
Solvent: dmso
Data collected on: Oct 23 2024



Type text here

Plotname: SG-60-FLUORINE_01_plot01--

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SG-60

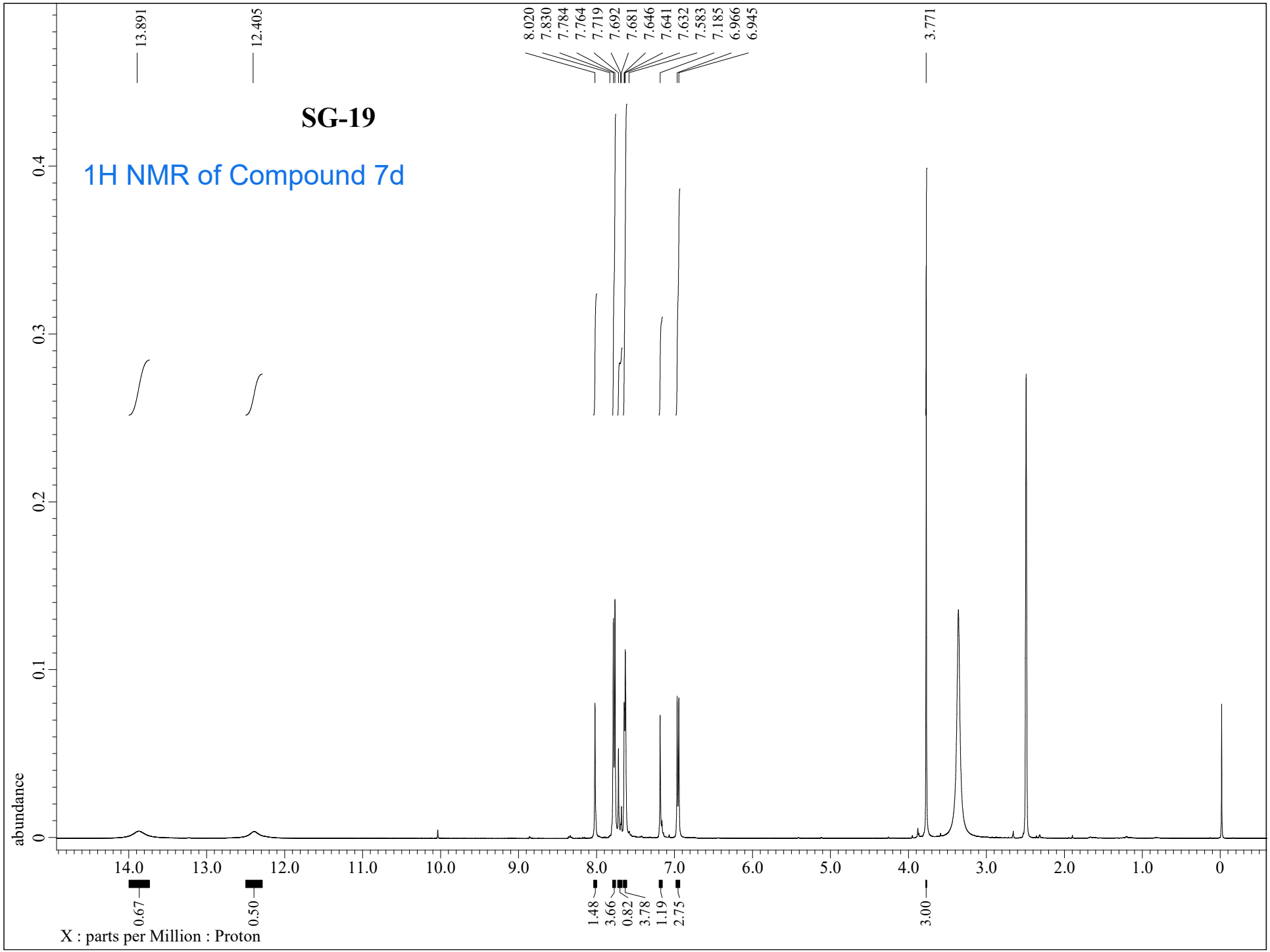
INTEGRAL VALUES

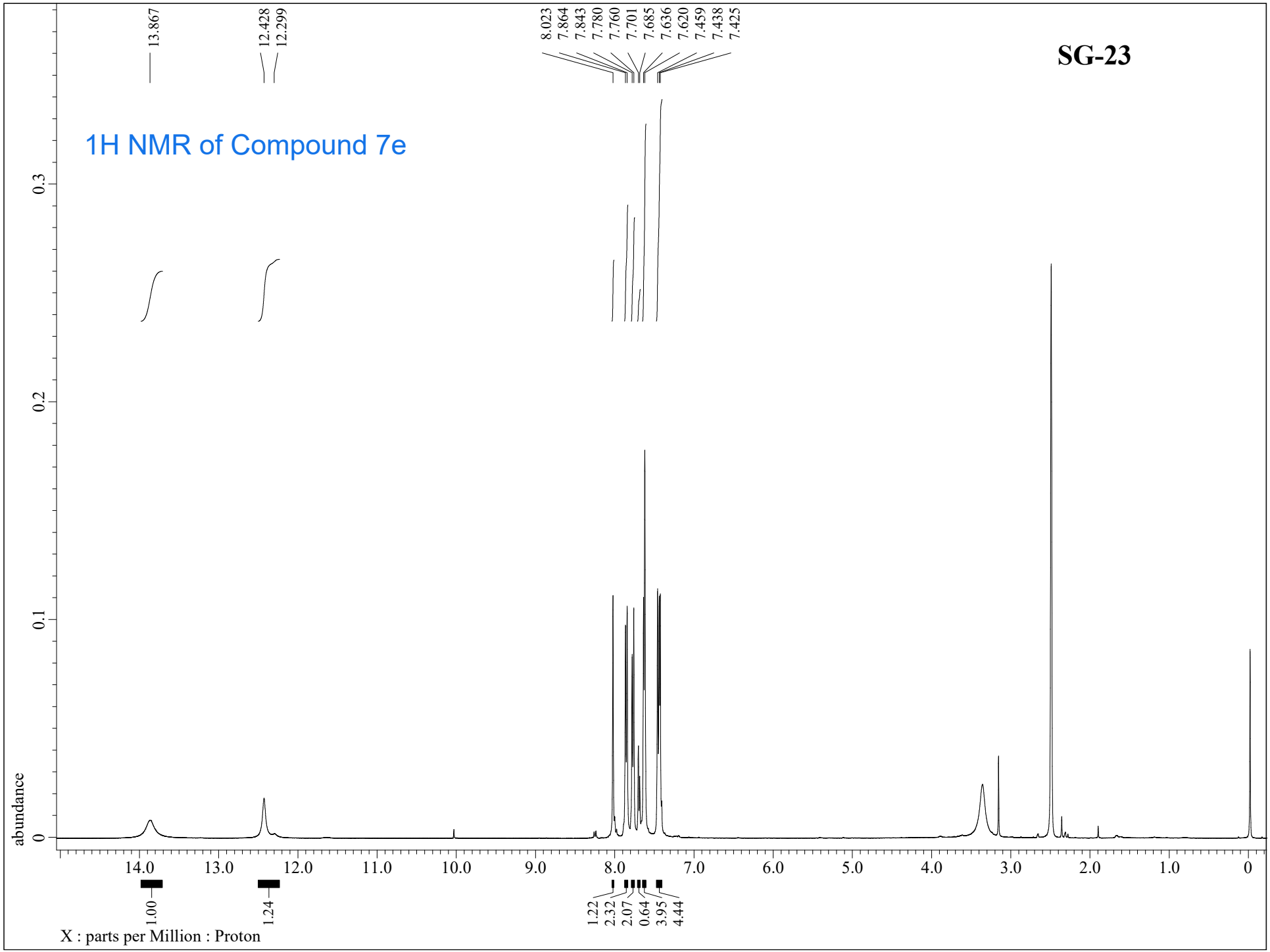
Integral	start(ppm)	end	value
1	33.656	-111.911	3.909
2	-111.911	-112.067	0.493
3	-112.067	-114.373	7.496
4	-114.373	-114.811	7.321
5	-114.811	-203.653	80.782

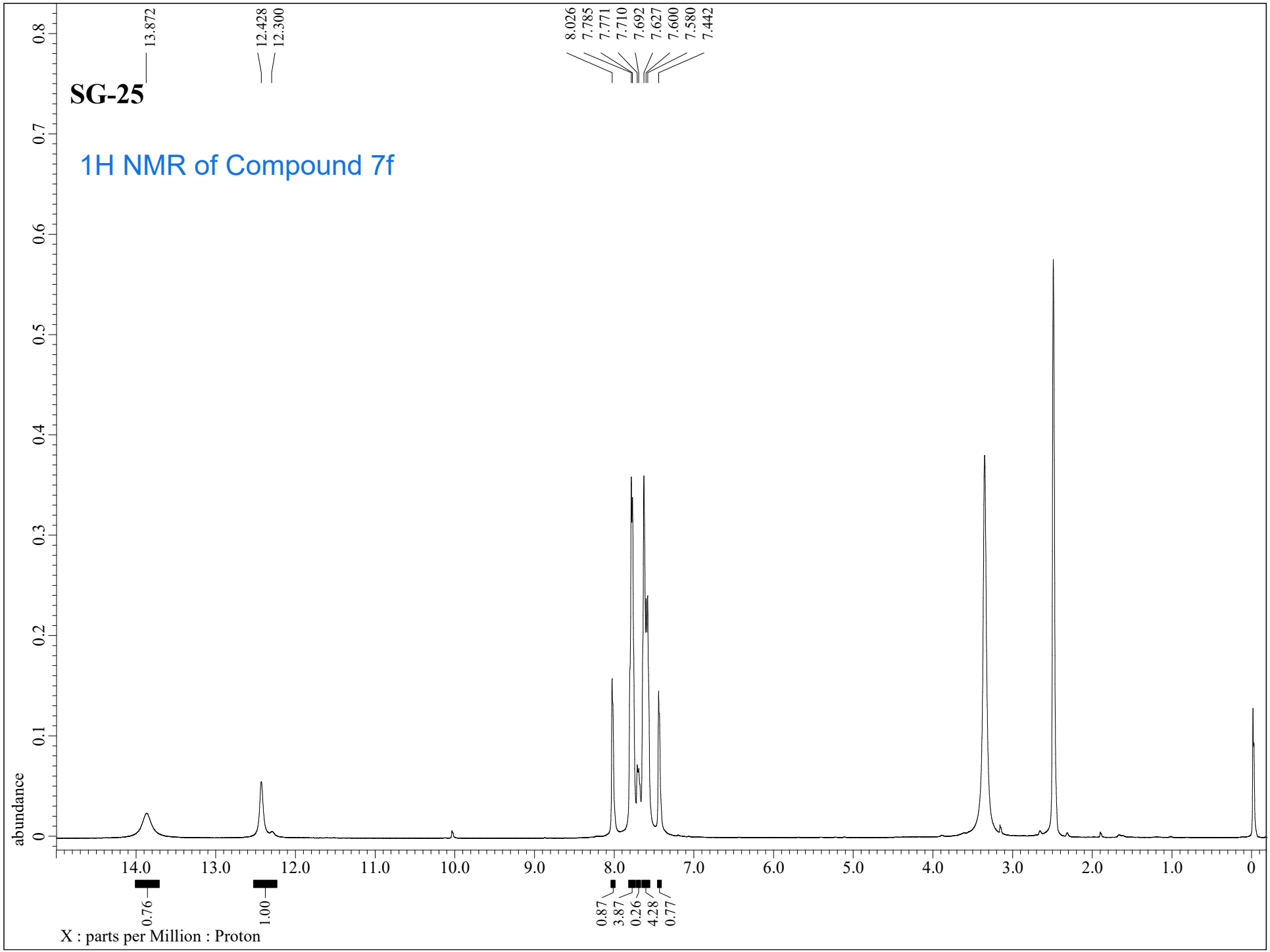
PEAK FREQUENCIES

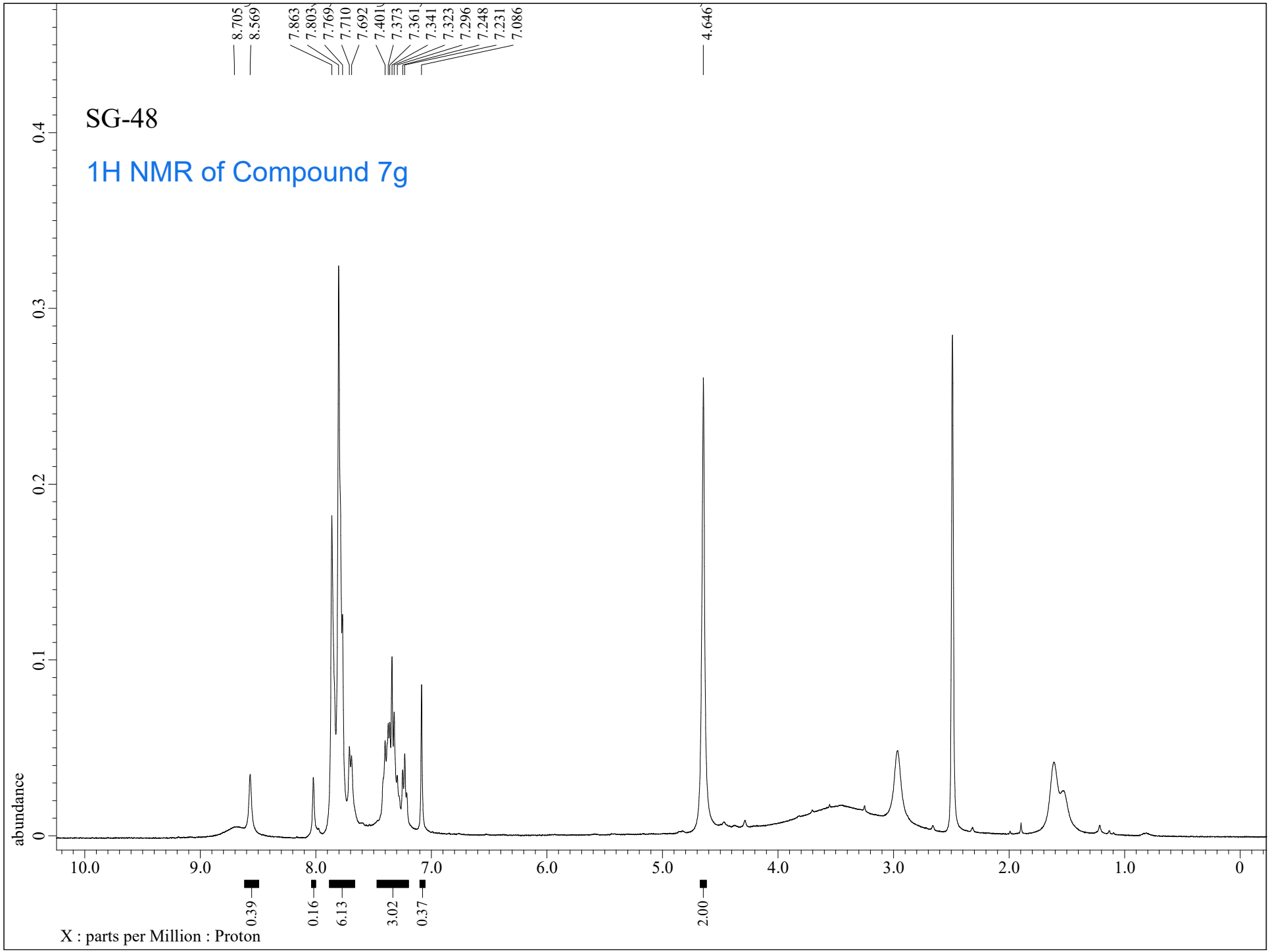
index	freq(ppm)	intensity
1	-114.556	37.6392

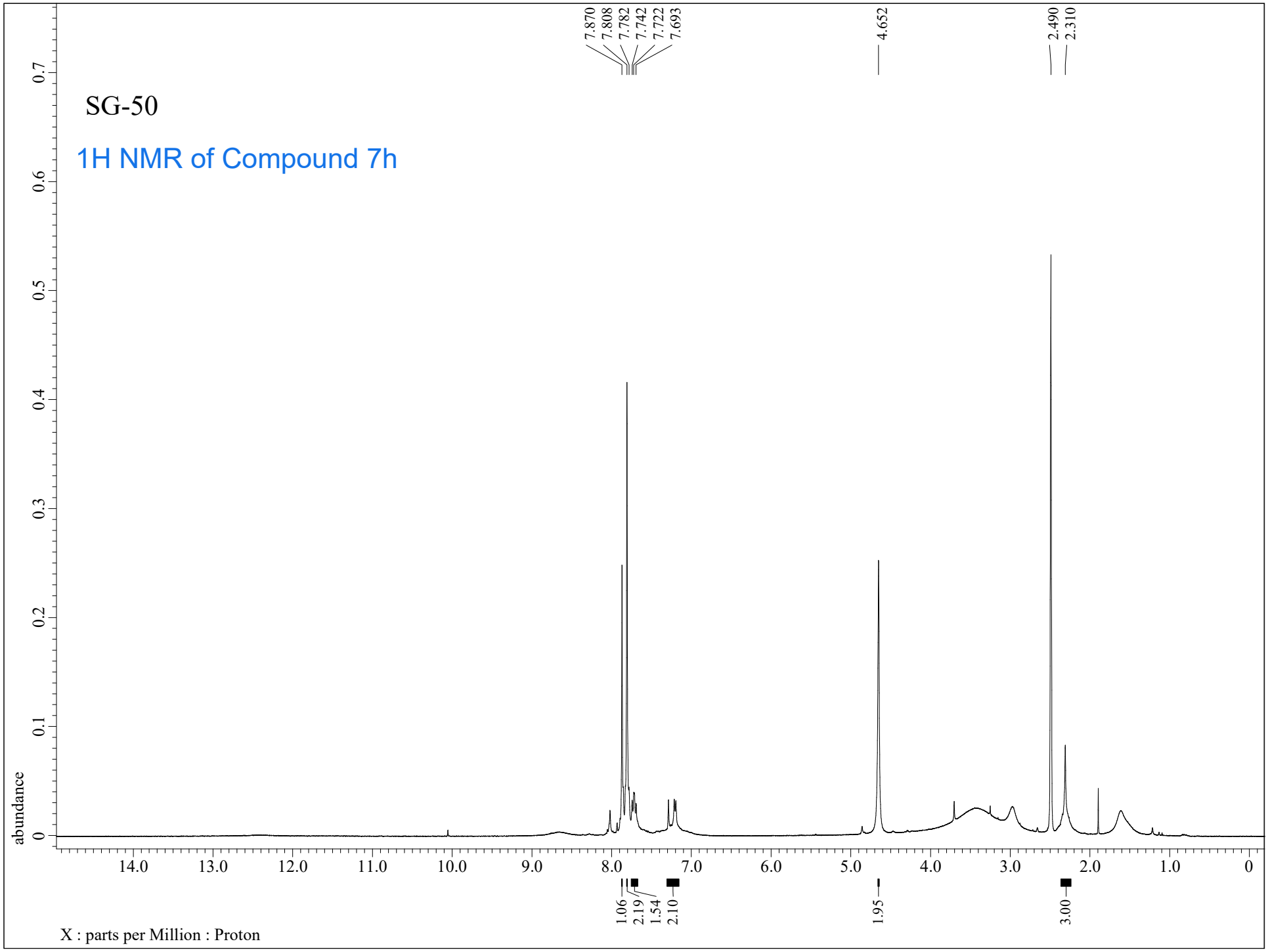
Plotname: SG-60-FLUORINE_01_plot02--


SG-19
1H NMR of Compound 7d
13.891
12.405
8.020
7.830
7.784
7.764
7.719
7.692
7.681
7.646
7.641
7.632
7.583
7.185
6.966
6.945
3.771
abundance
0
0.1
0.2
0.3
0.4
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.67
0.50
1.48
3.66
0.82
3.78
1.19
2.75
3.00
X : parts per Million : Proton


SG-23
1H NMR of Compound 7e
13.867
12.428
12.299
8.023
7.864
7.843
7.780
7.760
7.701
7.685
7.636
7.620
7.459
7.438
7.425
abundance
0
0.1
0.2
0.3
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
1.24
1.22
2.32
2.07
0.64
3.95
4.44
X : parts per Million : Proton

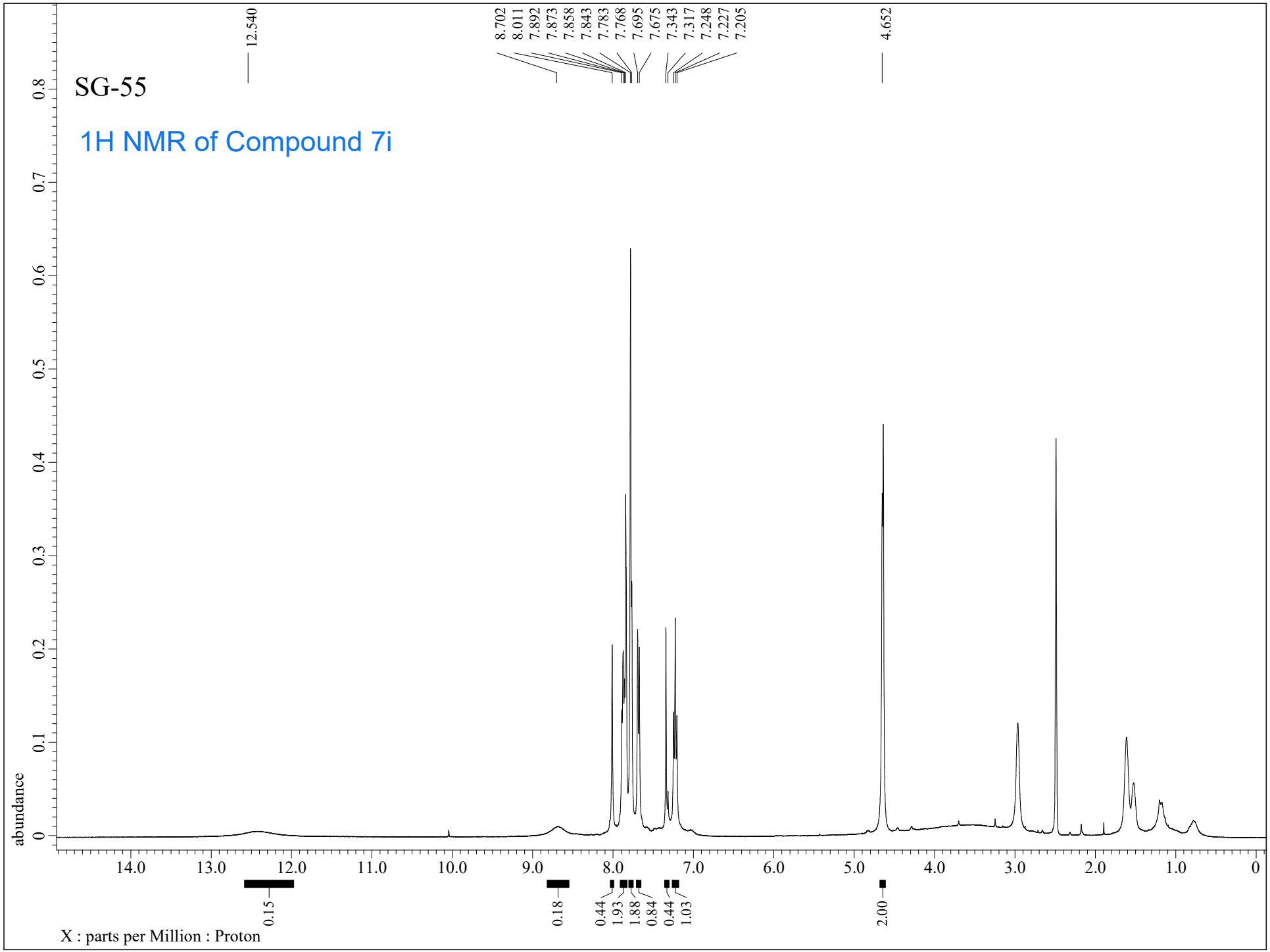

SG-25
1H NMR of Compound 7f
13.872
12.428
12.300
8.026
7.785
7.771
7.710
7.692
7.627
7.600
7.580
7.442
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.76
1.00
0.87
3.87
0.26
4.28
0.77
X : parts per Million : Proton


8.705
8.569
7.863
7.803
7.769
7.710
7.692
7.401
7.373
7.361
7.341
7.323
7.296
7.248
7.231
7.086
4.646
SG-48
1H NMR of Compound 7g
abundance
0.4
0.3
0.2
0.1
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.39
0.16
6.13
3.02
0.37
2.00
X : parts per Million : Proton


SG-50
1H NMR of Compound 7h
7.870
7.808
7.782
7.742
7.722
7.693
4.652
2.490
2.310
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.06
2.19
1.54
2.10
1.95
3.00
X : parts per Million : Proton

SG-55

1H NMR of Compound 7i

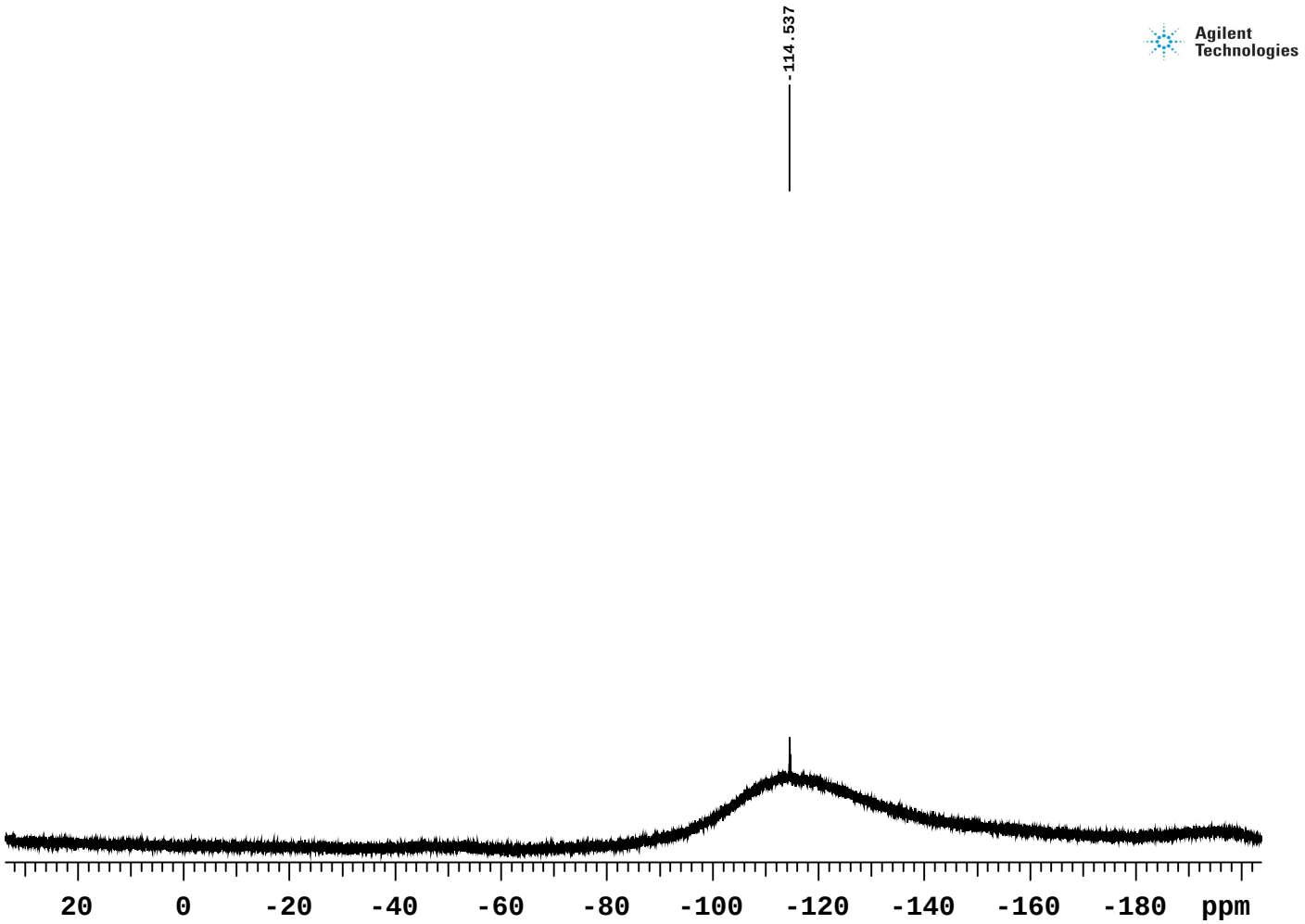


19F NMR of Compound 7i

SG-55

Sample Name:
SG-55
Data Collected on:
localhost.localdomain-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2024/Oct/20241023
Sample directory:
SG-55_20241023_01
FidFile: SG-55-FLUORINE_02

Pulse Sequence: FLUORINE (s2pul)
Solvent: dmso
Data collected on: Oct 23 2024



Plotname: SG-55-FLUORINE_02_plot01--

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SG-55

INTEGRAL VALUES

Integral	start(ppm)	end	value
1	33.656	-203.653	100.000

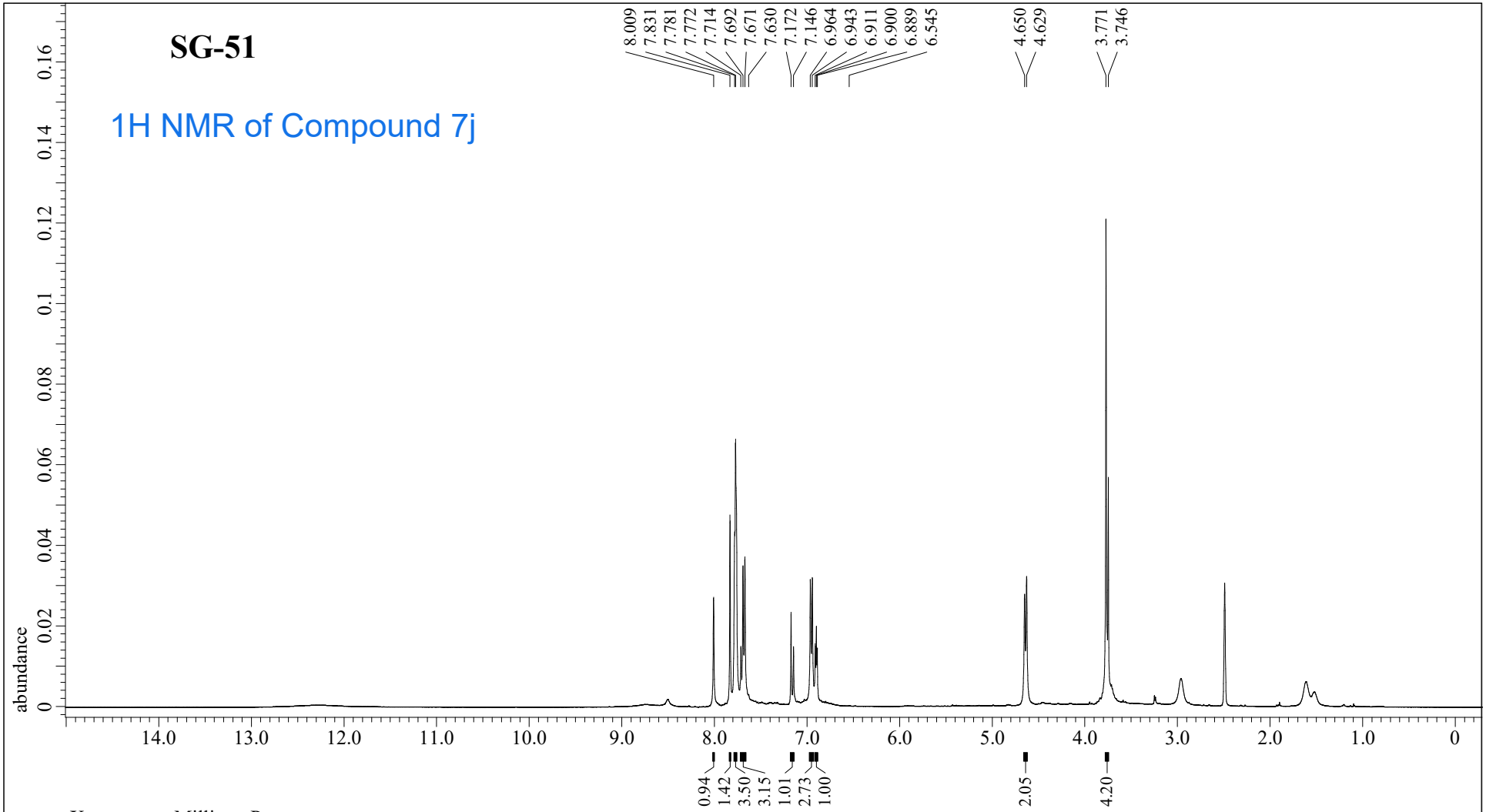
PEAK FREQUENCIES

index	freq(ppm)	intensity
1	-114.537	15.8254

Plotname: SG-55-FLUORINE_02_plot02--

SG-51

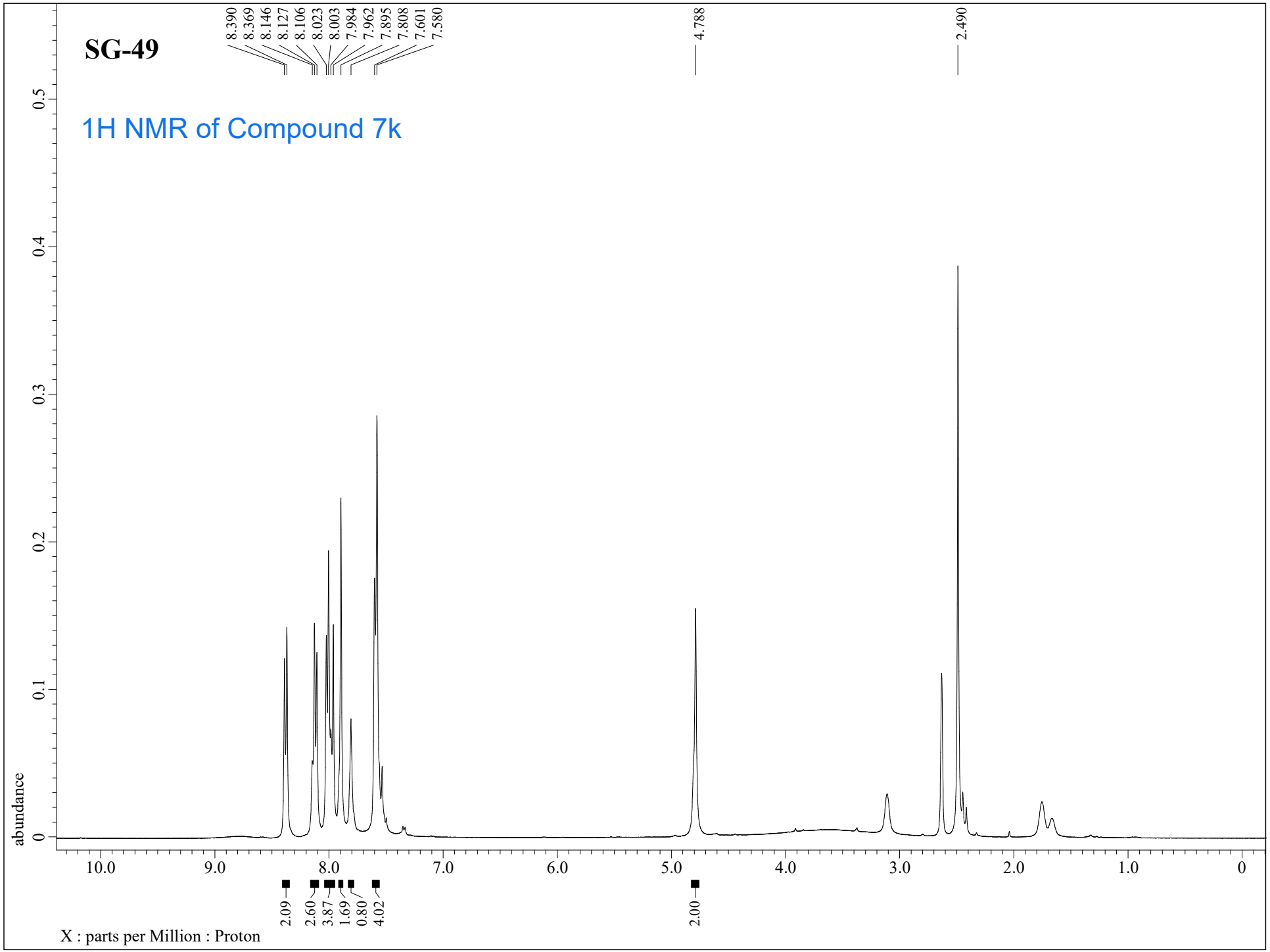
1H NMR of Compound 7j

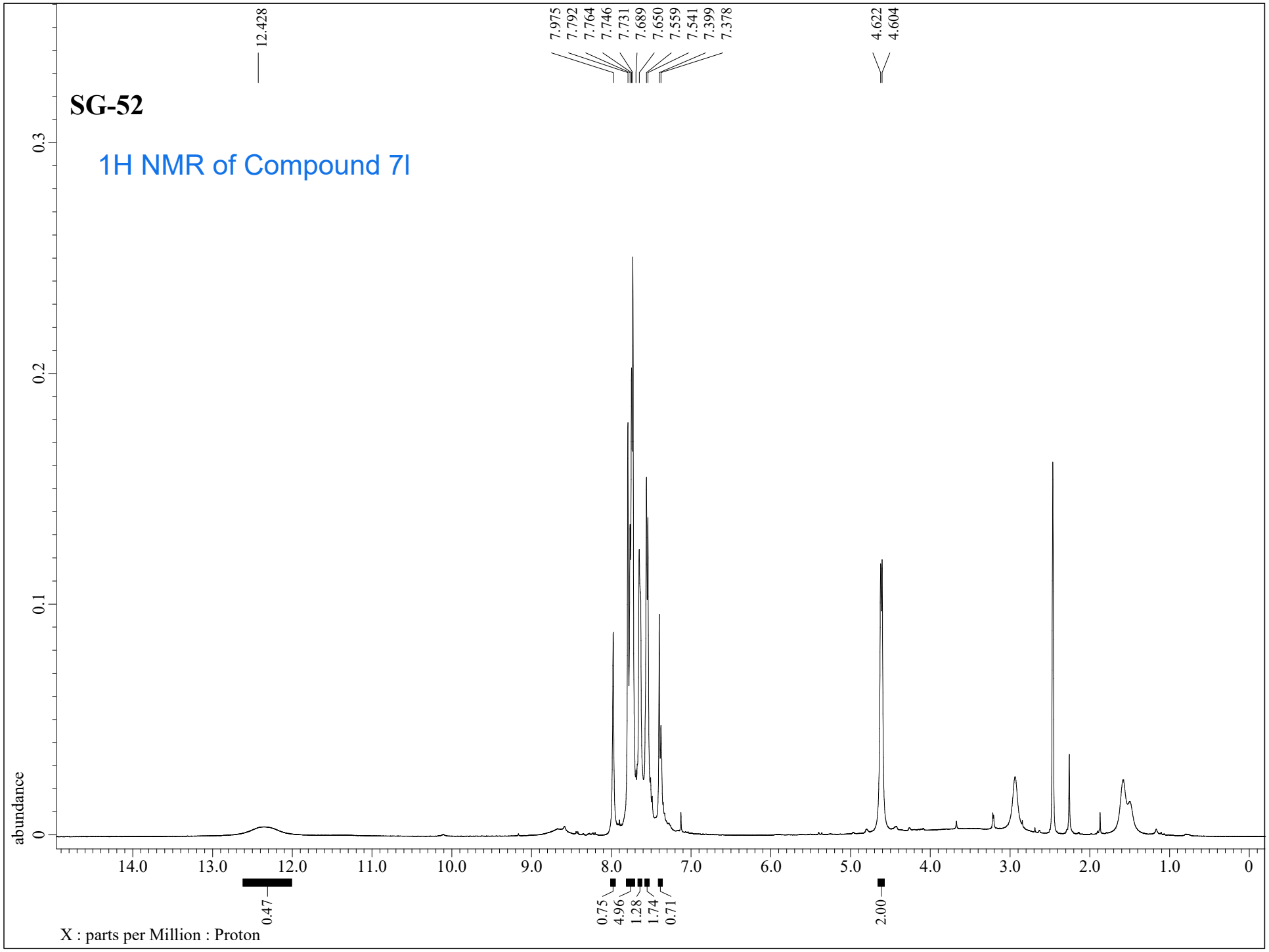


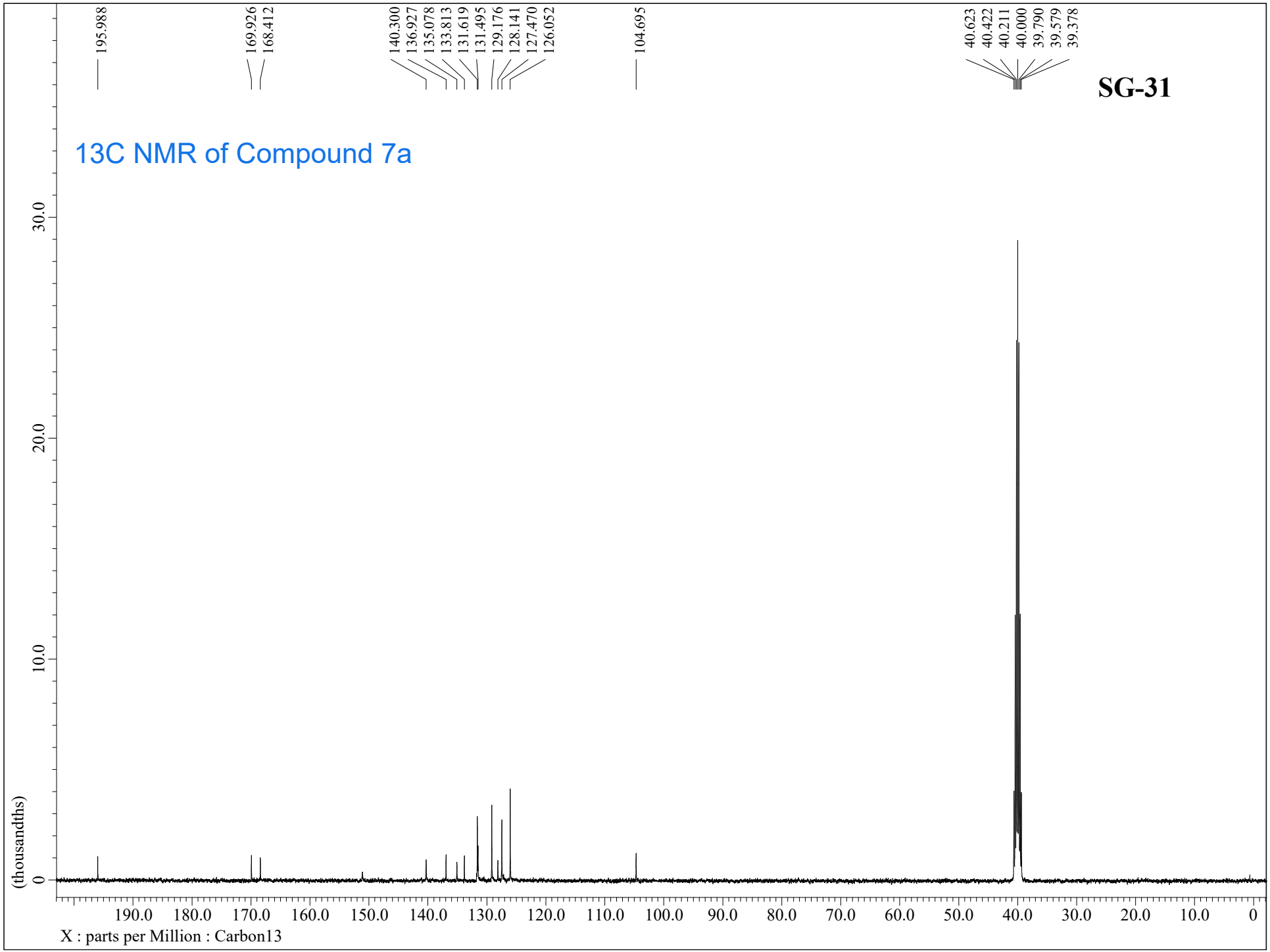
X : parts per Million : Proton

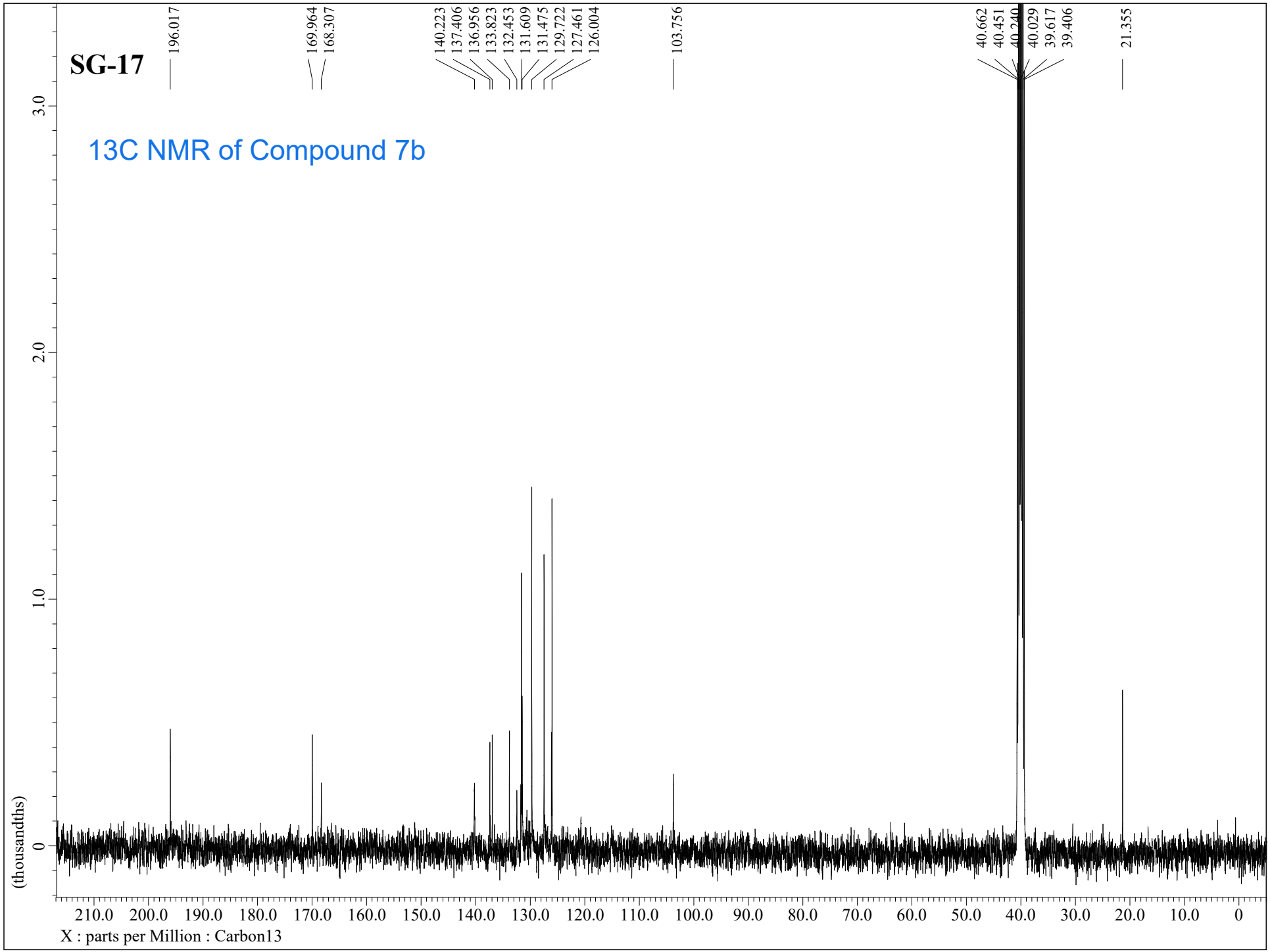
Filename	= SR_SG 51_Proton-1-2.j	Field_Strength	= 9.39094035[T] (400[MH	---- PROCESSING PARAMETERS ----	
Author	= default	X_Acq_Duration	= 1.63577856[s]	sexp(0.4[Hz], 0.0[s])	
Experiment	= proton.jxp	X_Domain	= 1H	trapezoid(0[%], 0[%], 80[%], 100[%])	
Sample_Id	= SR/SG 51	X_Freq	= 399.83219794[MHz]	zerofill(4)	
Solvent	= DMSO-D6	X_Offset	= 5[ppm]	fft(1, TRUE, TRUE)	
Creation_Time	= 8-MAY-2024 18:38:36	X_Points	= 16384	machinephase	
Revision_Time	= 10-MAY-2024 19:17:55	X_Prescans	= 1	ppm	
Current_Time	= 10-MAY-2024 19:18:10	X_Resolution	= 0.61132969[Hz]		
		X_Sweep	= 10.01602564[kHz]	Derived from: SR_SG 51_Proton-1-1.jdf	
Comment	= single_pulse	X_Sweep_Clipped	= 8.01282051[kHz]		
Data_Format	= 1D COMPLEX	Irr_Domain	= Proton		
Dim_Size	= 52429	Irr_Freq	= 399.83219794[MHz]		
Dim_Title	= Proton	Irr_Offset	= 5[ppm]		
Dim_Units	= [ppm]	Tri_Domain	= Proton		
Dimensions	= X	Tri_Freq	= 399.83219794[MHz]		
Spectrometer	= DELTA2_NMR	Tri_Offset	= 5[ppm]		
		Blanking	= 2[us]		

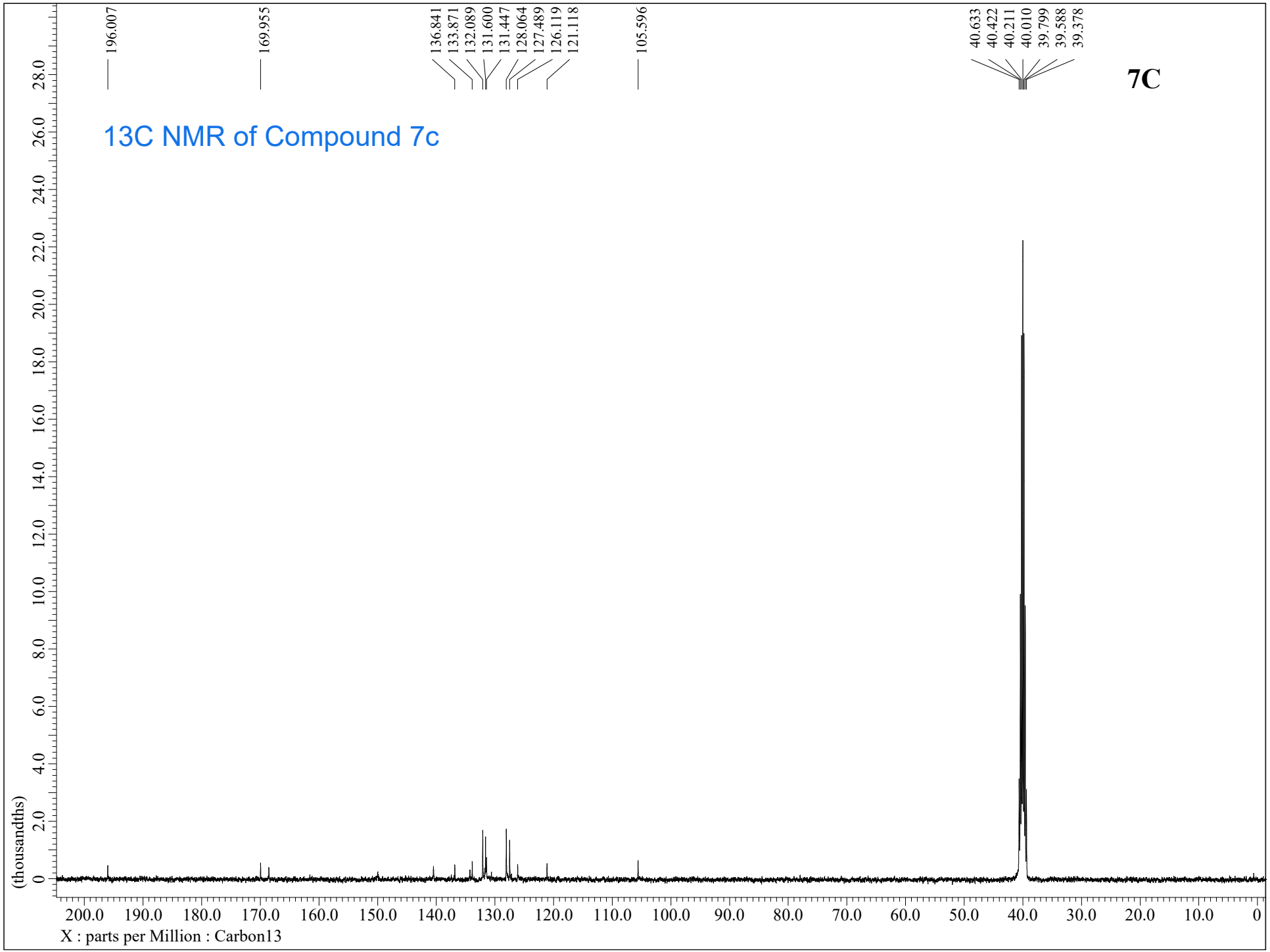
JEOL
Solutions for Innovation

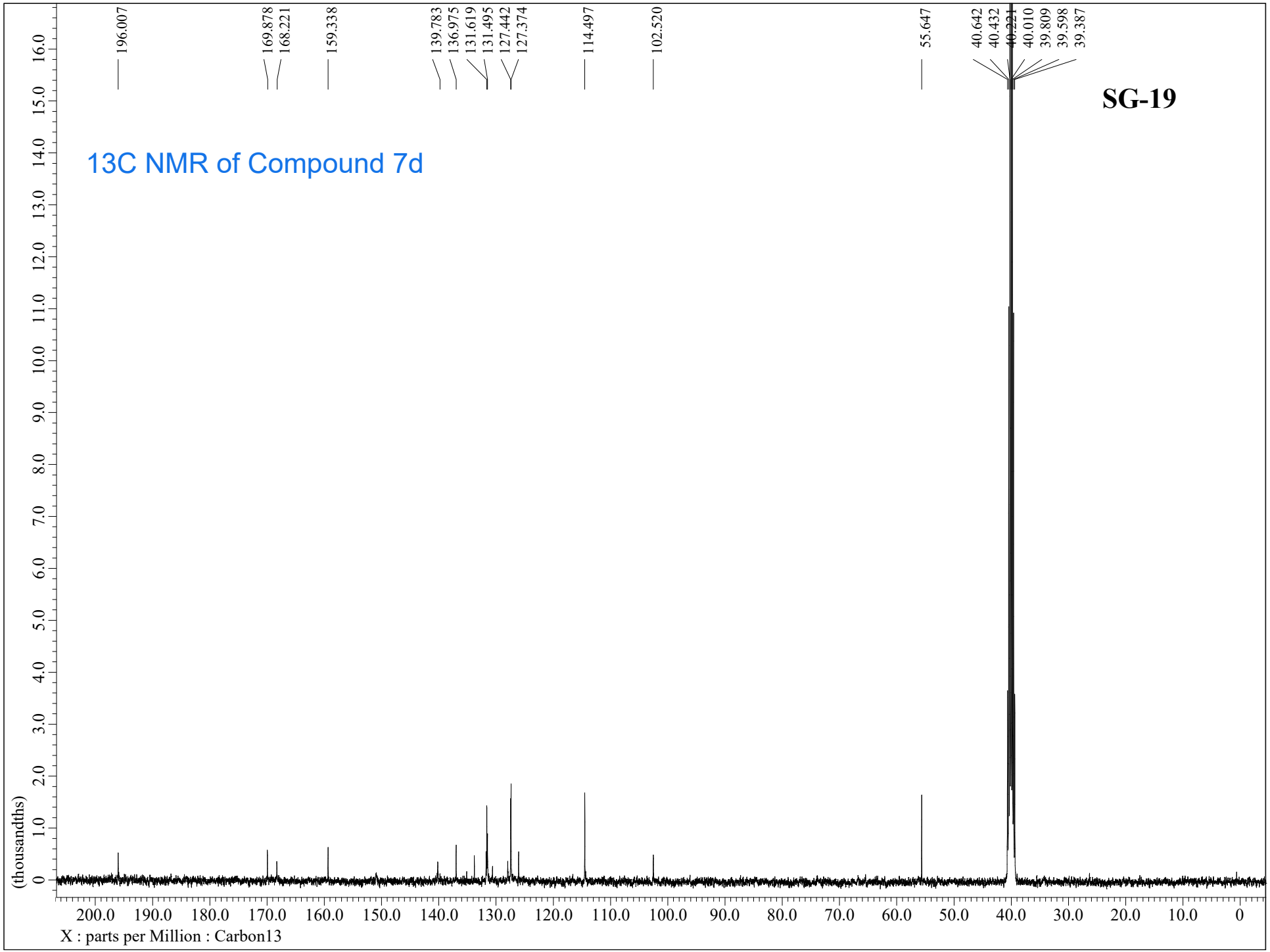

SG-49
1H NMR of Compound 7k
8.390
8.369
8.146
8.127
8.106
8.023
8.003
7.984
7.962
7.895
7.808
7.601
7.580
4.788
2.490
abundance
0
0.1
0.2
0.3
0.4
0.5
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.09
2.60
3.87
1.69
0.80
4.02
2.00
X : parts per Million : Proton

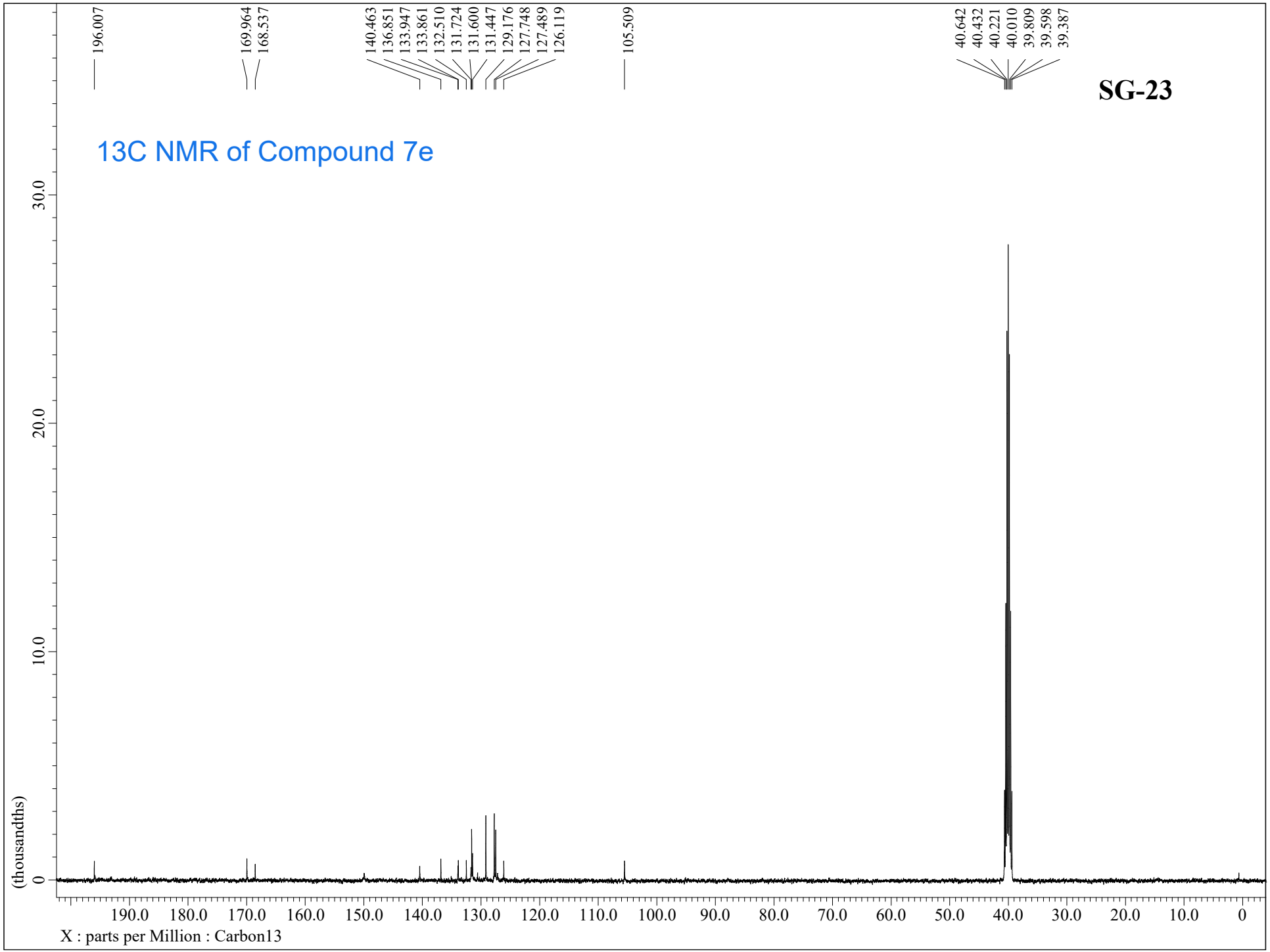

SG-52
1H NMR of Compound 7l
12.428
7.975
7.792
7.764
7.746
7.731
7.689
7.650
7.559
7.541
7.399
7.378
4.622
4.604
abundance
0.3
0.2
0.1
0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.47
0.75
4.96
1.28
1.74
0.71
2.00
X : parts per Million : Proton

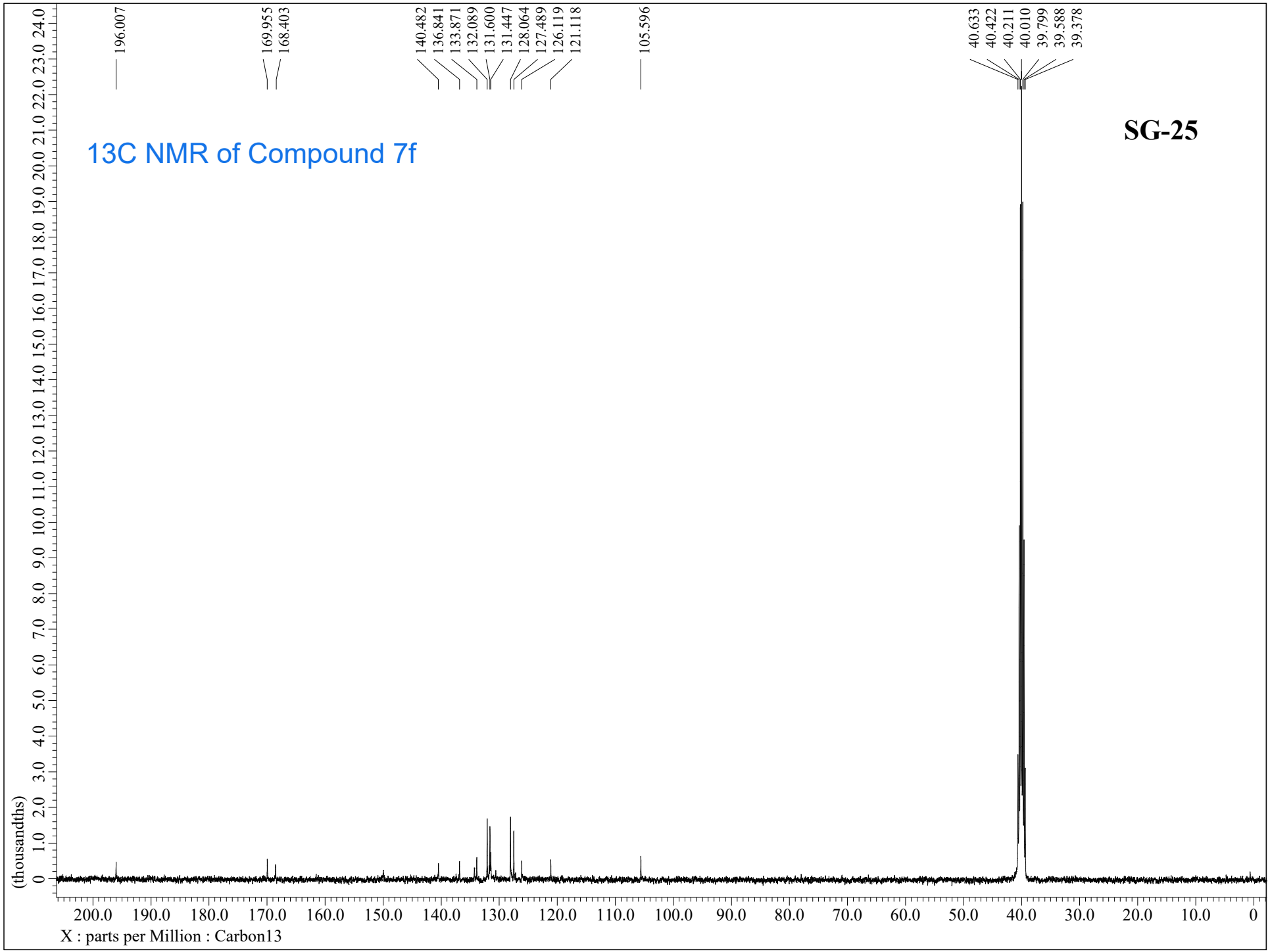

195.988
169.926
168.412
140.300
136.927
135.078
133.813
131.619
131.495
129.176
128.141
127.470
126.052
104.695
40.623
40.422
40.211
40.000
39.790
39.579
39.378
SG-31
13C NMR of Compound 7a
30.0
20.0
10.0
0
(thousandths)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
X : parts per Million : Carbon13

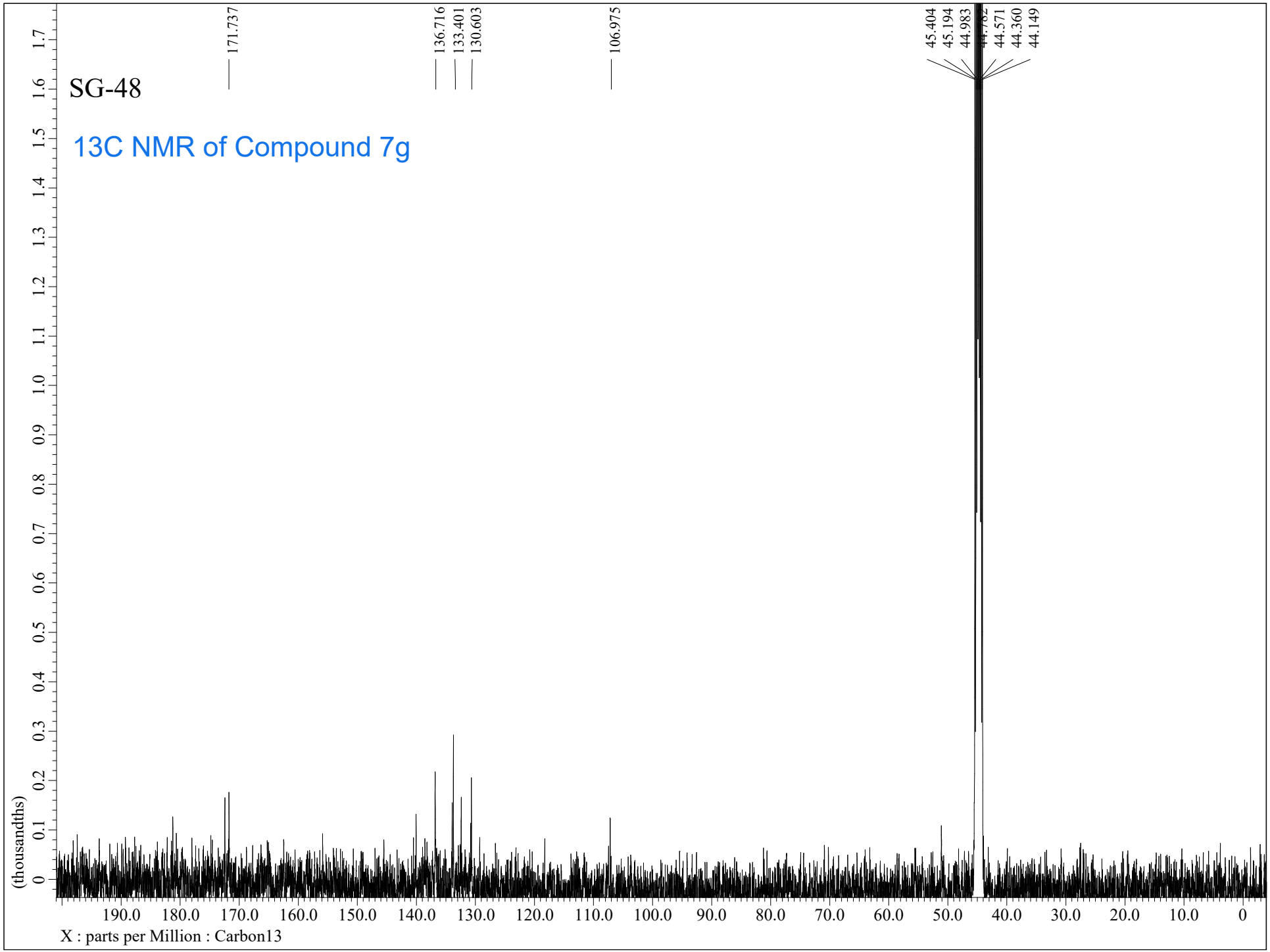

SG-17
196.017
169.964
168.307
140.223
137.406
136.956
133.823
132.453
131.609
131.475
129.722
127.461
126.004
103.756
40.662
40.451
40.240
40.029
39.617
39.406
21.355
13C NMR of Compound 7b
3.0
2.0
1.0
0
(thousandths)
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : Carbon13

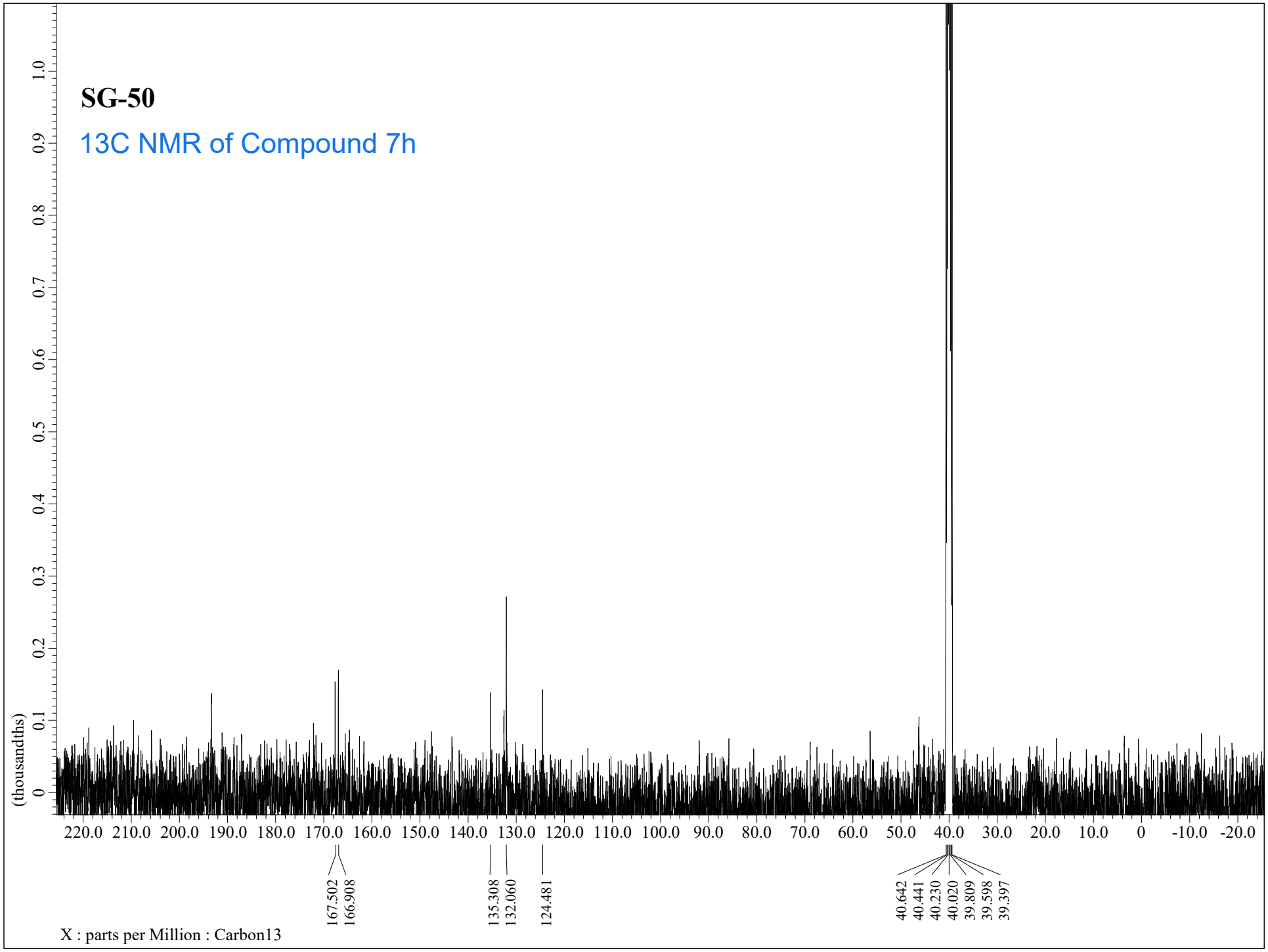

196.007
169.955
136.841
133.871
132.089
131.600
131.447
128.064
127.489
126.119
121.118
105.596
40.633
40.422
40.211
40.010
39.799
39.588
39.378
7C
13C NMR of Compound 7c
(thousandths)
X : parts per Million : Carbon13

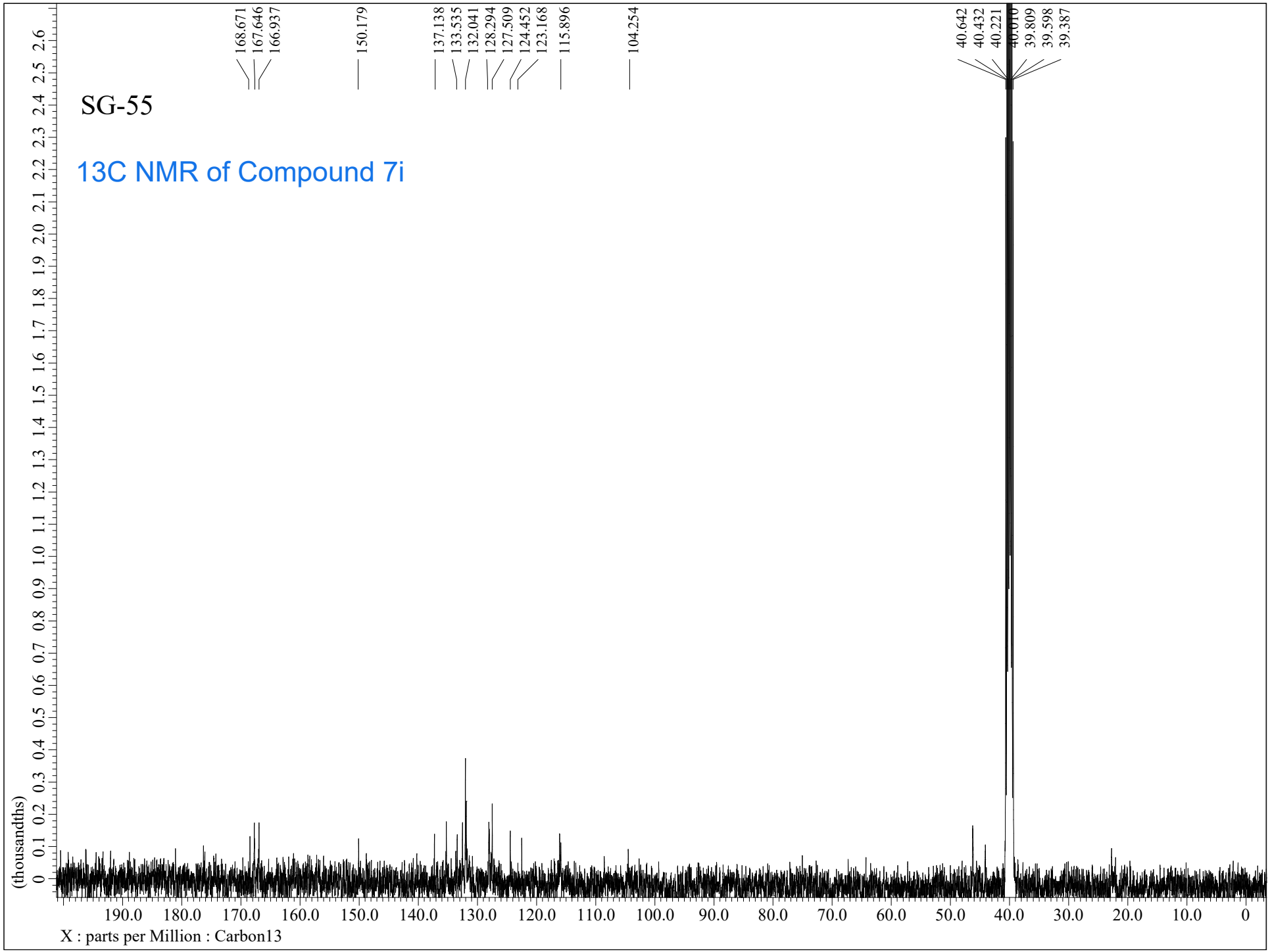

196.007
169.878
168.221
159.338
139.783
136.975
131.619
131.495
127.442
127.374
114.497
102.520
55.647
40.642
40.432
40.221
40.010
39.809
39.598
39.387
SG-19
13C NMR of Compound 7d
(thousandths)
X : parts per Million : Carbon13

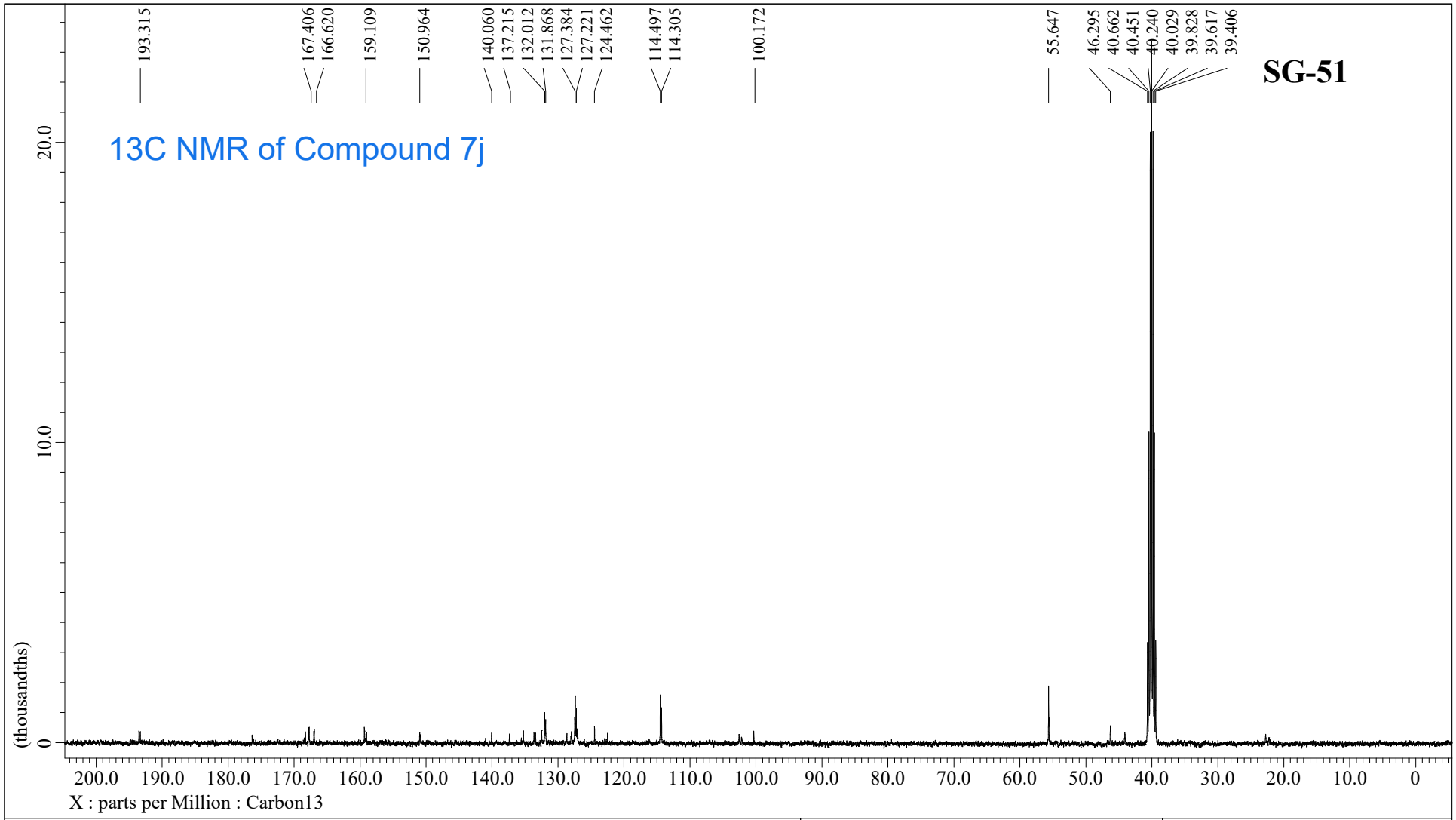

196.007
169.964
168.537
140.463
136.851
133.947
133.861
132.510
131.724
131.600
131.447
129.176
127.748
127.489
126.119
105.509
40.642
40.432
40.221
40.010
39.809
39.598
39.387
SG-23
13C NMR of Compound 7e
30.0
20.0
10.0
0
(thousandths)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
X : parts per Million : Carbon13


196.007
169.955
168.403
140.482
136.841
133.871
132.089
131.600
131.447
128.064
127.489
126.119
121.118
105.596
40.633
40.422
40.211
40.010
39.799
39.588
39.378
SG-25
13C NMR of Compound 7f
(thousandths)
X : parts per Million : Carbon13


SG-48
13C NMR of Compound 7g
171.737
136.716
133.401
130.603
106.975
45.404
45.194
44.983
44.571
44.360
44.149
(thousandths)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
X : parts per Million : Carbon13


SG-50
13C NMR of Compound 7h
(thousandths)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
167.502
166.908
135.308
132.060
124.481
40.642
40.441
40.230
40.020
39.809
39.598
39.397
X : parts per Million : Carbon13


SG-55
13C NMR of Compound 7i
168.671
167.646
166.937
150.179
137.138
133.535
132.041
128.294
127.509
124.452
123.168
115.896
104.254
40.642
40.432
40.221
40.010
39.809
39.598
39.387
(thousandths)
X : parts per Million : Carbon13



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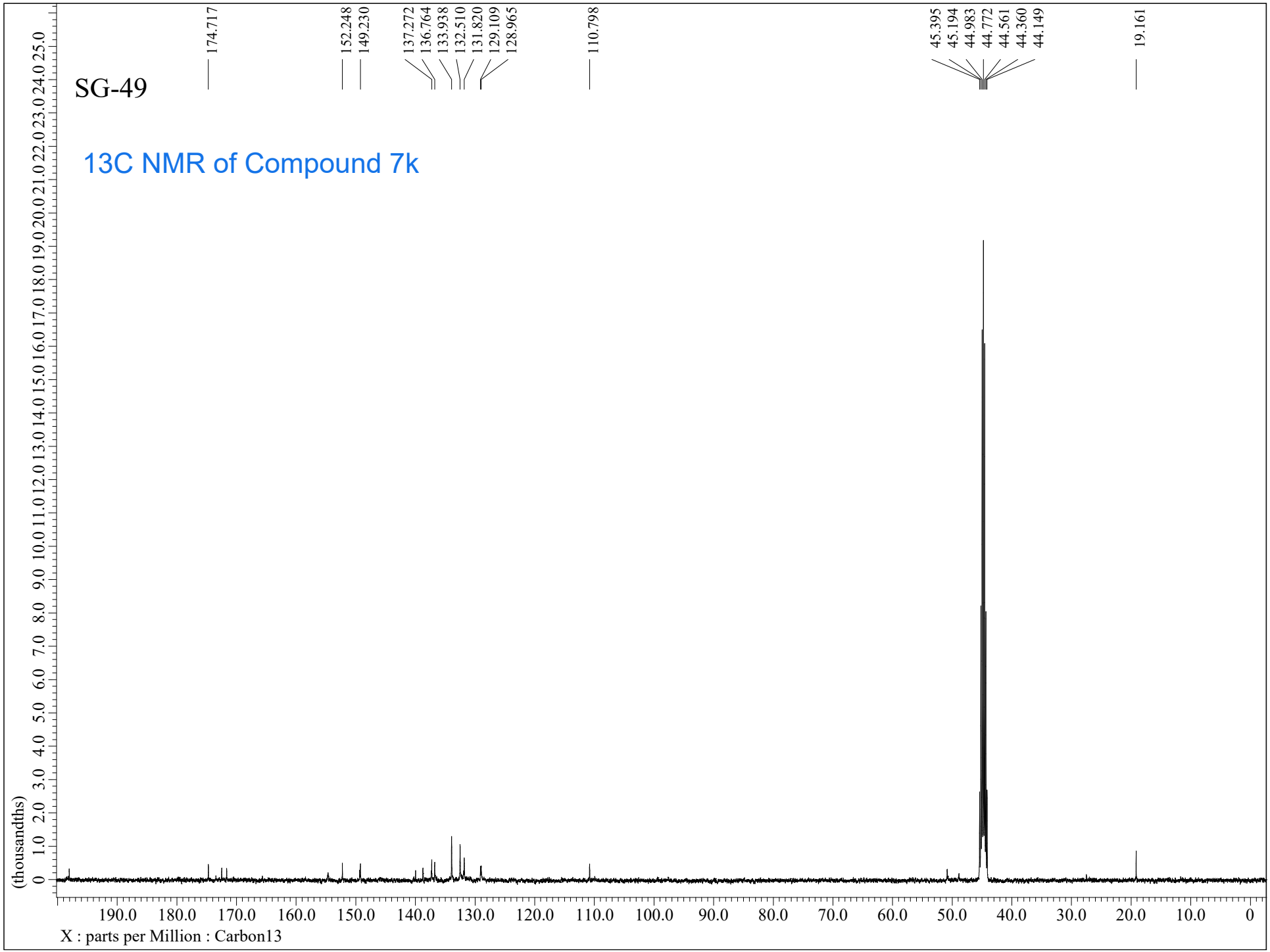
Author	= default	X_Acq_Duration	= 1.03809024[s]
Experiment	= carbon.jxp	X_Domain	= 13C
Sample_Id	= SR/SG 51	X_Freq	= 100.53787572[MHz]
Solvent	= DMSO-D6	X_Offset	= 100[ppm]
Creation_Time	= 8-MAY-2024 18:42:	X_Points	= 32768
Revision_Time	= 10-MAY-2024 19:22:	X_Prescans	= 4
Current_Time	= 10-MAY-2024 19:23:	X_Resolution	= 0.96330739[Hz]
		X_Sweep	= 31.56565657[kHz]
Comment	= single pulse decou	X_Sweep_Clipped	= 25.25252525[kHz]
Data_Format	= 1D COMPLEX	Irr_Domain	= Proton
Dim_Size	= 26214	Irr_Freq	= 399.83219794[MHz]
Dim_Title	= Carbon13	Irr_Offset	= 5[ppm]
Dim_Units	= [ppm]	Blanking	= 5[us]
Dimensions	= X	Clipped	= FALSE
Spectrometer	= DELTA2_NMR	Decimation_Reg	= r: 198(197),g: 39
		Scans	= 512

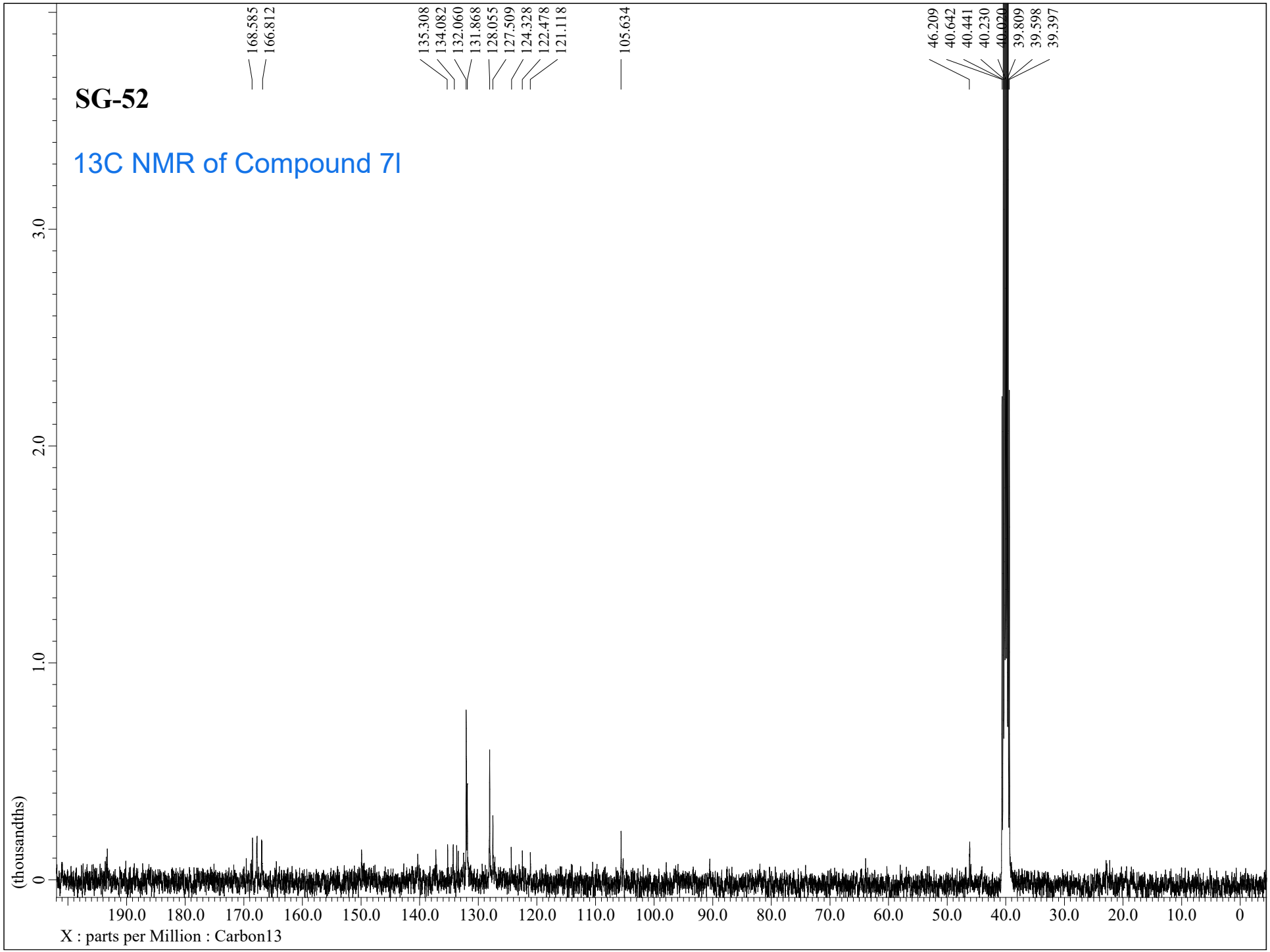
```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: SR_SG 51_Carbon-1-1.jdf
```

JEOL
Solutions for Innovation

SG-49

13C NMR of Compound 7k




SG-52
13C NMR of Compound 7l
168.585
166.812
135.308
134.082
132.060
131.868
128.055
127.509
124.328
122.478
121.118
105.634
46.209
40.642
40.441
40.230
40.020
39.809
39.598
39.397
(thousandths)
3.0
2.0
1.0
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
X : parts per Million : Carbon13

HRMS of 7a (ESI) m/z calcd for C20H14N4OS3 [M+H] + , 422.54; found, 423.03.

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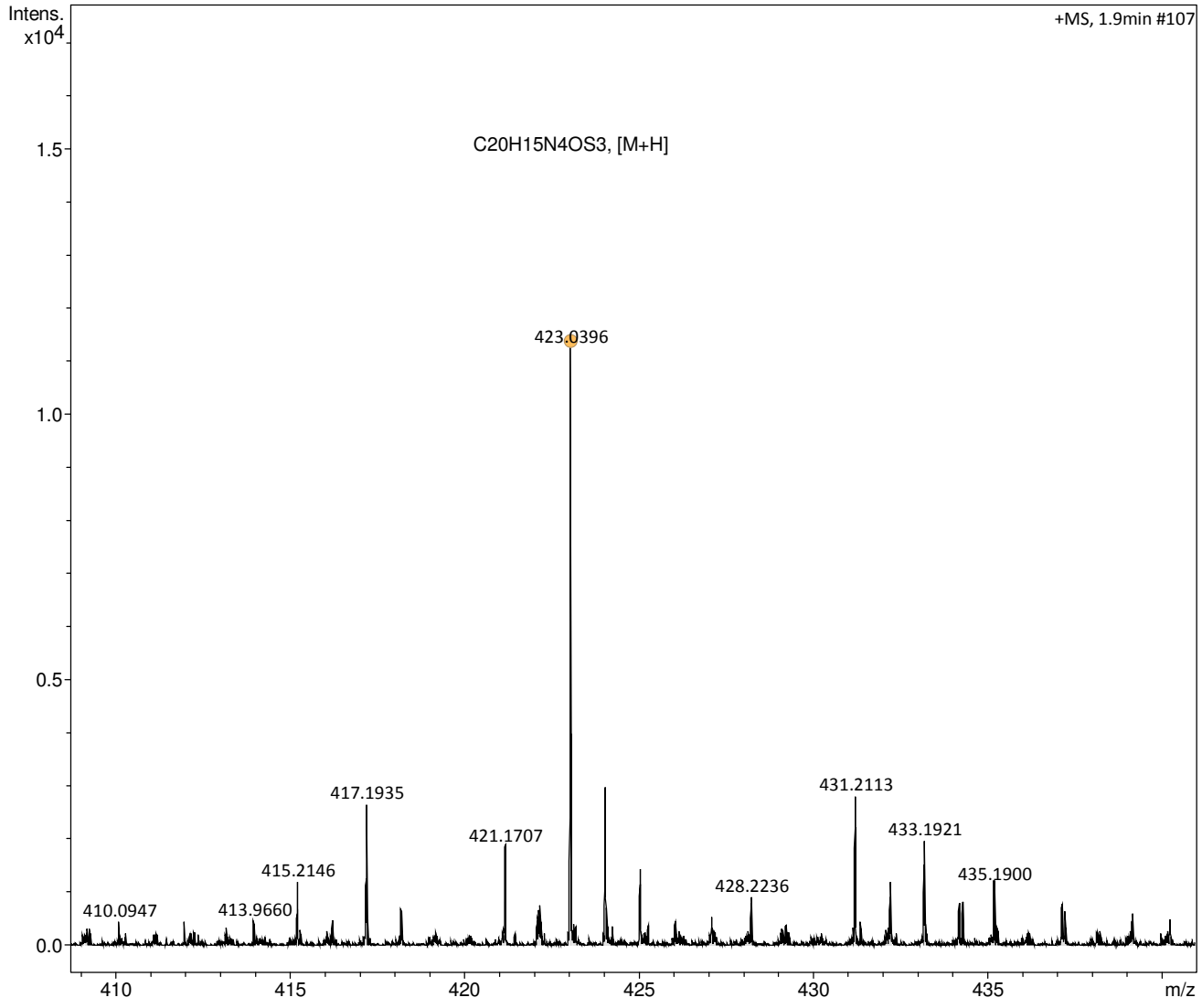
Analysis Info

Acquisition Date	8/16/2024 7:11:32 PM		
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG31_RA8_01_7865.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG31	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
423.039565	1	C20H15N4OS3	100.00	423.040251	0.7	1.6	18.6	15.5	even	ok	M+H

HRMS of 7b (ESI) m/z calcd for C21H16N4OS3 [M+H] + , 436.57; found, 437.05.

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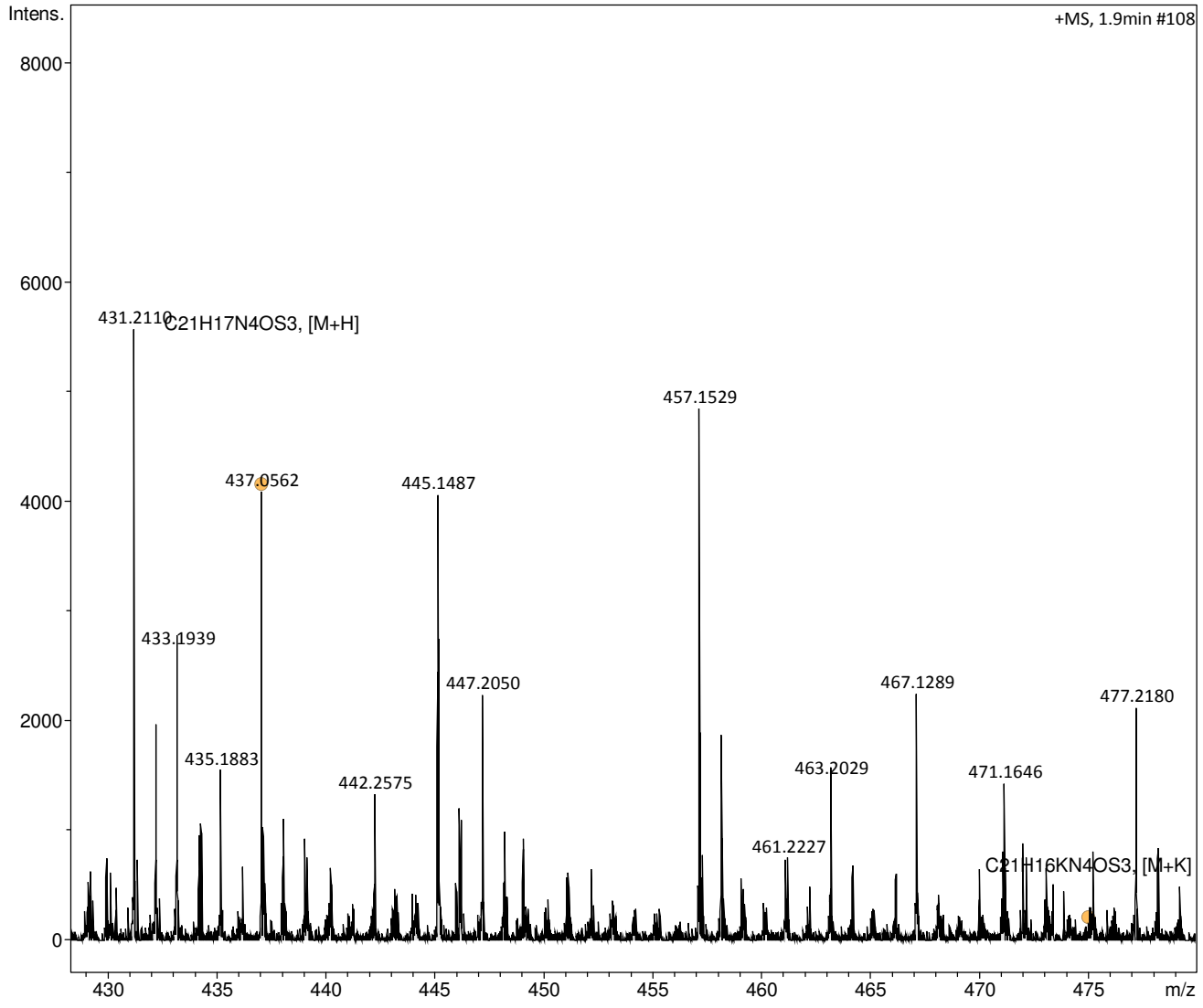
Analysis Info

Acquisition Date	8/16/2024 5:56:50 PM		
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG17_RA1_01_7858.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG17	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
437.056248	1	C21H17N4OS3	100.00	437.055901	-0.3	-0.8	26.2	15.5	even	ok	M+H
475.013241	1	C21H16KN4OS3	100.00	475.011782	-1.5	-3.1	364.5	15.5	even	ok	M+K

HRMS of 7c (ESI) m/z calcd for C21H13FN4OS3 [M+H] + , 440.53; found, 441.03.

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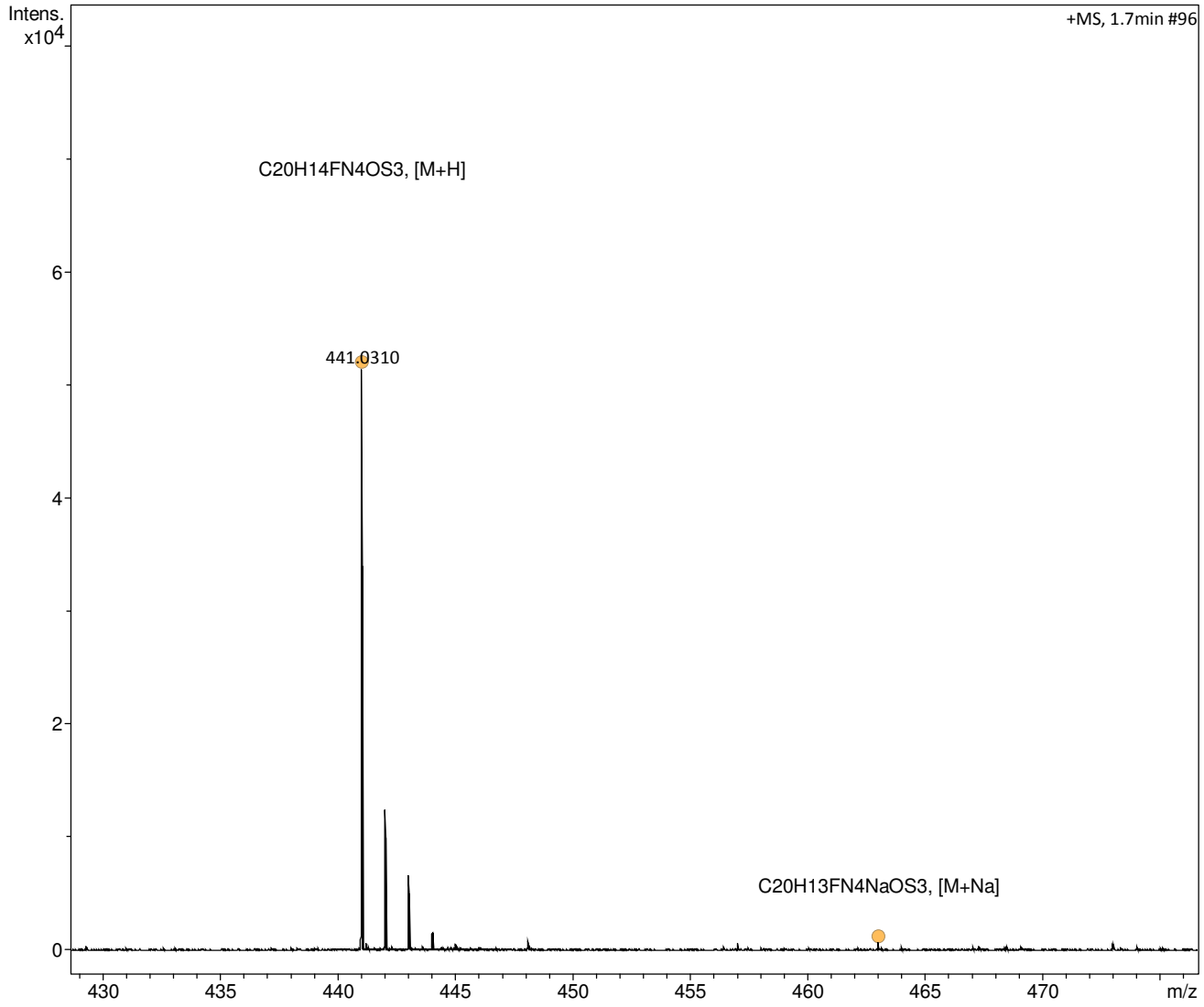
Analysis Info

Acquisition Date	8/31/2024 6:55:50 PM		
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG-60_RC2_01_7972.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG-60	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
441.031020	1	C20H14FN4OS3	100.00	441.030829	-0.2	-0.4	19.4	15.5	even	ok	M+H
463.012543	1	C20H13FN4NaOS3	100.00	463.012773	0.2	0.5	81.6	15.5	even	ok	M+Na

HRMS of 7d (ESI) m/z calcd for C21H16N4O2S3 [M+H] + , 452.57; found, 453.05.

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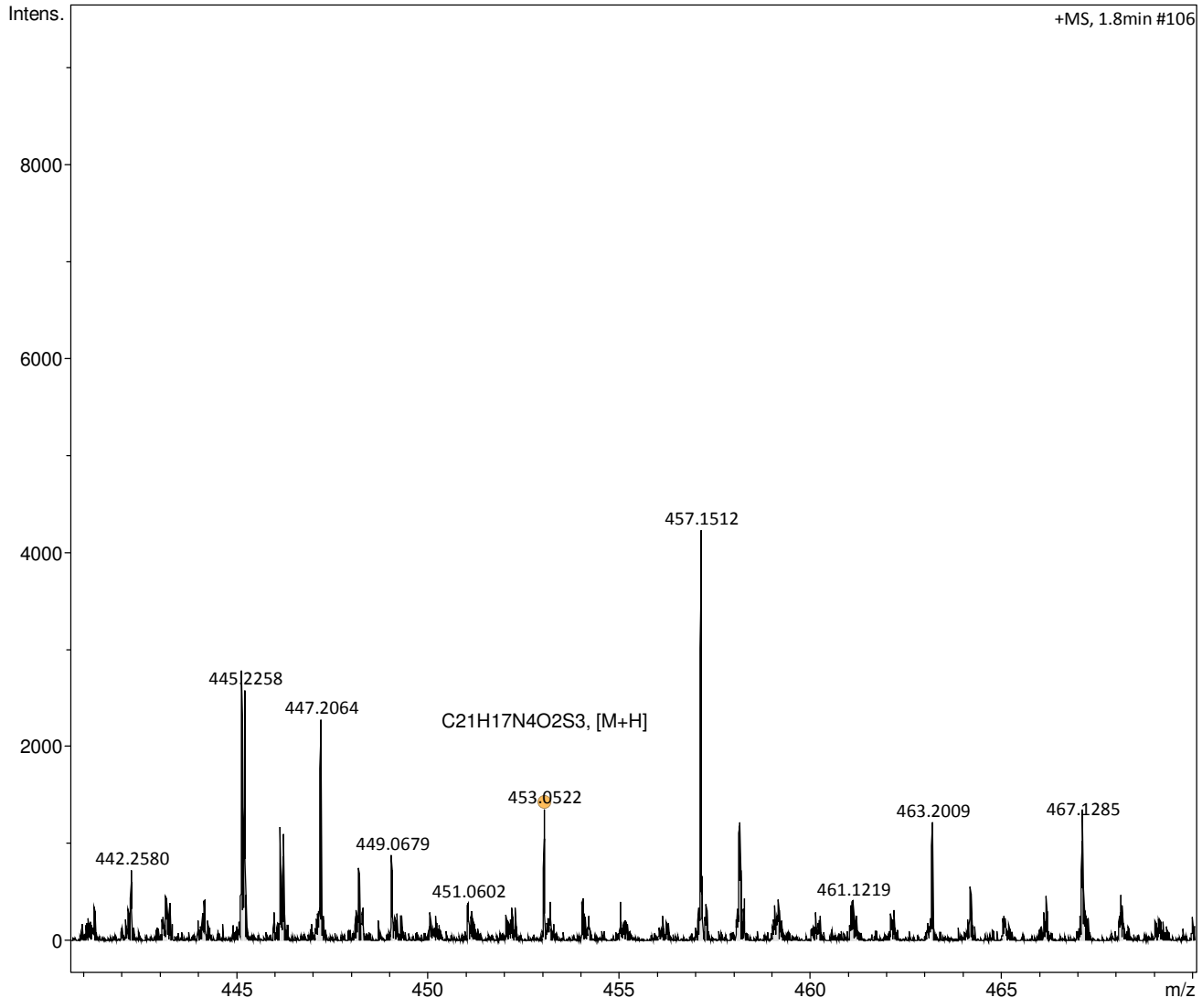
Analysis Info

Acquisition Date	8/16/2024 6:28:52 PM		
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG19_RA4_01_7861.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG19	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
453.052229	1	C21H17N4O2S3	100.00	453.050815	-1.4	-3.1	63.3	15.5	even	ok	M+H

HRMS of 7e (ESI) m/z calcd for C20H13ClN4OS3 [M+H] + , 456.98; found, 457.15.

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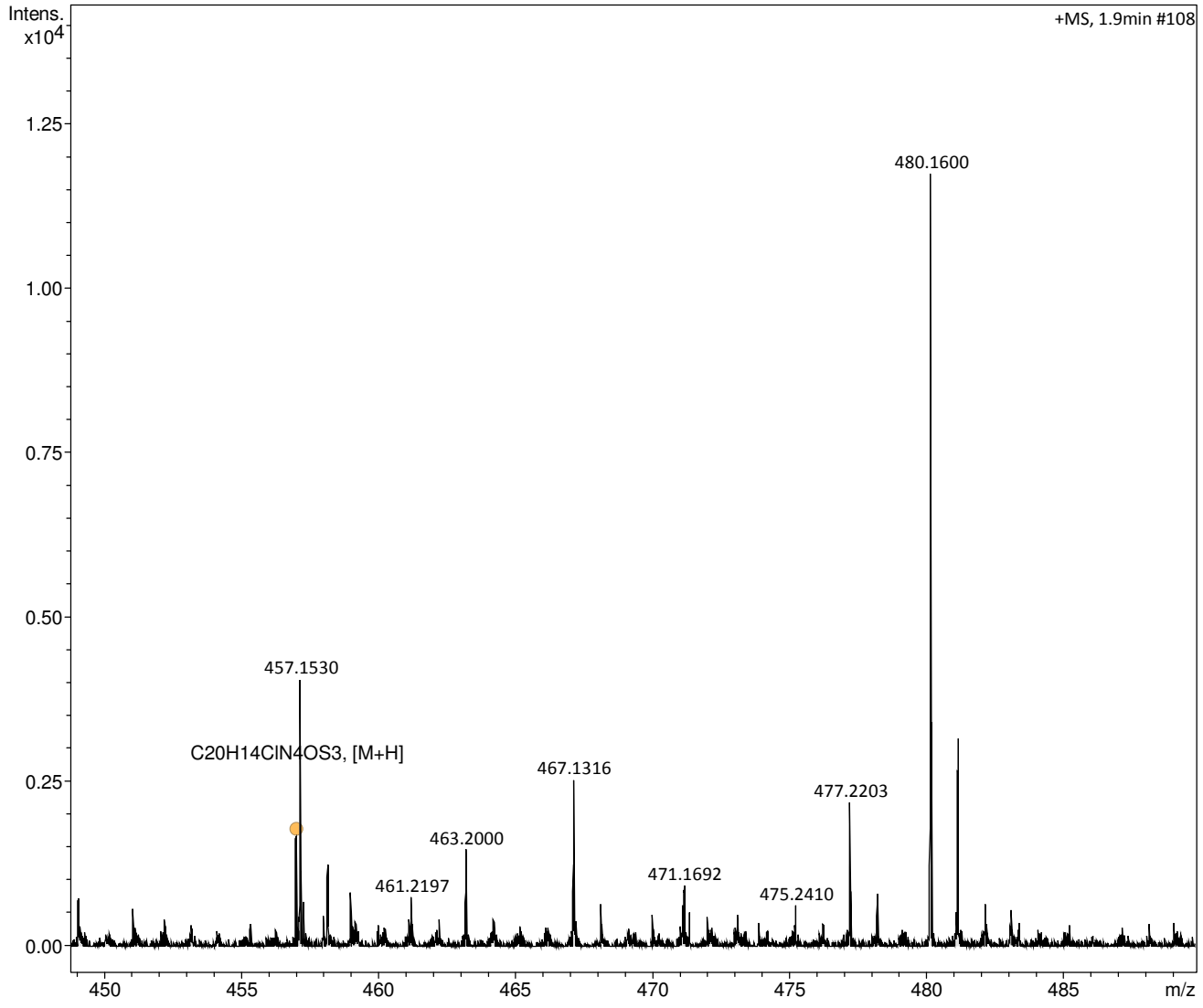
Analysis Info

Acquisition Date	8/16/2024 6:07:30 PM		
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG23_RA2_01_7859.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG23	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
457.002552	1	C20H14ClN4OS3	100.00	457.001278	-1.3	-2.8	54.6	15.5	even	ok	M+H

HRMS of 7f (ESI) m/z calcd for C20H13BrN4OS3 [M+H] + , 501.44; found, 500.95.

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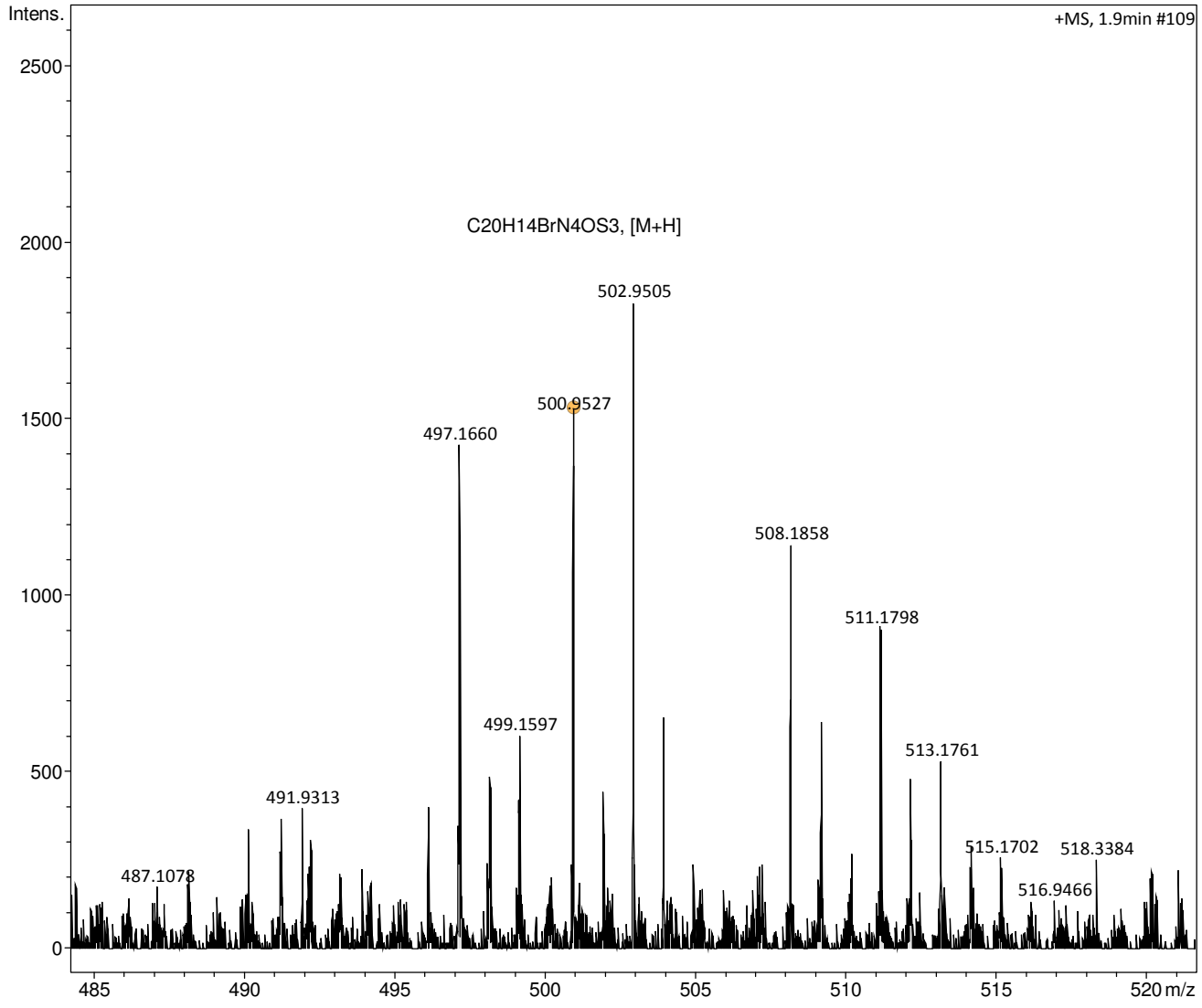
Analysis Info

Acquisition Date	8/16/2024 7:54:13 PM		
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG25_RB4_01_7869.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG25	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
500.952739	1	C20H14BrN4OS3	100.00	500.950763	-2.0	-3.9	55.2	15.5	even	ok	M+H

HRMS of 7g (ESI) m/z calcd for C22H16N4O3S3 [M+H] + , 480.58; found, 481.045.

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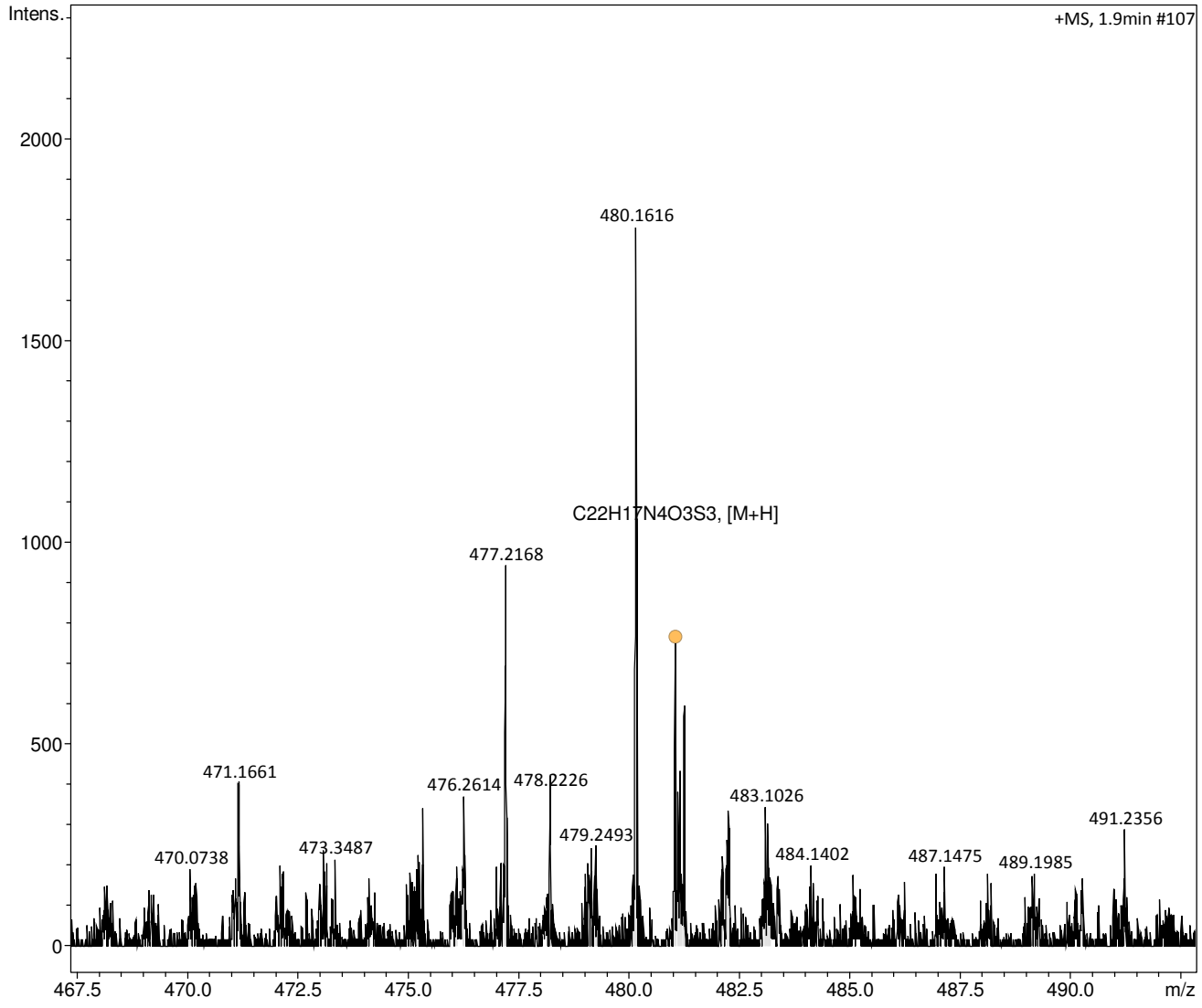
Analysis Info

Acquisition Date	8/16/2024 9:19:35 PM		
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG48_RC4_01_7877.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG48	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
481.048586	1	C22H17N4O3S3	100.00	481.045730	-2.9	-5.9	n.a.	16.5	even	ok	M+H

HRMS of 7h (ESI) m/z calcd for C23H18N4O3S3 [M+H] + , 494.60; found, , 495.06.

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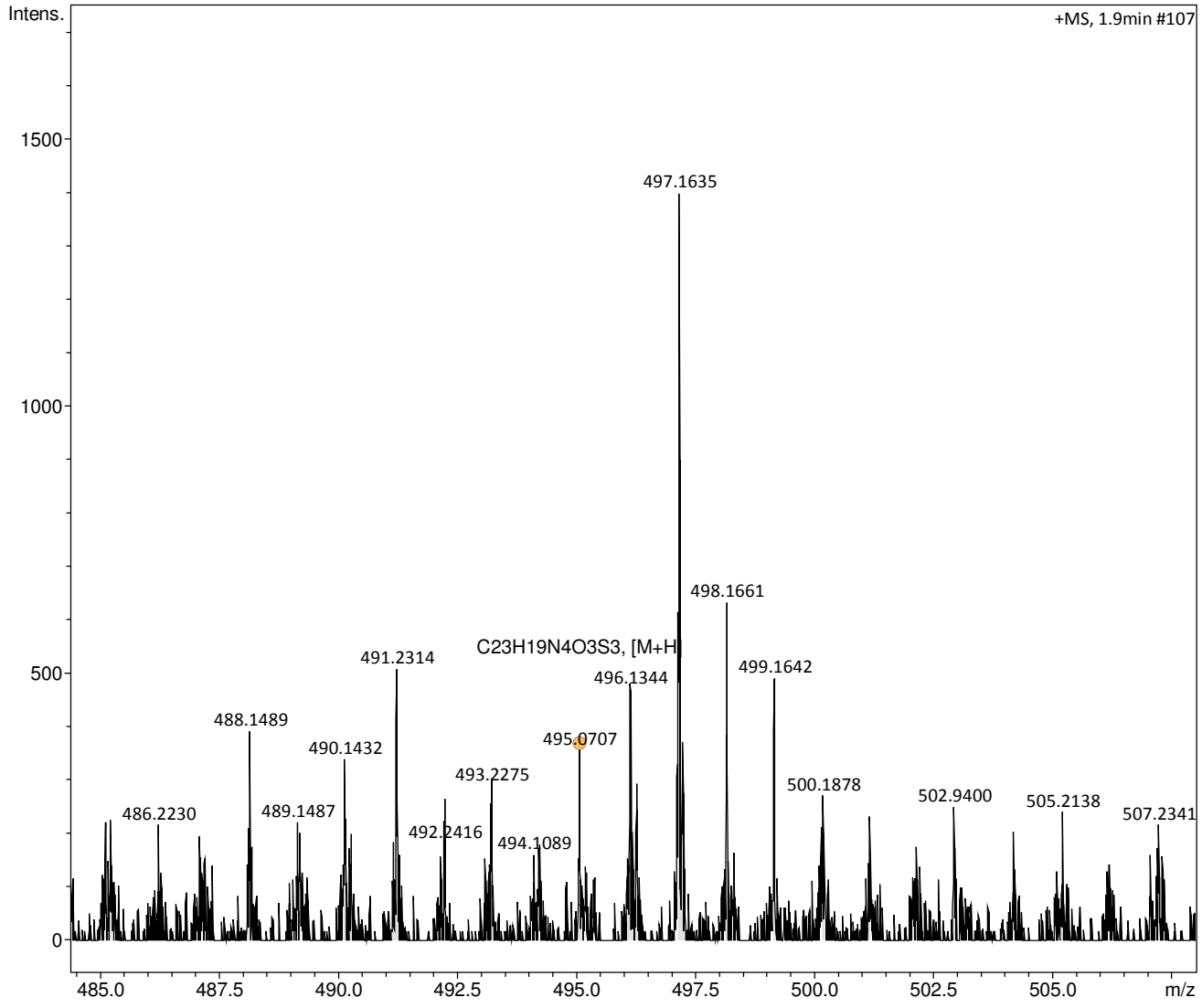
Analysis Info

Acquisition Date	8/16/2024 7:22:12 PM		
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG50_RB1_01_7866.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG50	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
495.070743	1	C23H19N4O3S3	100.00	495.061380	-9.4	-18.9	95.3	16.5	even	ok	M+H

HRMS of 7i (ESI) m/z calcd for C22H15FN4O3S3 [M+H] + , 498.57; found, 499.03.

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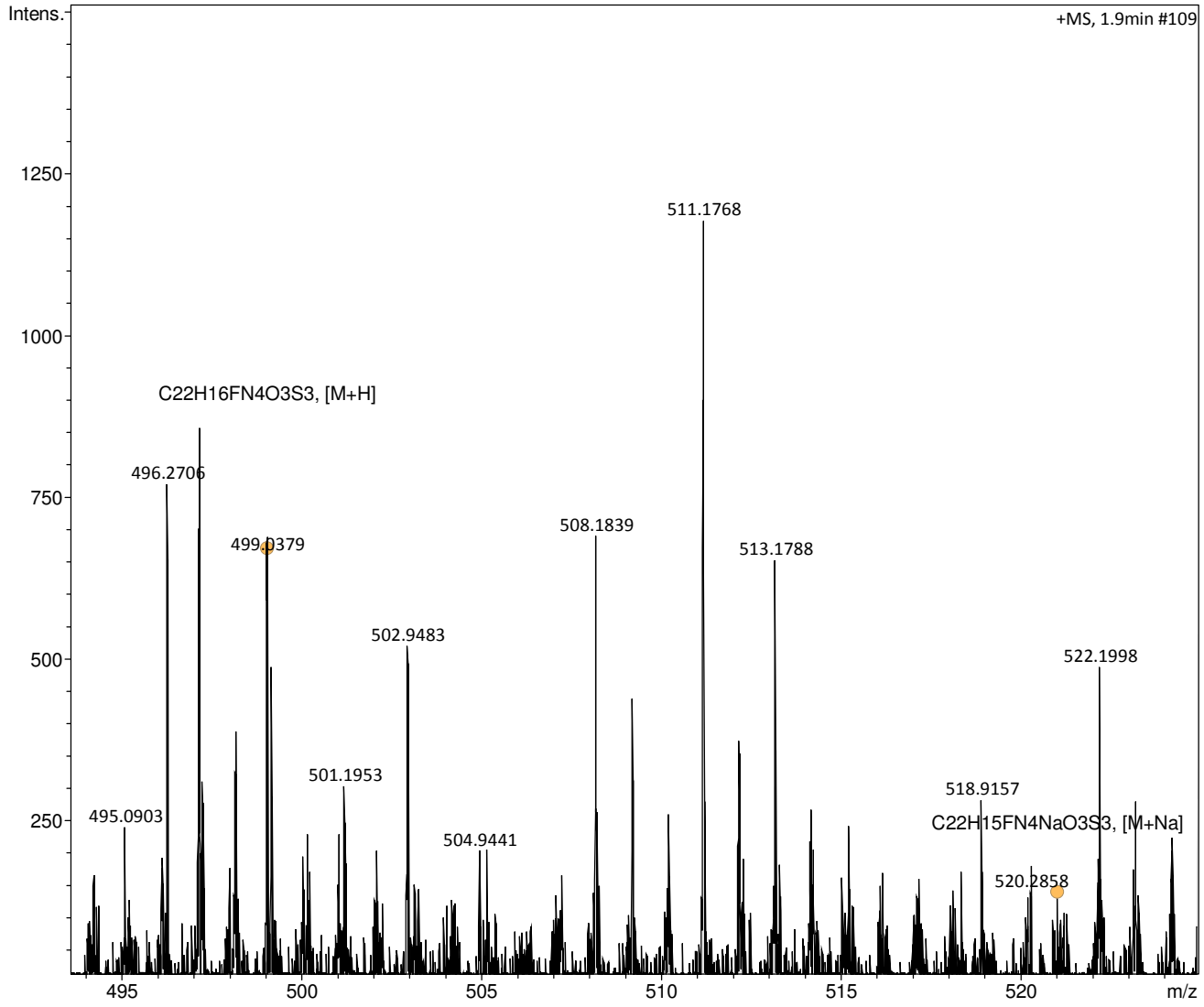
Analysis Info

Acquisition Date	8/16/2024 8:04:51 PM		
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG55_RB5_01_7870.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG55	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
499.037945	1	C22H16FN4O3S3	100.00	499.036308	-1.6	-3.3	102.8	16.5	even	ok	M+H
521.017335	1	C22H15FN4NaO3S3	100.00	521.018252	0.9	1.8	466.2	16.5	even	ok	M+Na
	1	C22H15FN4NaO3S3	100.00	521.018252	0.9	1.8	466.2	16.5	even	ok	M+Na

HRMS of 7j (ESI) m/z calcd for C23H18N4O4S3 [M+H] + , 510.60; found, 511.05.

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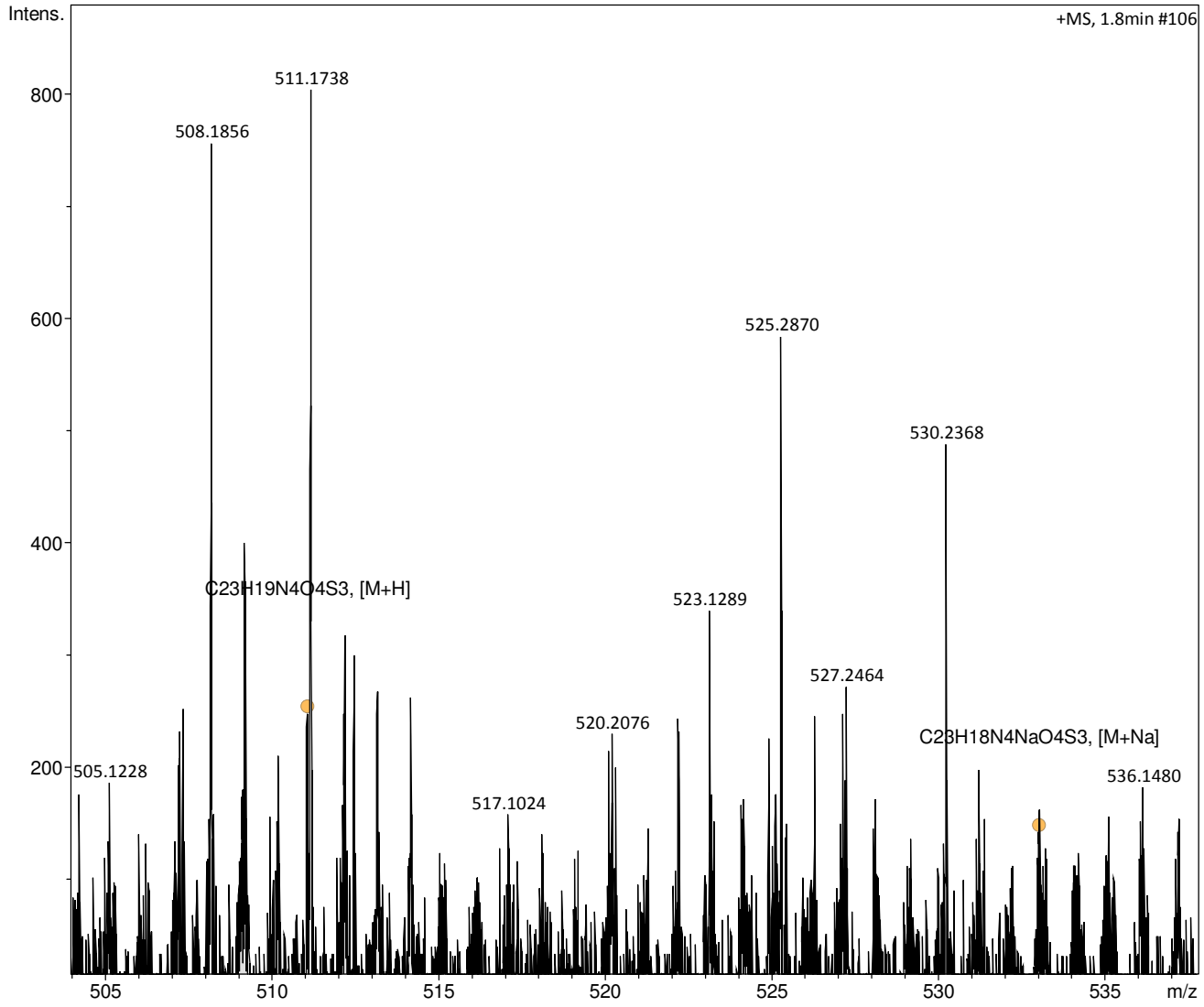
Analysis Info

		Acquisition Date	8/16/2024 9:08:54 PM
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG51_RC3_01_7876.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG51	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
511.060893	1	C23H19N4O4S3	100.00	511.056295	-4.6	-9.0	120.8	16.5	even	ok	M+H
533.029607	1	C23H18N4NaO4S3	100.00	533.038239	8.6	16.2	384.1	16.5	even	ok	M+Na
	1	C23H18N4NaO4S3	100.00	533.038239	8.6	16.2	384.1	16.5	even	ok	M+Na

HRMS of 7k (ESI) m/z calcd for C22H15ClN4O3S3 [M+H] + , 515.02; found, 515.06.

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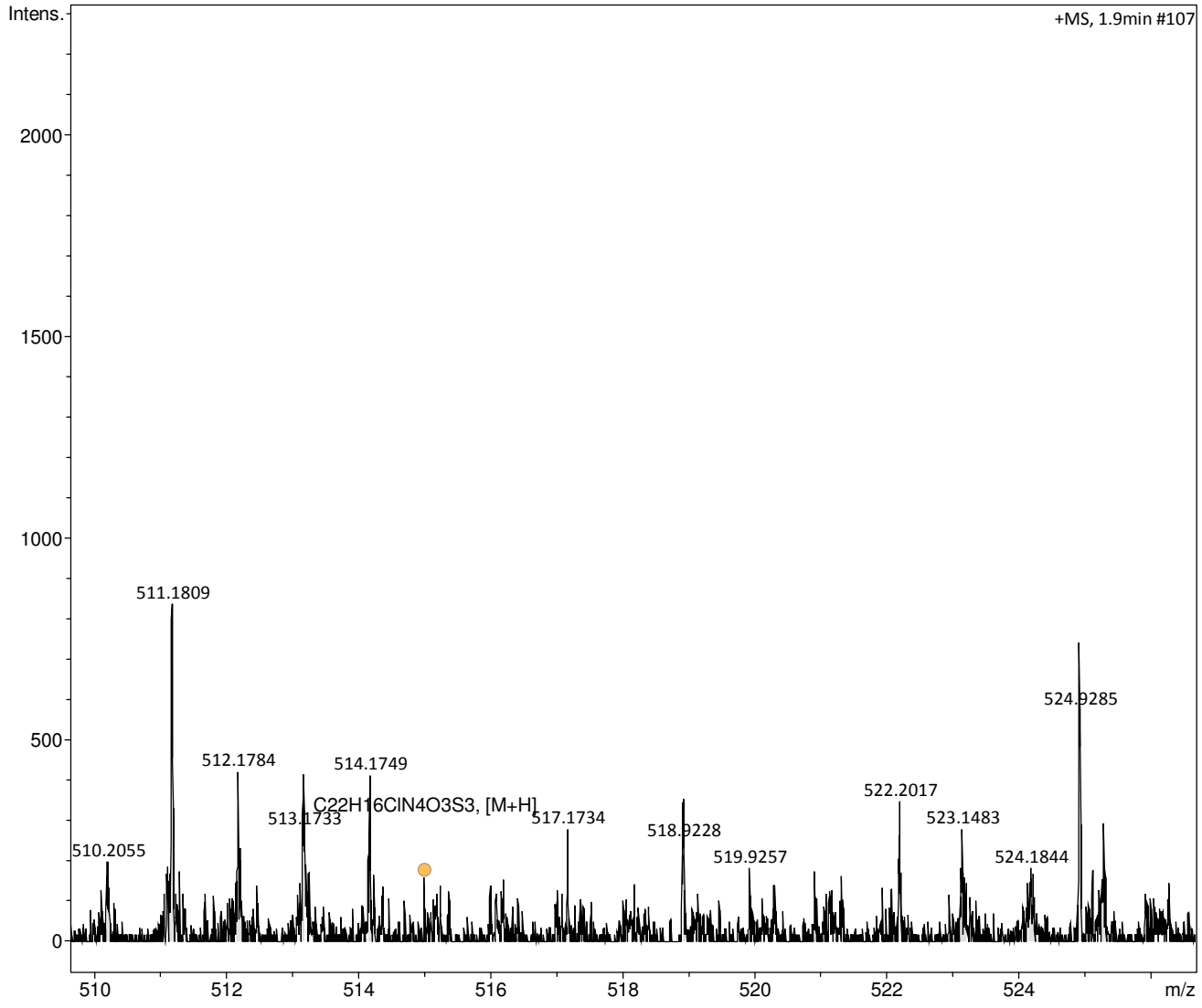
Analysis Info

Acquisition Date	8/16/2024 8:26:12 PM		
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG49_RB7_01_7872.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG49	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
515.002975	1	C22H16ClN4O3S3	100.00	515.006757	3.8	7.3	n.a.	16.5	even	ok	M+H

HRMS of 7l (ESI) m/z calcd for C22H15BrN4O3S3 [M+H] + , 559.47; found, 558.95.

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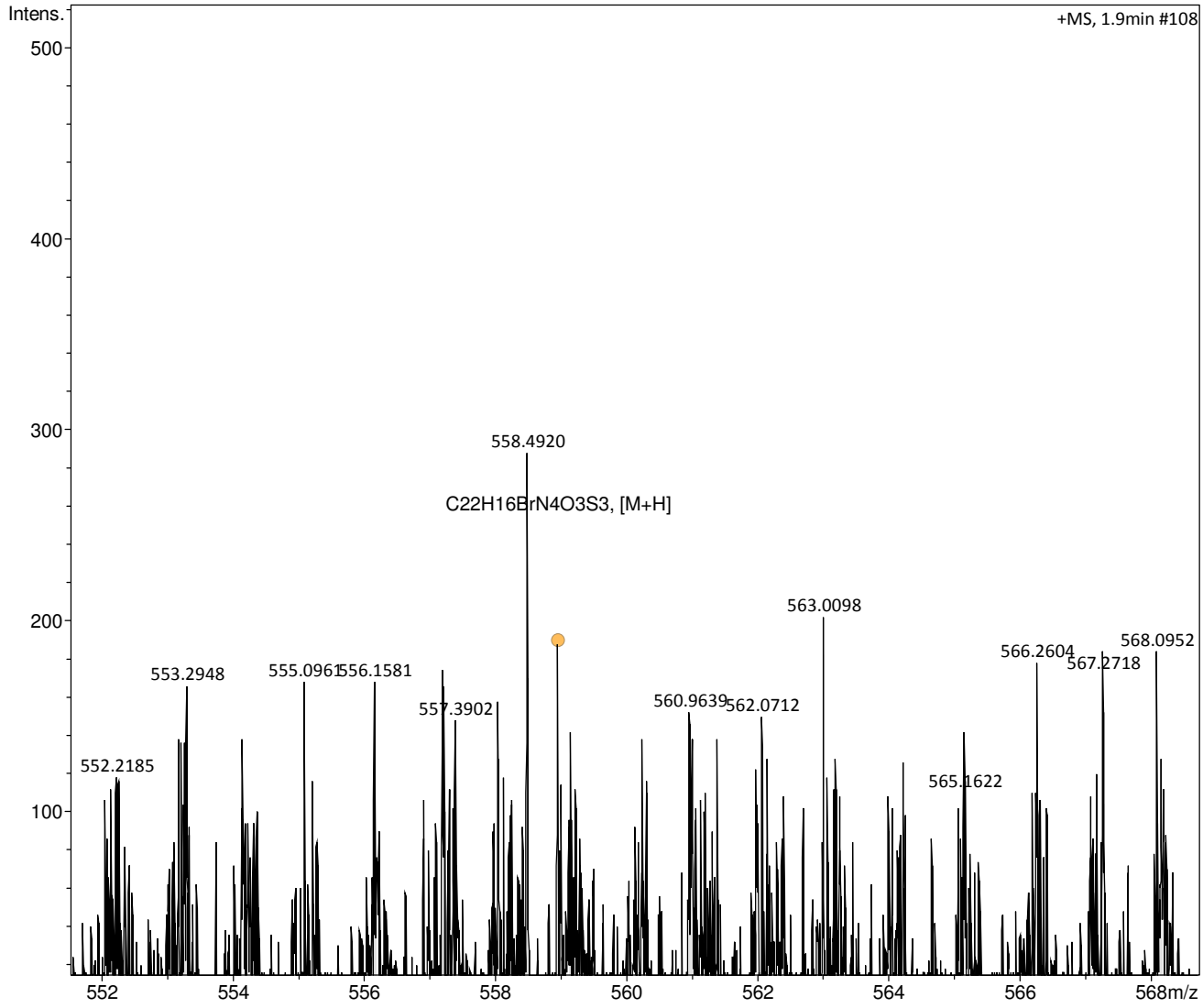
Analysis Info

		Acquisition Date	8/16/2024 6:50:12 PM
Analysis Name	D:\Data\2024\AUG\SPPU COLLEGE\S. P. COLLEGE\PROF. PRAVIN MHASKE\SG52_RA6_01_7863.d		
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_july 2024.m	Analyst :	Nitin S. Kadam CIF
Sample Name	SG52	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.9 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
558.953197	1	C22H16BrN4O3S3	100.00	558.956242	3.0	5.4	187.4	16.5	even	ok	M+H

HPLC chromatogram of Blank

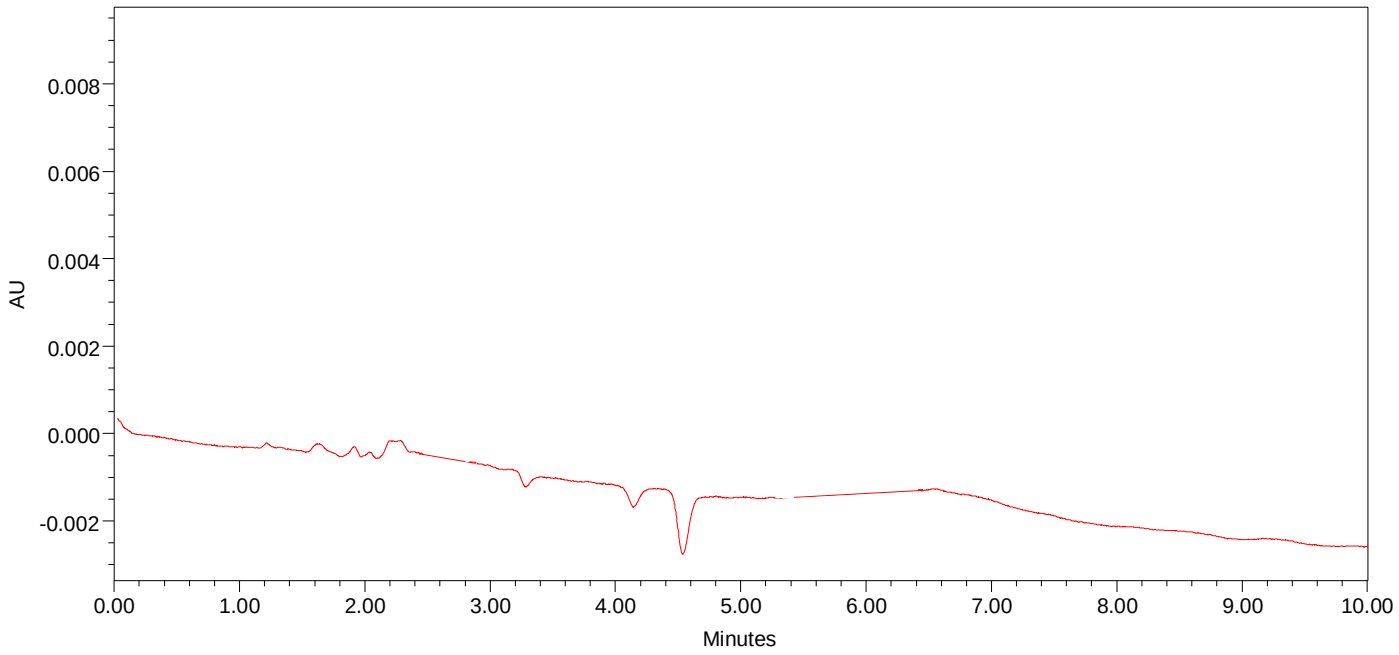
HPLC chromatogram of 7aHPLC chromatogram of 7a

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	Blank	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	1	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method	Blank Processing
Injection Volume:	10.00 ul	Channel Name:	223.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.0 nm (2998
Date Acquired:	23-10-2024 11:03:20 AM IST		
Date Processed:	25-10-2024 09:50:17 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area

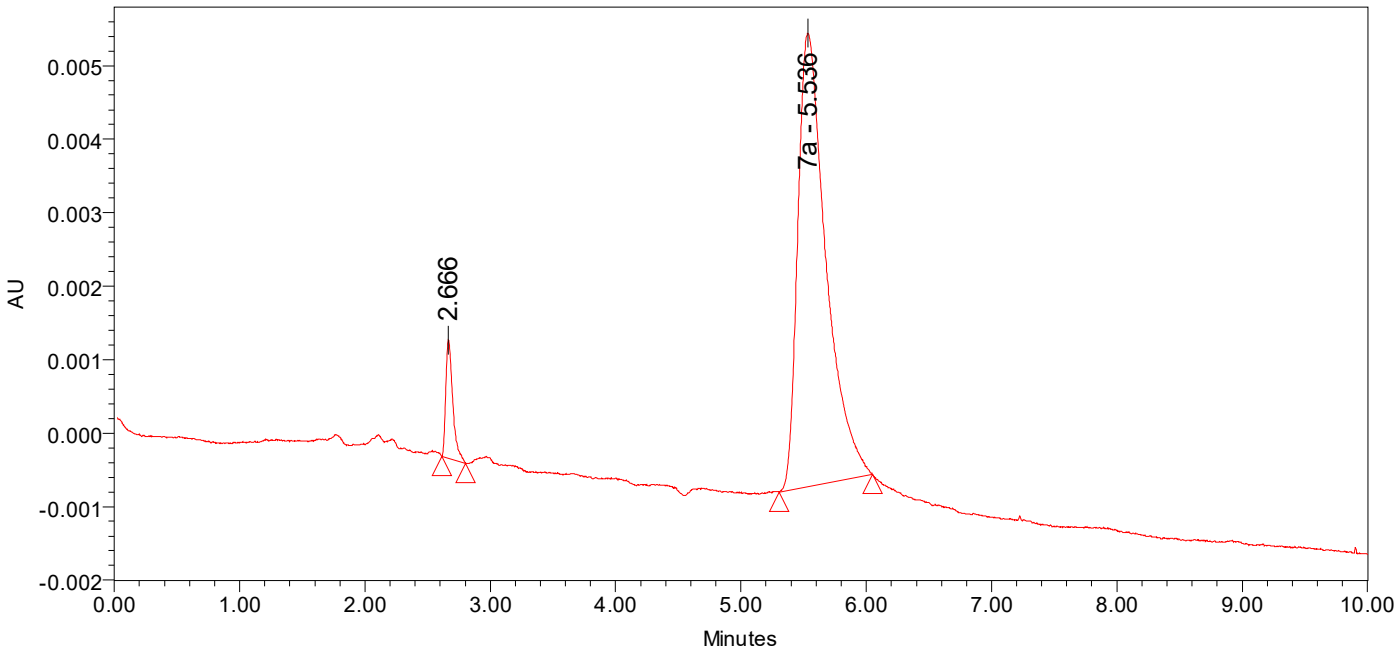
HPLC chromatogram of 7a

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7a	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	2	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7a Processing
Injection Volume:	10.00 ul	Channel Name:	223.0nm@2
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.0 nm (2998
Date Acquired:	23-10-2024 11:14:02 AM IST		
Date Processed:	23-10-2024 02:01:01 PM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.666	6166	6.01
2	7a	5.536	96359	93.99

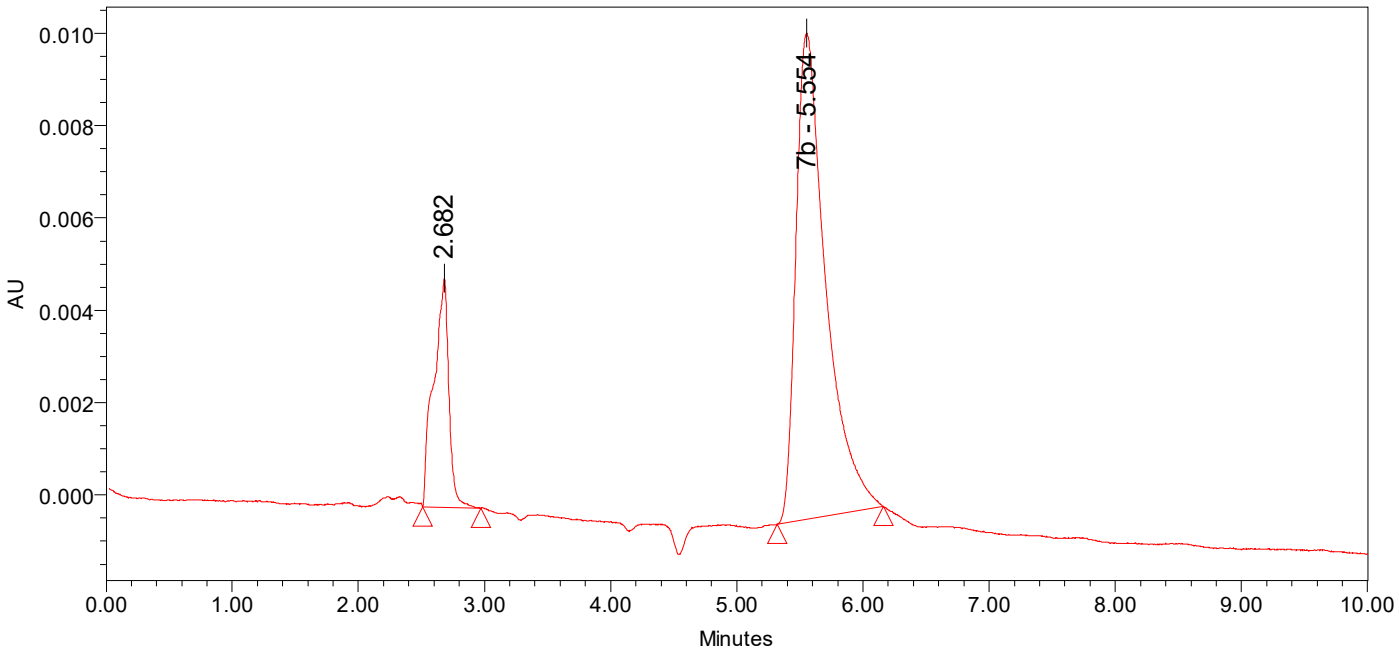
HPLC chromatogram of 7b

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7b	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	3	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7b Processing
Injection Volume:	10.00 ul	Channel Name:	223.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.0 nm (2998
Date Acquired:	23-10-2024 11:24:41 AM IST		
Date Processed:	24-10-2024 09:04:13 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.682	41639	19.30
2	7b	5.554	174055	80.70

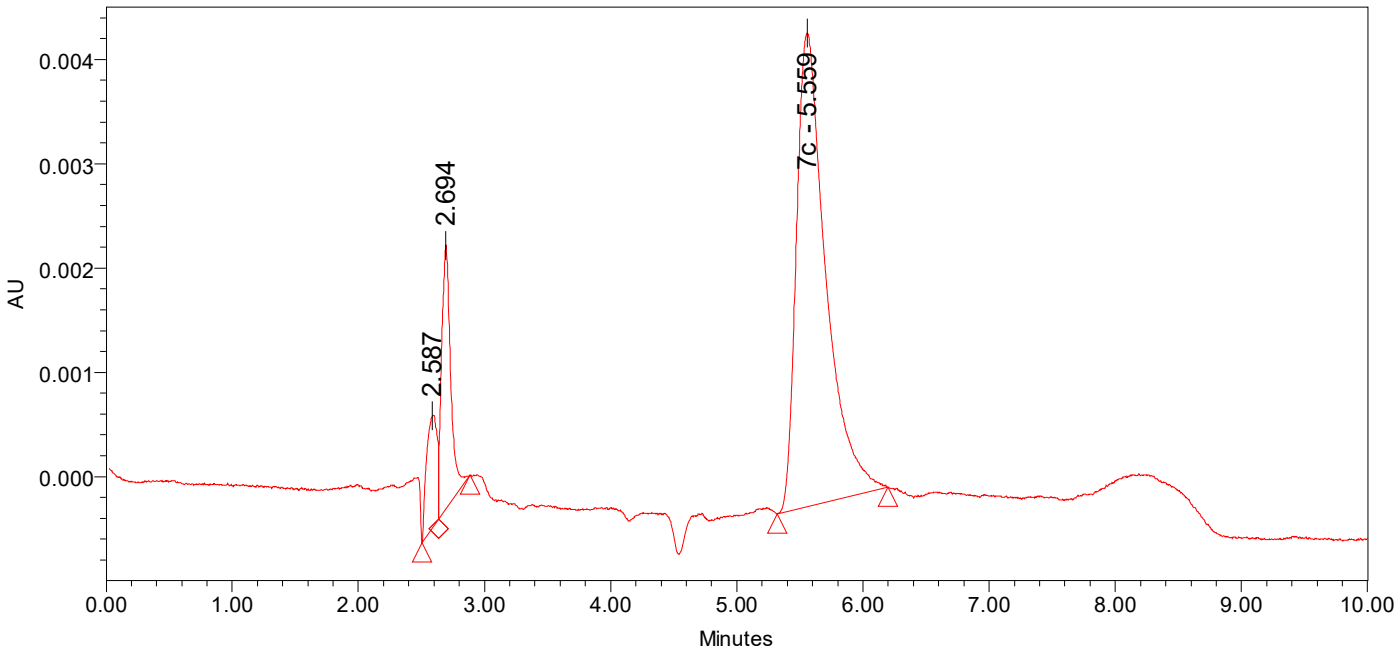
HPLC chromatogram of 7c

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7c	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	4	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7c Processing
Injection Volume:	10.00 ul	Channel Name:	232.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 232.0 nm (2998
Date Acquired:	23-10-2024 11:35:21 AM IST		
Date Processed:	24-10-2024 09:10:32 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.587	6364	6.85
2		2.694	12714	13.69

	Name	RT	Area	% Area
3	7c	5.559	73771	79.45

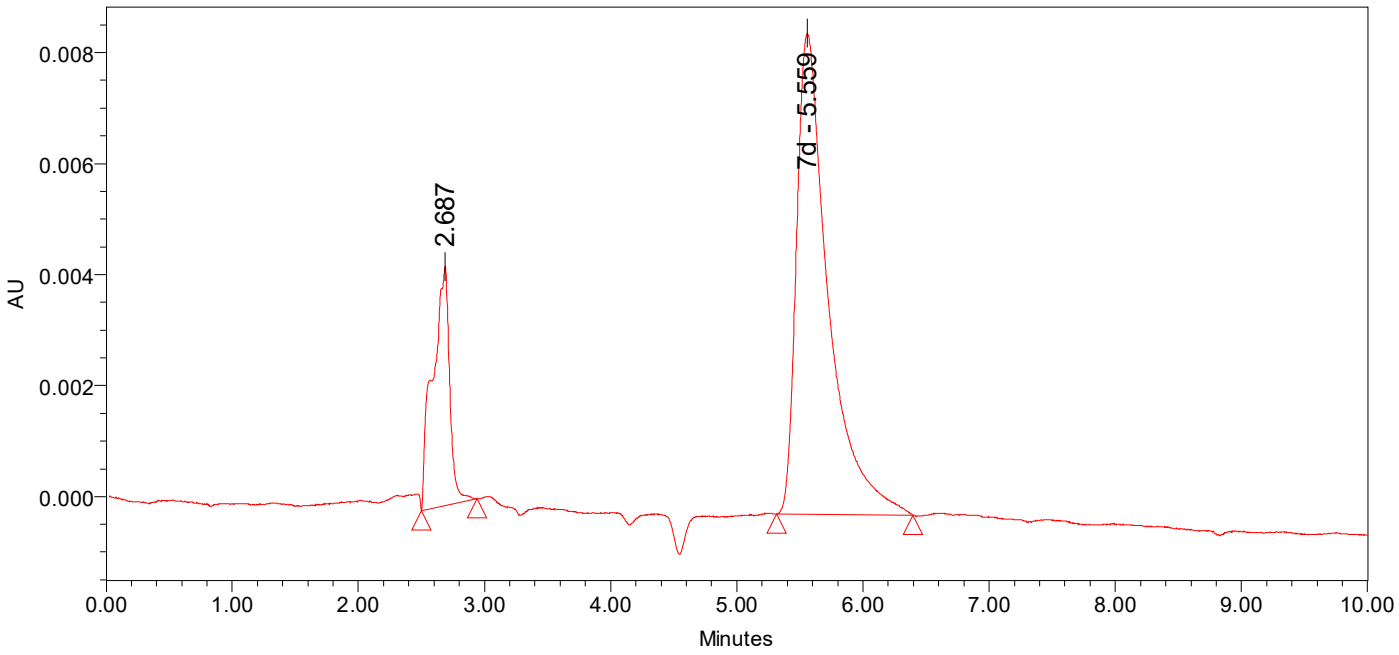
HPLC chromatogram of 7d

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7d	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	5	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7d Processing
Injection Volume:	10.00 ul	Channel Name:	223.5nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.5 nm (2998
Date Acquired:	23-10-2024 11:46:05 AM IST		
Date Processed:	25-10-2024 09:16:27 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.687	40146	20.91
2	7d	5.559	151855	79.09

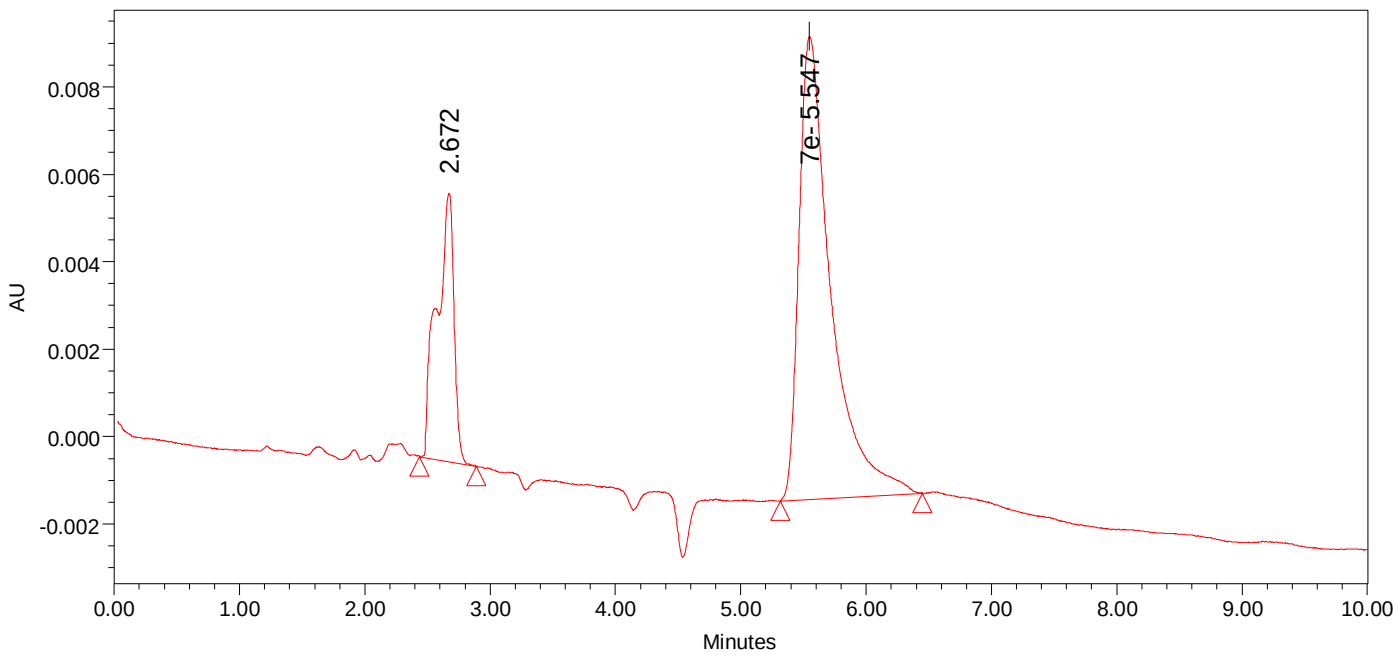
HPLC chromatogram of 7e

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

S A M P L E I N F O R M A T I O N

Sample Name:	7e	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	1	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method	7e Processing
Injection Volume:	10.00 ul	Channel Name:	223.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.0 nm (2998
Date Acquired:	23-10-2024 11:56:45 AM IST		
Date Processed:	25-10-2024 09:59:15 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.672	58185	23.73
2	7e	5.547	187038	76.27

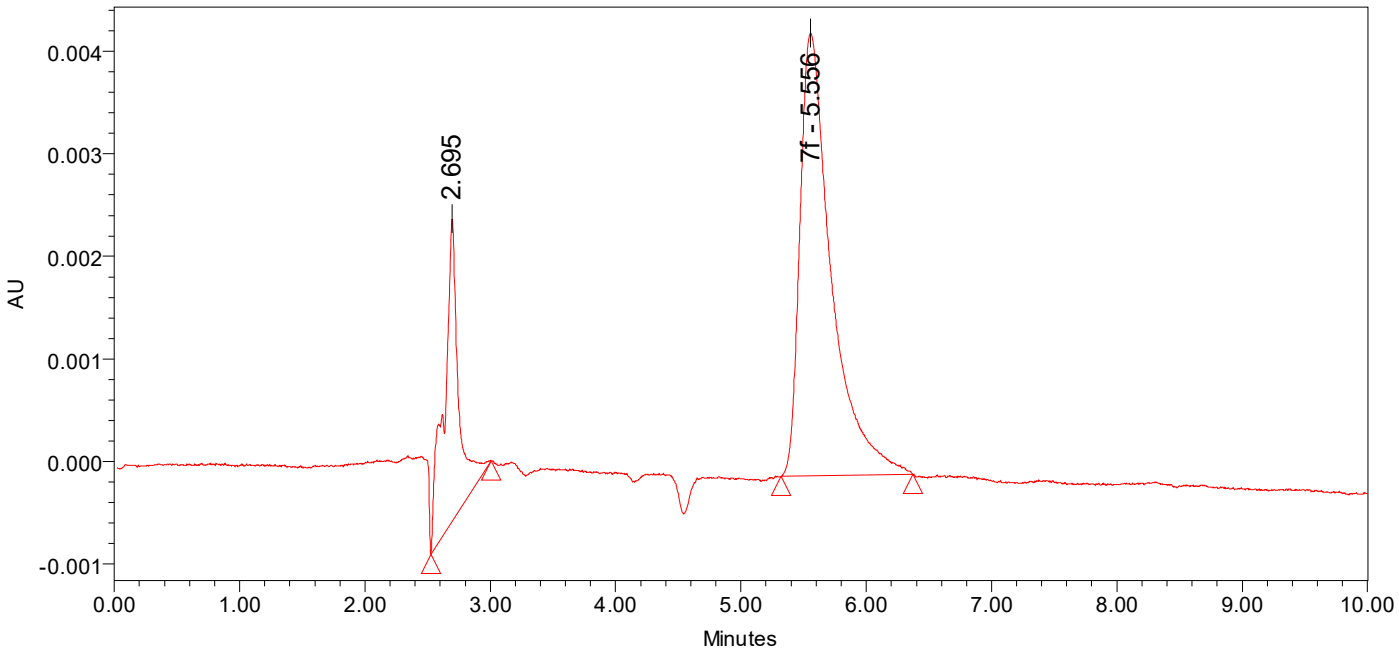
HPLC chromatogram of 7f

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7f	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	7	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7f processing
Injection Volume:	10.00 ul	Channel Name:	232.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 232.0 nm (2998
Date Acquired:	23-10-2024 12:07:26 PM IST		
Date Processed:	24-10-2024 09:58:47 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.695	23818	24.05
2	7f	5.556	75212	75.95

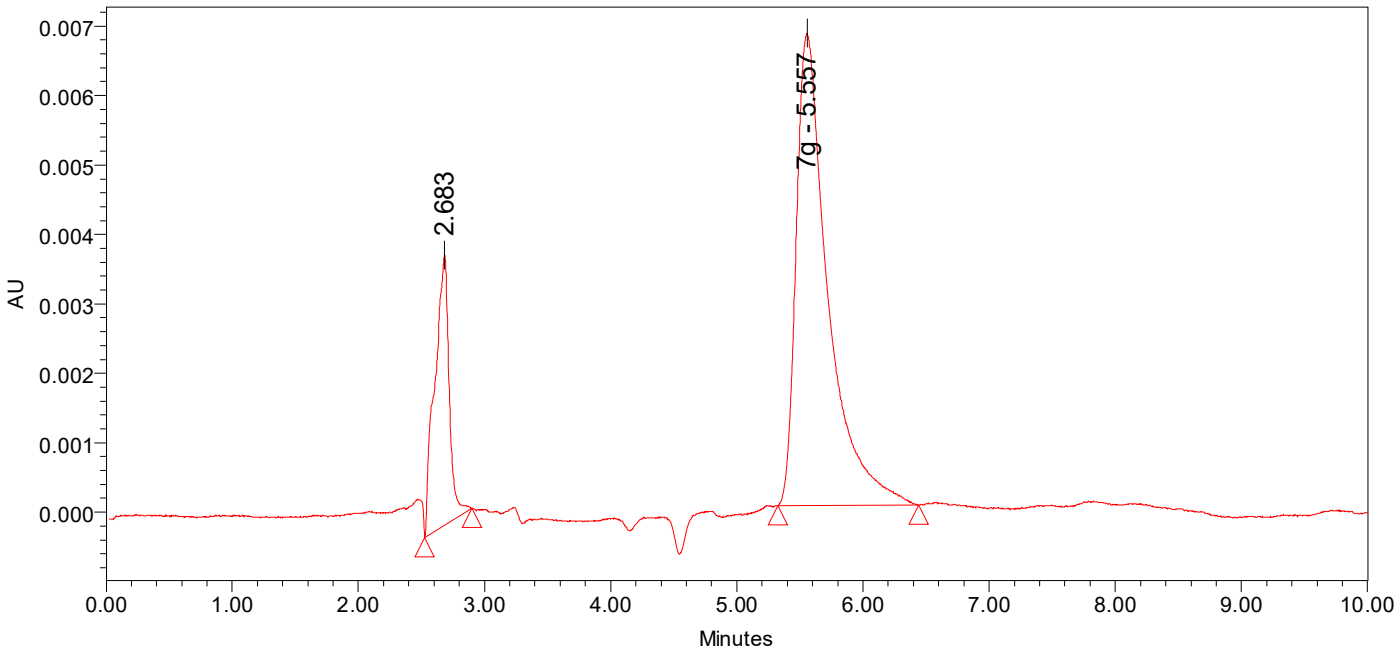
HPLC chromatogram of 7g

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7g	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	8	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7g processing
Injection Volume:	10.00 ul	Channel Name:	223.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.0 nm (2998
Date Acquired:	23-10-2024 12:18:07 PM IST		
Date Processed:	25-10-2024 09:24:58 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.683	31120	20.72
2	7g	5.557	119107	79.28

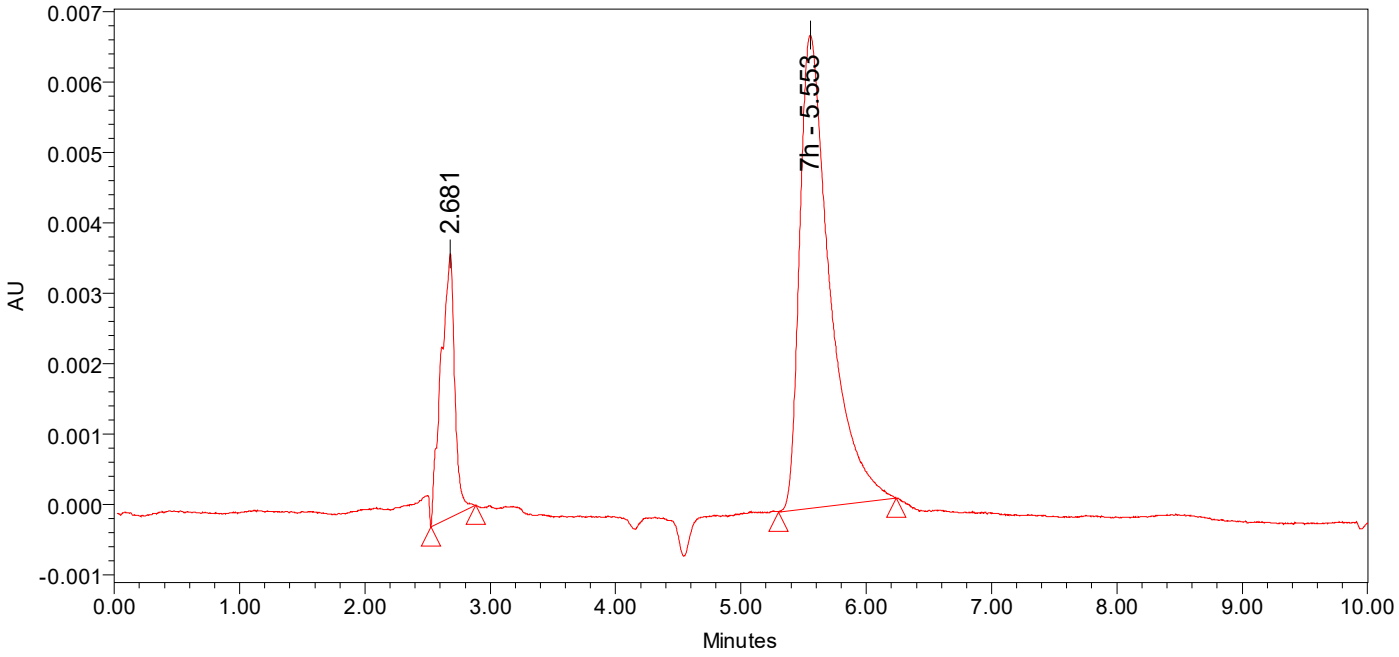
HPLC chromatogram of 7h

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7h	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	9	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7h Processing
Injection Volume:	10.00 ul	Channel Name:	223.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.0 nm (2998
Date Acquired:	23-10-2024 12:28:47 PM IST		
Date Processed:	25-10-2024 09:27:27 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.681	28132	20.02
2	7h	5.553	112377	79.98

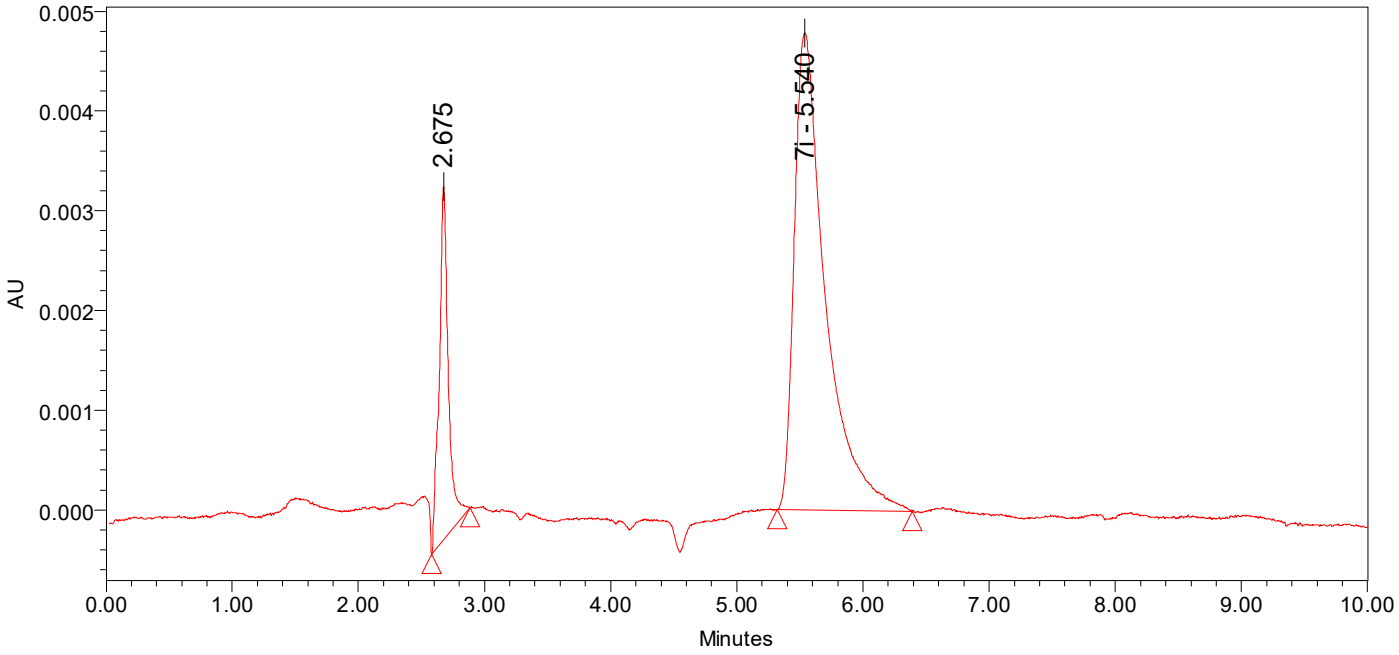
HPLC chromatogram of 7i

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7i	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	10	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7i Processing
Injection Volume:	10.00 ul	Channel Name:	223.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.0 nm (2998
Date Acquired:	23-10-2024 12:39:28 PM IST		
Date Processed:	25-10-2024 09:35:10 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.675	17805	17.86
2	7i	5.540	81889	82.14

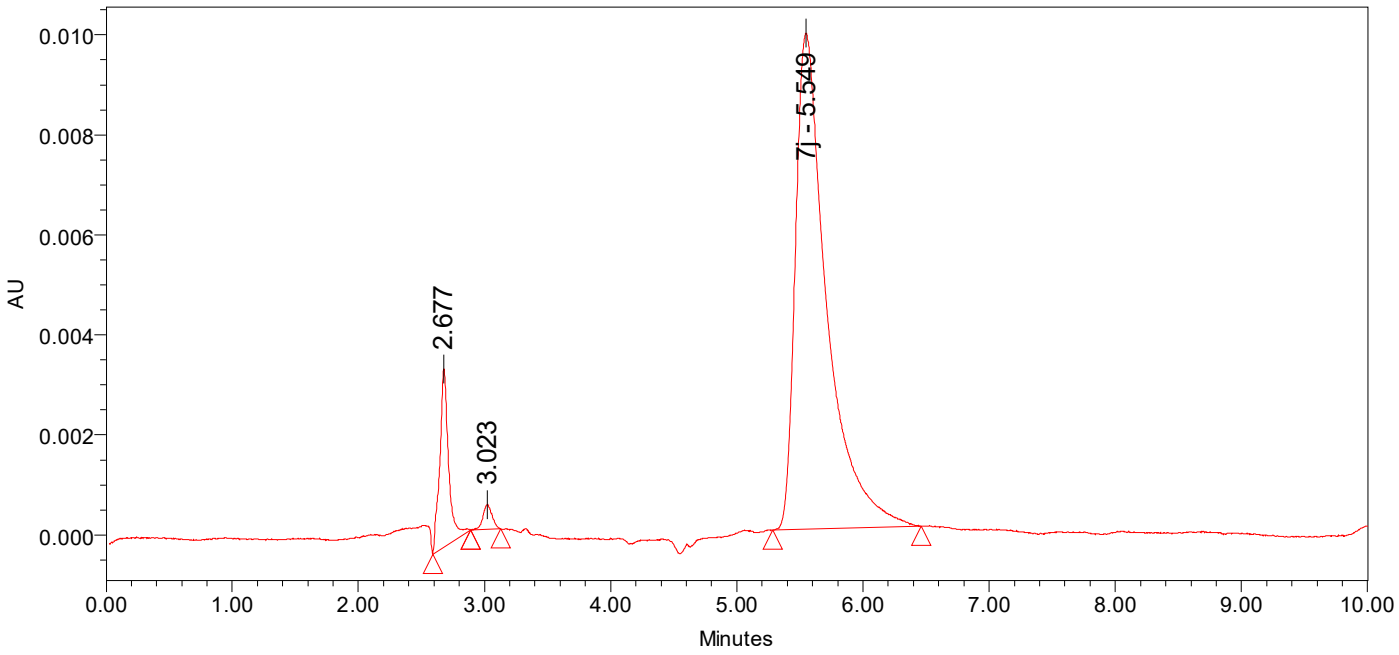
HPLC chromatogram of 7j

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7j	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	11	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7j
Injection Volume:	10.00 ul	Channel Name:	223.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.0 nm (2998
Date Acquired:	23-10-2024 12:50:09 PM IST		
Date Processed:	25-10-2024 09:56:46 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.677	17499	9.14
2		3.023	2554	1.33

	Name	RT	Area	% Area
3	7j	5.549	171486	89.53

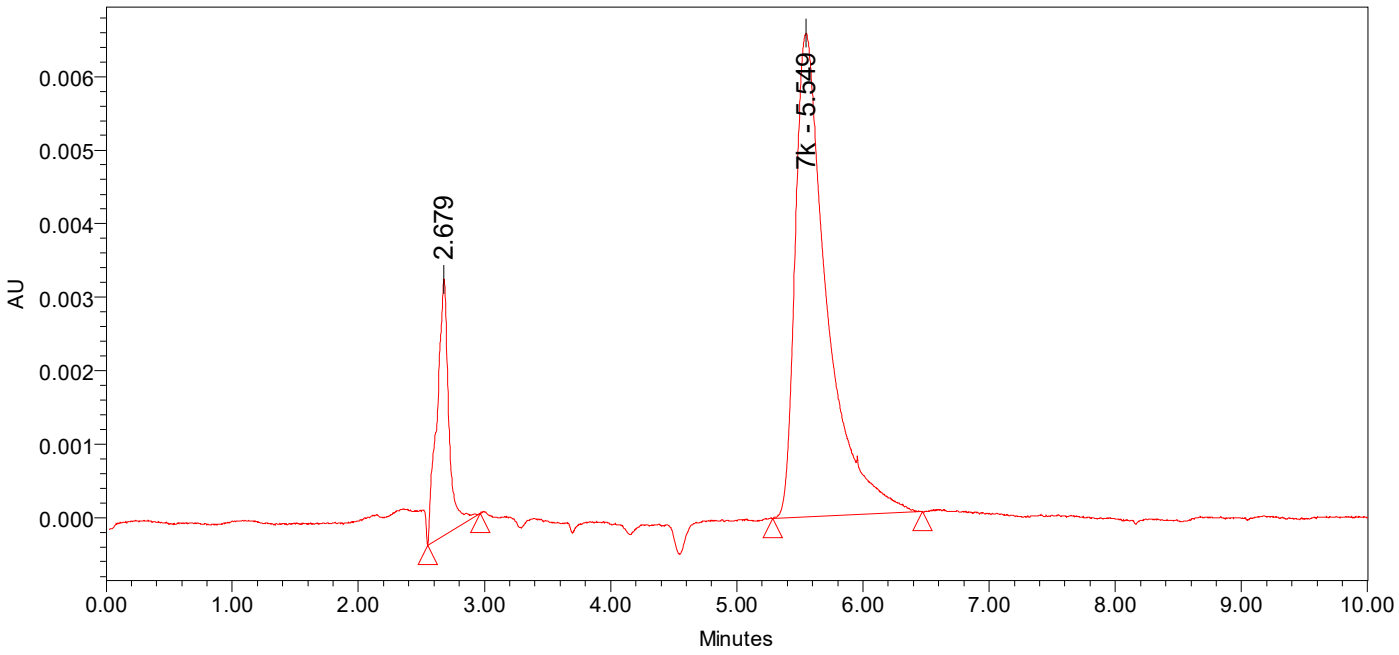
HPLC chromatogram of 7k

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7k	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	12	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7k
Injection Volume:	10.00 ul	Channel Name:	223.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.0 nm (2998
Date Acquired:	23-10-2024 01:00:51 PM IST		
Date Processed:	25-10-2024 09:37:41 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.679	22804	16.55
2	7k	5.549	115001	83.45

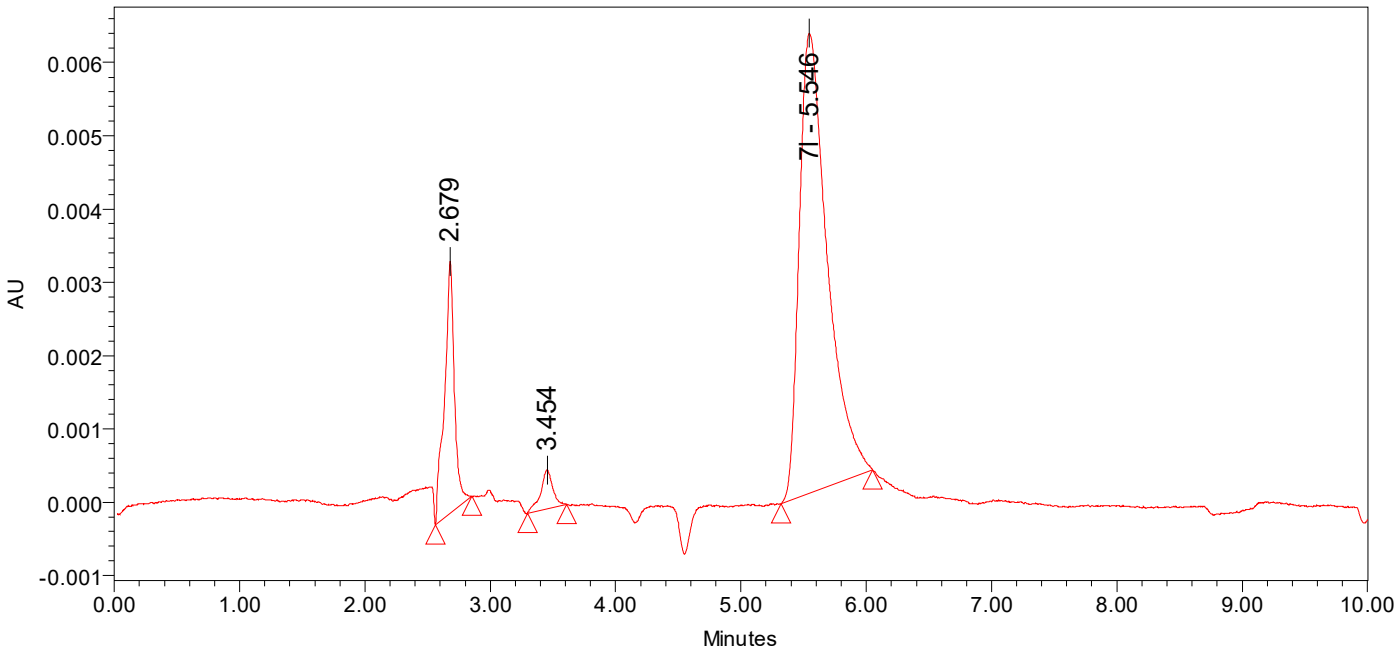
HPLC chromatogram of 7l

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY
KLE COLLEGE OF PHARMACY, BELAGAVI

SAMPLE INFORMATION

Sample Name:	7l	Acquired By:	User_1
Sample Type:	Unknown	Sample Set Name:	Trial1_23102024_SS
Vial:	13	Acq. Method Set:	Trial1_23102024_MS
Injection #:	1	Processing Method:	7l Processing
Injection Volume:	10.00 ul	Channel Name:	223.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 223.0 nm (2998
Date Acquired:	23-10-2024 01:11:30 PM IST		
Date Processed:	25-10-2024 09:40:36 AM IST		

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		2.679	18760	15.61
2		3.454	3559	2.96
3	7l	5.546	97847	81.43