

SUPPORTING INFORMATION

DESIGN, BIOLOGICAL EVALUATION, AND COMPUTER-AIDED ANALYSIS OF DIHYDROTHIAZEPINES AS SELECTIVE ANTICHLAMYDIAL AGENTS

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Table S1. Detailing of the Antichlamydial potency in different unit measures.

ID	IC₅₀ (µg/mL)	IC₅₀ (µM)	pIC₅₀
5a	1.61	4.40	5.36
5b	3.32	8.94	5.05
5c	4.69	12.57	4.90
5e	5.18	12.65	4.90
5d	4.79	12.77	4.89
11b	6.93	14.19	4.85
5g	6.37	15.51	4.81
11a	6.53	15.72	4.80
5f	6.35	16.43	4.78
5k	7.44	17.50	4.76
5h	6.59	17.54	4.76
5l	7.50	17.84	4.75
5j	7.18	17.97	4.75
5i	6.72	18.90	4.72
5y	7.36	21.19	4.67
5n	9.00	23.30	4.63
5m	9.00	24.57	4.61
5o	10.21	27.87	4.56
11c	12.30	27.99	4.55
7a	10.00	28.79	4.54
5q	14.69	39.55	4.40
5p	14.41	40.32	4.40
13a	14.99	44.32	4.35
344	16.53	46.24	4.34
6a	17.63	49.45	4.31
9a	16.08	49.73	4.30
5s	22.76	50.86	4.29
13c	22.60	53.91	4.27
9b	21.35	57.35	4.24
13b	20.88	59.77	4.22
9c	21.45	69.78	4.16
11d	0.70	1.61	5.79
11e	1.08	2.46	5.60
5x	2.78	7.82	5.10

Table S2. Detailing of the prediction accuracy of KPLS-radial 2D QSAR Model (radial 13).

ID	Set	Y(Exp)	Y(Pred)	Error
5a	train	5.36	5.14	-0.22
5b	train	5.05	5.04	-0.01
5c	test	4.90	4.89	-0.01
5e	train	4.90	4.90	0.00
5d	test	4.89	4.77	-0.12
11b	train	4.85	4.75	-0.10
5g	train	4.81	4.97	0.16
11a	train	4.80	4.91	0.11
5f	train	4.78	4.74	-0.05
5k	train	4.76	4.66	-0.10
5h	test	4.76	4.63	-0.13
5l	train	4.75	4.63	-0.12
5j	train	4.75	4.56	-0.19
5i	train	4.72	4.52	-0.20
5y	train	4.67	4.80	0.13
5n	test	4.63	4.59	-0.04
5m	train	4.61	4.72	0.11
5o	train	4.56	4.52	-0.03
11c	train	4.55	4.58	0.03
7a	test	4.54	4.51	-0.03
5q	train	4.40	4.46	0.06
5p	test	4.40	4.44	0.05
13a	train	4.35	4.35	-0.01
344	train	4.34	4.59	0.25
6a	train	4.31	4.44	0.14
9a	train	4.30	4.16	-0.14
5s	train	4.29	4.41	0.12
13c	test	4.27	4.37	0.10
9b	train	4.24	4.23	-0.01
13b	train	4.22	4.32	0.10
9c	train	4.16	4.13	-0.03

*Biological activity displayed (both experimental and predicted) are presented in pIC₅₀ format.

Table S3. Statistical parameters of the model generated by AutoQSAR Fingerprint (radial 13) - Kernel based partial least square regression.

	Training set			Test set	
	Score	SD	R ²	RMSE	Q ²
Model KPLS - radial 13	0.83	0.13	0.83	0.08	0.87
Reference Value	-	-	>0.6	-	>0.5

As presented in Table S3, the obtained model displays satisfactory statistical results. The correlation coefficient (R^2) is a measure of the data explained by the model. The acceptable R^2 value for regression models is >0.6 (more than 60% of the explained variance).¹ The predictability of the model in the test set was tested by the coefficient of determination between the observed and predicted biological activities for the test set (Q^2).² This last parameter should have a minimum acceptable value of 0.5 indicating 50% prediction of variability. The difference between R^2 and Q^2 should be less than 0.1 because higher values may indicate overfitting of the model.³ Further, the standard deviation of the regression (SD) calculated based on the training set and the root mean square error in the test set predictions (RMSE)⁴ expresses the variability not explained by the model, and thus should have the lowest possible value.^{4,5} The score value presented in Table 5 is an internal parameter from AutoQSAR calculated by the software to guide the user decision regarding the best model among the ones generated.⁶

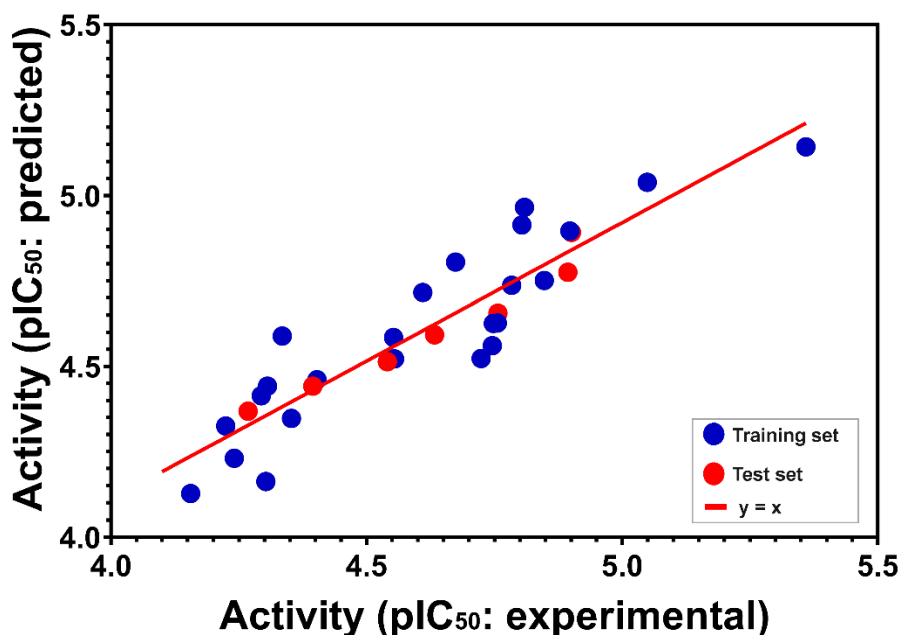
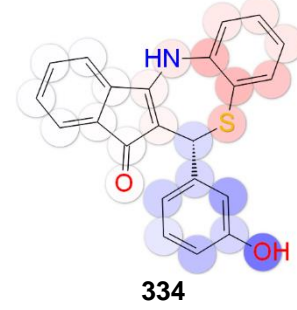
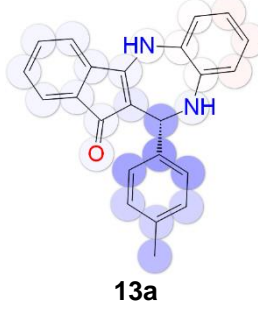
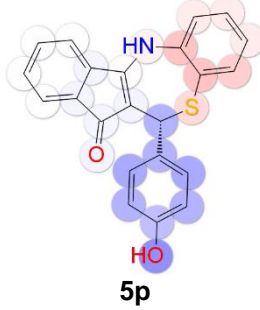
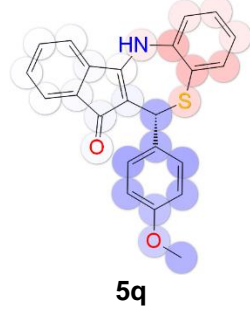
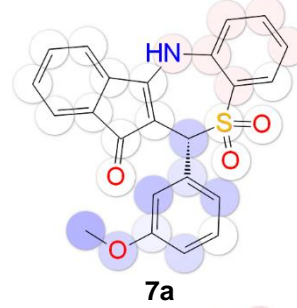
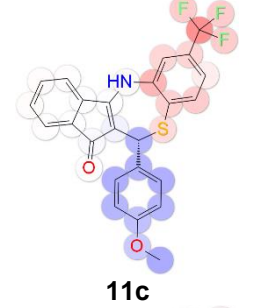
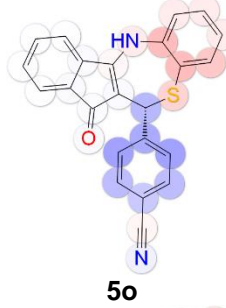
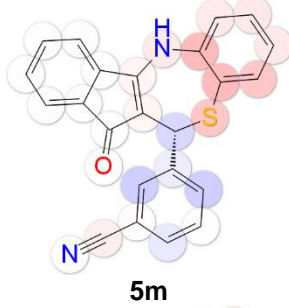
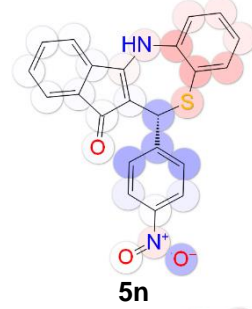
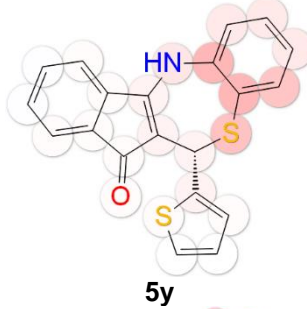
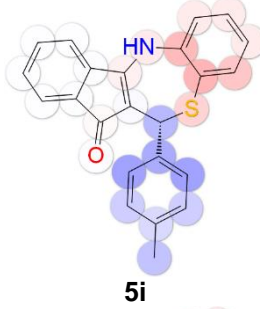
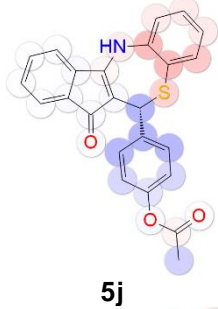
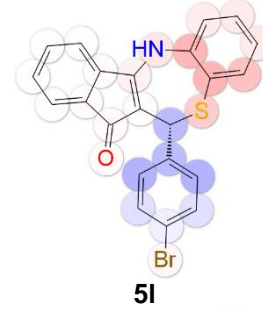
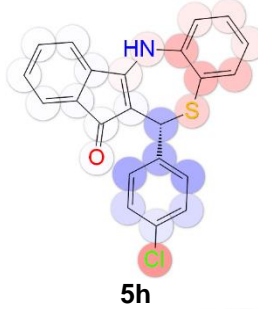
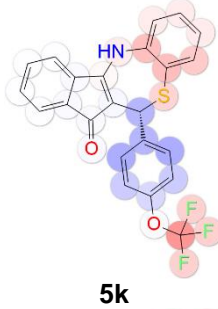
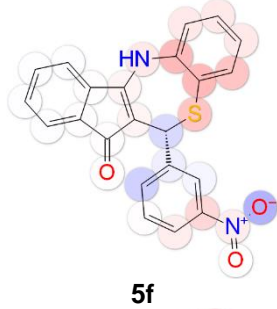
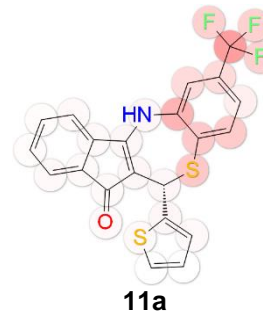
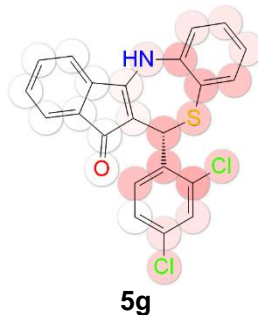
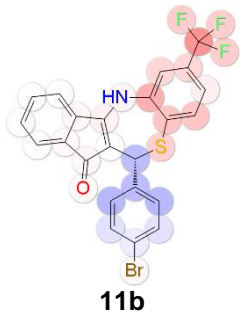
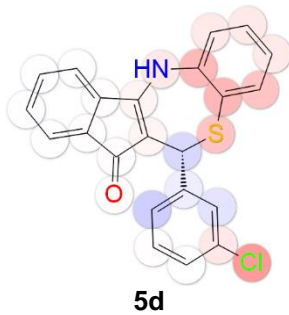
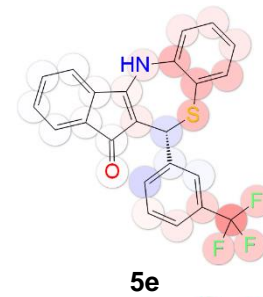
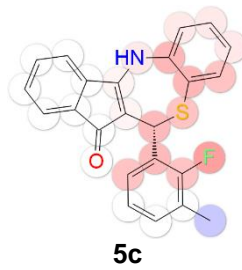
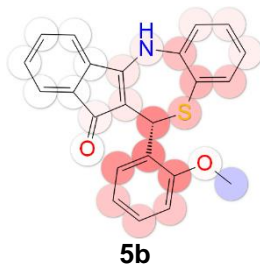
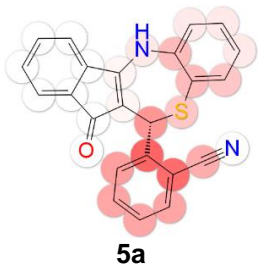


Figure S1. Experimental versus KPLS-radial 2D QSAR model (radial 13) predicted values of antichlamydial activity (pIC_{50}).



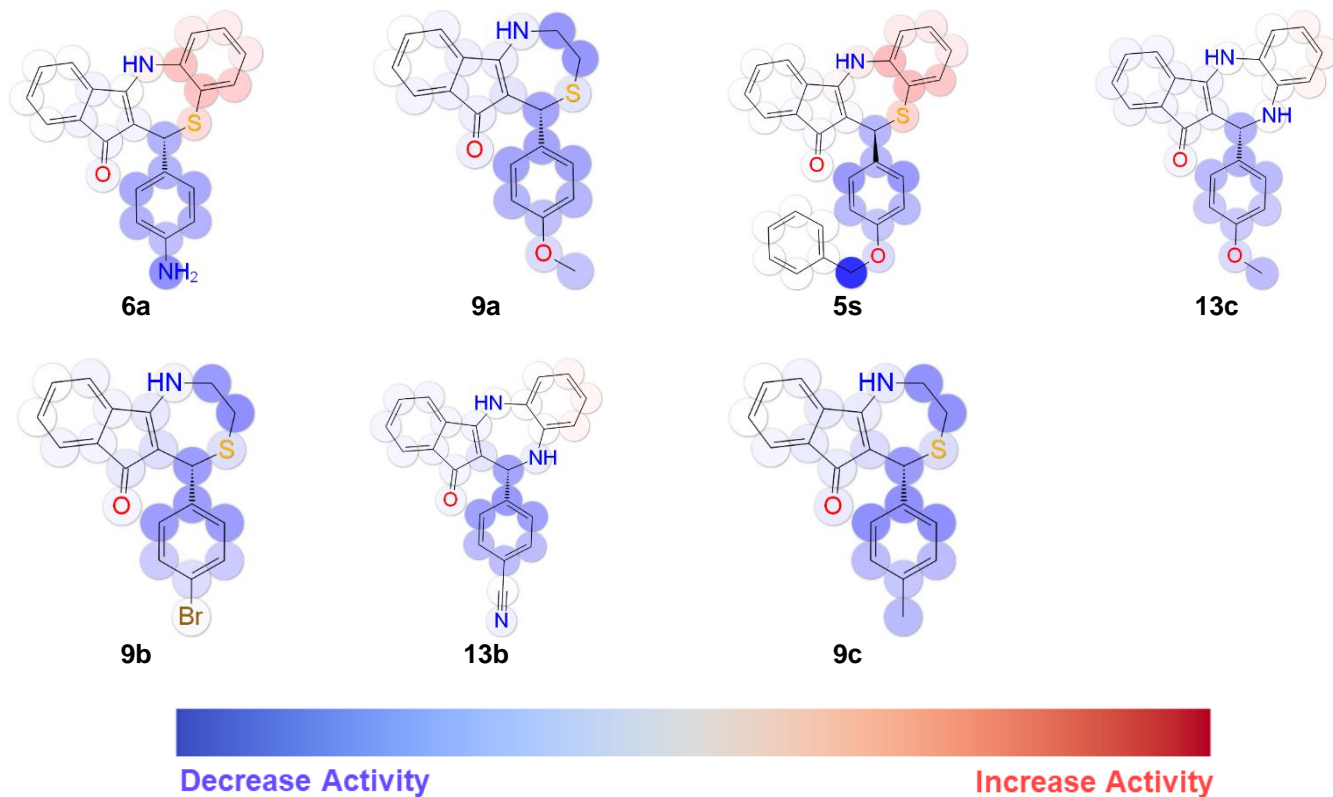


Figure S2. Color maps for the 2D fingerprint (radial 13) QSAR model for all the molecules used to generate the QSAR model. Atoms that display a favorable contribution to the antichlamydial activity are colored red and unfavorable are colored blue. Color intensity reflects the strength of the effect. Note₁: stereochemistry is displayed because the molecules are drawn as 3D form, which is required for Maestro software to display the QSAR color maps. However, stereochemistry is not considered in the generation of the 2D descriptors used to build the model. Note₂: Only molecules with a determined value of antichlamydial activity were used to generate the QSAR model. Therefore, molecules with no inhibition seen within the concentration range tested (25 -0.39 $\mu\text{g/mL}$) are not included.

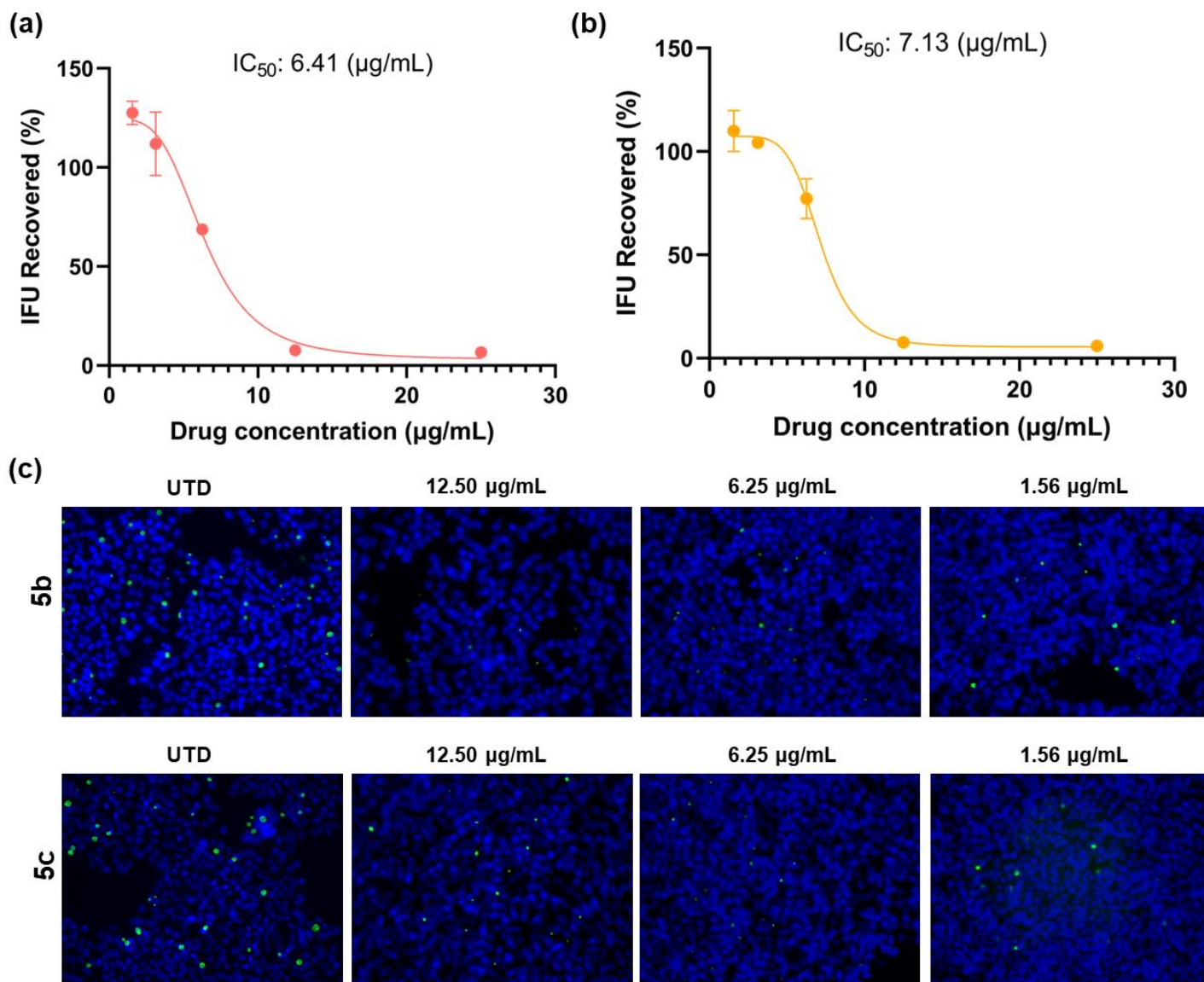


Figure S3. Dose–response curves for the effect of **5b** (a) and **5c** (b) reported as % of recovered IFU. Error bars report SEM (N = 3). (c): immunofluorescence images of **5b** and **5c** inhibitory effect. Chlamydial inclusions are displayed in green (MOMP - Ctr L2) and HEP-2 cell nuclei in blue (DAPI). Images were acquired on 20x magnification using an Olympus CKX53 fluorescence microscope with EP50 camera. Channel merge was processed using ImageJ software. UTD: untreated; AZM: Azithromycin. Omitted error bars indicates a SD value shorter than the size of the symbol presented in the plots.

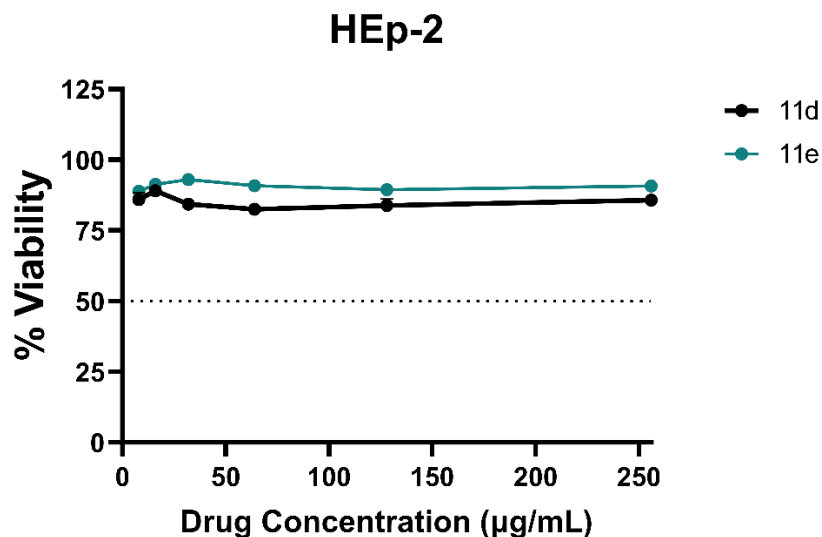
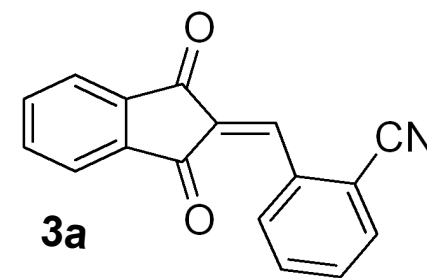
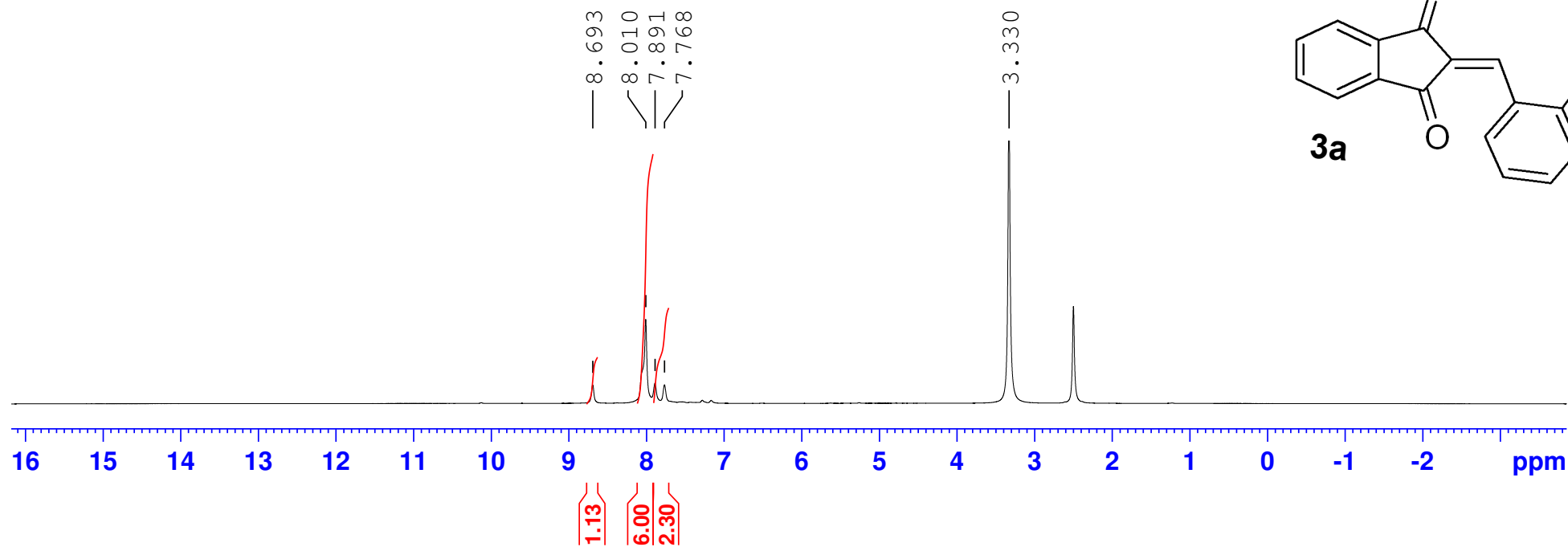
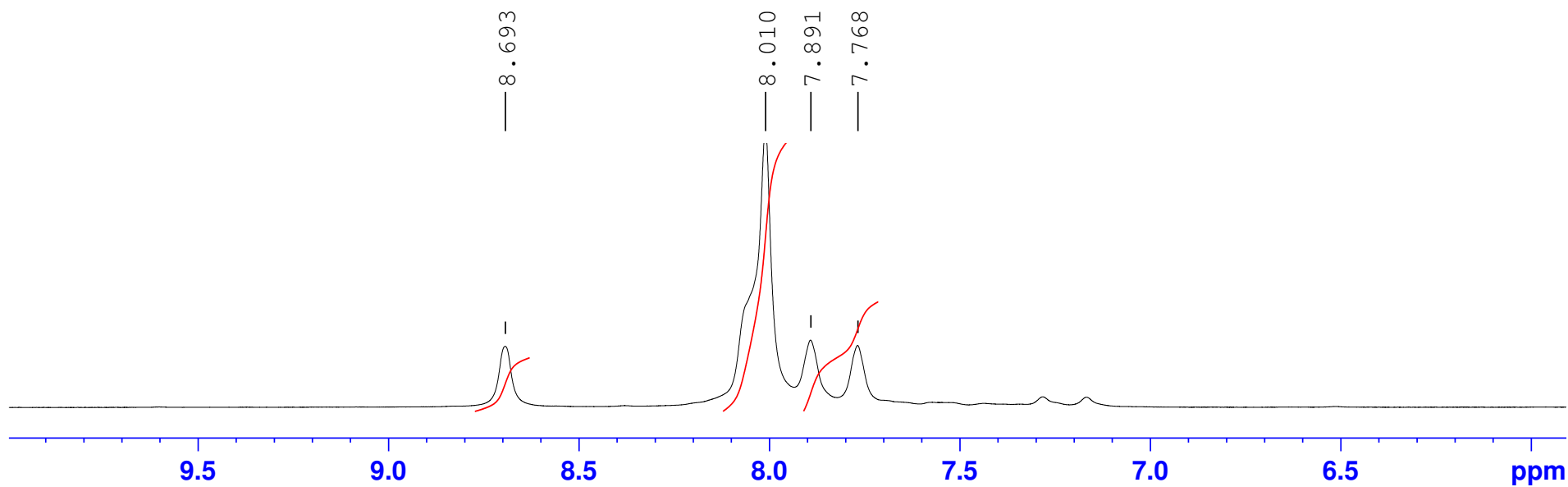
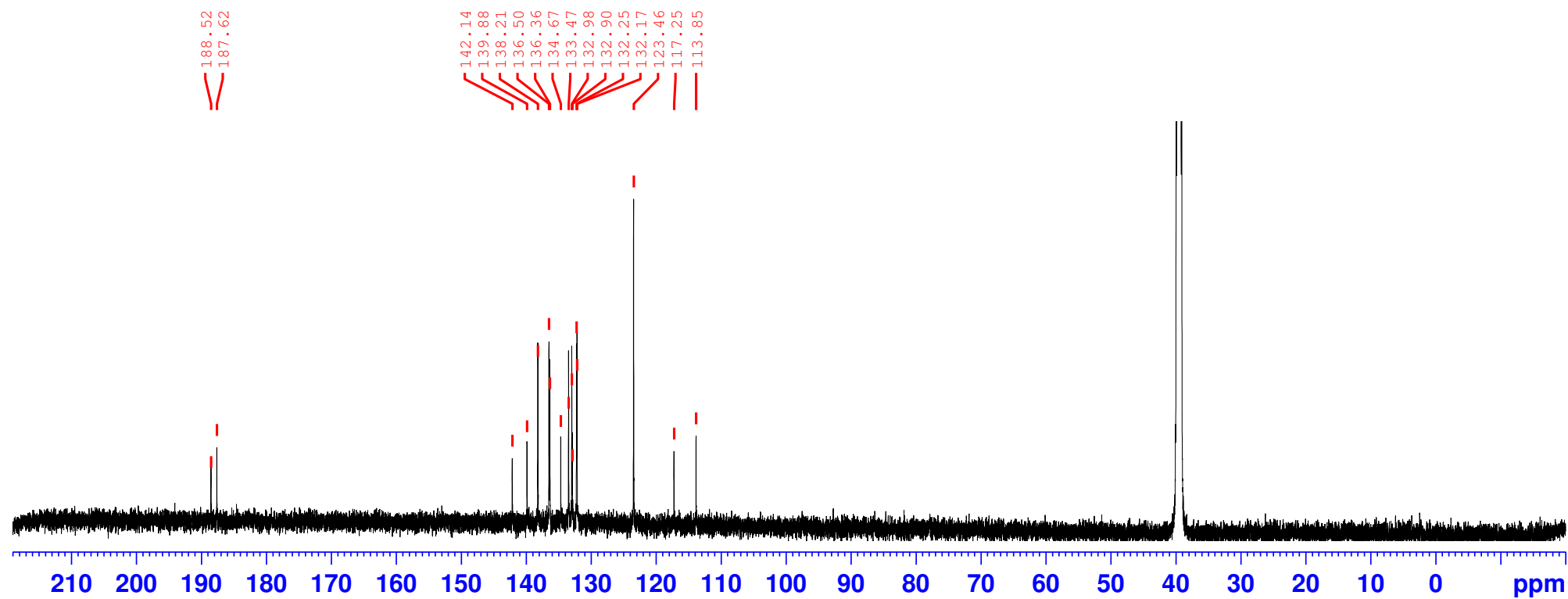
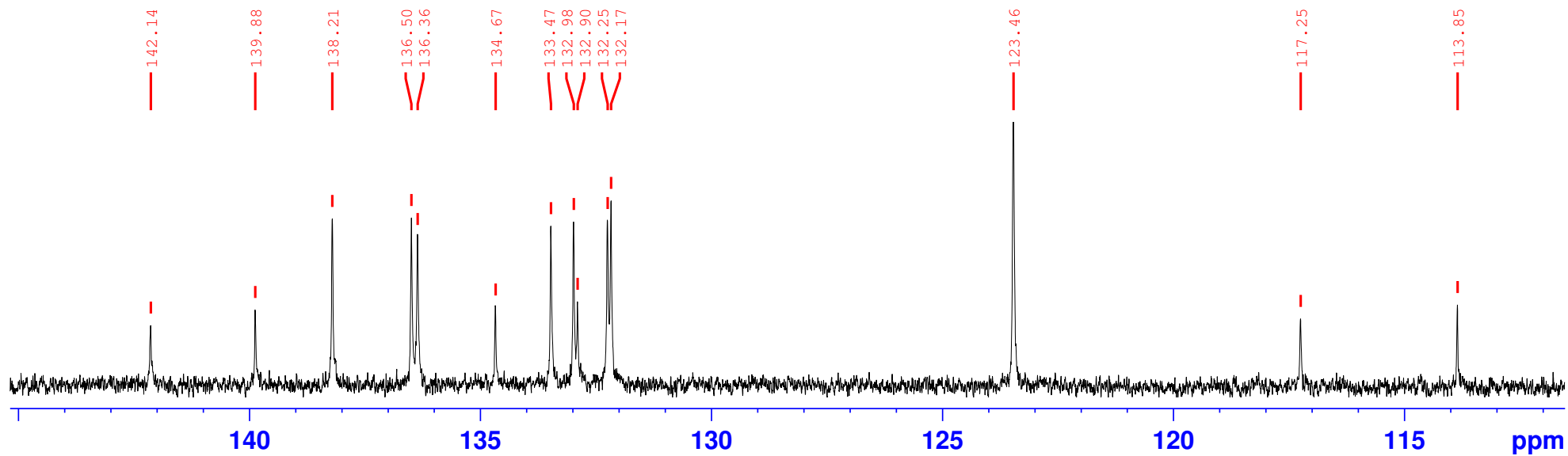


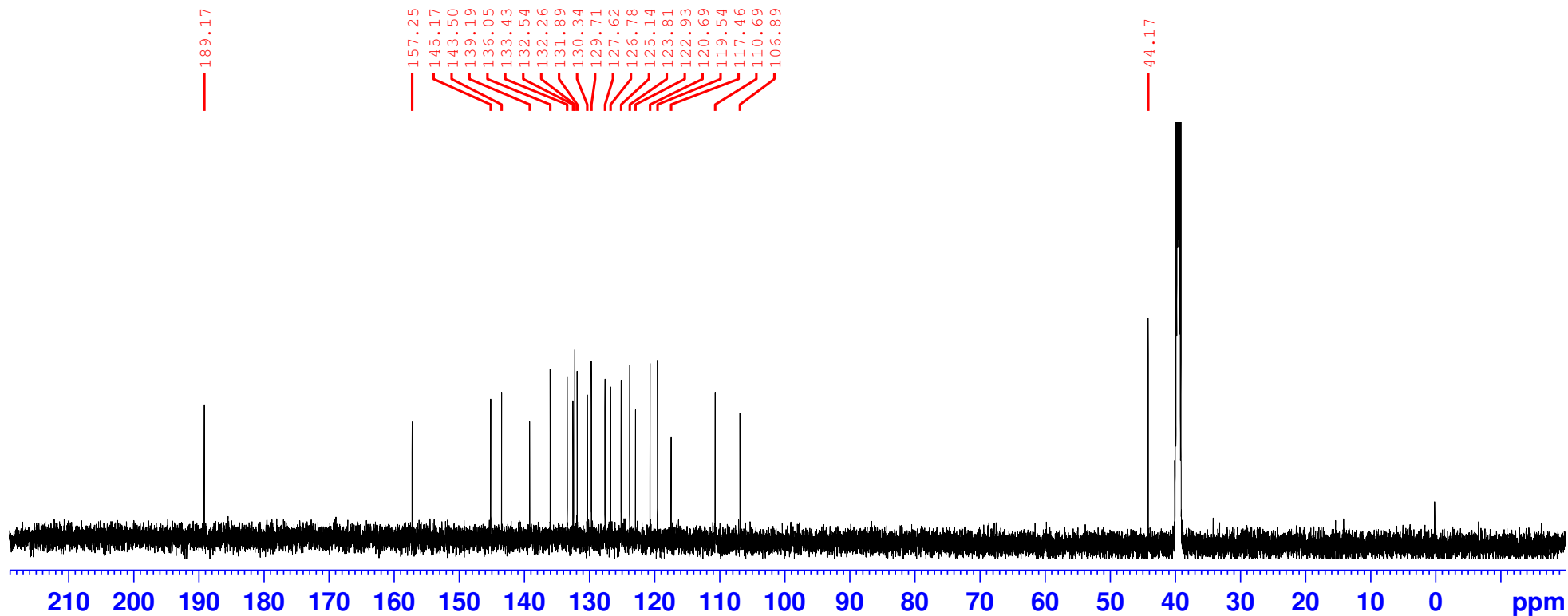
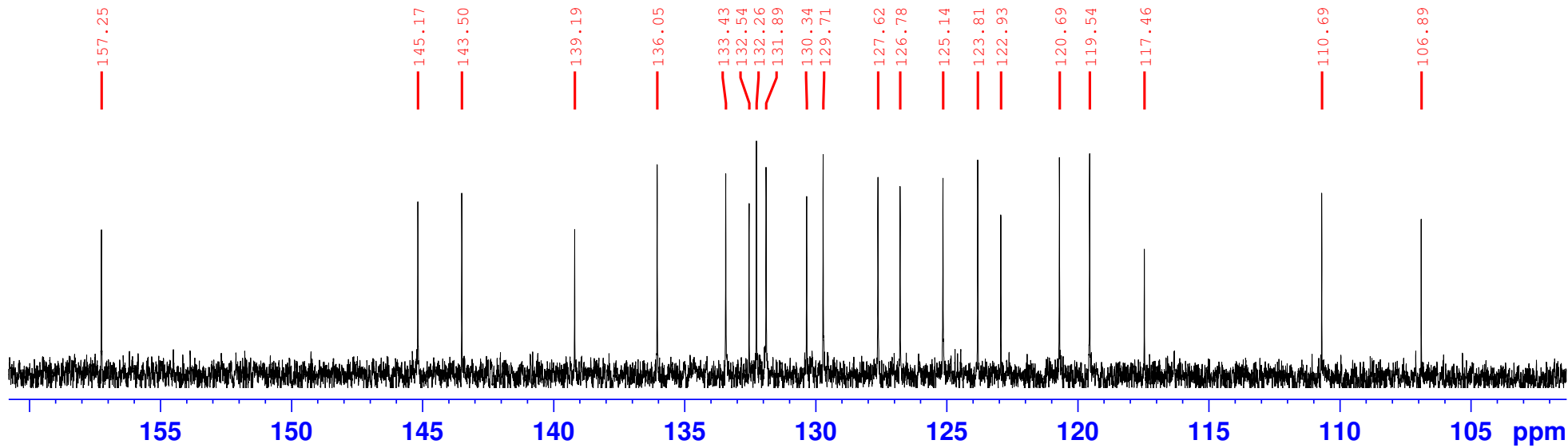
Figure S4. Viability analysis for molecules **11d** and **11e** against HEp-2 cell line. Error bars report SEM (N = 3). Each experiment included technical replicates. Omitted error bars indicates a SD value shorter than the size of the symbol presented in the plots.

REFERENCES

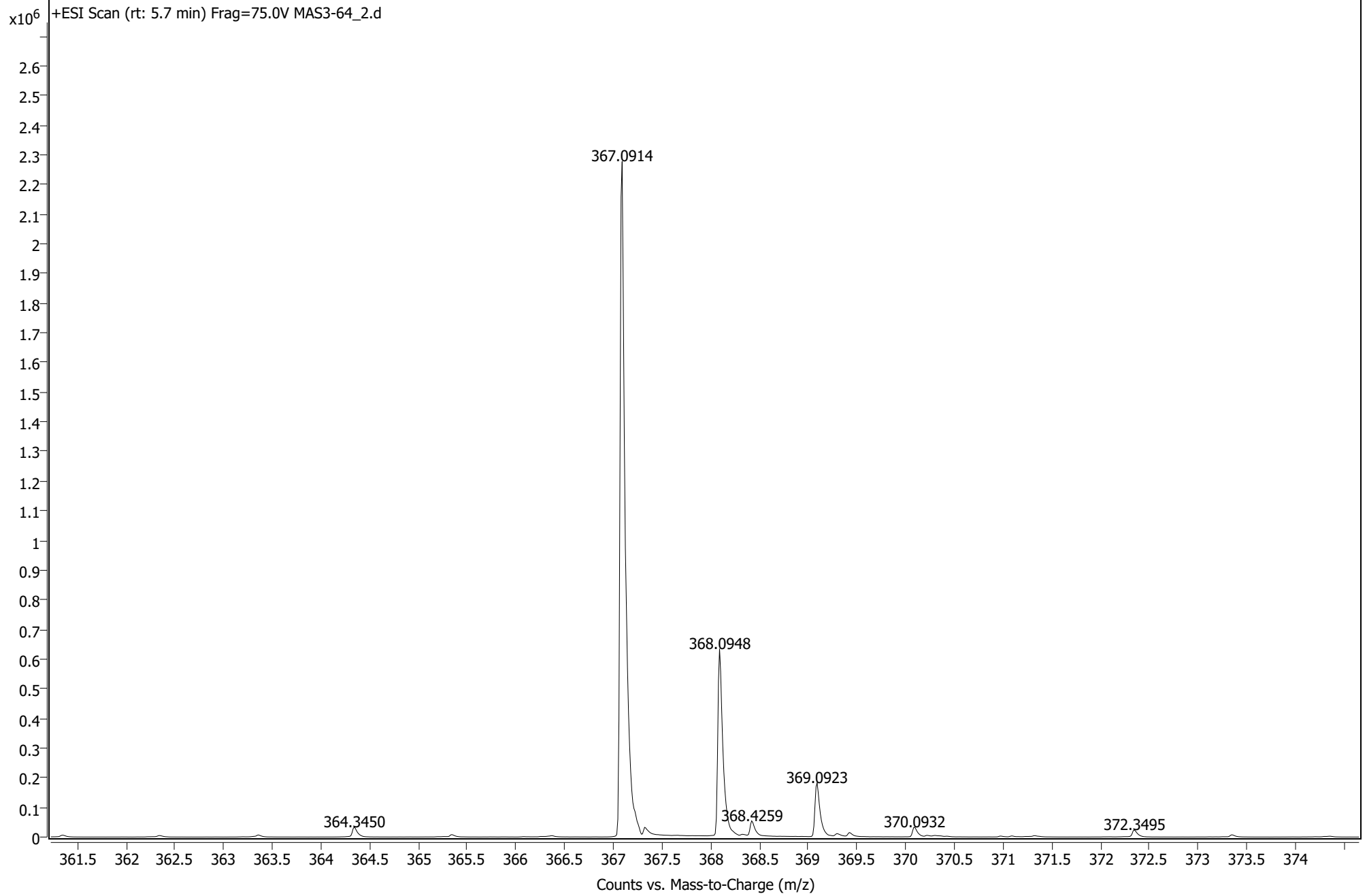
- (1) Alexander, D. L. J.; Tropsha, A.; Winkler, D. A. Beware of R²: Simple, Unambiguous Assessment of the Prediction Accuracy of QSAR and QSPR Models. *J. Chem. Inf. Model.* **2015**, *55* (7), 1316-1322.
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- (4) Gramatica, P. Principles of QSAR models validation: internal and external. *QSAR & Comb. Sci.* **2007**, *26* (5), 694-701.
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- (6) Dixon, S. L.; Duan, J.; Smith, E.; Barga, C. D. V.; Sherman, W.; Repasky, M. P. AutoQSAR: an automated machine learning tool for best-practice quantitative structure–activity relationship modeling. *Future Med. Chem.* **2016**, *8* (15), 1825-1839.







User Spectrum Plot Report



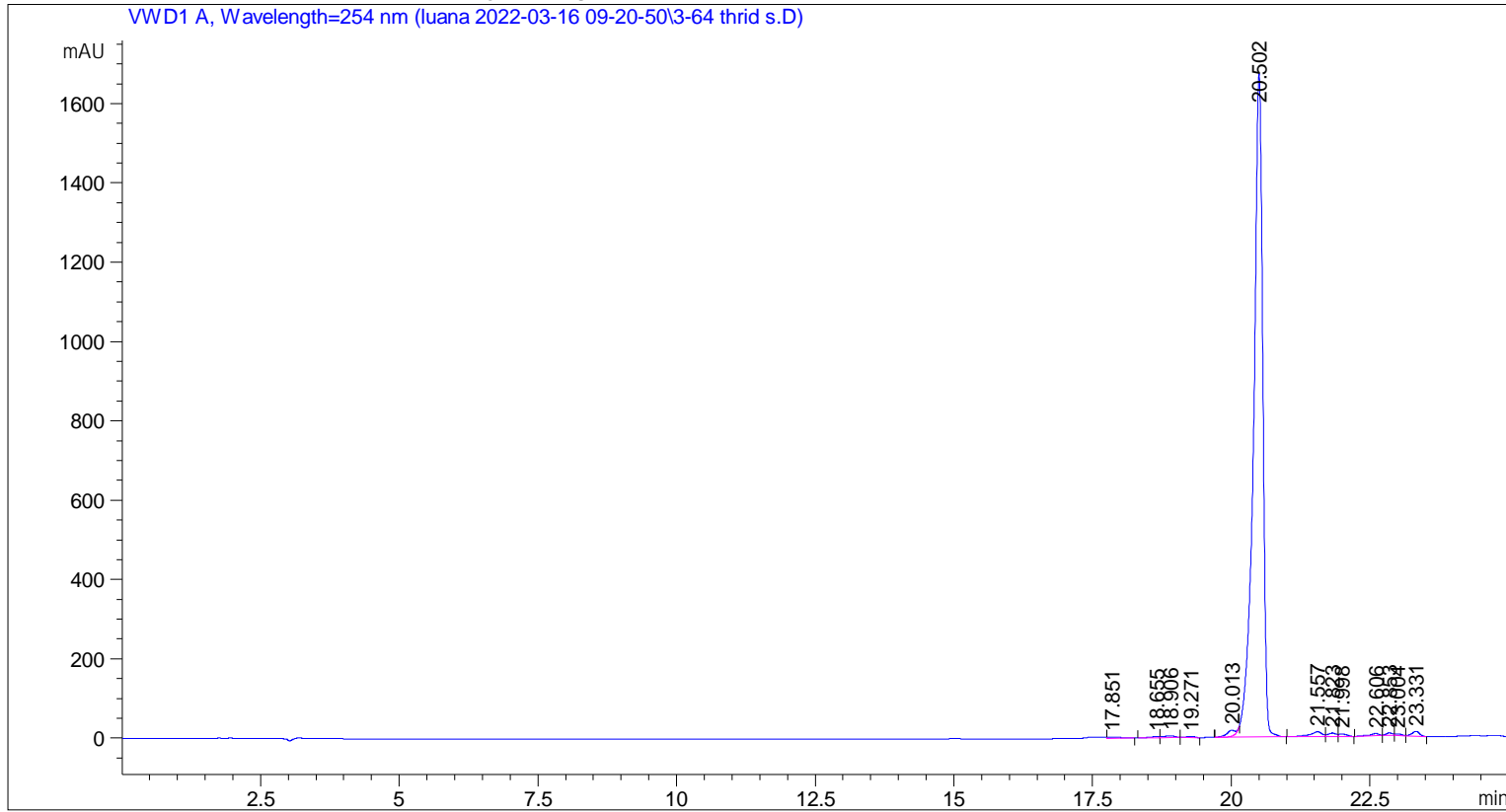
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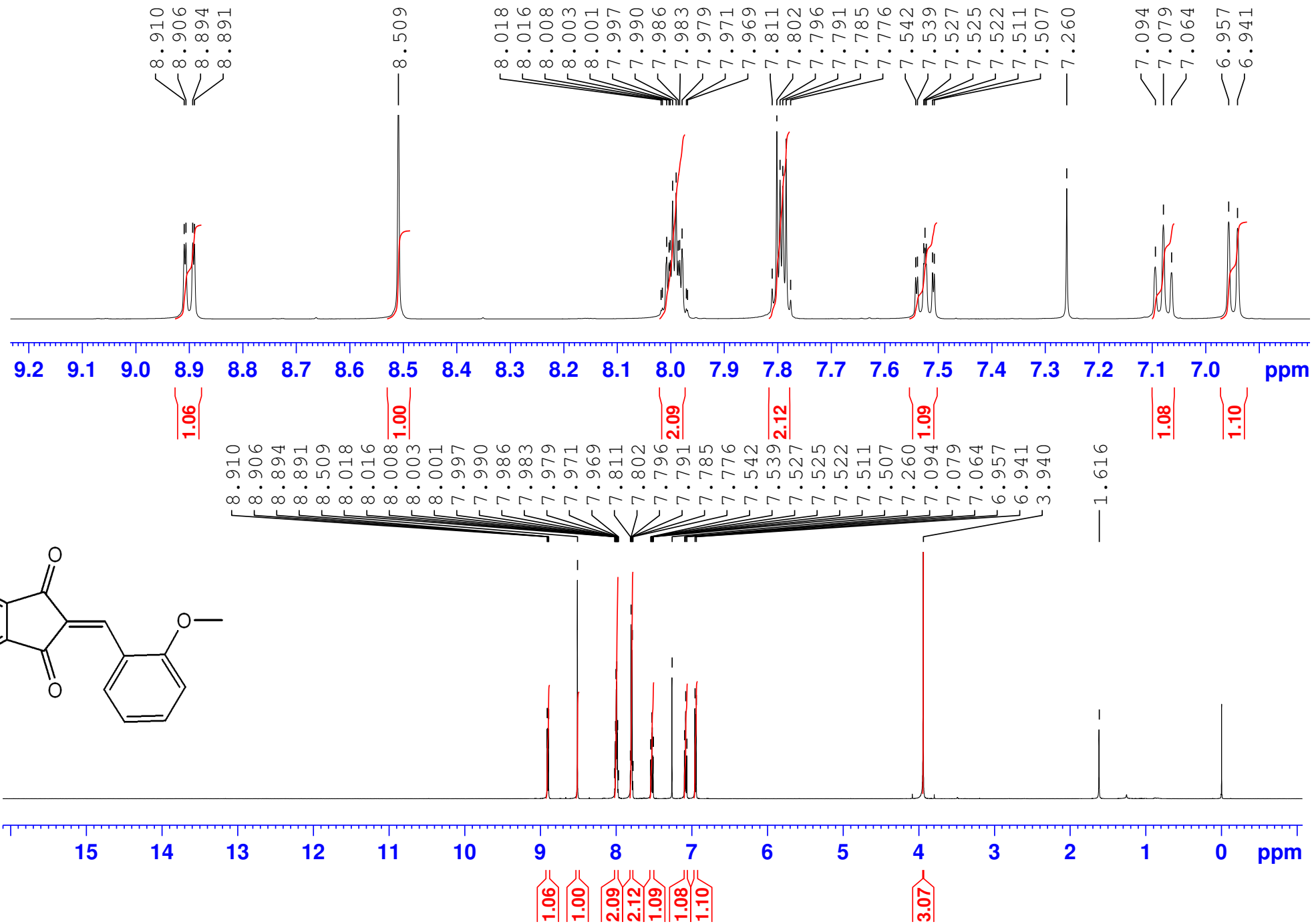
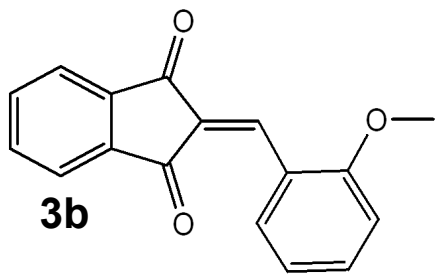
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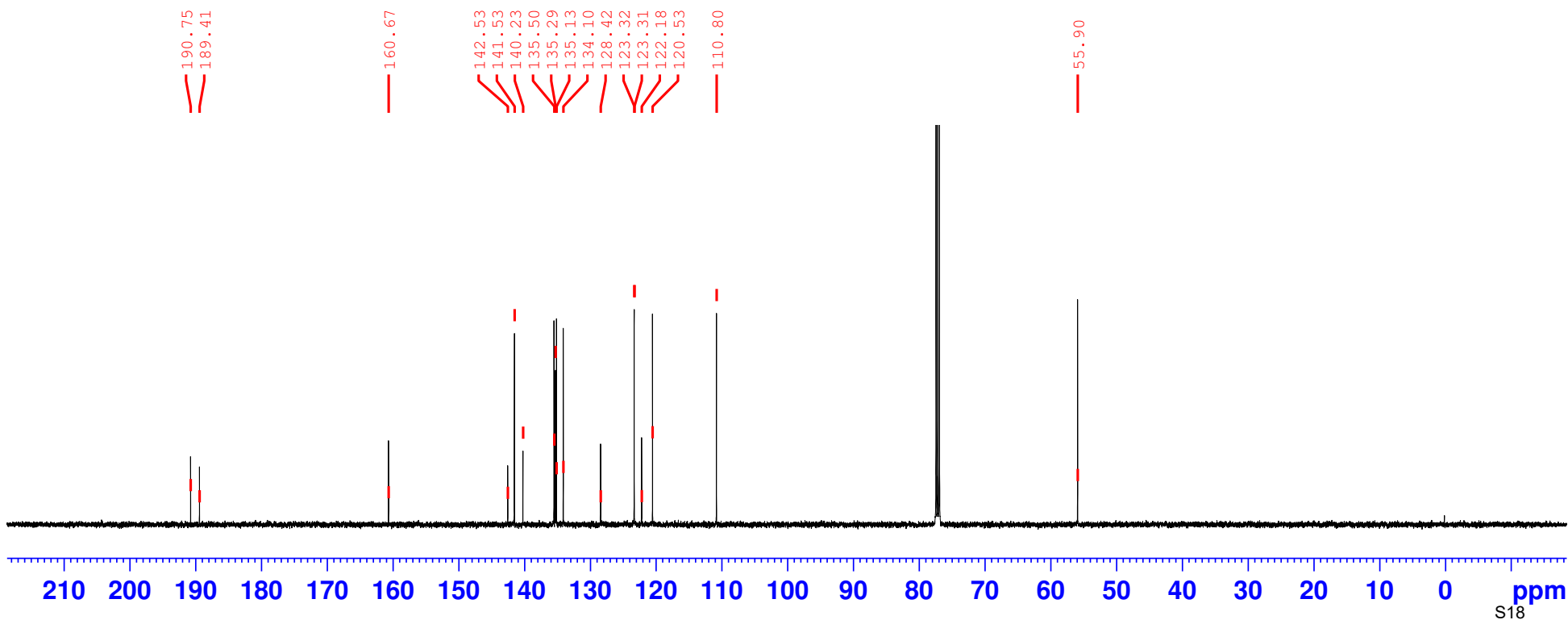
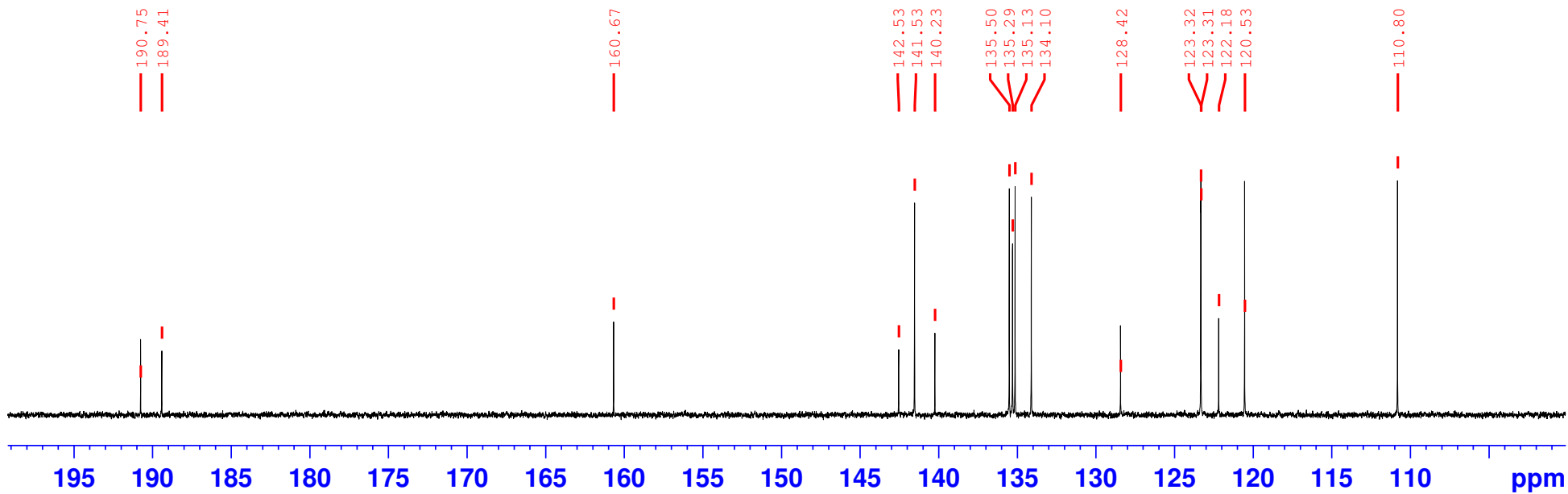
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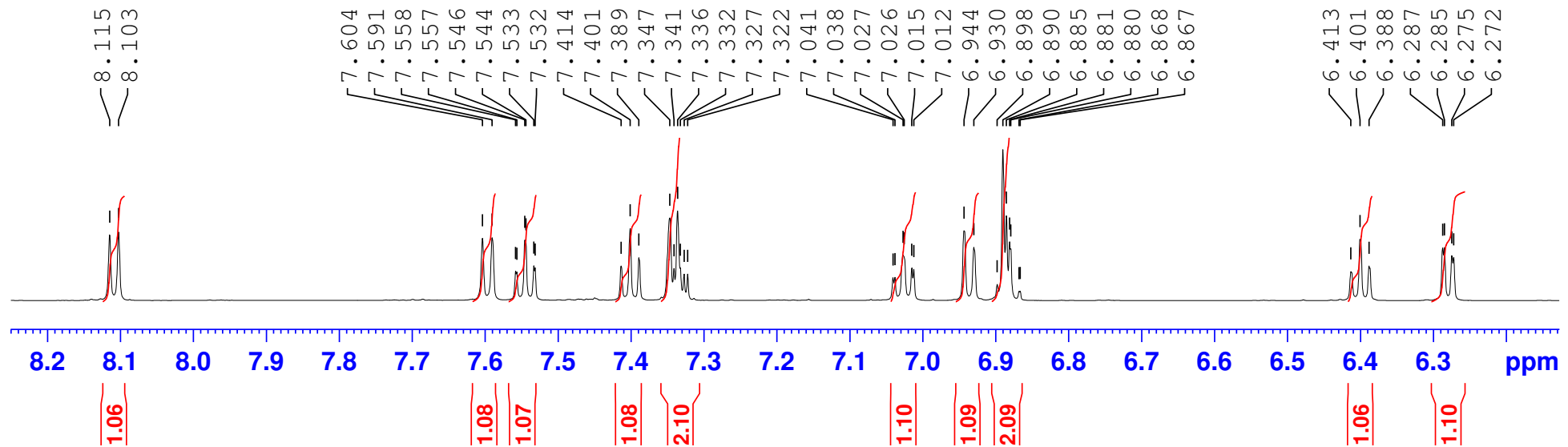
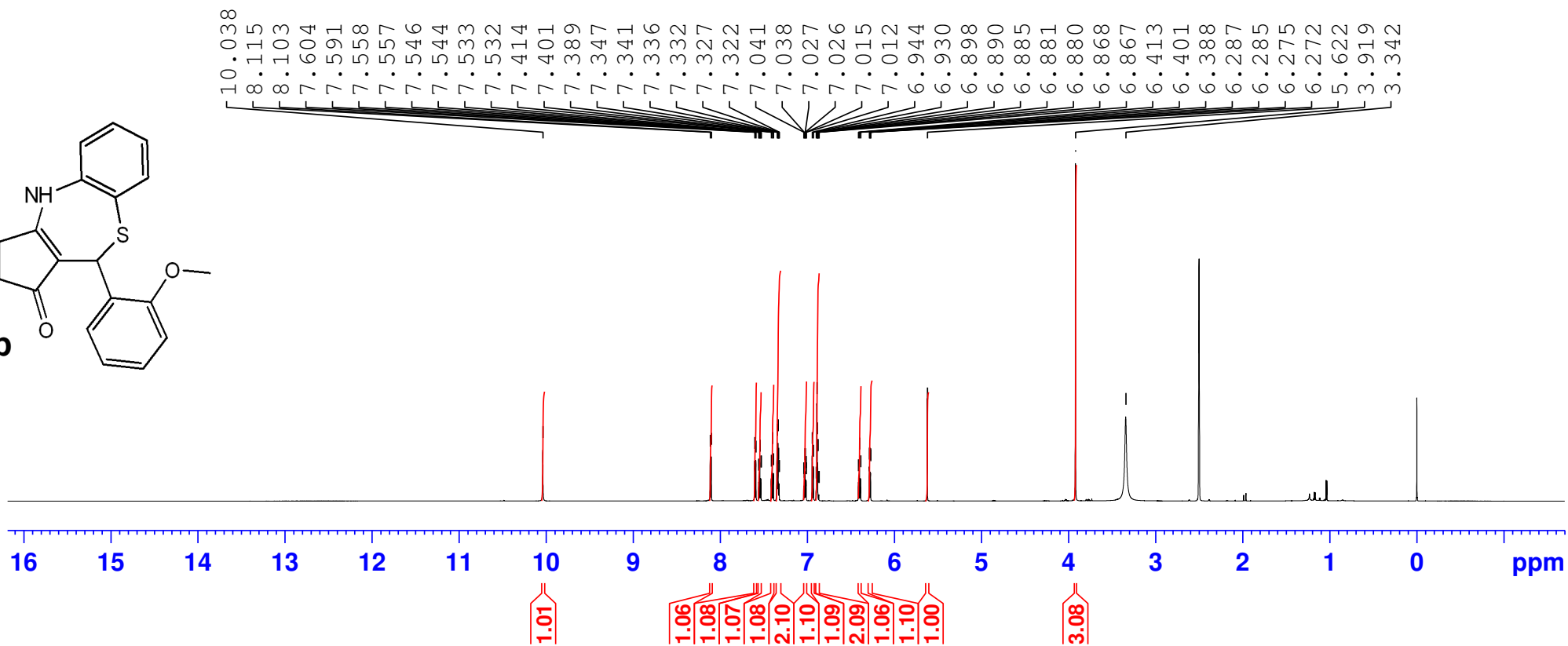
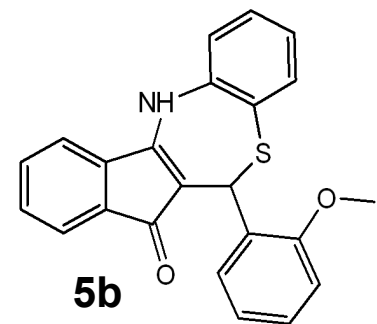
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7	21.557	BV	0.2184	197.02502	12.53508	0.9675
8	21.823	VV	0.1556	94.62735	8.93035	0.4647
9	21.998	VB	0.1626	63.78162	6.27615	0.3132
10	22.606	BB	0.1515	53.95757	5.31438	0.2650
11	22.853	BV	0.1274	52.95997	6.40889	0.2601
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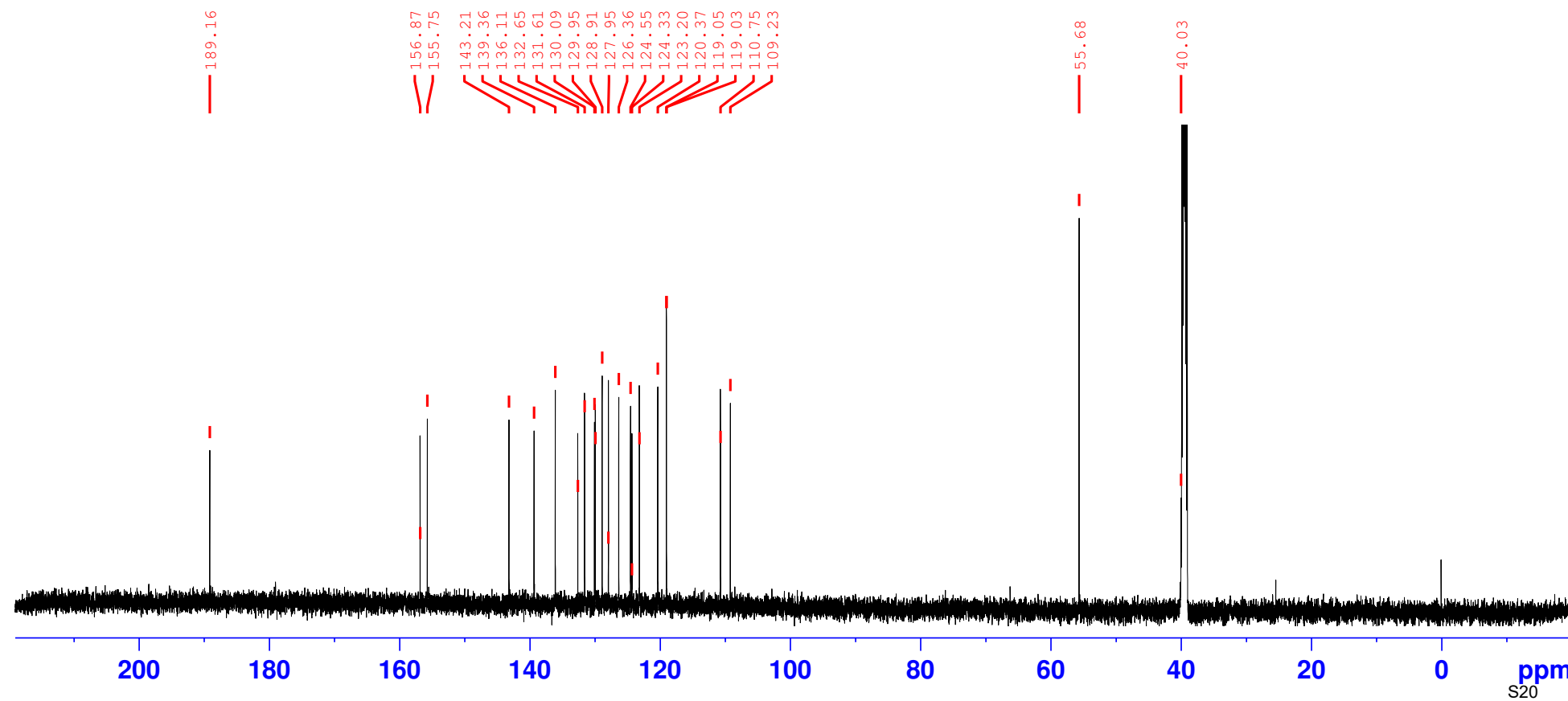
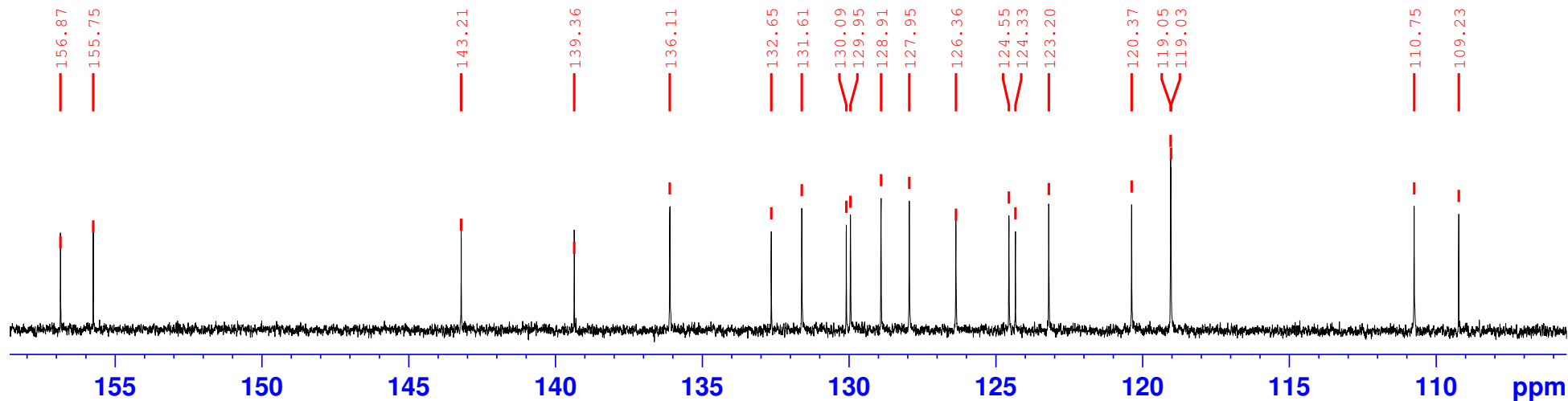
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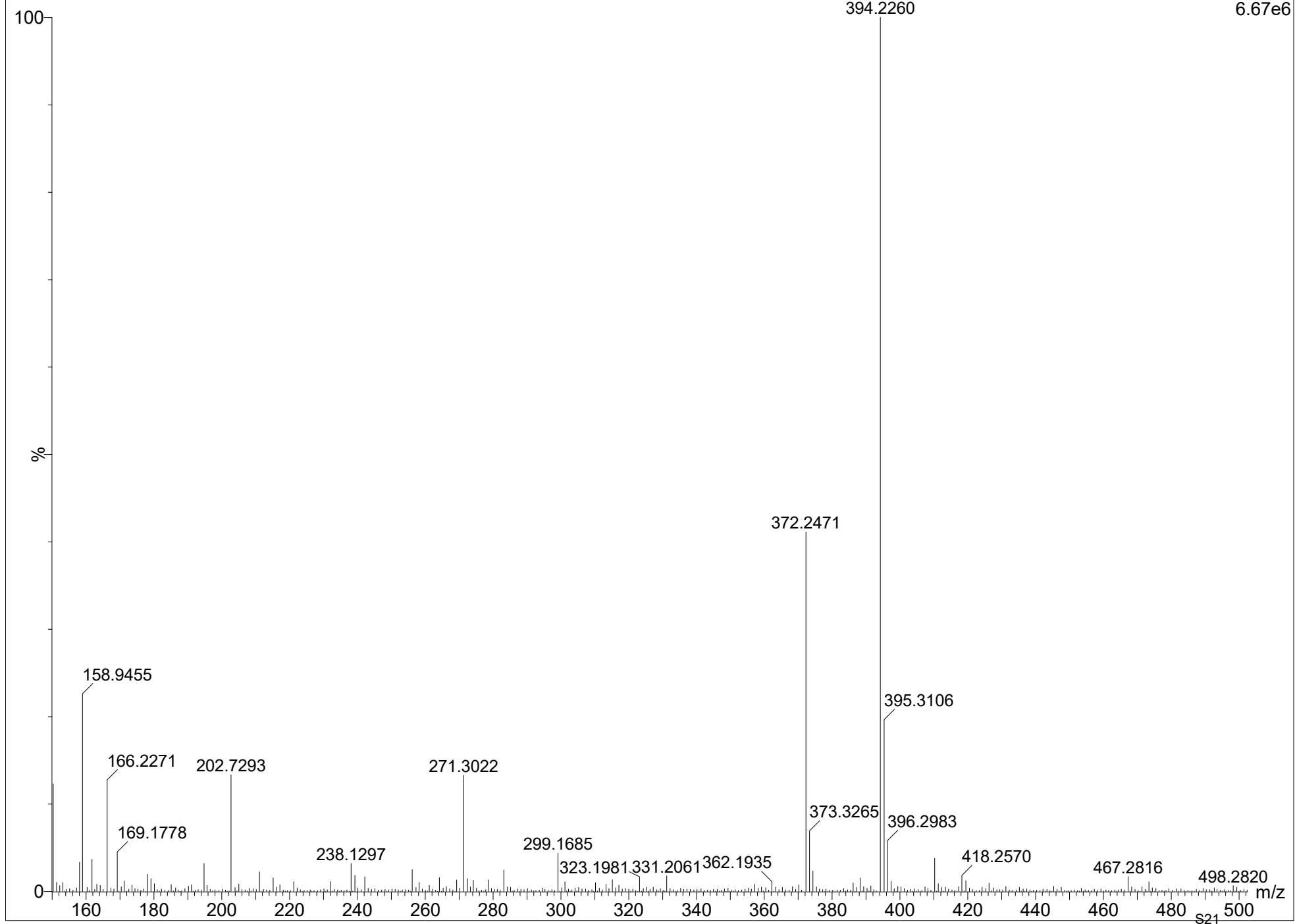






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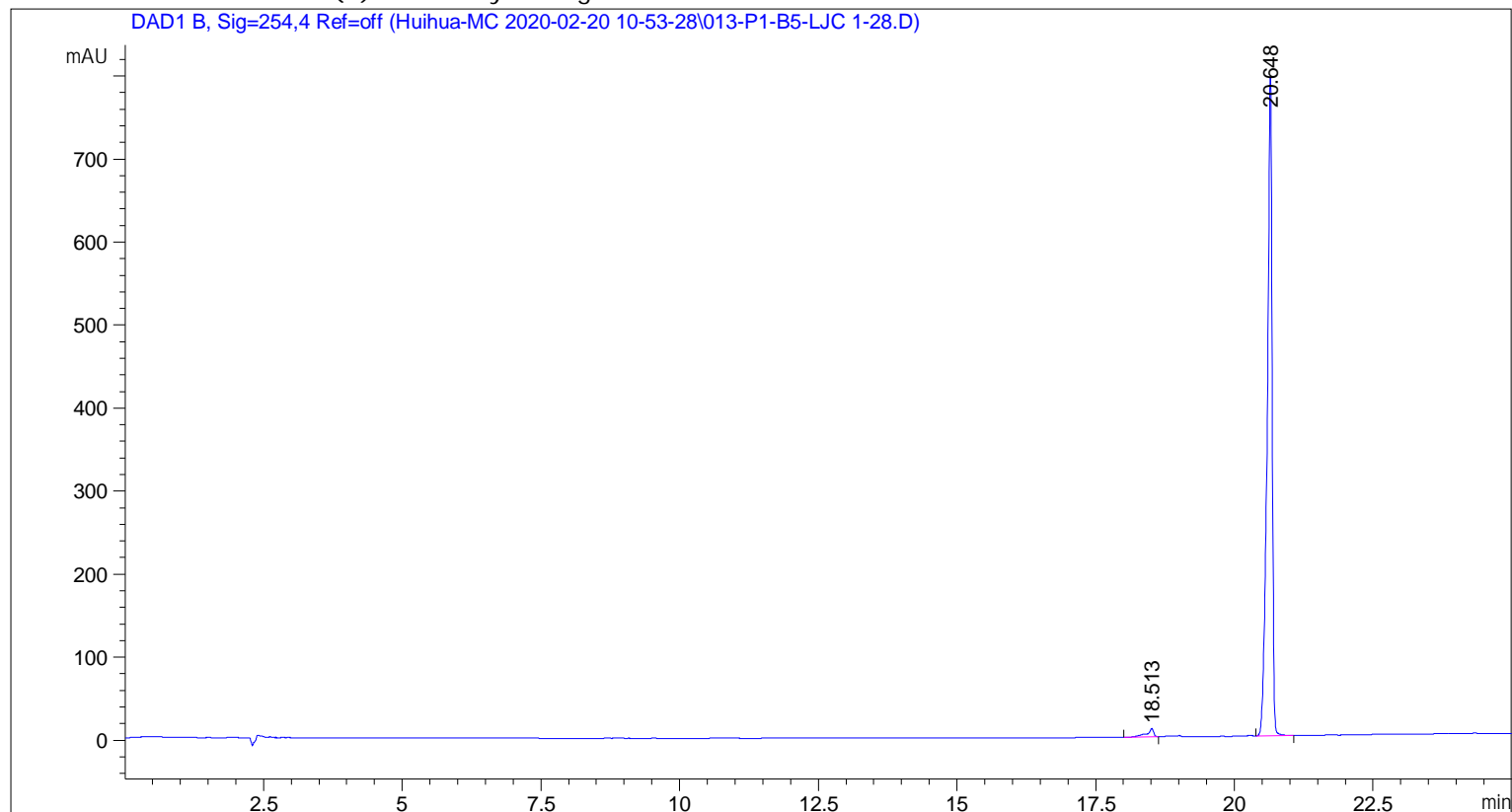


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Use Multiplier & Dilution Factor with ISTDs

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Signal 1: DAD1 B, Sig=254,4 Ref=off

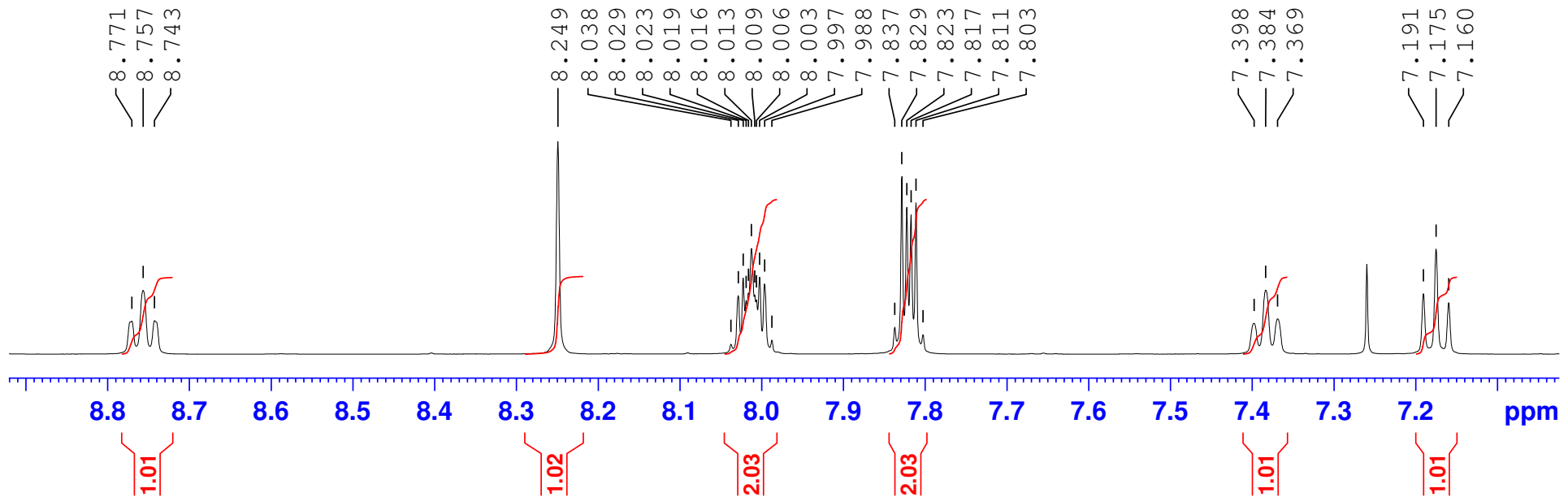
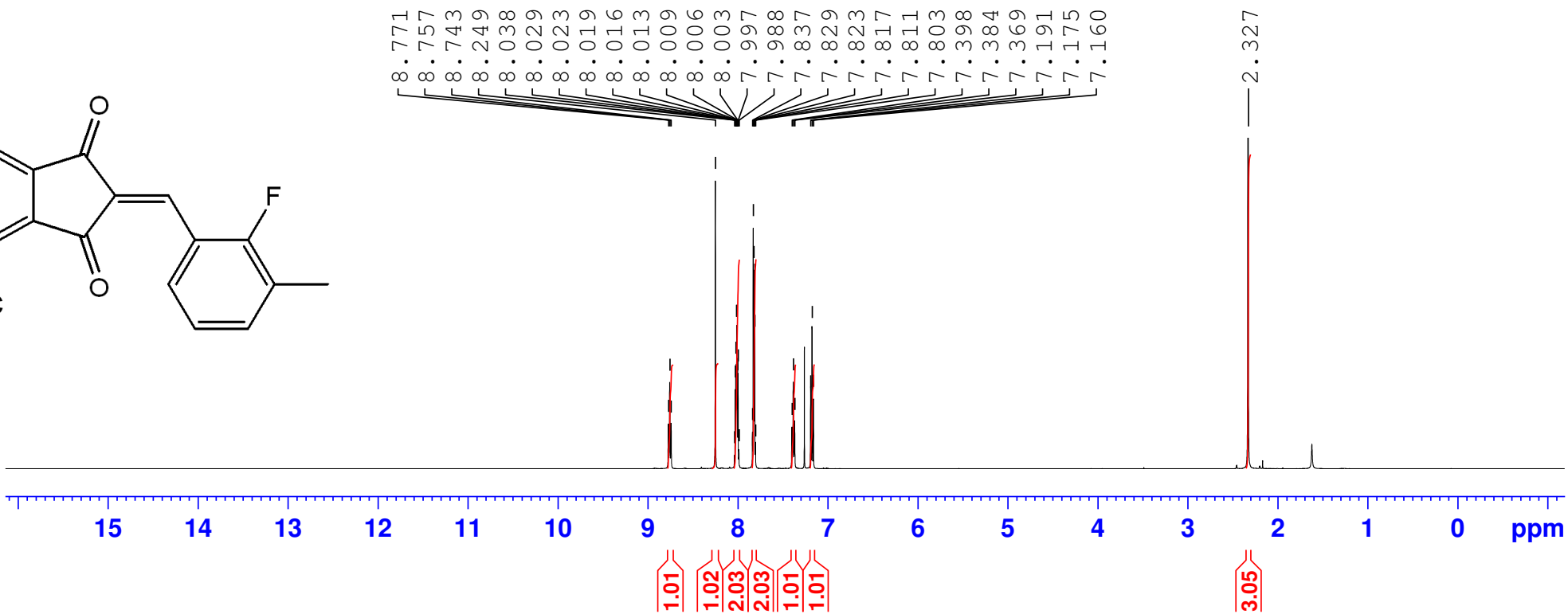
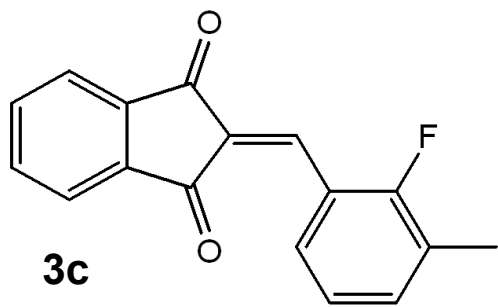
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.513	BB	0.1180	84.43469	9.84892	1.7142
2	20.648	VB	0.0893	4841.26465	792.19861	98.2858

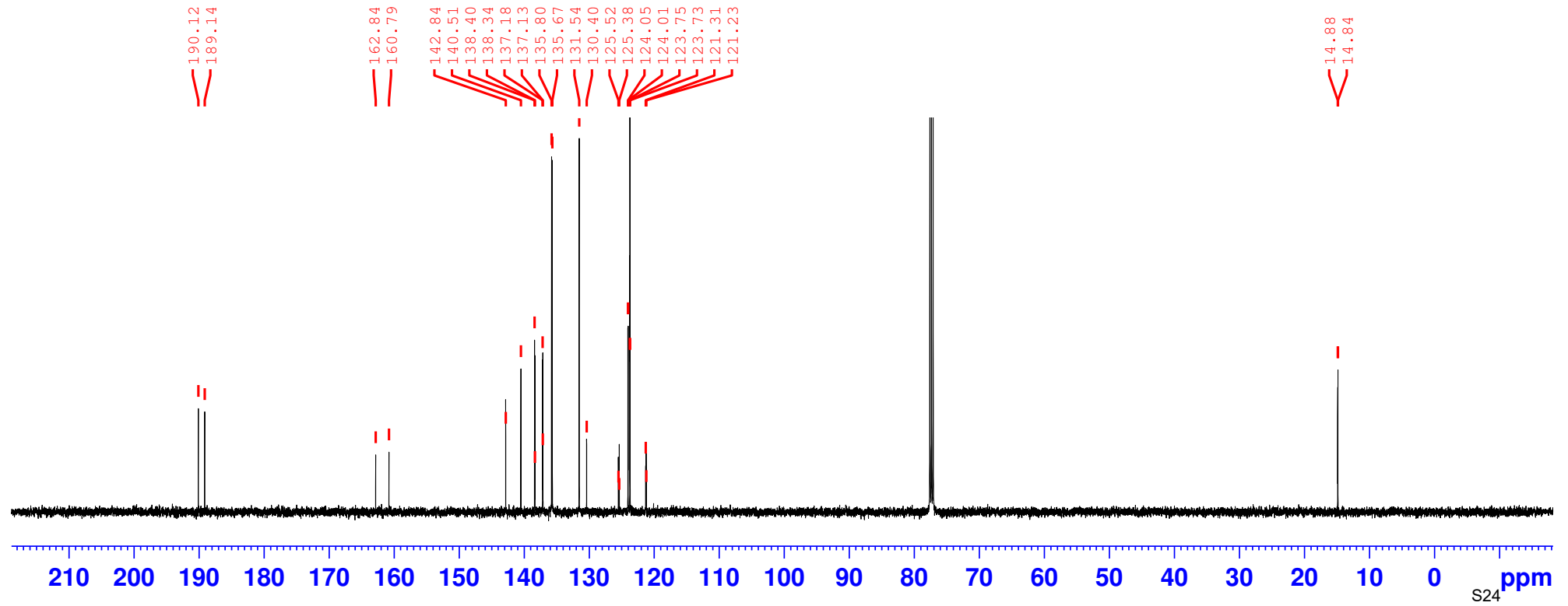
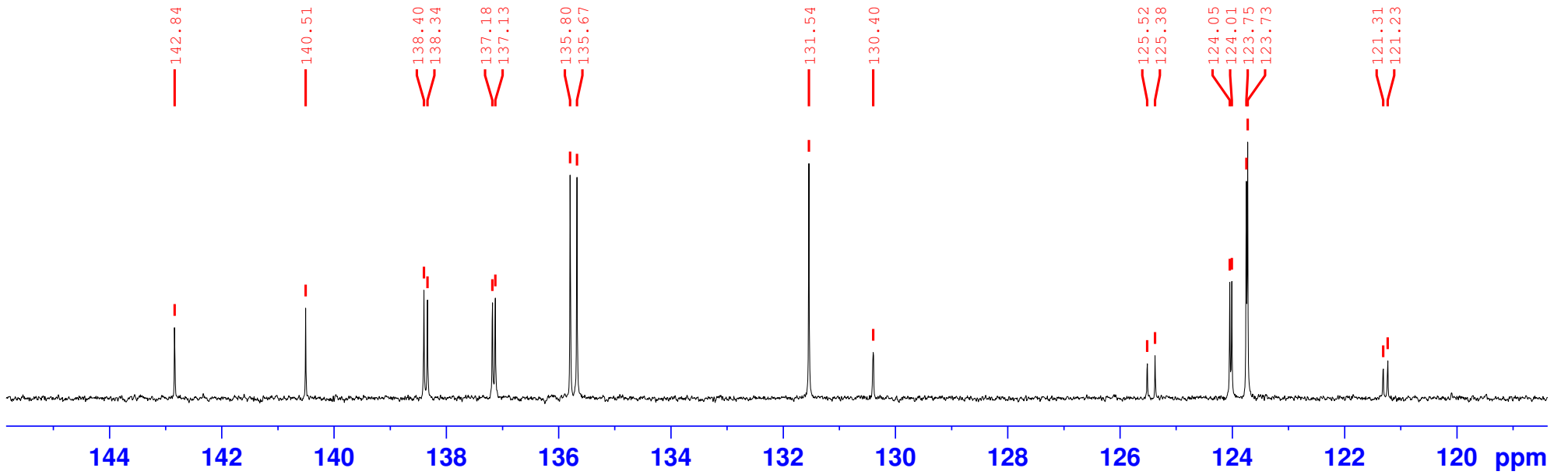
```
Totals :                4925.69934  802.04752
```

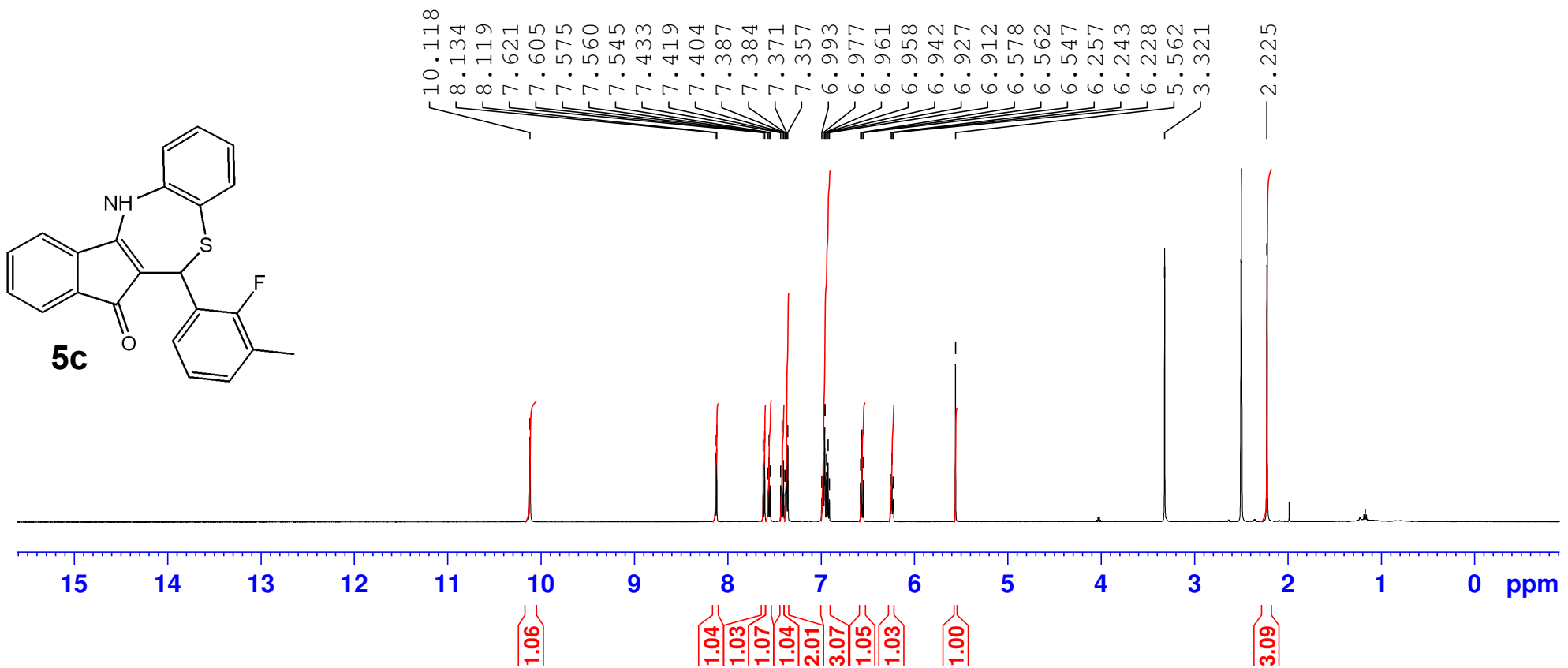
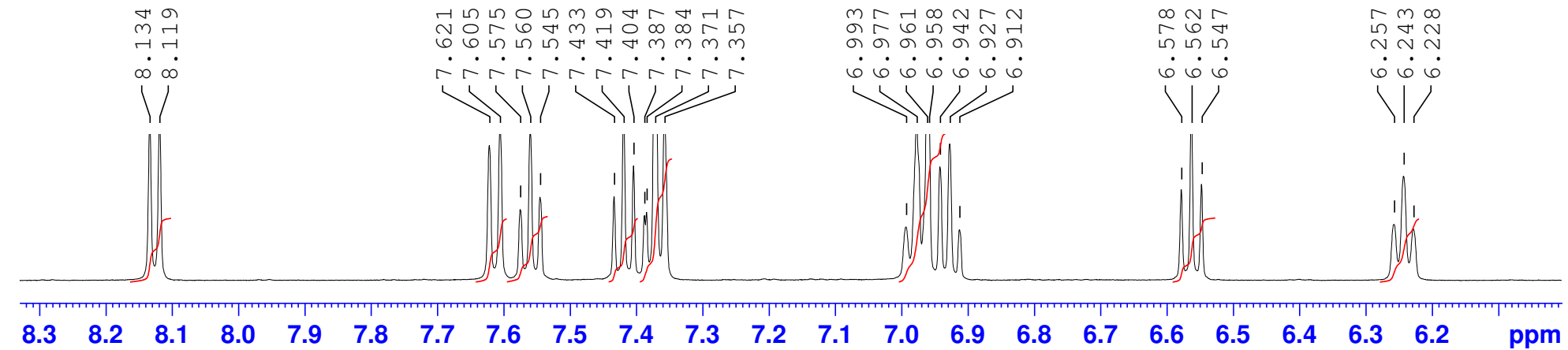
```

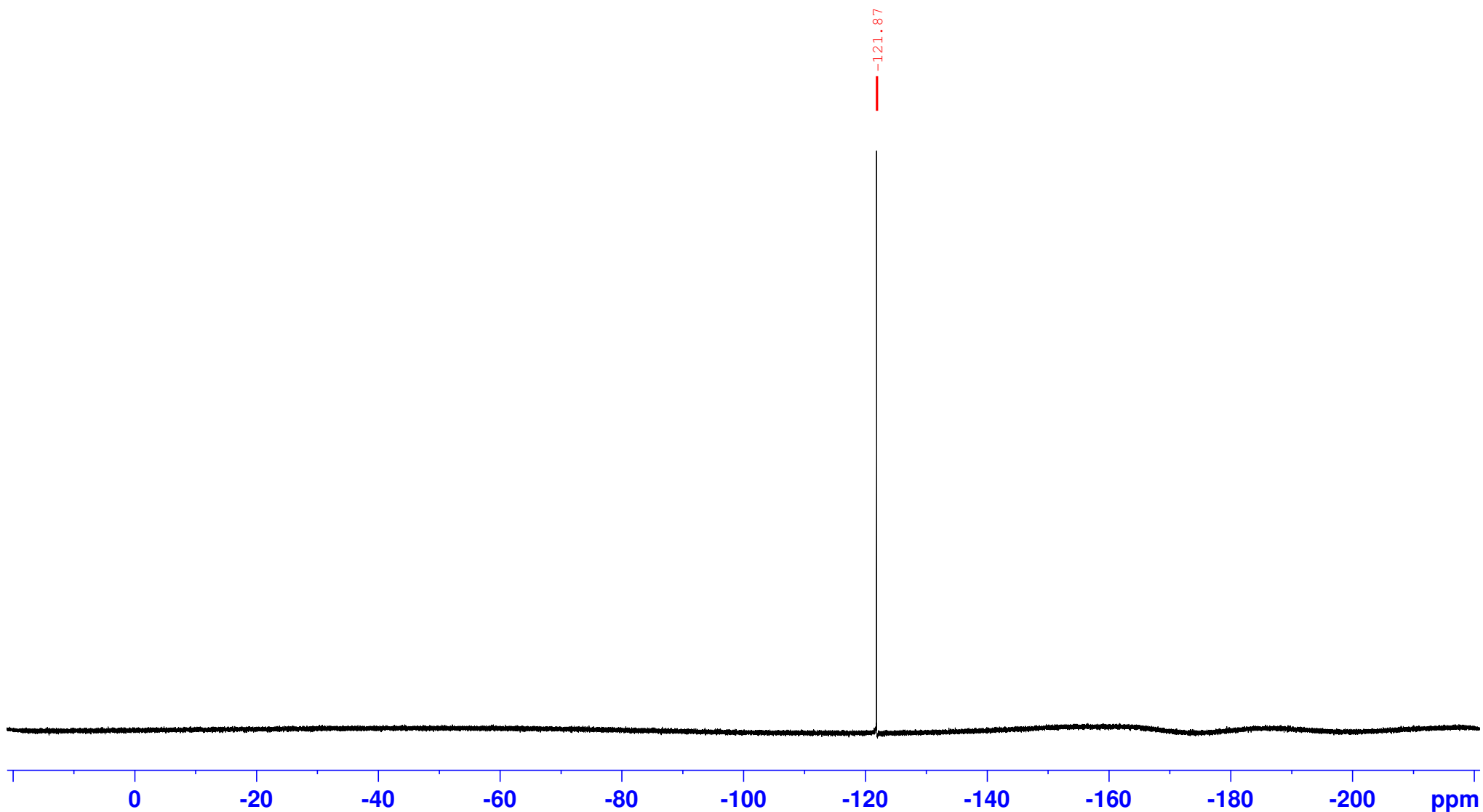
=====
*** End of Report ***

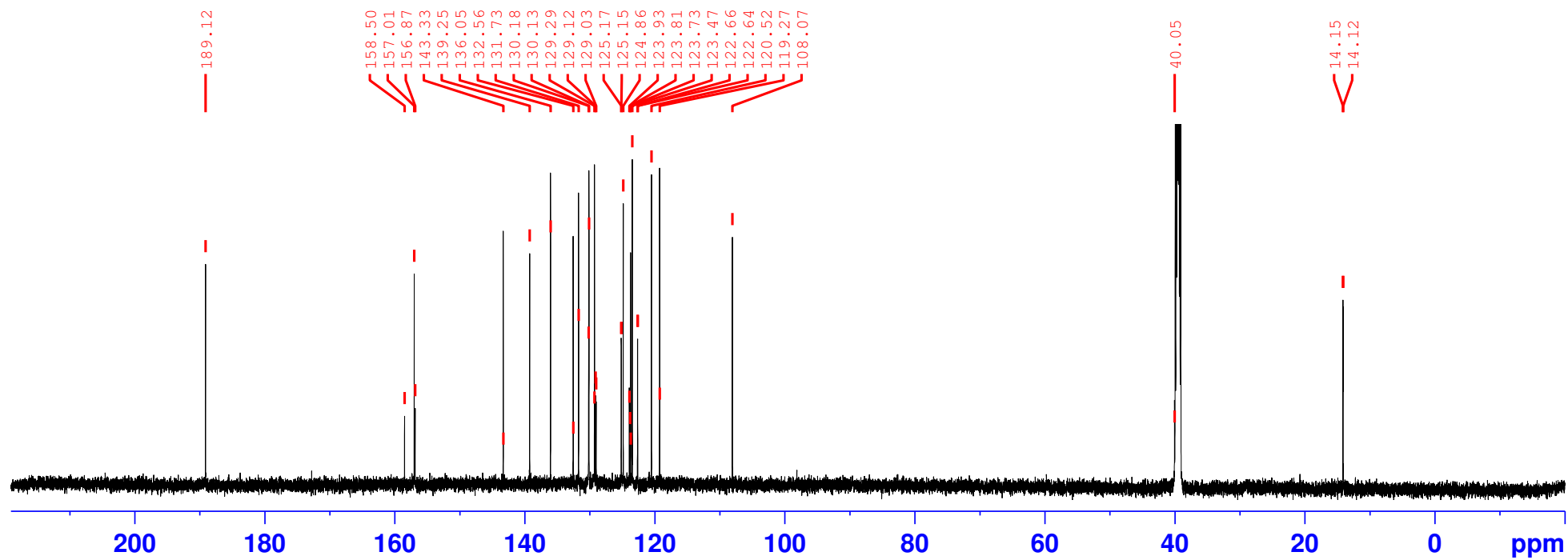
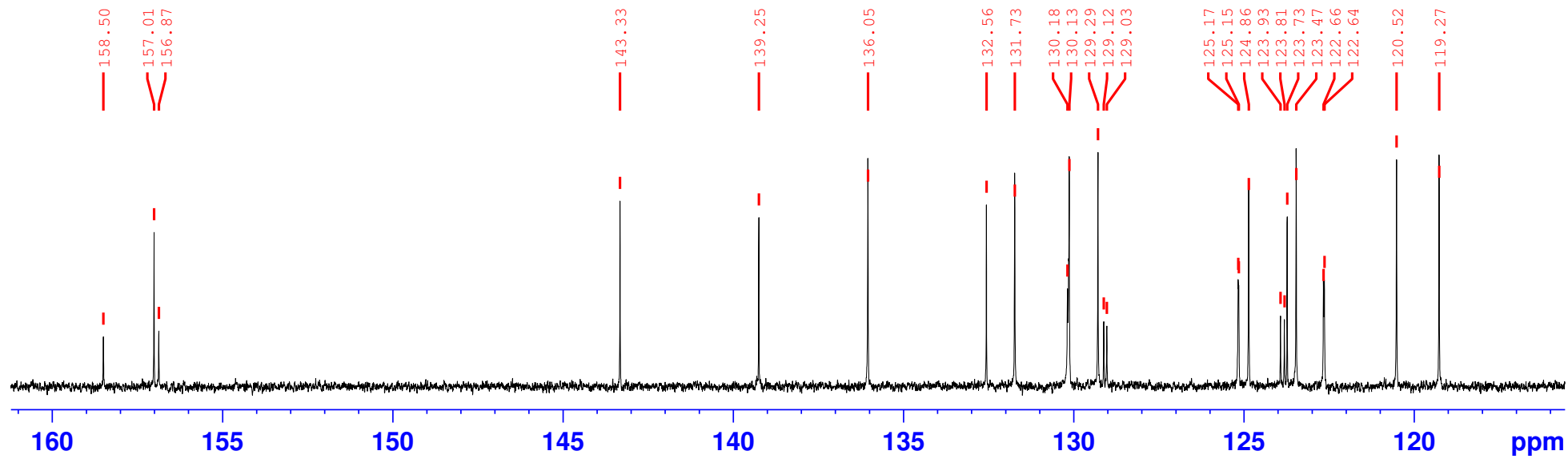
```



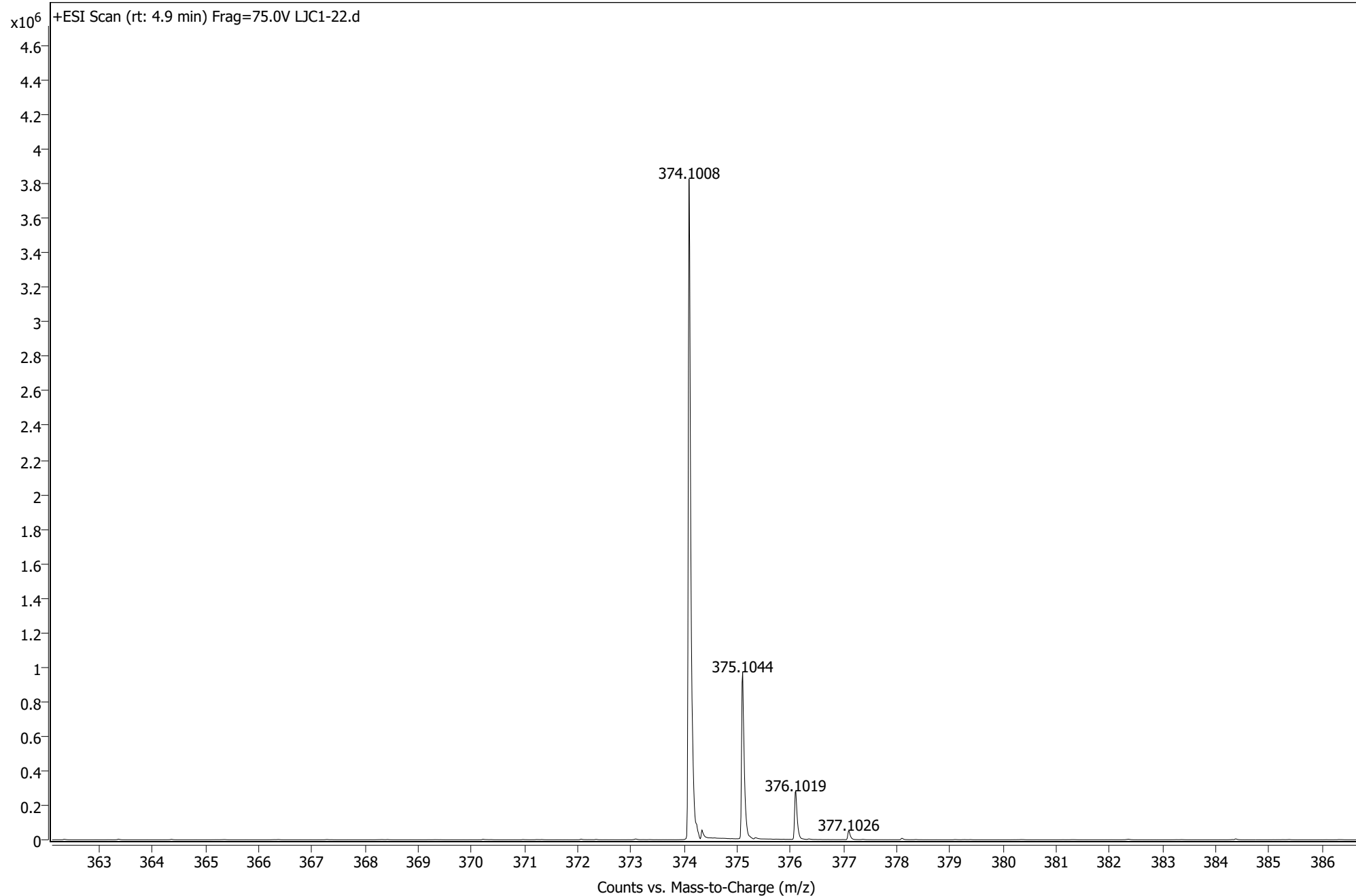








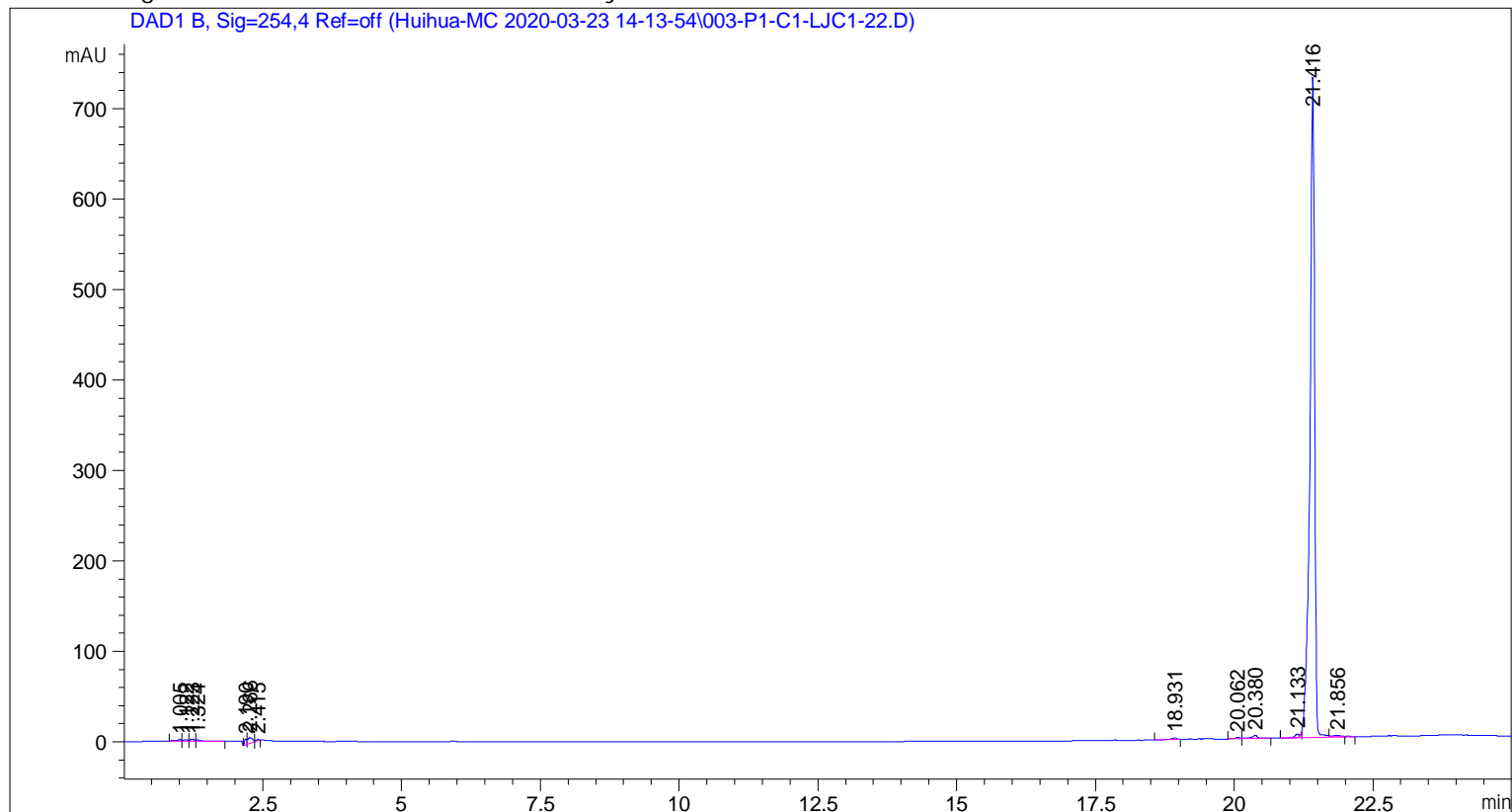
User Spectrum Plot Report



```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    3
Sample Operator : SYSTEM
Acq. Instrument : 1260Infini ty2             Locati on :   P1-C-01
Injection Date  : 3/23/2020 2:58:08 PM       Inj       :    1
                                           Inj Volume: 50.000 µl

Method         : C:\Users\Public\Documents\ChemStation\1\Data\Huihua-MC 2020-03-23 14-13-54
                \MC-SMALL MOLE.M (Sequence Method)
Last changed   : 2/19/2020 11:54:04 AM by SYSTEM
  
```



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

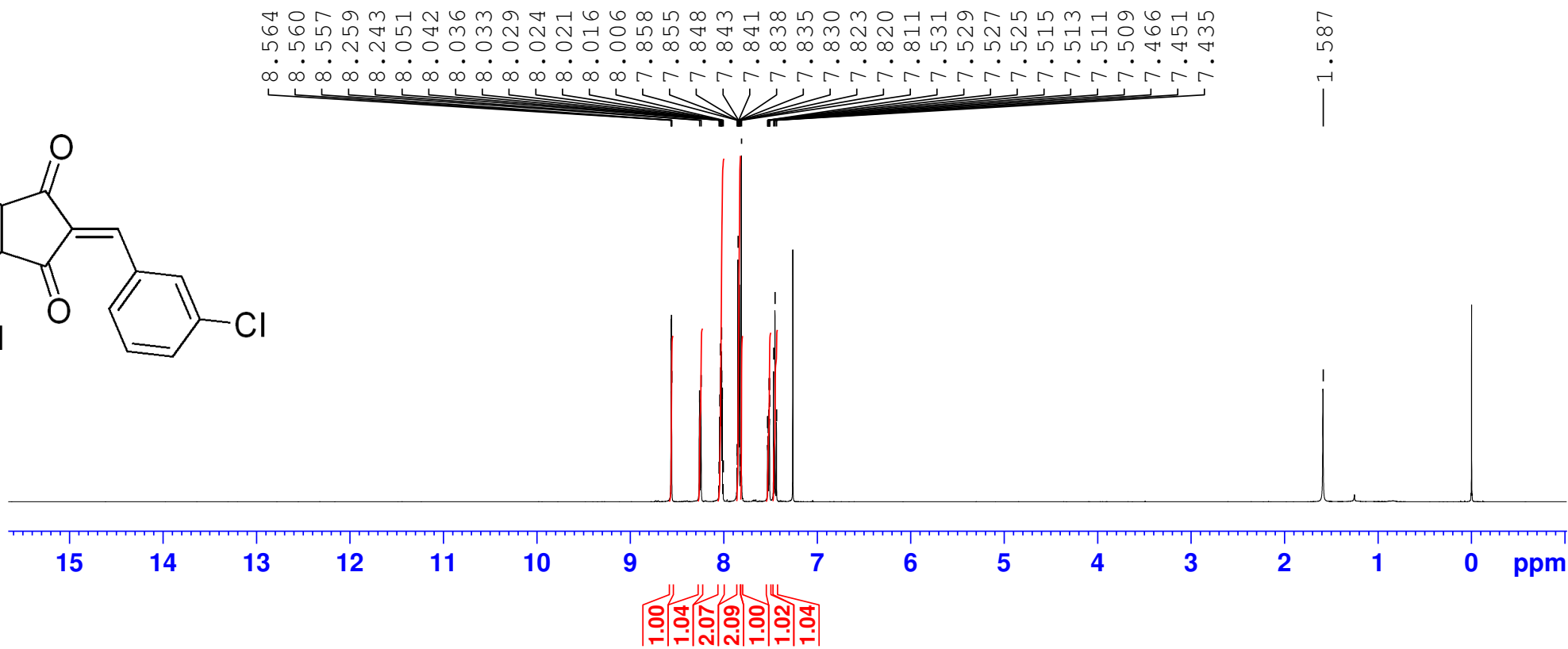
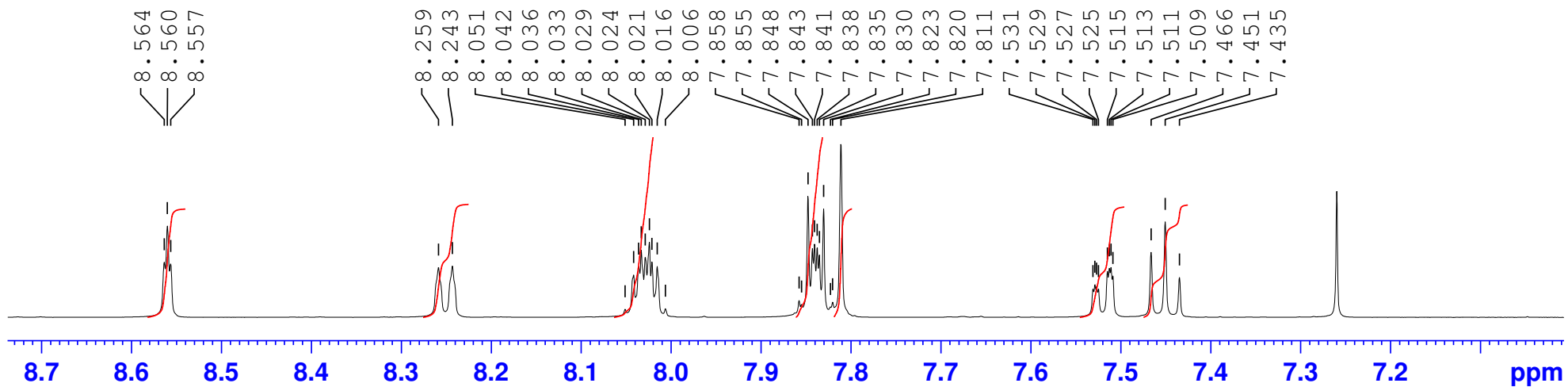
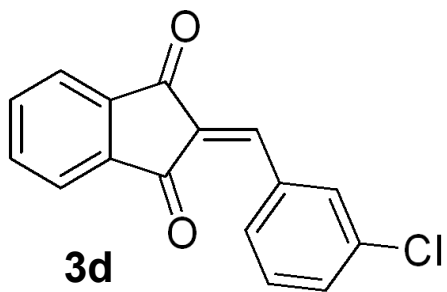
Signal 1: DAD1 B, Sig=254,4 Ref=off

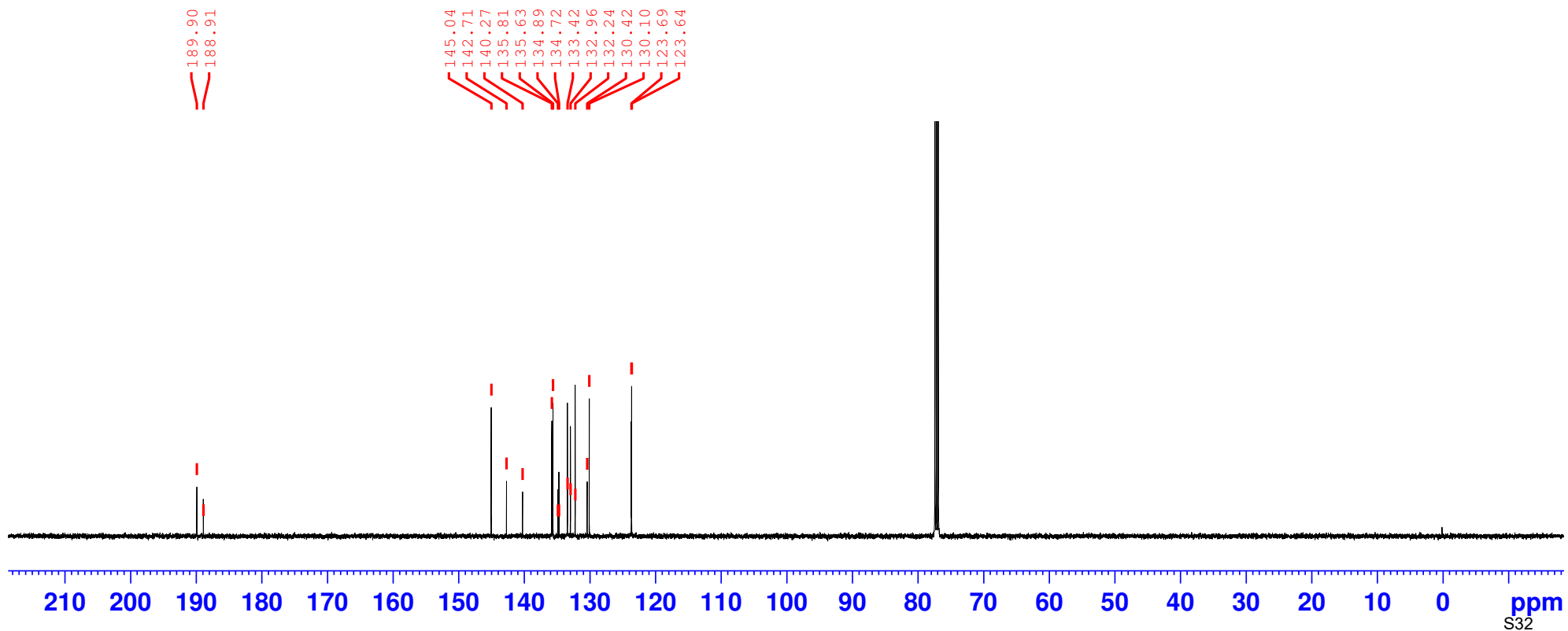
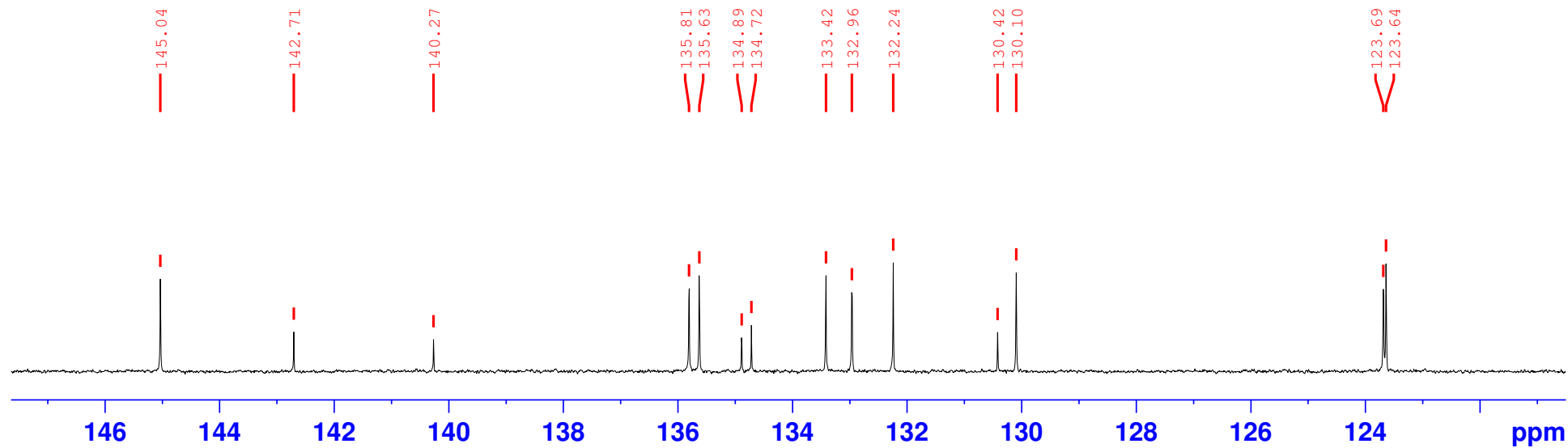
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.005	BV	0.0513	7.06923	2.09814	0.1569
2	1.122	VV	0.0779	7.80227	1.42504	0.1732
3	1.223	VV	0.0699	10.57917	2.05994	0.2348
4	1.324	VB	0.0864	6.30973	1.04606	0.1401
5	2.190	BV	0.0360	14.94652	6.22738	0.3318
6	2.266	VV	0.0818	38.18400	6.37926	0.8476
7	2.415	VB	0.0634	6.31446	1.49156	0.1402
8	18.931	BB	0.1081	16.73990	2.16868	0.3716
9	20.062	BV	0.0902	8.46999	1.33149	0.1880

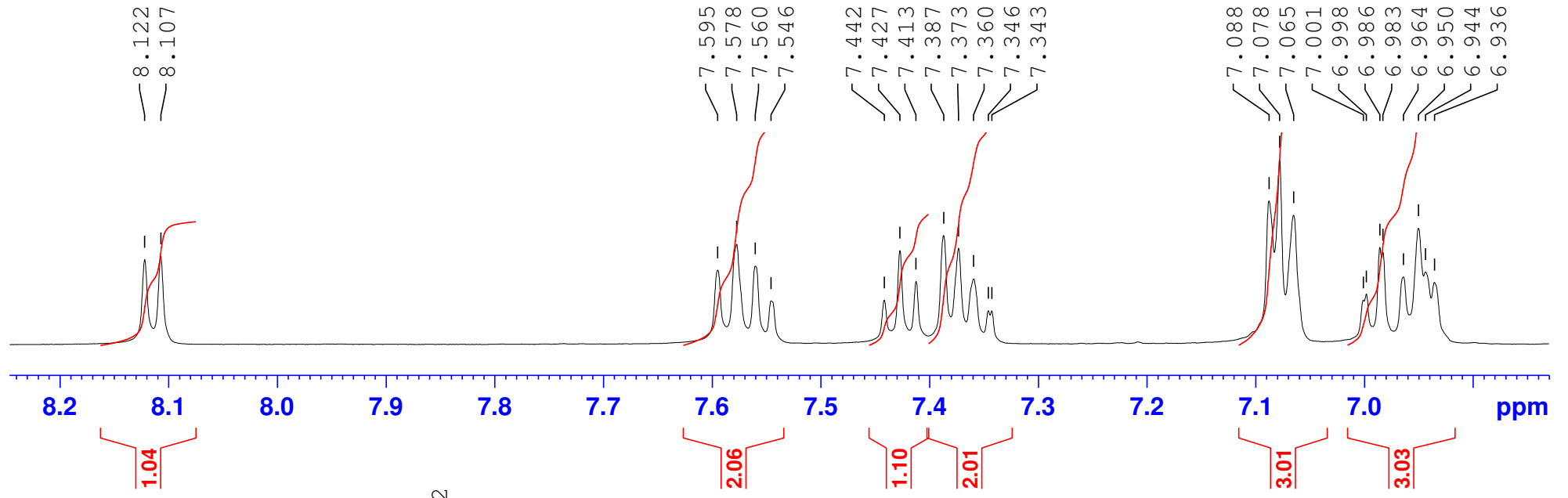
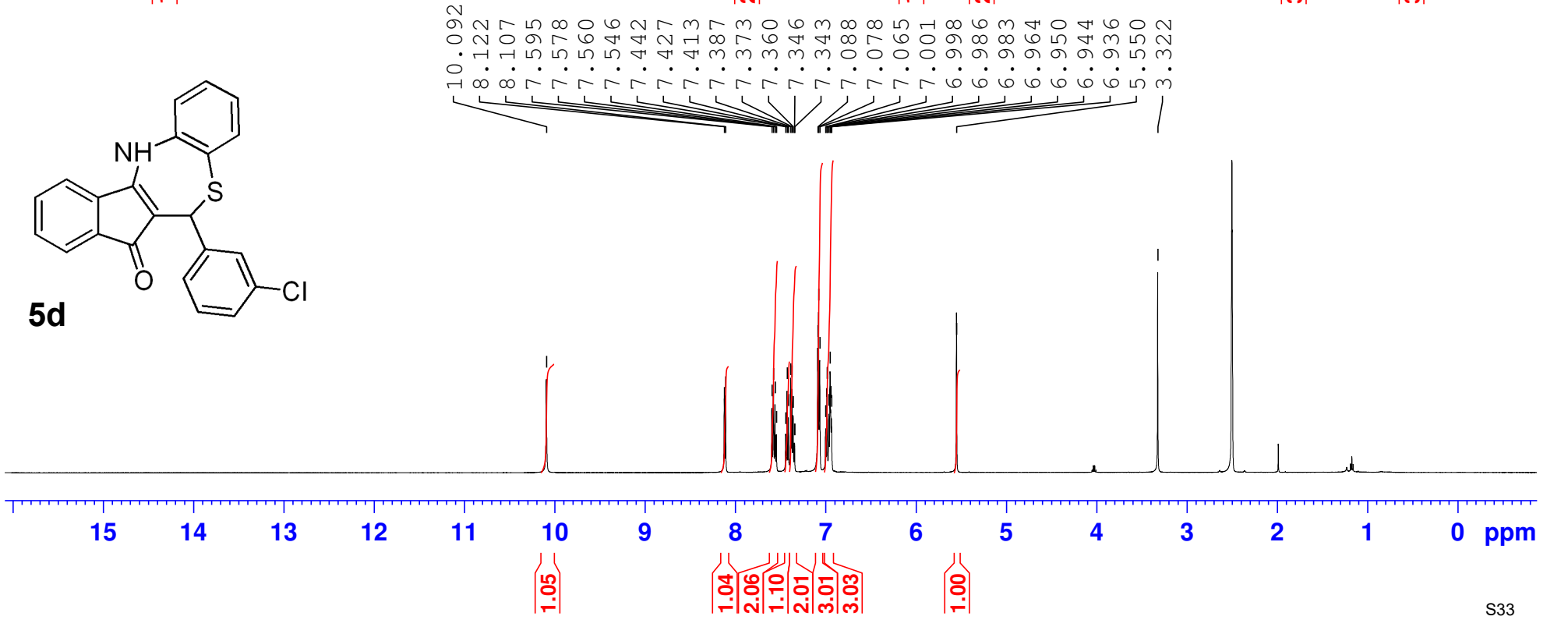
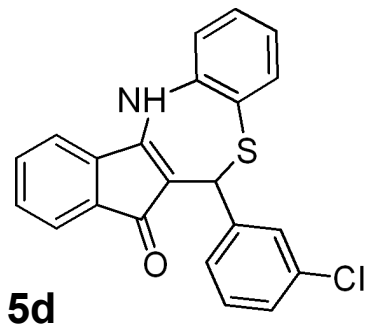
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
10	20.380	VV R	0.1213	31.83788	3.59509	0.7068
11	21.133	BV E	0.0870	23.94049	4.04545	0.5314
12	21.416	VV R	0.0869	4314.00391	730.46741	95.7640
13	21.856	VV E	0.1301	18.63017	1.84068	0.4136

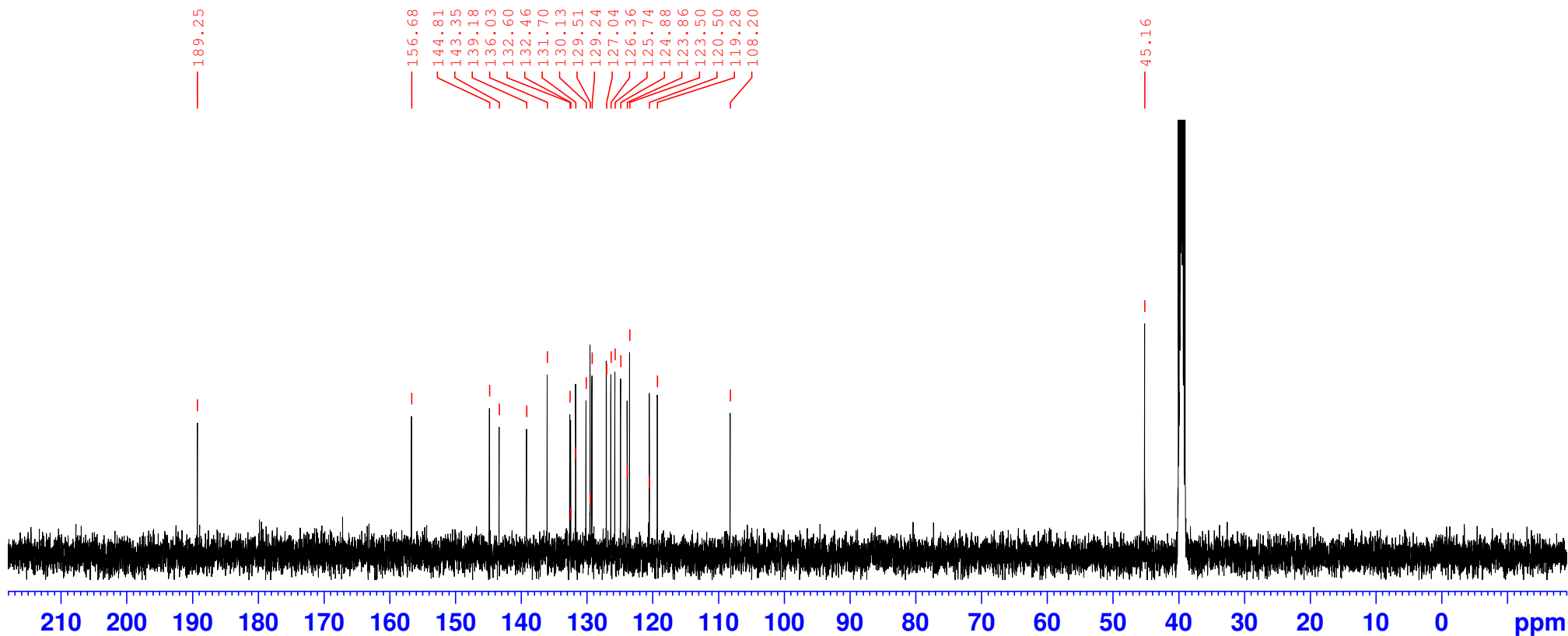
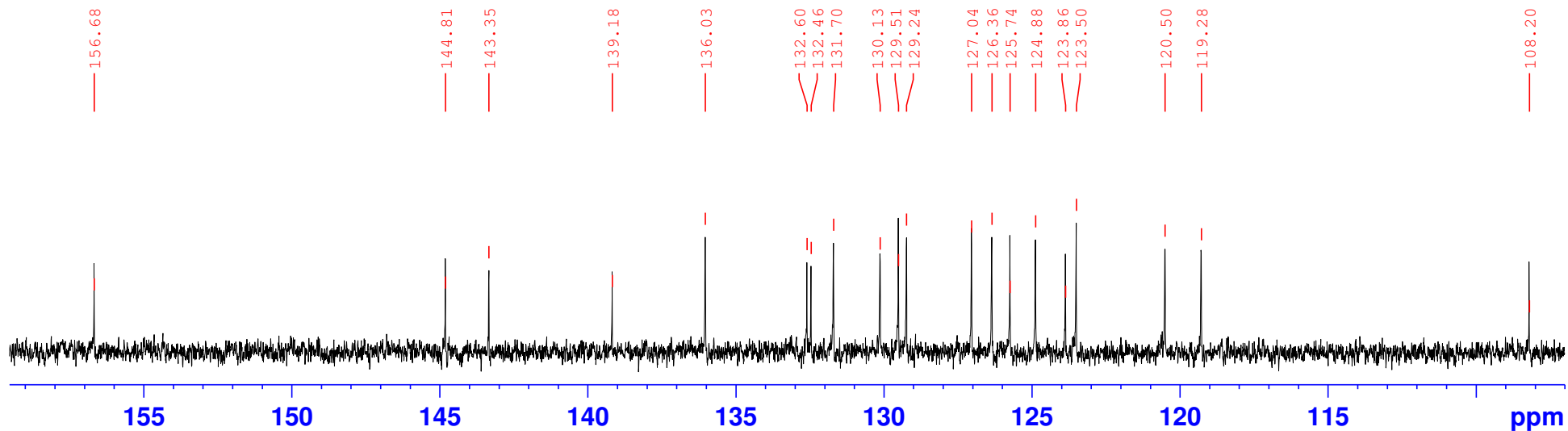
Totals : 4504.82773 764.17618

=====
*** End of Report ***

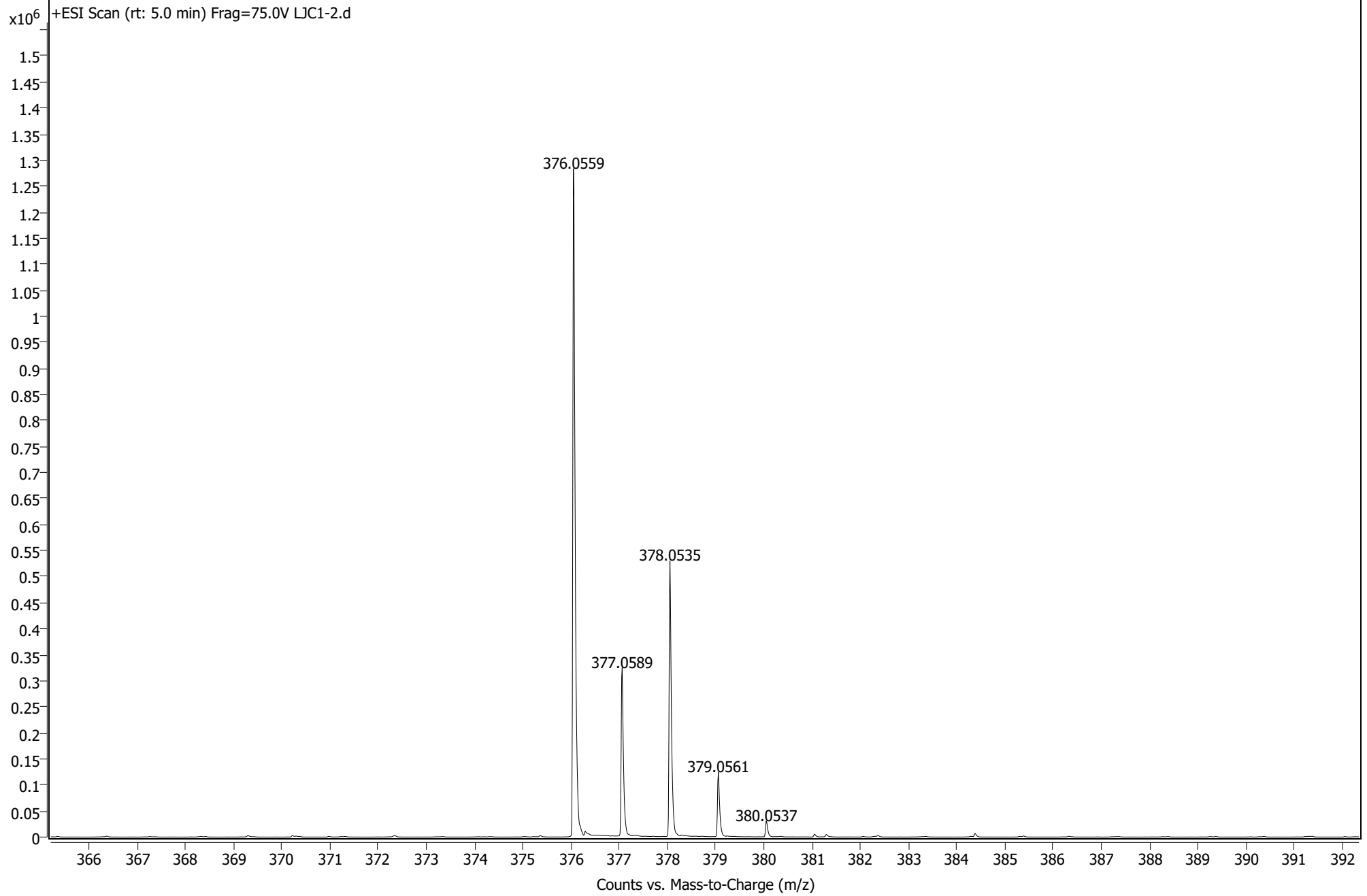








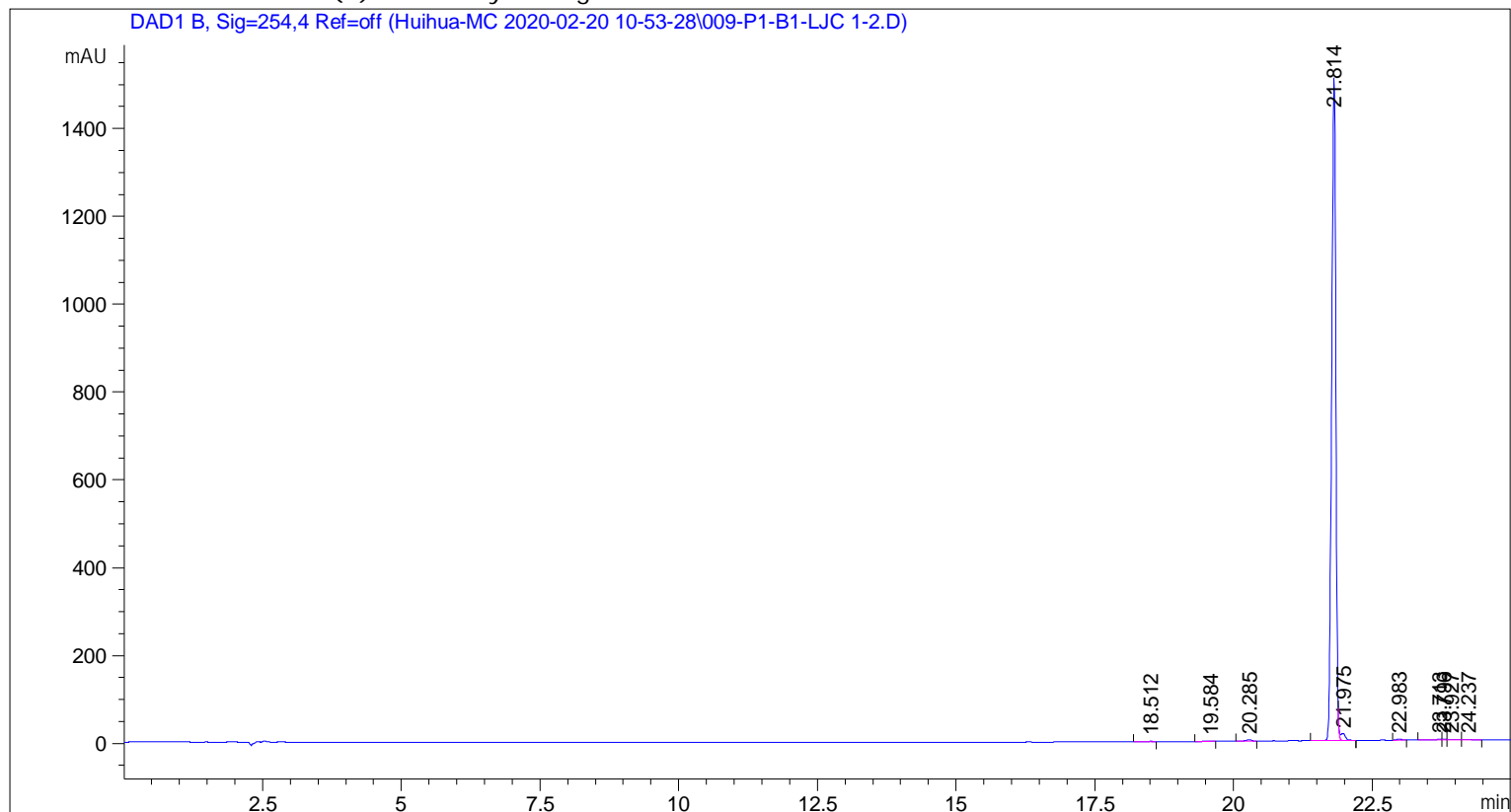
User Spectrum Plot Report



```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    9
Sample Operator : SYSTEM
Acq. Instrument : 1260Infinity2              Location  : P1-B-01
Injection Date  : 2/20/2020 2:26:03 PM       Inj       :    1
                                           Inj Volume: 50.000 µl

Method          : C:\Users\Public\Documents\ChemStation\1\Data\Huihua-MC 2020-02-20 10-53-28
                  \MC-SMALL MOLE.M (Sequence Method)
Last changed    : 2/19/2020 11:54:04 AM by SYSTEM
Additional Info  : Peak(s) manually integrated
  
```



=====
 Area Percent Report
 =====

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

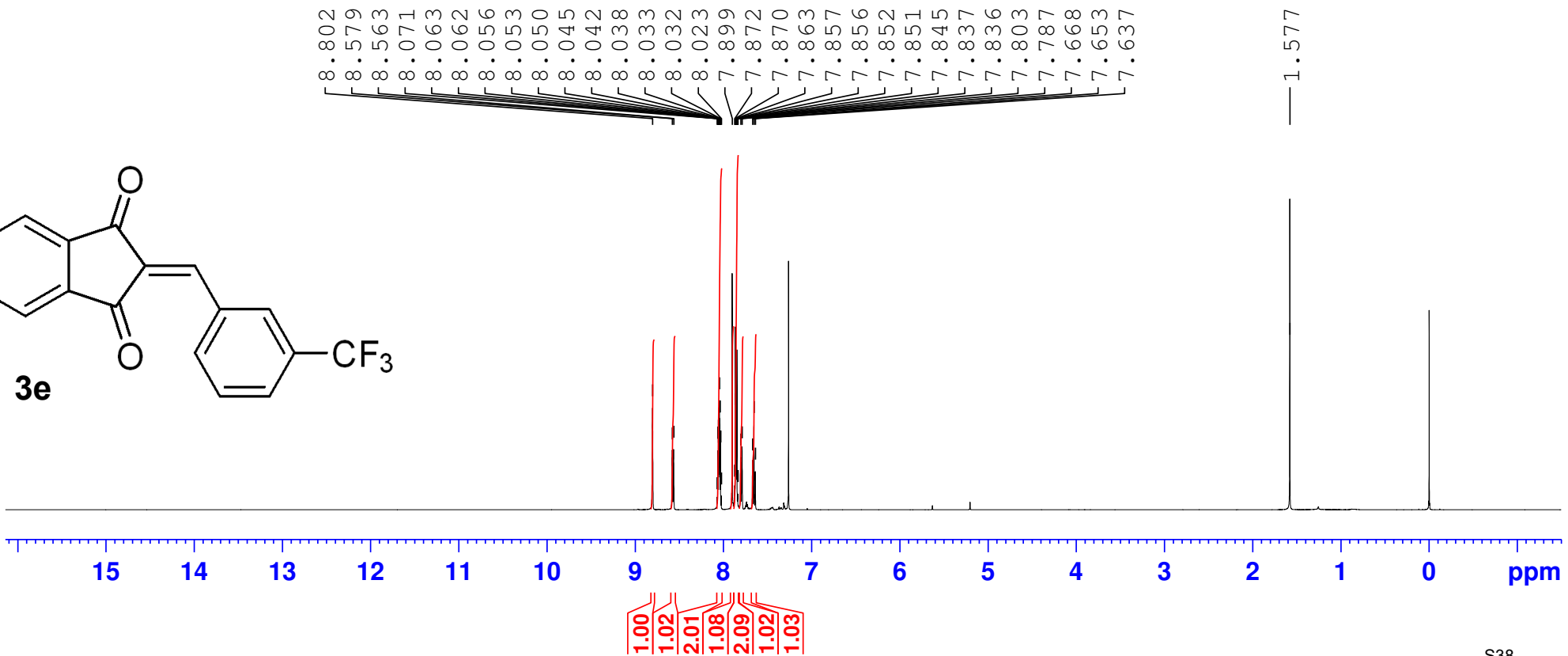
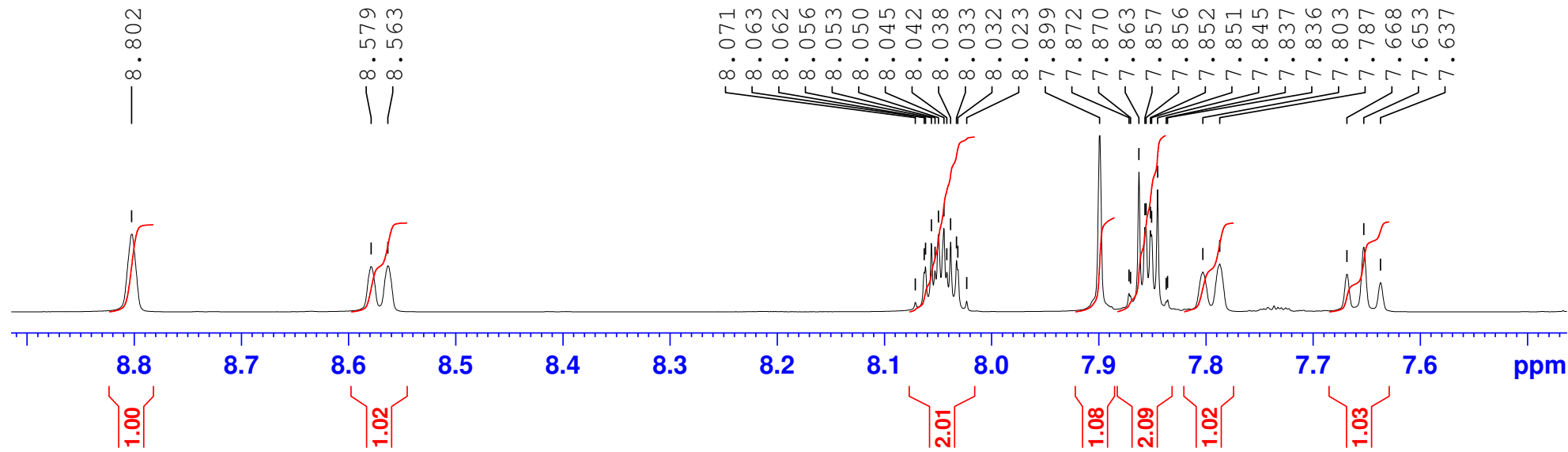
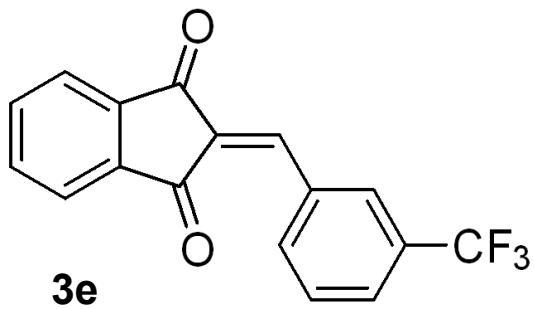
Signal 1: DAD1 B, Sig=254,4 Ref=off

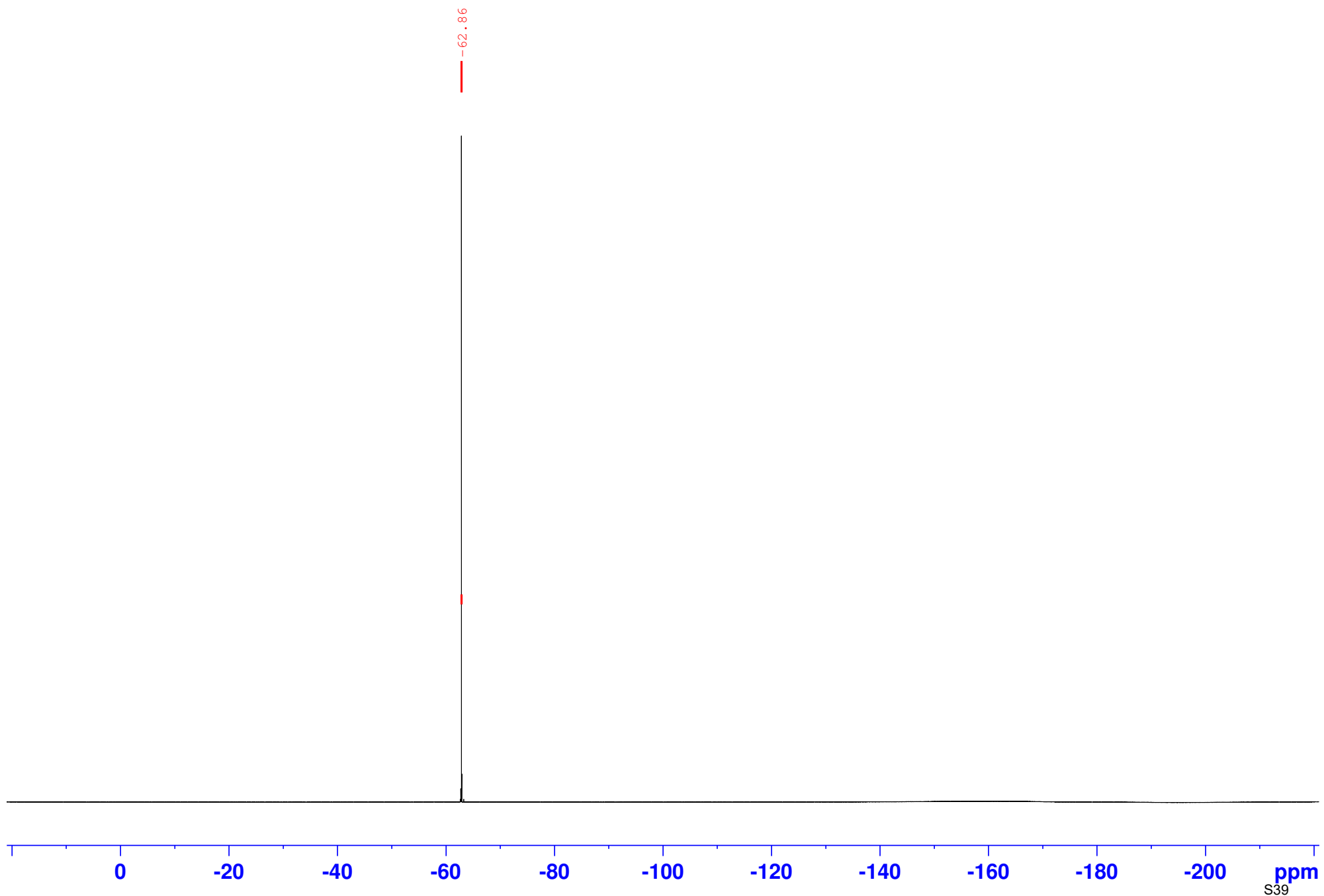
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.512	BB	0.1047	8.14009	1.09586	0.1013
2	19.584	BB	0.0948	7.19604	1.12263	0.0895
3	20.285	BB	0.1072	24.30151	3.49124	0.3023
4	21.814	BV R	0.0806	7830.76221	1508.22754	97.4197
5	21.975	VB E	0.0917	96.65552	15.72954	1.2025
6	22.983	BB	0.0878	15.89518	2.73559	0.1977
7	23.713	BV	0.1234	16.67326	1.81107	0.2074
8	23.796	VV	0.0712	6.57142	1.34045	0.0818

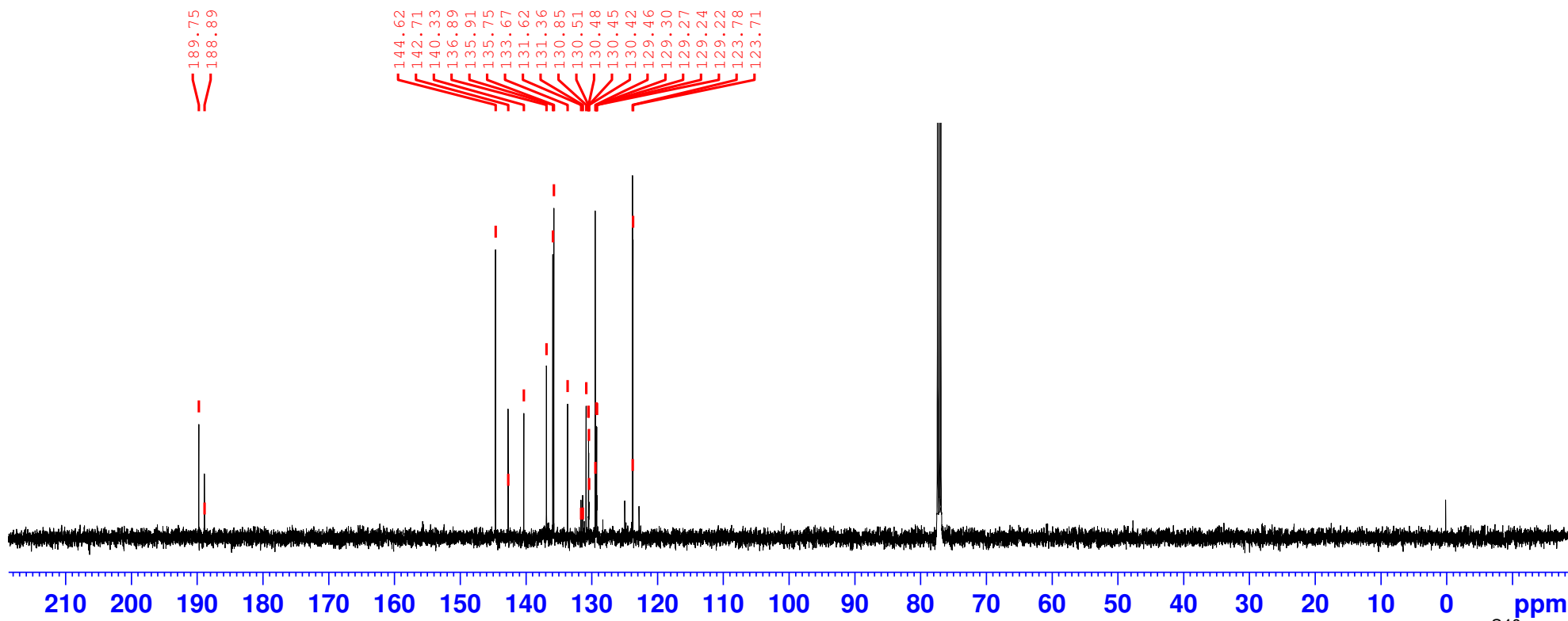
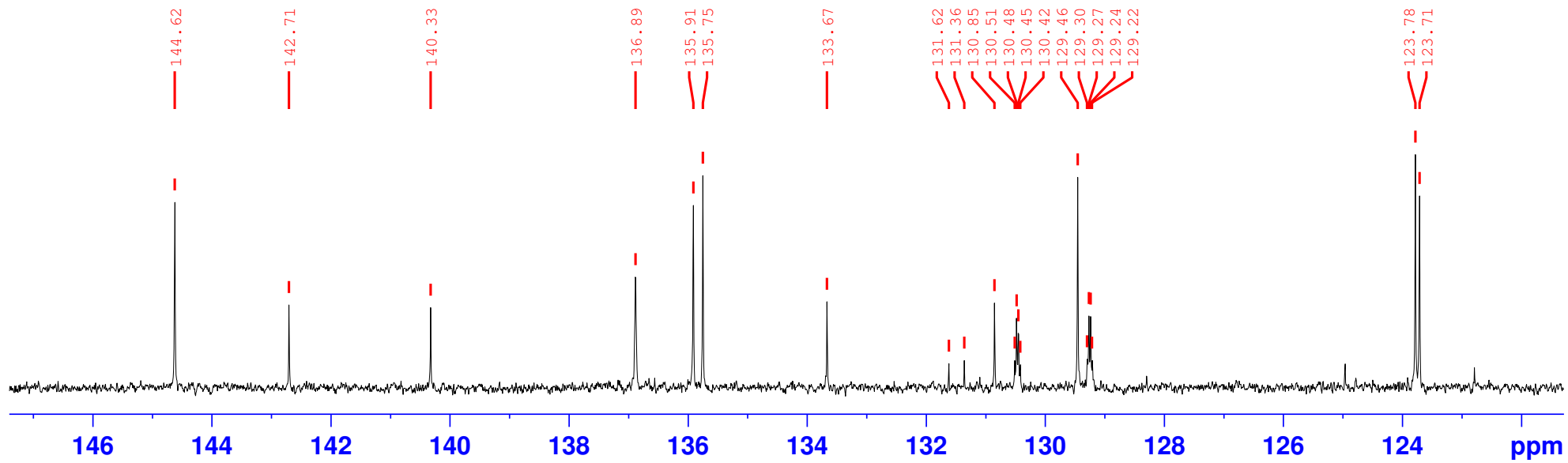
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
9	23.927	VV	0.1472	15.77227	1.40241	0.1962
10	24.237	VB	0.1176	16.20648	1.86166	0.2016

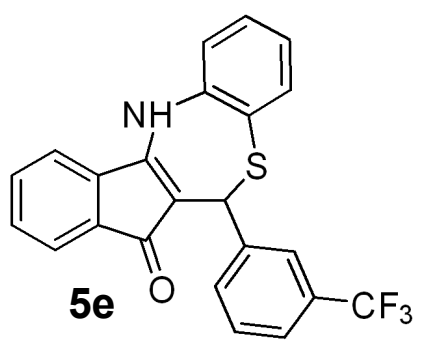
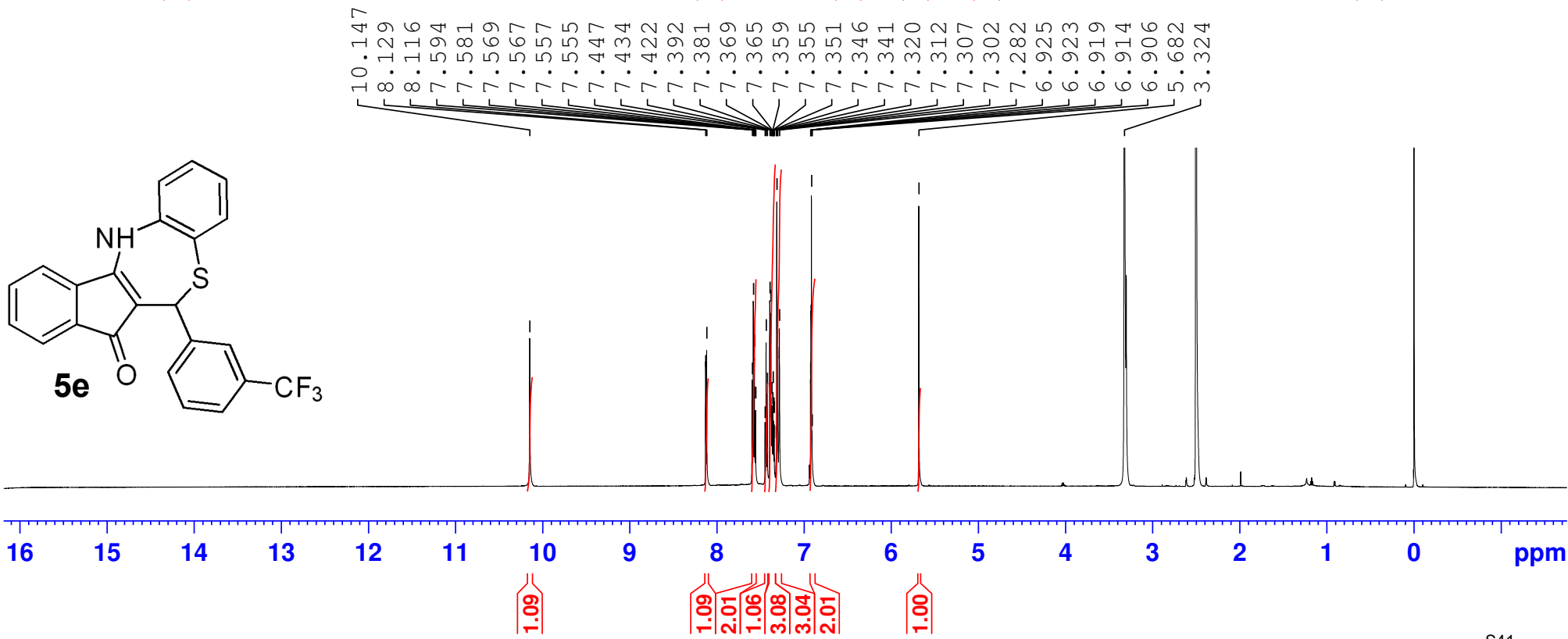
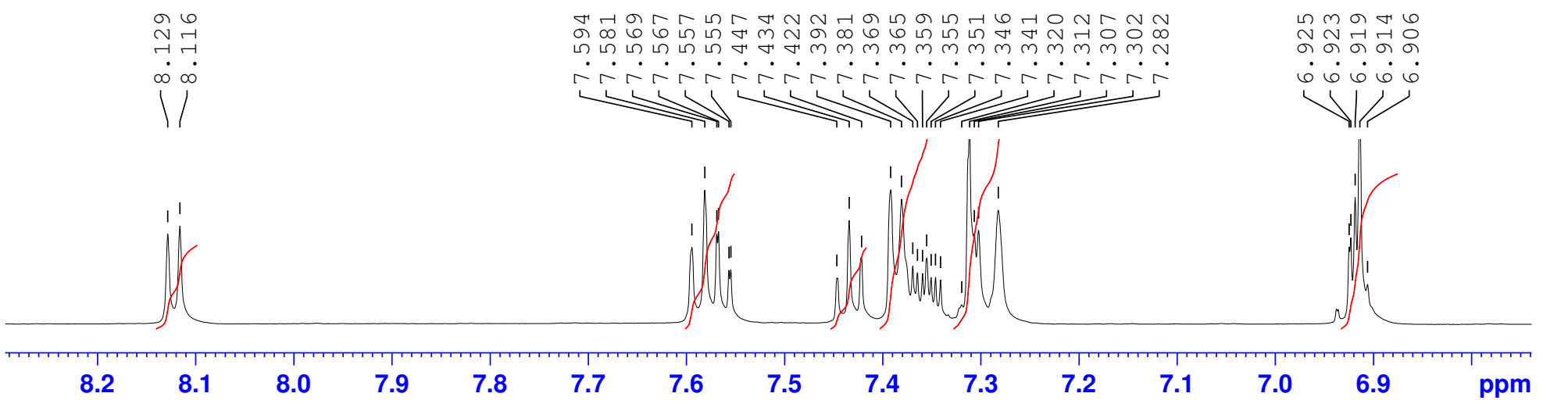
Totals : 8038.17398 1538.81798

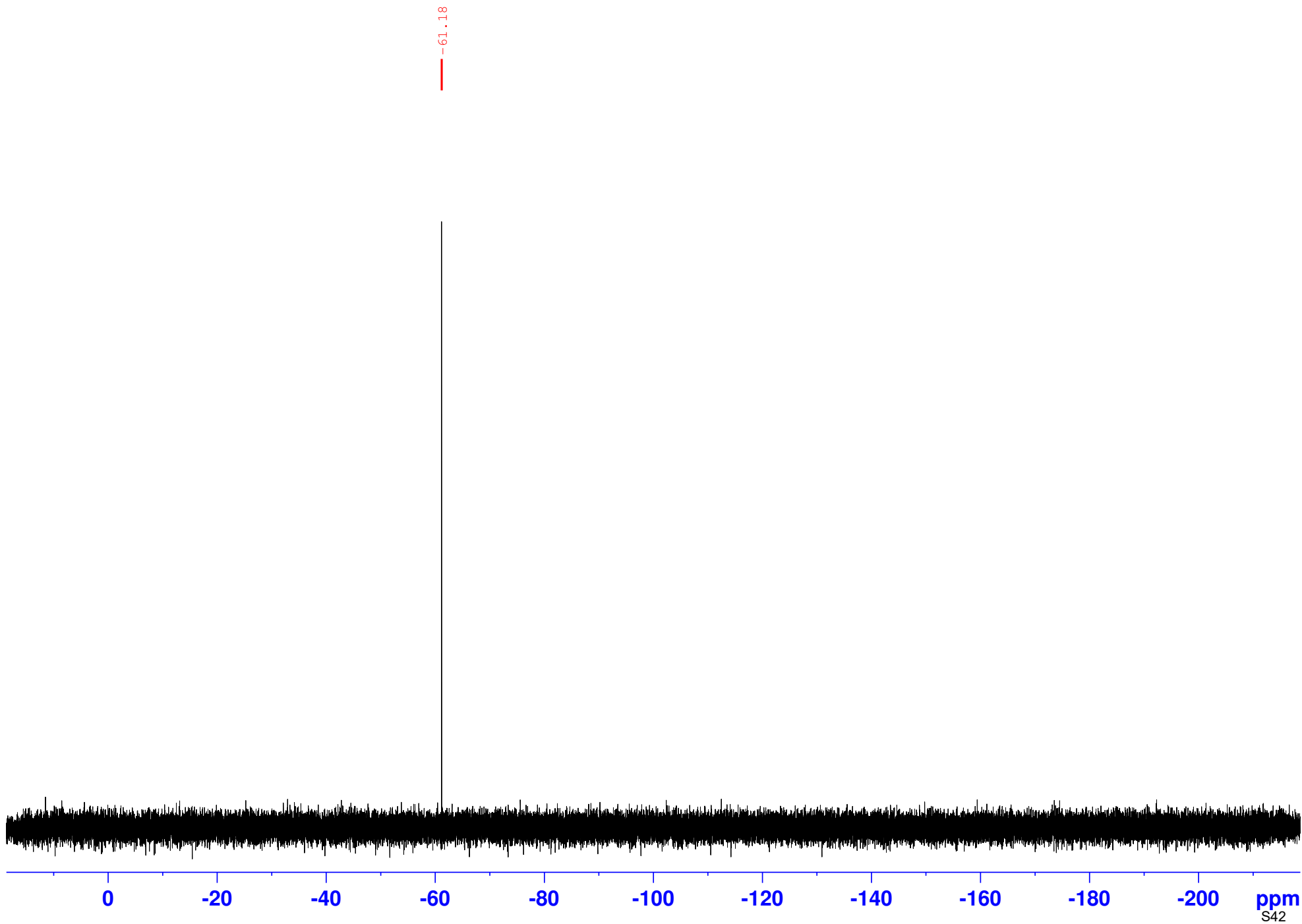
=====
*** End of Report ***

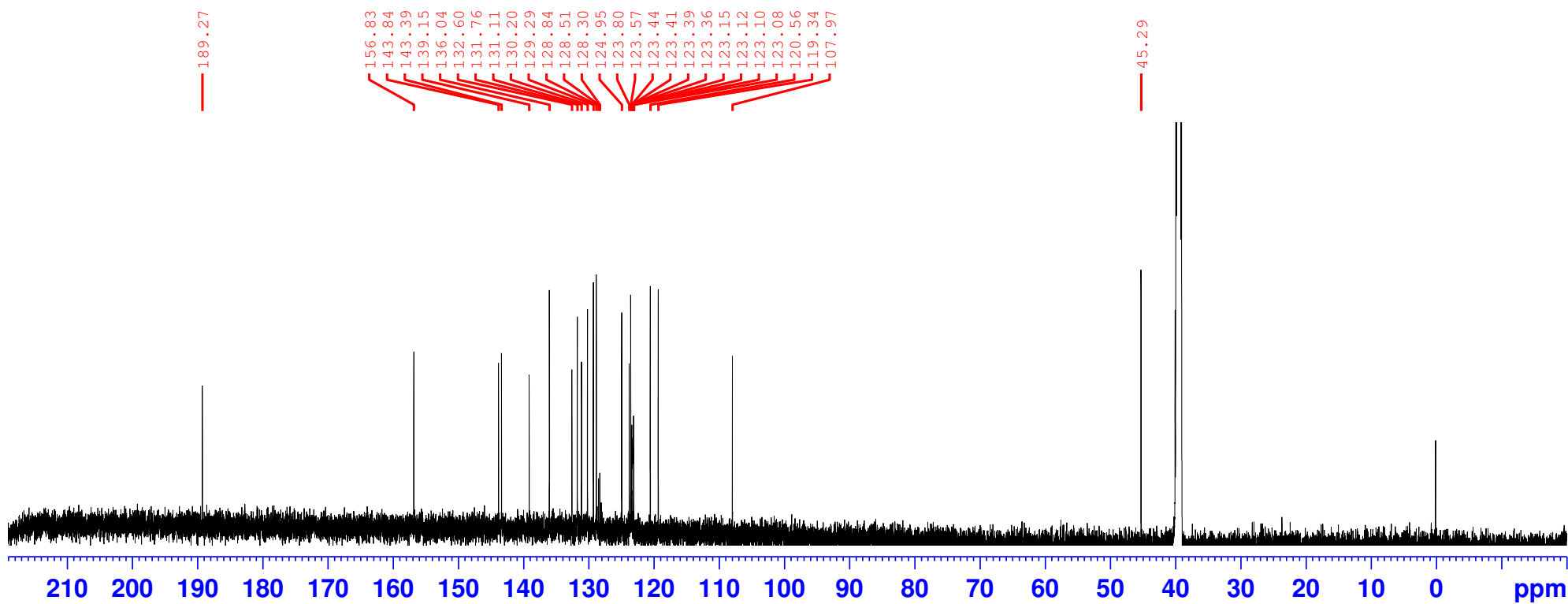
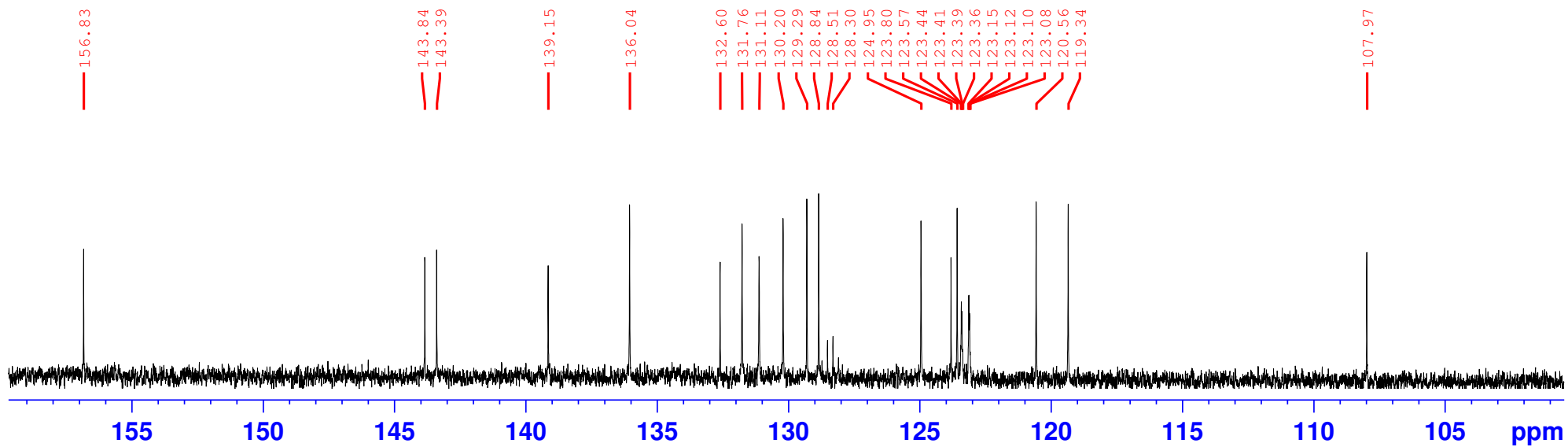


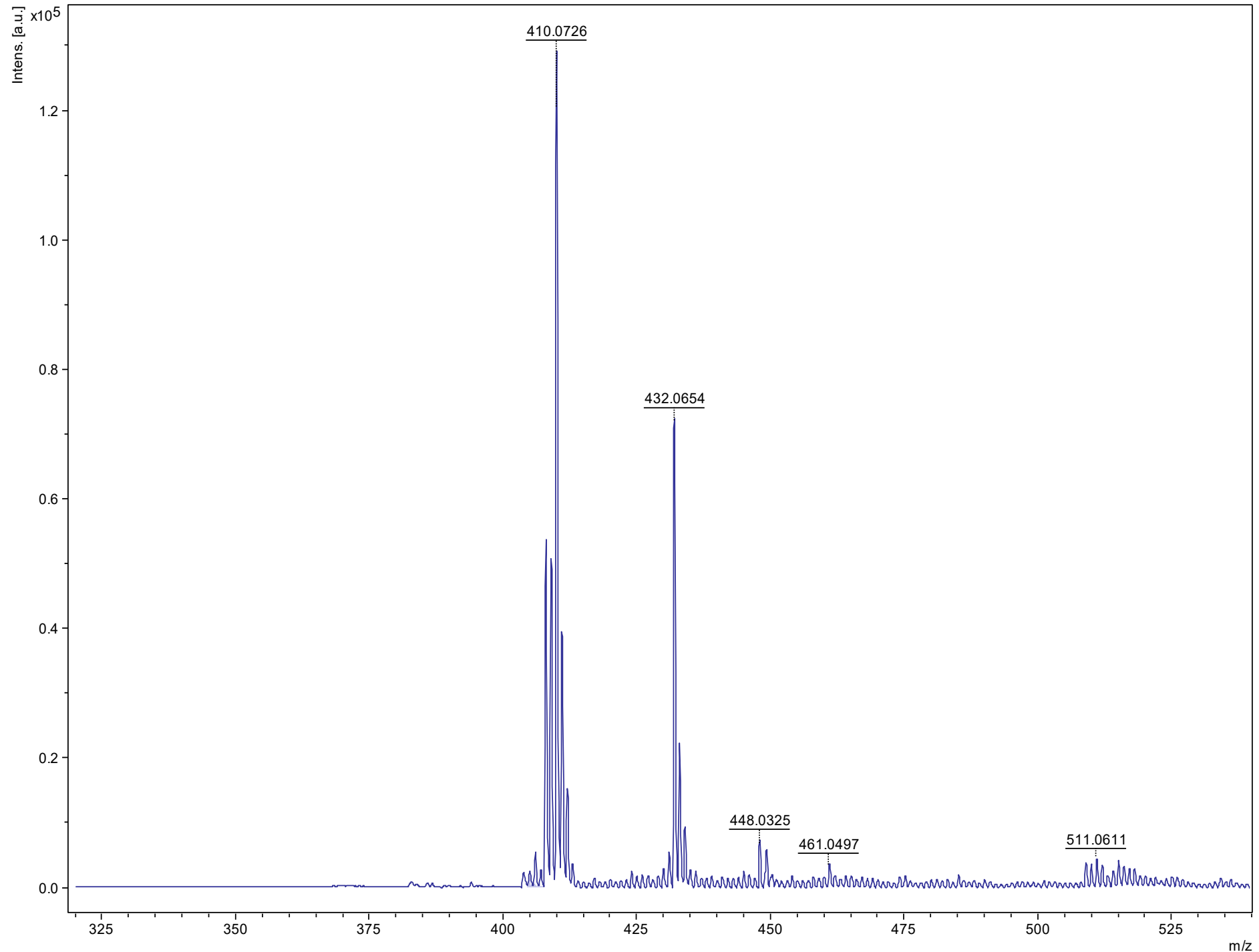










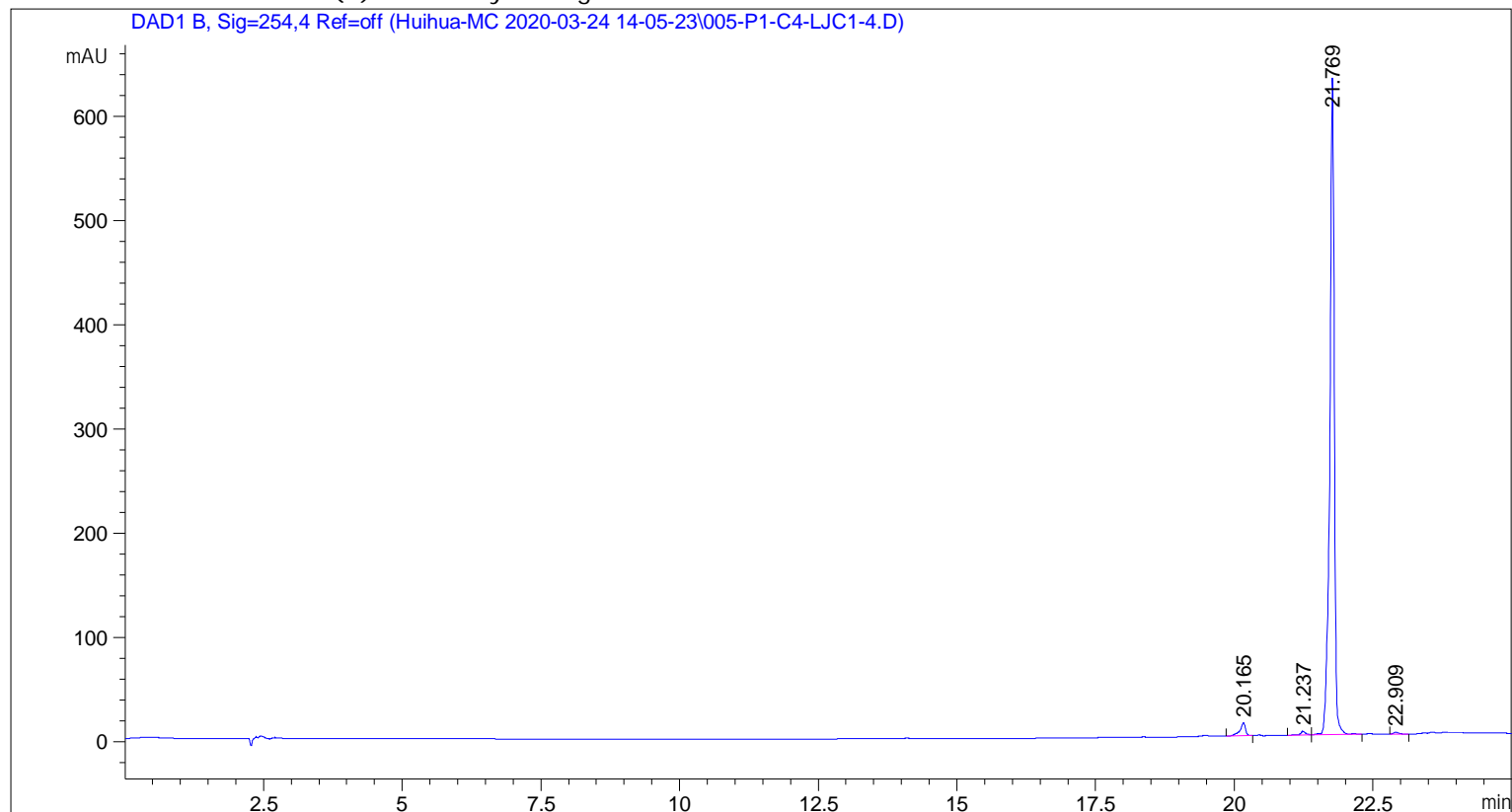


Sample Name: LJC1-4

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    5
Sample Operator : SYSTEM
Acq. Instrument : 1260Infinity2              Location  : P1-C-04
Injection Date  : 3/24/2020 3:47:35 PM      Inj       :    1
                                           Inj Volume: 50.000 µl
Method          : C:\Users\Public\Documents\ChemStation\1\Data\Huihua-MC 2020-03-24 14-05-23
                  \MC-SMALL MOLE.M (Sequence Method)
Last changed    : 2/19/2020 11:54:04 AM by SYSTEM
Additional Info : Peak(s) manually integrated
=====

```



```

=====
                          Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

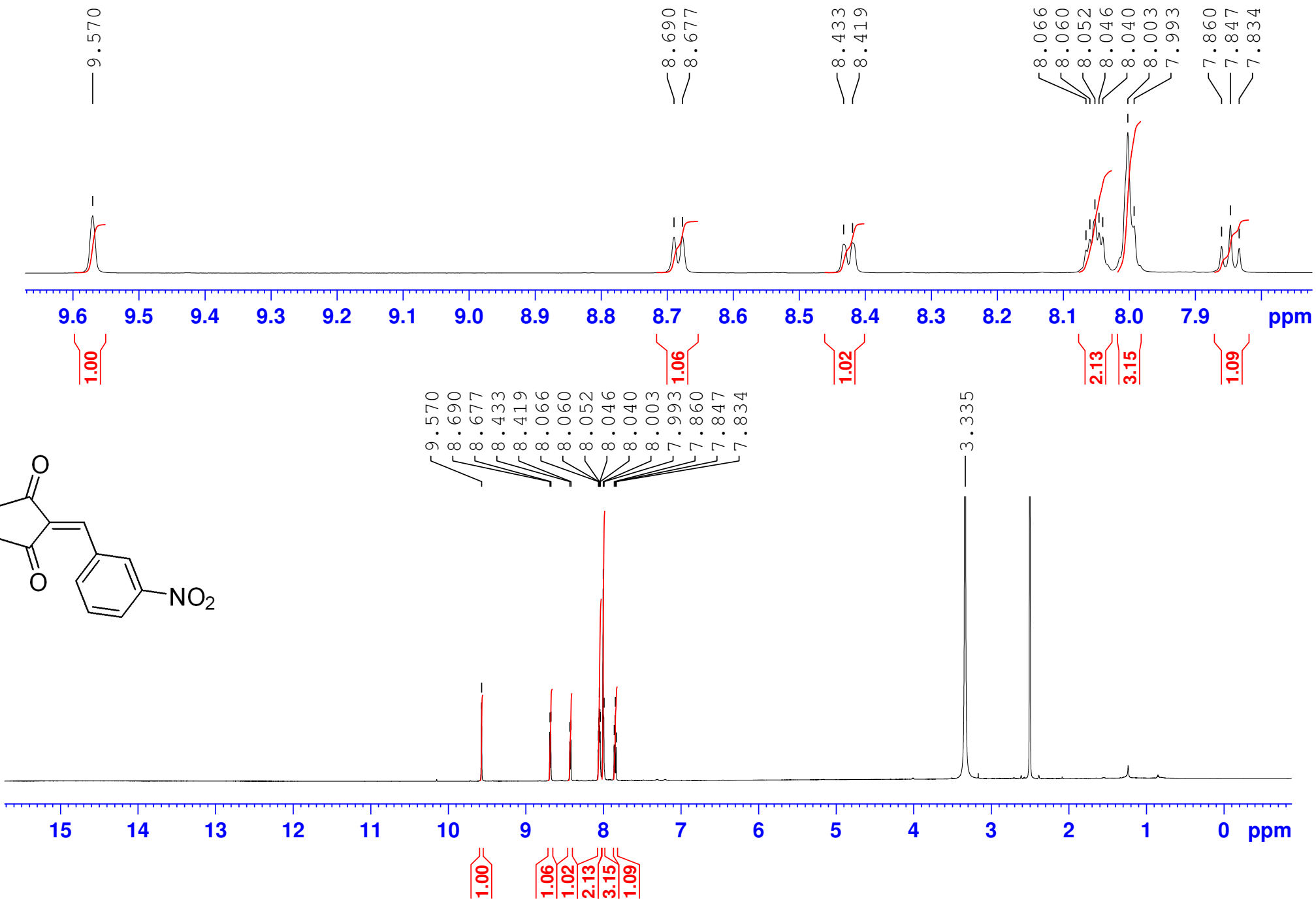
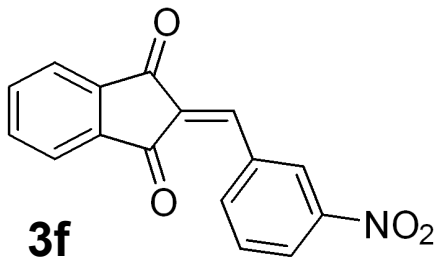
```

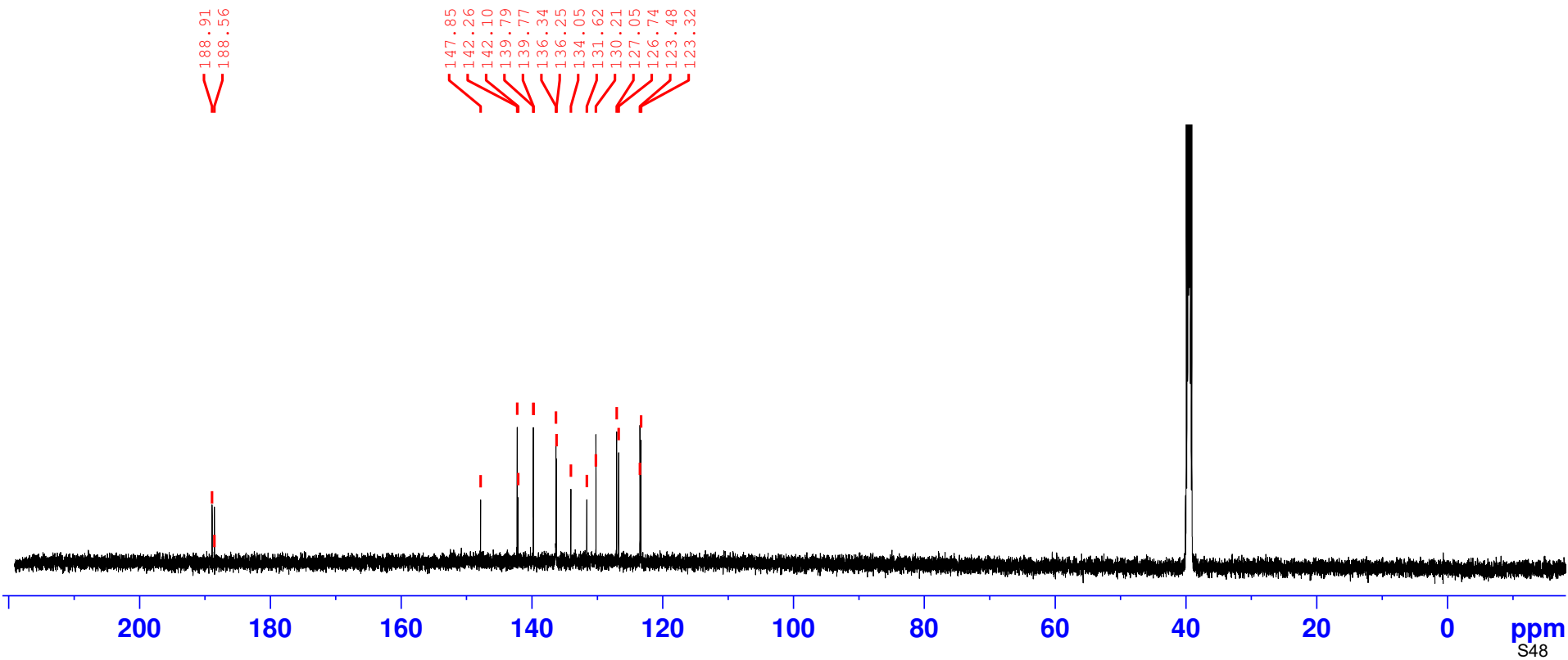
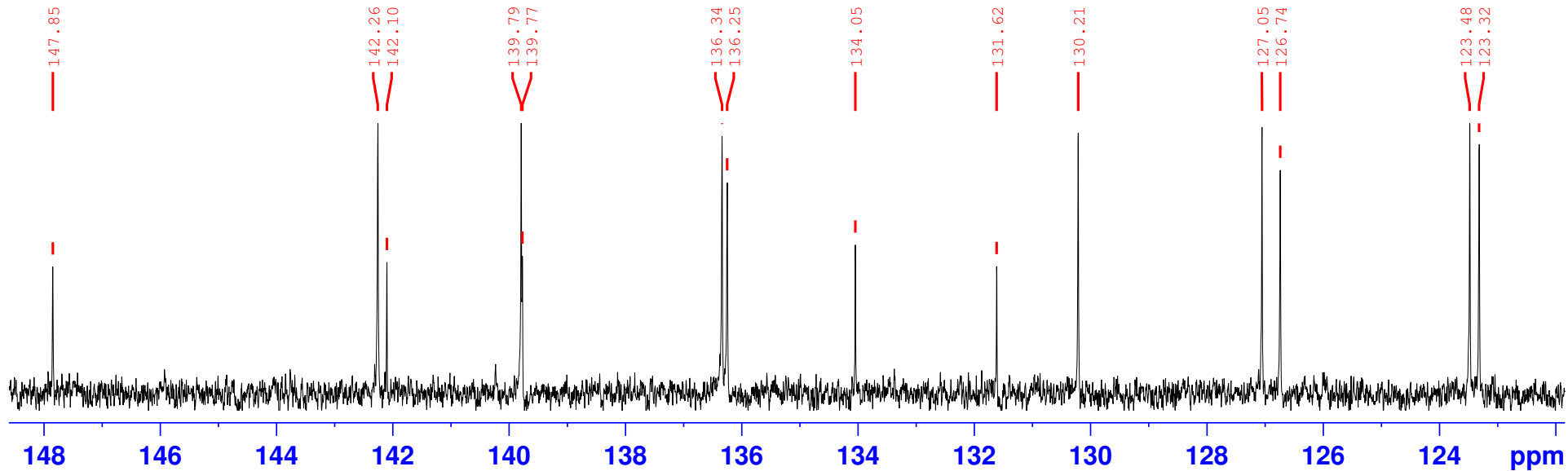
Signal 1: DAD1 B, Sig=254,4 Ref=off

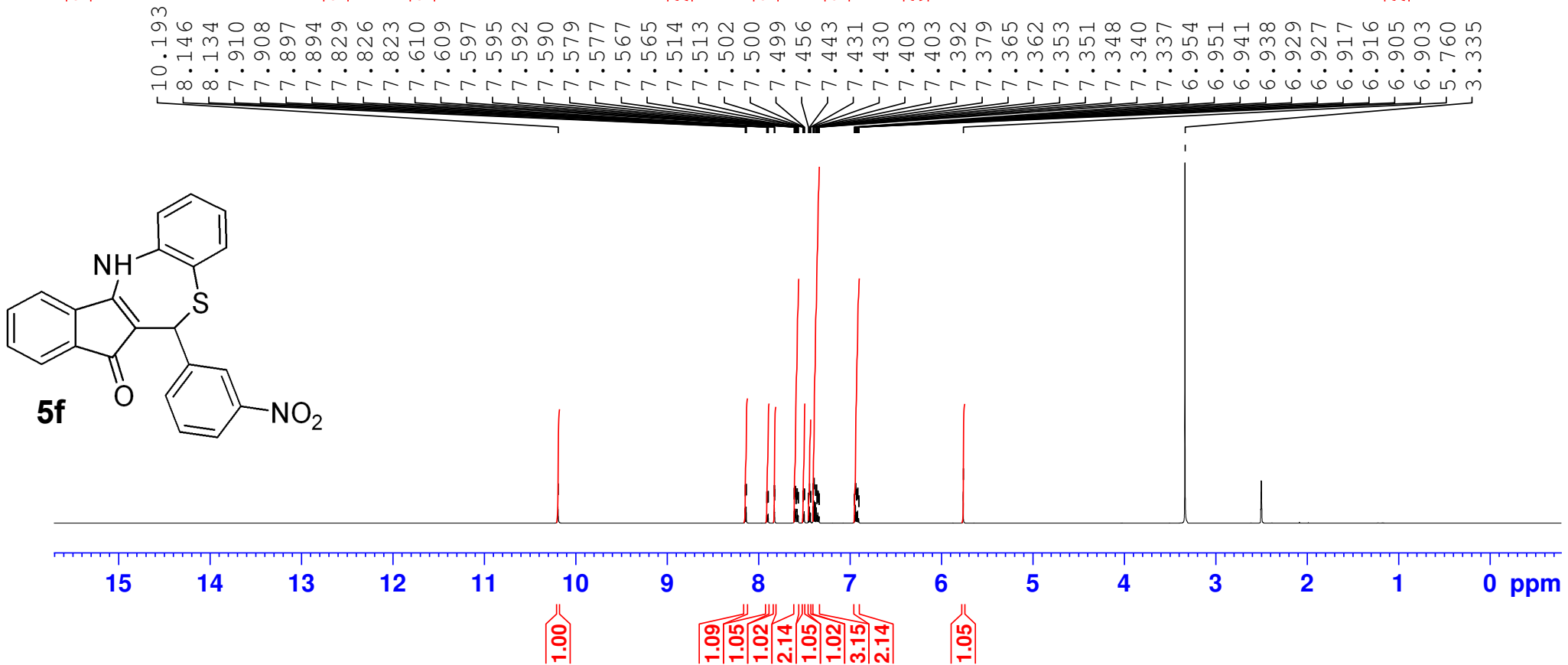
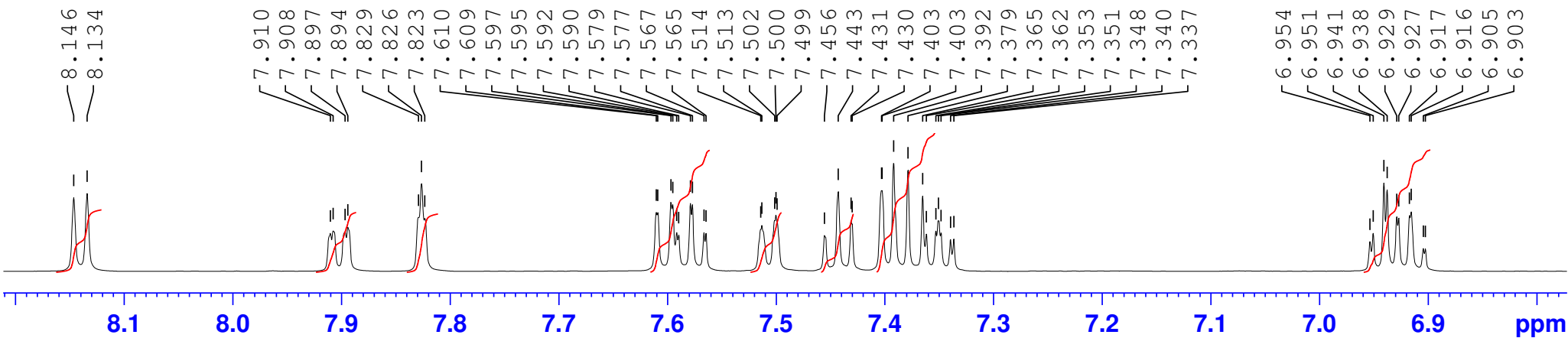
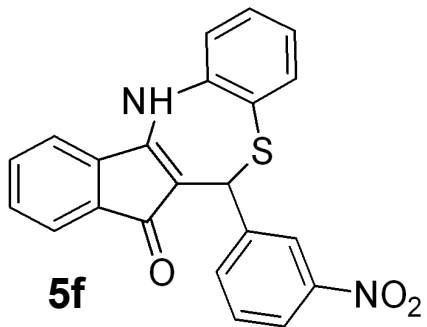
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.165	BB	0.0998	87.45600	12.47928	2.3975
2	21.237	BB	0.0884	20.89450	3.46431	0.5728
3	21.769	VV R	0.0834	3528.32349	629.36877	96.7267
4	22.909	BB	0.0939	11.04991	1.74431	0.3029

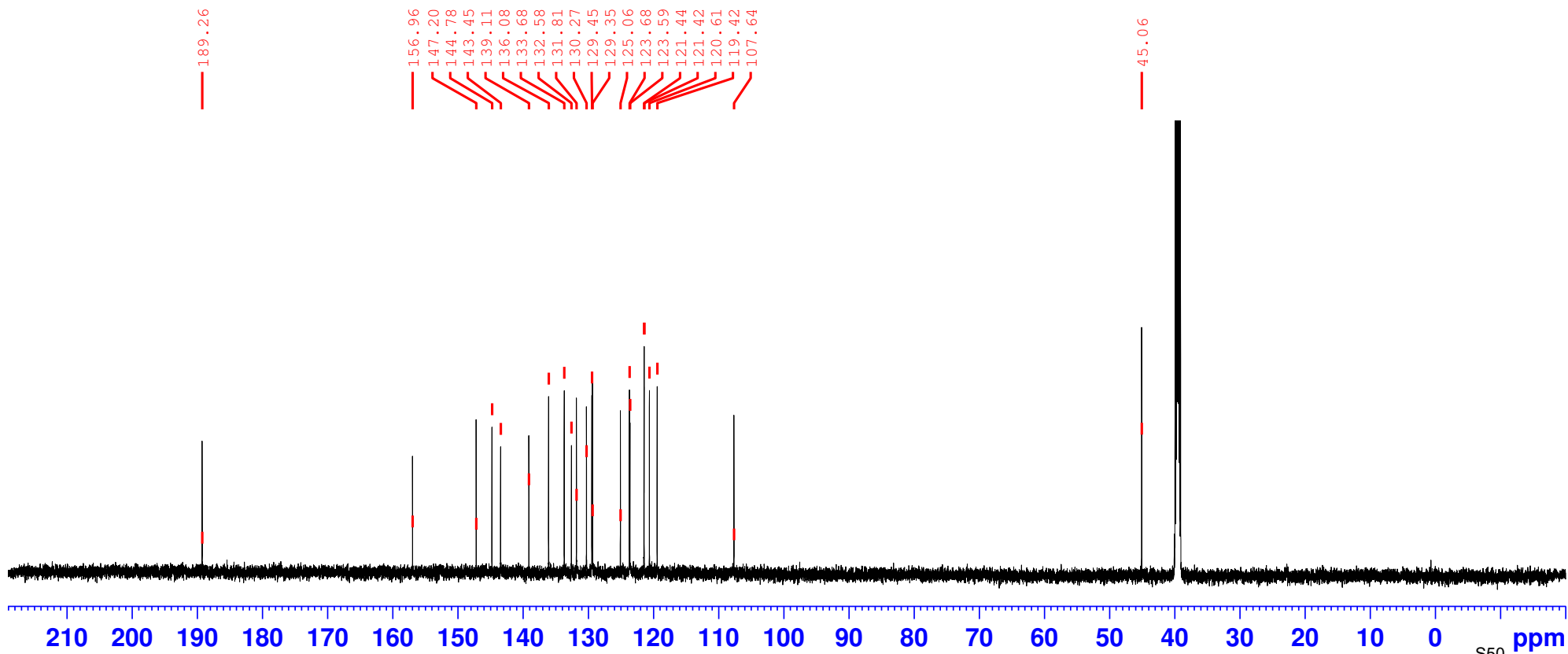
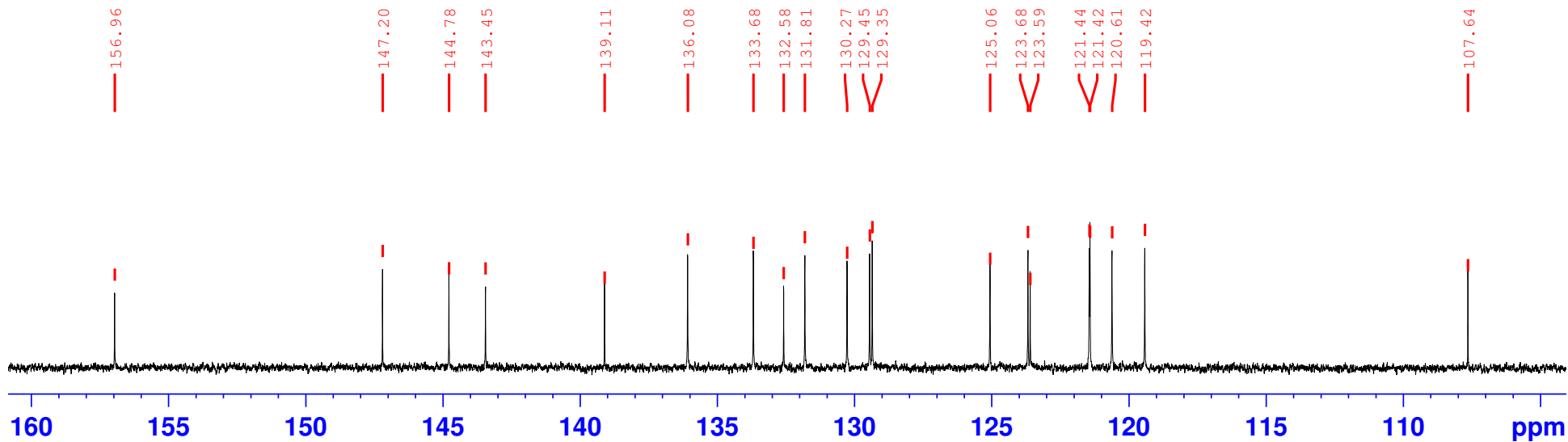
```
Totals :                      3647.72389  647.05667
```

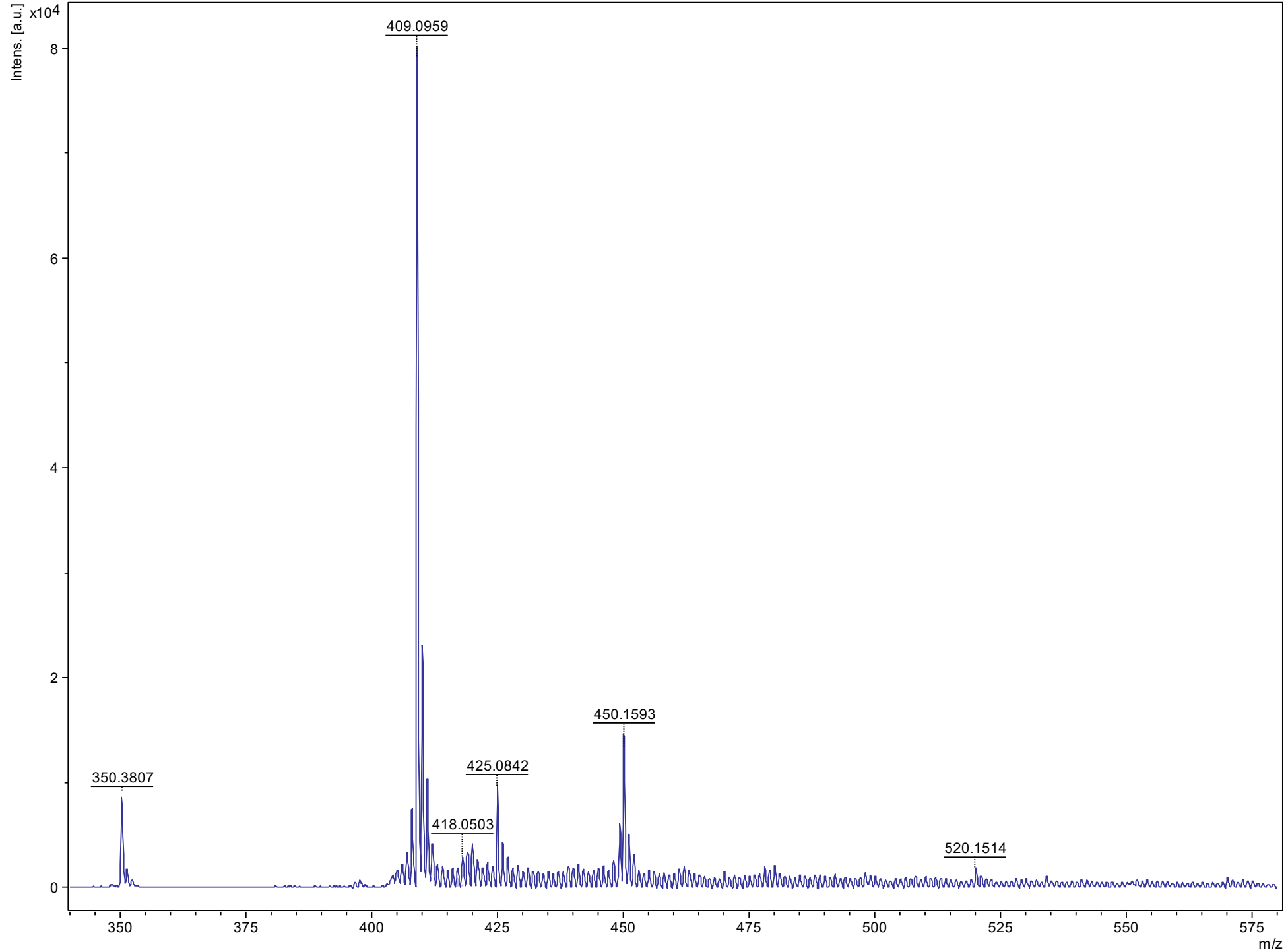
=====
*** End of Report ***











Sample Name: MAS 3-62

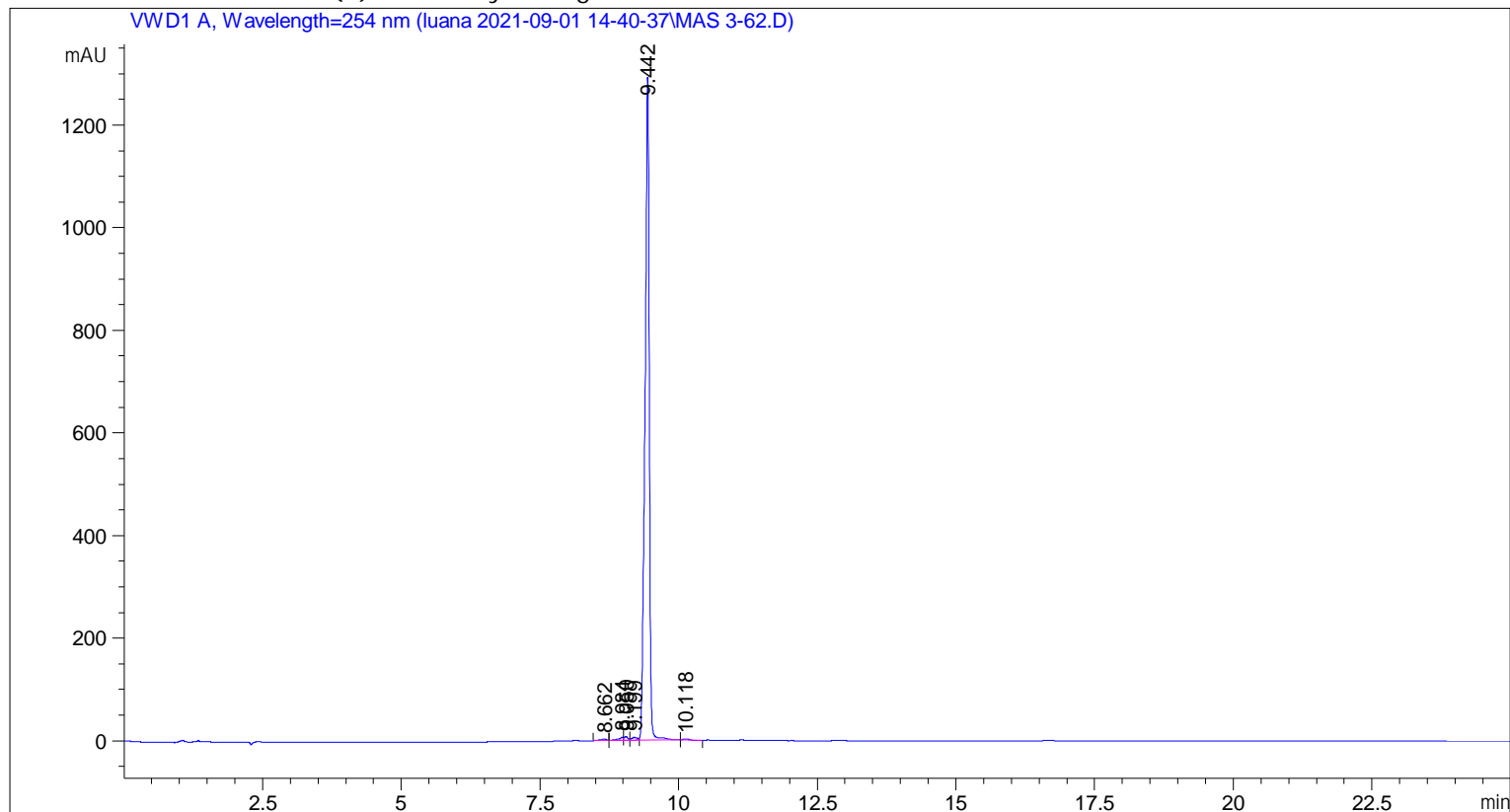
```

=====
Acq. Operator   : SYSTEM                               Seq. Line :    5
Acq. Instrument : 1220 HPLC                             Location  :   65
Injection Date  : 9/1/2021 4:13:08 PM                  Inj       :    1
                                                    Inj Volume: 50.000 µl

Acq. Method     : C:\Chem32\1\Data\luana 2021-09-01 14-40-37\Luana_small_molecule.M
Last changed    : 9/1/2021 3:22:09 PM by SYSTEM
Analysis Method : C:\Chem32\1\Data\luana 2021-09-01 14-40-37\Luana_small_molecule.M (Sequence
Method)
Last changed    : 9/1/2021 3:44:43 PM by SYSTEM
Method Info     : MeOH/water

Sample Info     : MAS 3-62
    
```

Additional Info : Peak(s) manually integrated



Area Percent Report

```

=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

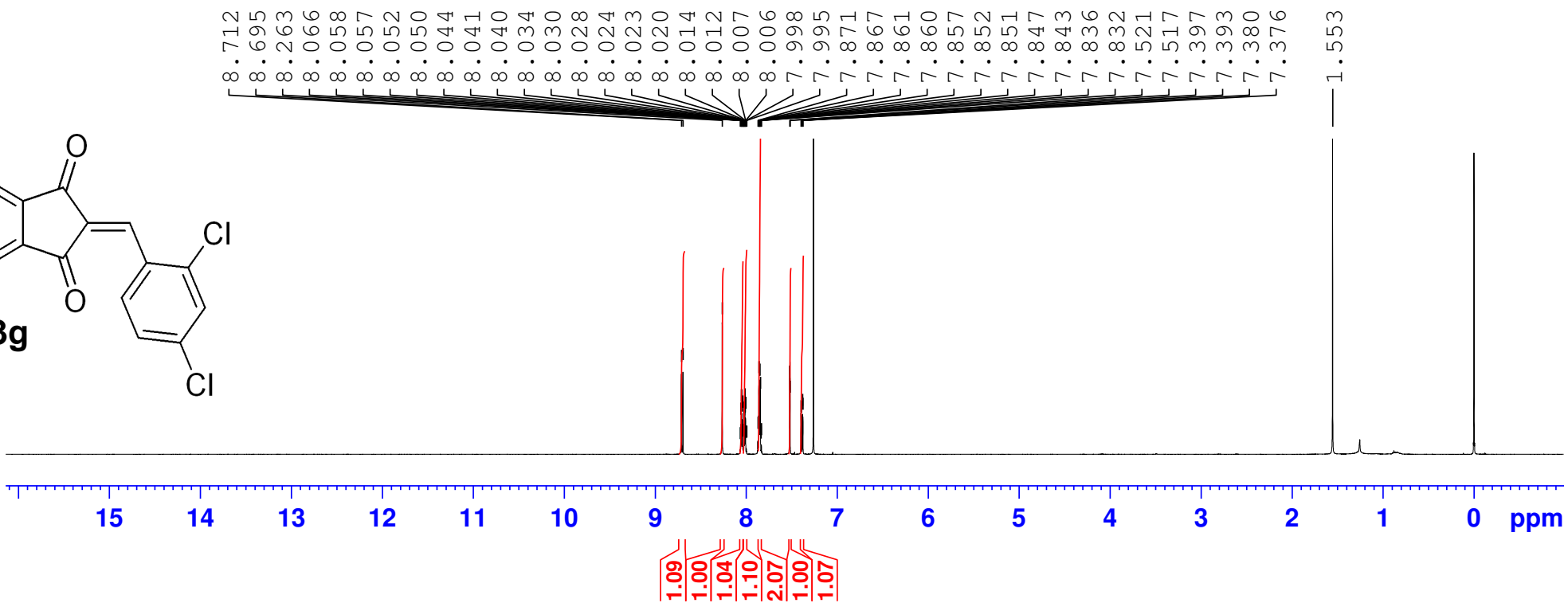
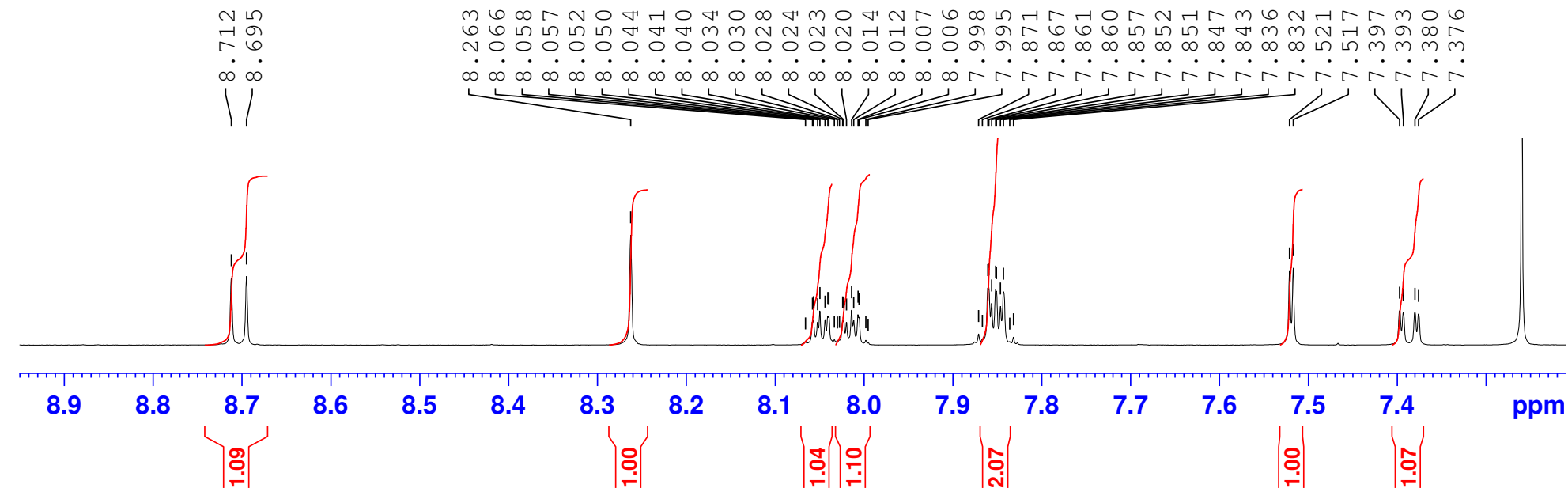
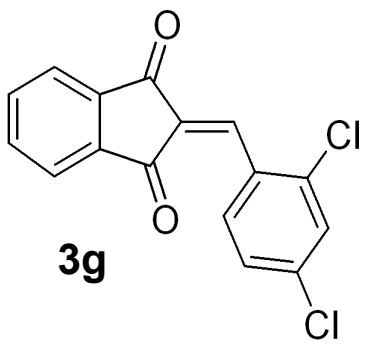
Signal 1: VWD1 A, Wavelength=254 nm

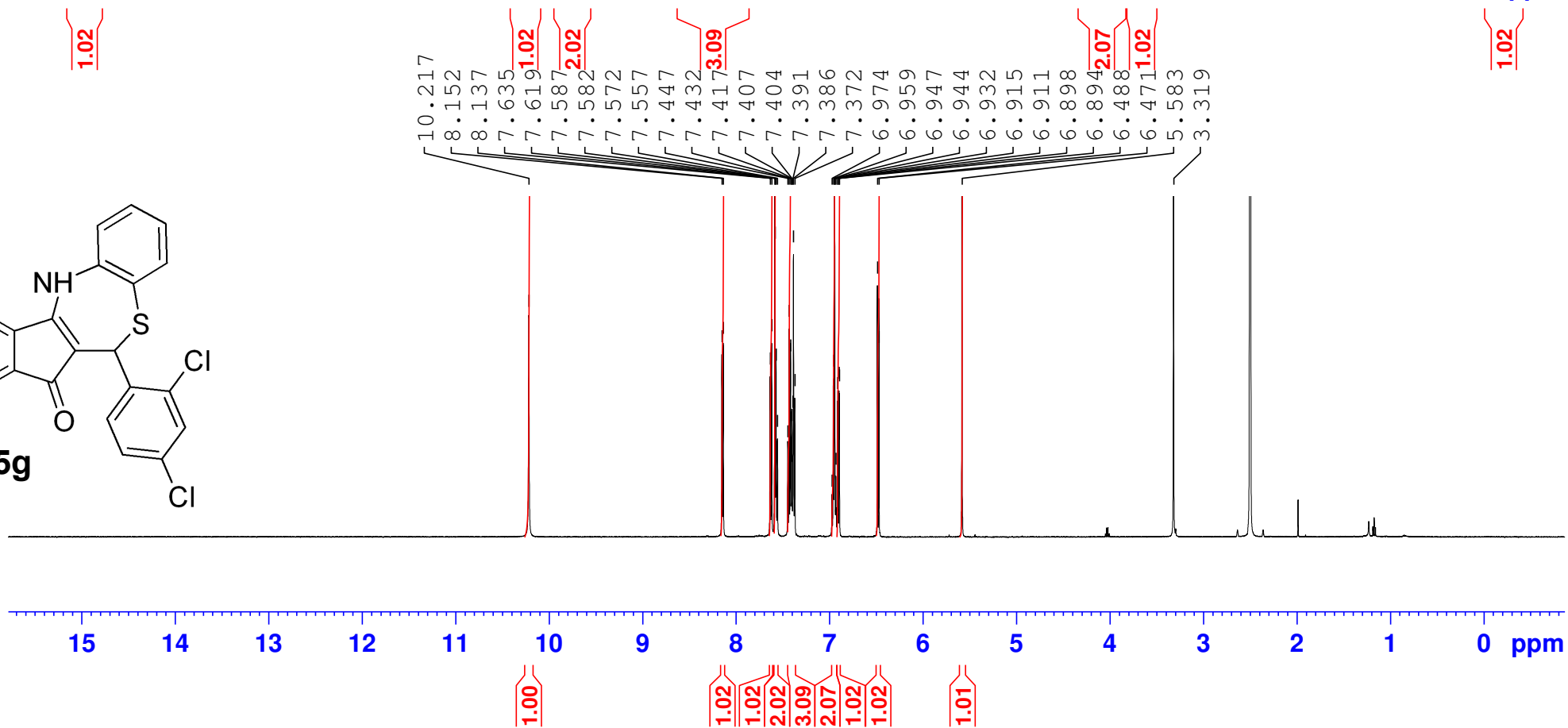
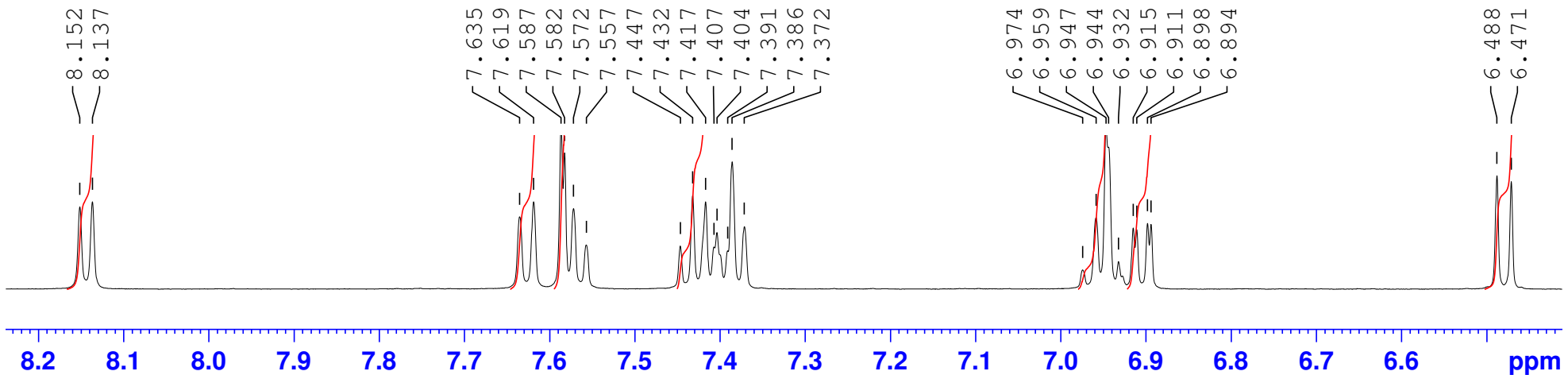
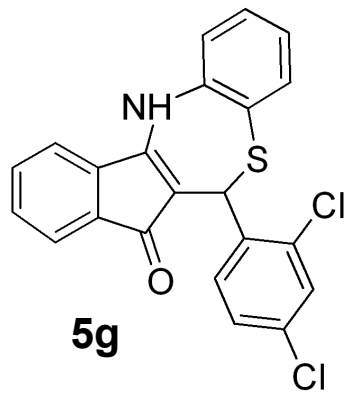
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.662	BB	0.1041	18.26989	2.47541	0.2613
2	8.984	BV E	0.0787	29.72317	5.27424	0.4251
3	9.050	VV E	0.0683	32.02338	6.75701	0.4580

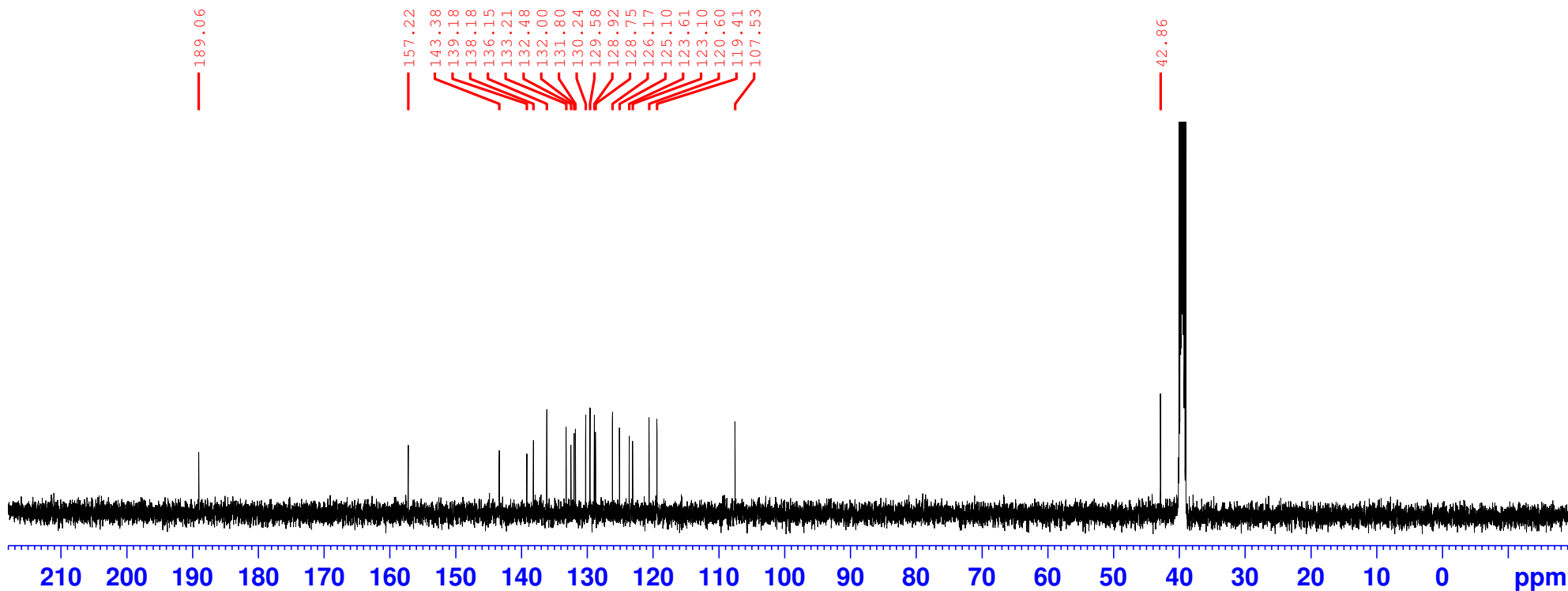
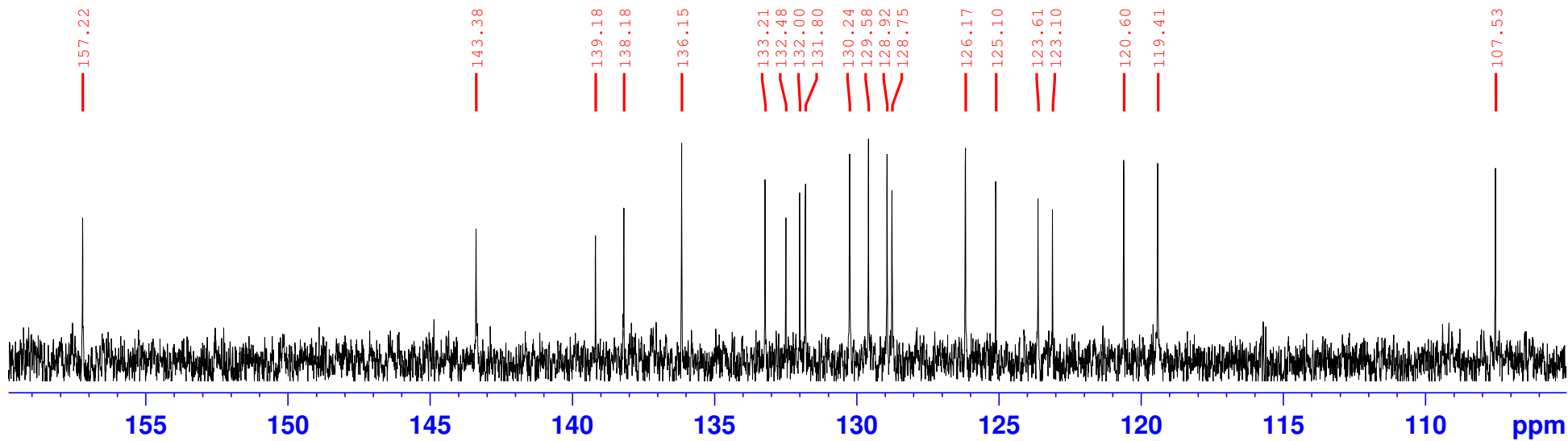
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
4	9.199	VV E	0.0972	37.04636	5.19777	0.5298
5	9.442	VV R	0.0759	6861.21191	1293.59338	98.1269
6	10.118	BV R	0.0976	13.91127	1.99002	0.1990

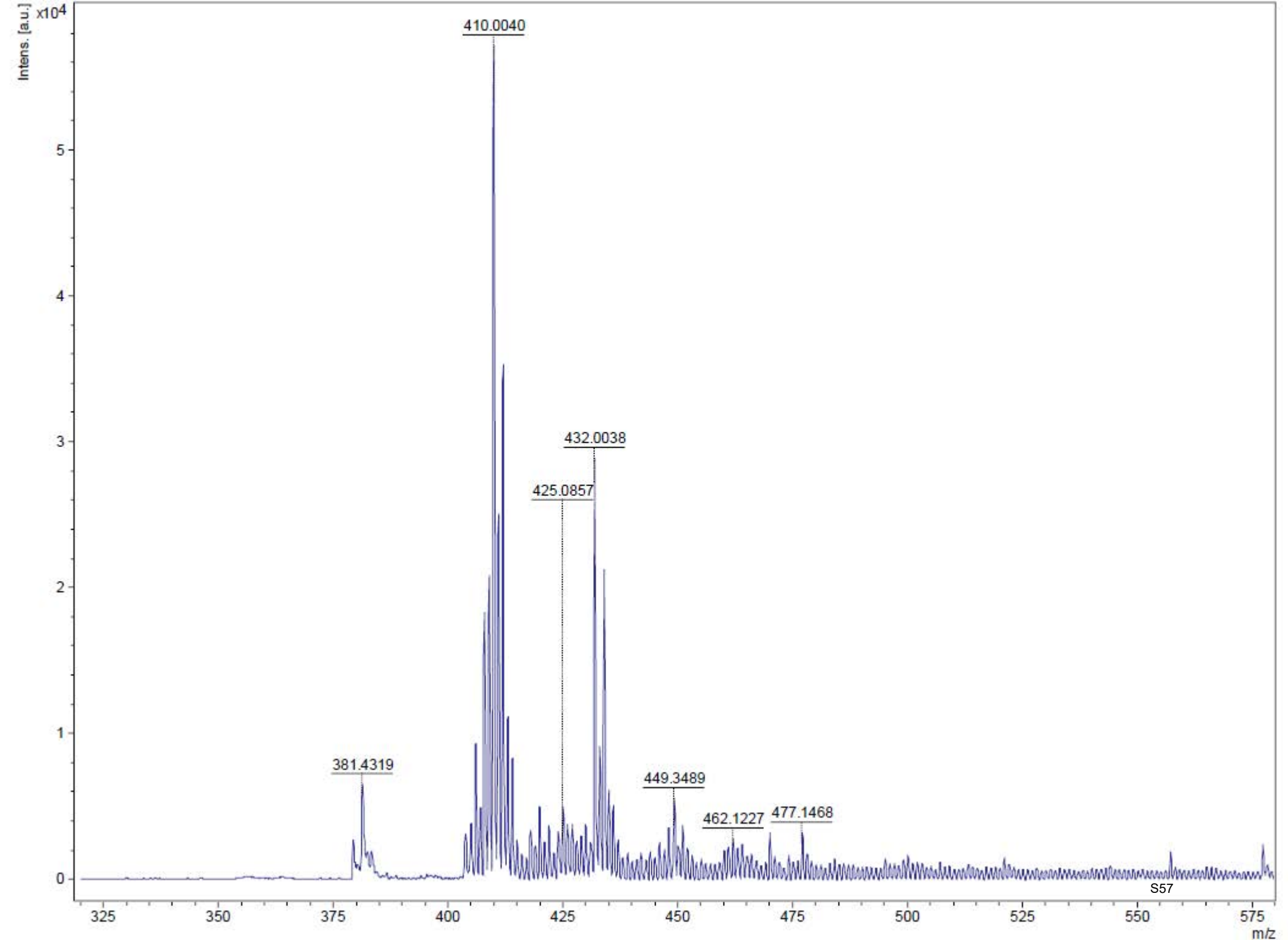
Totals : 6992.18599 1315.28784

=====
*** End of Report ***



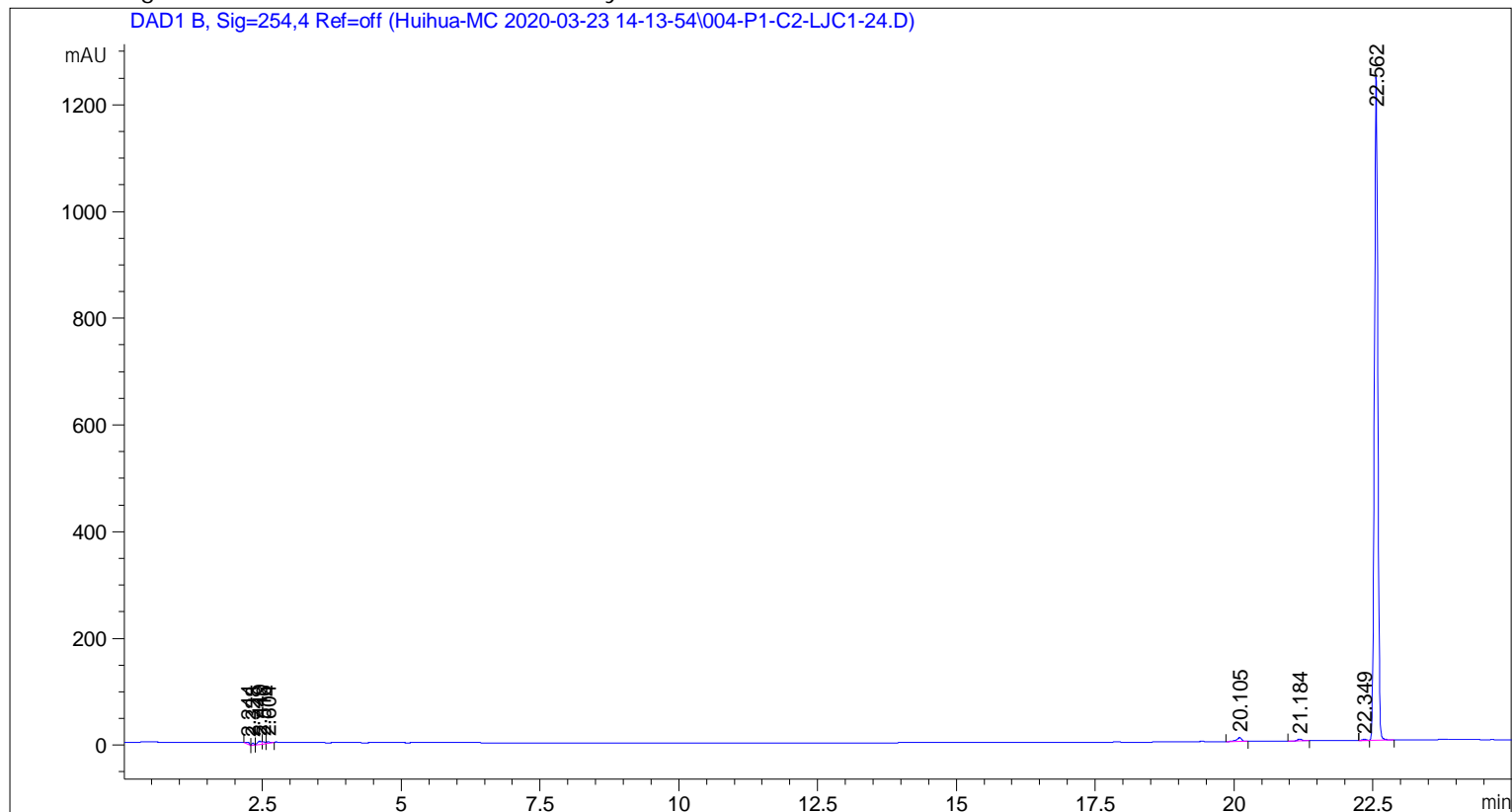






```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    4
Sample Operator : SYSTEM
Acq. Instrument : 1260Infinite2              Location  : P1-C-02
Injection Date  : 3/23/2020 3:24:33 PM       Inj       :    1
                                                Inj Volume: 50.000 µl
Method          : C:\Users\Public\Documents\ChemStation\1\Data\Huihua-MC 2020-03-23 14-13-54
                 \MC-SMALL MOLE.M (Sequence Method)
Last changed    : 2/19/2020 11:54:04 AM by SYSTEM
  
```



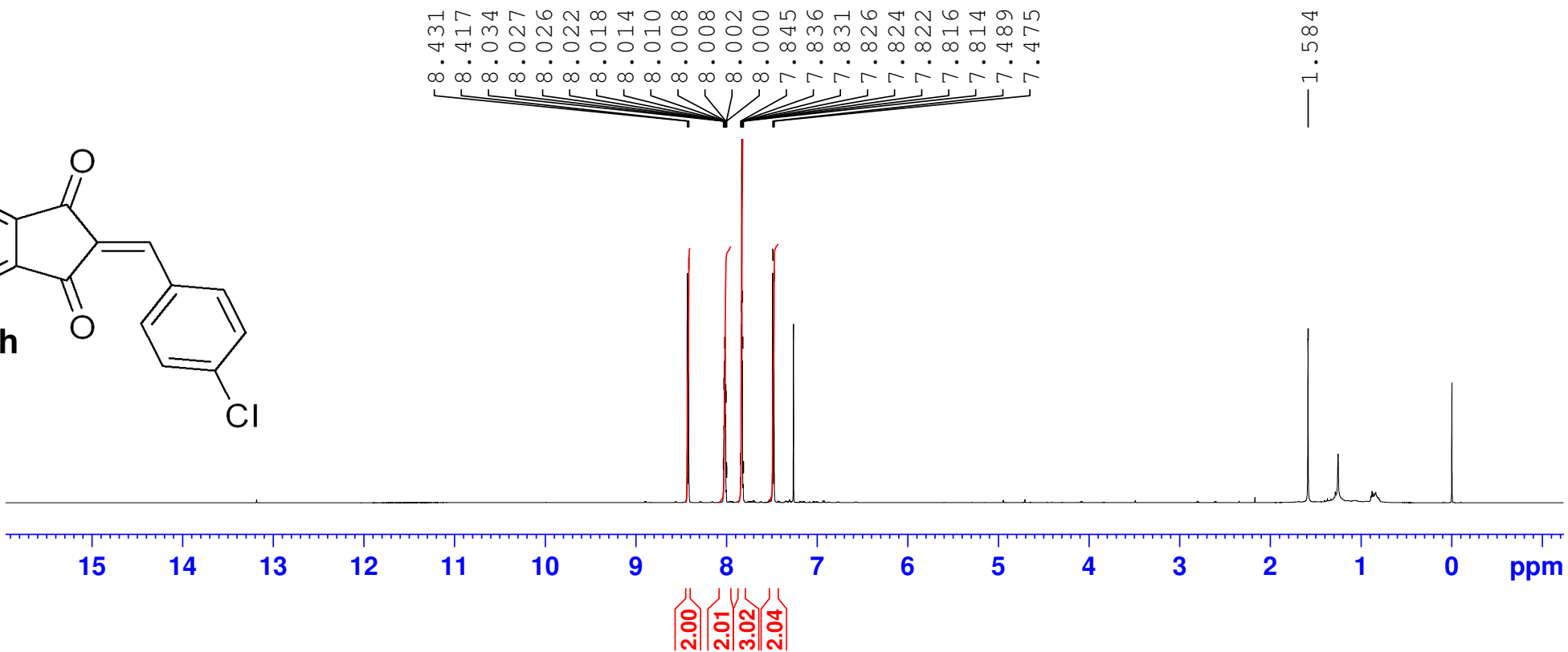
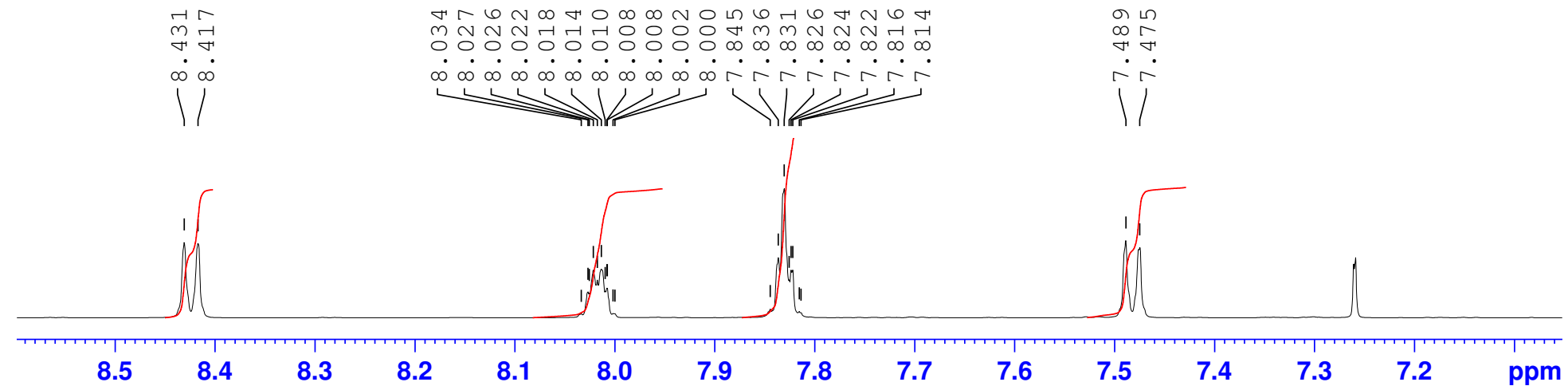
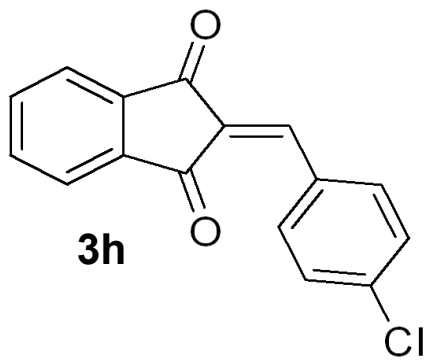
=====
 Area Percent Report
 =====

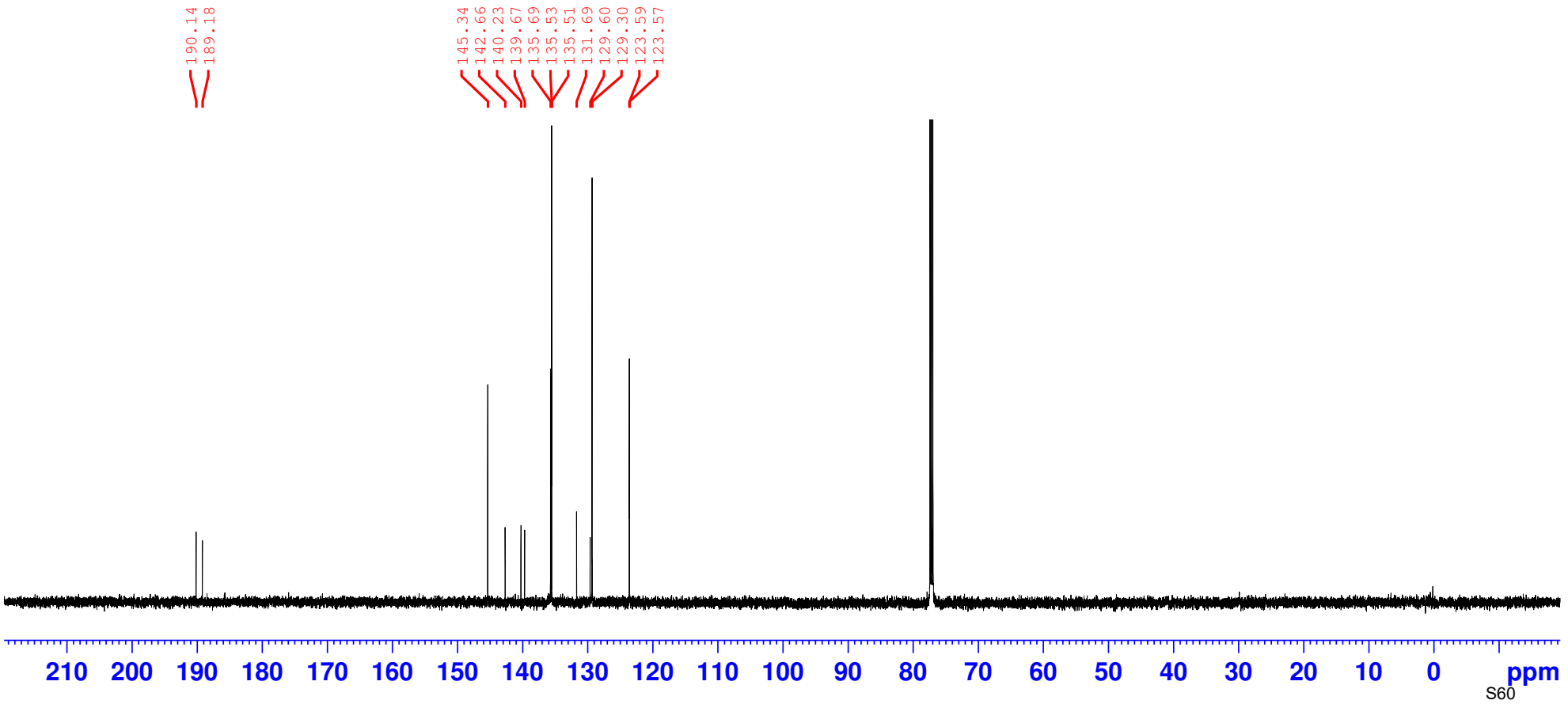
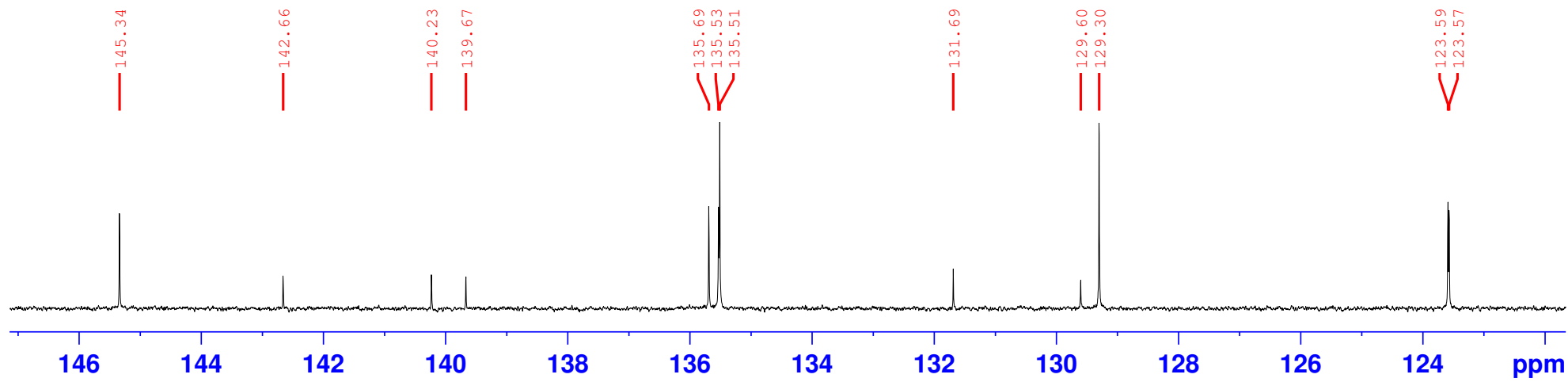
```

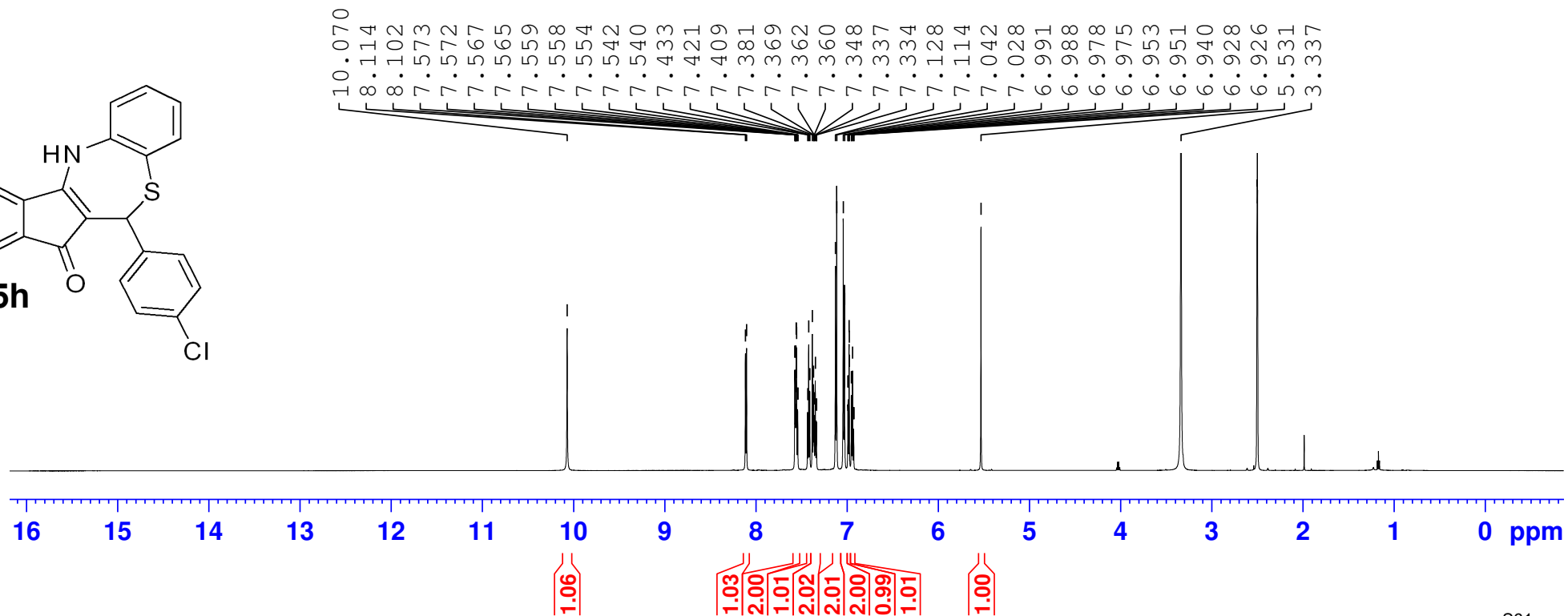
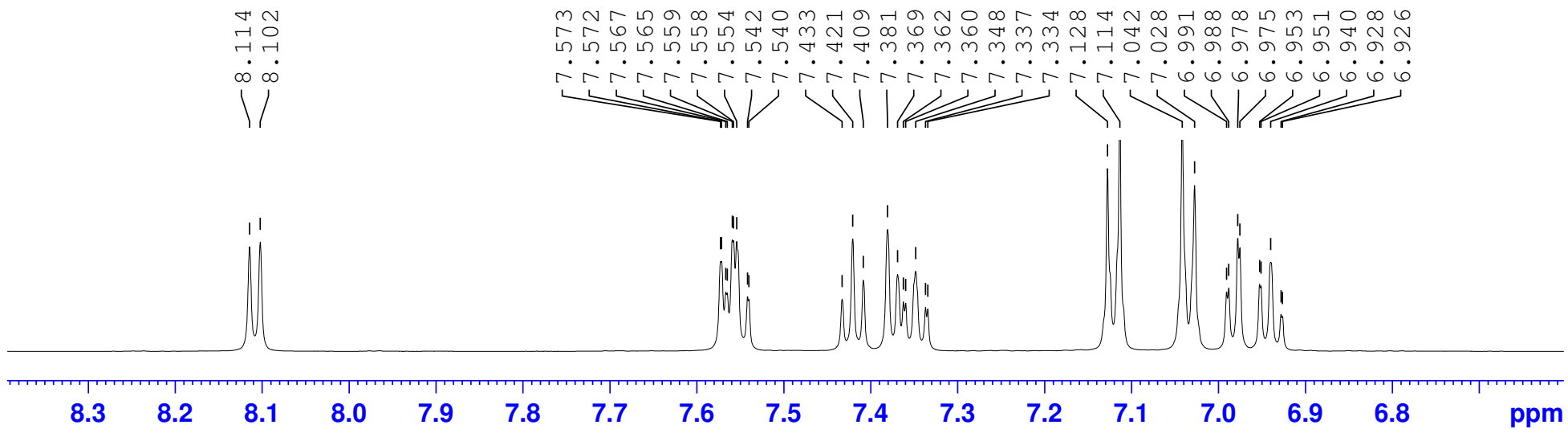
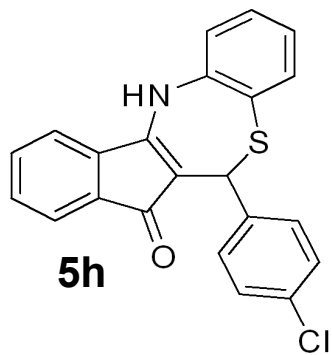
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

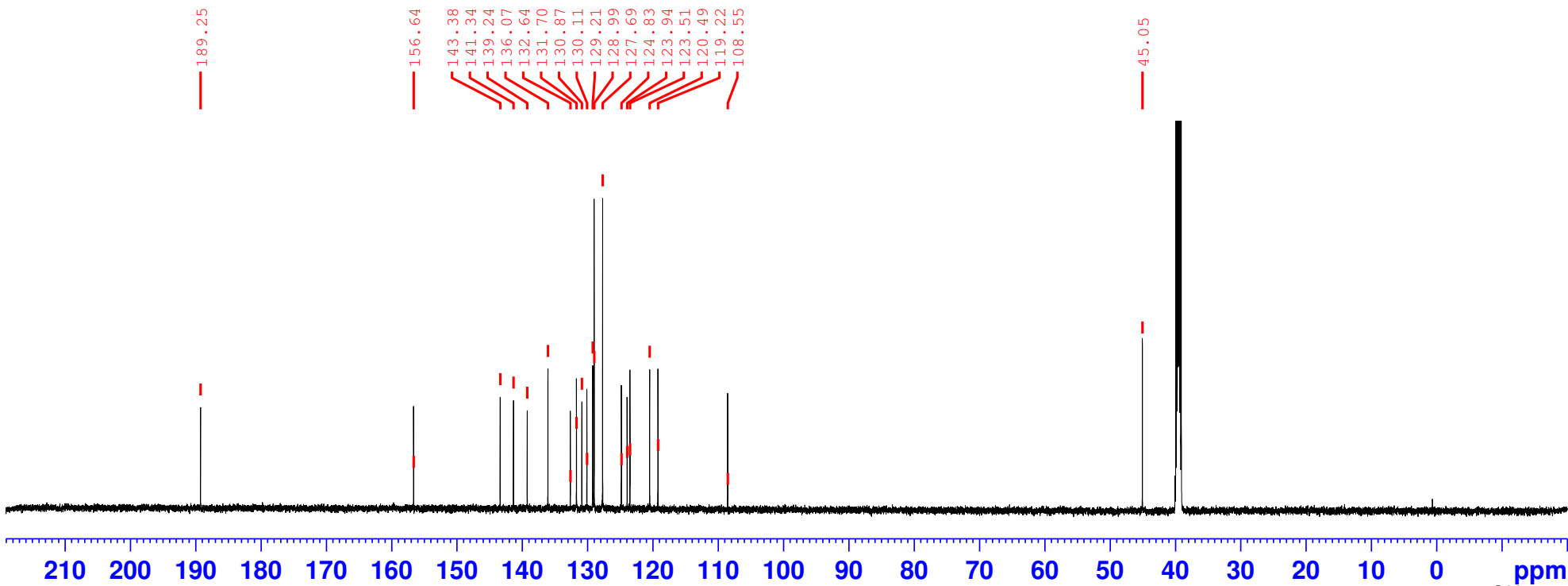
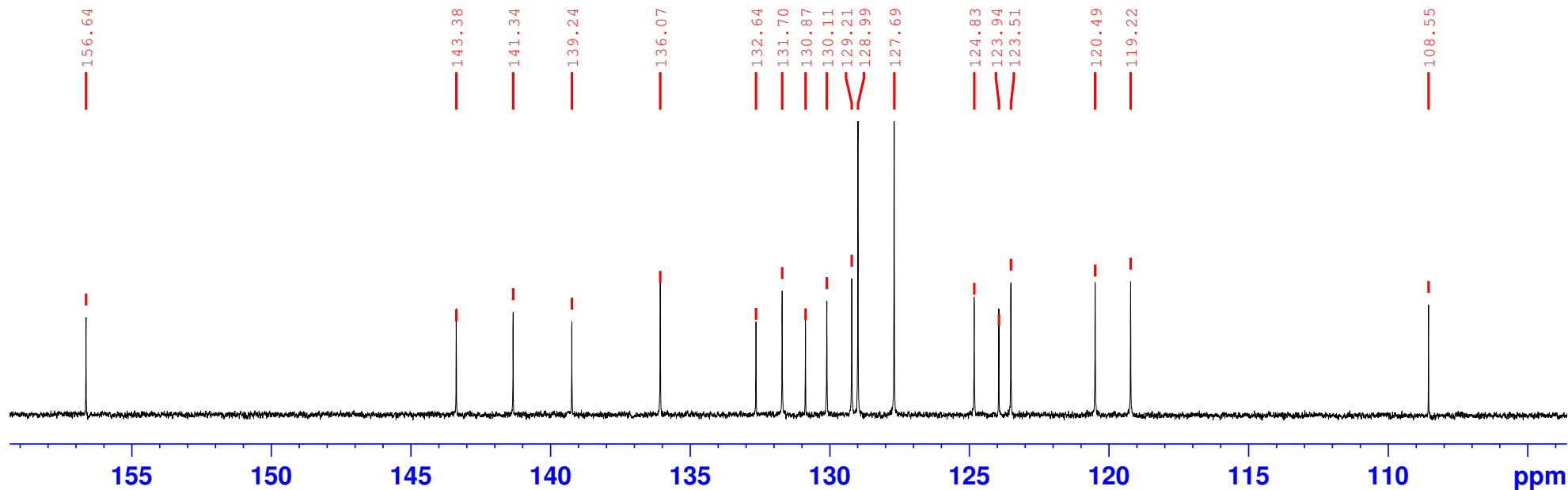
Signal 1: DAD1 B, Sig=254, 4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.244	BB	0.0527	14.43443	3.76618	0.2594
2	2.328	BB	0.0438	11.32773	4.42787	0.2035
3	2.449	BV	0.0799	31.01915	6.25525	0.5573
4	2.516	VV	0.0532	14.17586	4.01256	0.2547
5	2.604	VB	0.0739	16.91662	3.19085	0.3040
6	20.105	BB	0.0936	46.56497	7.18940	0.8367
7	21.184	BB	0.0878	21.39718	3.68343	0.3845
8	22.349	BV E	0.0736	10.60570	2.22393	0.1906
9	22.562	VB R	0.0665	5399.10205	1247.41296	97.0094

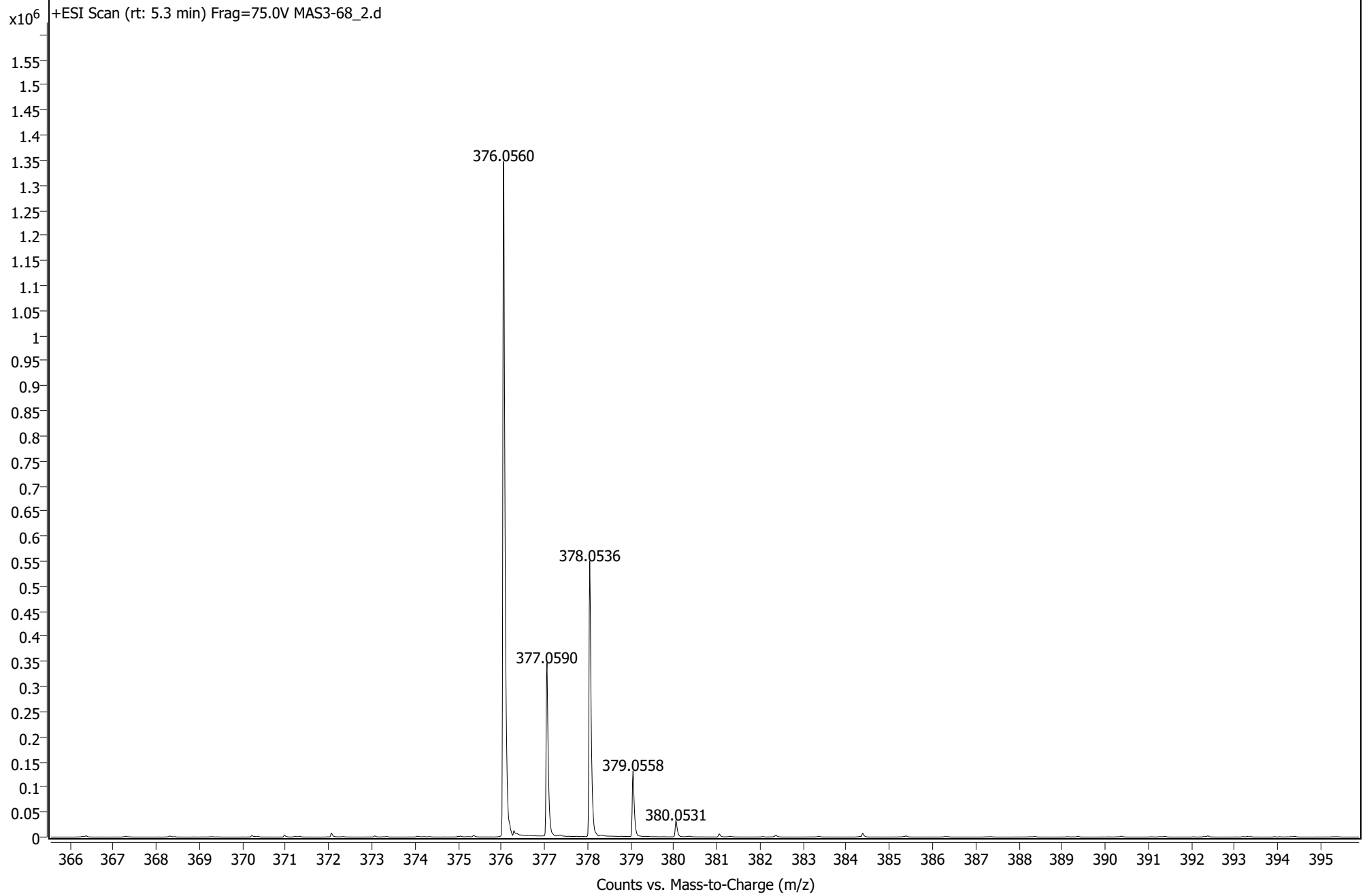








User Spectrum Plot Report



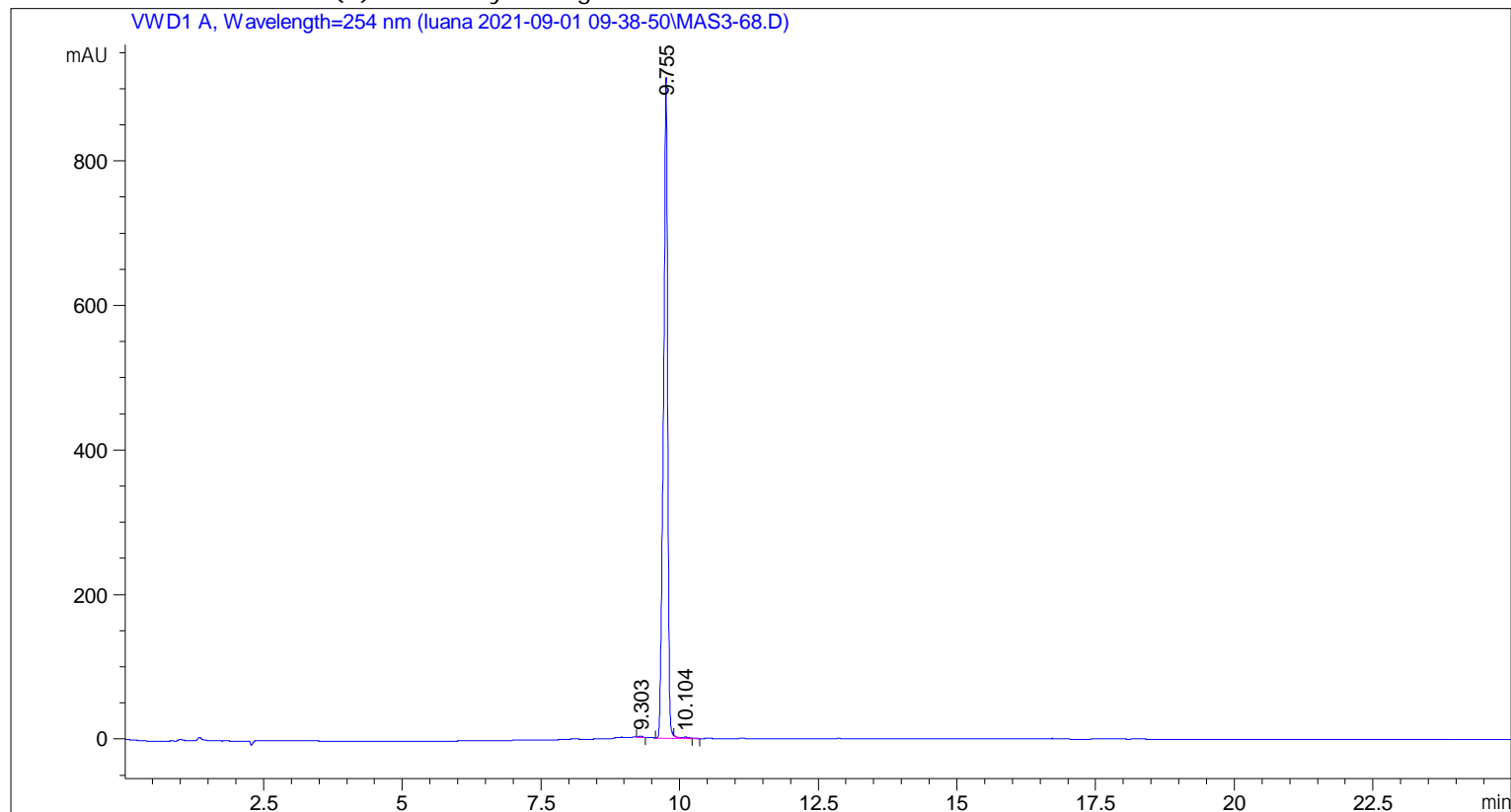
Sample Name: MAS3-68

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :   10
Acq. Instrument : 1220 HPLC                   Location  :   61
Injection Date  : 9/1/2021 1:16:36 PM        Inj       :    1
                                           Inj Volume: 50.000 µl
Method          : C:\Chem32\1\Data\luana 2021-09-01 09-38-50\Luana_small_molecule.M (Sequence
                :                               Method)
Last changed    : 9/1/2021 9:41:46 AM by SYSTEM
Method Info     : MeOH/water

Sample Info     : MAS3-68
  
```

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====
  
```

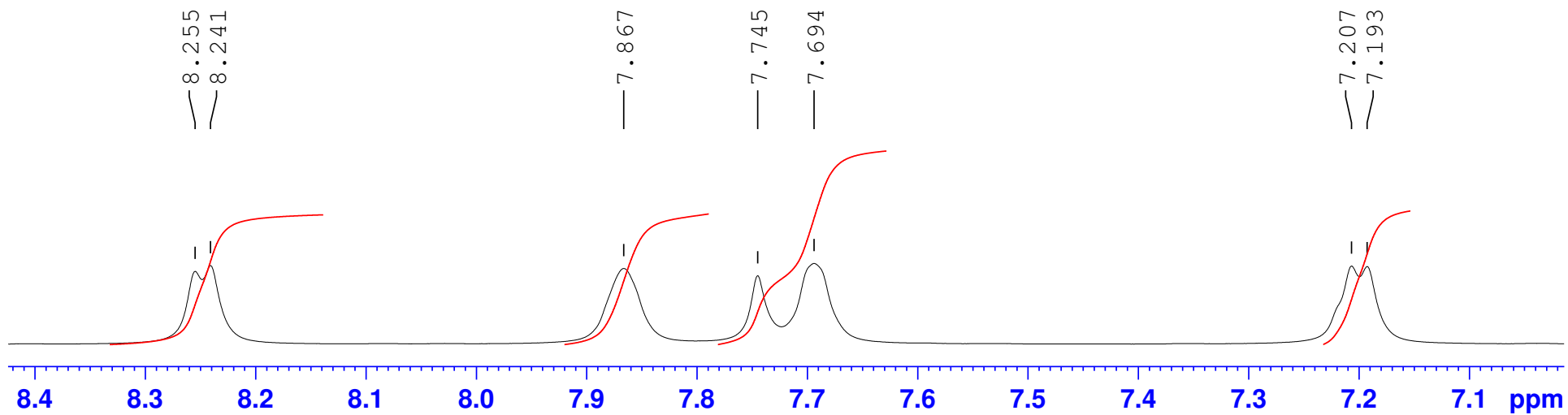
```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: VWD1 A, Wavelength=254 nm

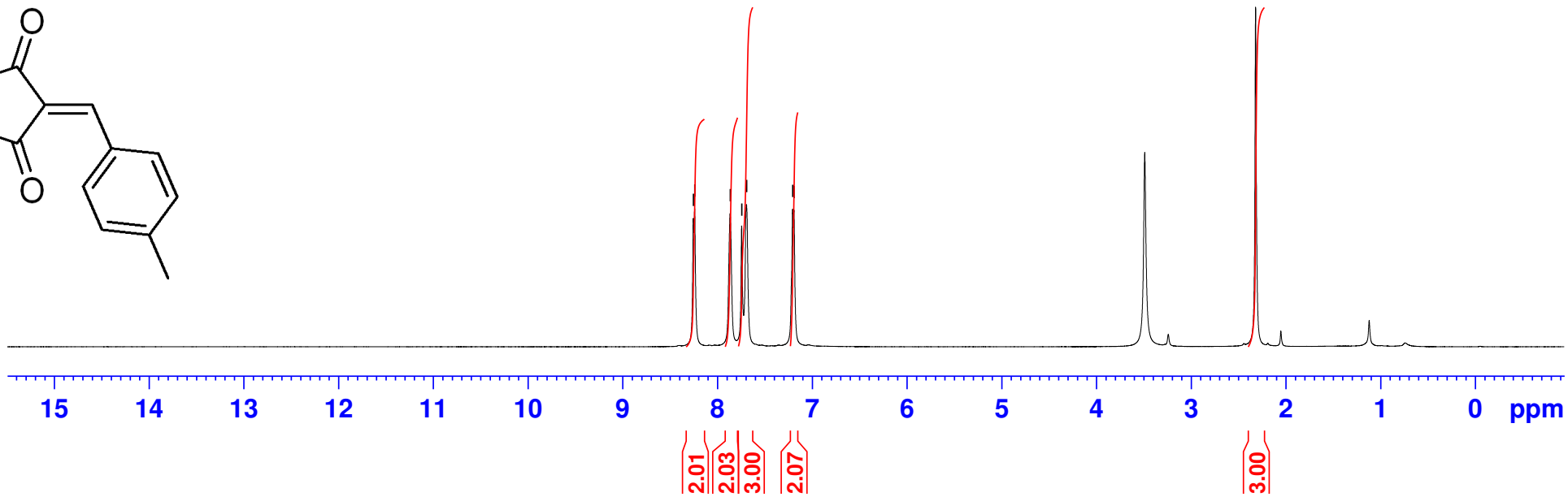
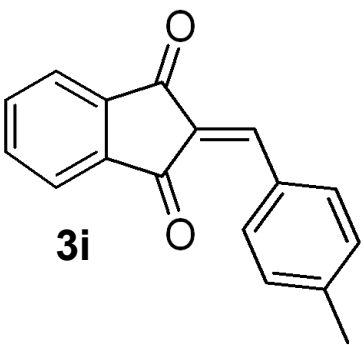
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.303	VB	0.0807	12.70151	2.32658	0.2624
2	9.755	BV R	0.0763	4813.19189	915.44733	99.4327
3	10.104	VV E	0.1108	14.76127	1.77888	0.3049

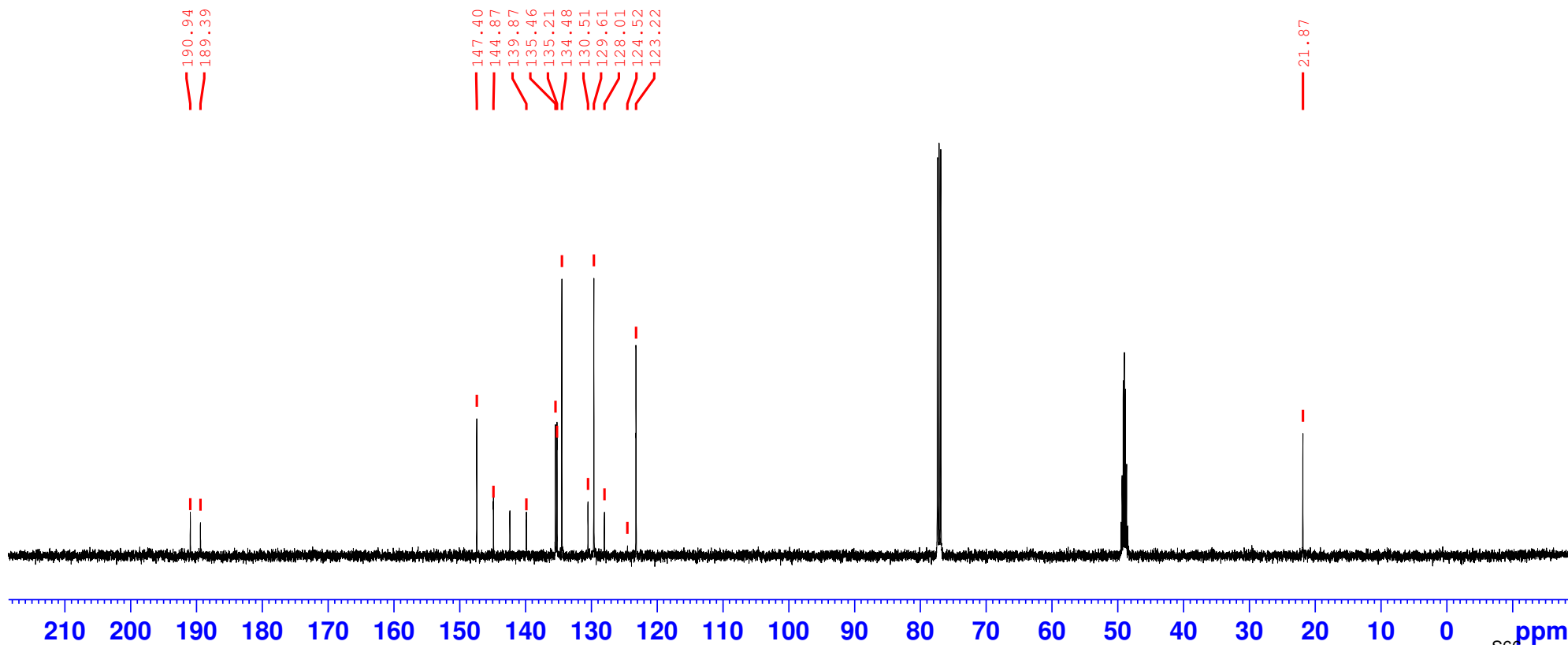
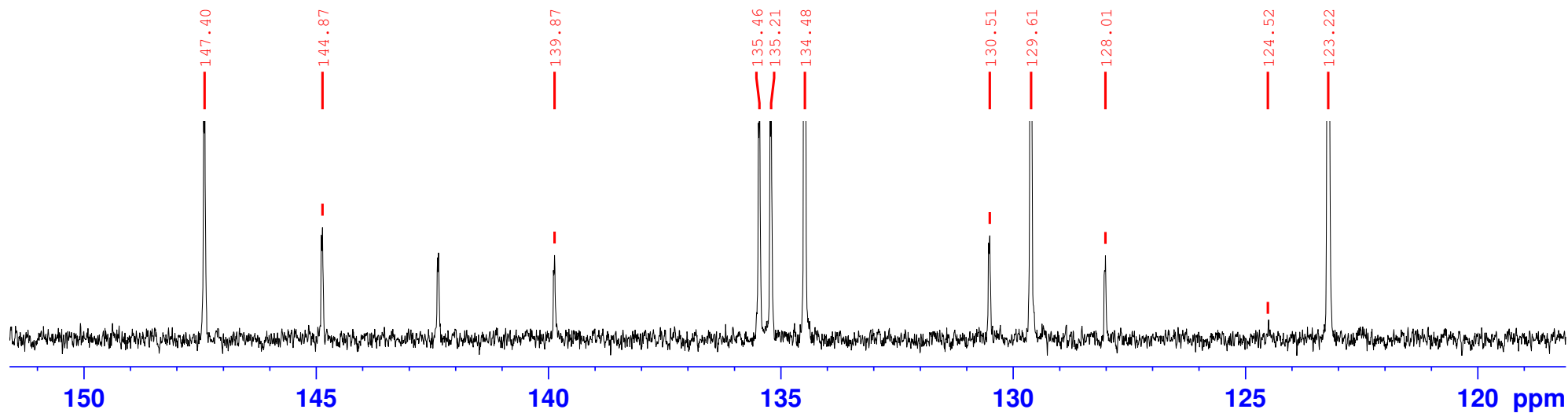
```
Totals :                      4840.65467  919.55279
```

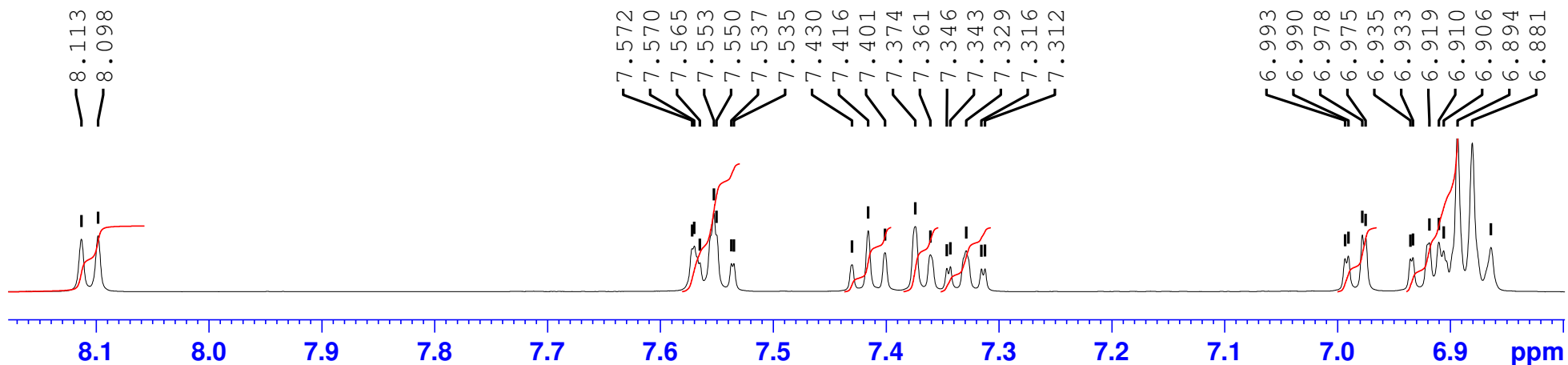
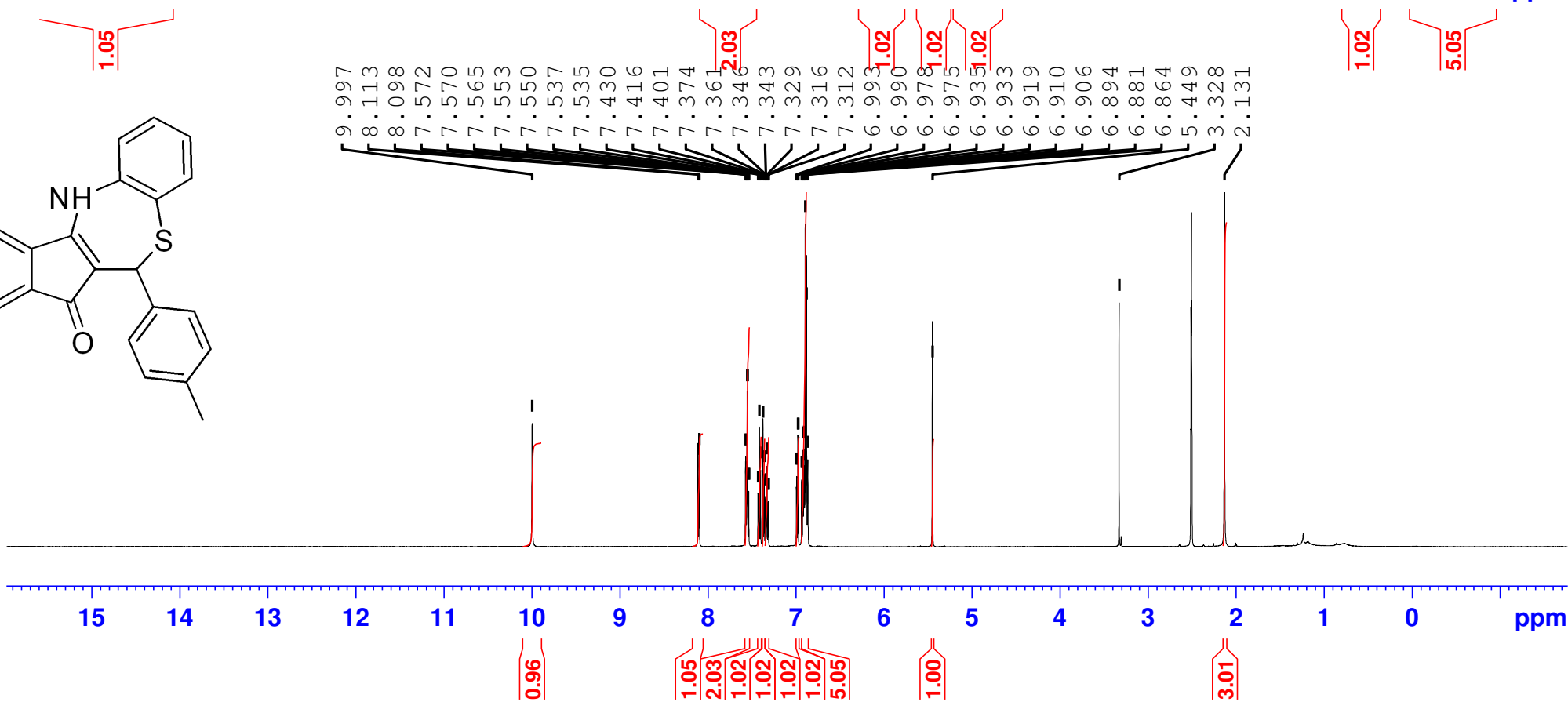
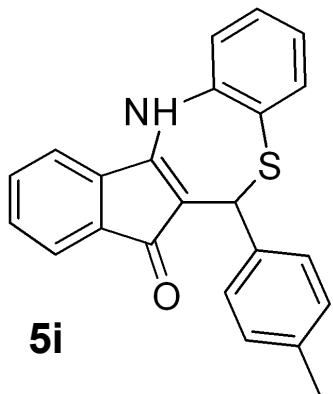



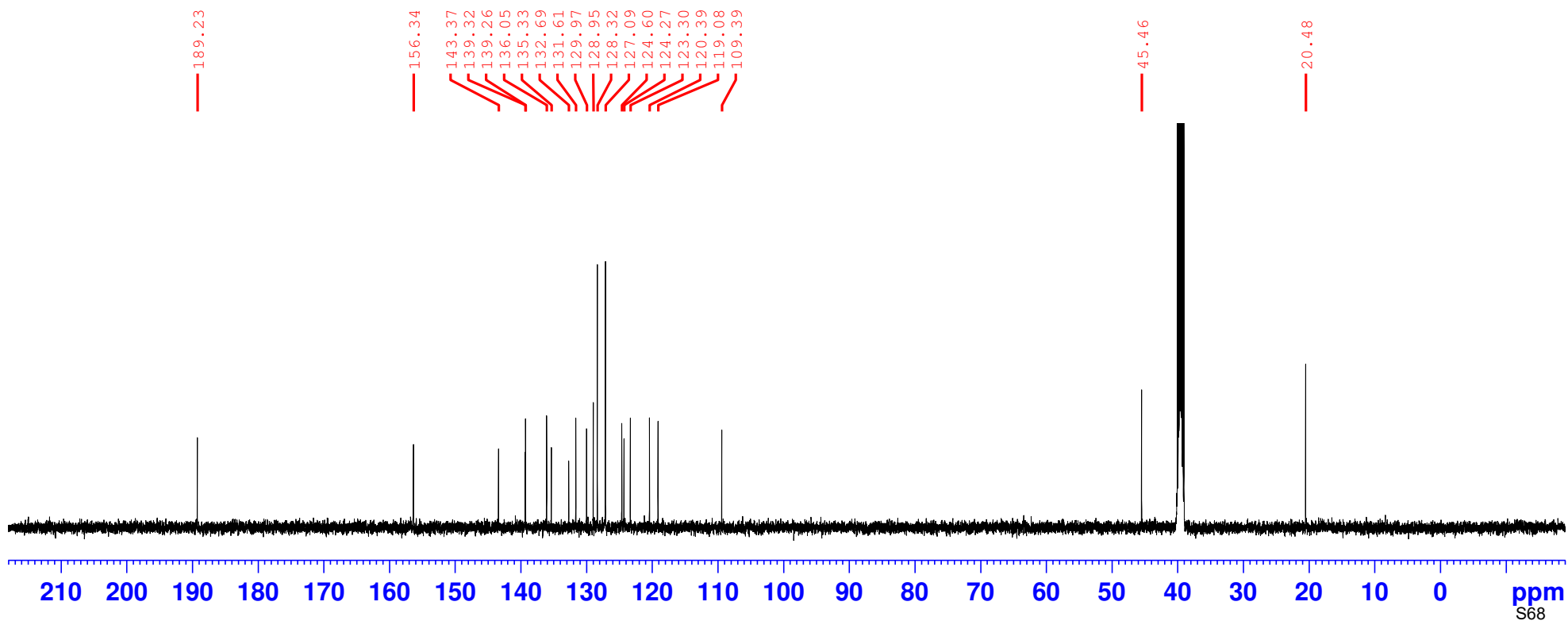
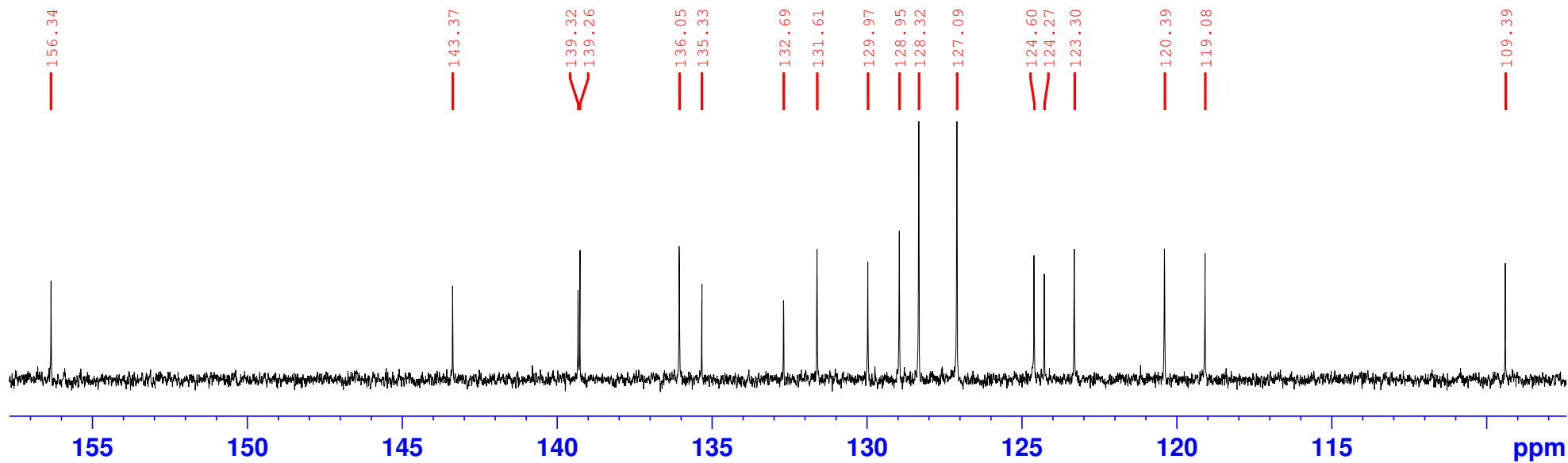
8.255
8.241
7.867
7.745
7.694
7.207
7.193

2.319

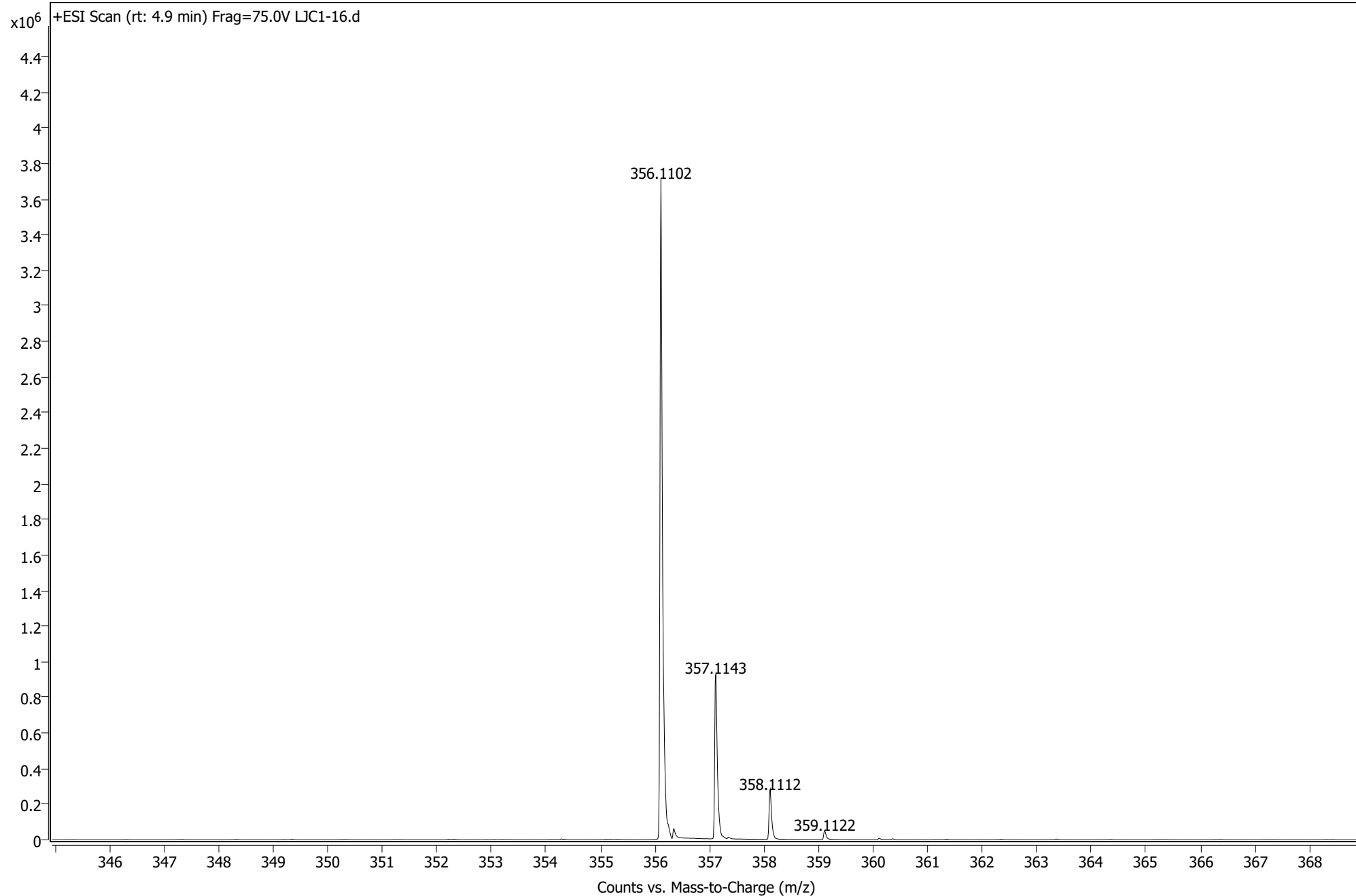








User Spectrum Plot Report



Sample Name: LJC 1-16

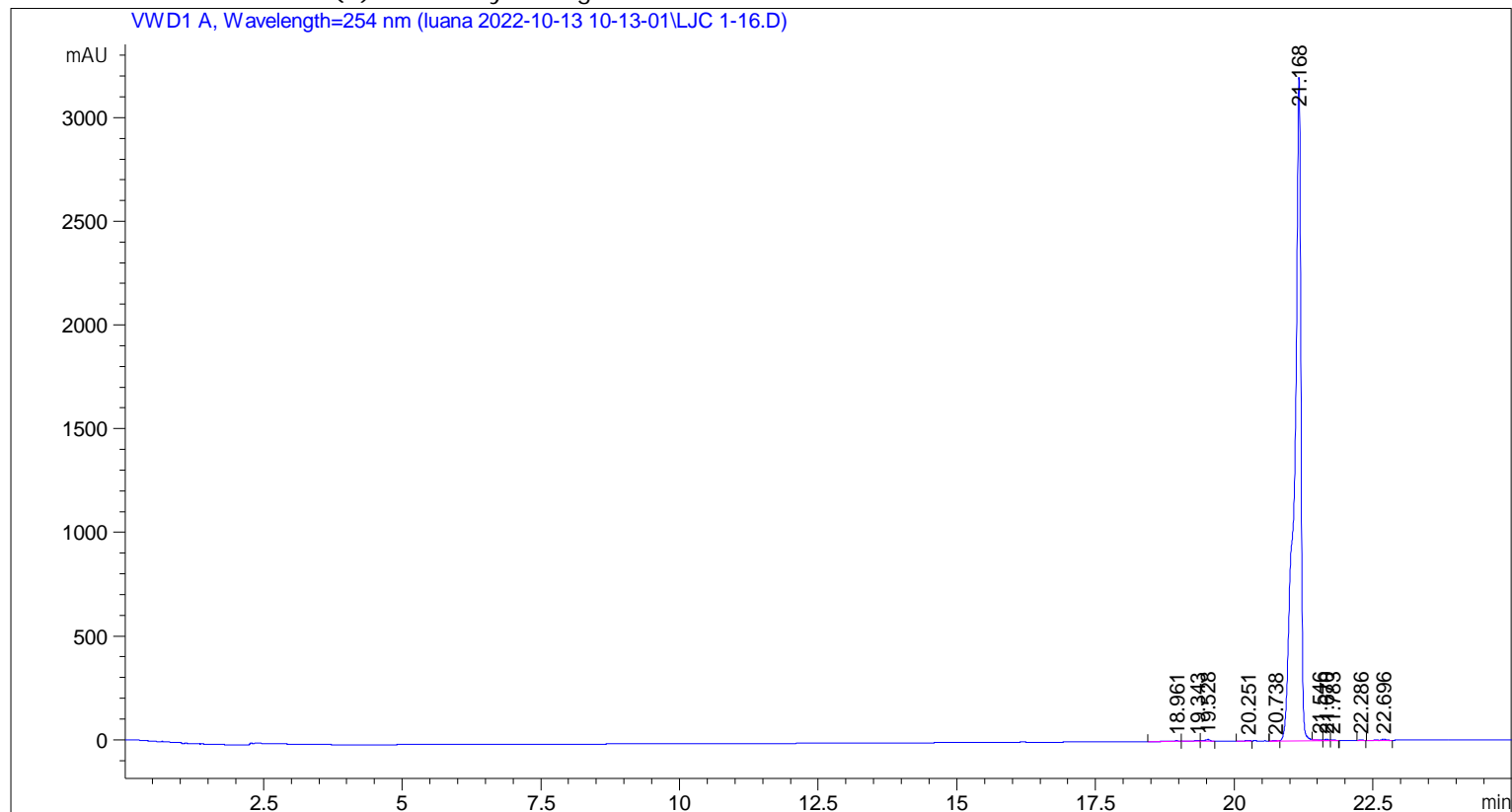
```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    2
Acq. Instrument : 1220 HPLC                     Location  :   82
Injection Date  : 10/13/2022 10:41:43 AM      Inj       :    1
                                           Inj Volume: 70.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2022-10-13 10-13-01\Luana_small_molecule.M (Sequence
                :                               Method)
Last changed    : 10/13/2022 10:13:06 AM by SYSTEM
Method Info     : MeOH/water

```

Sample Info : LJC 1-16

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

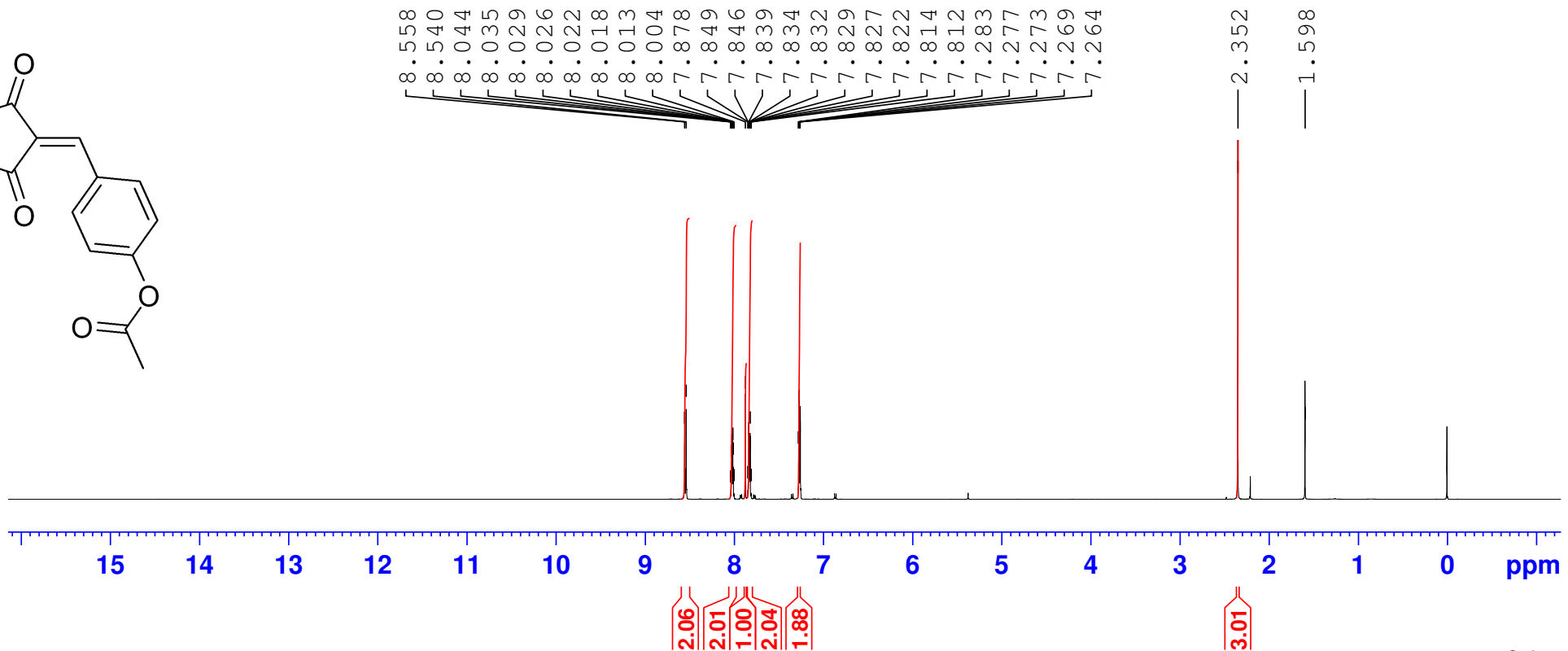
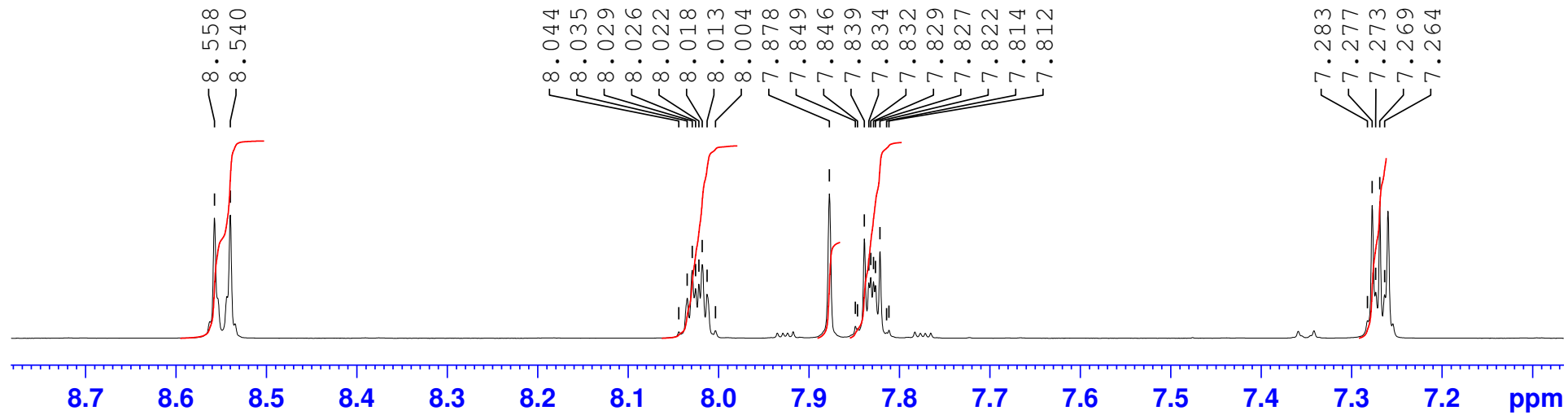
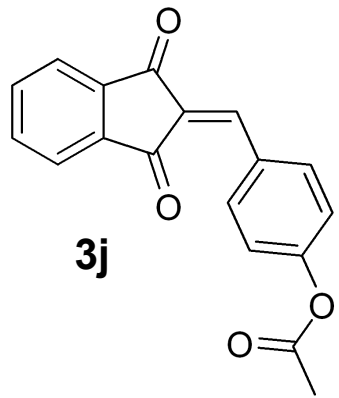
Signal 1: VWD1 A, Wavelength=254 nm

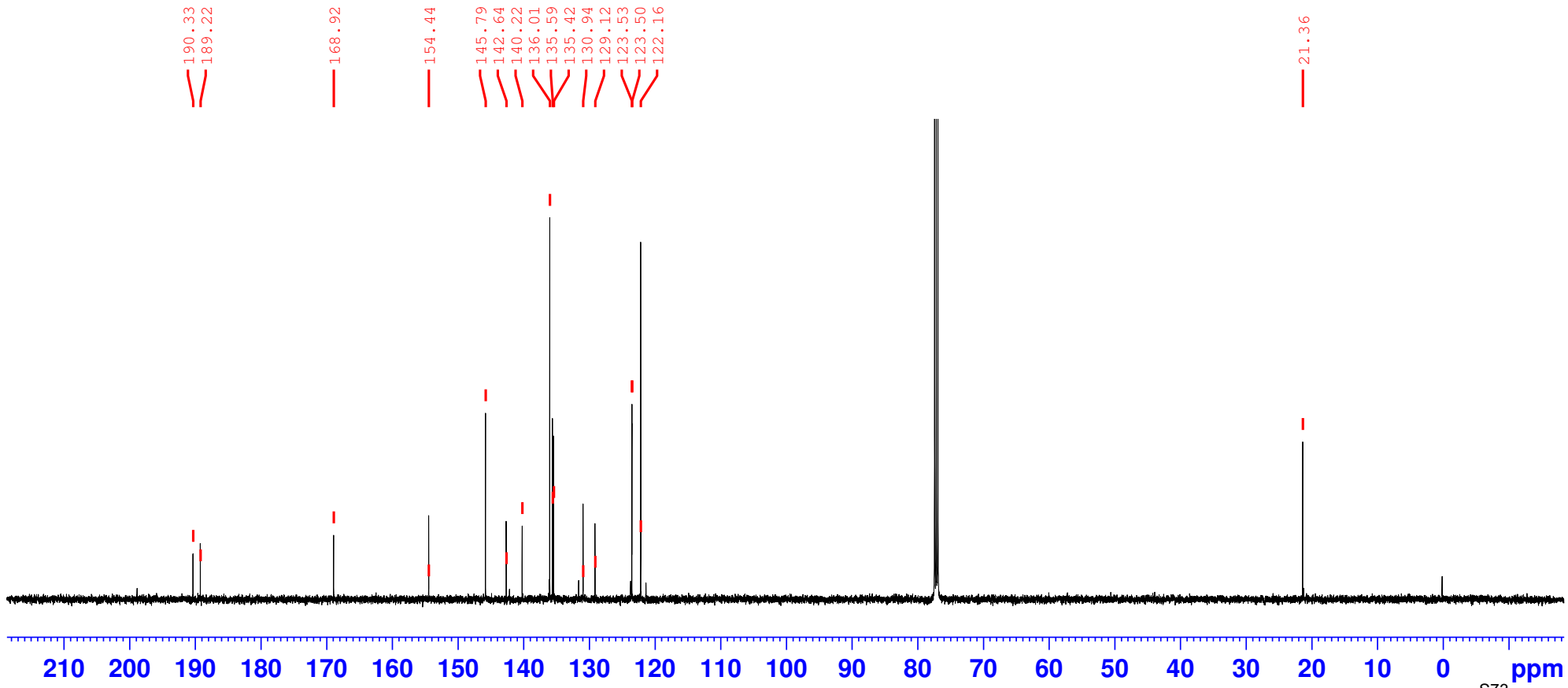
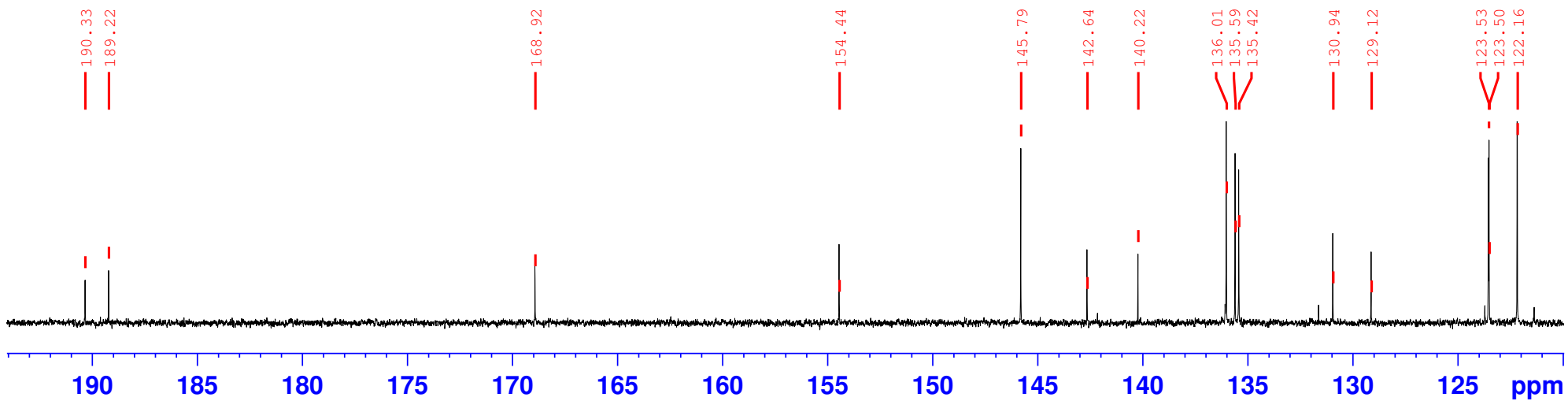
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.961	BV	0.1473	42.43138	3.85711	0.1646
2	19.343	VV	0.1368	38.71626	3.86751	0.1501
3	19.528	VB	0.1094	67.21614	8.67919	0.2607
4	20.251	BV	0.1107	17.27770	2.24765	0.0670

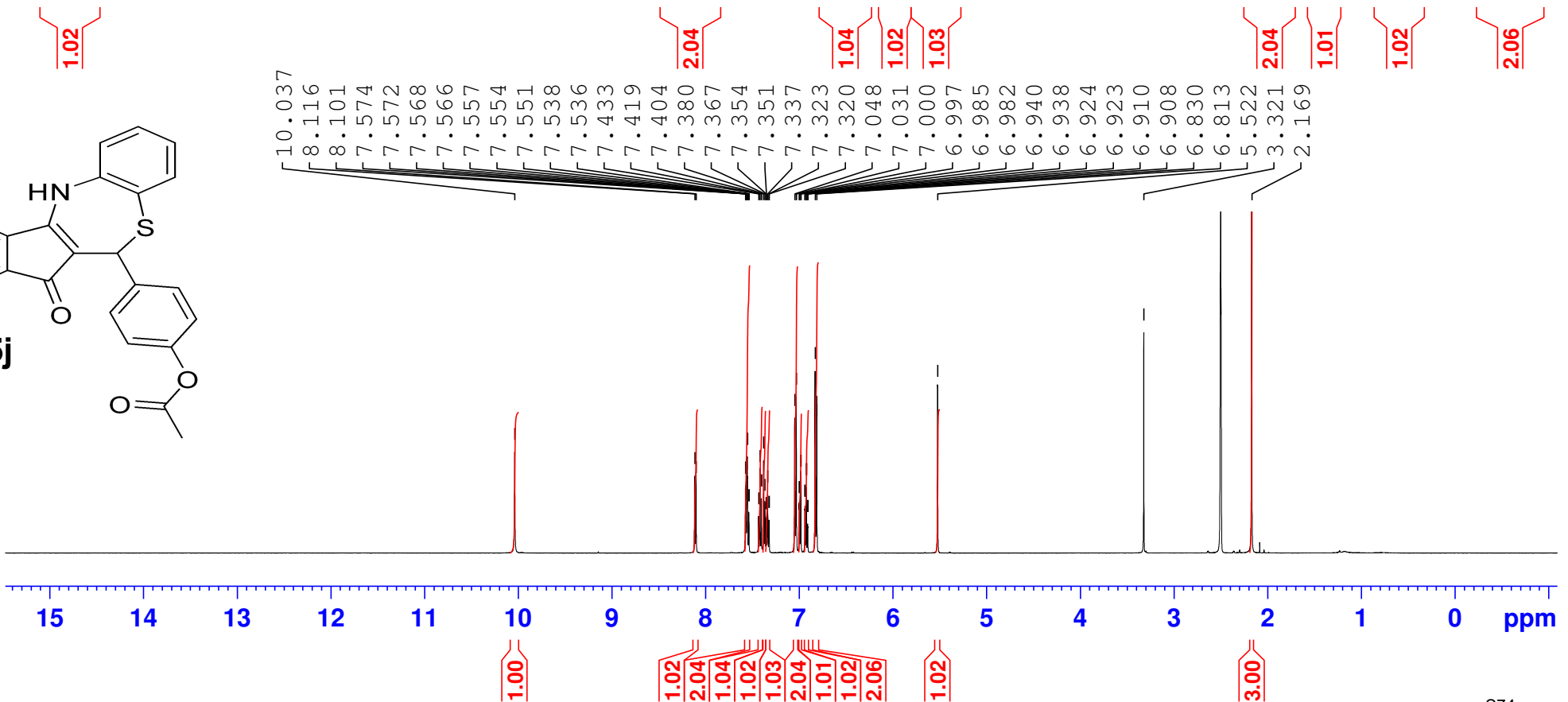
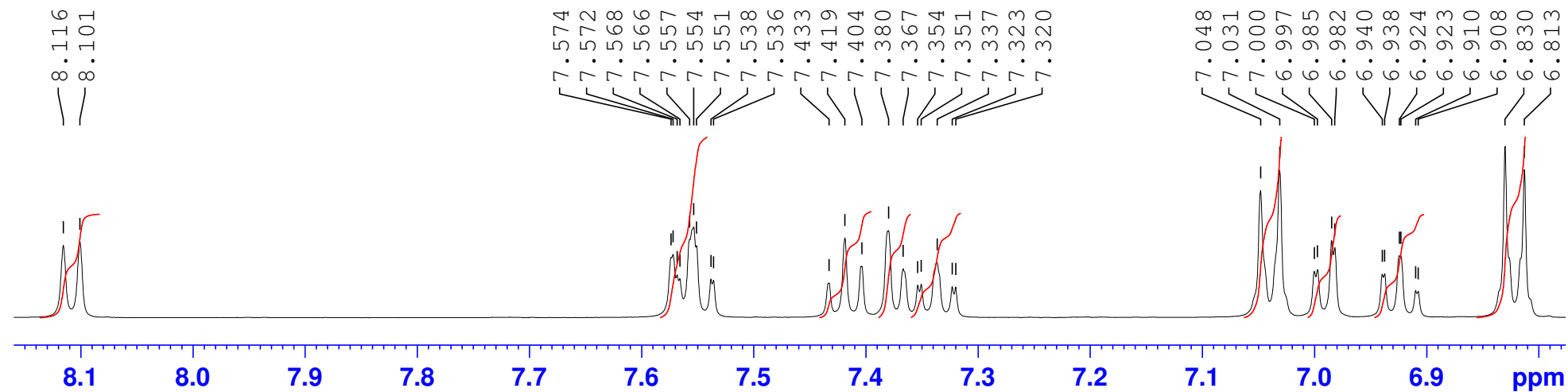
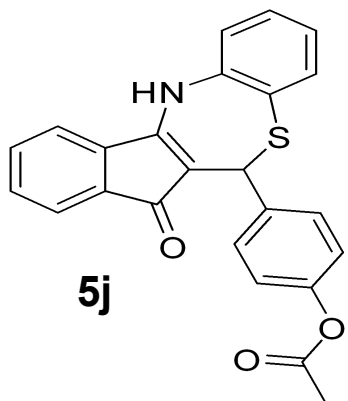
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	20.738	BV E	0.0749	10.98089	2.21383	0.0426
6	21.168	VV R	0.1110	2.55137e4	3199.24023	98.9471
7	21.546	VV E	0.0833	14.64745	2.50039	0.0568
8	21.670	VV E	0.0839	28.88376	4.96104	0.1120
9	21.783	VB E	0.0711	16.66855	3.52928	0.0646
10	22.286	VB	0.0634	7.36391	1.81084	0.0286
11	22.696	VB R	0.0743	27.31478	5.46726	0.1059

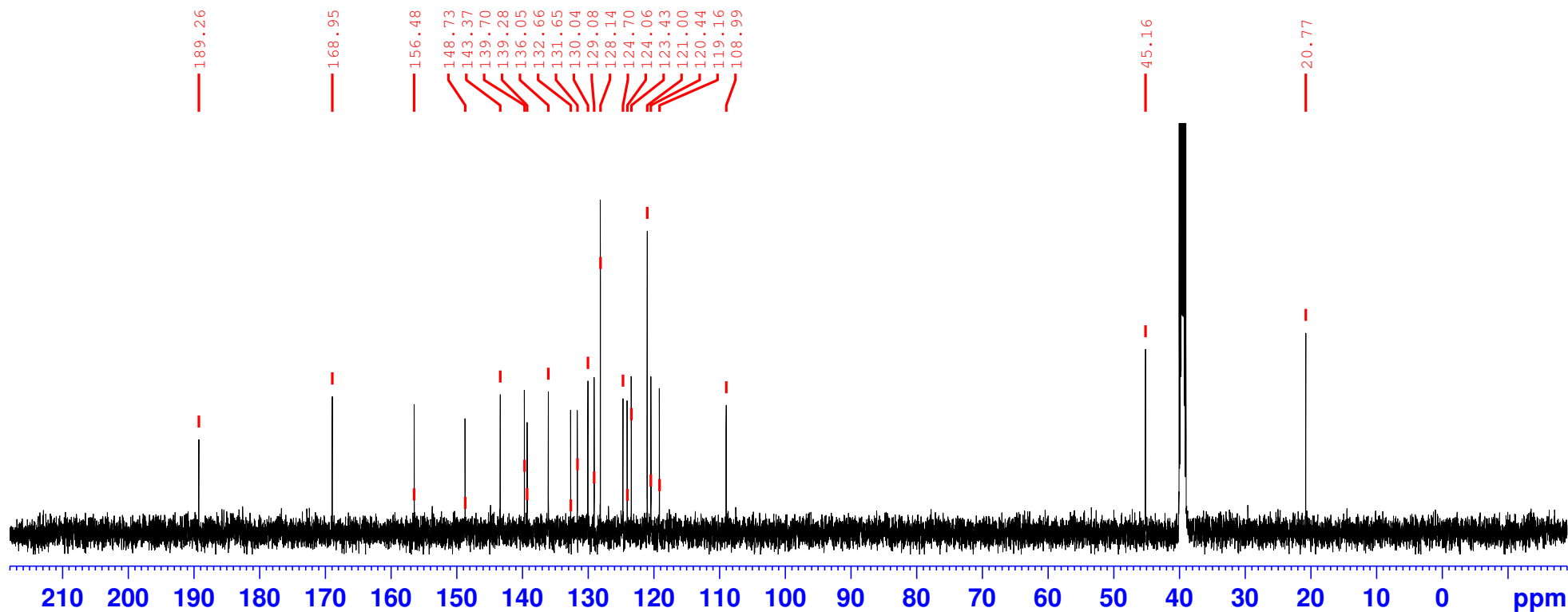
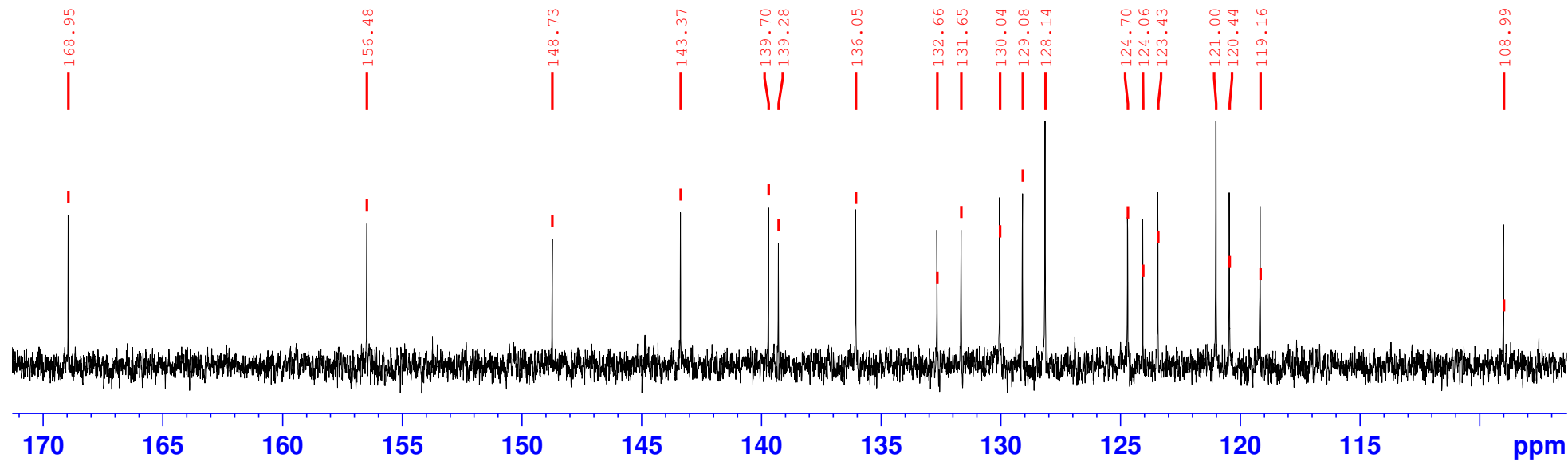
Totals : 2.57852e4 3238.37434

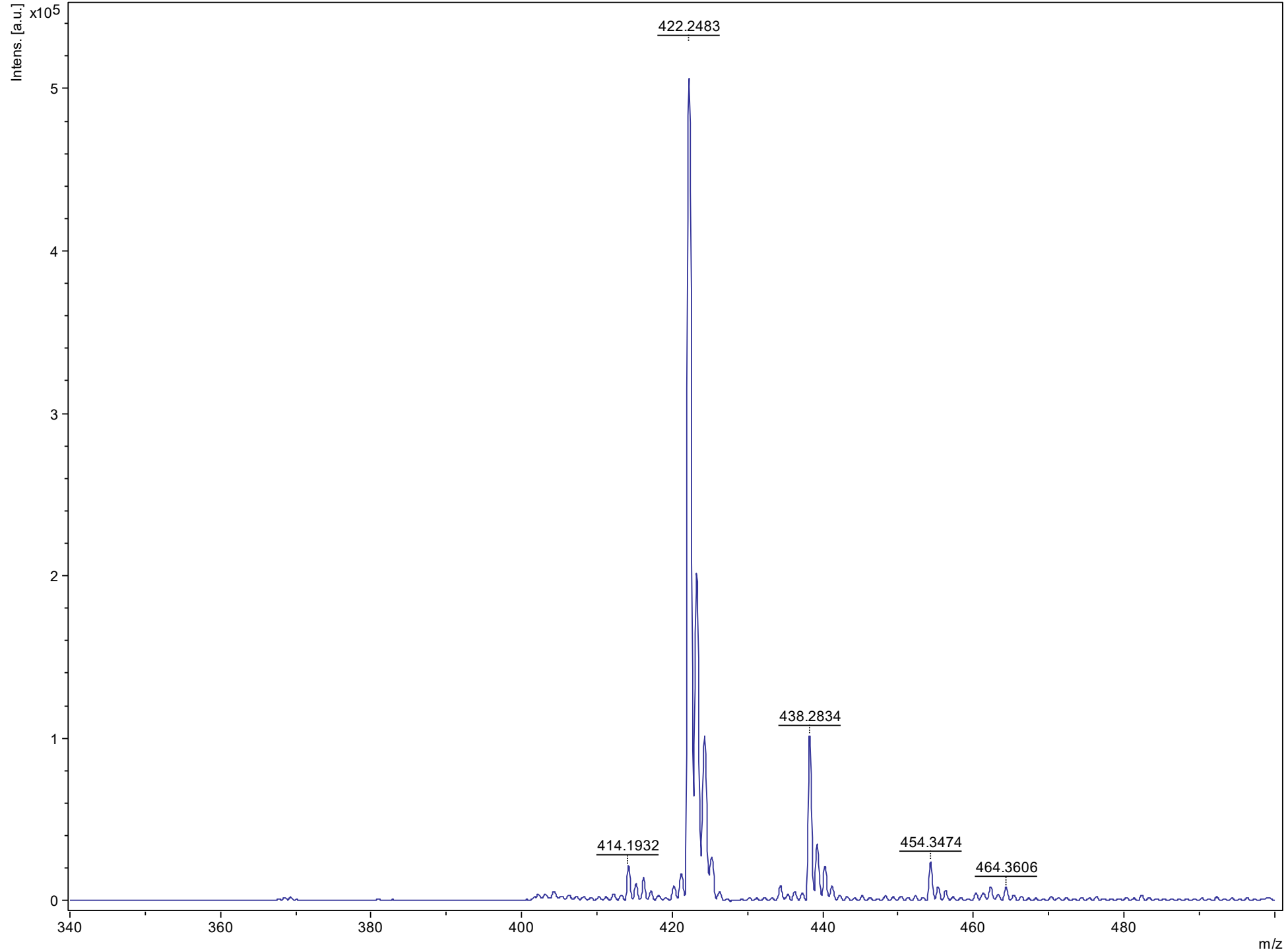
=====
*** End of Report ***











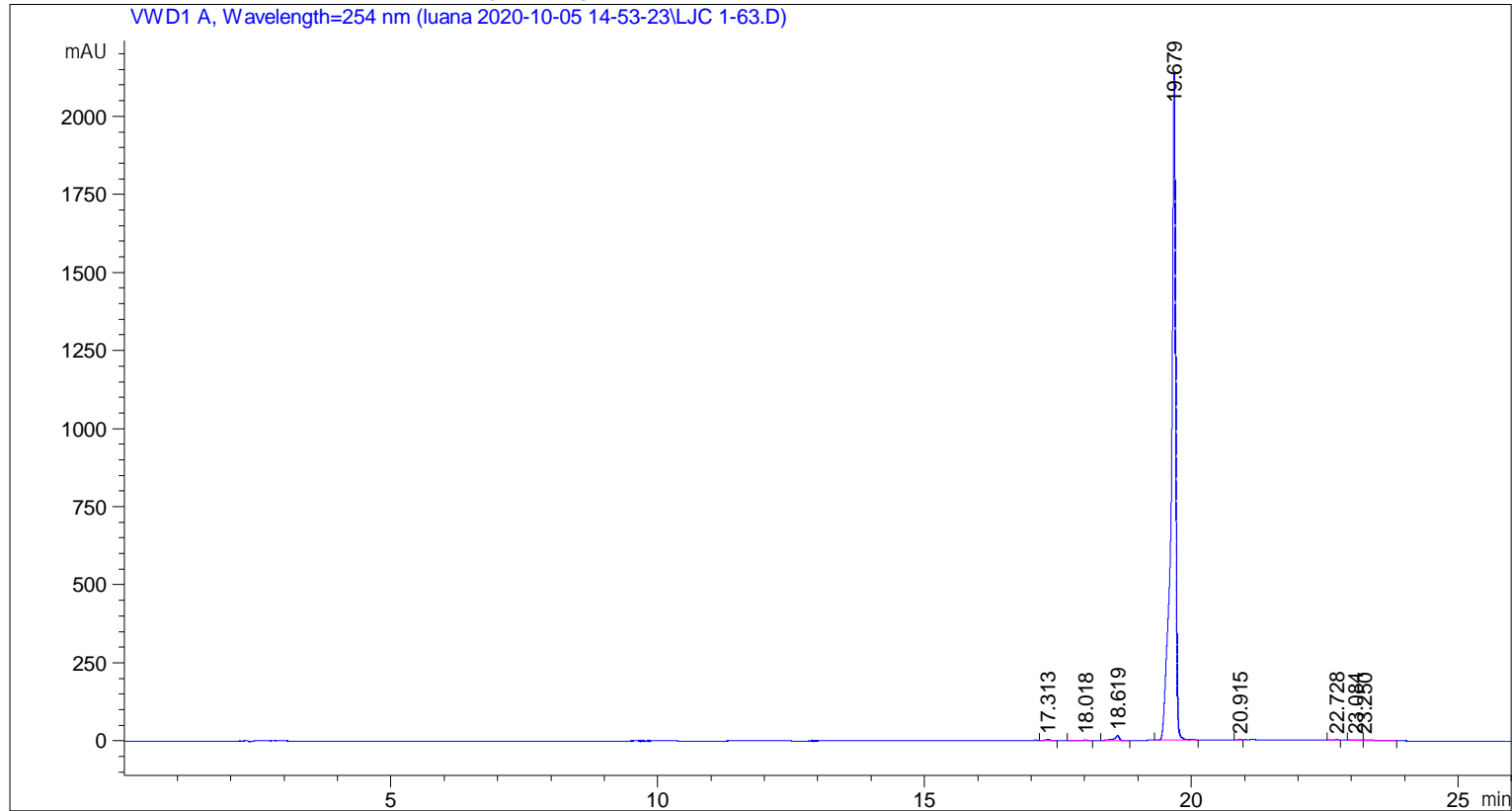
Sample Name: LJC 1-63

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    3
Acq. Instrument : 1220 HPLC                   Location  :    3
Injection Date  : 10/5/2020 3:48:36 PM      Inj       :    1
                                                Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-10-05 14-53-23\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 10/5/2020 2:58:07 PM by SYSTEM
Method Info     : Water/MeOH

Sample Info     : LJC 1-63
    
```

Additional Info : Peak(s) manually integrated



Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

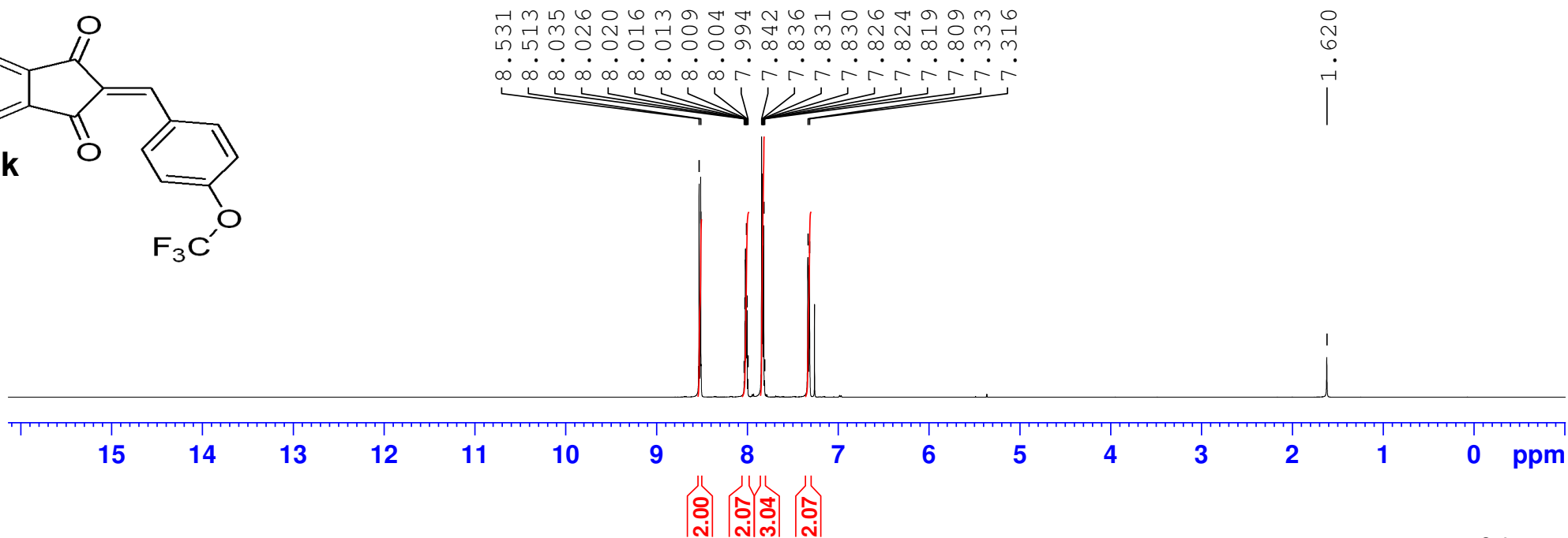
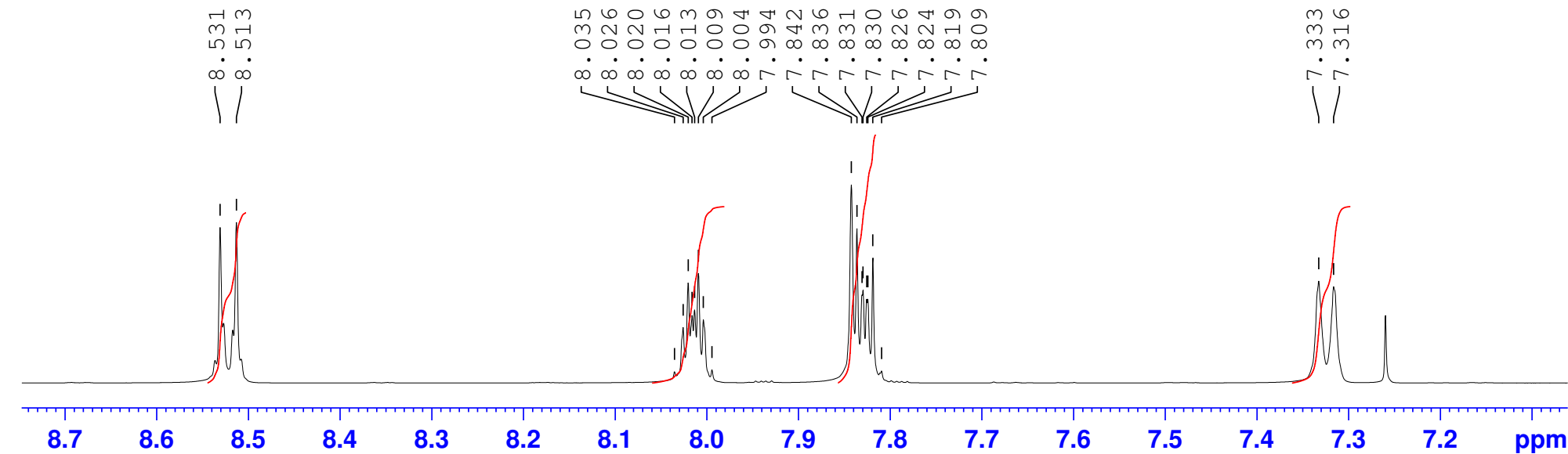
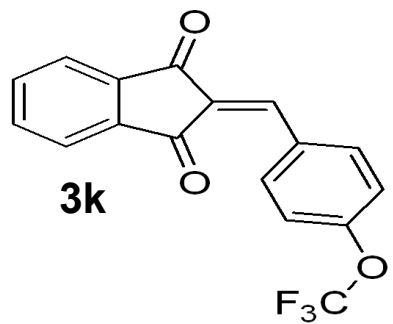
Signal 1: VWD1 A, Wavelength=254 nm

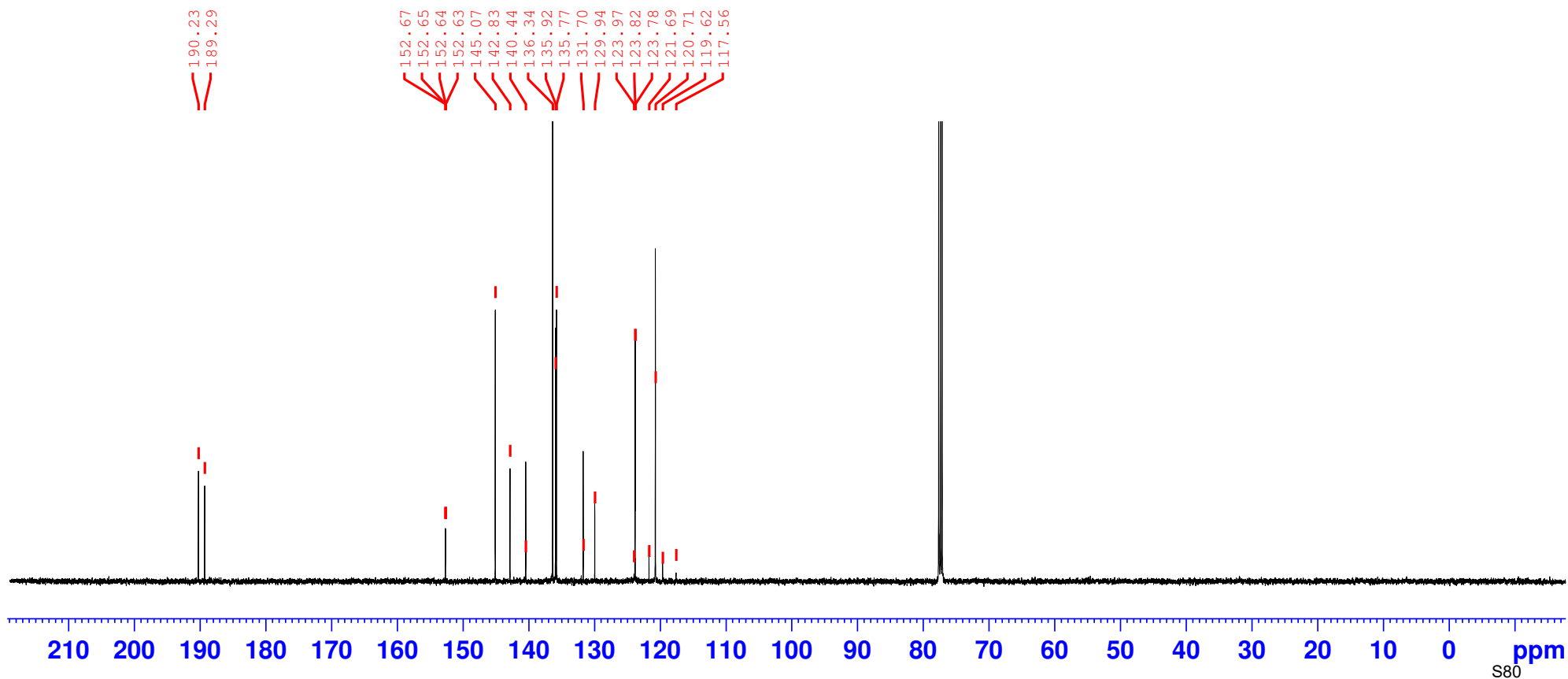
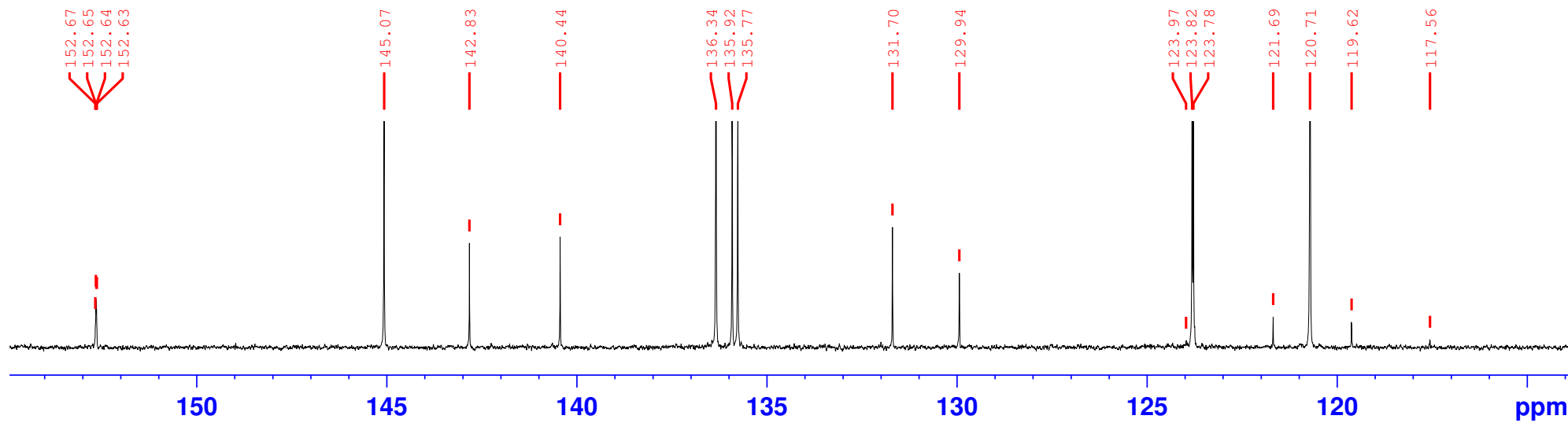
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.313	VB	0.0849	26.59534	4.31320	0.2114
2	18.018	BV	0.0954	13.68562	2.01119	0.1088
3	18.619	BV R	0.0921	108.80461	16.35528	0.8649
4	19.679	BV R	0.0815	1.23551e4	2134.36719	98.2076

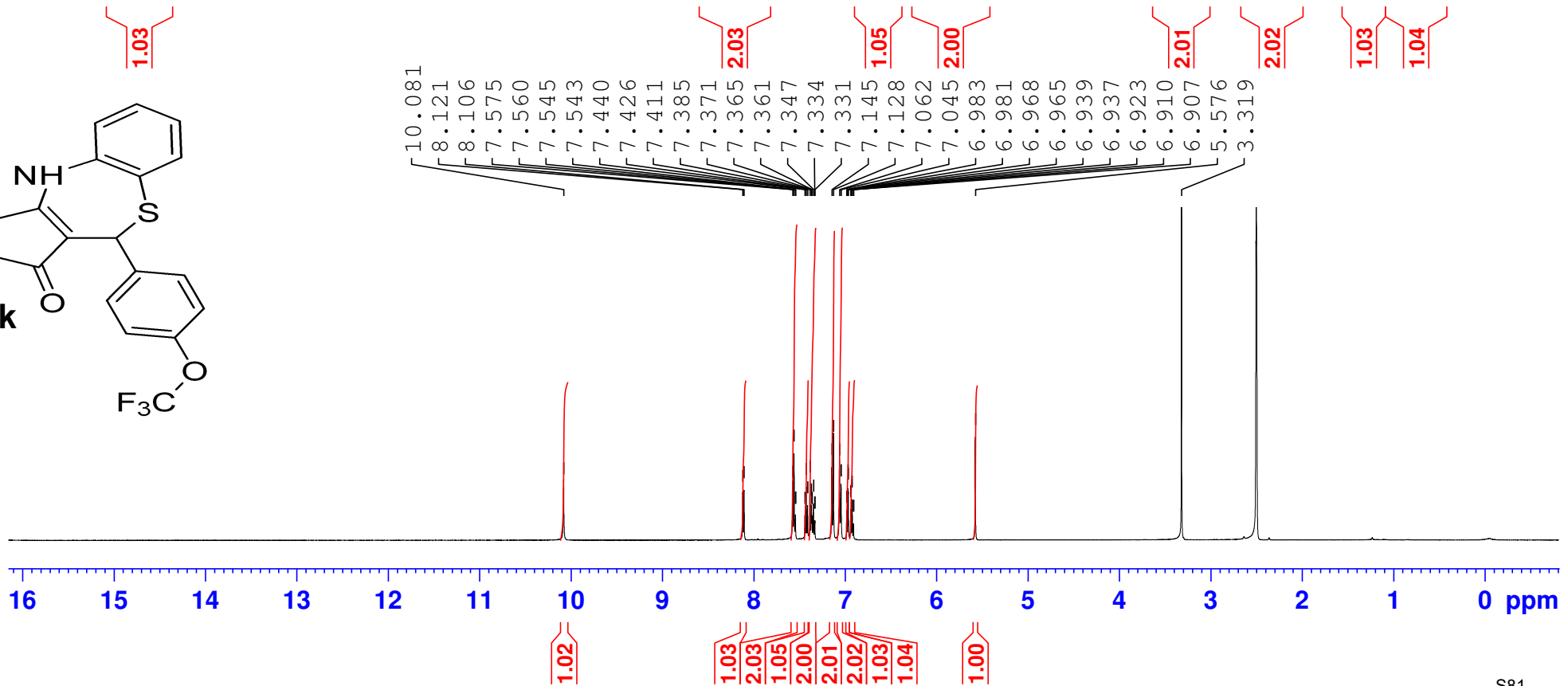
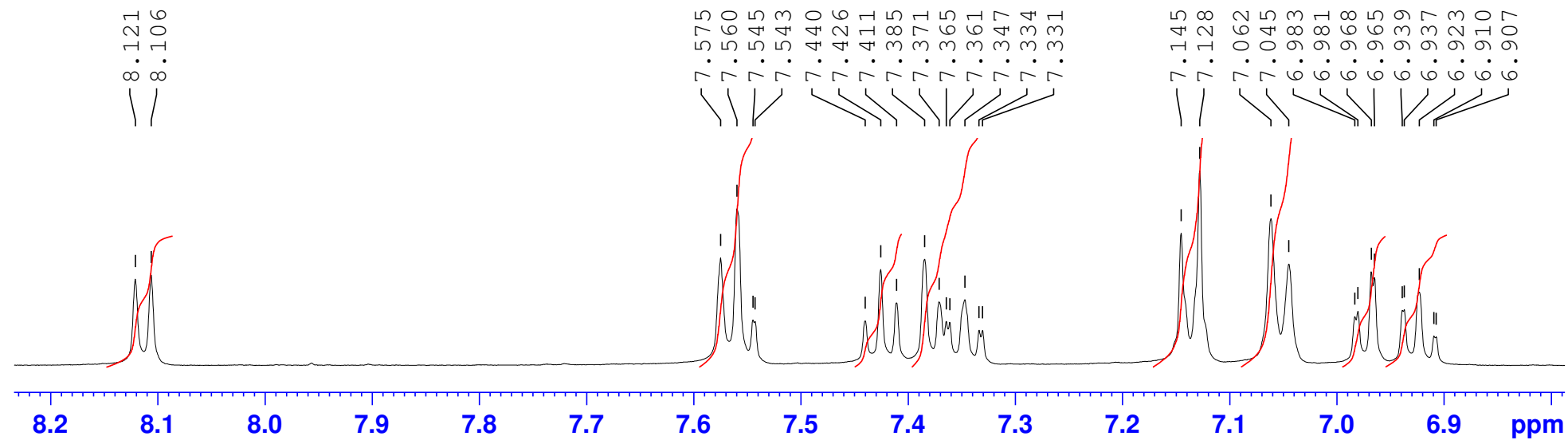
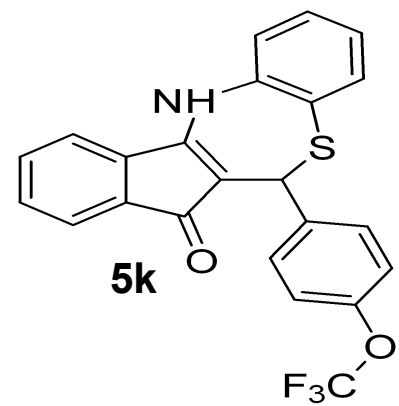
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	20.915	VV	0.0822	12.76791	2.10826	0.1015
6	22.728	BV	0.0756	11.00524	1.88531	0.0875
7	23.084	VV	0.1904	28.53626	1.76667	0.2268
8	23.250	VB	0.1524	24.09718	1.87609	0.1915

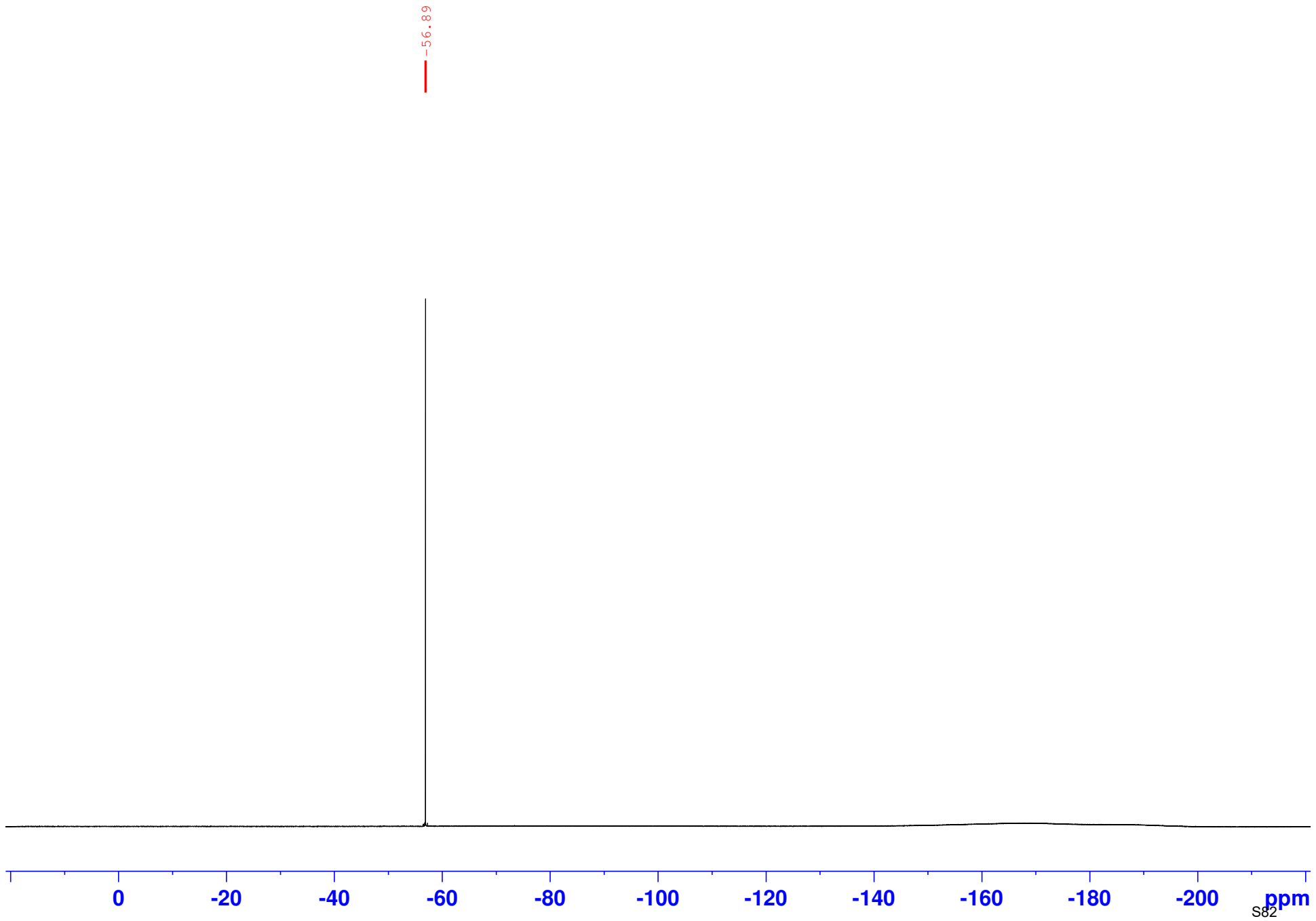
Totals : 1.25806e4 2164.68319

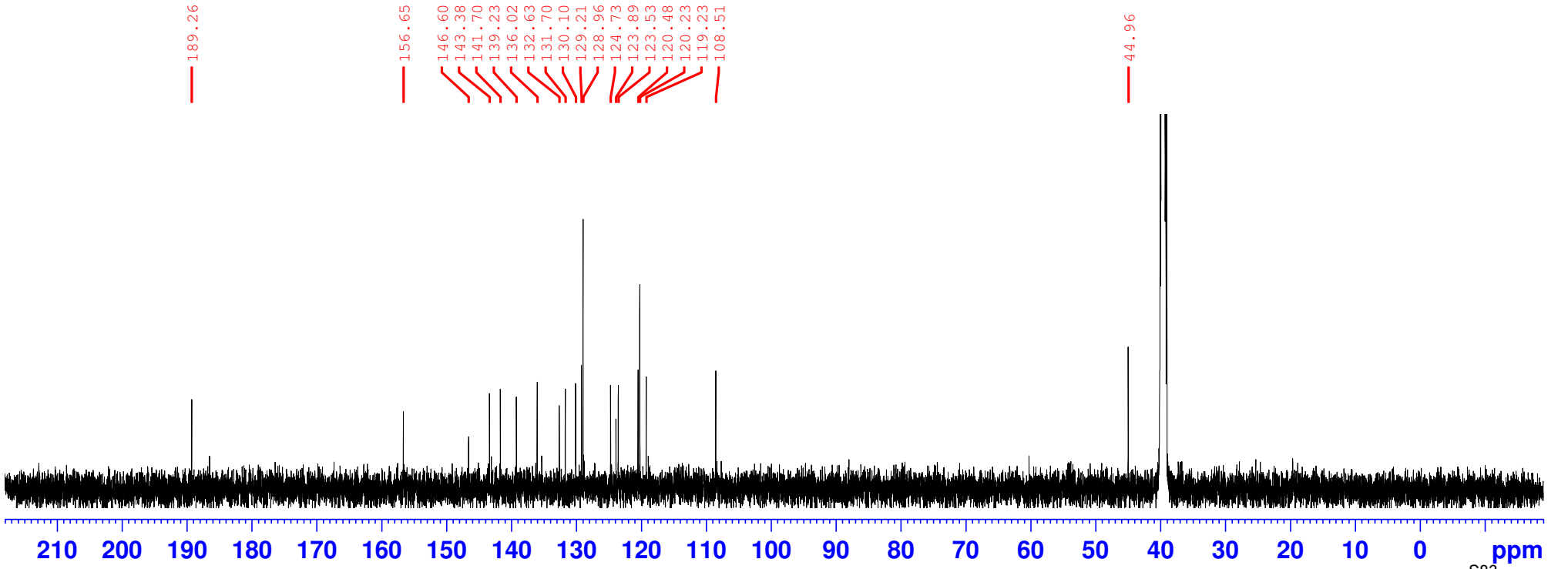
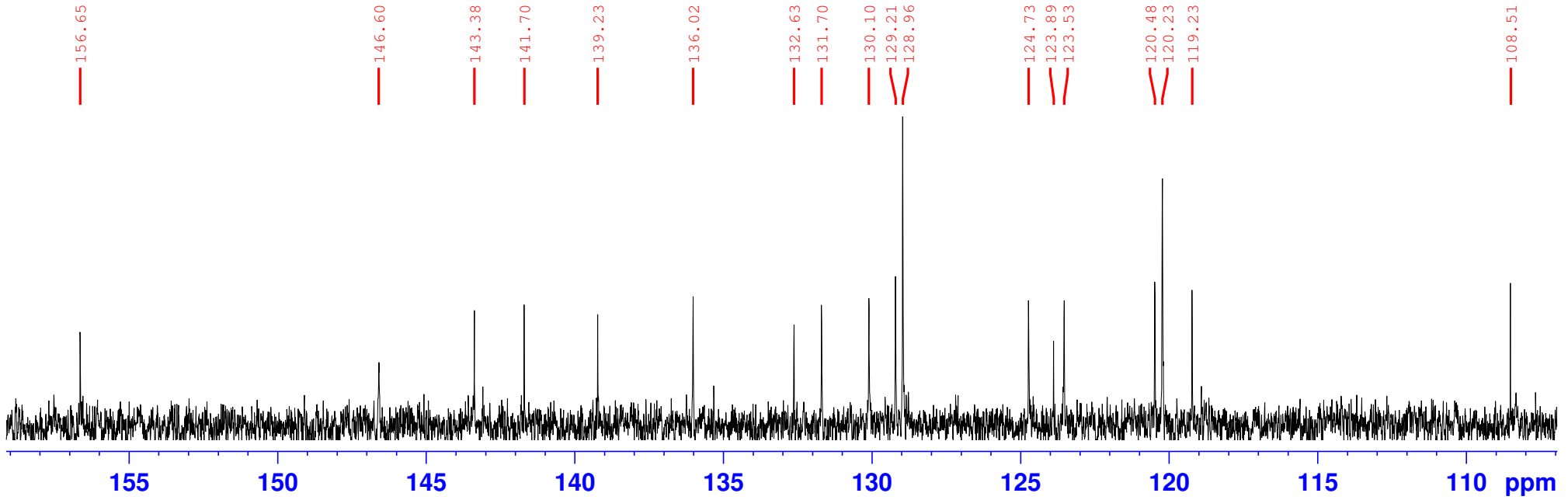
=====
*** End of Report ***

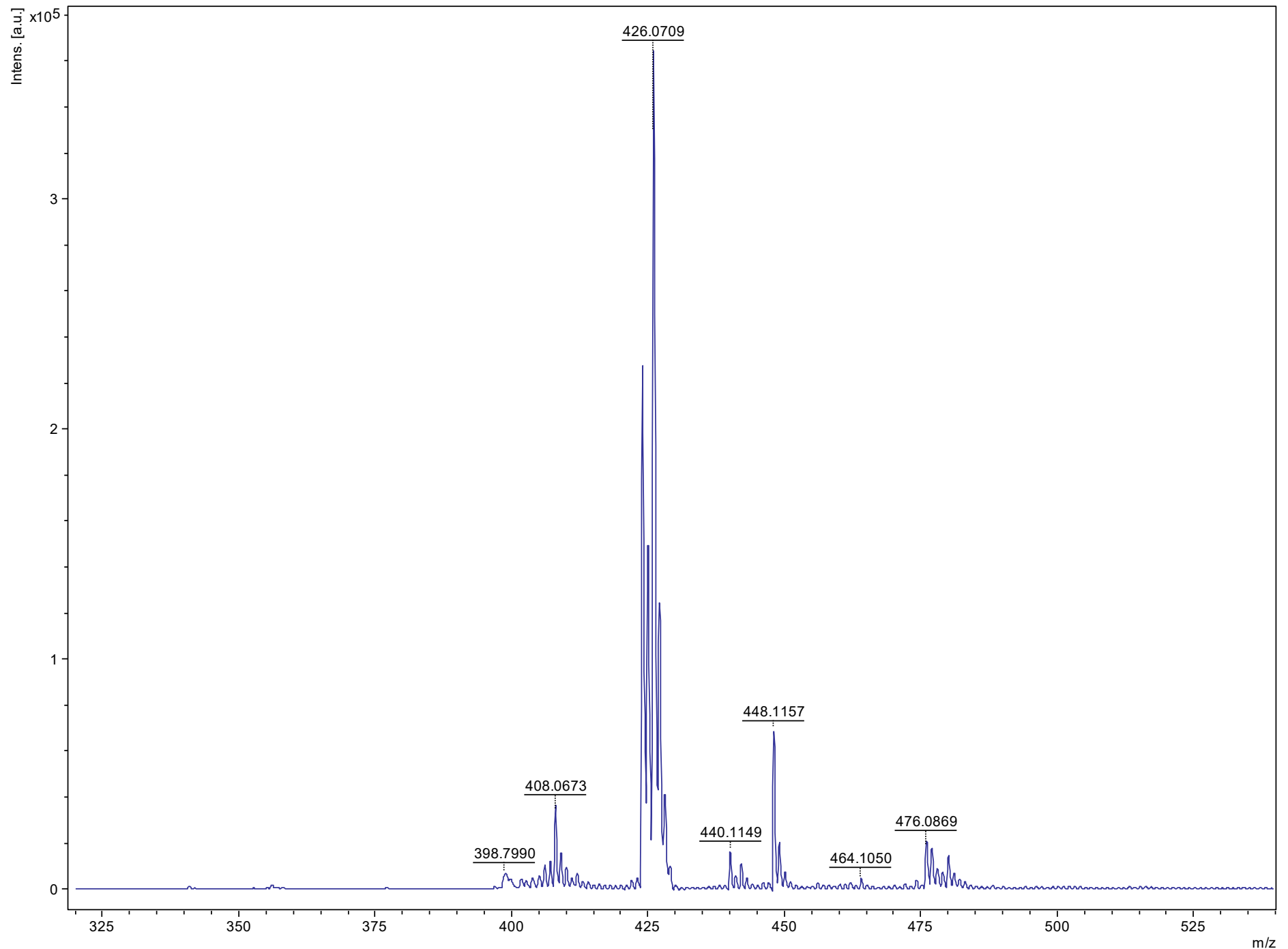












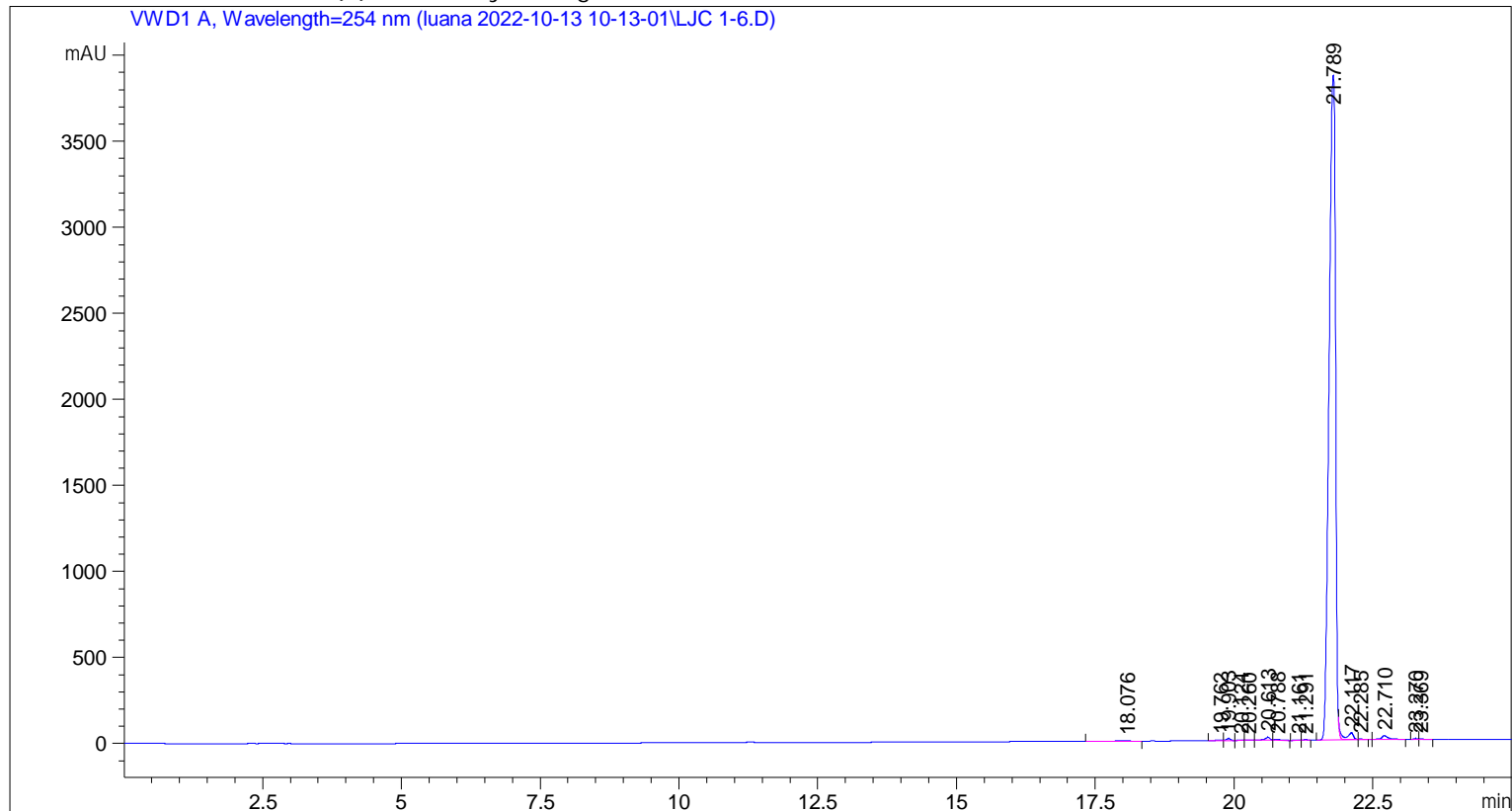
Sample Name: LJC 1-6

```

=====
Acq. Operator   : SYSTEM                               Seq. Line :    1
Acq. Instrument : 1220 HPLC                            Location  :   81
Injection Date  : 10/13/2022 10:14:32 AM              Inj       :    1
                                                    Inj Volume: 70.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2022-10-13 10-13-01\Luana_small_molecule.M (Sequence
                Method)
Last changed    : 10/13/2022 10:13:06 AM by SYSTEM
Method Info     : MeOH/water

Sample Info     : LJC 1-6
    
```

Additional Info : Peak(s) manually integrated



Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

Signal 1: VWD1 A, Wavelength=254 nm

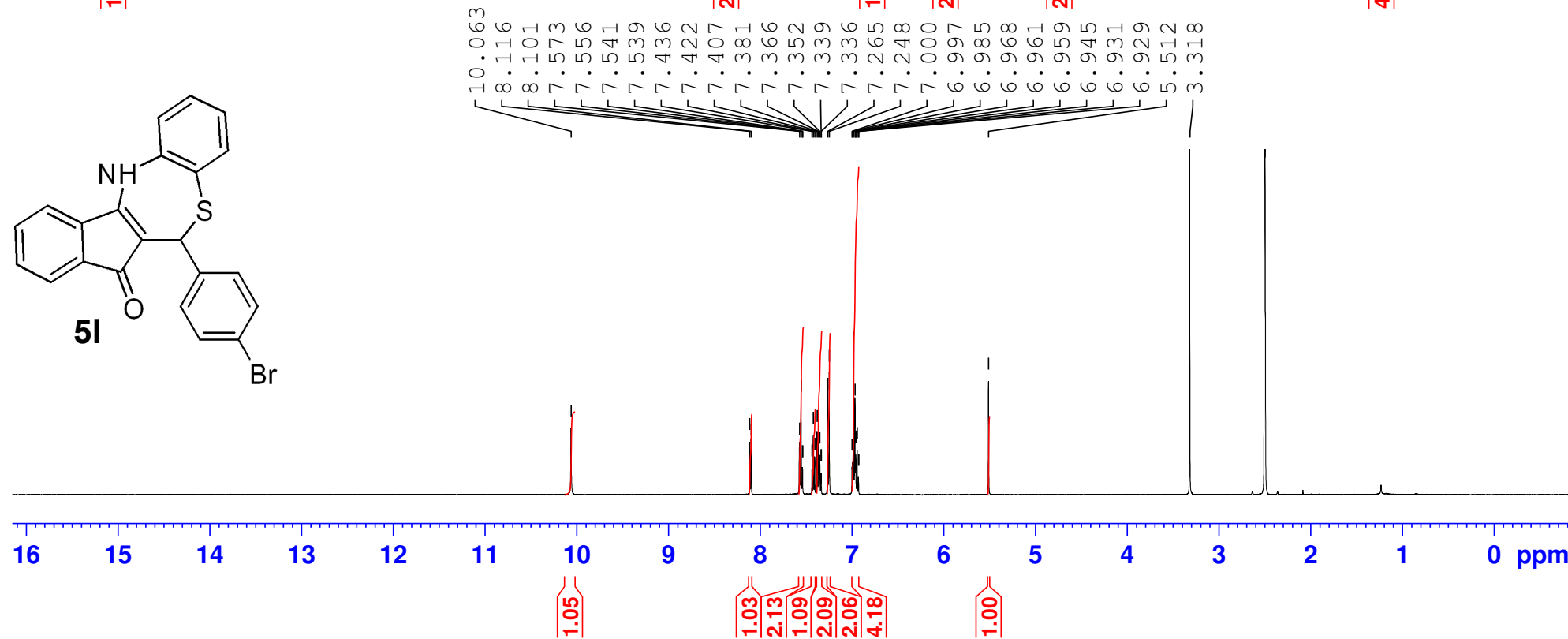
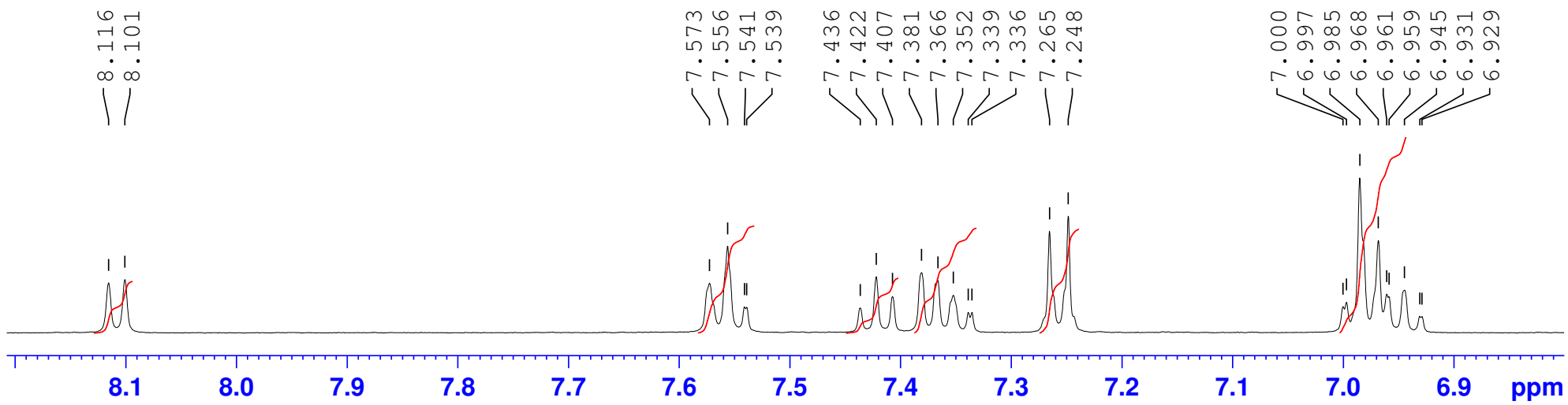
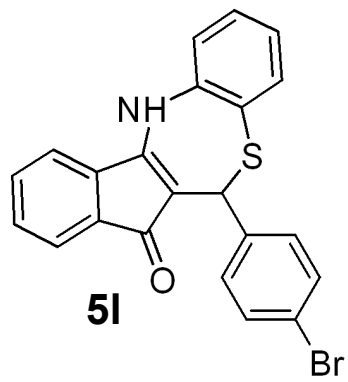
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.076	VV R	0.2002	54.79712	3.48981	0.1709
2	19.762	BV	0.1113	36.27752	4.58555	0.1131
3	19.903	VB	0.0777	63.20223	12.14047	0.1971
4	20.124	BV	0.0755	16.75923	3.33963	0.0523

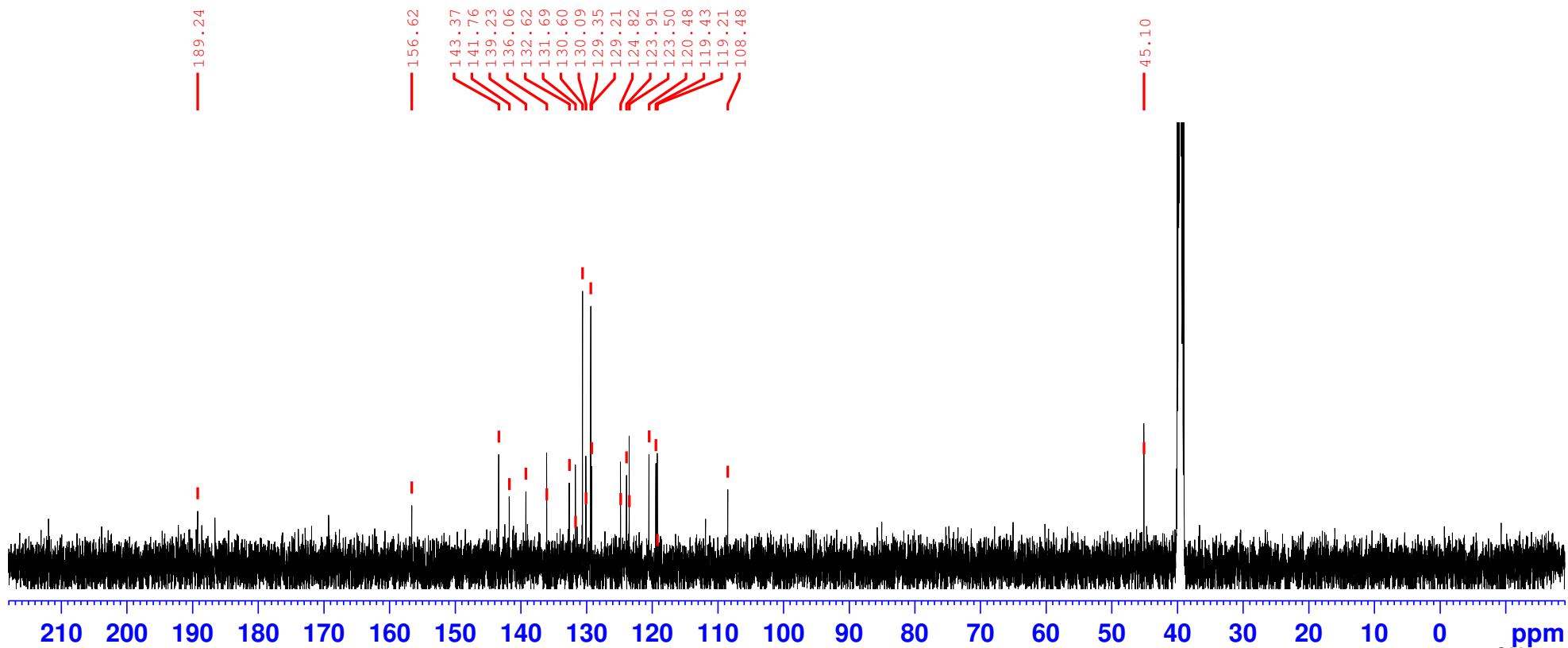
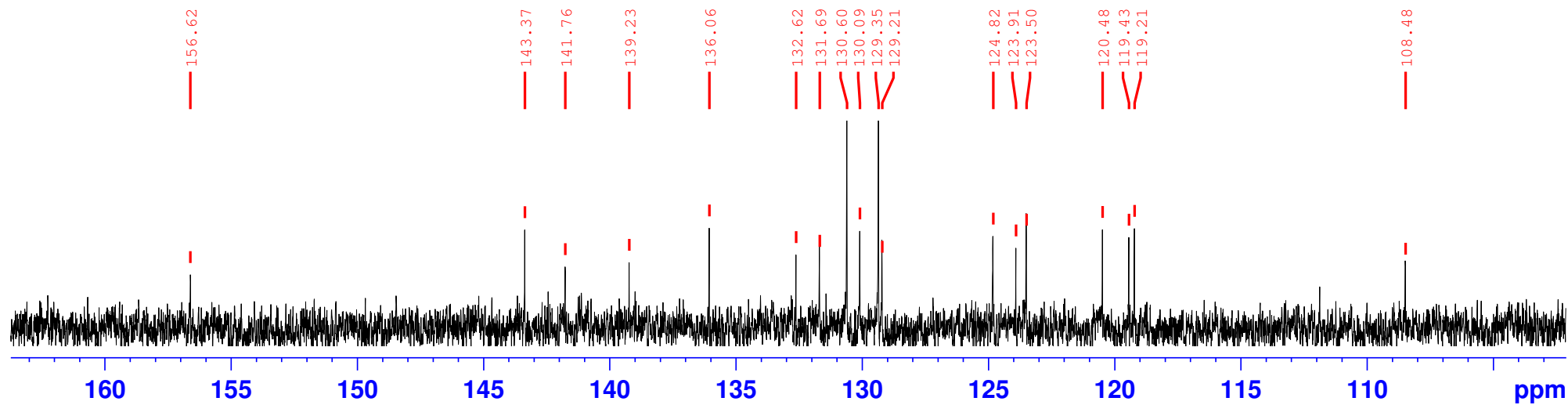
Sample Name: LJC 1-6

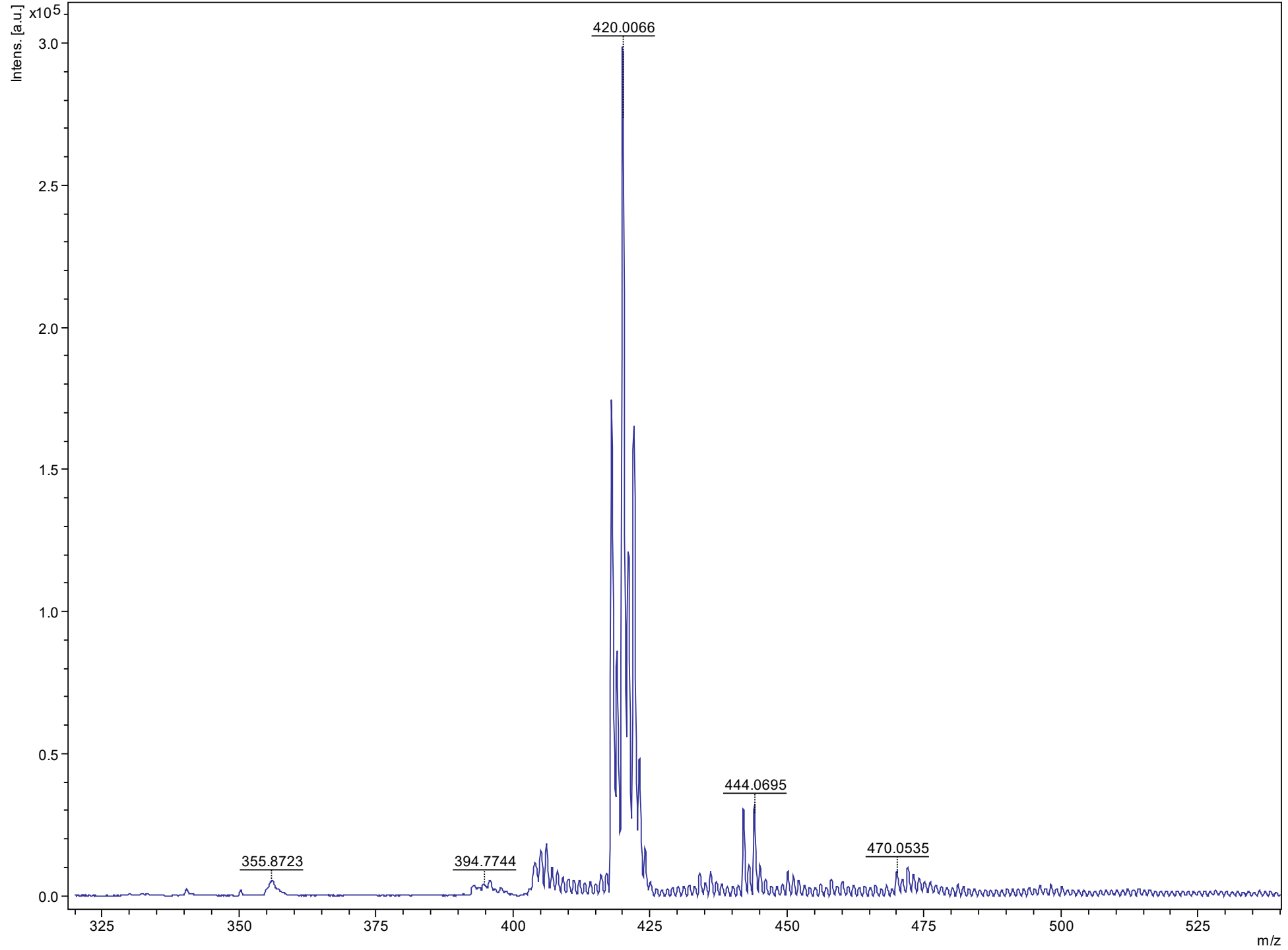
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	20.260	VB	0.0883	12.79254	2.06380	0.0399
6	20.613	BV	0.0949	121.01133	18.12976	0.3774
7	20.788	VB	0.1076	47.65682	6.06828	0.1486
8	21.161	BV	0.0878	14.07956	2.35262	0.0439
9	21.291	VB	0.0806	20.27028	3.72081	0.0632
10	21.789	BV R	0.1237	3.10069e4	3860.99536	96.7049
11	22.117	VV E	0.1358	401.01624	40.05136	1.2507
12	22.285	VV E	0.0894	19.76507	3.05993	0.0616
13	22.710	BB	0.1252	194.15594	22.17187	0.6055
14	23.270	BV	0.0674	28.24593	6.41218	0.0881
15	23.369	VB	0.0942	26.48766	3.90199	0.0826

Totals : 3.20634e4 3992.48341

=====
*** End of Report ***



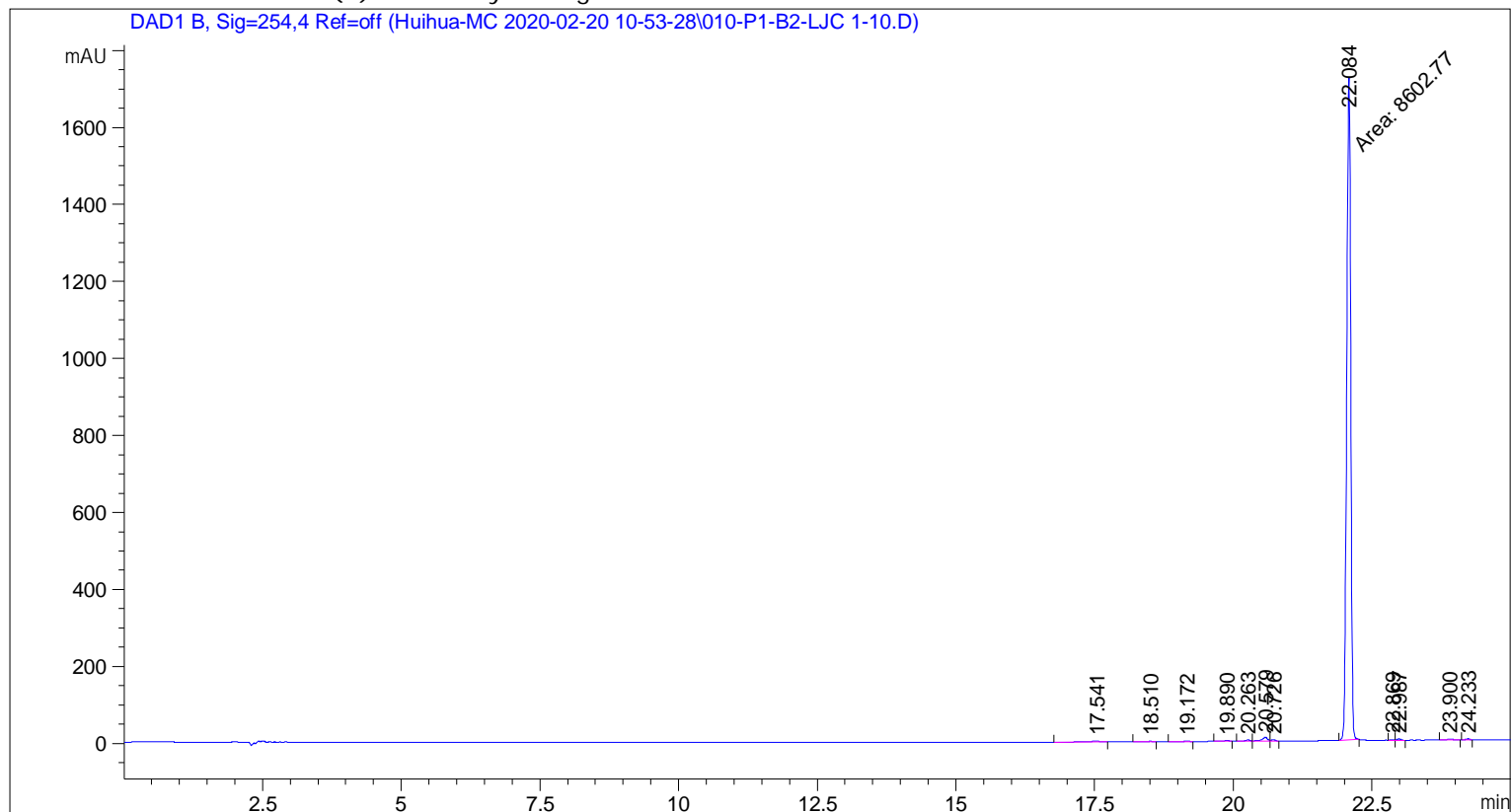




```

=====
Acq. Operator   : SYSTEM                      Seq. Line :   10
Sample Operator : SYSTEM
Acq. Instrument : 1260Infinity2              Location  : P1-B-02
Injection Date  : 2/20/2020 2:52:28 PM       Inj       :    1
                                           Inj Volume: 50.000 µl

Method          : C:\Users\Public\Documents\ChemStation\1\Data\Huihua-MC 2020-02-20 10-53-28
                  \MC-SMALL MOLE.M (Sequence Method)
Last changed    : 2/19/2020 11:54:04 AM by SYSTEM
Additional Info : Peak(s) manually integrated
  
```



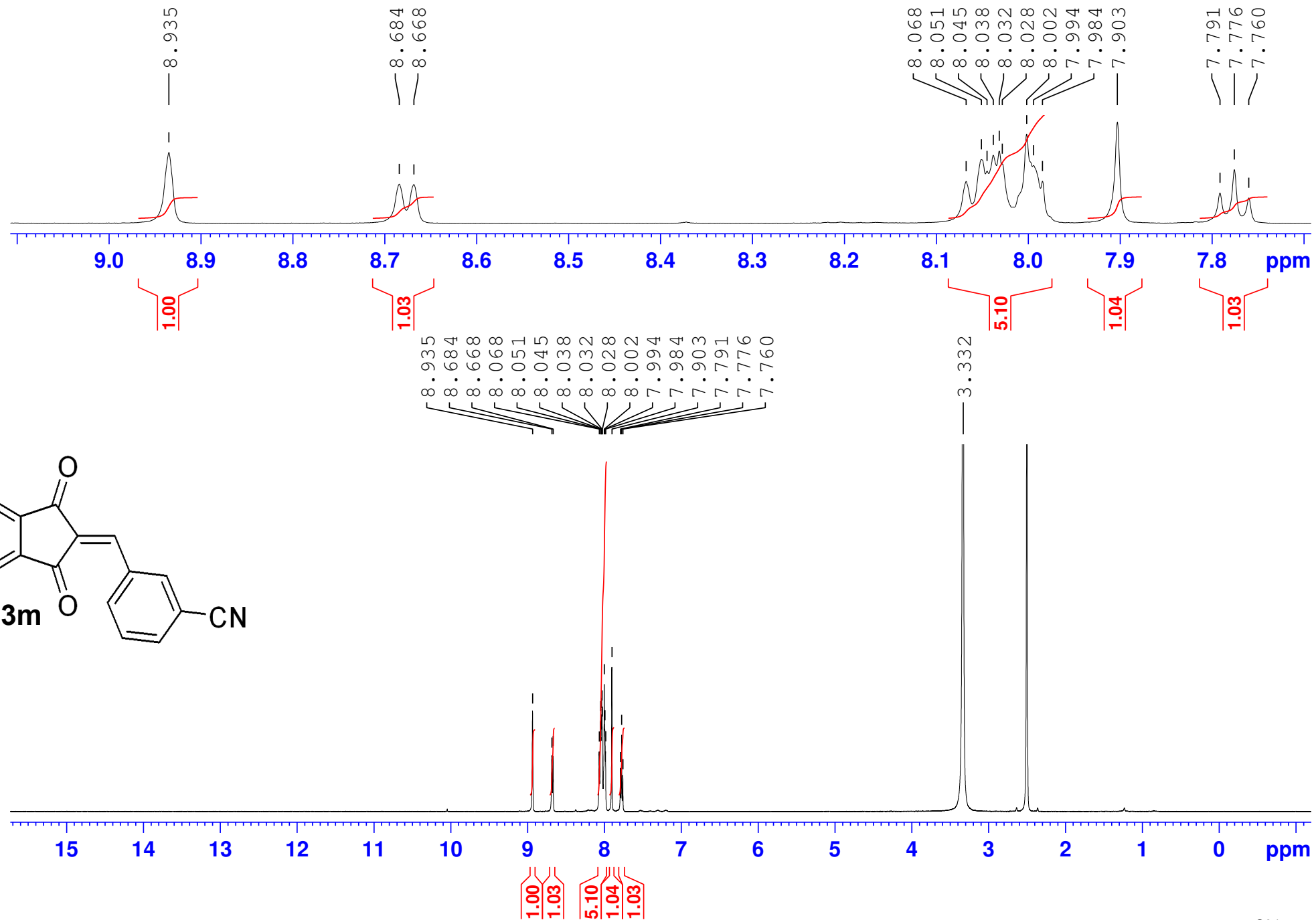
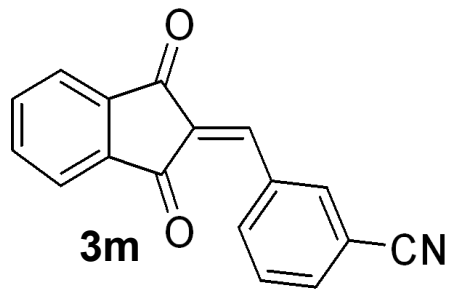
Area Percent Report

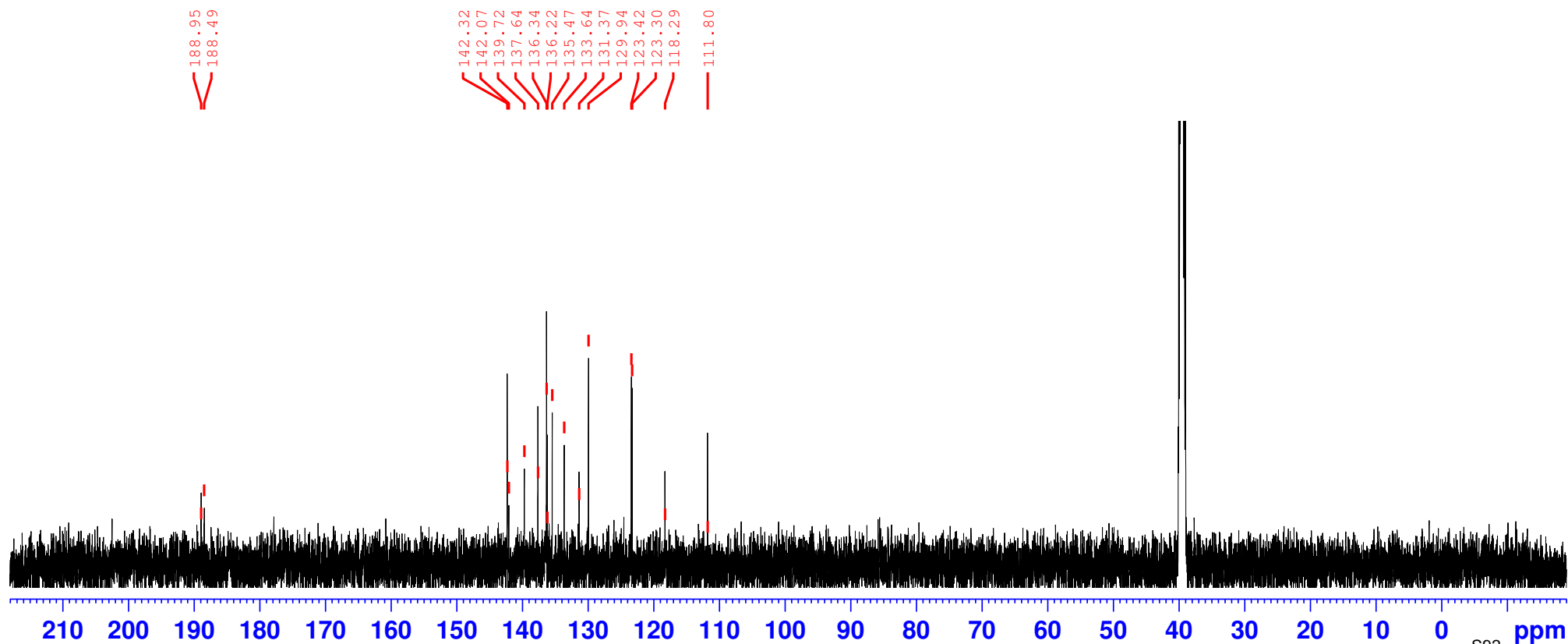
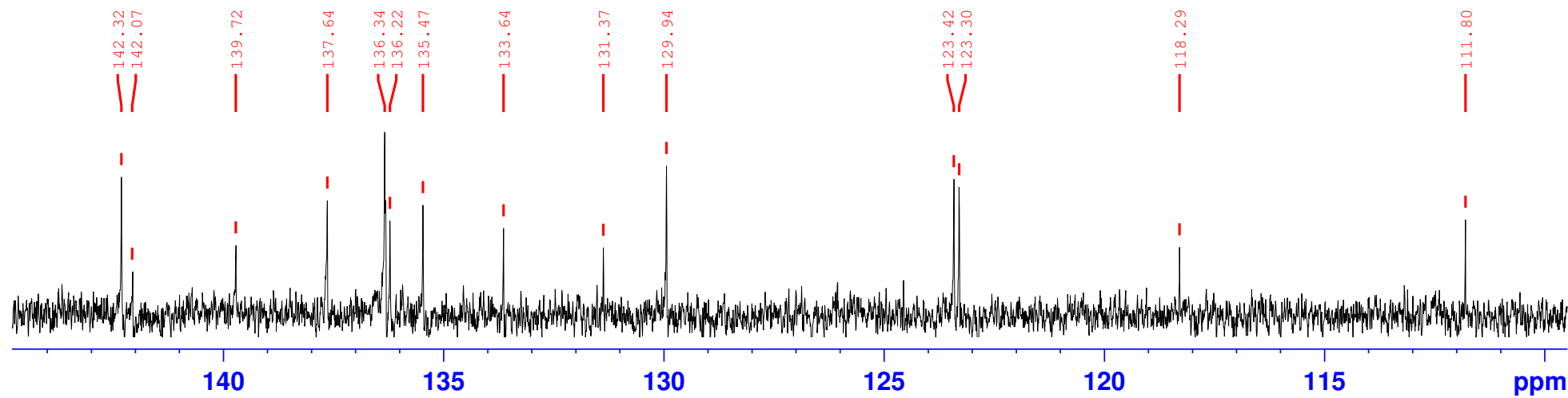
```

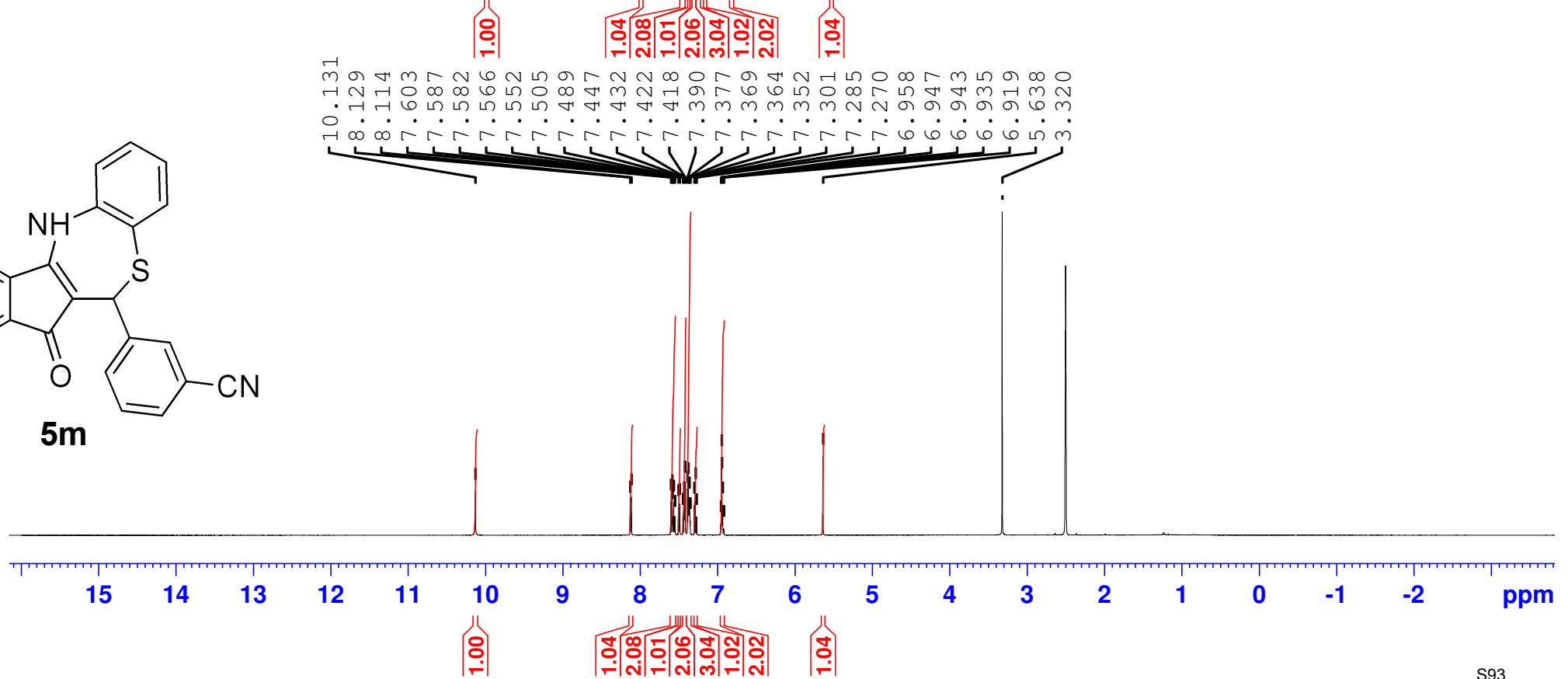
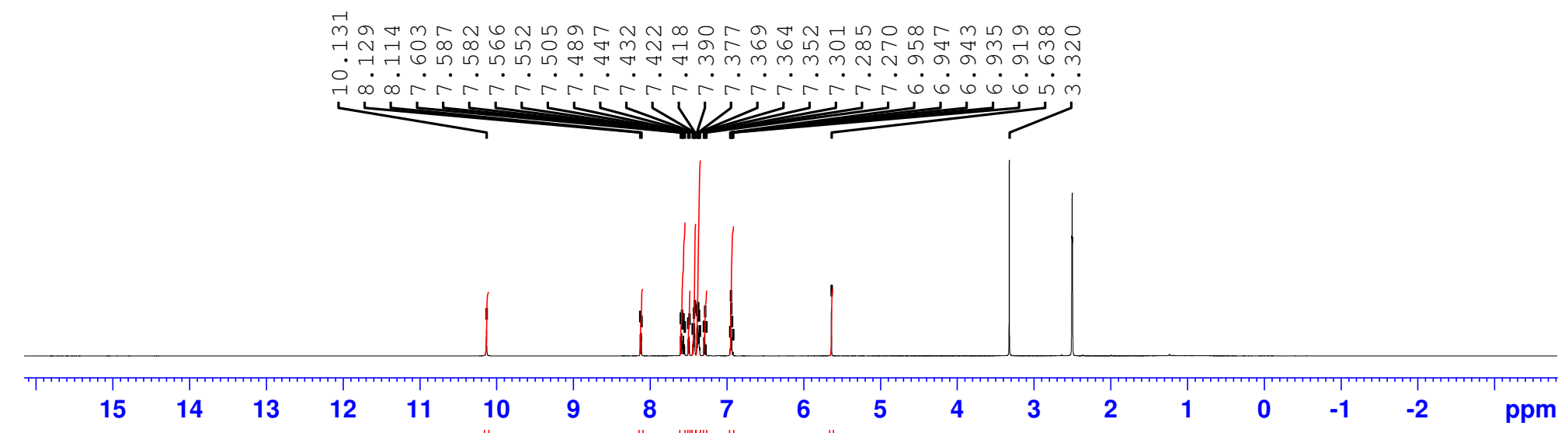
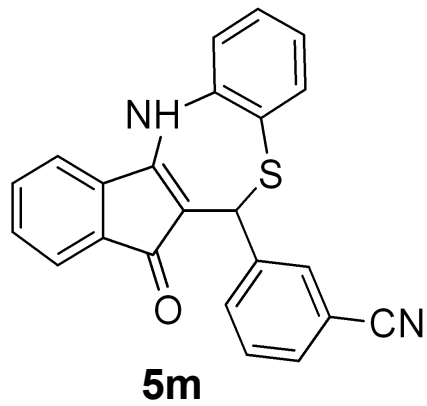
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

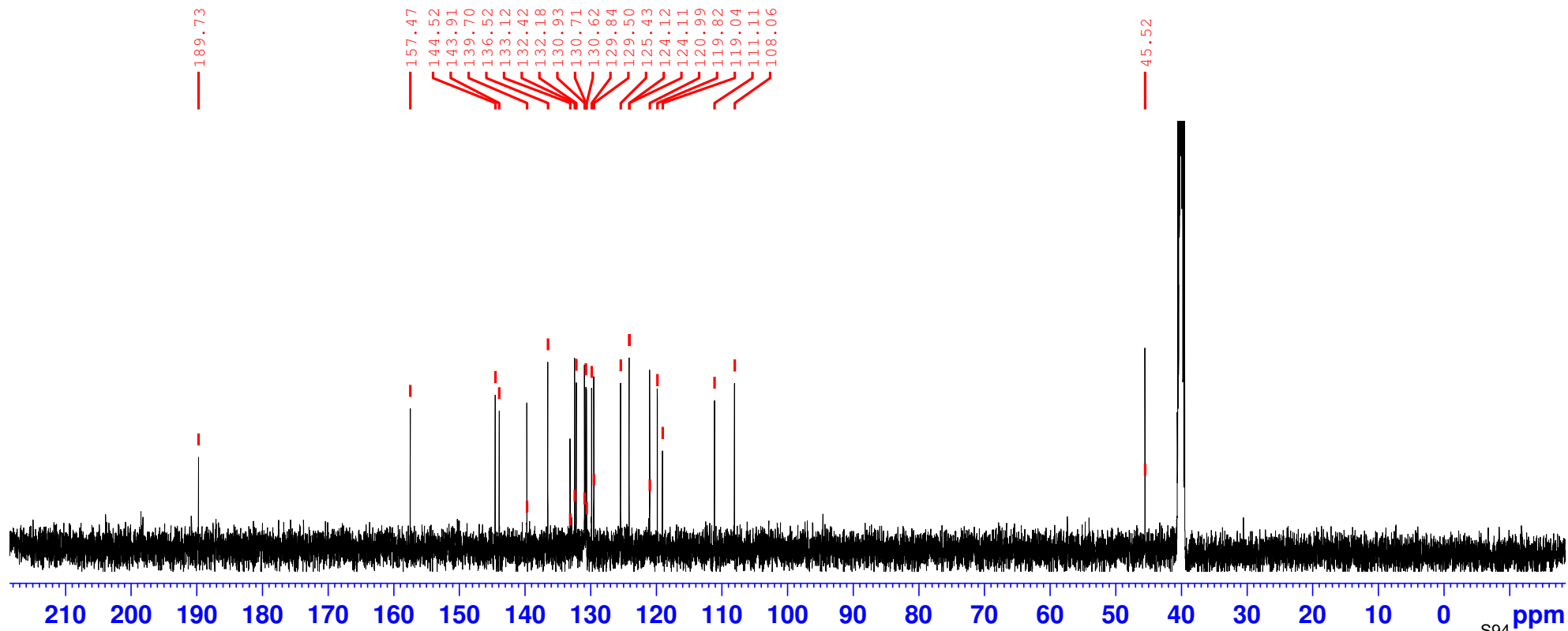
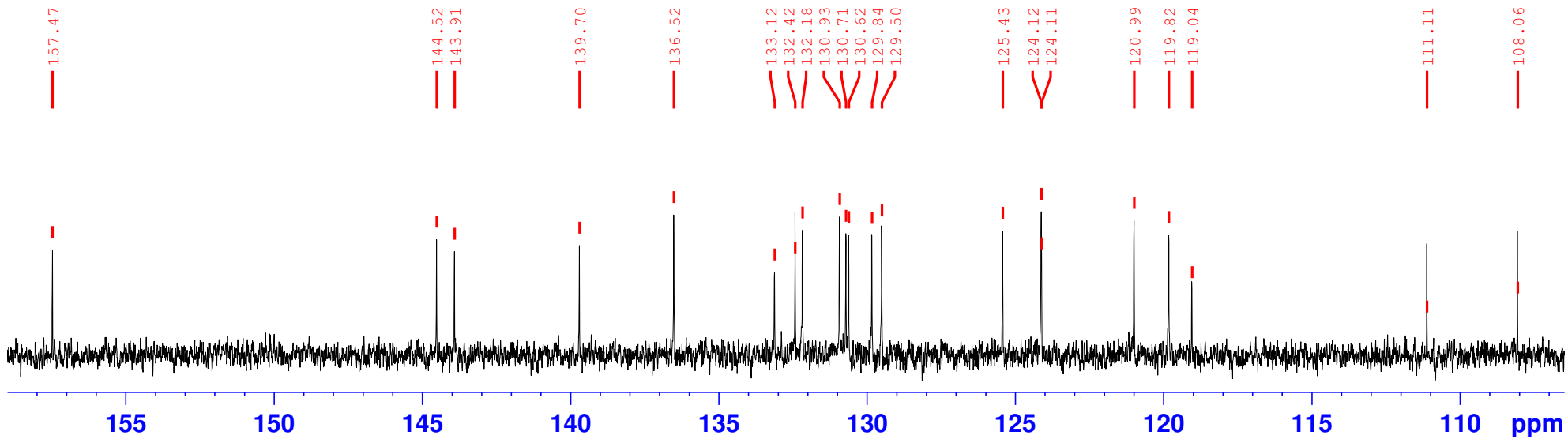
Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.541	BB	0.1958	32.40498	2.17484	0.3661
2	18.510	BB	0.0951	8.37263	1.26717	0.0946
3	19.172	BB	0.0995	13.87209	1.98501	0.1567
4	19.890	BB	0.1008	19.03114	2.74774	0.2150
5	20.263	BV	0.0961	23.47944	3.50729	0.2653
6	20.579	VV	0.1021	76.04619	10.29921	0.8592
7	20.726	VB	0.0802	17.80149	3.23307	0.2011
8	22.084	MM	0.0832	8602.76563	1723.17896	97.2016

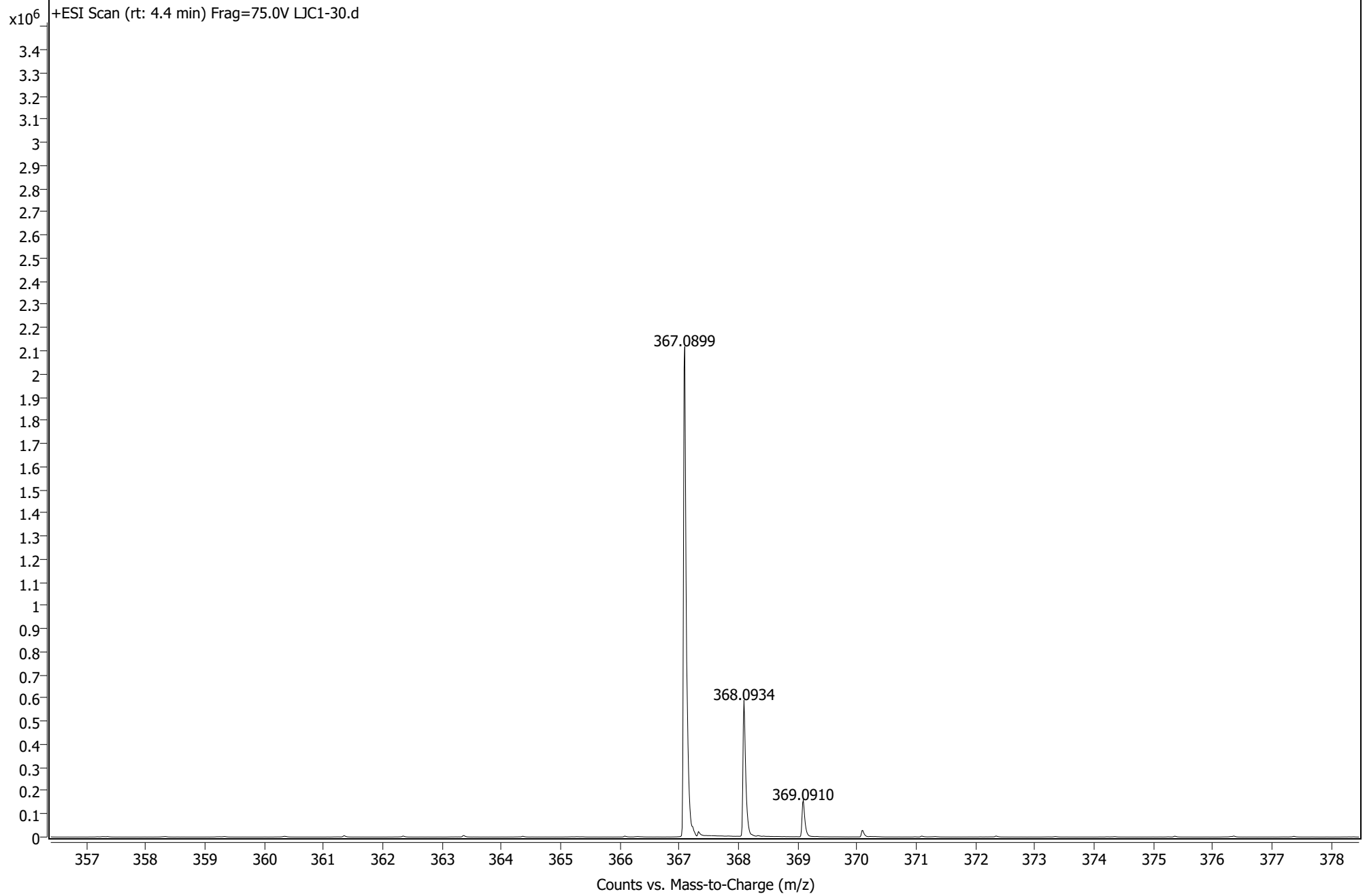








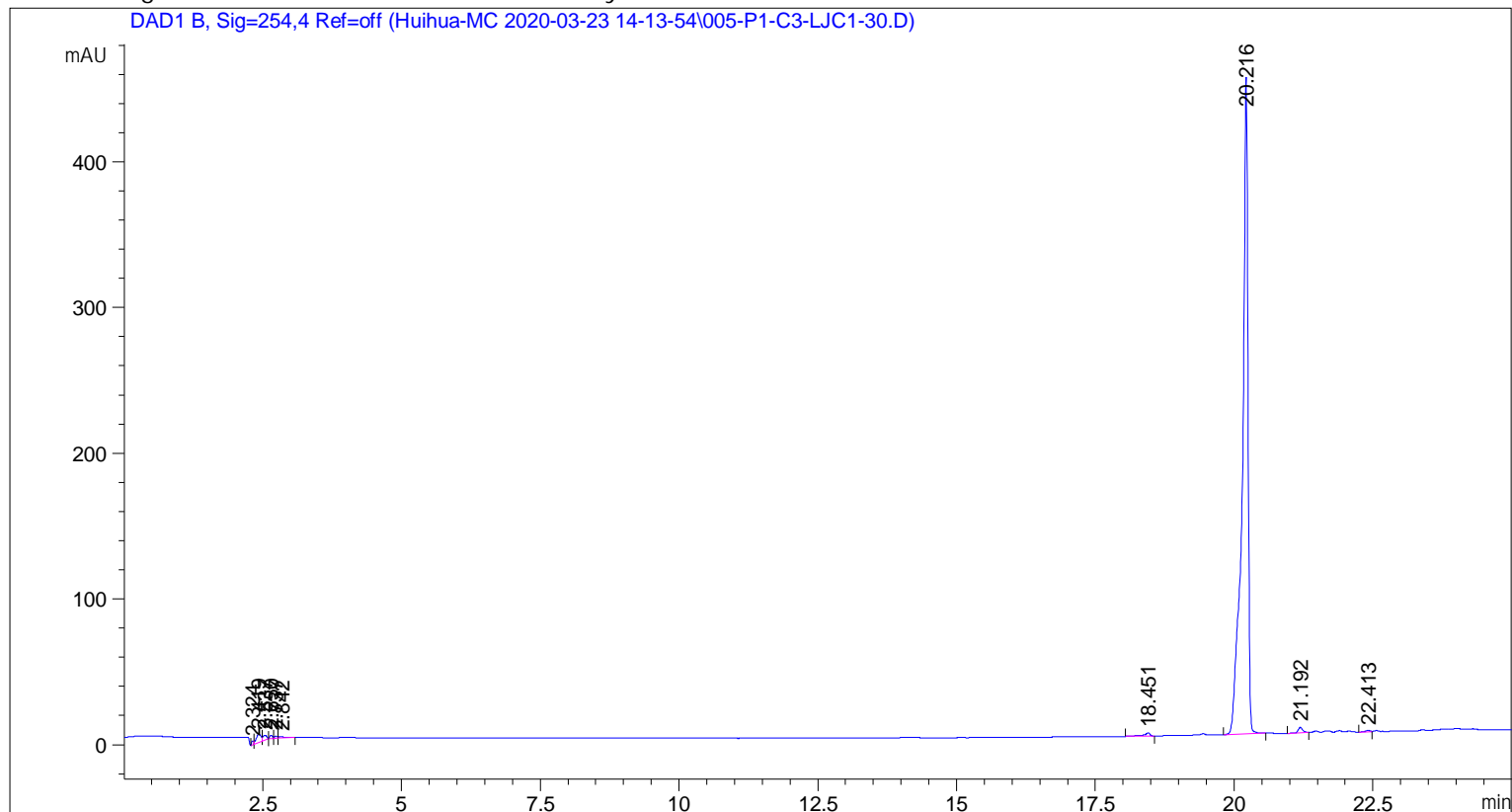
User Spectrum Plot Report



```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    5
Sample Operator : SYSTEM
Acq. Instrument : 1260Infini ty2             Locati on :   P1-C-03
Injection Date  : 3/23/2020 3:51:00 PM      Inj       :    1
                                           Inj Volume: 50.000 µl

Method         : C:\Users\Public\Documents\ChemStation\1\Data\Huihua-MC 2020-03-23 14-13-54
                \MC-SMALL MOLE.M (Sequence Method)
Last changed   : 2/19/2020 11:54:04 AM by SYSTEM
  
```



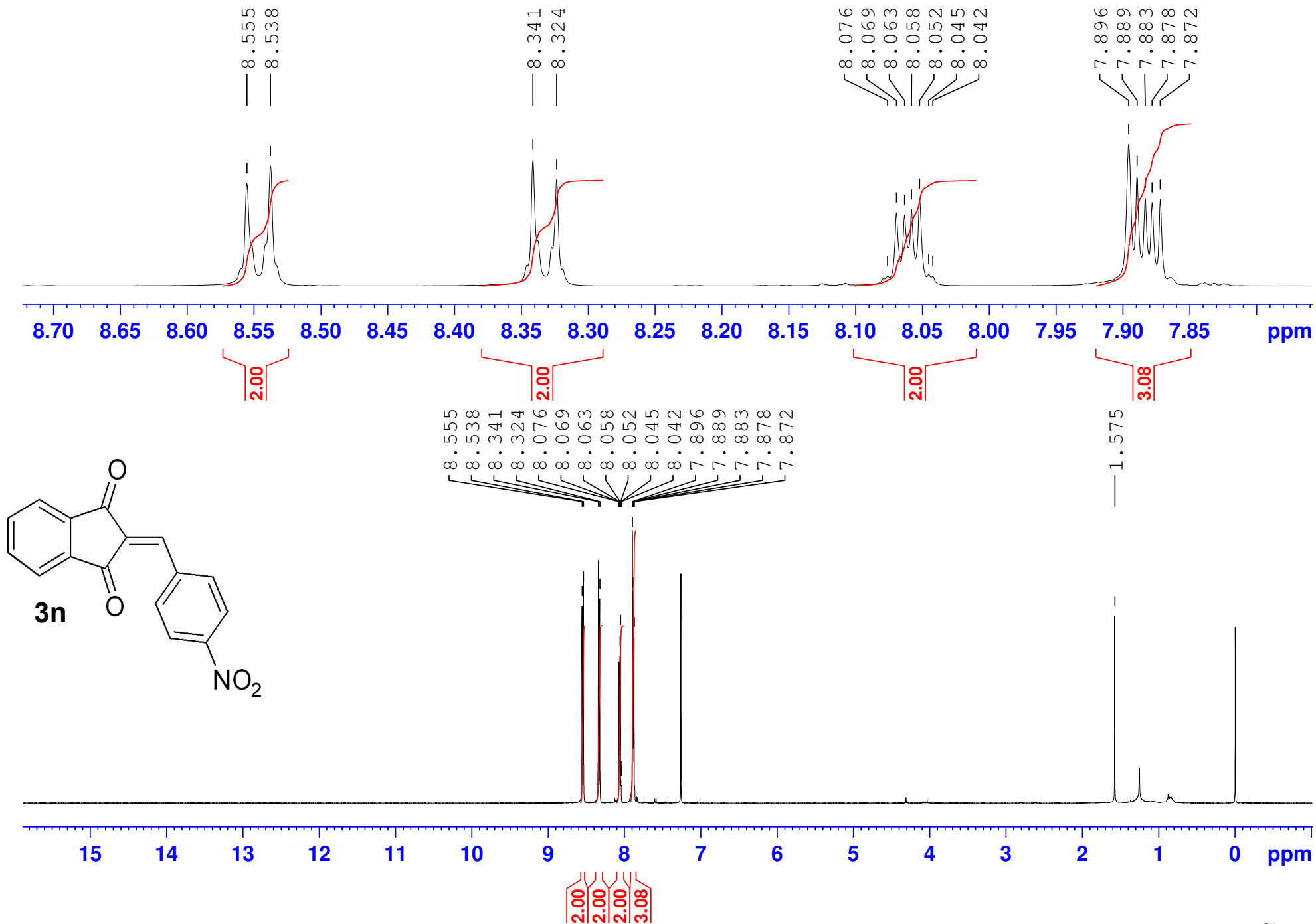
=====
 Area Percent Report
 =====

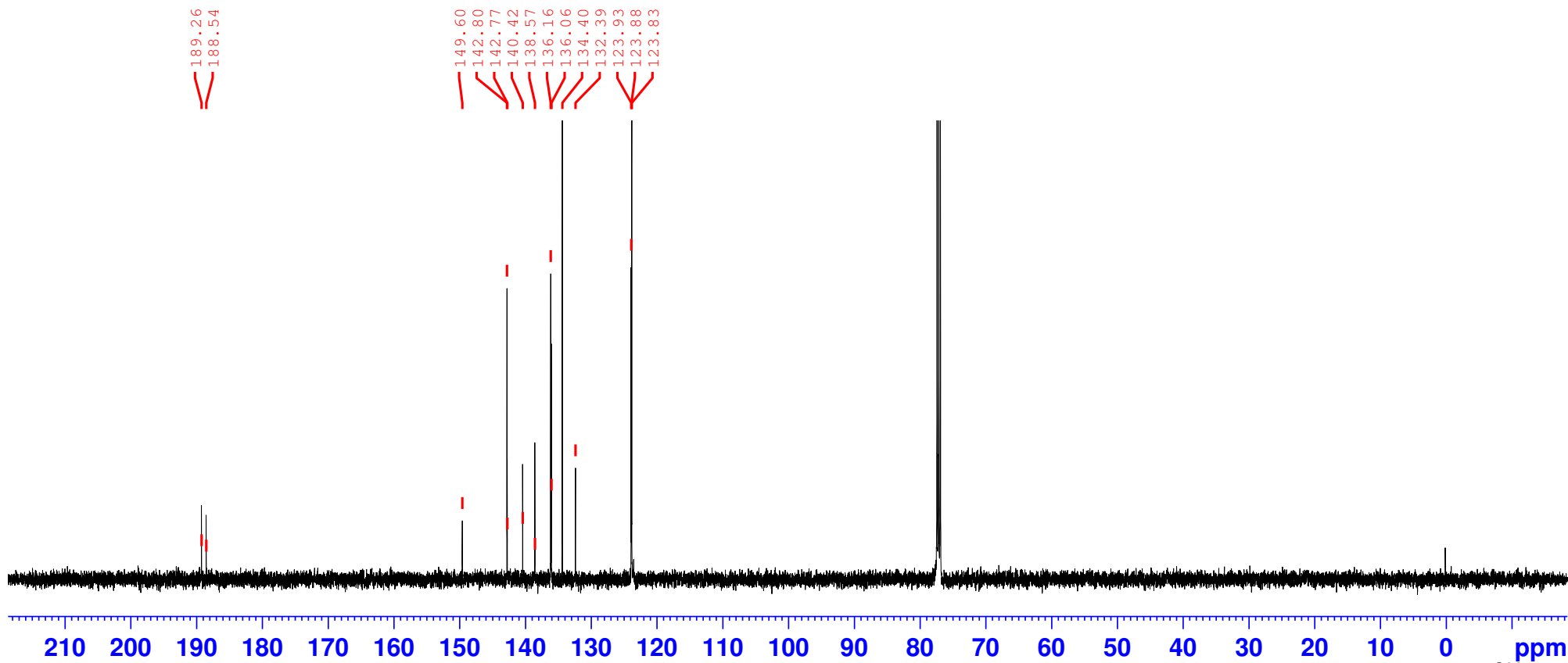
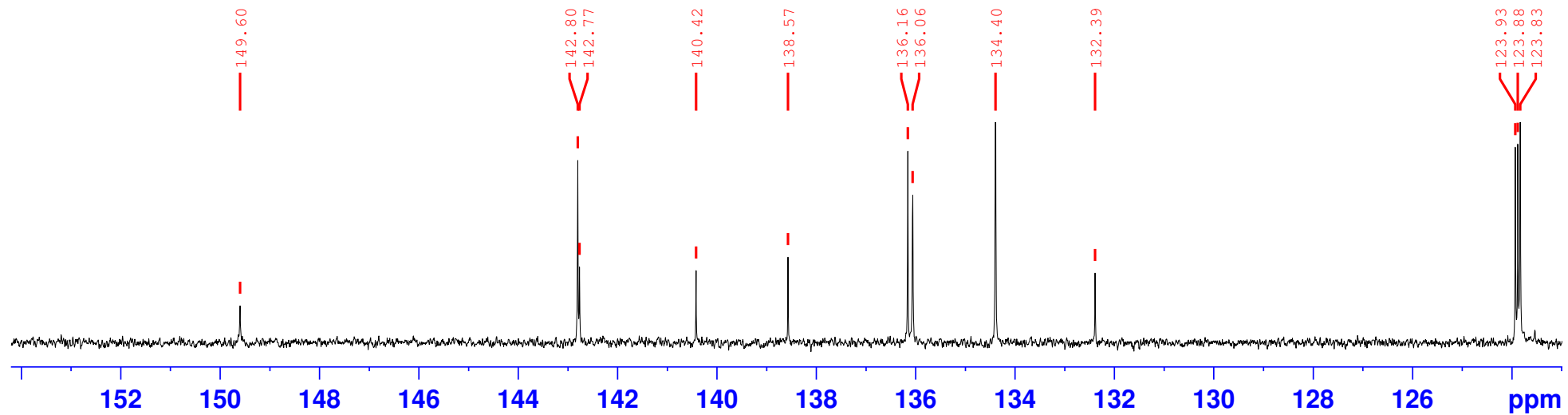
```

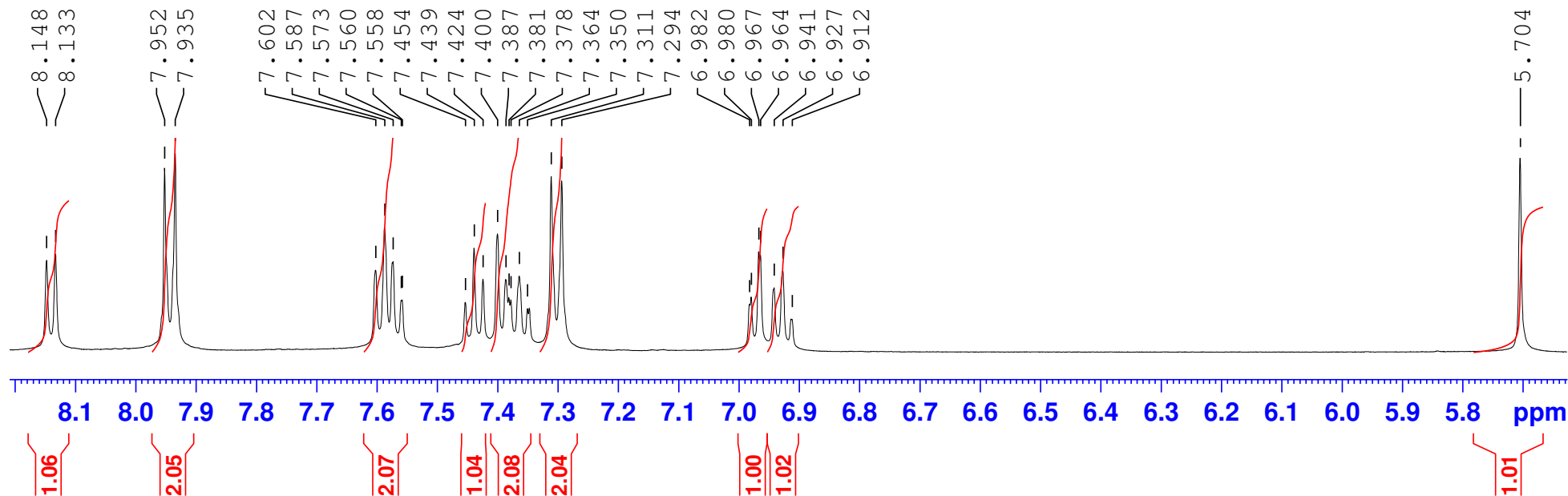
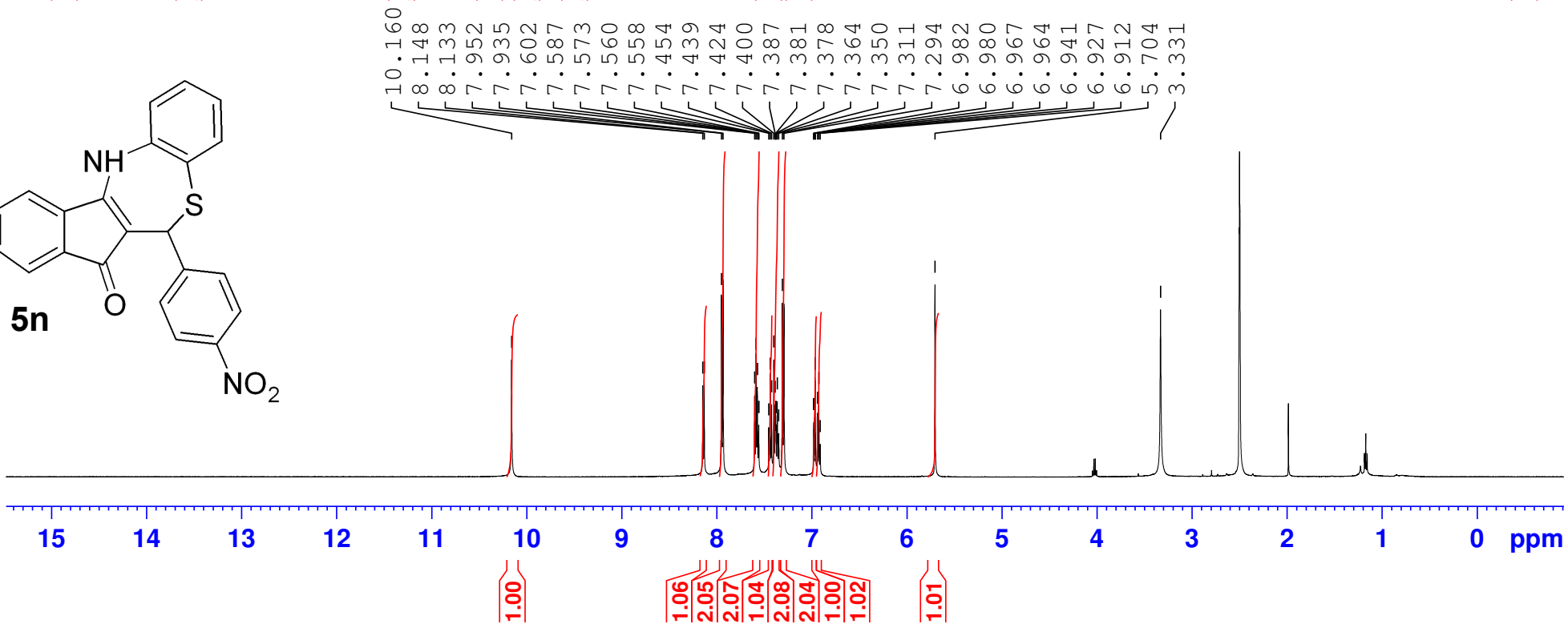
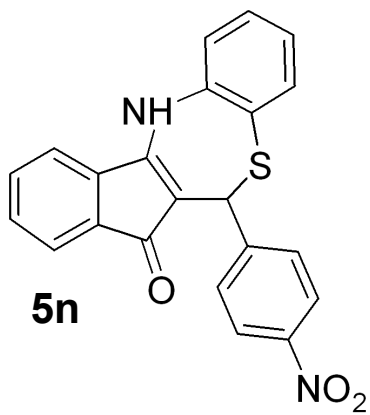
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

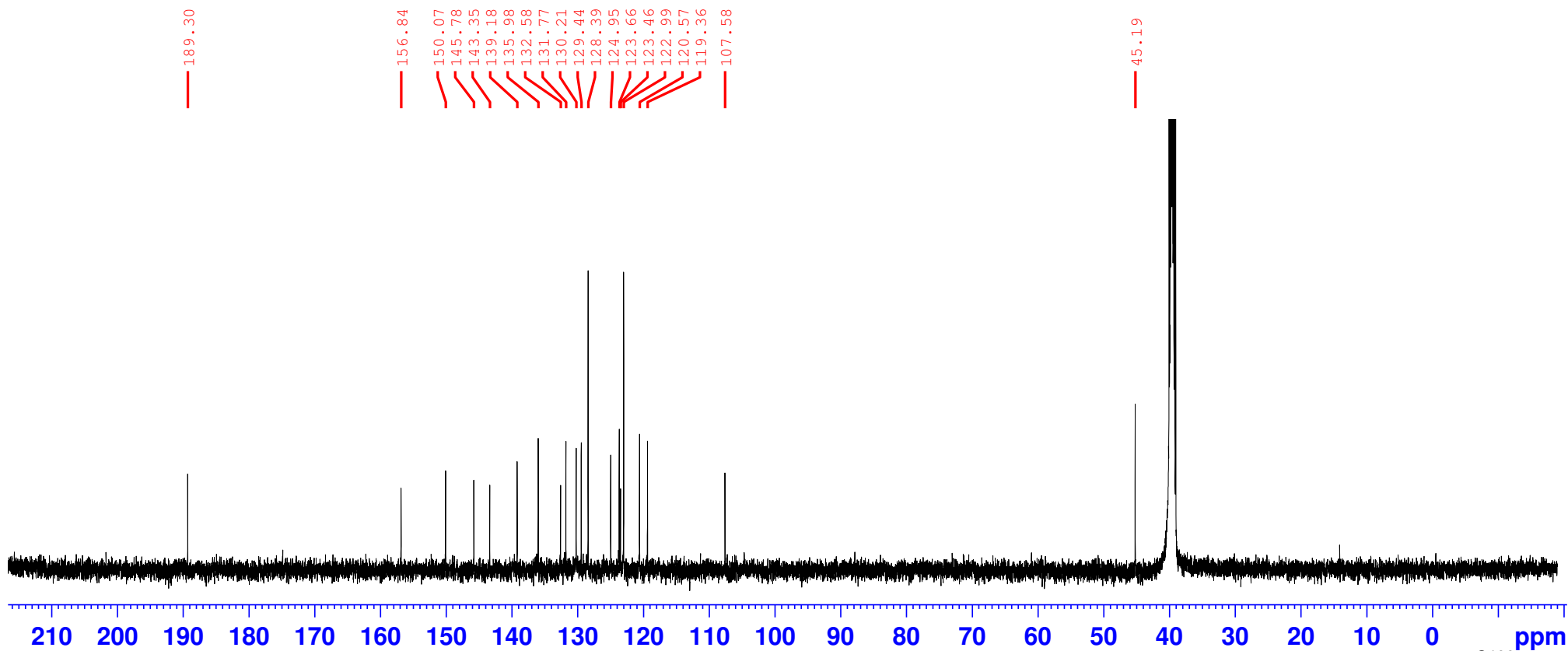
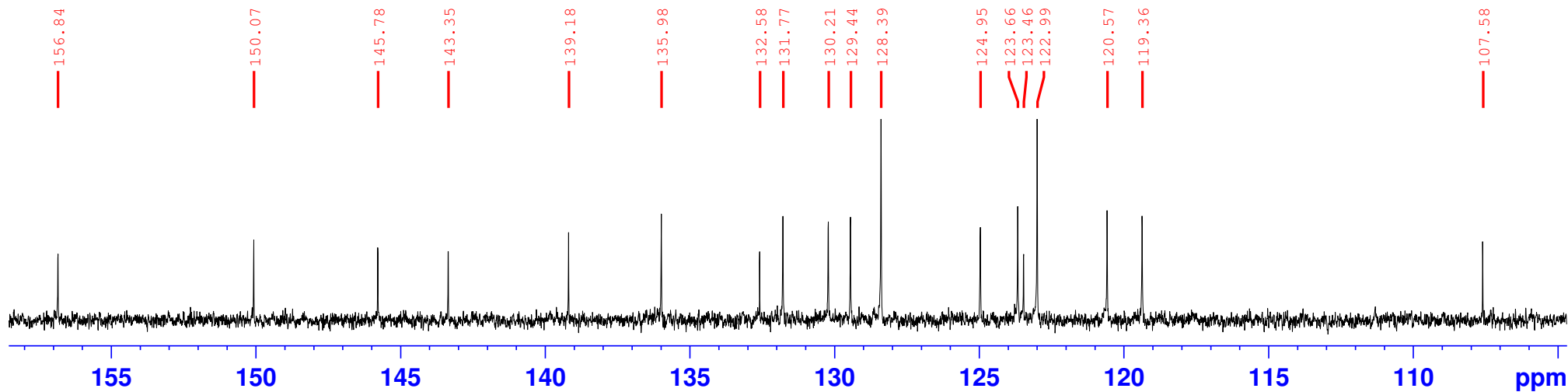
Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.324	BV	0.0440	6.67127	2.43366	0.2030
2	2.419	VV	0.0833	33.35941	5.45547	1.0152
3	2.537	VB	0.0674	15.37650	3.23788	0.4679
4	2.650	BV	0.0486	7.10886	2.26824	0.2163
5	2.737	VV	0.0603	5.41211	1.36257	0.1647
6	2.842	VB	0.0946	7.40014	1.09833	0.2252
7	18.451	BB	0.1138	18.00785	2.14840	0.5480
8	20.216	BB	0.1000	3166.03979	450.58041	96.3498
9	21.192	BB	0.0825	20.62754	3.73076	0.6277

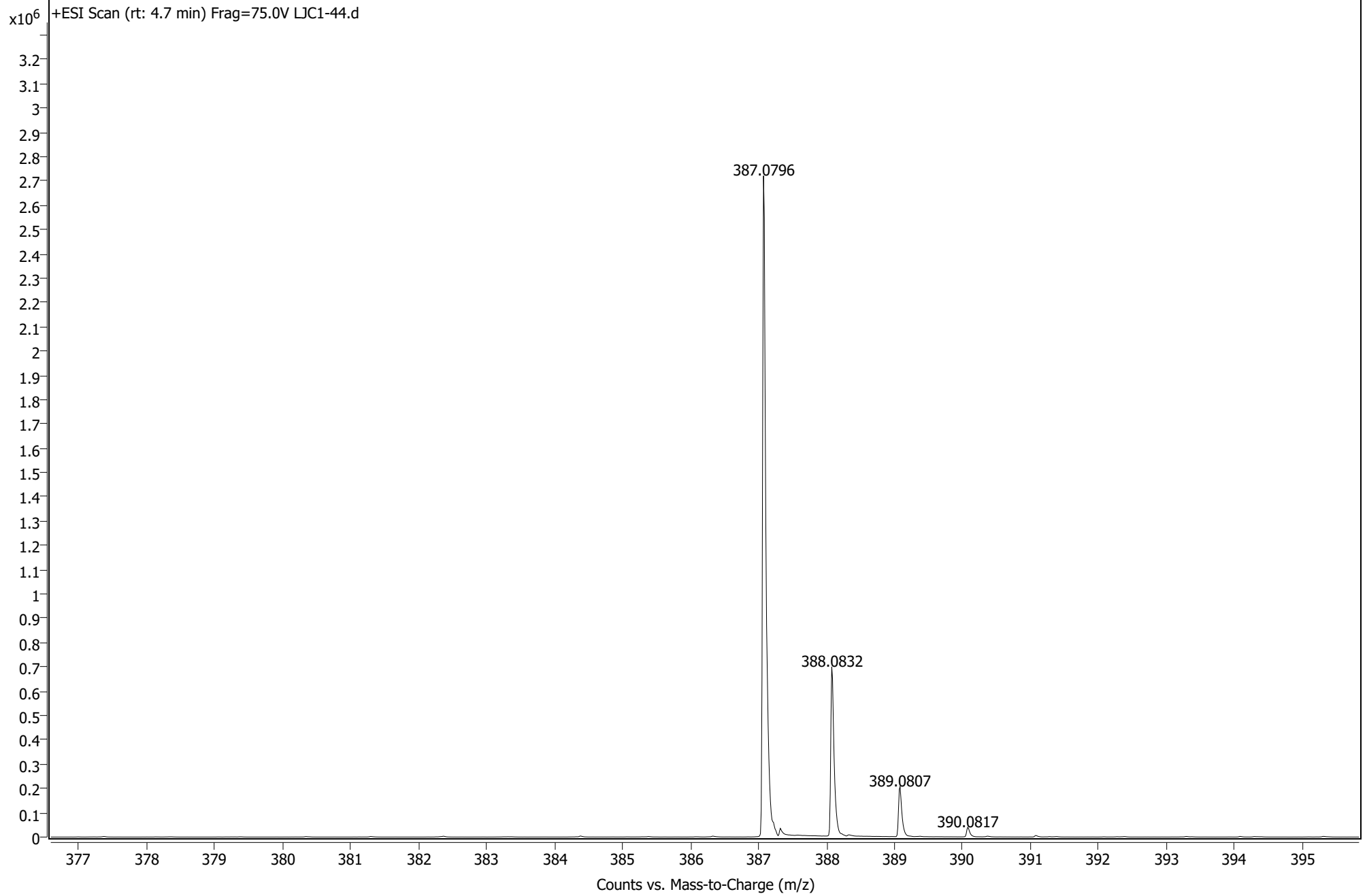








User Spectrum Plot Report

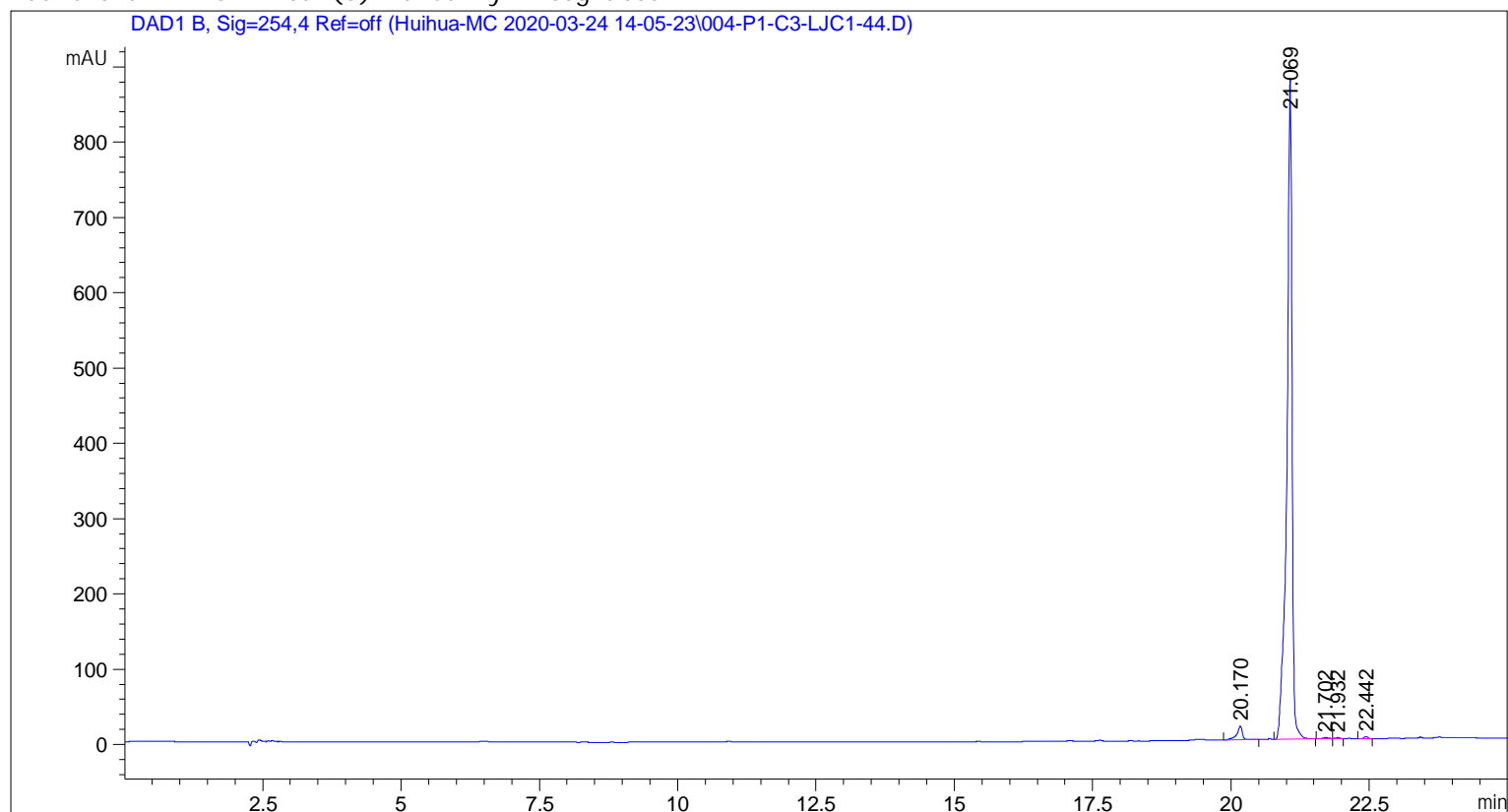


Sample Name: LJC1-44

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    4
Sample Operator : SYSTEM
Acq. Instrument : 1260Infinity2              Location  : P1-C-03
Injection Date  : 3/24/2020 3:21:09 PM       Inj       :    1
                                           Inj Volume: 50.000 µl
Method          : C:\Users\Public\Documents\ChemStation\1\Data\Huihua-MC 2020-03-24 14-05-23
                  \MC-SMALL MOLE.M (Sequence Method)
Last changed    : 2/19/2020 11:54:04 AM by SYSTEM
Additional Info : Peak(s) manually integrated
=====

```



```

=====
                          Area Percent Report
=====

```

```

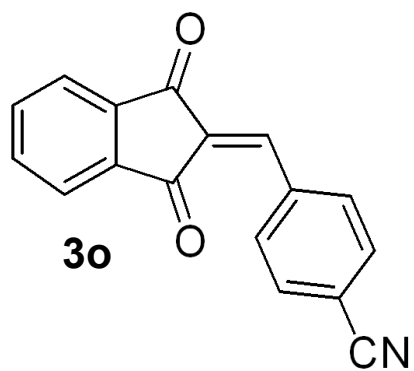
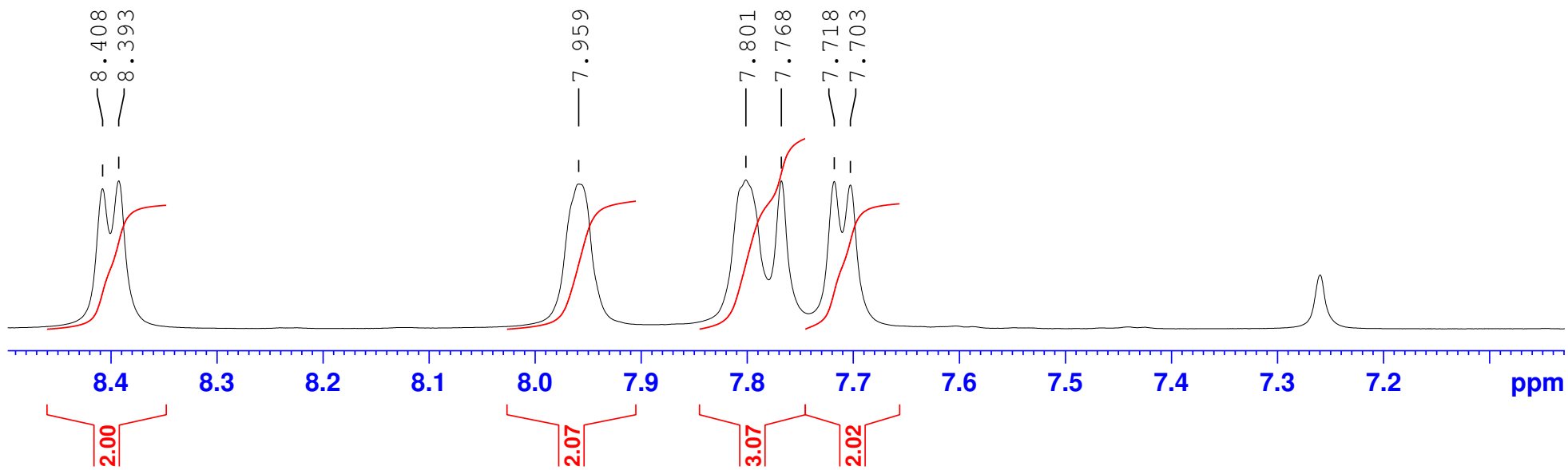
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

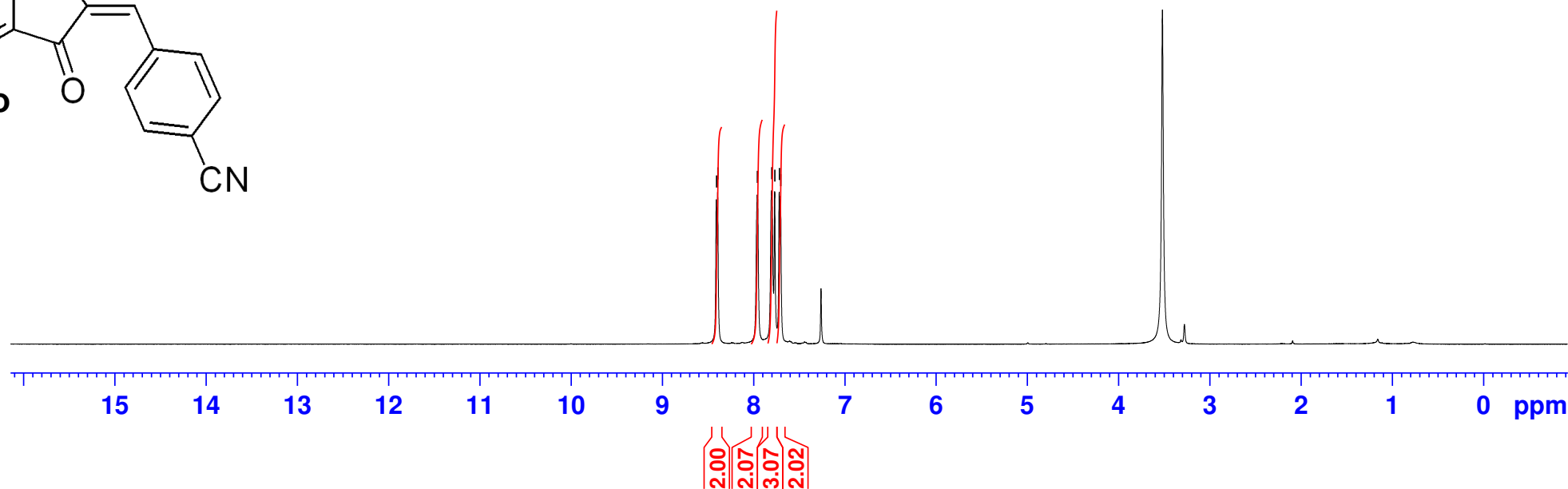
Signal 1: DAD1 B, Sig=254,4 Ref=off

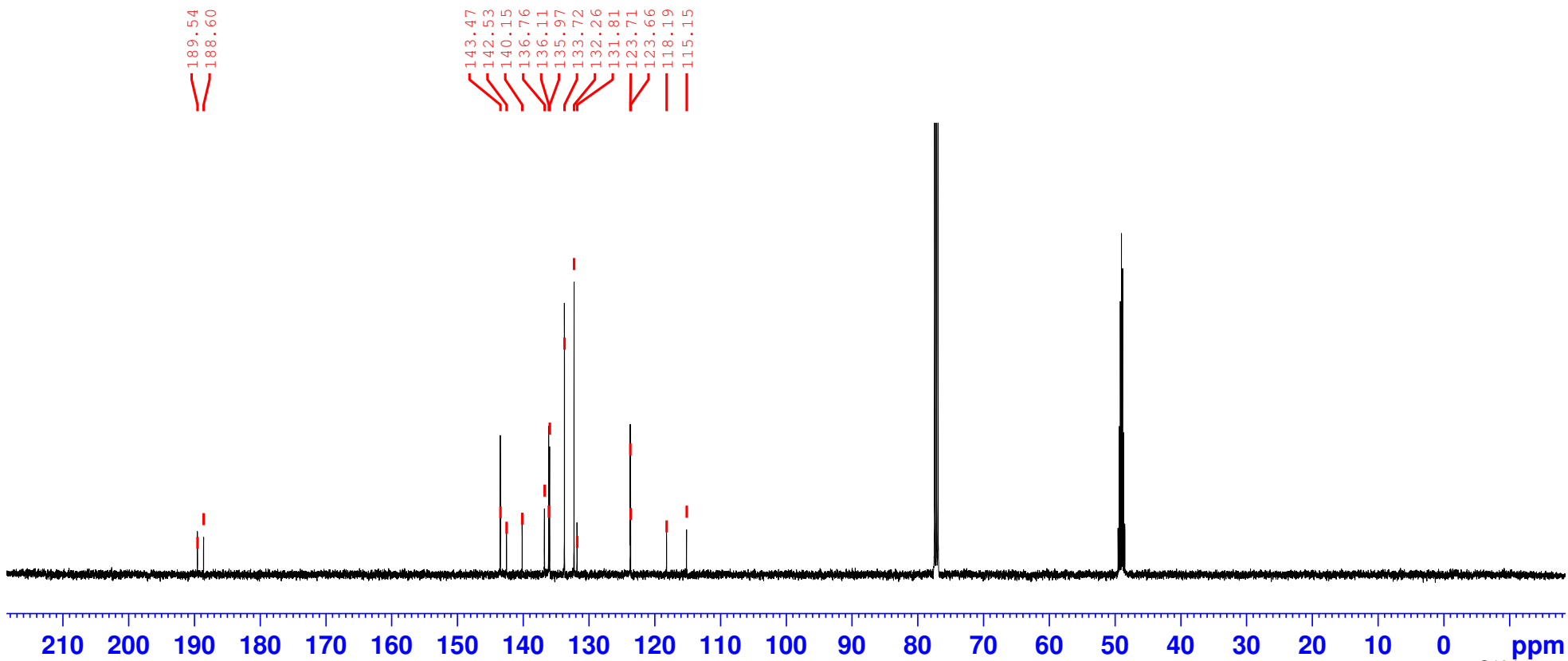
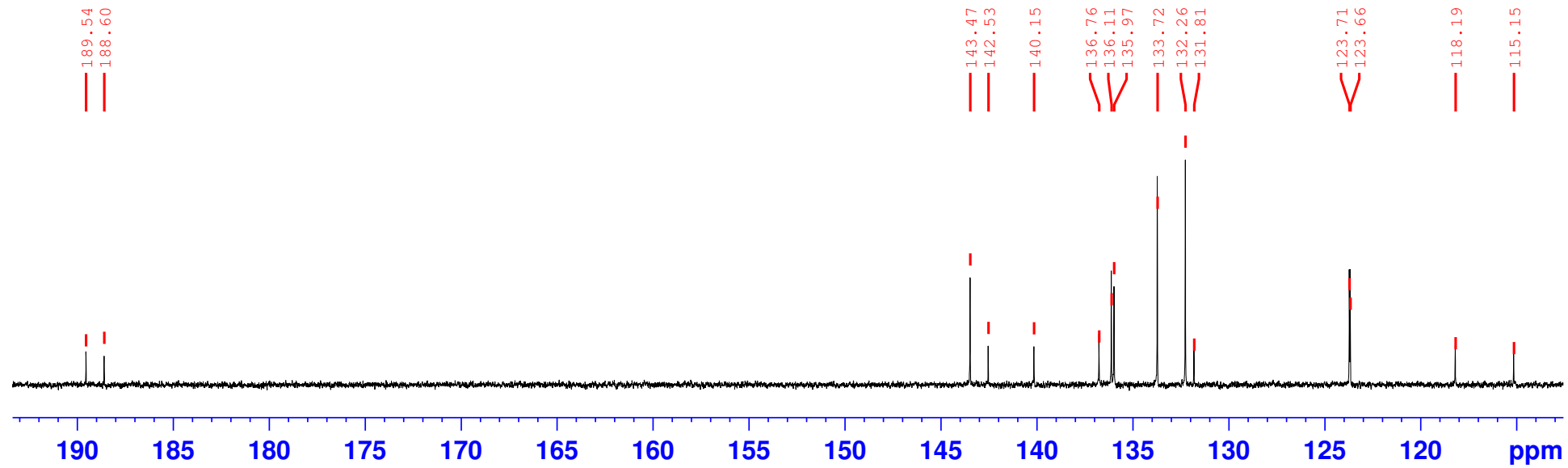
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.170	BV R	0.1018	131.25250	18.27964	2.2326
2	21.069	BB	0.0939	5708.81201	877.07391	97.1056
3	21.702	BV	0.1138	13.58999	1.62136	0.2312
4	21.932	VV	0.1097	10.36470	1.51650	0.1763
5	22.442	BB	0.0768	14.95388	2.96631	0.2544

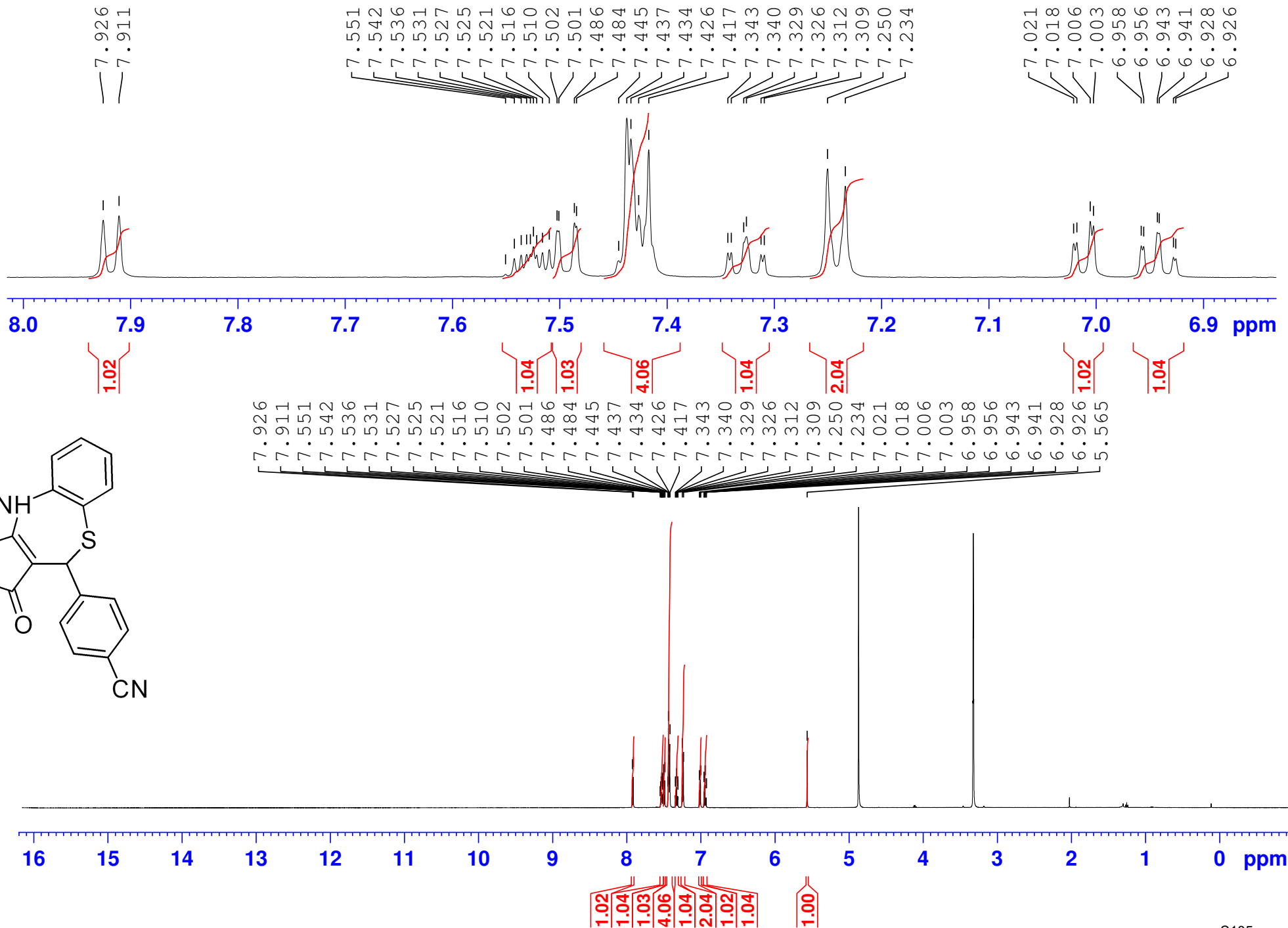
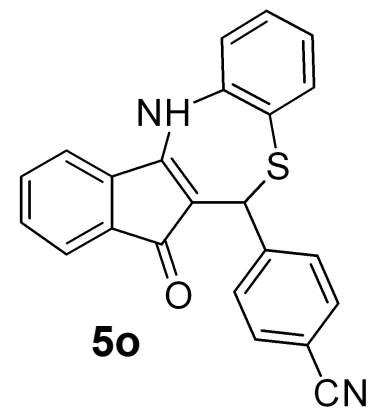
```
Totals :                      5878.97308  901.45772
```

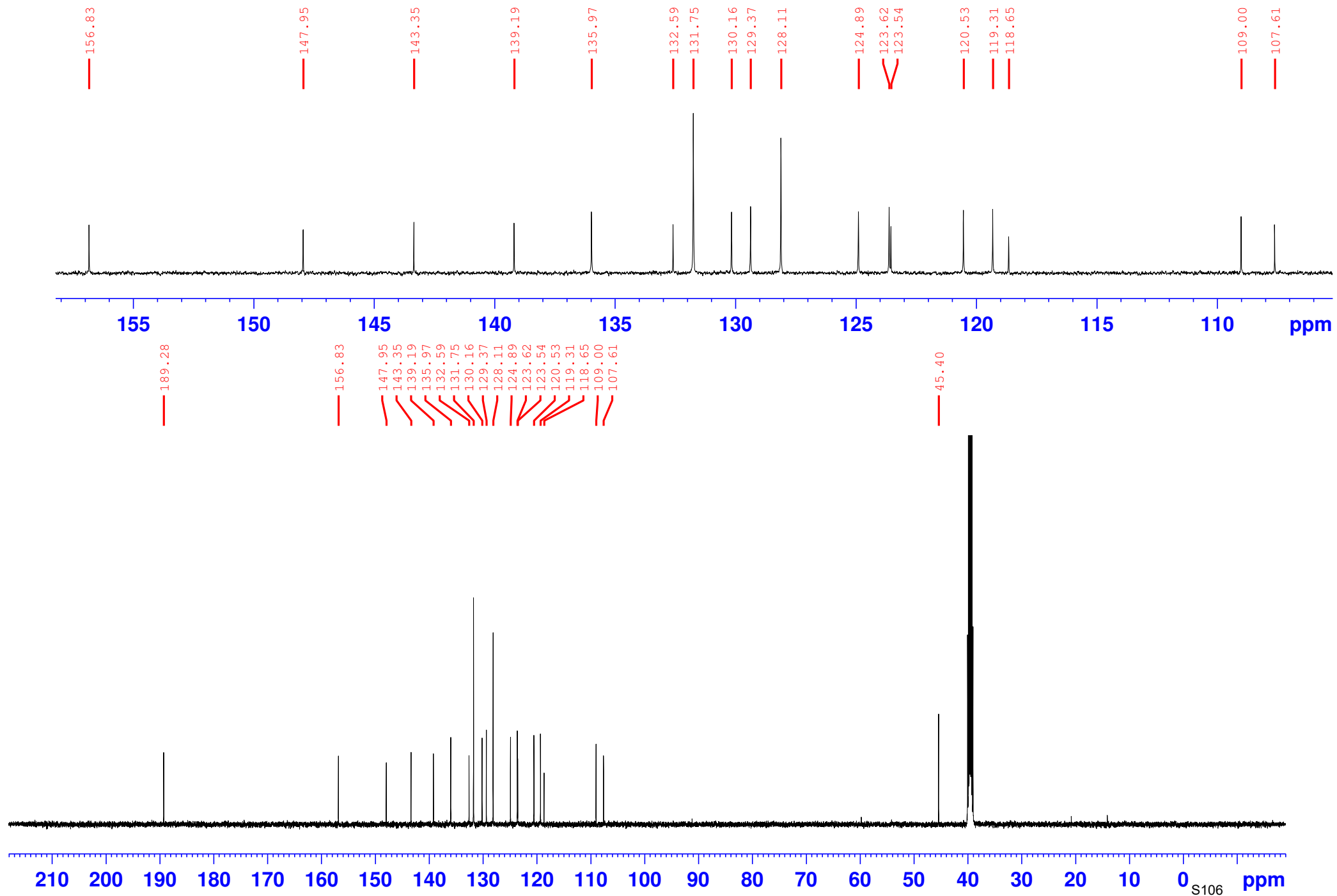


8.408
8.393
7.959
7.801
7.768
7.718
7.703

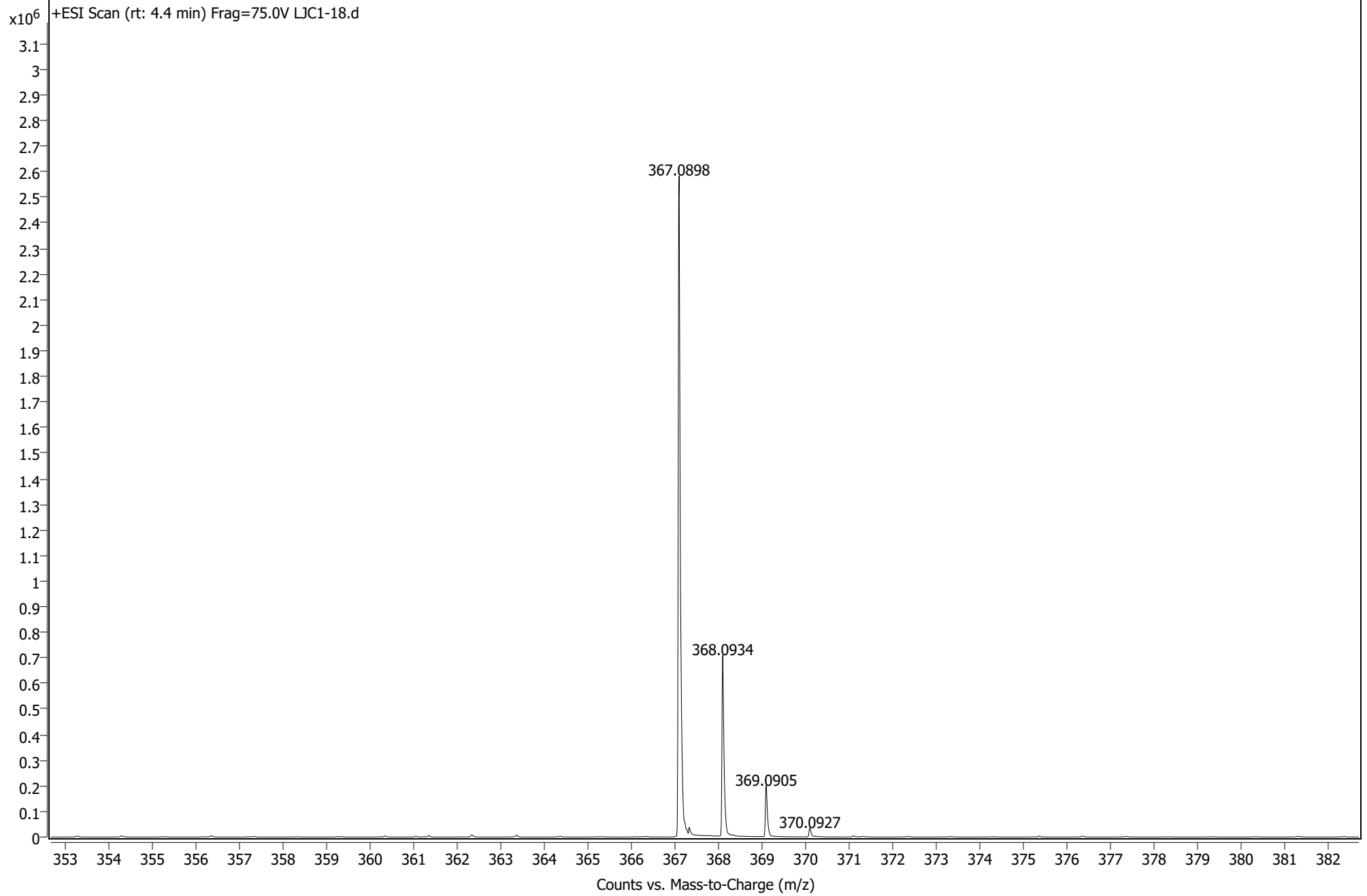








User Spectrum Plot Report

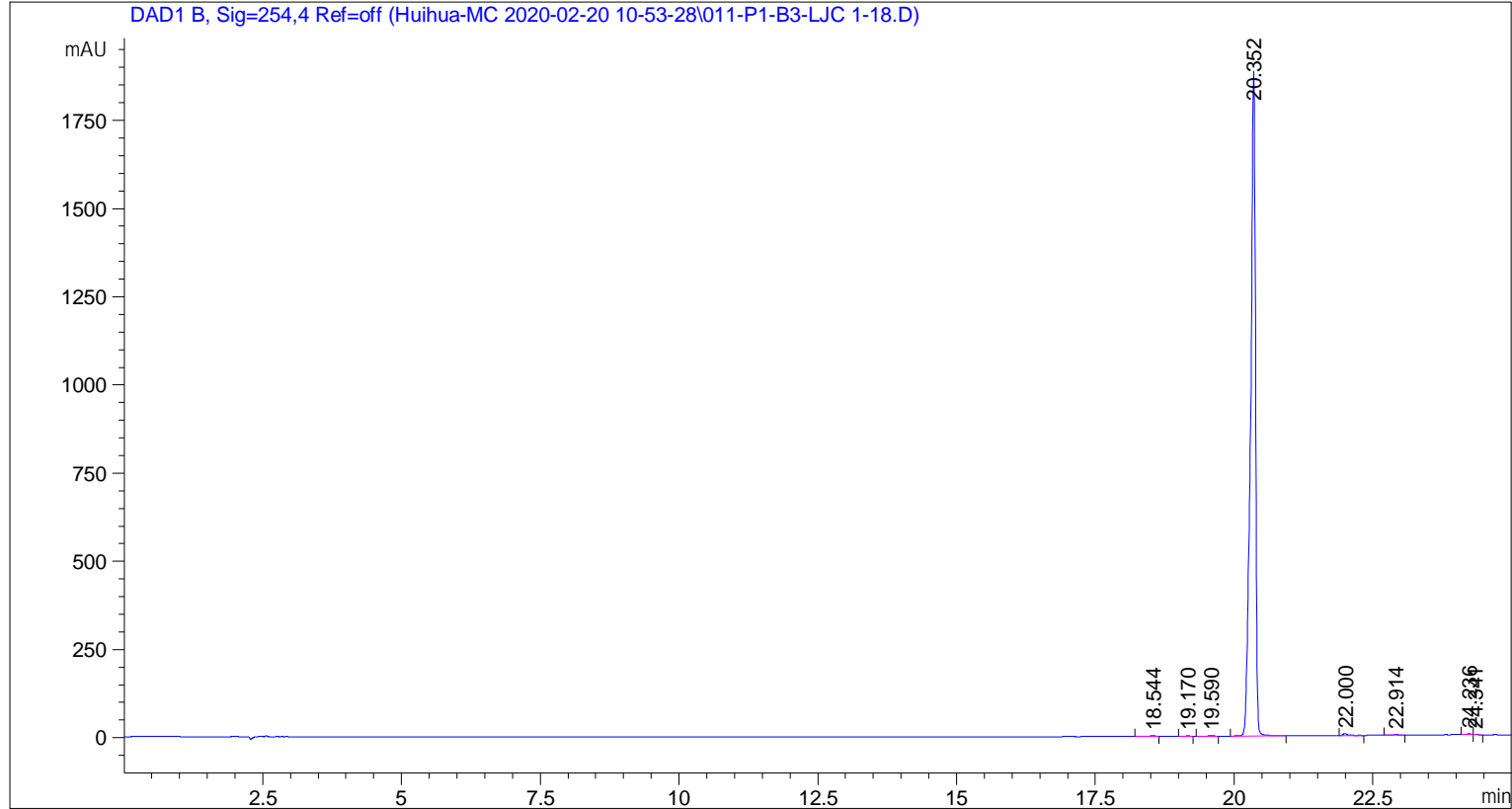


Sample Name: LJC 1-18

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :   11
Sample Operator : SYSTEM
Acq. Instrument : 1260Infinity2              Location  : P1-B-03
Injection Date  : 2/20/2020 3:18:51 PM       Inj       :    1
                                           Inj Volume: 50.000 µl

Method          : C:\Users\Public\Documents\ChemStation\1\Data\Huihua-MC 2020-02-20 10-53-28
                  \MC-SMALL MOLE.M (Sequence Method)
Last changed    : 2/19/2020 11:54:04 AM by SYSTEM
Additional Info  : Peak(s) manually integrated
    
```



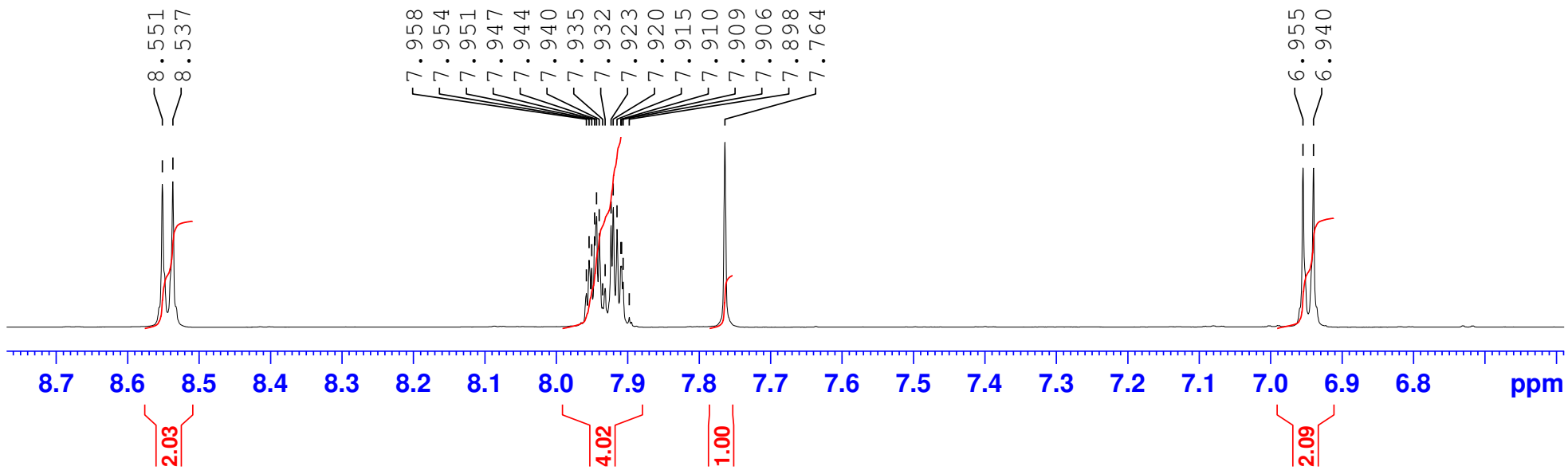
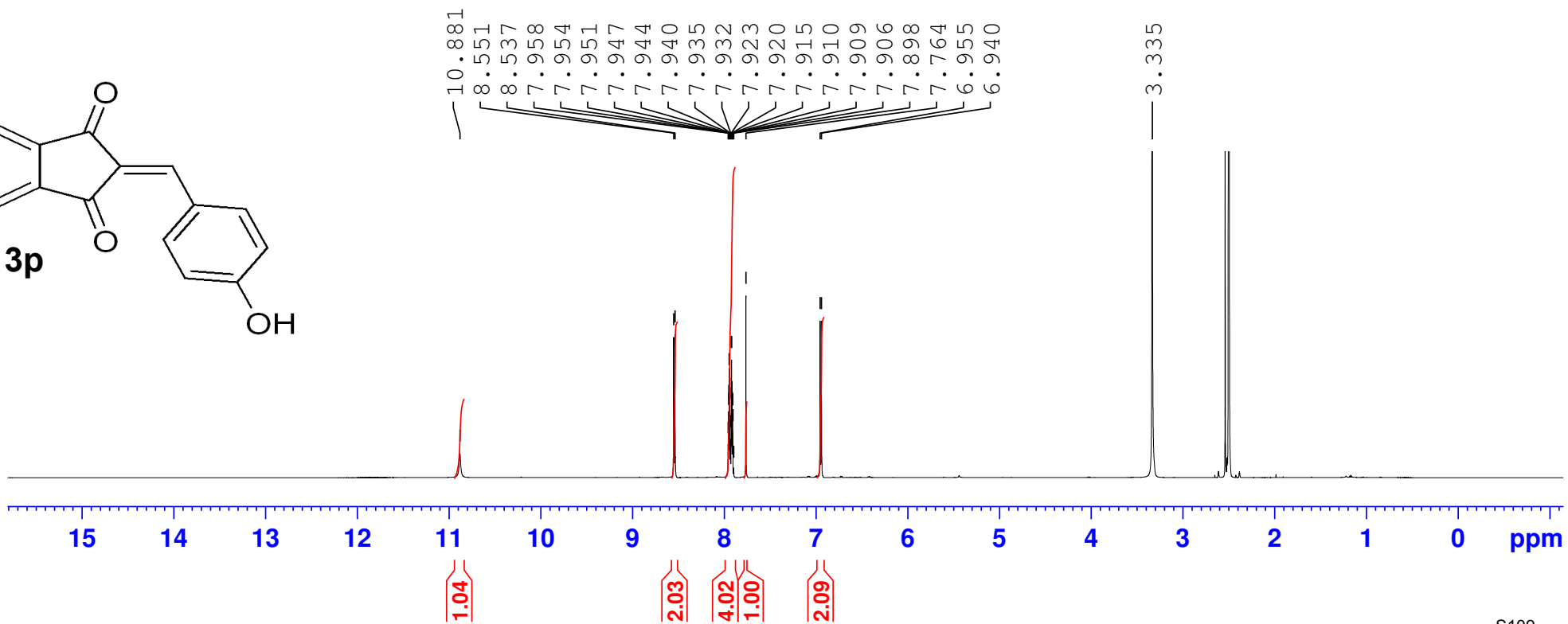
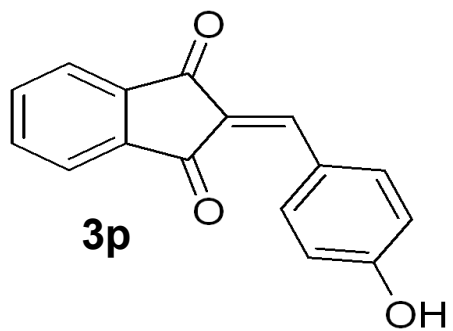
=====
 Area Percent Report
 =====

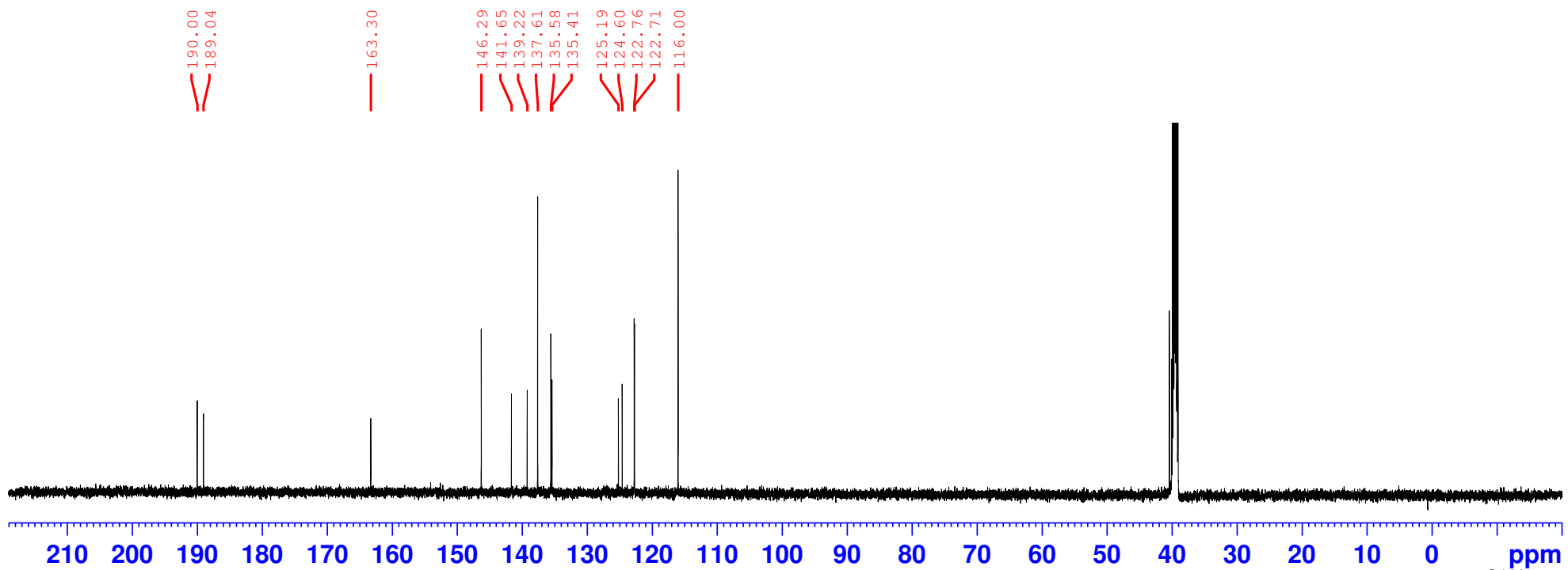
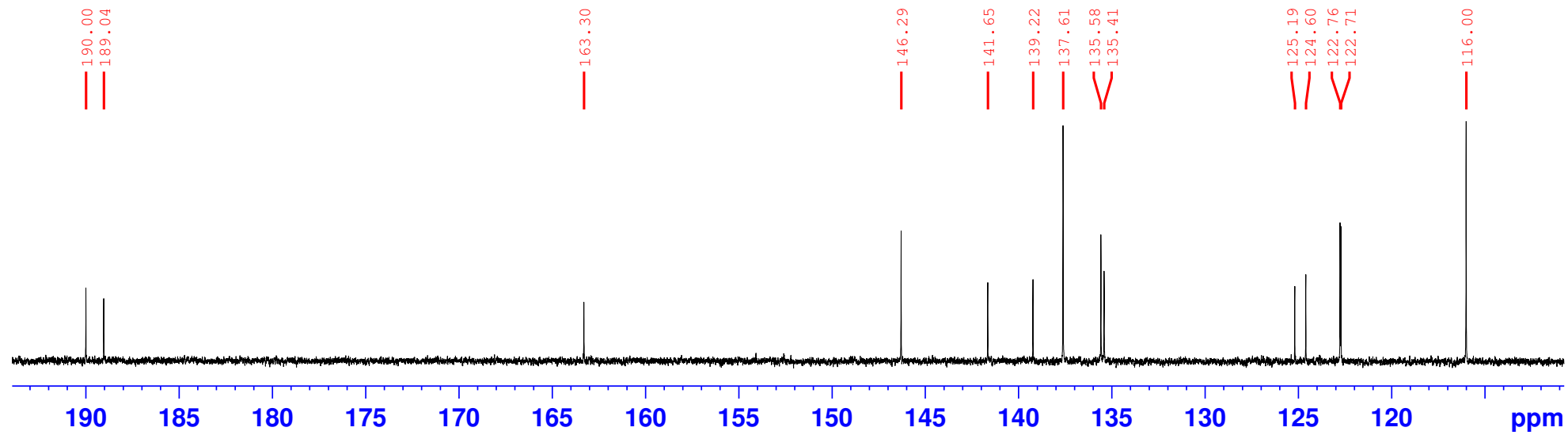
```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.544	BB	0.1038	14.88345	2.02333	0.1274
2	19.170	BB	0.0829	6.15387	1.10693	0.0527
3	19.590	BB	0.0915	9.87105	1.56649	0.0845
4	20.352	BB	0.0895	1.15841e4	1889.74011	99.1602
5	22.000	BV R	0.0809	30.08016	5.40855	0.2575
6	22.914	BB	0.0760	16.19878	3.14833	0.1387
7	24.236	BV	0.0726	15.81355	3.15030	0.1354
8	24.341	VB	0.0748	5.10453	1.04887	0.0437





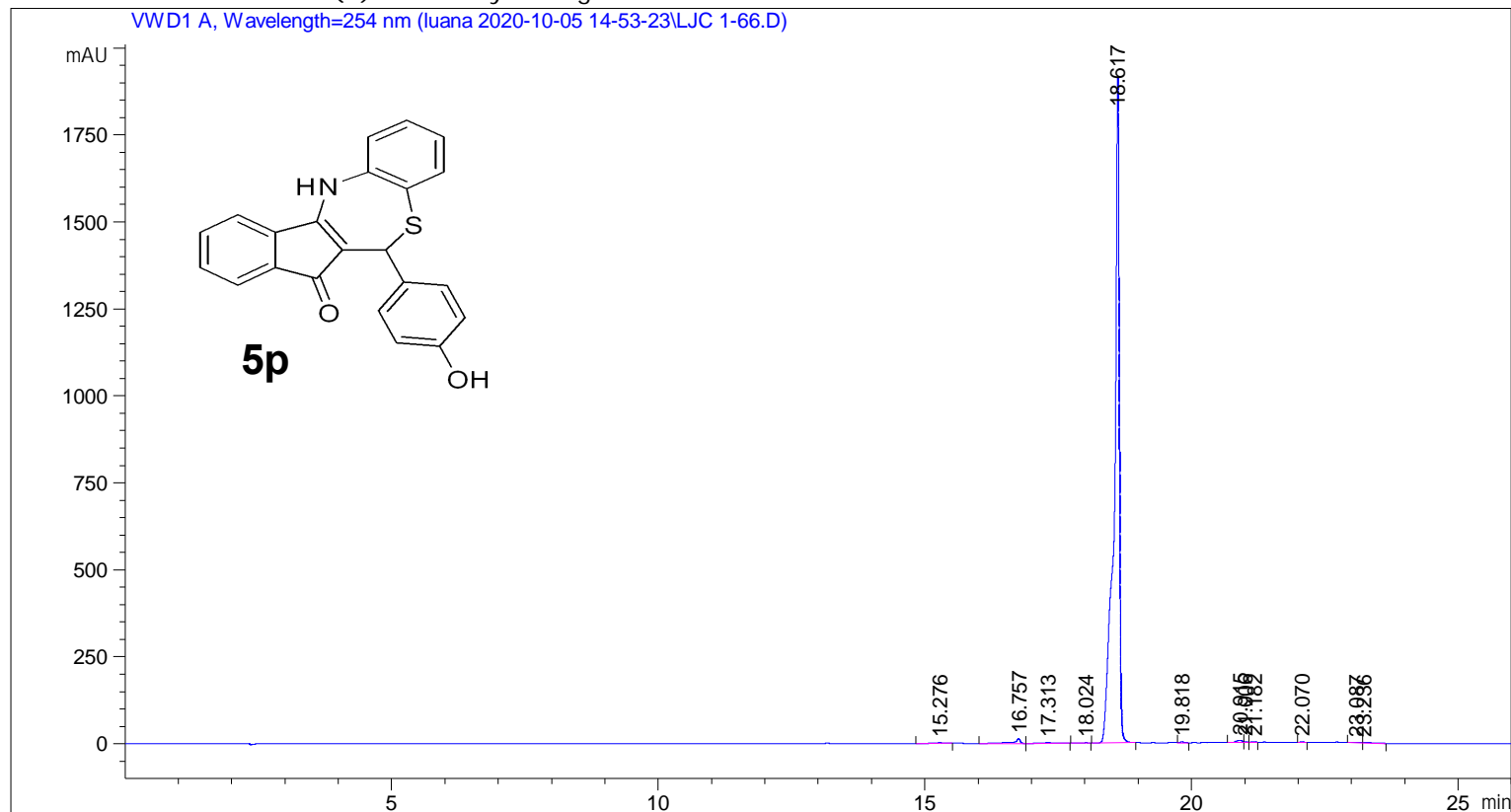
Sample Name: LJC 1-66

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    4
Acq. Instrument : 1220 HPLC                    Location  :    4
Injection Date  : 10/5/2020 4:16:18 PM      Inj       :    1
                                           Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-10-05 14-53-23\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 10/5/2020 2:58:07 PM by SYSTEM
Method Info     : Water/MeOH

Sample Info     : LJC 1-66
  
```

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====
  
```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: VWD1 A, Wavelength=254 nm

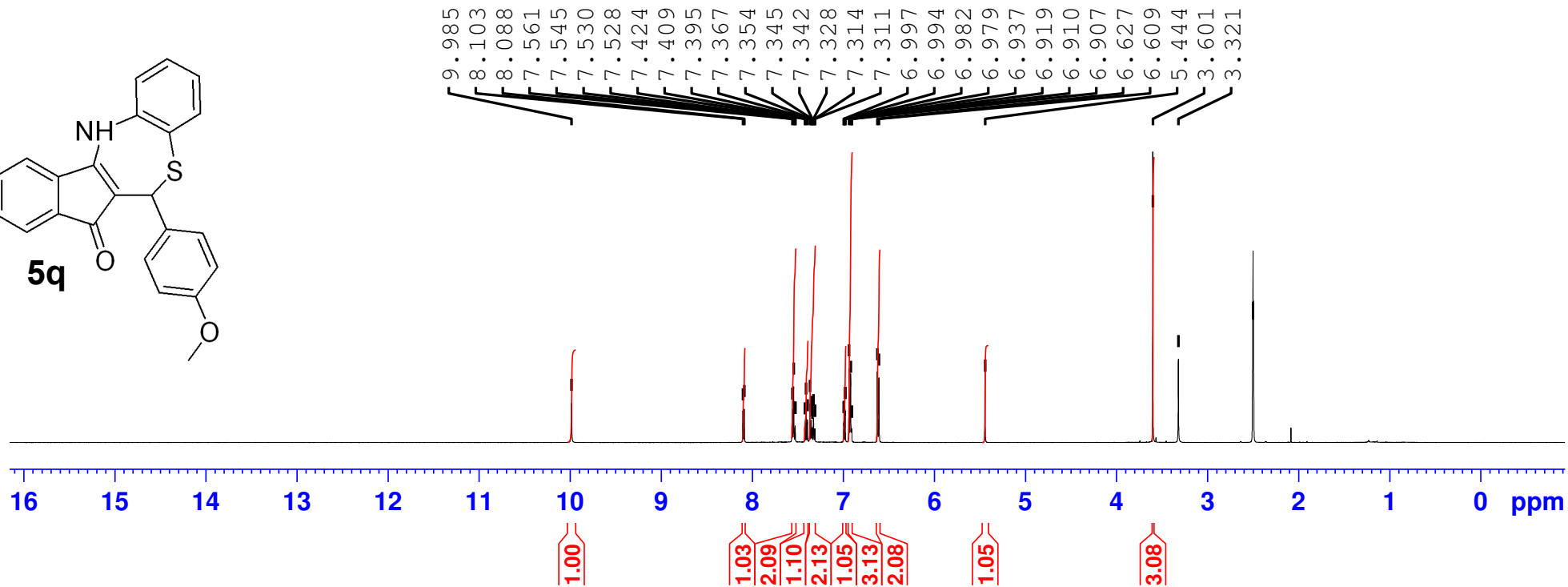
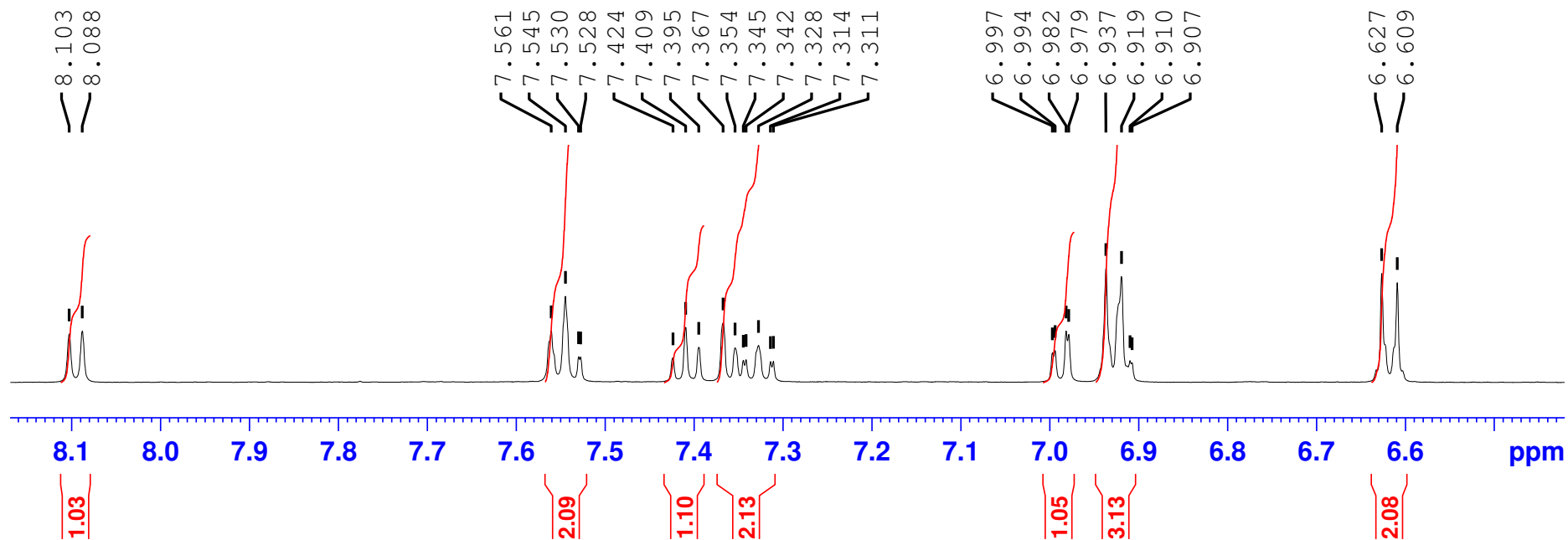
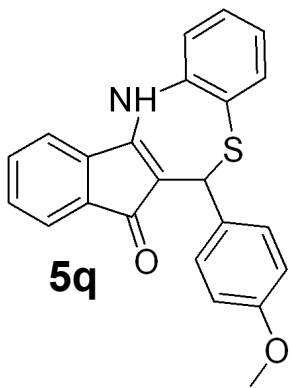
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.276	BV R	0.1073	23.01365	2.90744	0.1781
2	16.757	BB	0.1236	123.40454	13.38598	0.9551
3	17.313	BV R	0.1104	30.63163	3.66825	0.2371
4	18.024	BB	0.0821	10.32845	1.80940	0.0799

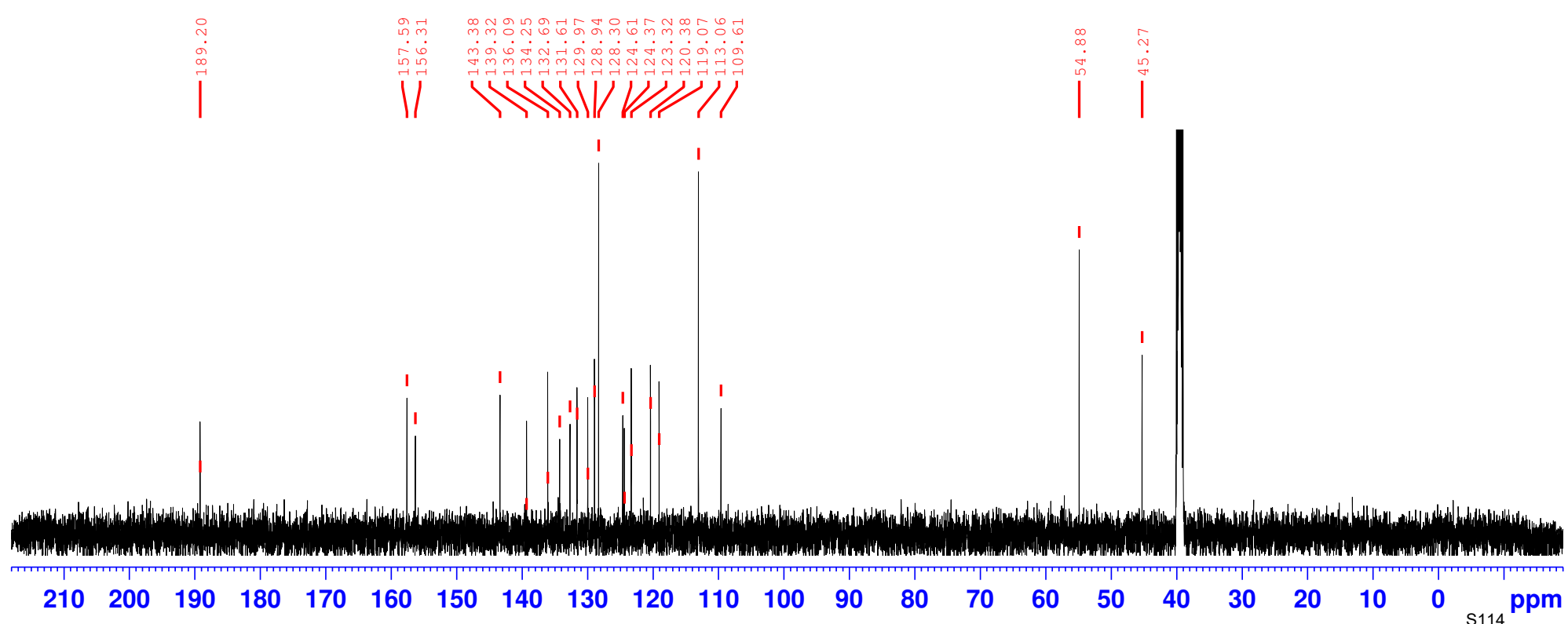
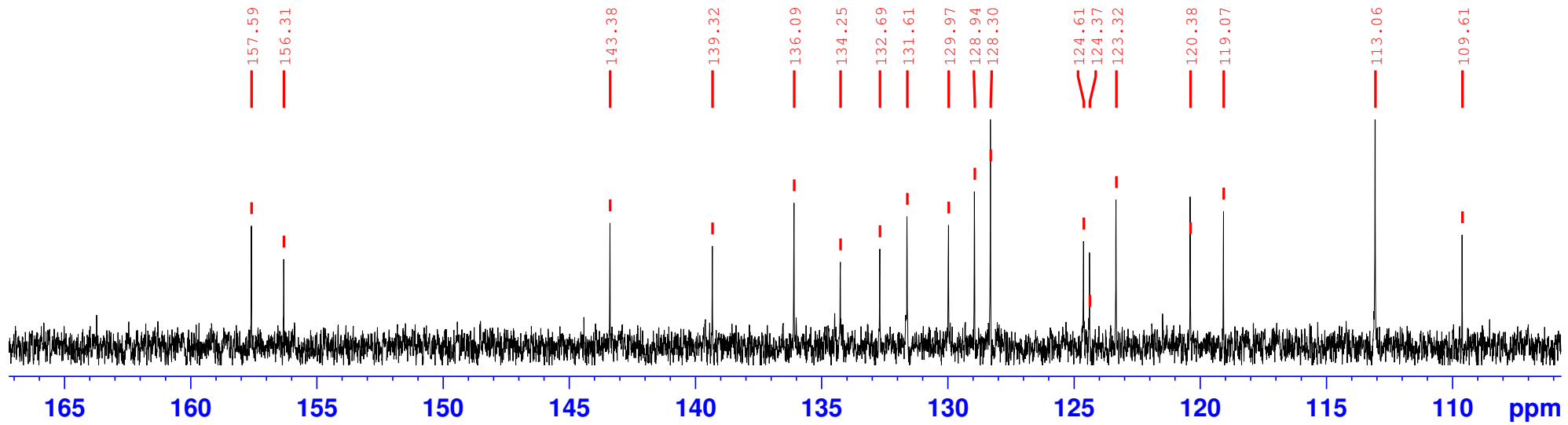
Sample Name: LJC 1-66

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	18.617	BB	0.0908	1.25792e4	1912.12598	97.3583
6	19.818	VB	0.0716	12.29644	2.48906	0.0952
7	20.915	BV	0.1053	52.01048	6.60877	0.4025
8	21.006	VV	0.0569	10.83188	2.81351	0.0838
9	21.182	VB	0.0808	15.29596	2.53902	0.1184
10	22.070	VB	0.0617	10.96301	2.76688	0.0848
11	23.087	VV	0.1879	28.83754	1.92394	0.2232
12	23.236	VB	0.1502	23.70951	1.95954	0.1835

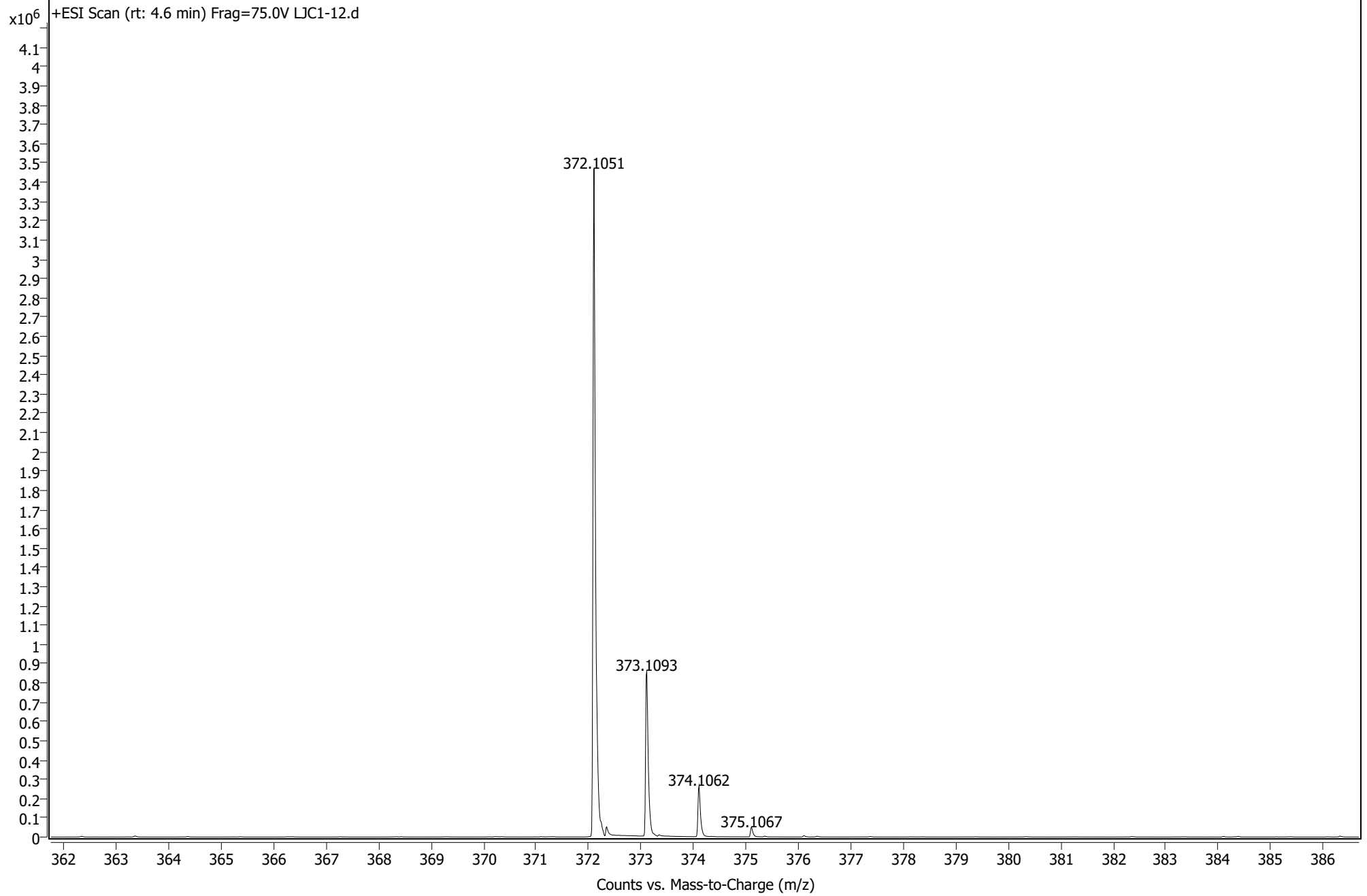
Totals : 1.29205e4 1954.99777

=====
*** End of Report ***





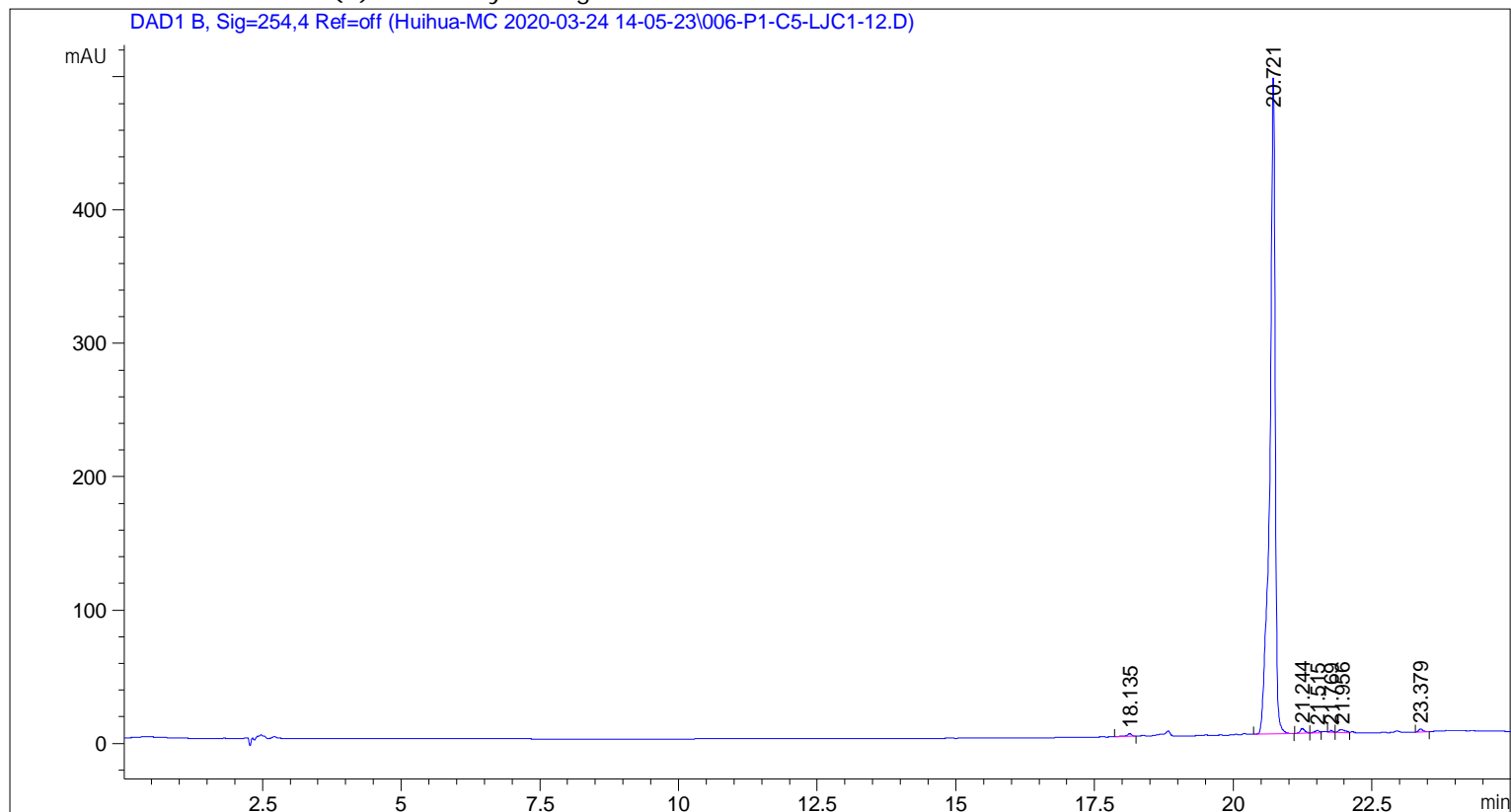
User Spectrum Plot Report



```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    6
Sample Operator : SYSTEM
Acq. Instrument : 1260Infinity2              Location  : P1-C-05
Injection Date  : 3/24/2020 4:14:01 PM       Inj       :    1
                                           Inj Volume: 50.000 µl

Method          : C:\Users\Public\Documents\ChemStation\1\Data\Huihua-MC 2020-03-24 14-05-23
                  \MC-SMALL MOLE.M (Sequence Method)
Last changed    : 2/19/2020 11:54:04 AM by SYSTEM
Additional Info  : Peak(s) manually integrated
  
```



=====
 Area Percent Report
 =====

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.135	BB	0.0924	12.62685	1.97890	0.3720
2	20.721	BB	0.0964	3318.05762	493.63647	97.7501
3	21.244	BB	0.0809	18.55090	3.44157	0.5465
4	21.515	BV	0.0808	9.00642	1.67240	0.2653
5	21.769	VB	0.0699	6.11392	1.32217	0.1801
6	21.956	BV	0.1342	19.27714	2.15768	0.5679
7	23.379	BB	0.0743	10.79699	2.23928	0.3181

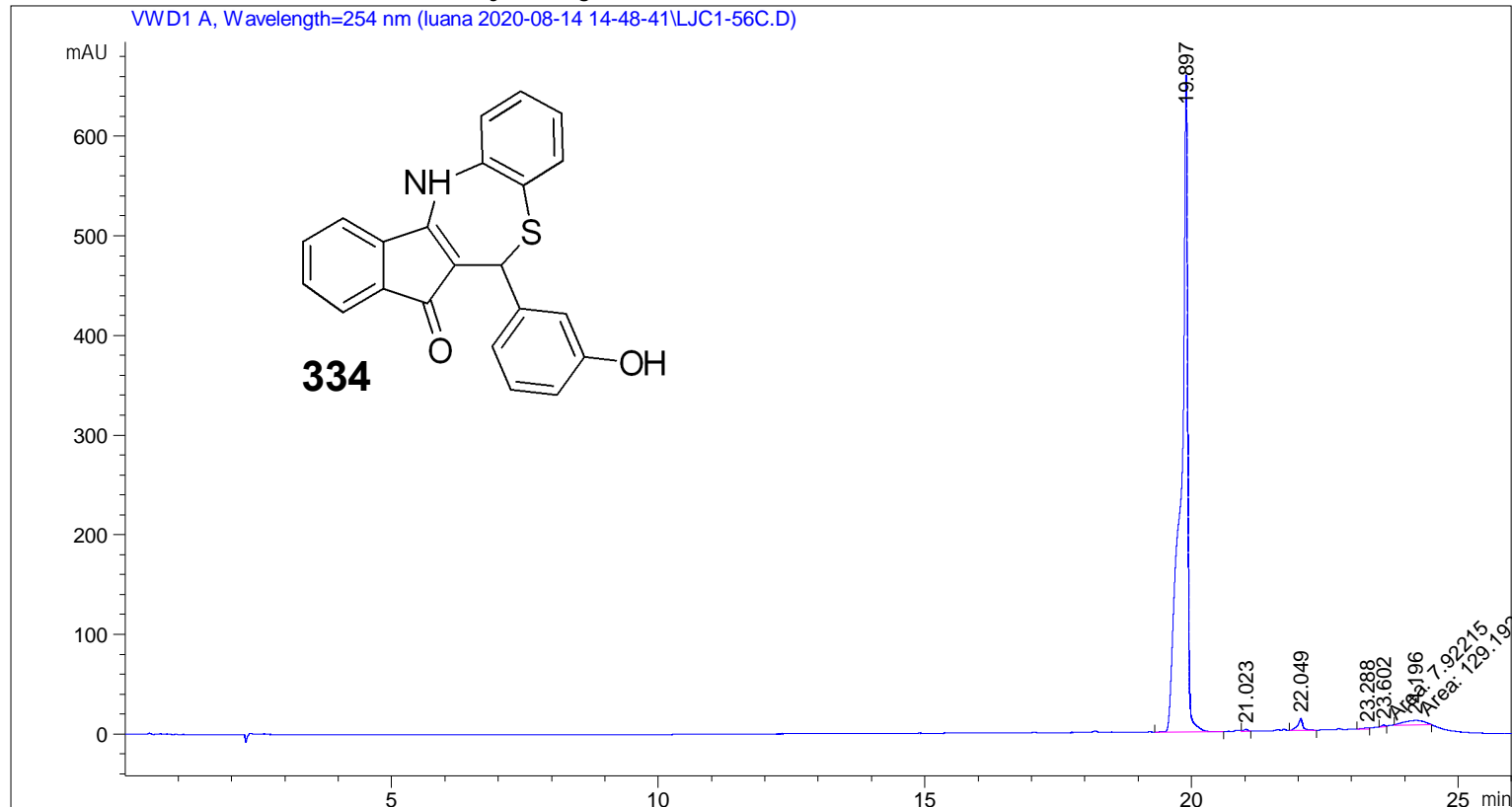
Sample Name: LJC1-56C

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    7
Acq. Instrument : 1220 HPLC                   Location  :   46
Injection Date  : 8/14/2020 5:35:56 PM      Inj       :    1
                                           Inj Volume: 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-08-14 14-48-41\MOHAMED-SMALL MOLECULE.M (
                : Sequence Method)
Last changed    : 8/14/2020 2:48:44 PM by SYSTEM
Sample Info     : LJC1-56C
=====

```

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====

```

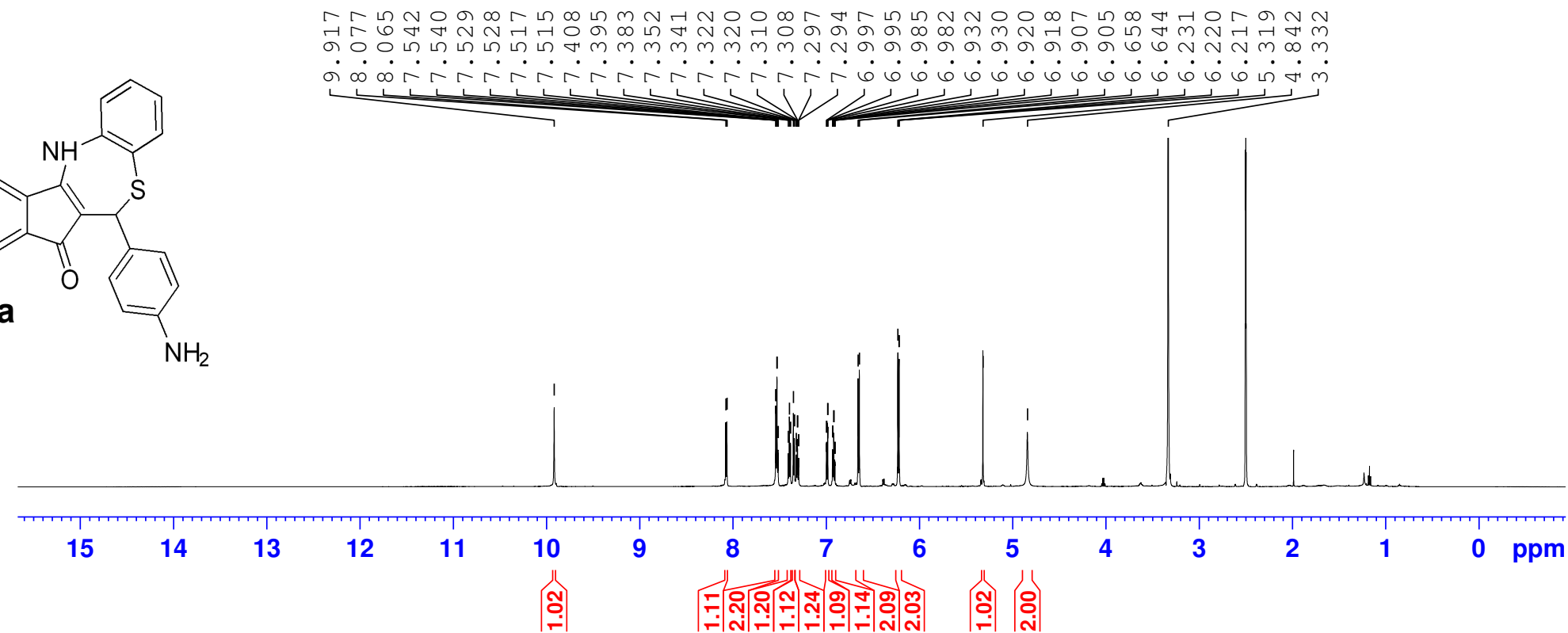
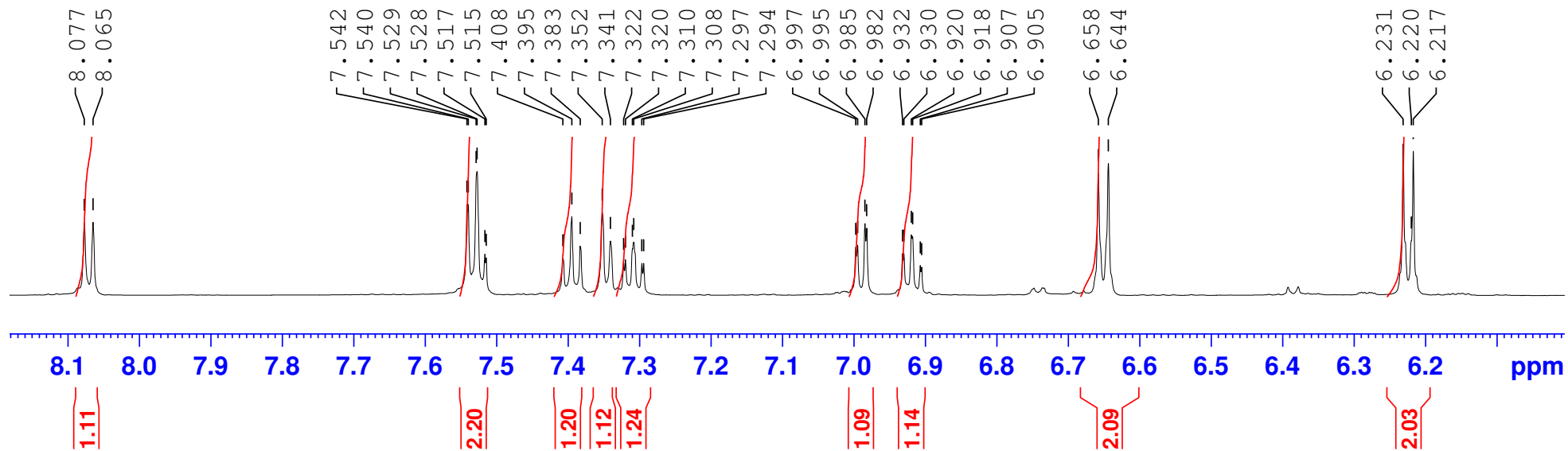
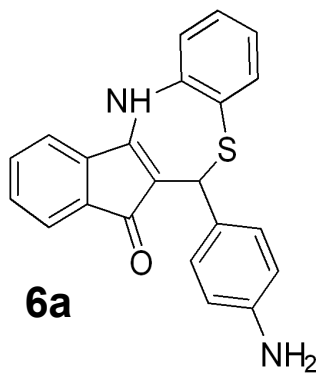
```

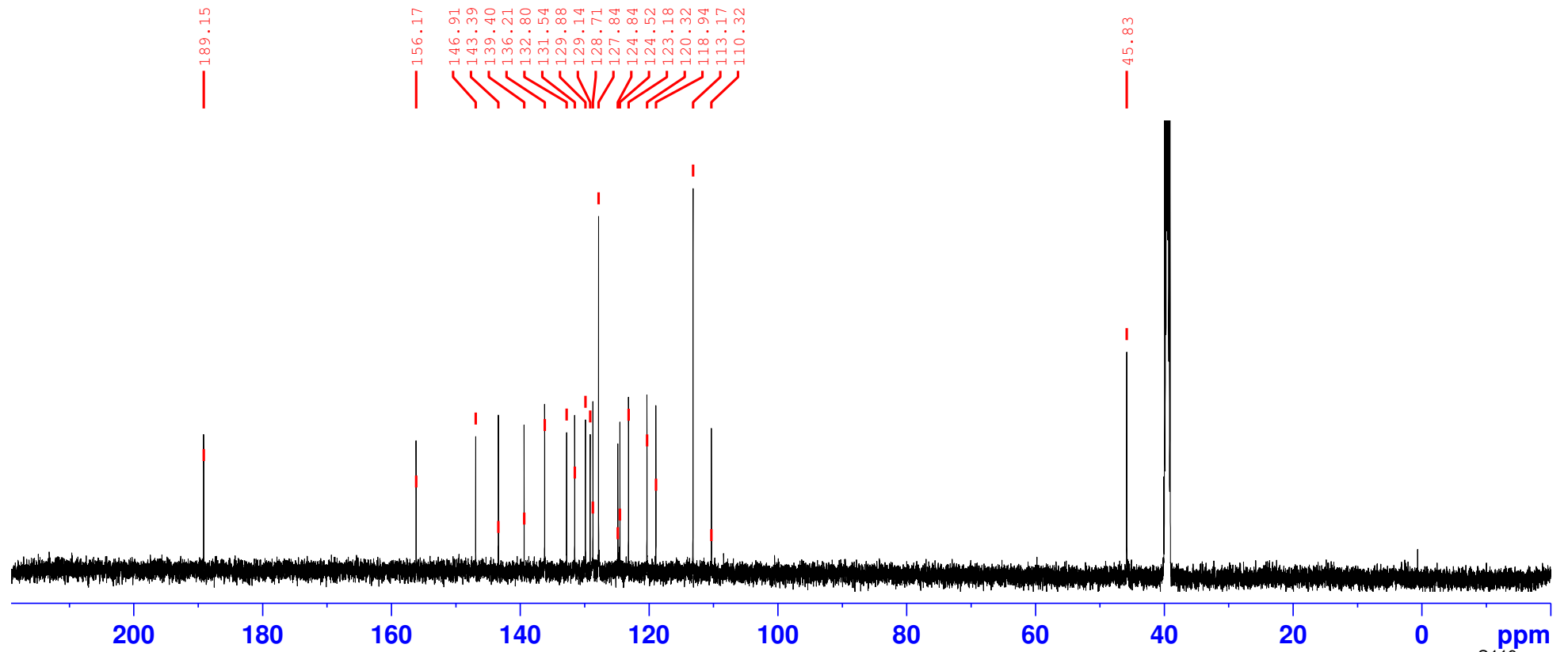
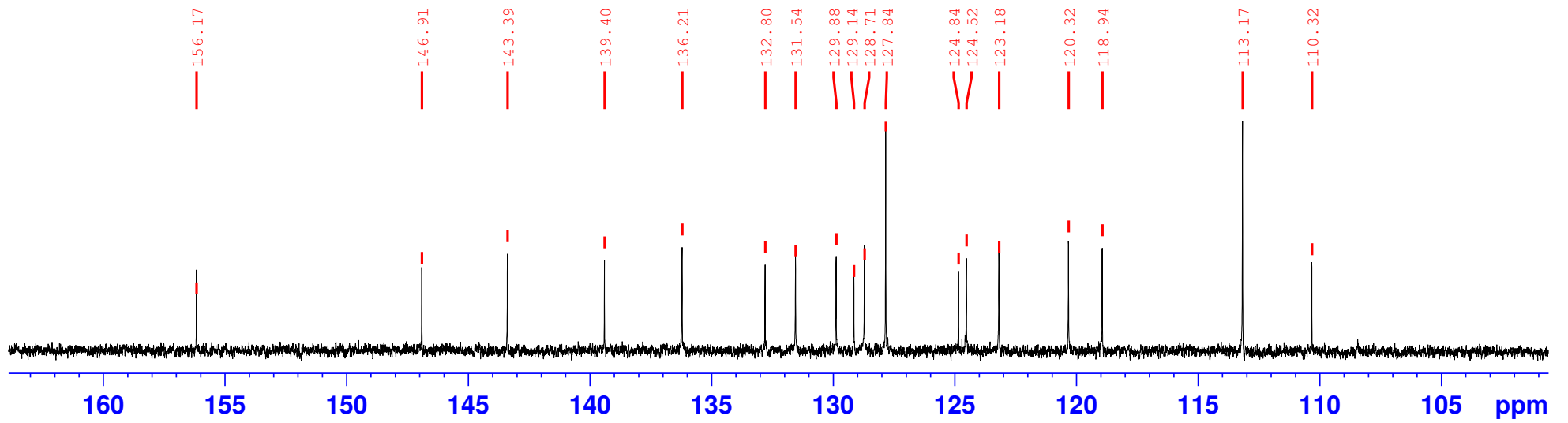
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

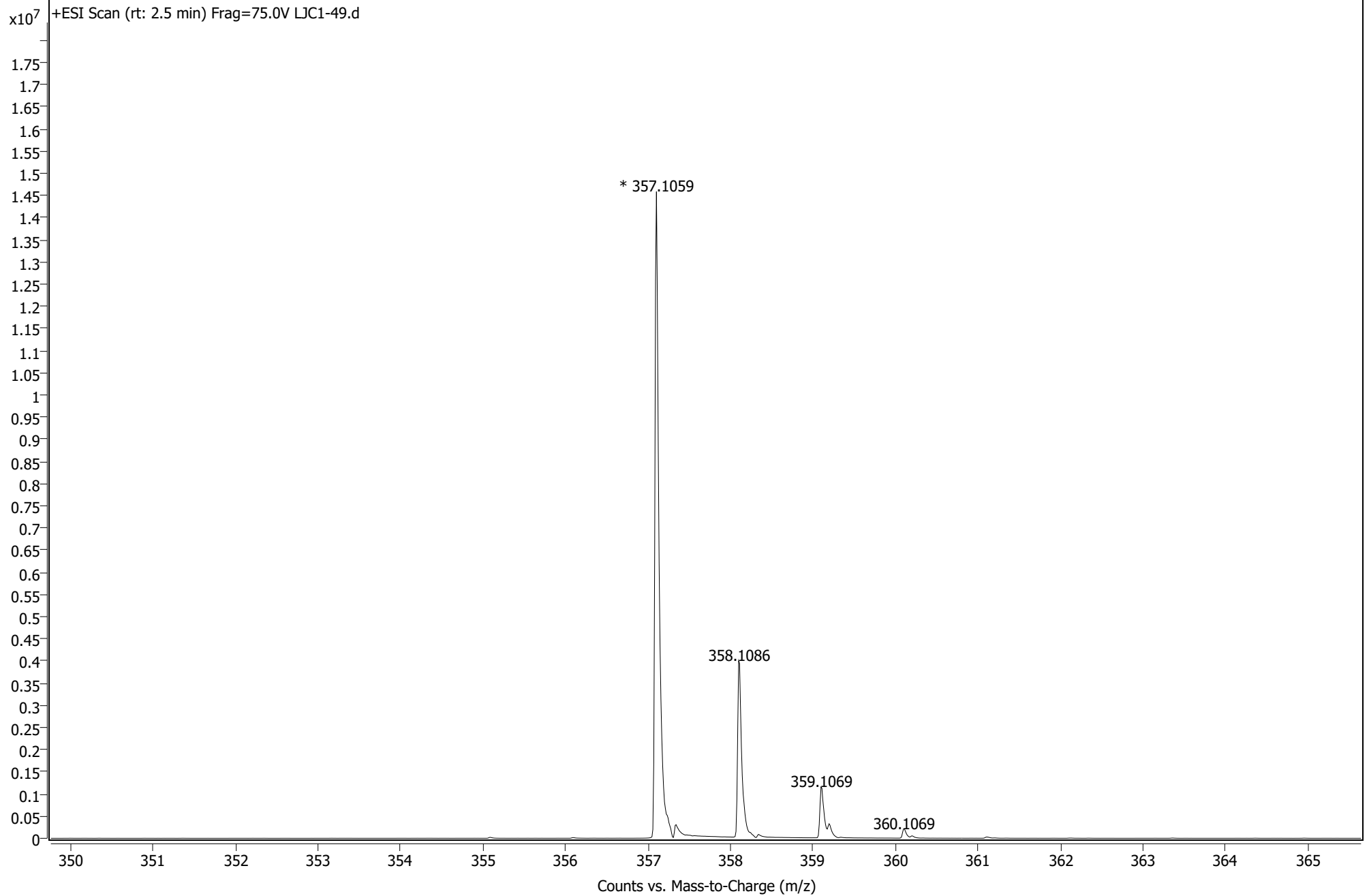
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.897	BV R	0.1140	5621.10010	659.25385	95.8936
2	21.023	VB	0.0778	10.87987	1.97471	0.1856
3	22.049	BB	0.0921	80.39686	11.93002	1.3715
4	23.288	BV	0.0913	12.31616	1.72462	0.2101
5	23.602	MM	0.0557	7.92215	1.70286	0.1351
6	24.196	MM	0.4624	129.19249	4.65623	2.2040





User Spectrum Plot Report

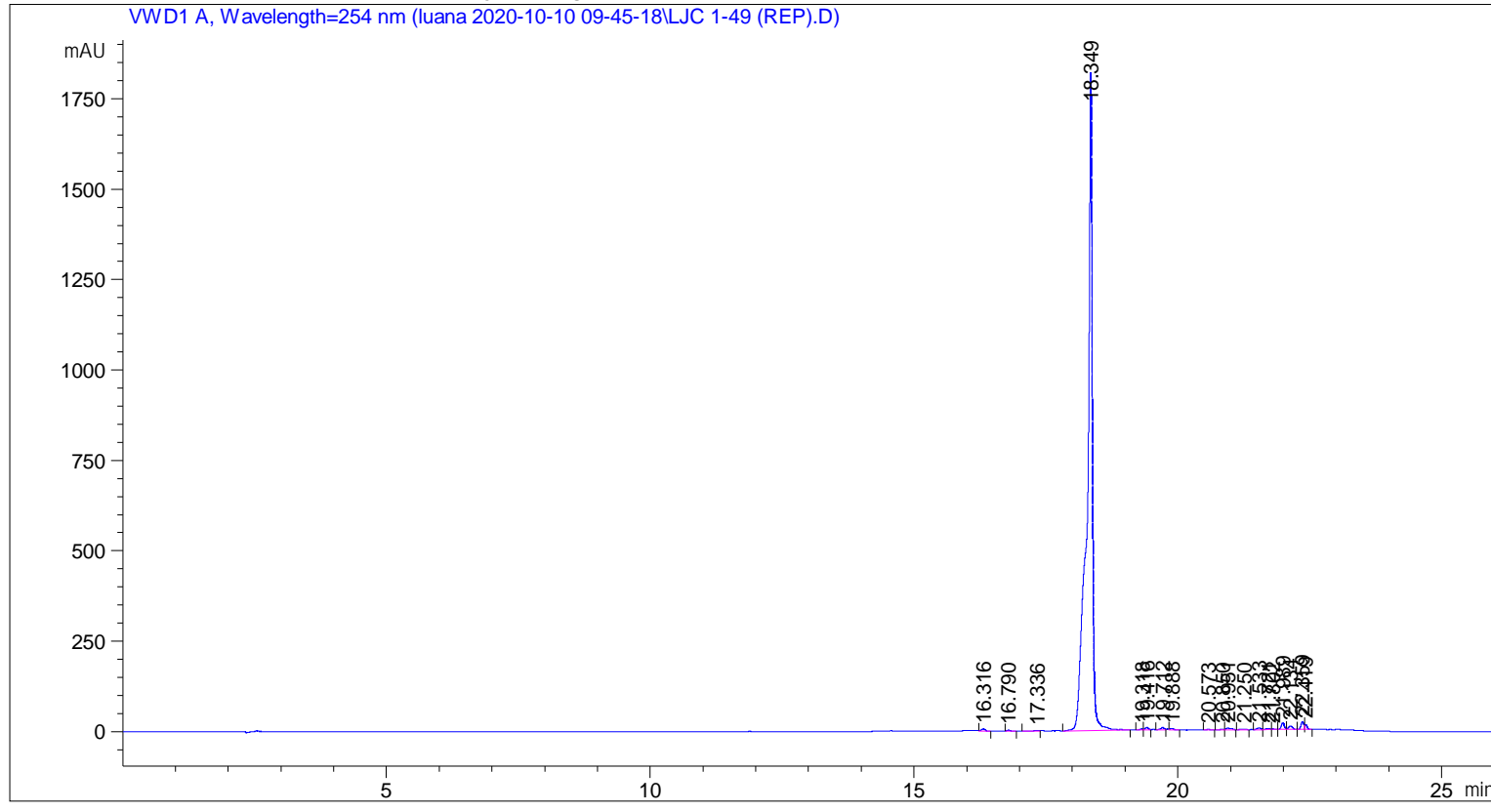



```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    4
Acq. Instrument : 1220 HPLC                   Location  :   12
Injection Date  : 10/10/2020 11:07:59 AM    Inj       :    1
                                           Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-10-10 09-45-18\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 10/10/2020 10:17:41 AM by SYSTEM
Method Info     : Water/MeOH

Sample Info     : LJC 1-49 (REP)
  
```

Additional Info : Peak(s) manually integrated



Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

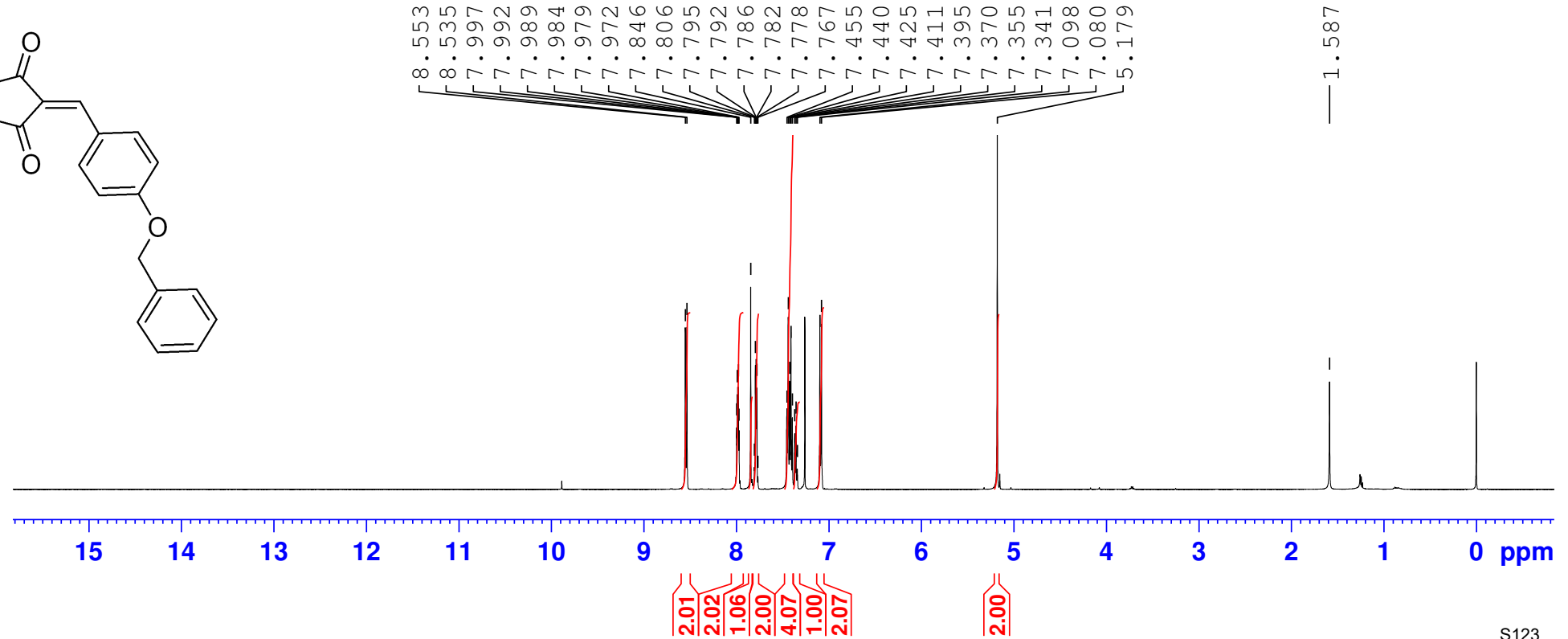
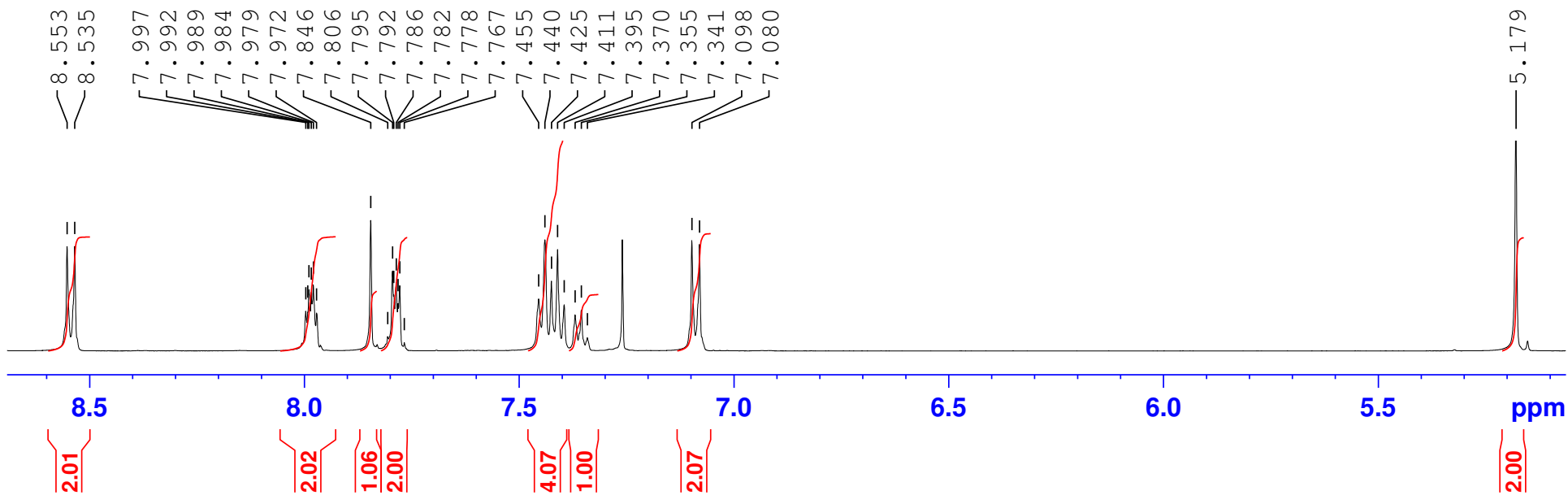
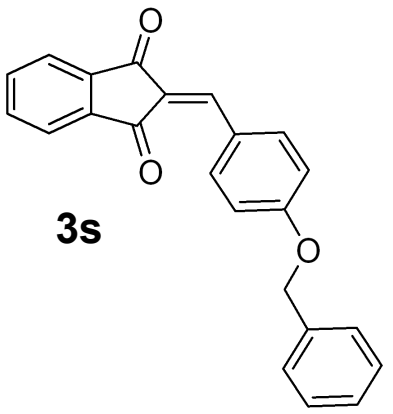
Signal 1: VWD1 A, Wavelength=254 nm

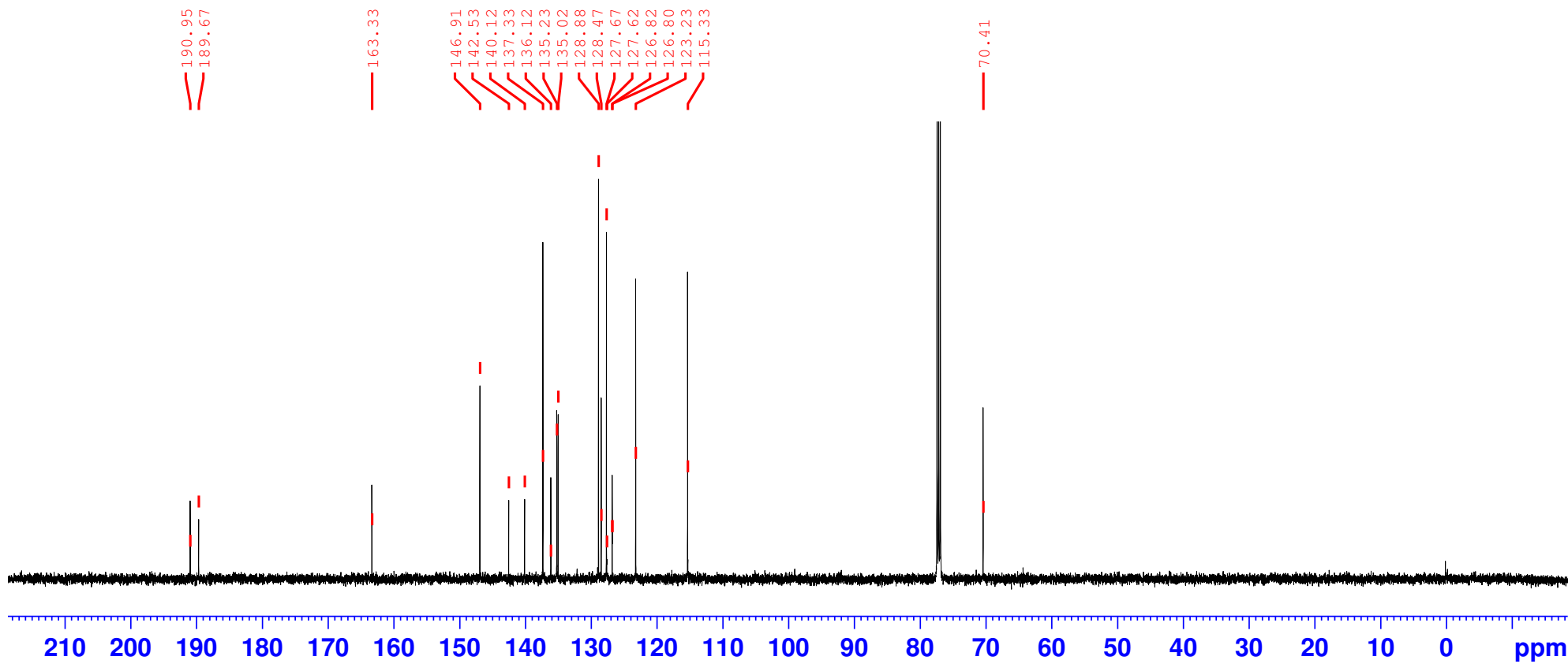
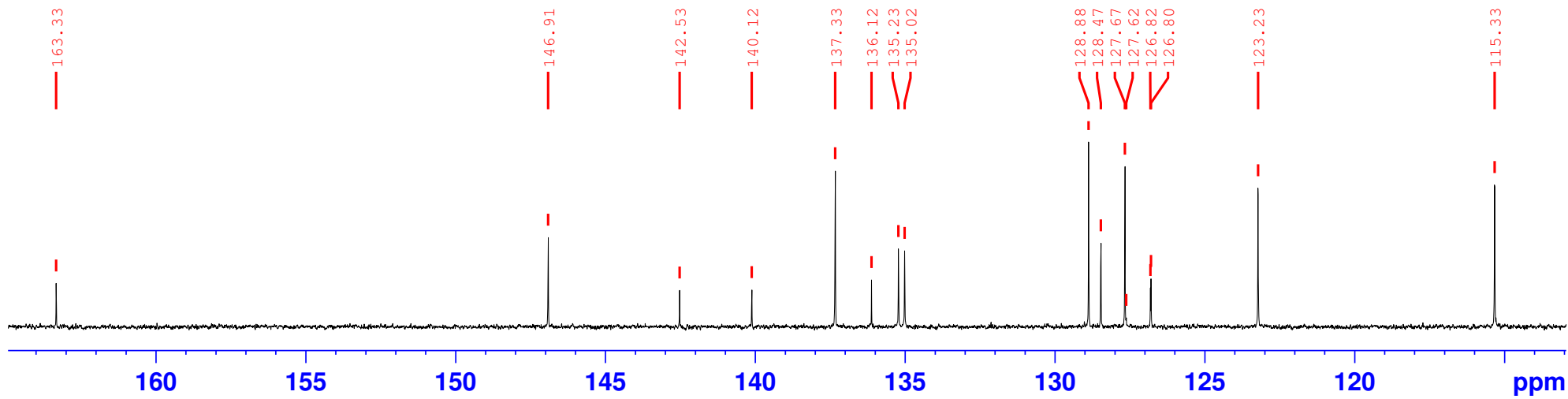
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.316	VB	0.0731	33.68761	6.71122	0.2624
2	16.790	VB	0.0623	12.18611	2.82564	0.0949
3	17.336	BV	0.0886	14.37601	2.04325	0.1120
4	18.349	BV R	0.0925	1.23141e4	1818.99268	95.9297

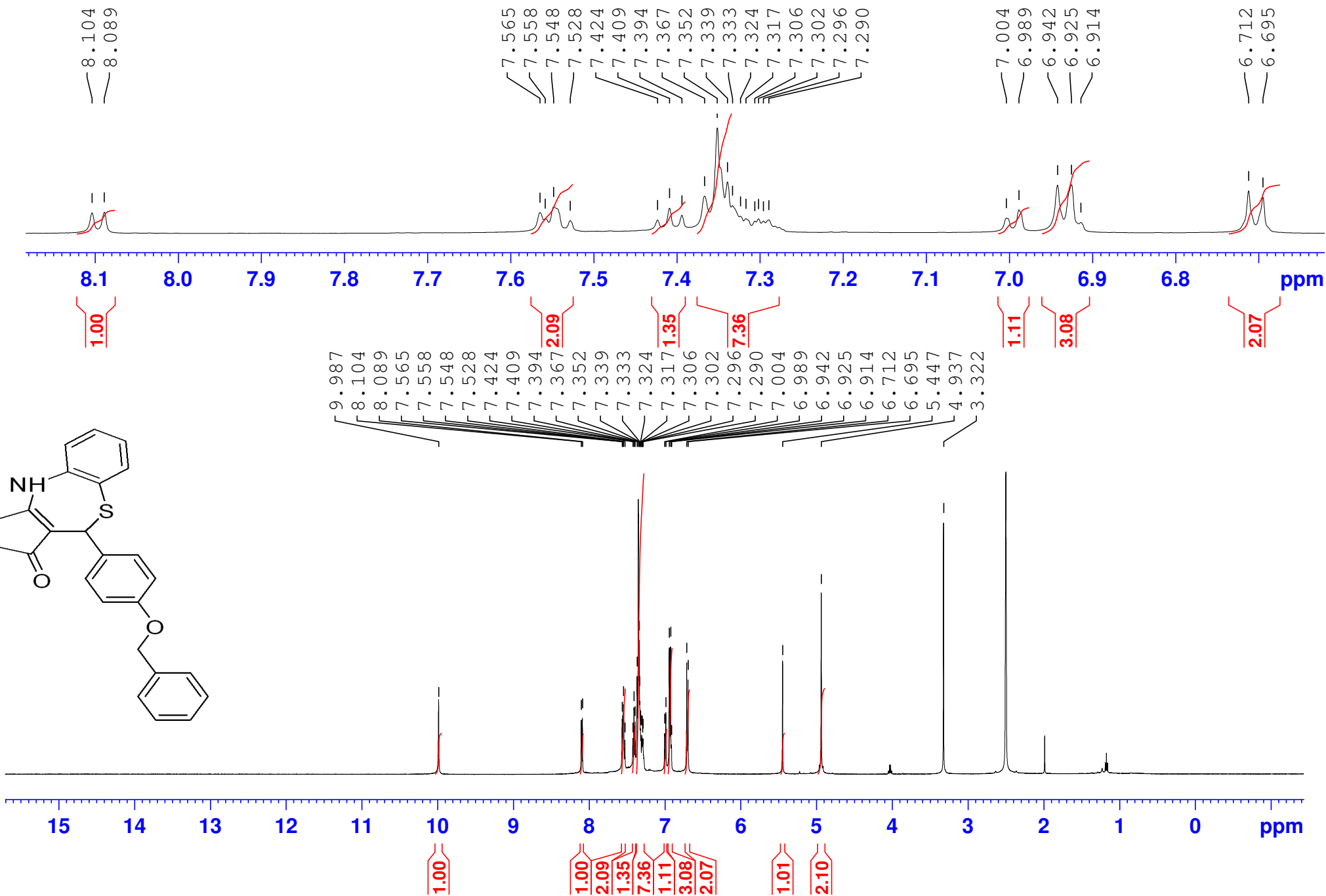
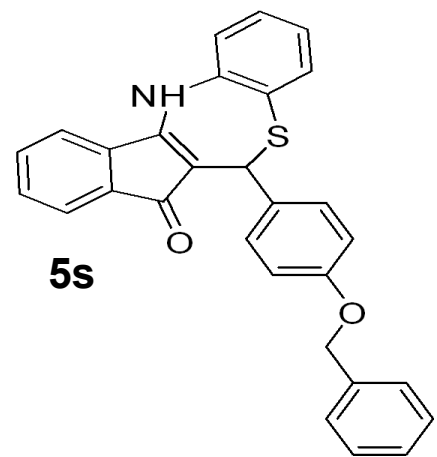
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	19.318	BV	0.0608	11.02094	2.58219	0.0859
6	19.416	VB	0.0648	29.12417	6.75608	0.2269
7	19.712	BV	0.0683	30.73411	6.60910	0.2394
8	19.888	VB	0.0768	19.16901	3.67528	0.1493
9	20.573	BB	0.0868	11.55071	1.97284	0.0900
10	20.850	BV	0.0754	12.73168	2.32569	0.0992
11	20.951	VB	0.1000	34.59518	4.61496	0.2695
12	21.250	BB	0.0961	13.58049	1.88486	0.1058
13	21.533	BV	0.0750	22.20419	4.54770	0.1730
14	21.721	VV	0.0848	17.24193	2.80103	0.1343
15	21.802	VB	0.0613	7.38845	1.73026	0.0576
16	21.989	BV	0.0623	75.02545	18.49339	0.5845
17	22.134	VB	0.0832	51.91785	9.90196	0.4045
18	22.359	BV	0.0558	82.77595	22.03440	0.6448
19	22.419	VB	0.0483	43.17870	13.51973	0.3364

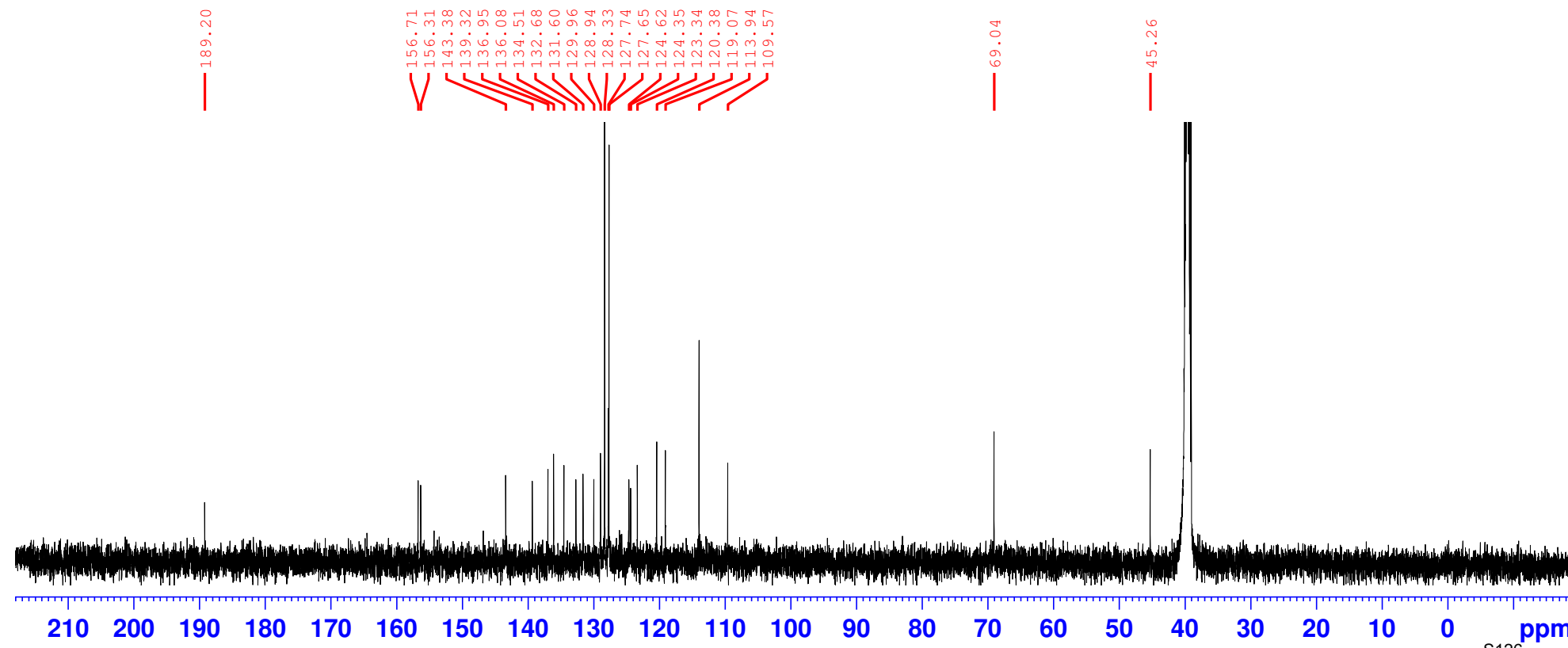
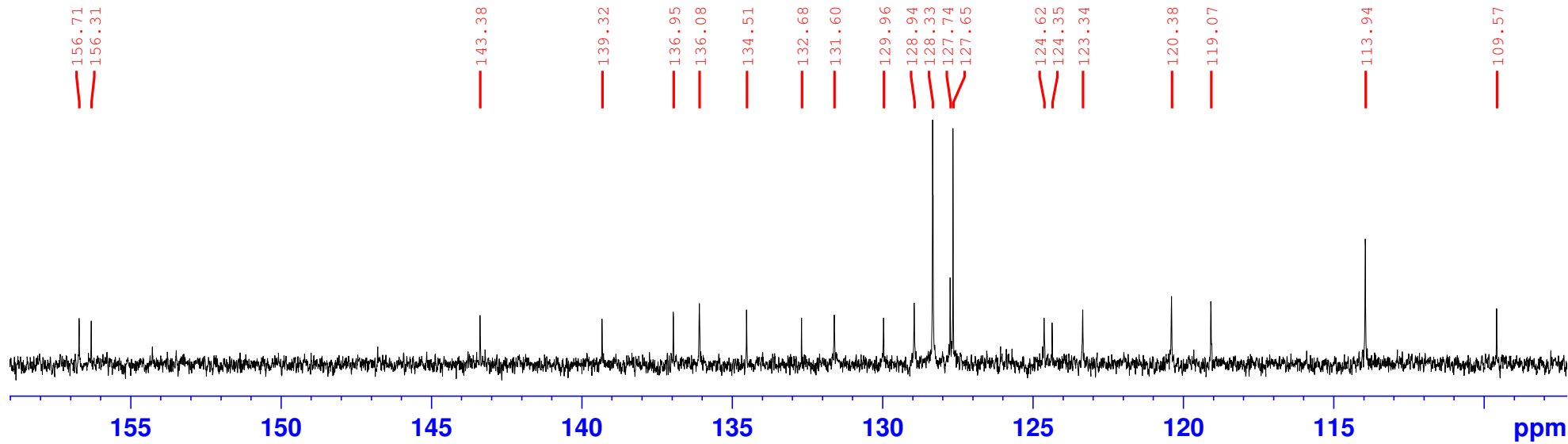
Totals : 1.28366e4 1934.02222

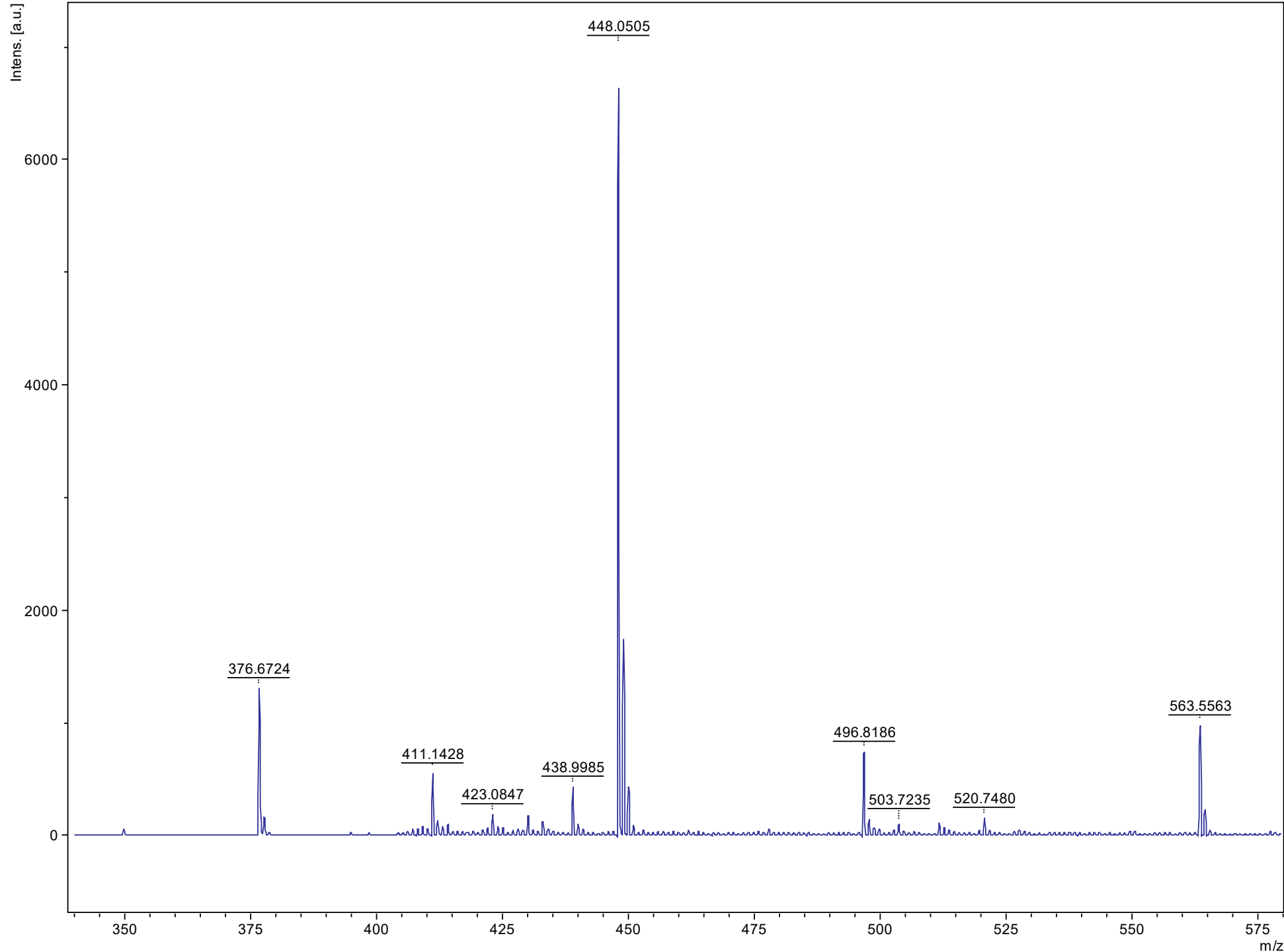
=====
*** End of Report ***









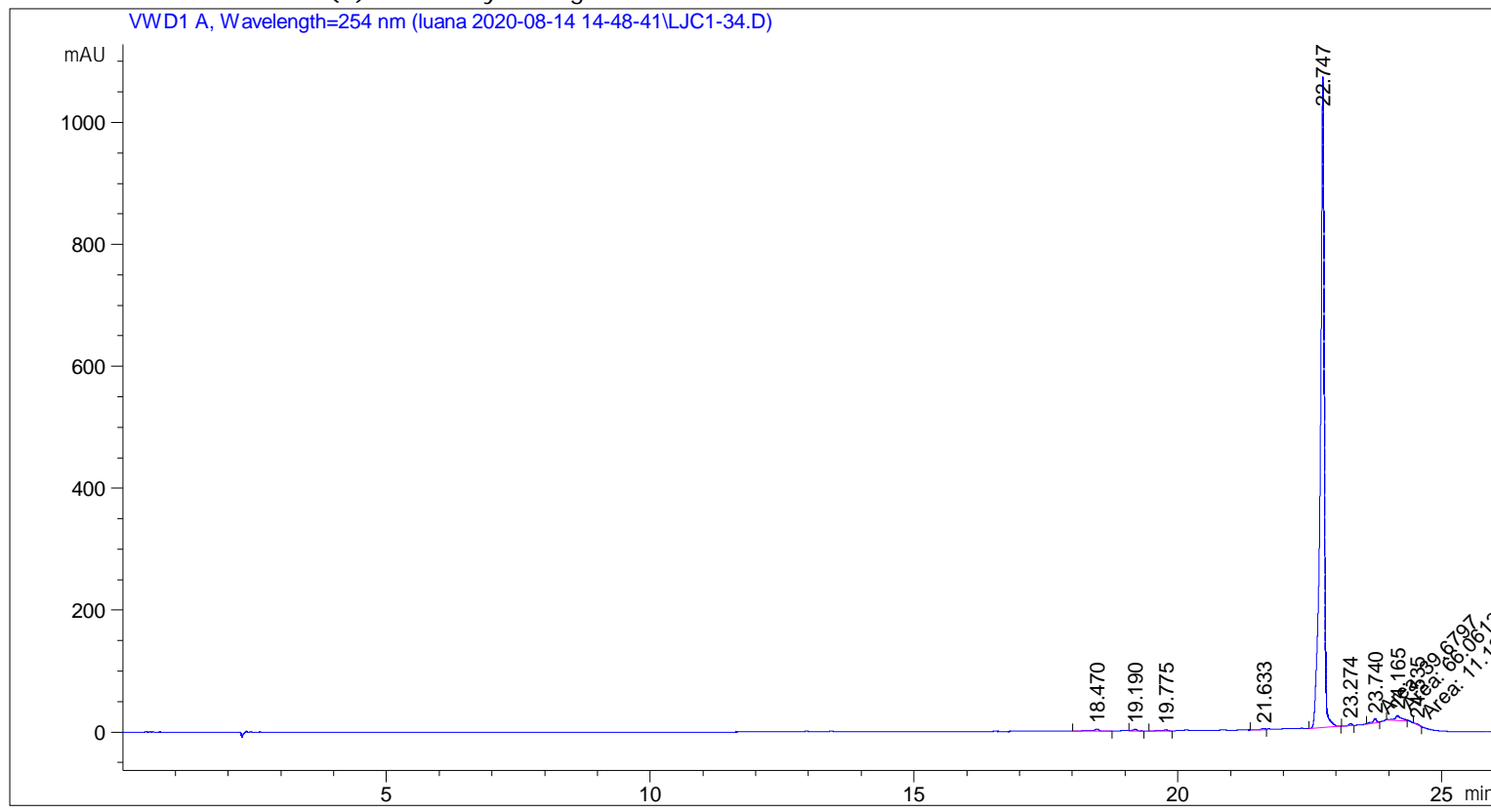


Sample Name: LJC1-34

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    3
Acq. Instrument : 1220 HPLC                   Location  :   43
Injection Date  : 8/14/2020 3:45:59 PM      Inj       :    1
                                           Inj Volume: 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-08-14 14-48-41\MOHAMED-SMALL MOLECULE.M (
                : Sequence Method)
Last changed    : 8/14/2020 2:48:44 PM by SYSTEM
Sample Info     : LJC1-34
    
```

Additional Info : Peak(s) manually integrated



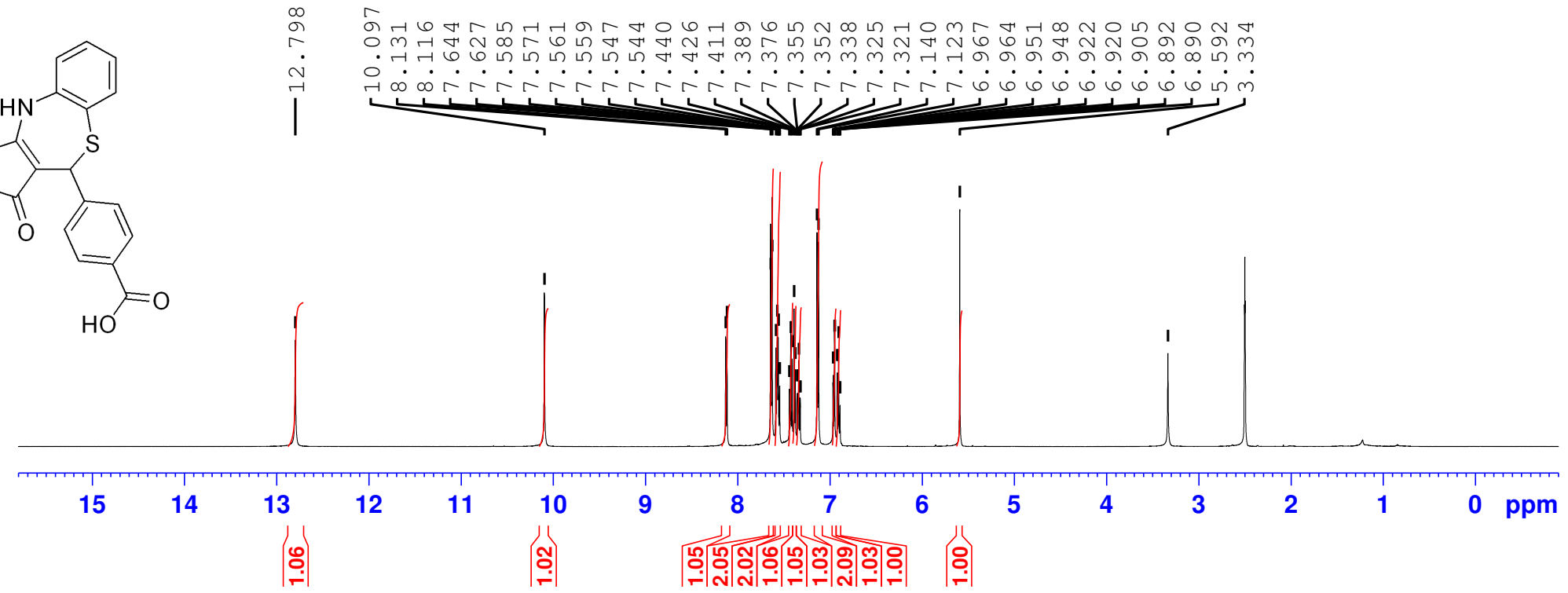
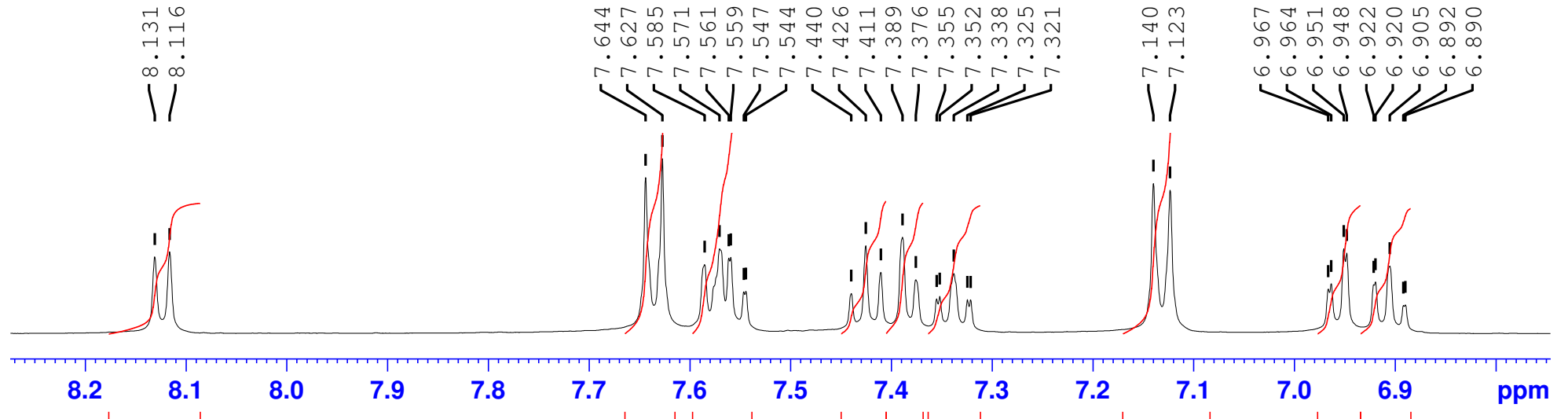
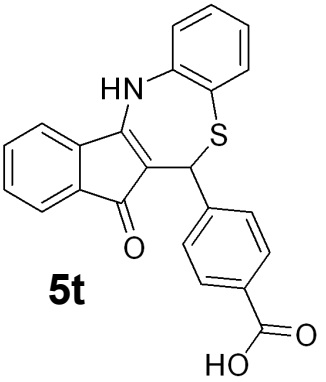
Area Percent Report

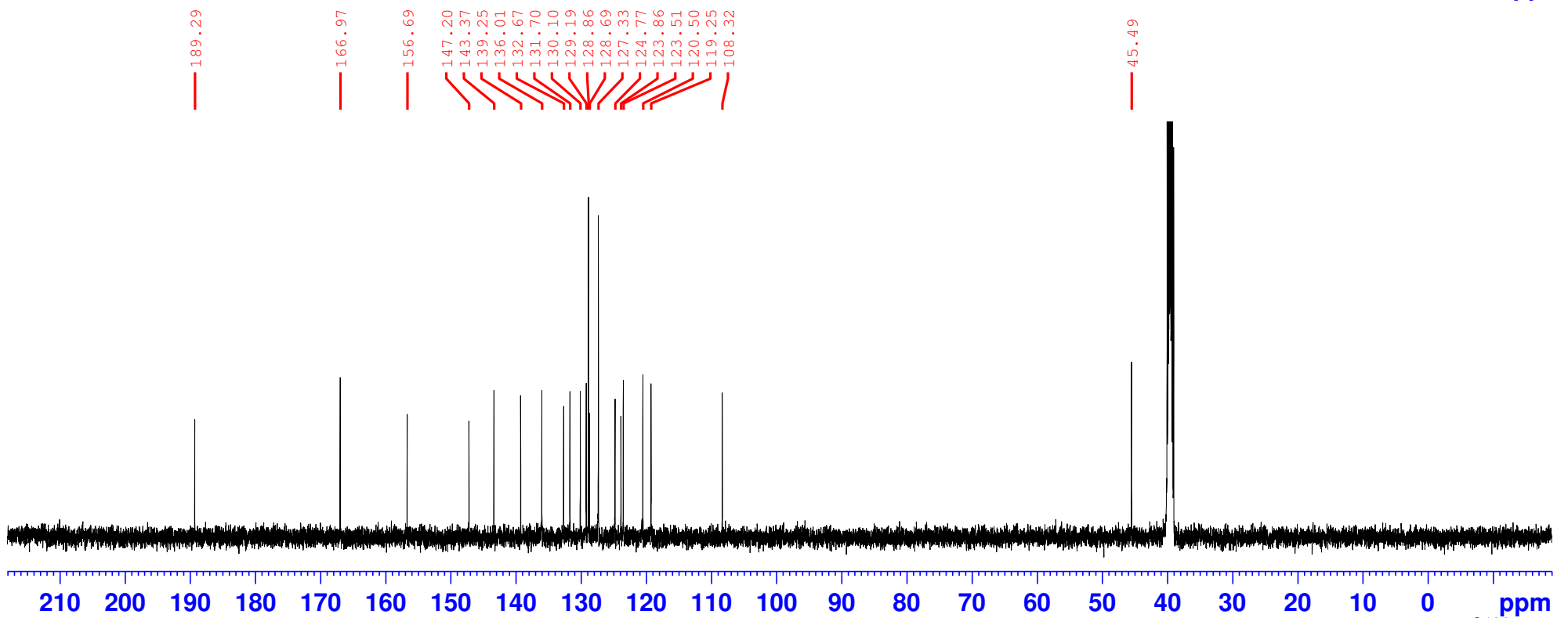
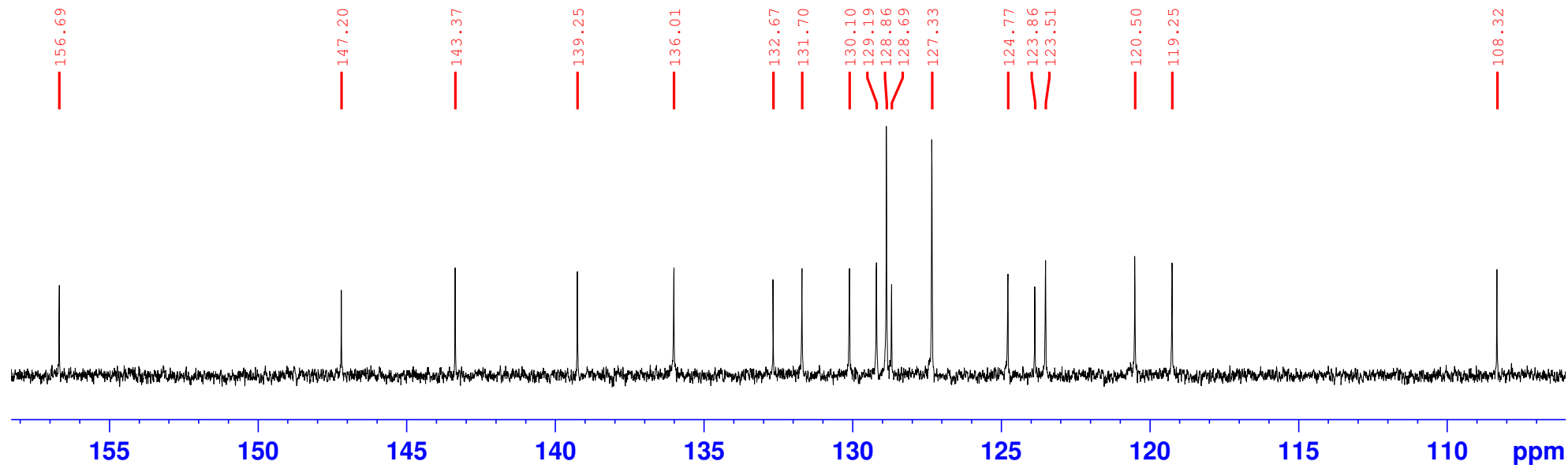
```

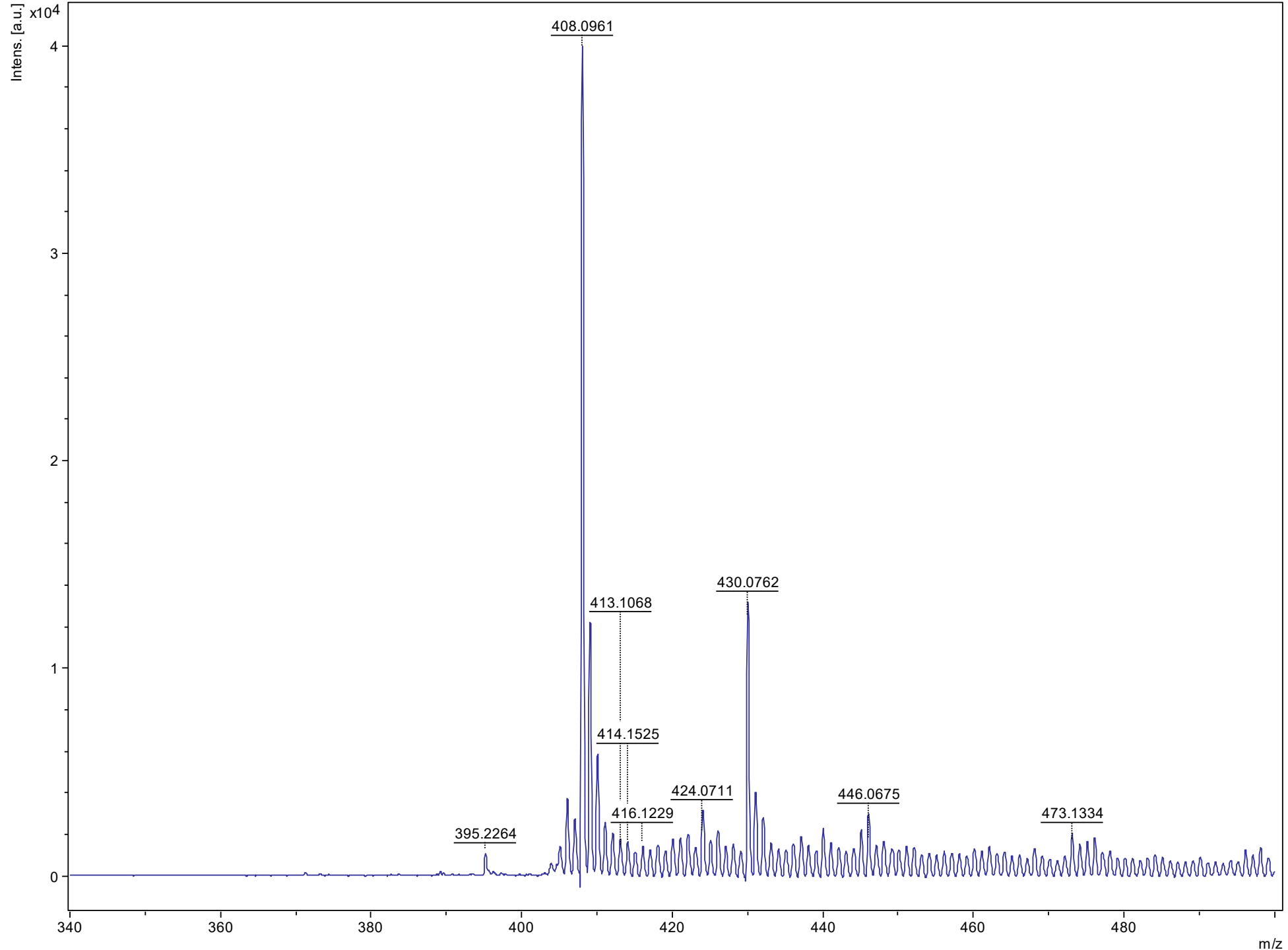
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.470	BV R	0.1257	33.29604	3.47731	0.5814
2	19.190	VV R	0.0837	17.15664	2.66021	0.2996
3	19.775	BB	0.0916	12.17624	1.72954	0.2126
4	21.633	BV	0.0753	11.09774	1.82887	0.1938
5	22.747	BB	0.0744	5522.29590	1066.95020	96.4195
6	23.274	VB R	0.0668	14.47833	3.19846	0.2528
7	23.740	MM	0.0897	39.67970	7.37479	0.6928





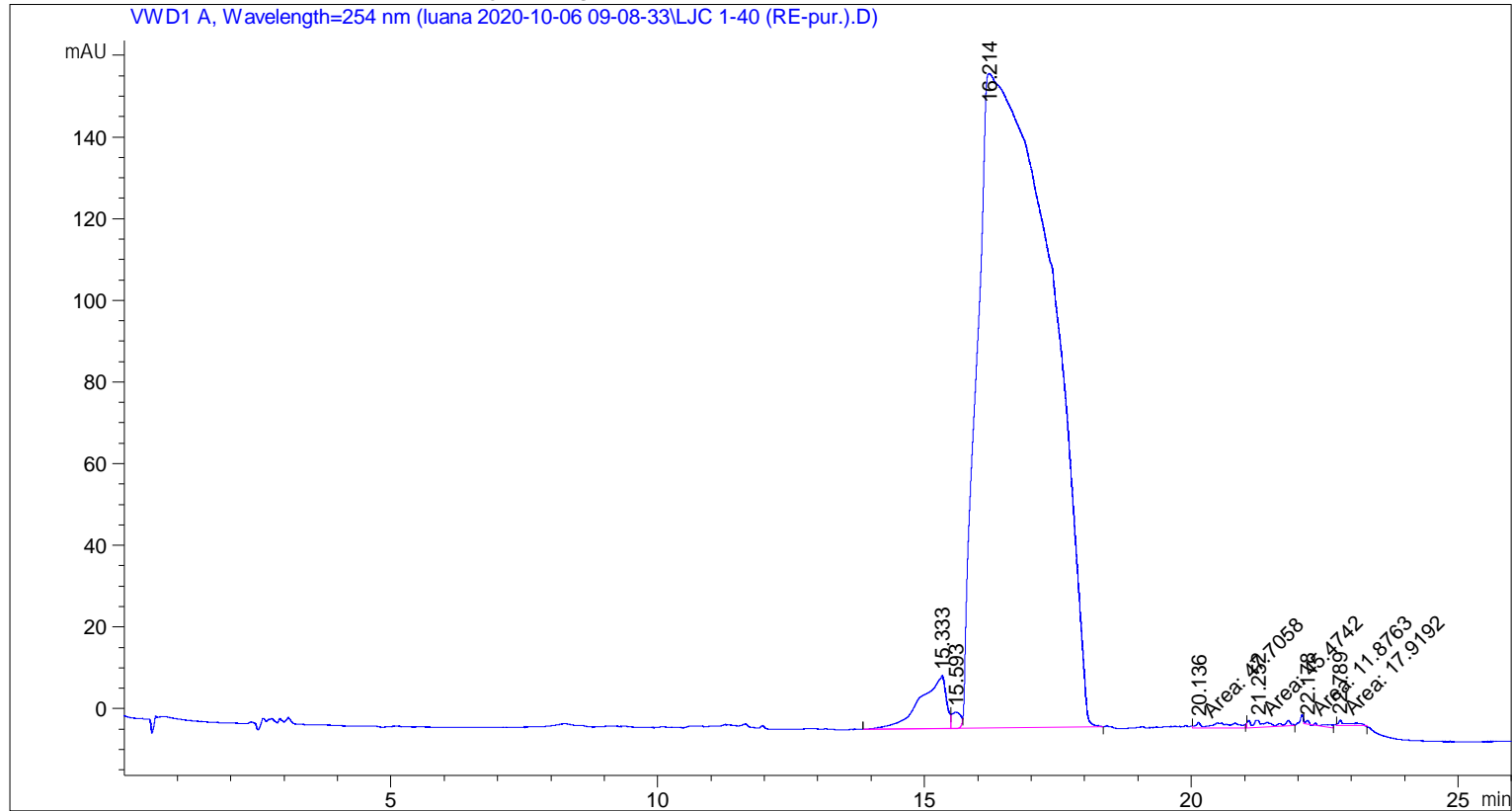


```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    1
Acq. Instrument : 1220 HPLC                   Location  :    7
Injection Date  : 10/6/2020 9:10:13 AM       Inj       :    1
                                           Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-10-06 09-08-33\MOHAMED-SMALL MOLECULE.M (
                : Sequence Method)
Last changed    : 10/6/2020 9:08:37 AM by SYSTEM
Method Info     : Water/MeOH

Sample Info     : LJC 1-40 (RE-pur.)
  
```

Additional Info : Peak(s) manually integrated



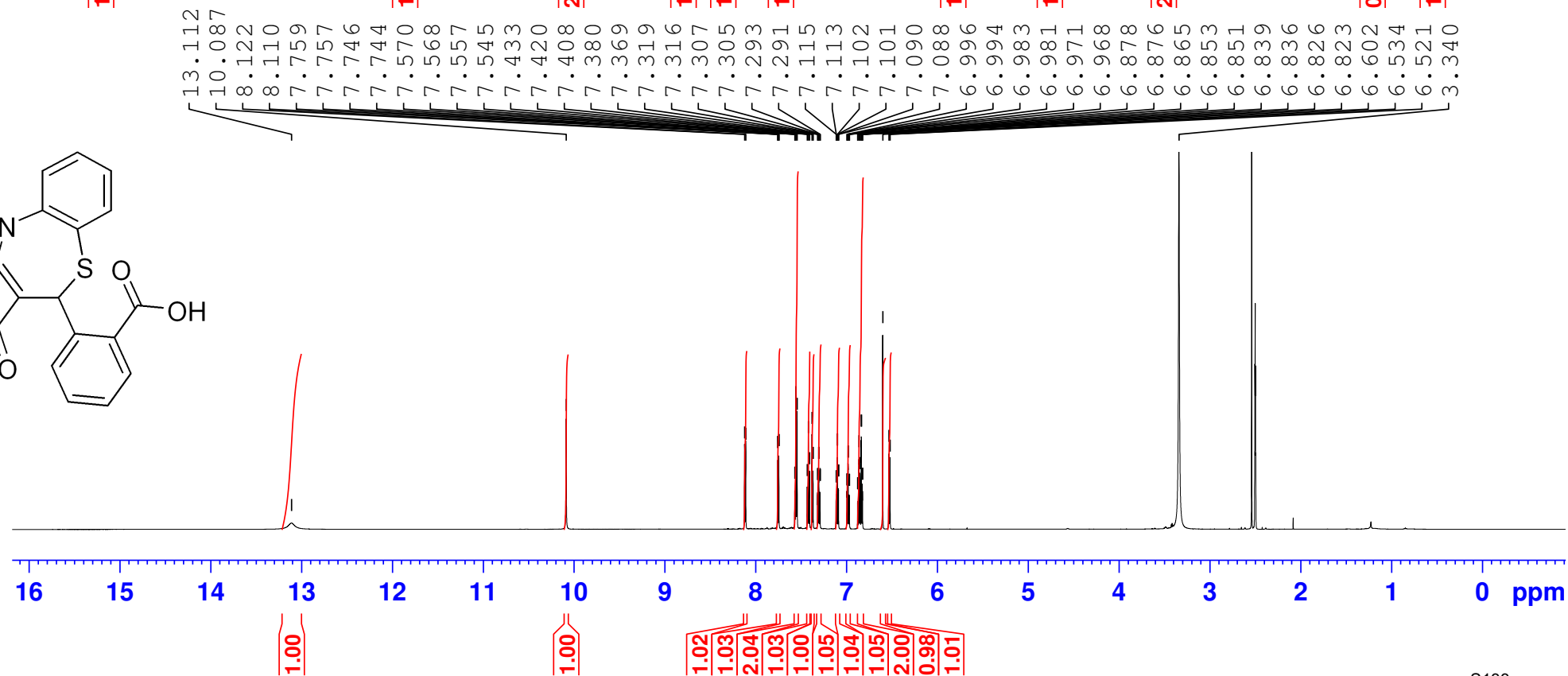
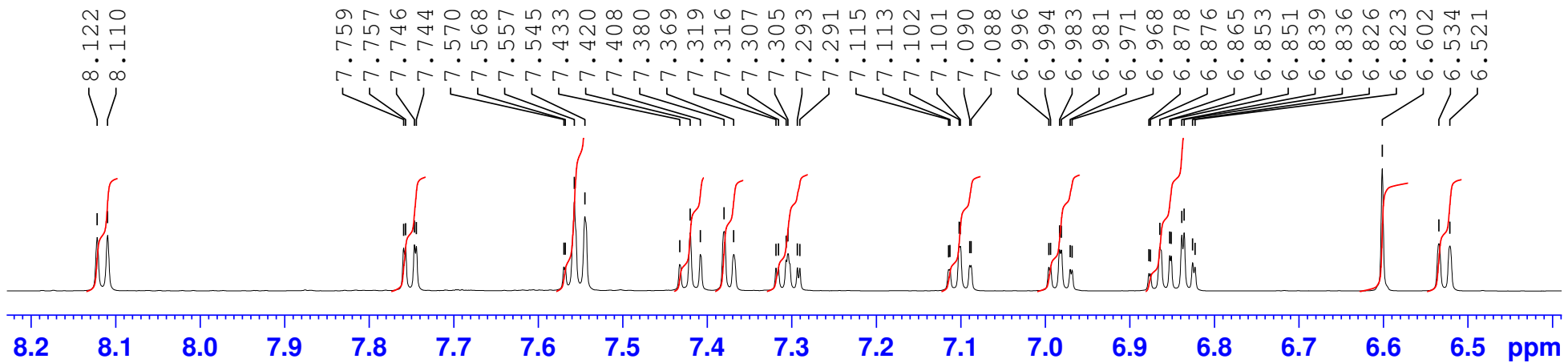
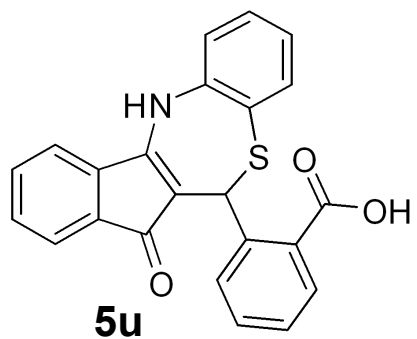
Area Percent Report

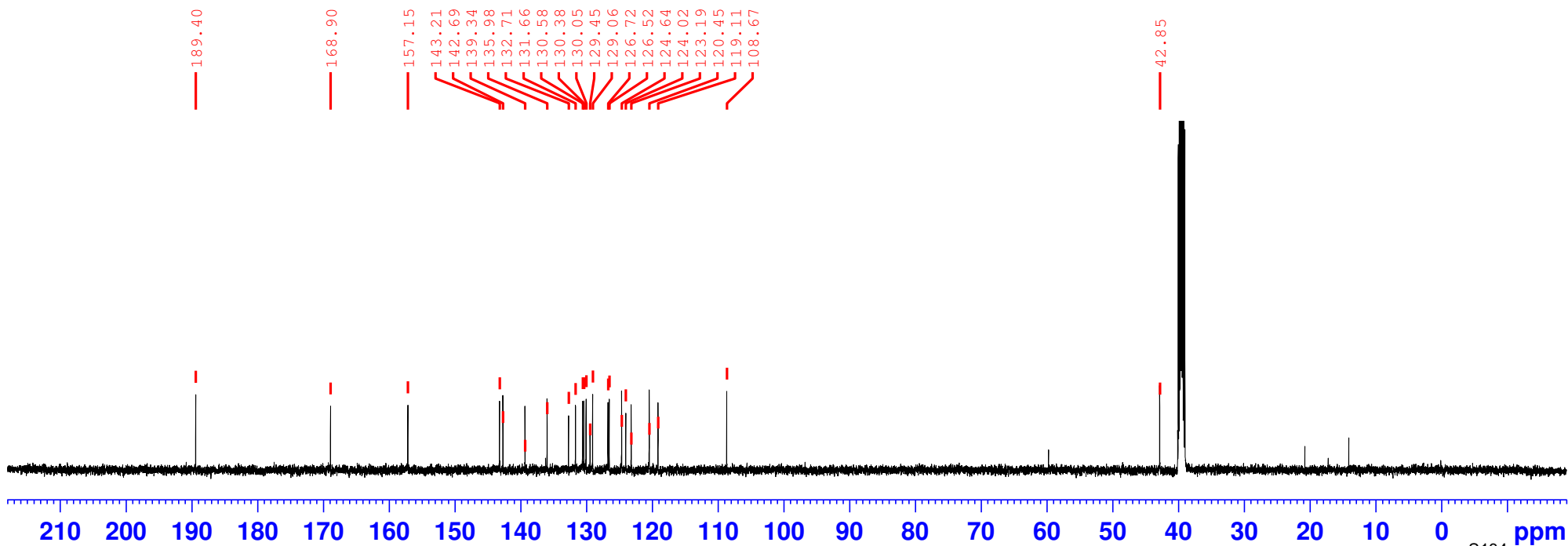
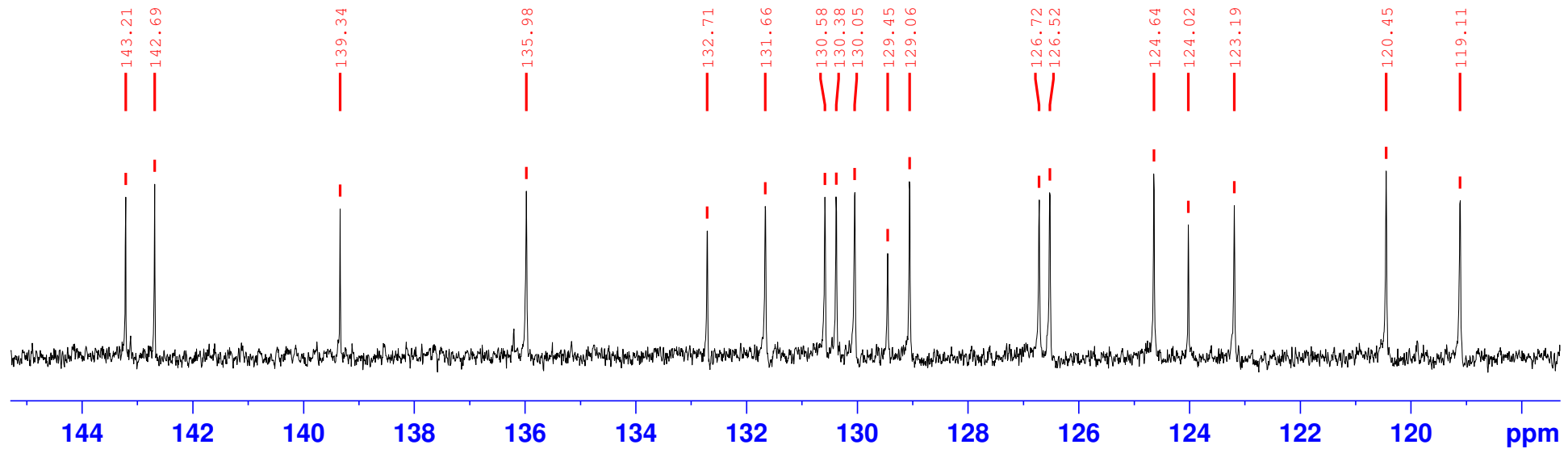
```

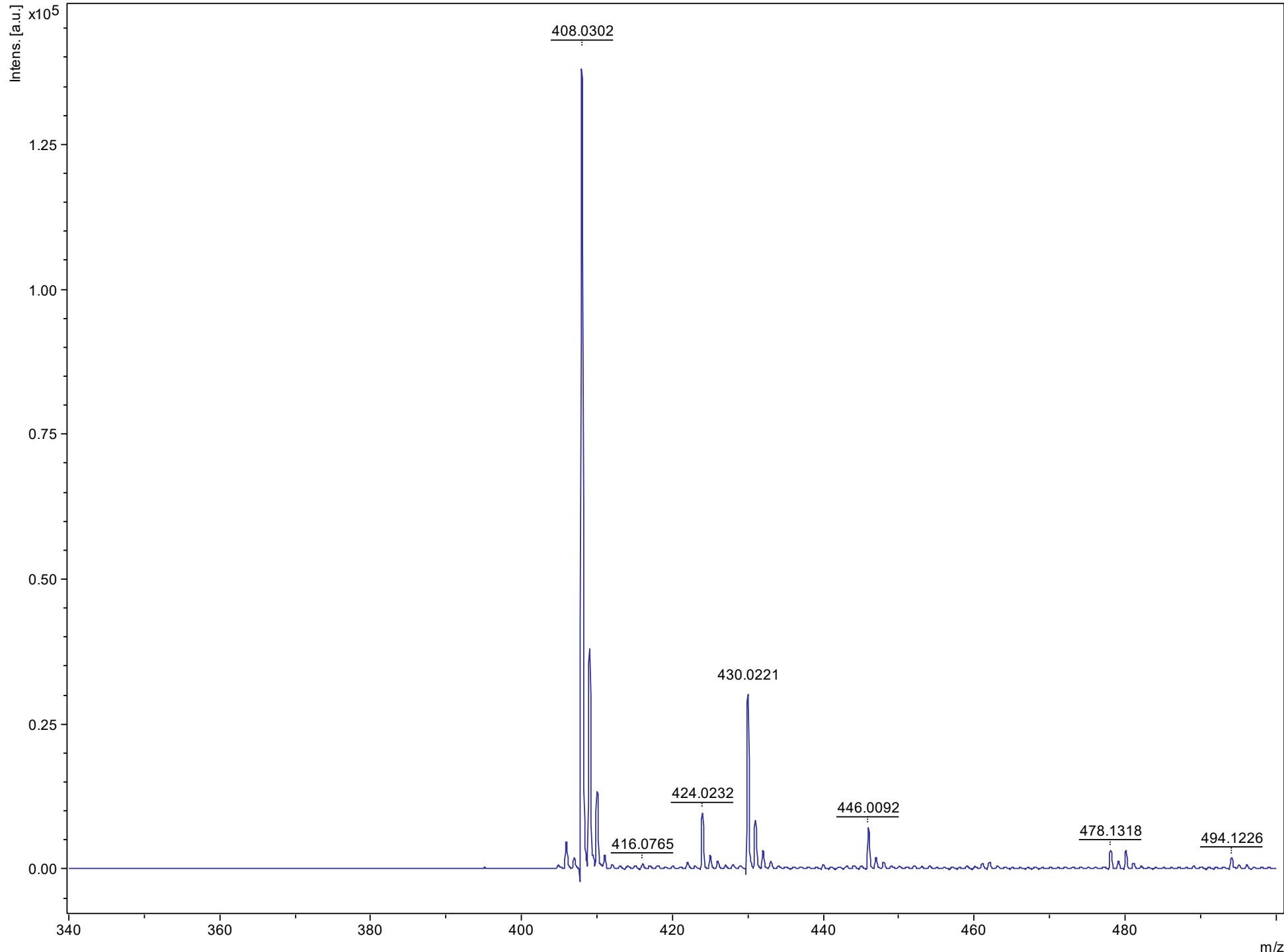
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.333	BV E	0.4104	437.84741	13.04955	2.7750
2	15.593	VV E	0.1271	43.01480	3.99643	0.2726
3	16.214	VB R	1.1059	1.51747e4	160.30304	96.1730
4	20.136	MM	0.5827	47.70582	1.36456	0.3023







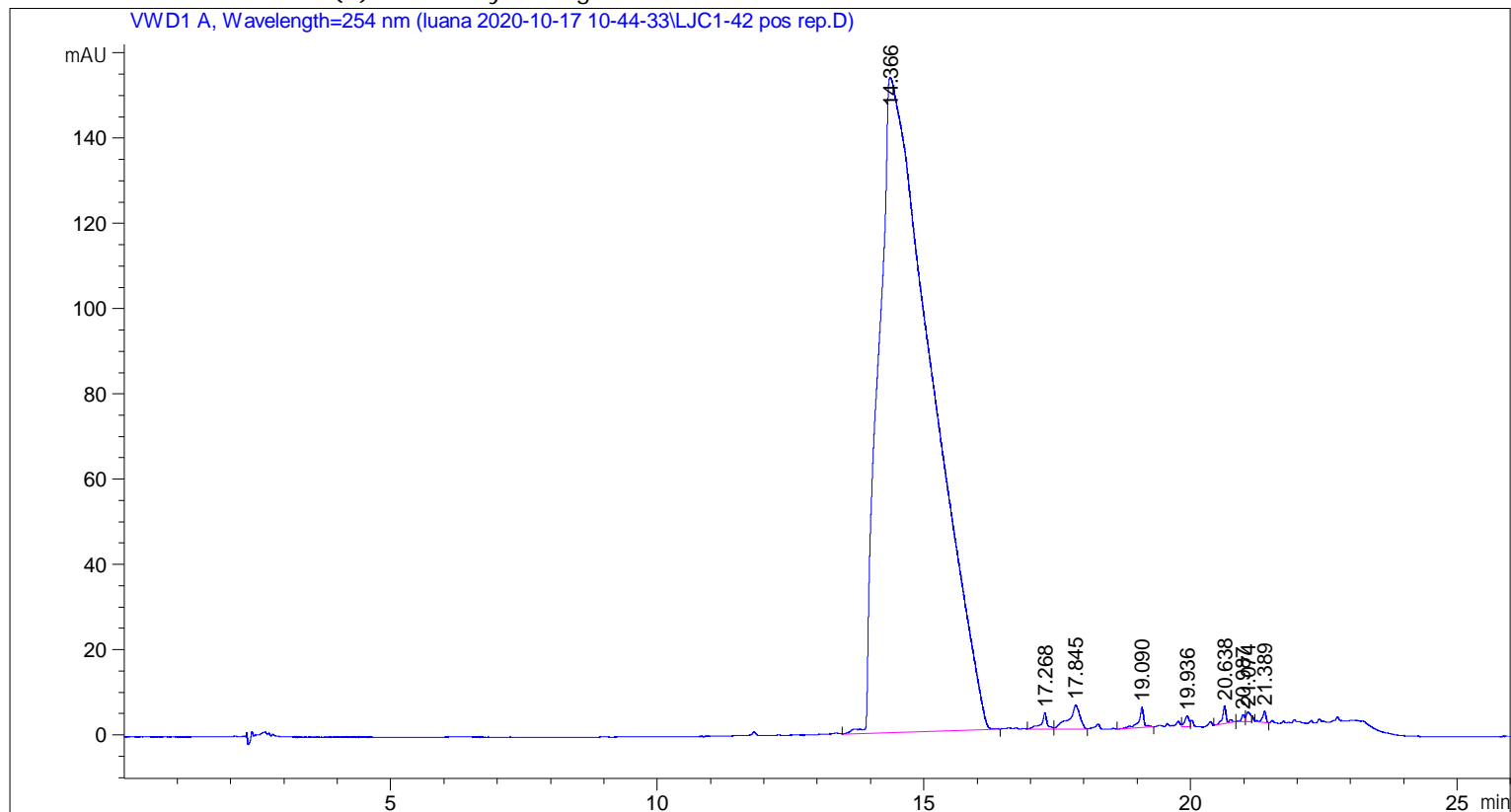
Sample Name: LJC1-42 pos rep

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    3
Acq. Instrument : 1220 HPLC                    Location  :   11
Injection Date  : 10/17/2020 11:39:45 AM      Inj       :    1
                                           Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-10-17 10-44-33\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 10/17/2020 11:15:13 AM by SYSTEM
Method Info     : Water/MeOH
    
```

Sample Info : LJC1-42 pos rep

Additional Info : Peak(s) manually integrated



Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

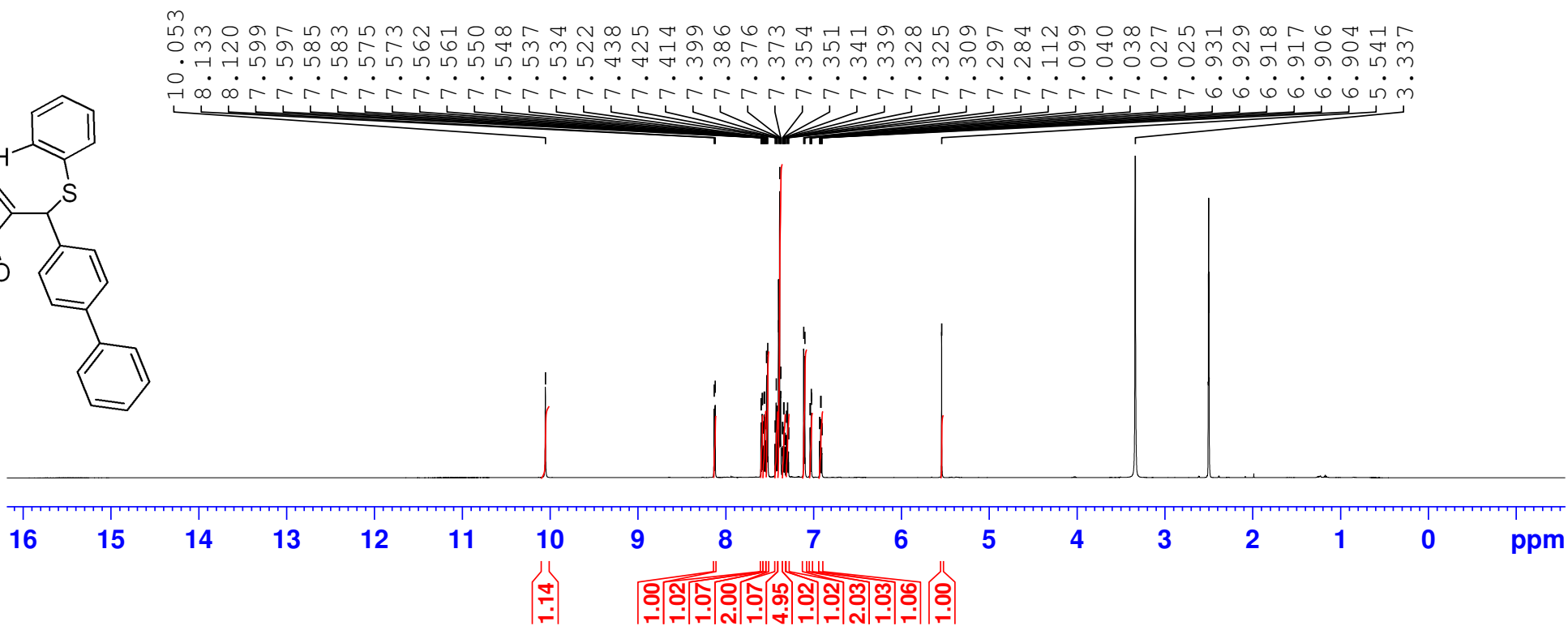
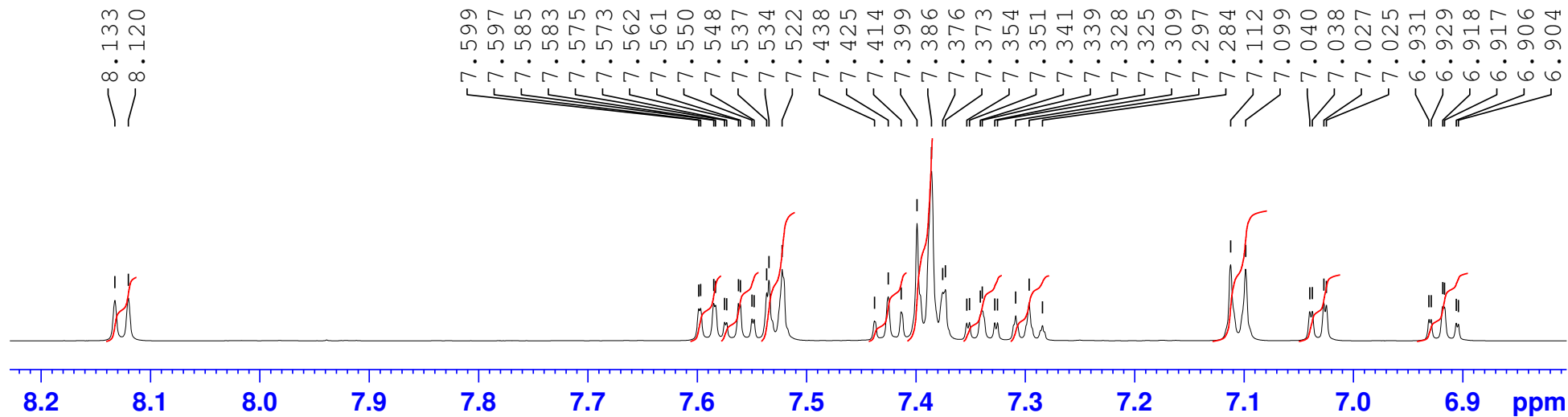
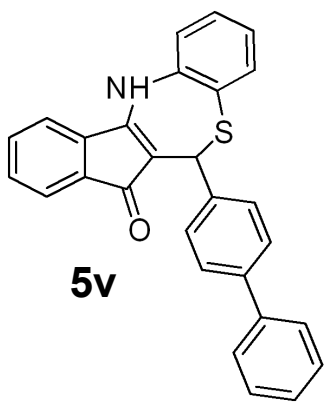
Signal 1: VWD1 A, Wavelength=254 nm

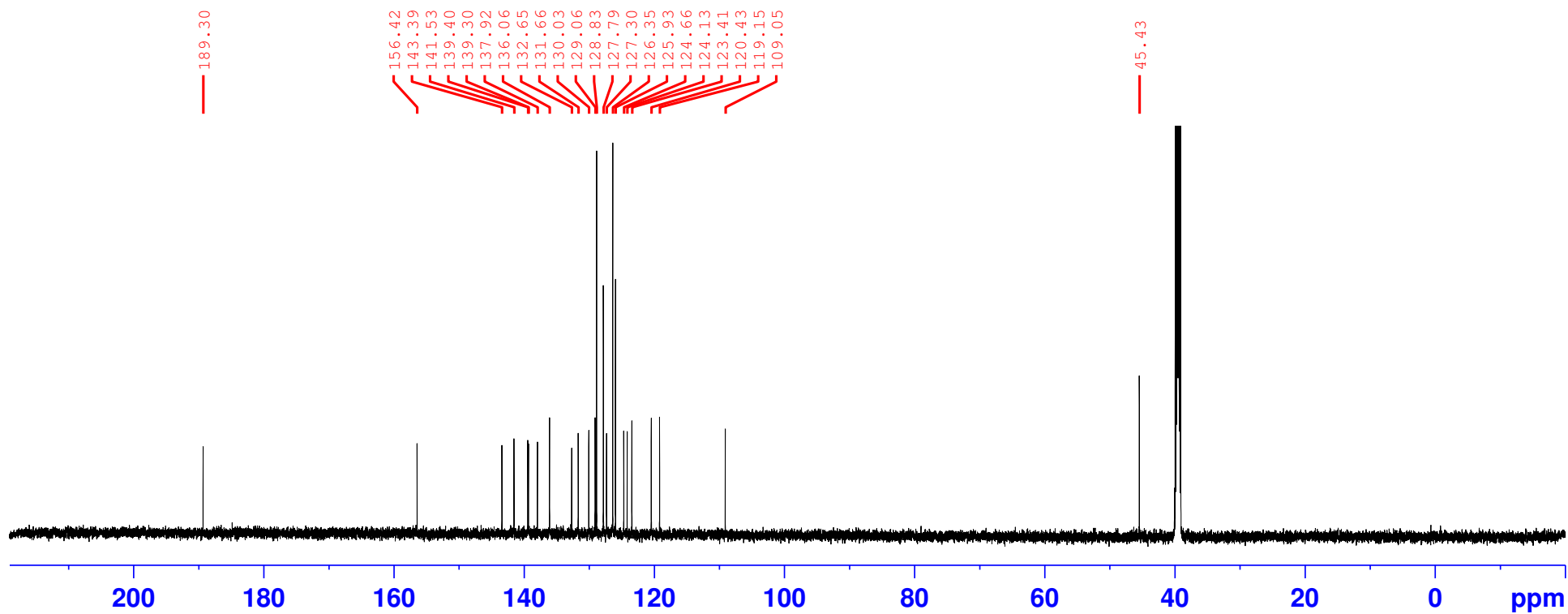
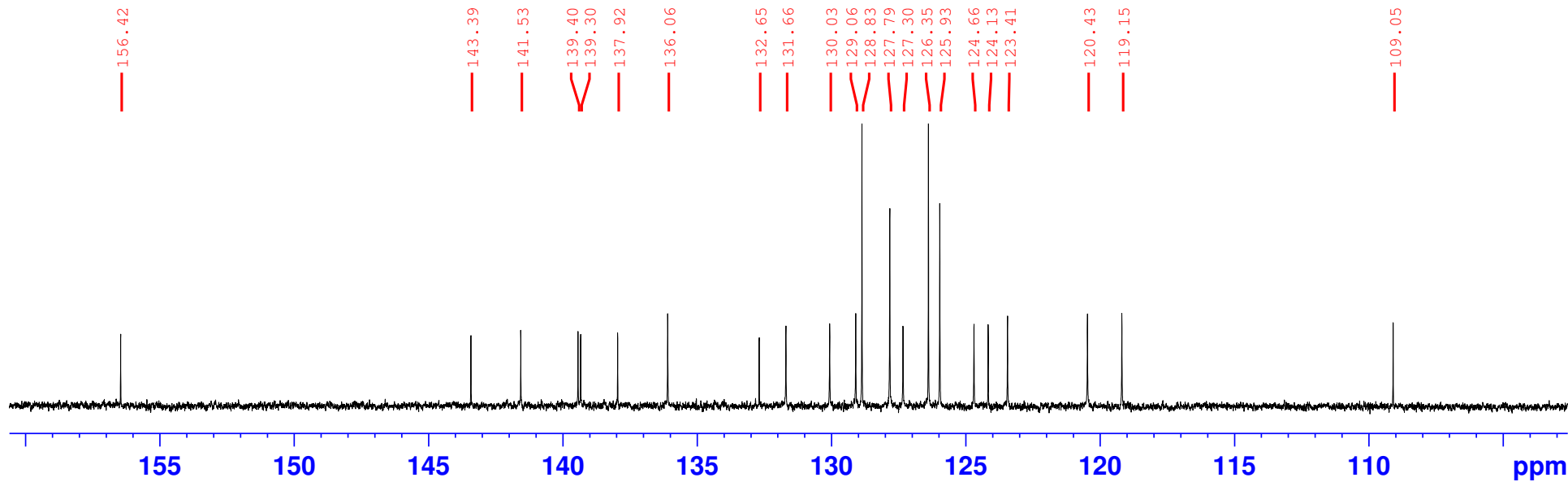
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.366	VV R	0.8197	1.05179e4	153.63815	97.9931
2	17.268	VV R	0.1030	30.27498	3.88028	0.2821
3	17.845	VV	0.1820	82.60709	5.60473	0.7696
4	19.090	VV R	0.0963	34.14436	4.84245	0.3181

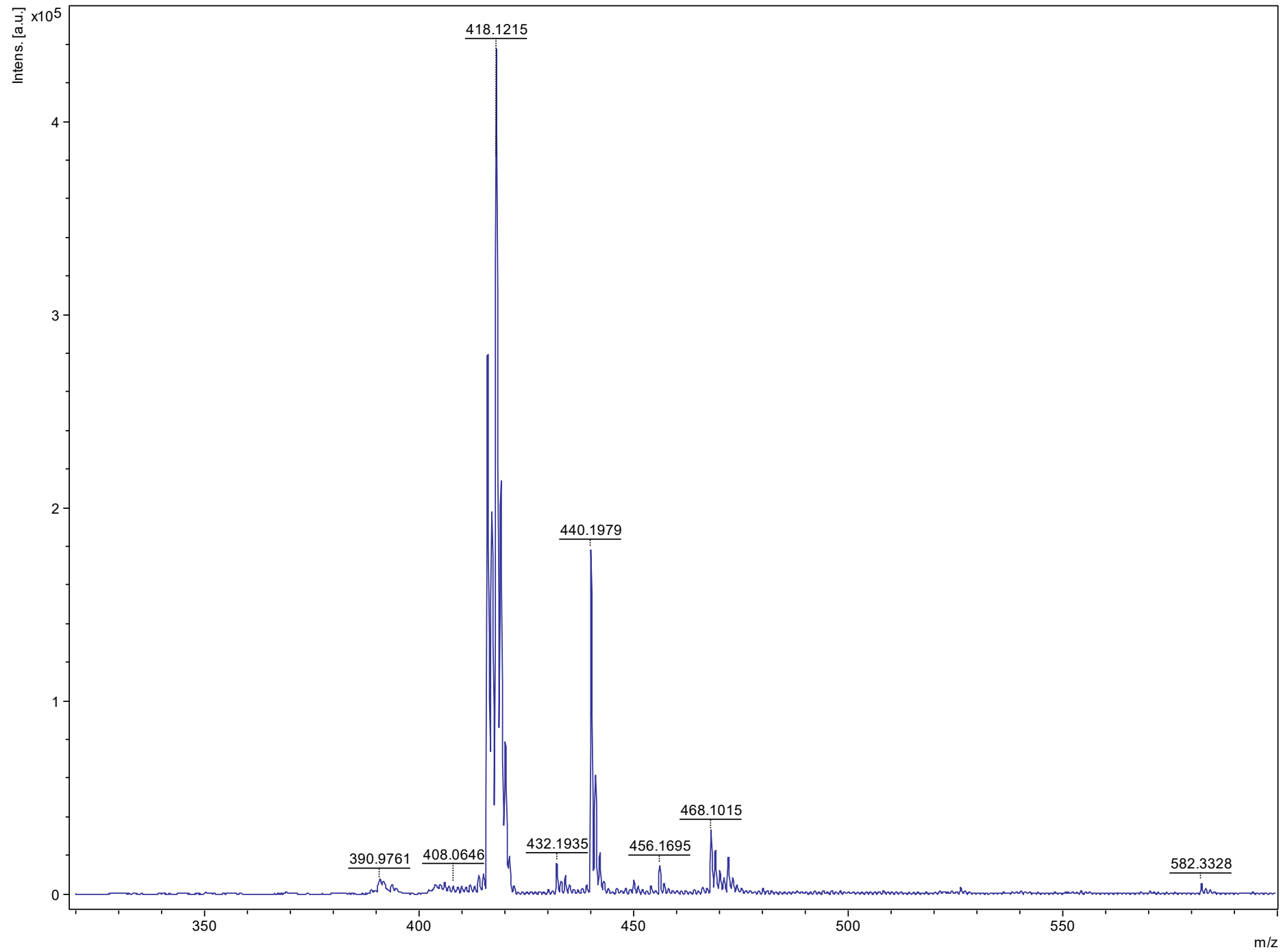
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	19.936	VV	0.0798	14.41827	2.53832	0.1343
6	20.638	VV R	0.0757	22.44223	4.24518	0.2091
7	20.987	BV	0.0580	6.96932	1.71201	0.0649
8	21.074	VV	0.0719	12.46015	2.29194	0.1161
9	21.389	VB R	0.0618	12.09581	2.72602	0.1127

Totals : 1.07333e4 181.47908

=====
*** End of Report ***







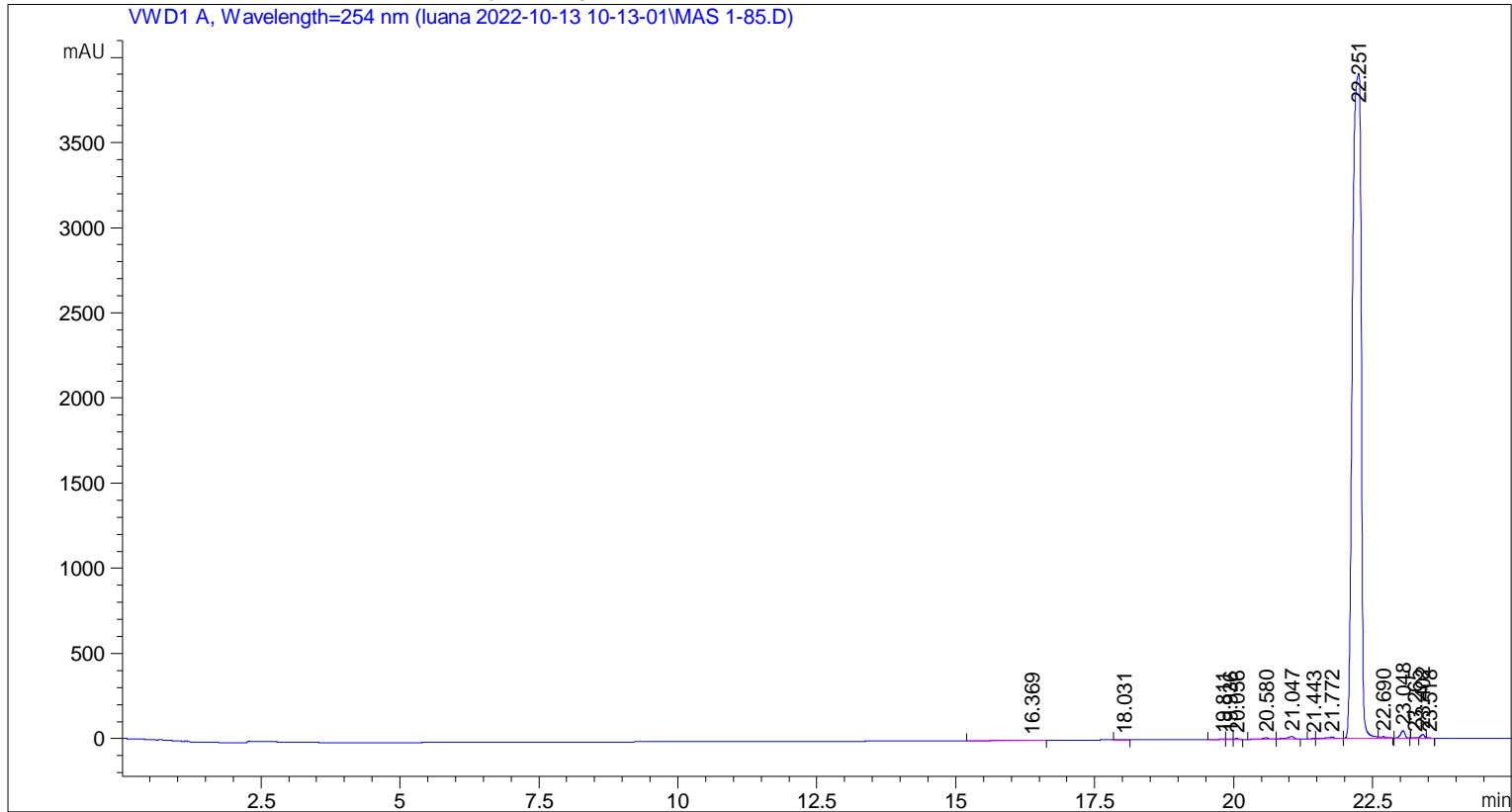
Sample Name: MAS 1-85

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    4
Acq. Instrument : 1220 HPLC                    Location  :   84
Injection Date  : 10/13/2022 11:36:02 AM      Inj       :    1
                                           Inj Volume: 70.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2022-10-13 10-13-01\Luana_small_molecule.M (Sequence
                :                               Method)
Last changed    : 10/13/2022 10:13:06 AM by SYSTEM
Method Info     : MeOH/water
    
```

Sample Info : MAS 1-85

Additional Info : Peak(s) manually integrated



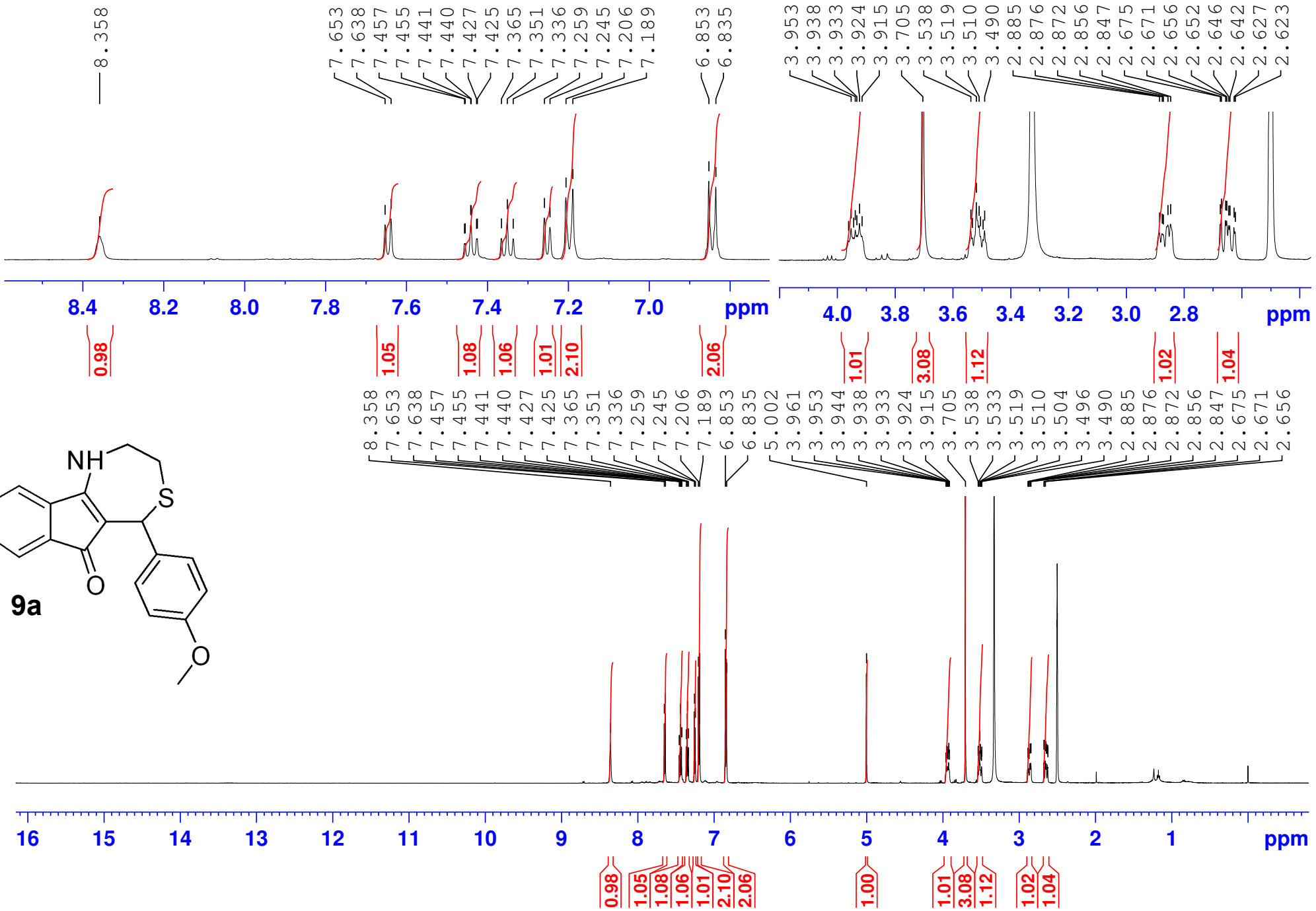
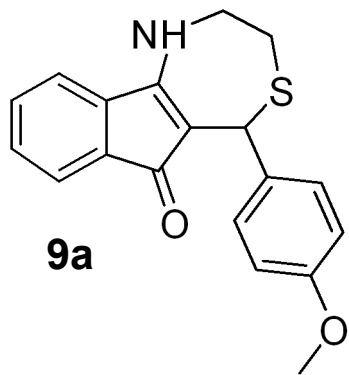
Area Percent Report

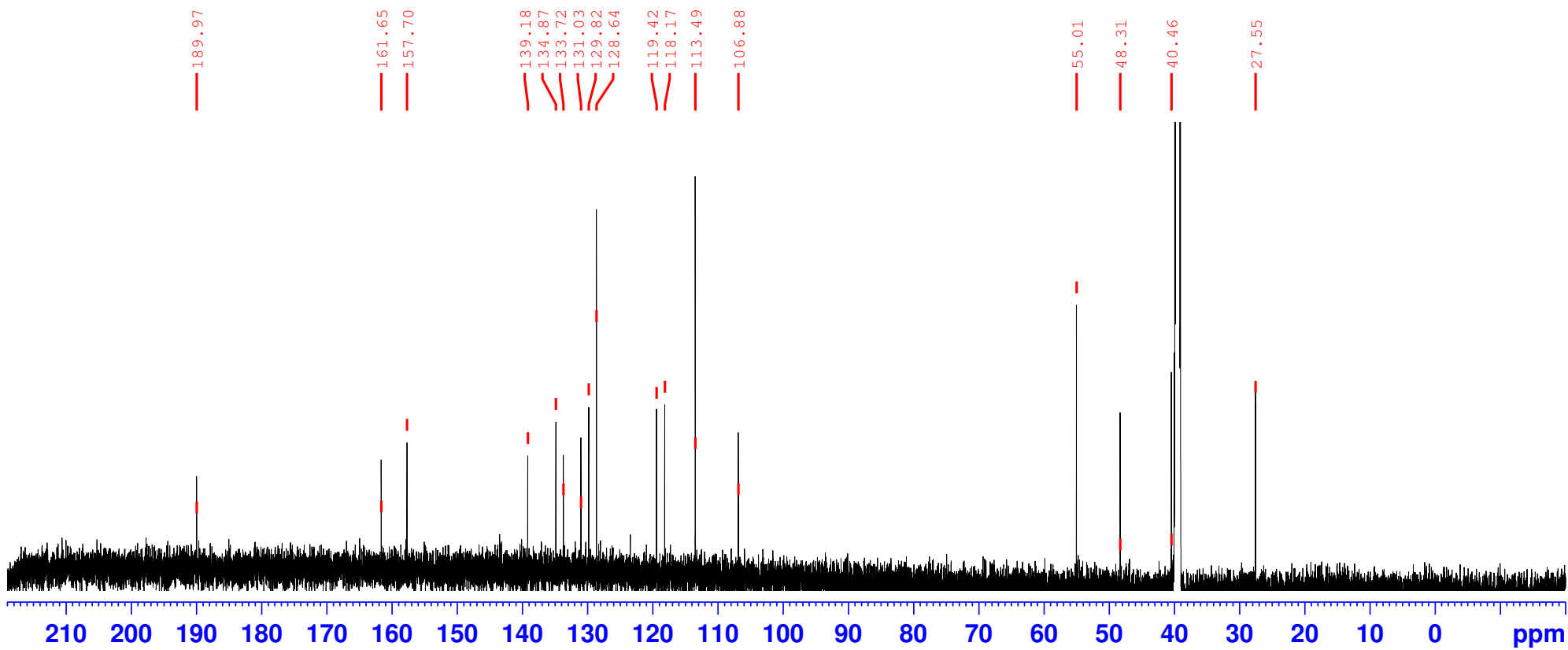
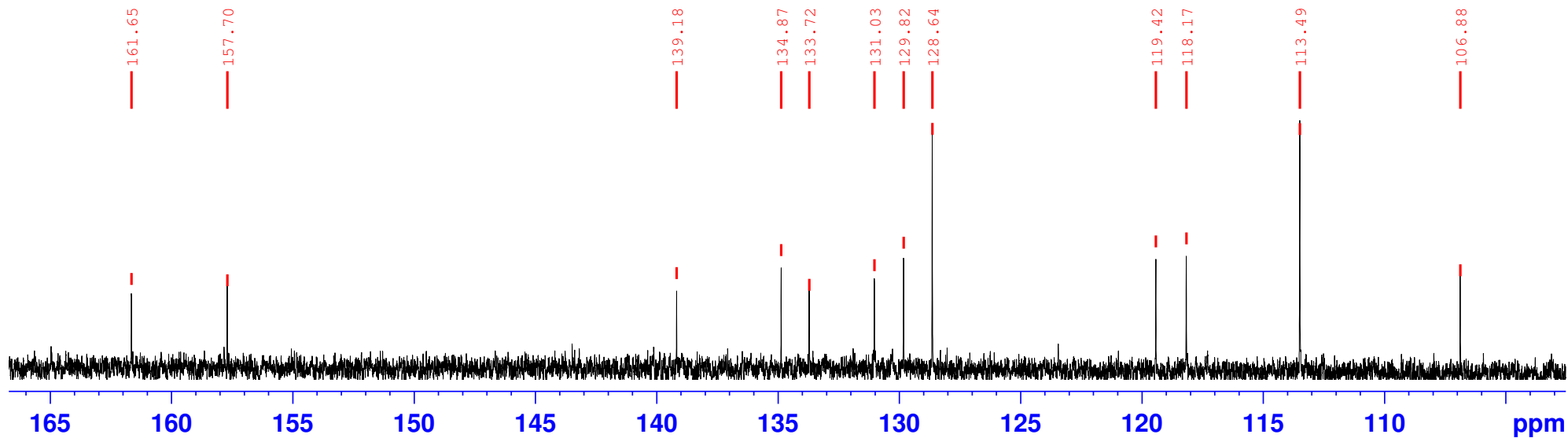
```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

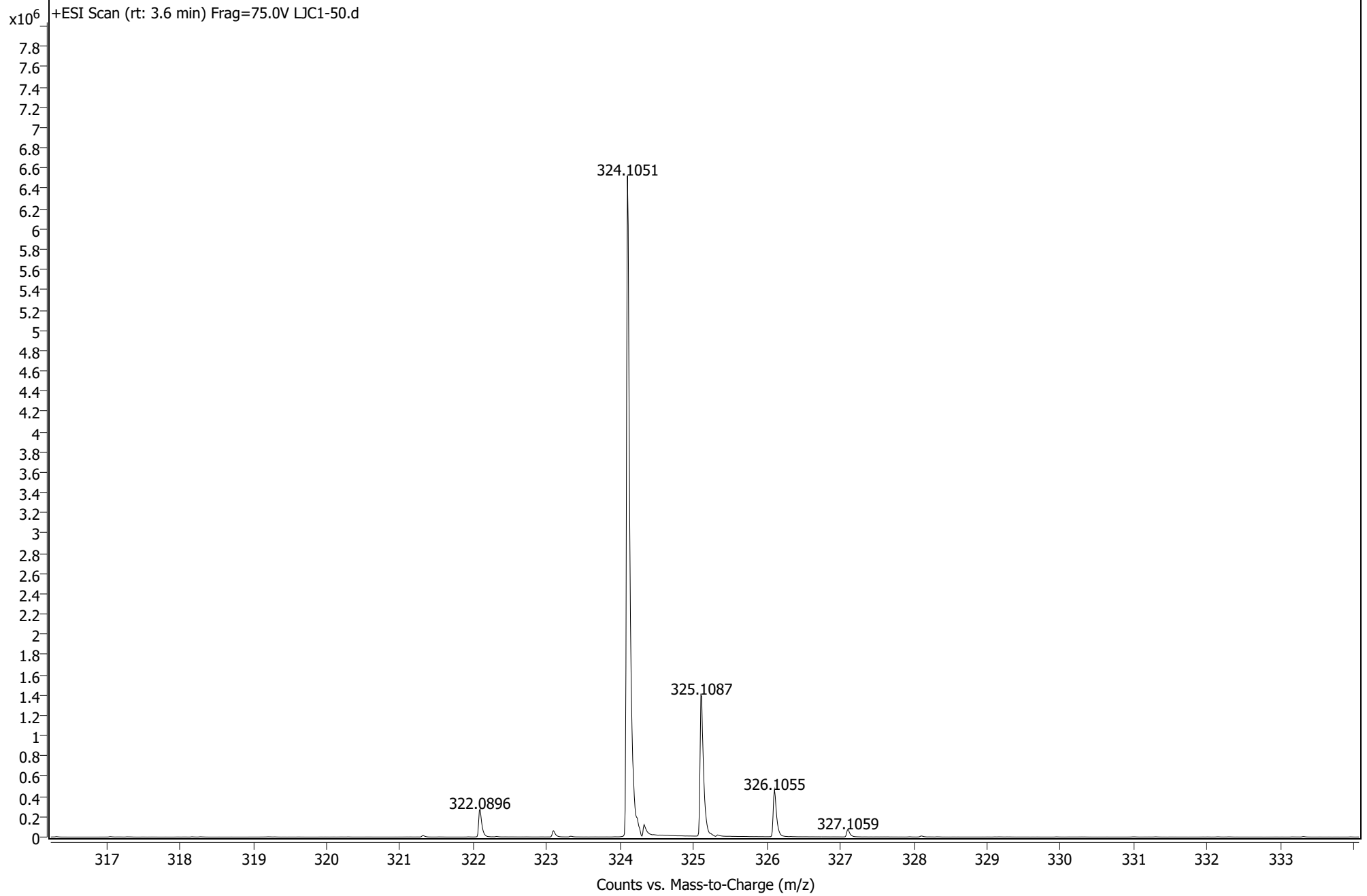
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.369	BB	0.4198	72.39281	2.36046	0.1680
2	18.031	VV	0.1560	31.03286	2.72306	0.0720
3	19.811	BV	0.1085	19.94106	2.59890	0.0463
4	19.936	VV	0.0891	24.77004	3.95412	0.0575





User Spectrum Plot Report



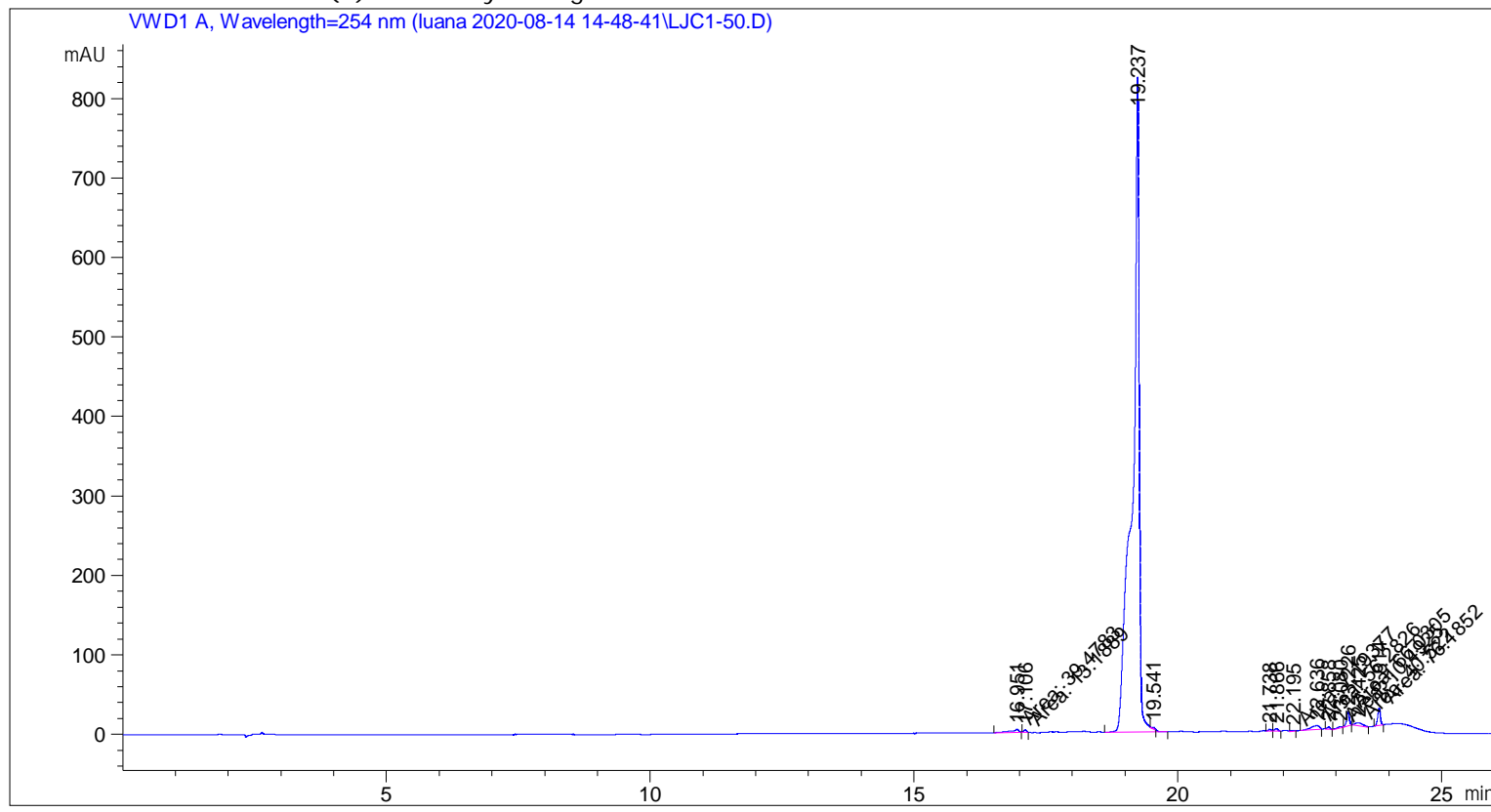
Sample Name: LJC1-50

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    6
Acq. Instrument : 1220 HPLC                   Location  :   45
Injection Date  : 8/14/2020 5:08:11 PM      Inj       :    1
                                           Inj Volume: 50.000 µl

Method          : C:\Chem32\1\Data\luana 2020-08-14 14-48-41\MOHAMED-SMALL MOLECULE.M (
                  Sequence Method)
Last changed    : 8/14/2020 2:48:44 PM by SYSTEM
Sample Info     : LJC1-50
    
```

Additional Info : Peak(s) manually integrated



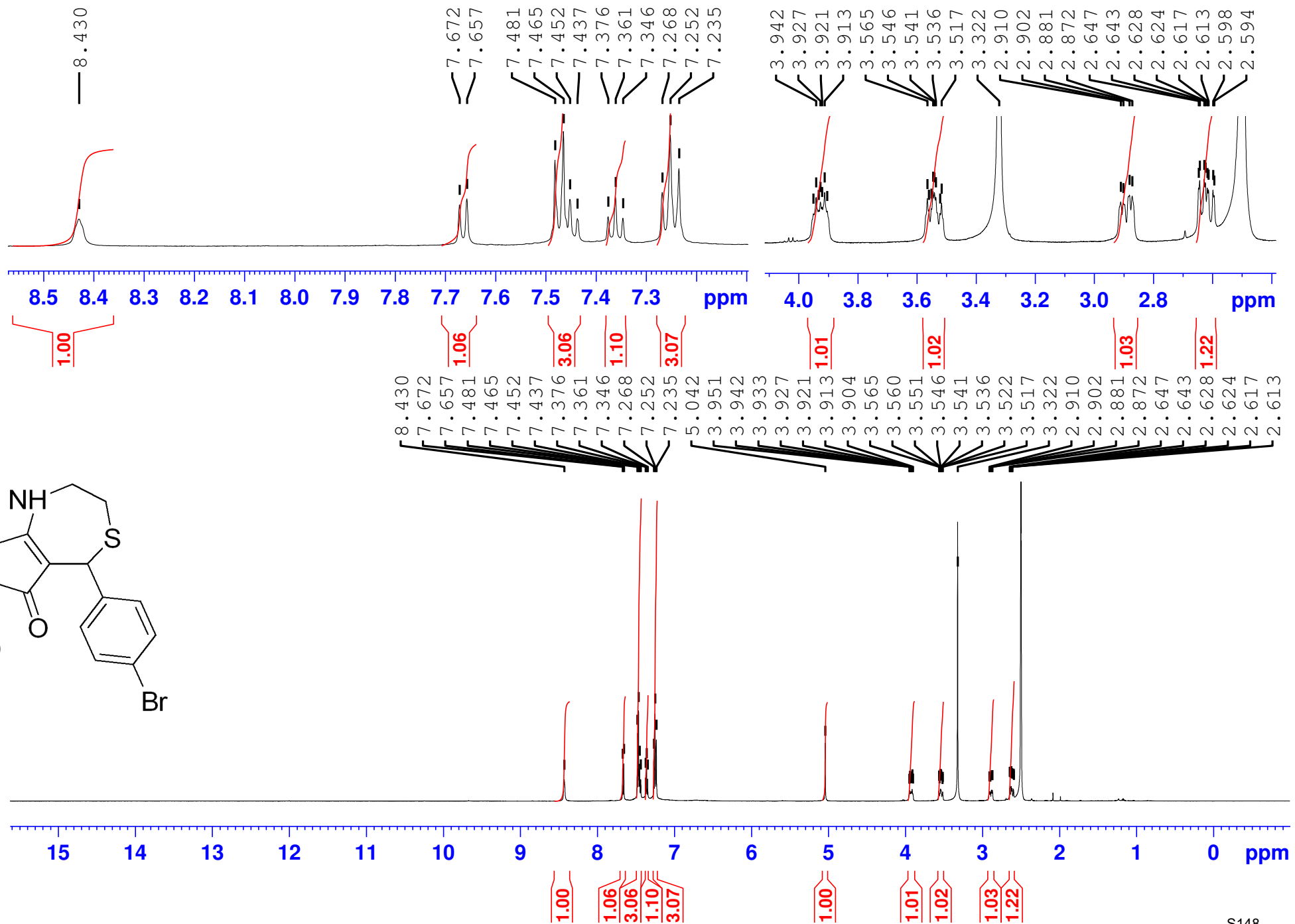
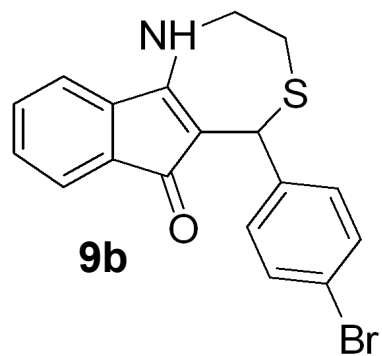
=====
 Area Percent Report
 =====

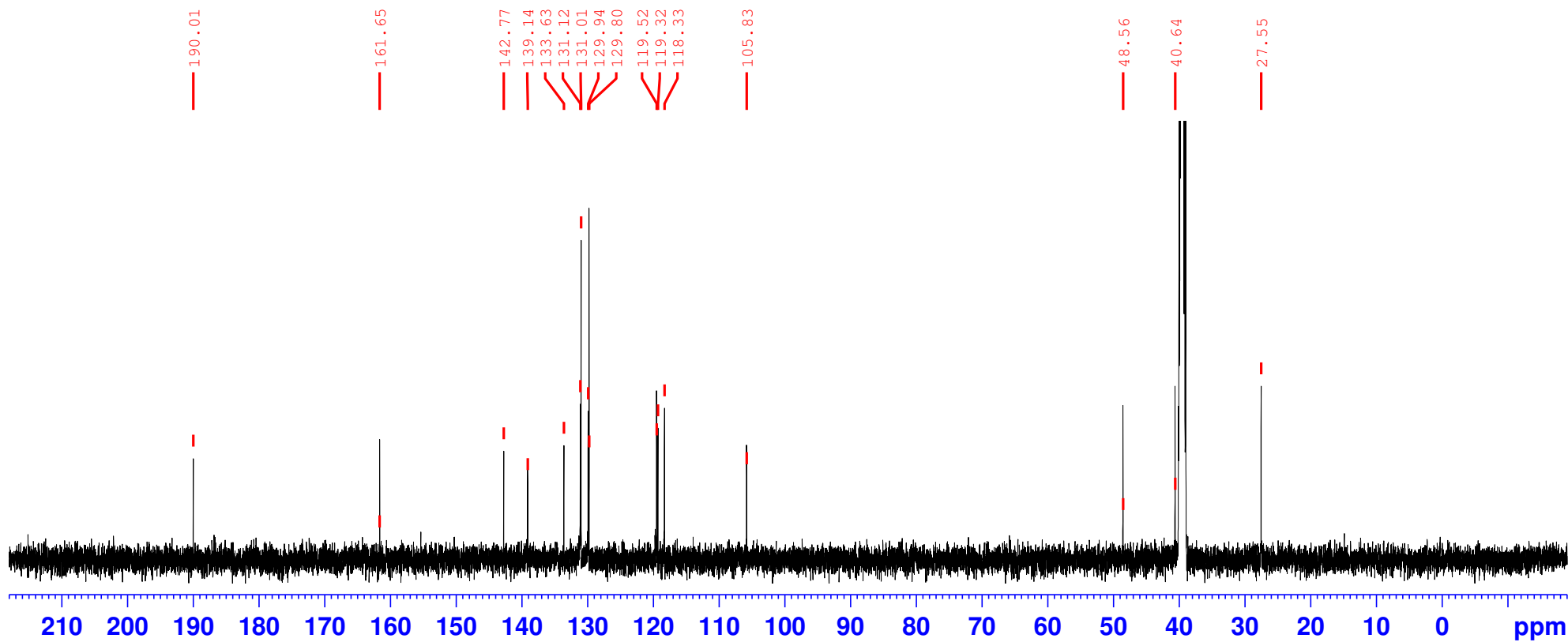
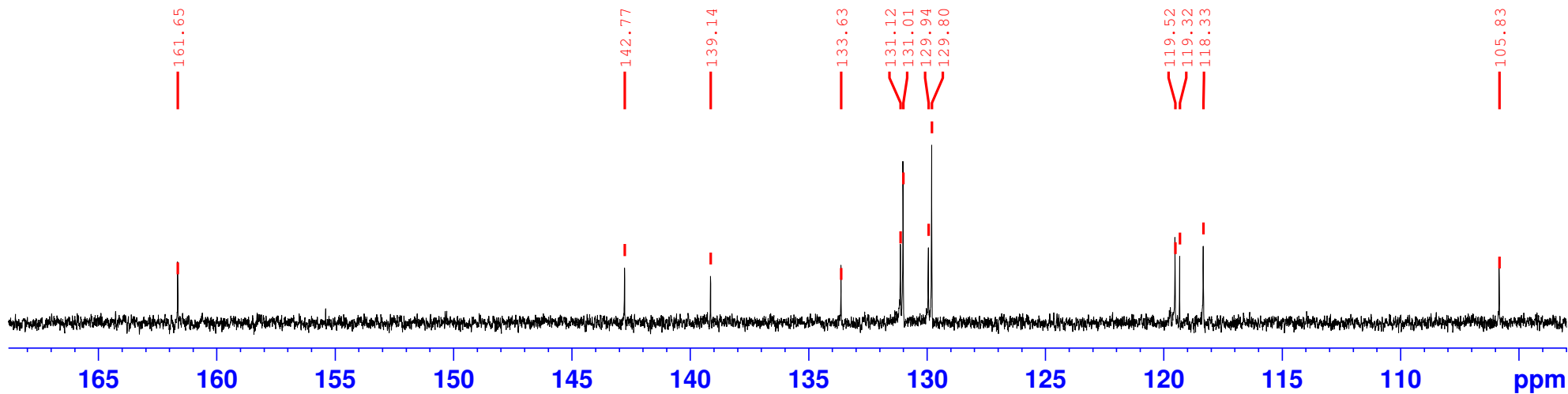
```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

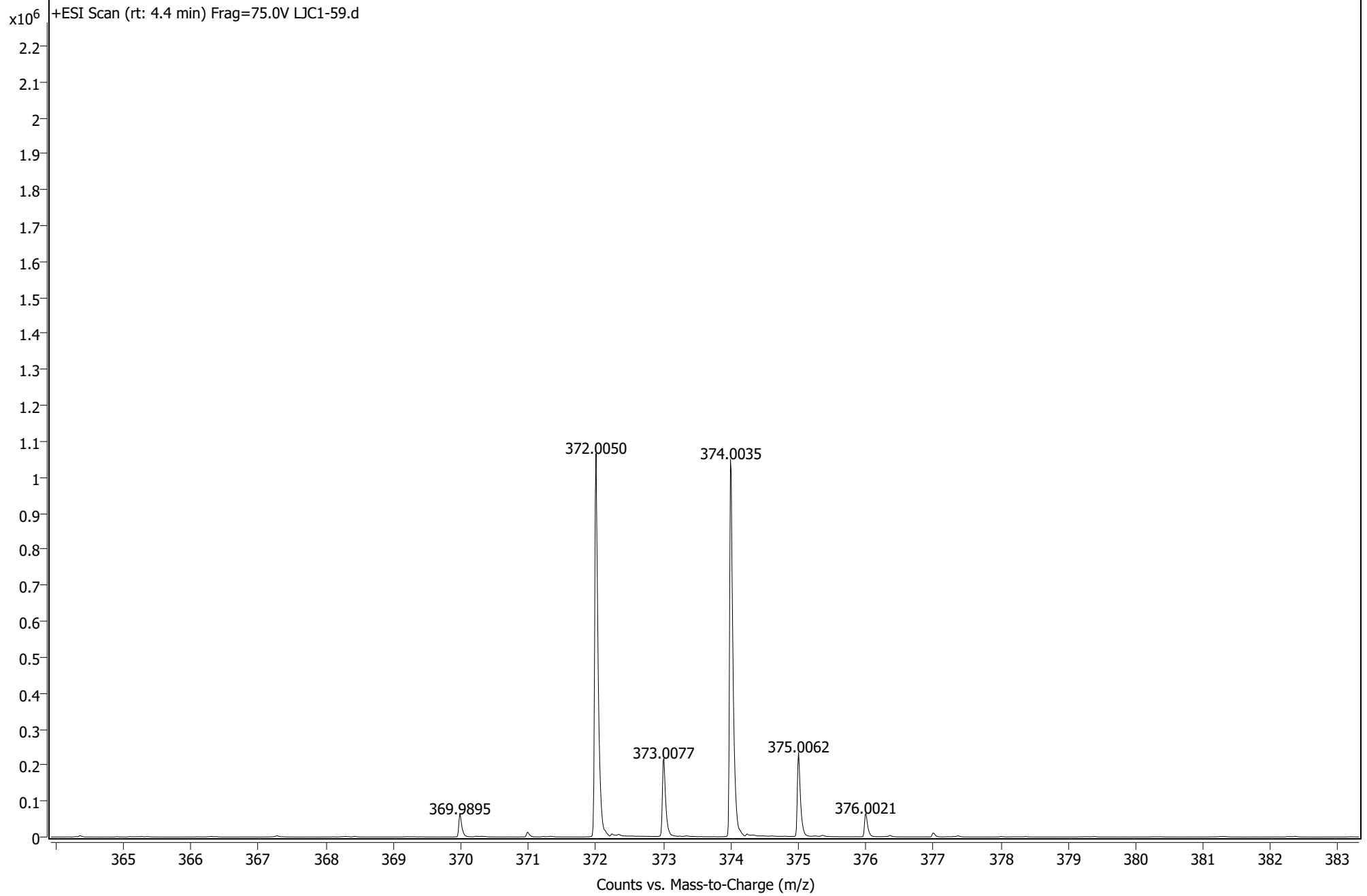
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.951	MM	0.1586	39.47832	4.14796	0.5122
2	17.106	MM	0.0707	13.18885	3.10871	0.1711
3	19.237	BV R	0.1191	7356.73584	824.14886	95.4403
4	19.541	VB E	0.0512	6.97107	2.15795	0.0904
5	21.738	VV	0.0649	10.06187	2.26236	0.1305
6	21.866	VB	0.0665	14.03131	3.08971	0.1820
7	22.195	MM	0.0709	7.19377	1.22277	0.0933





User Spectrum Plot Report



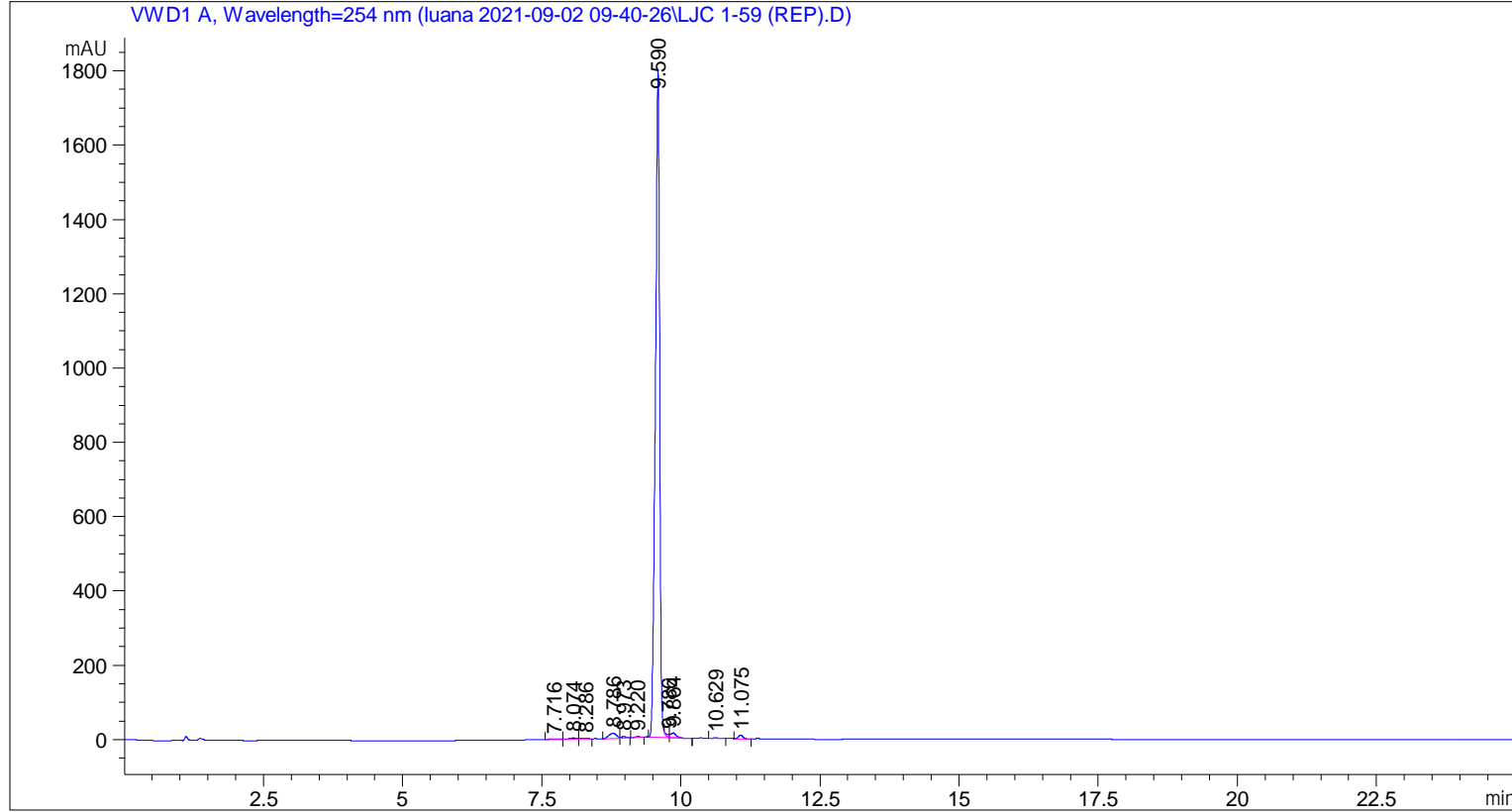
Sample Name: LJC 1-59 (REP)

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    8
Acq. Instrument : 1220 HPLC                    Location  :   72
Injection Date  : 9/2/2021 12:33:01 PM       Inj       :    1
                                           Inj Volume: 50.000 µl
Method          : C:\Chem32\1\Data\luana 2021-09-02 09-40-26\Luana_small_molecule.M (Sequence Method)
Last changed    : 9/2/2021 10:25:25 AM by SYSTEM
Method Info     : MeOH/water

Sample Info     : LJC 1-59 (REP)
    
```

Additional Info : Peak(s) manually integrated



Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

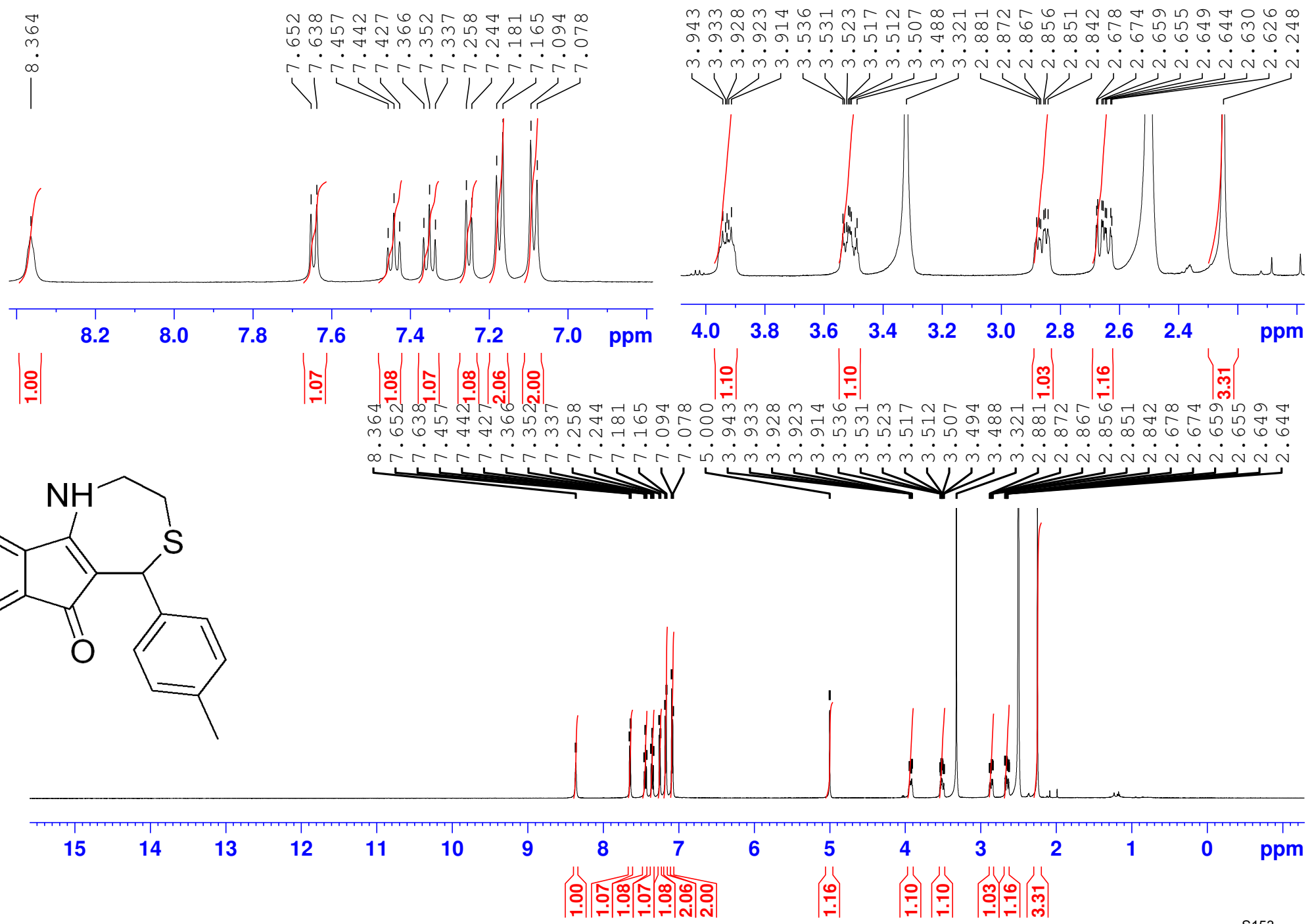
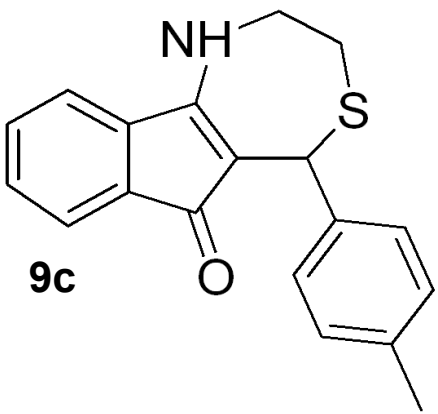
Signal 1: VWD1 A, Wavelength=254 nm

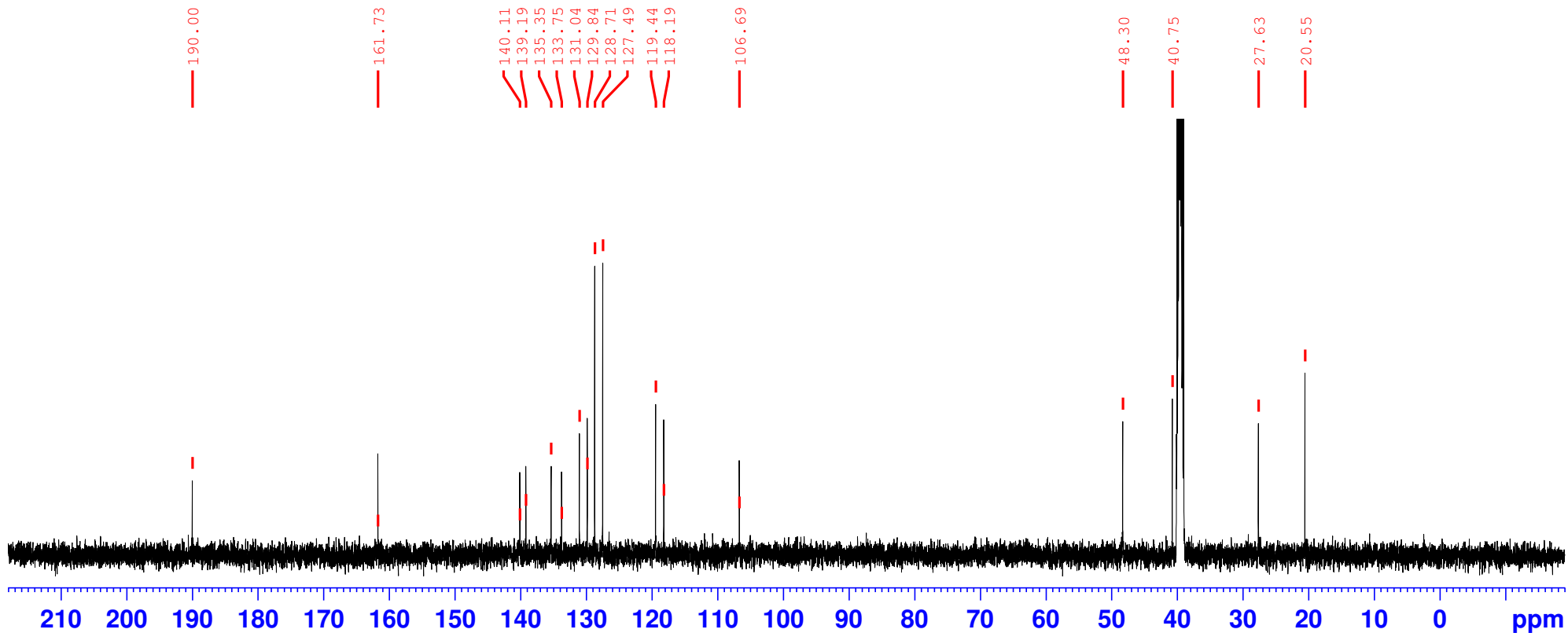
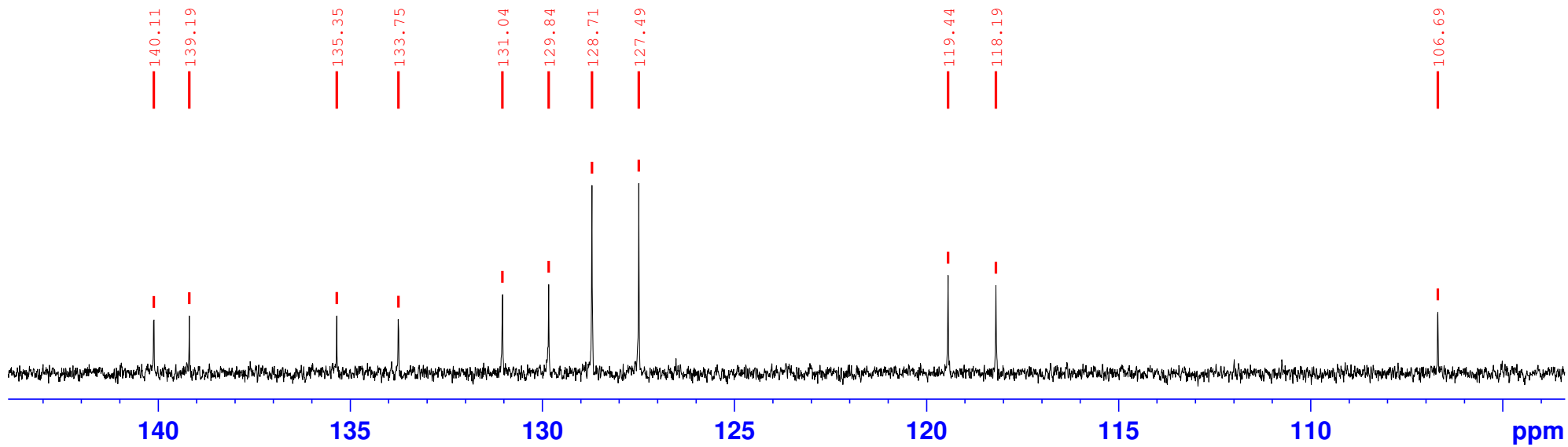
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.716	BV	0.1854	24.60387	1.93446	0.2465
2	8.074	VV	0.1478	35.60102	3.40983	0.3567
3	8.286	VV	0.1514	21.95141	1.96416	0.2199
4	8.786	BV	0.1595	133.35028	13.59041	1.3360
5	8.973	VB	0.0948	29.69850	4.34042	0.2975

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
6	9.220	BV	0.0961	19.68749	2.83234	0.1972
7	9.590	BV R	0.0760	9528.49805	1794.37732	95.4608
8	9.786	VV E	0.0462	25.50038	7.78751	0.2555
9	9.864	VB E	0.1006	93.23138	13.16180	0.9340
10	10.629	VV	0.1326	16.81372	1.94994	0.1684
11	11.075	BB	0.0778	52.65031	10.27224	0.5275

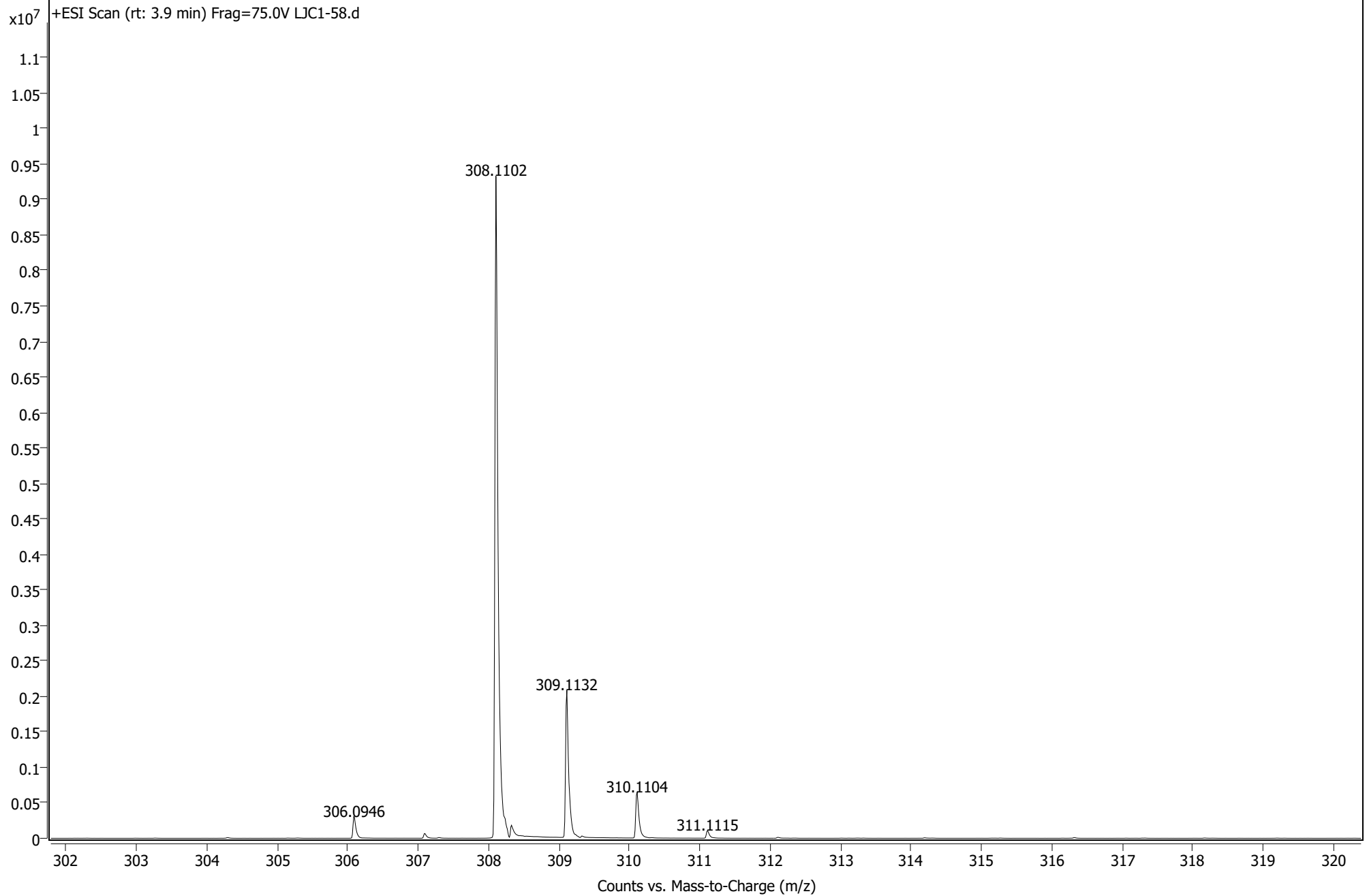
Totals : 9981.58639 1855.62043

=====
*** End of Report ***





User Spectrum Plot Report



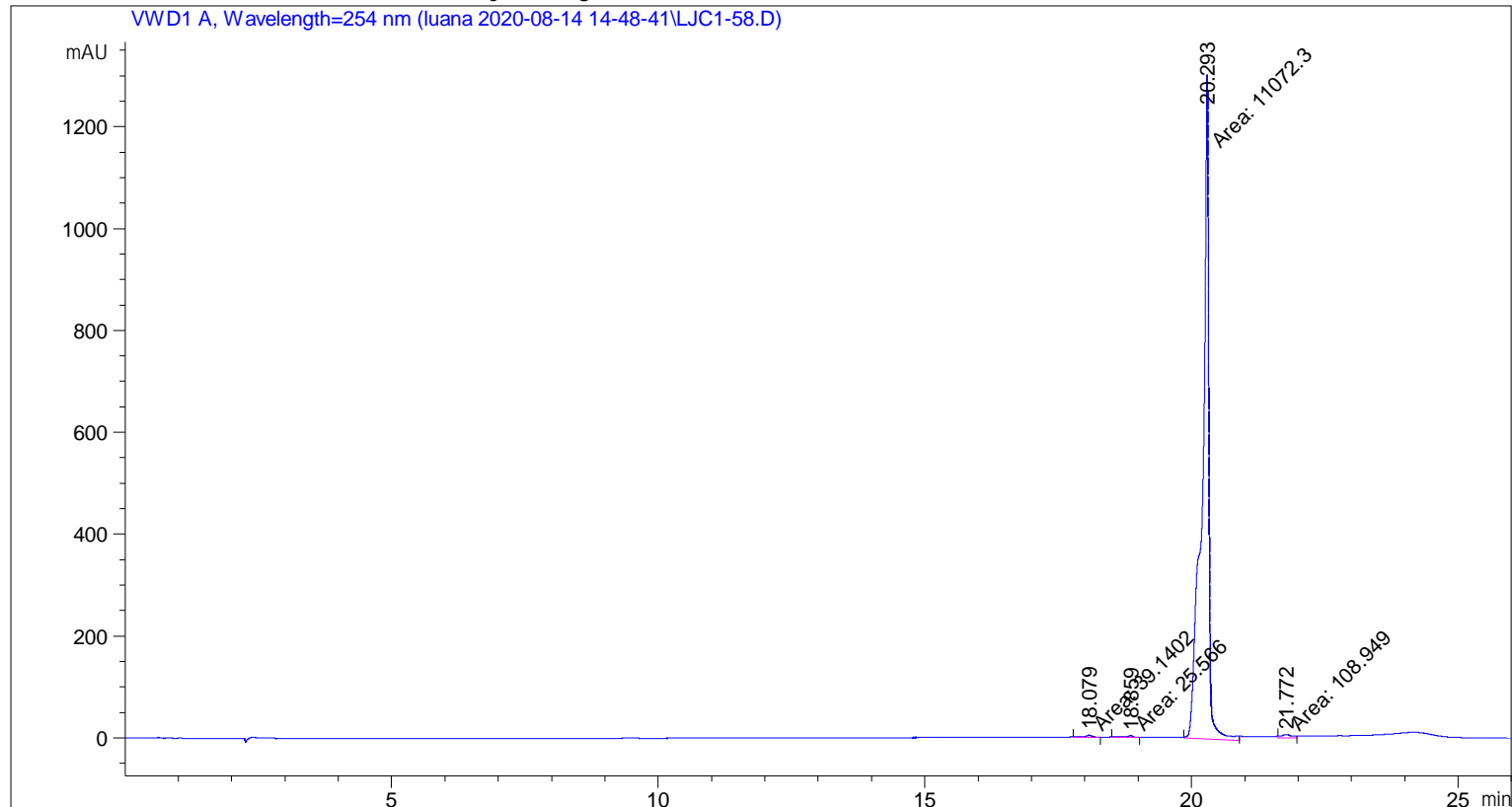
Sample Name: LJC1-58

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    8
Acq. Instrument : 1220 HPLC                   Location  :   47
Injection Date  : 8/14/2020 6:03:40 PM      Inj       :    1
                                           Inj Volume: 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-08-14 14-48-41\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 8/14/2020 2:48:44 PM by SYSTEM
Sample Info     : LJC1-58
=====

```

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====

```

```

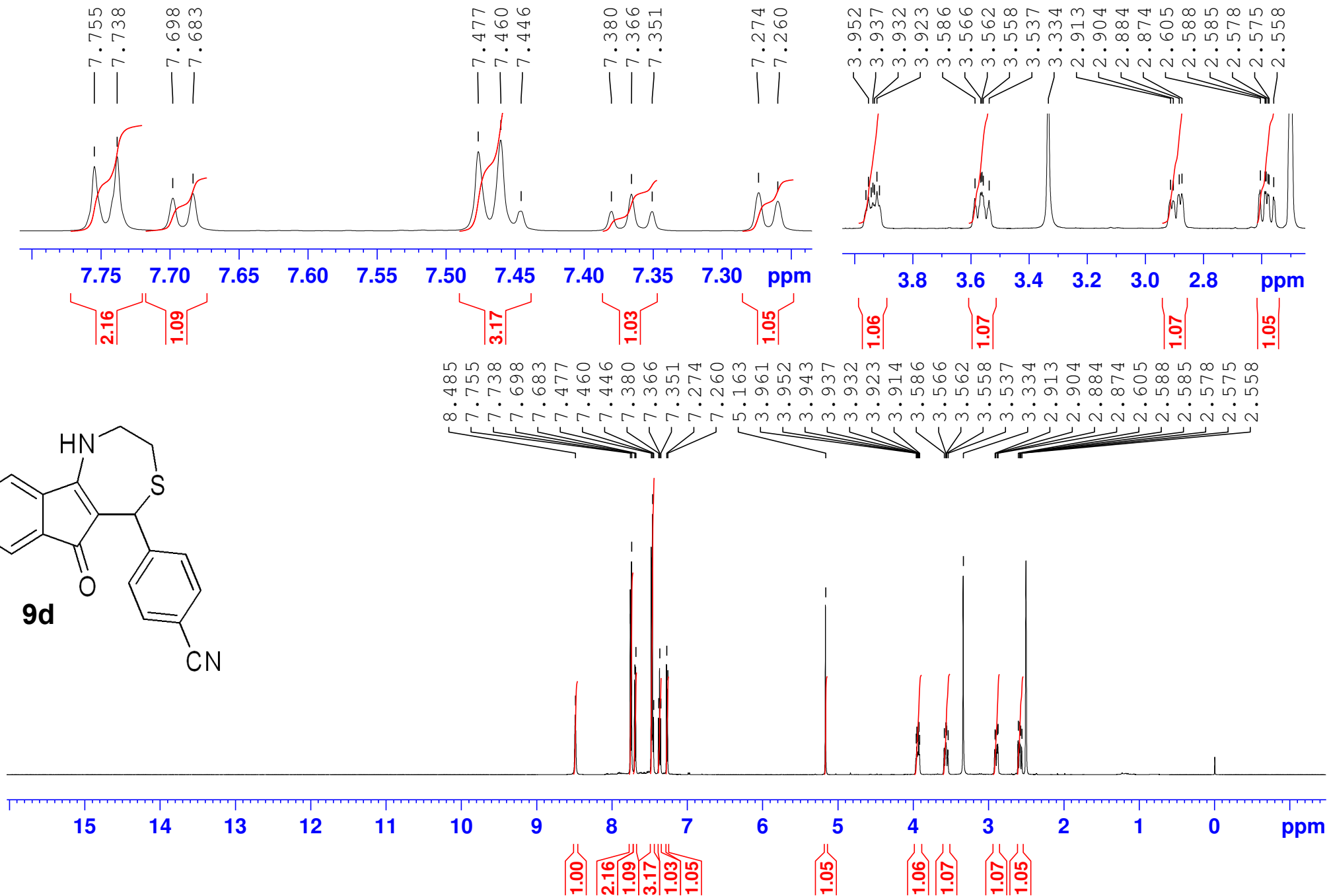
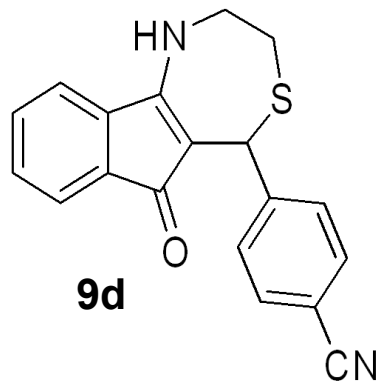
Sorted By           :      Signal
Multiplier          :      1.0000
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs

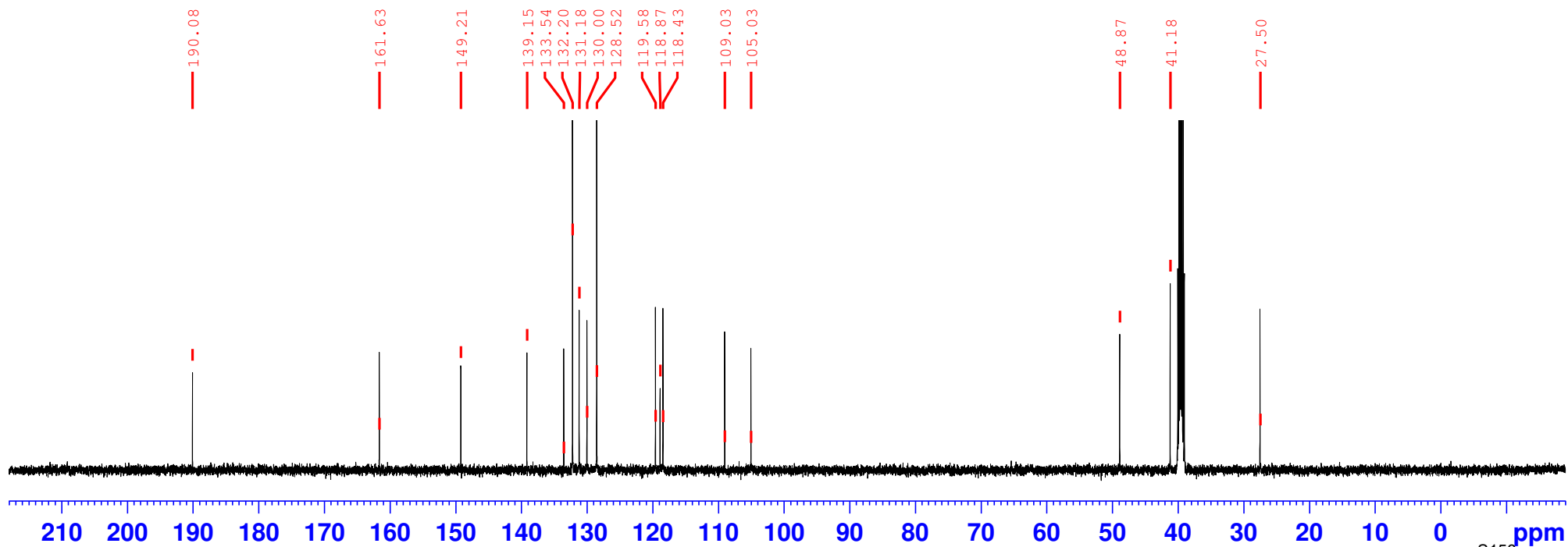
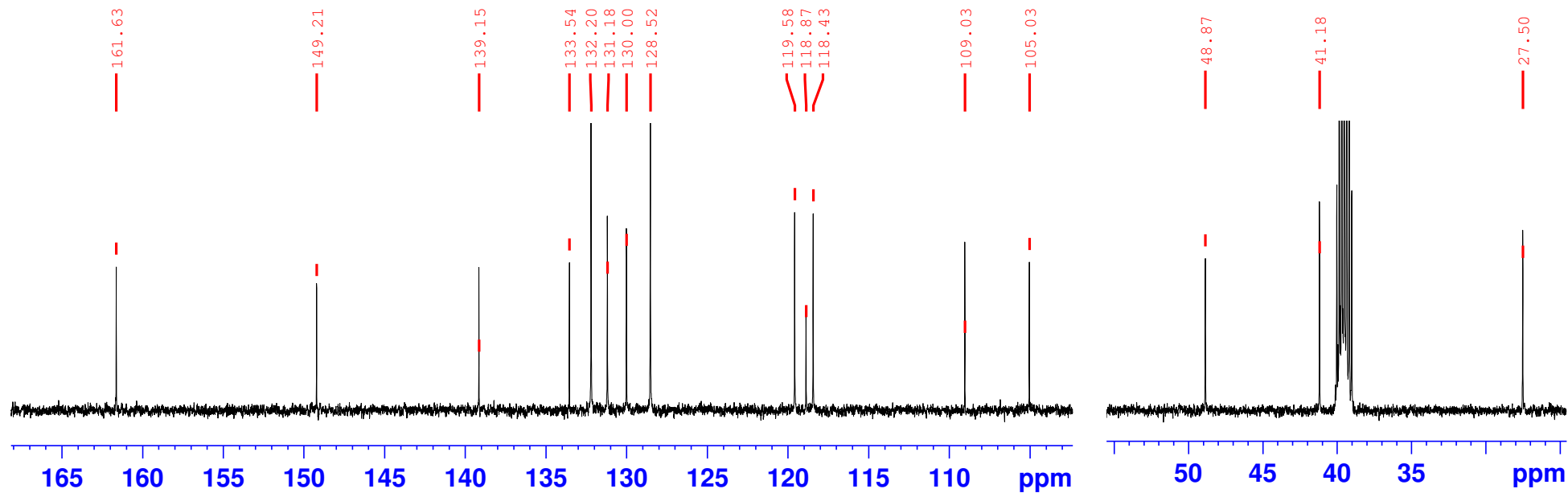
```

Signal 1: VWD1 A, Wavelength=254 nm

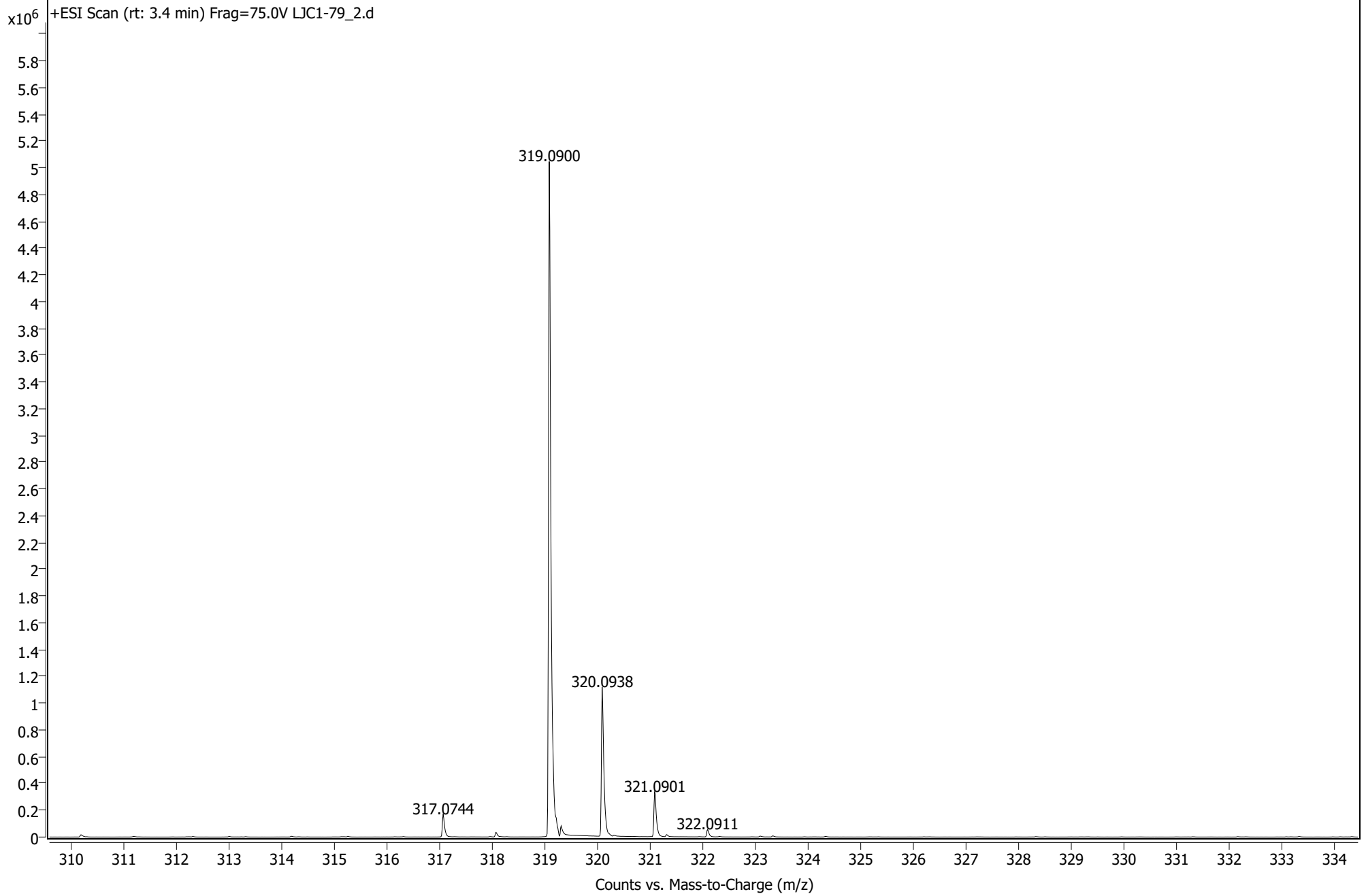
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.079	MM	0.1651	39.14021	3.95049	0.3480
2	18.859	MM	0.1416	25.56603	3.00918	0.2273
3	20.293	MM	0.1415	1.10723e4	1303.77124	98.4558
4	21.772	MM	0.2519	108.94907	7.20898	0.9688

```
Totals :                      1.12459e4  1317.93989
```





User Spectrum Plot Report



Sample Name: LJC 1-79

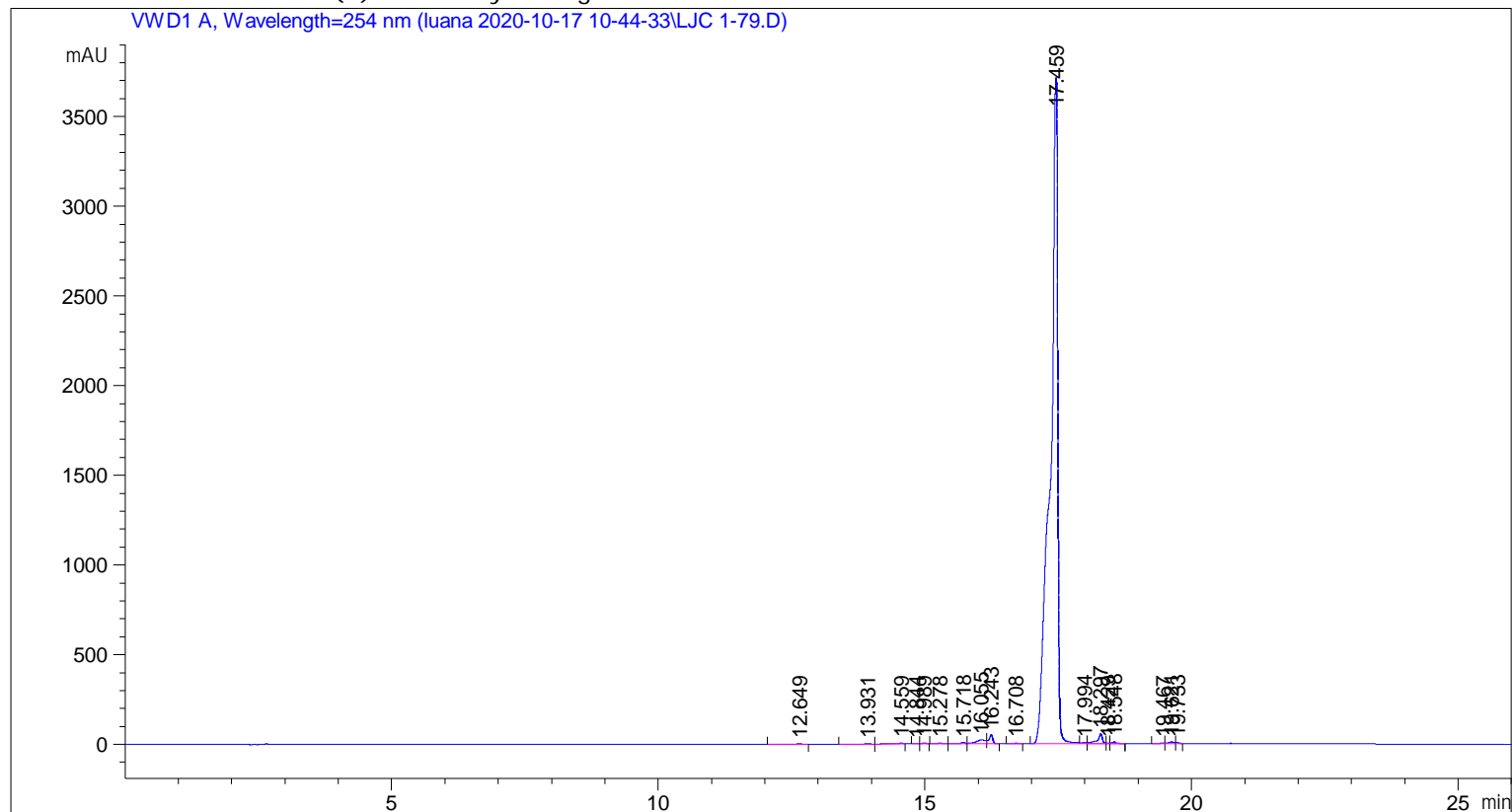
```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    5
Acq. Instrument : 1220 HPLC                     Location  :   13
Injection Date  : 10/17/2020 12:35:09 PM      Inj       :    1
                                           Inj Volume : 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-10-17 10-44-33\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 10/17/2020 11:15:13 AM by SYSTEM
Method Info     : Water/MeOH

Sample Info     : LJC 1-79

```

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====

```

```

Sorted By       :      Signal
Multiplier      :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 1: VWD1 A, Wavelength=254 nm

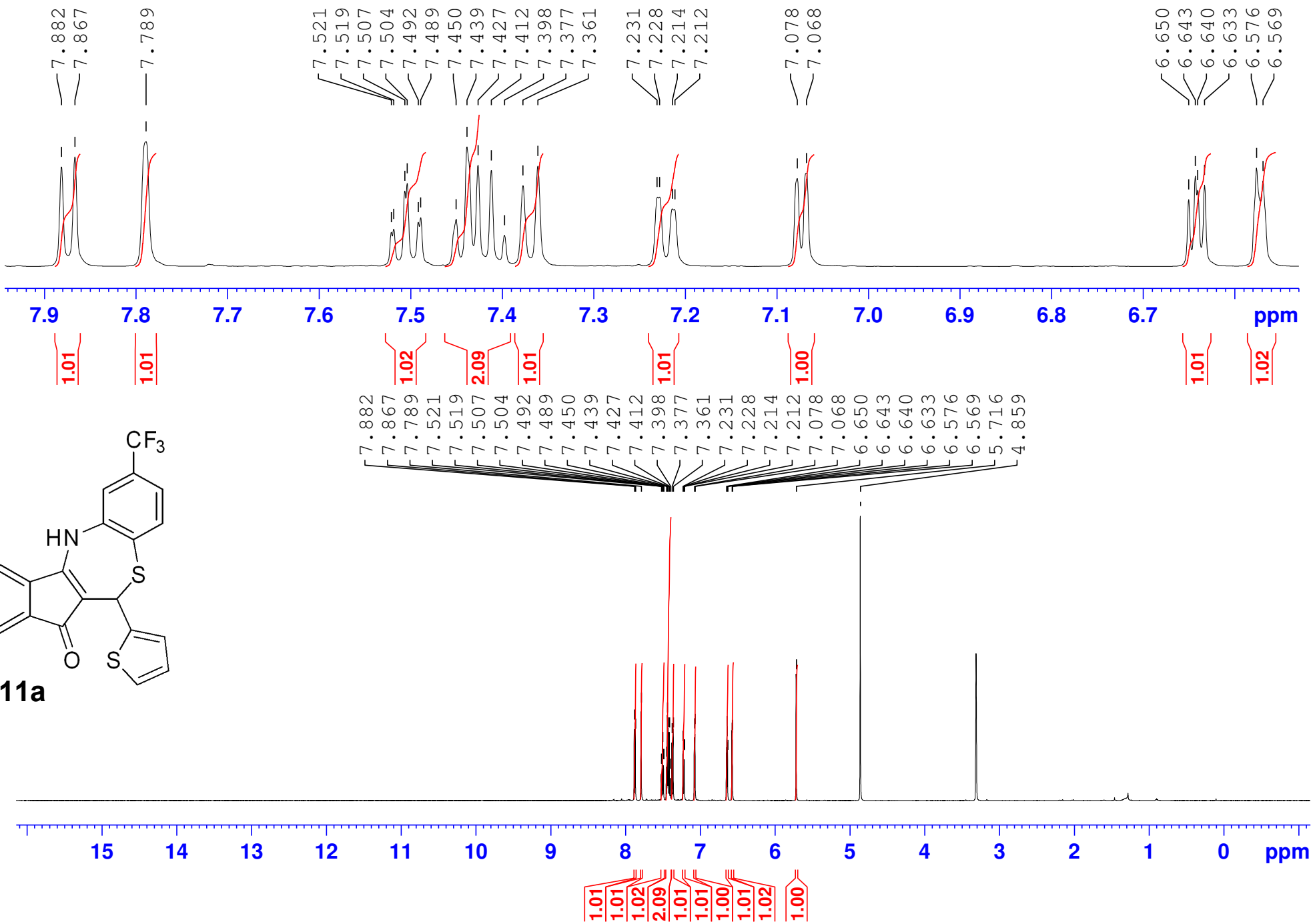
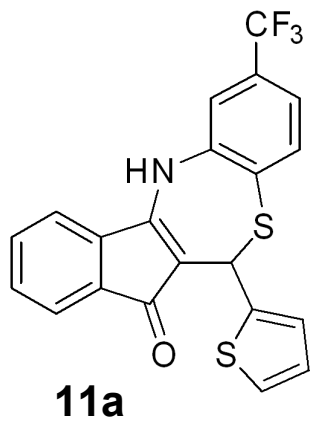
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.649	BB	0.1226	20.55055	2.09135	0.0555
2	13.931	VB R	0.0908	21.93307	3.28732	0.0592
3	14.559	BV	0.0928	33.31458	4.93156	0.0899
4	14.844	VV	0.0821	12.82092	2.10325	0.0346

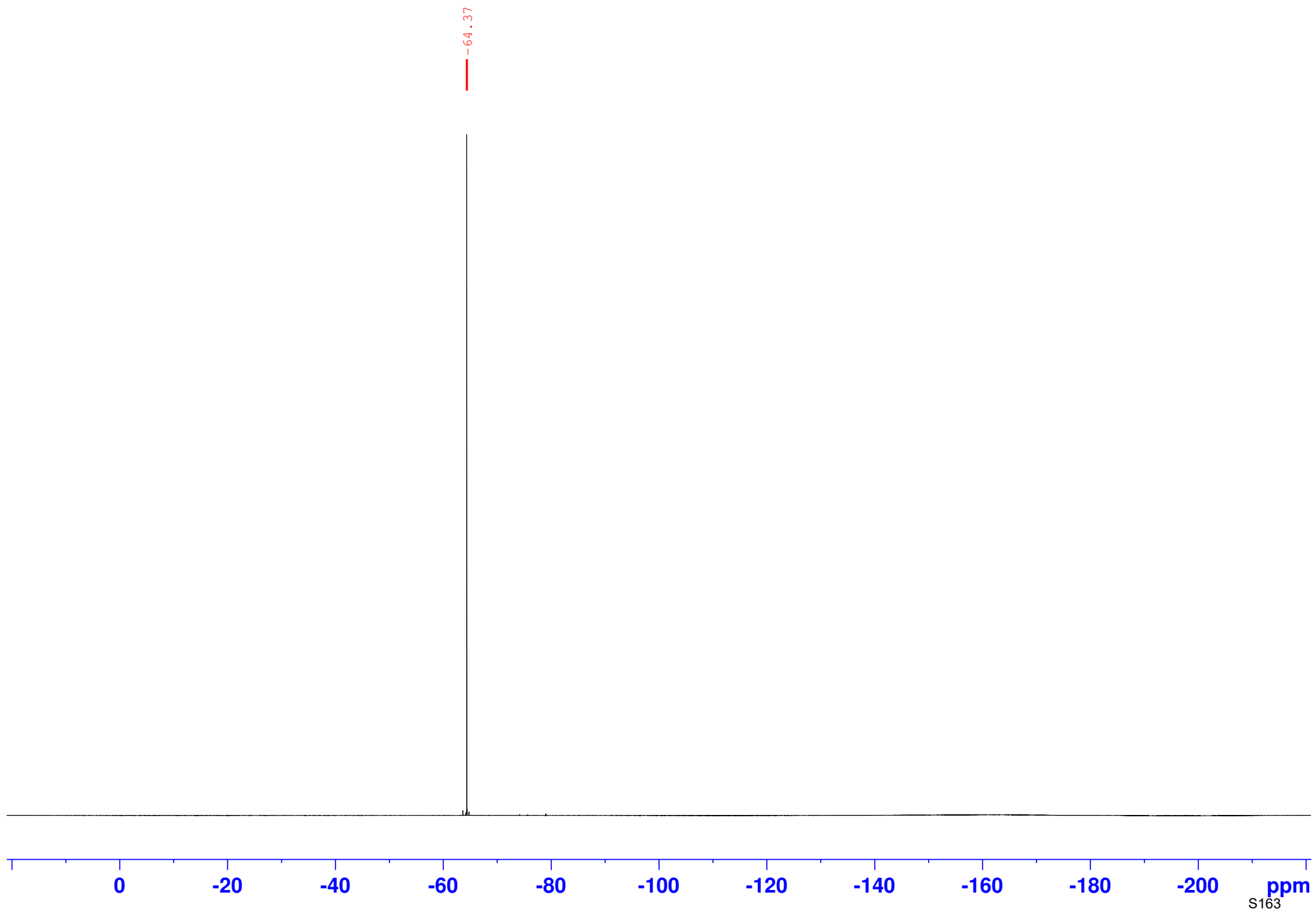
Sample Name: LJC 1-79

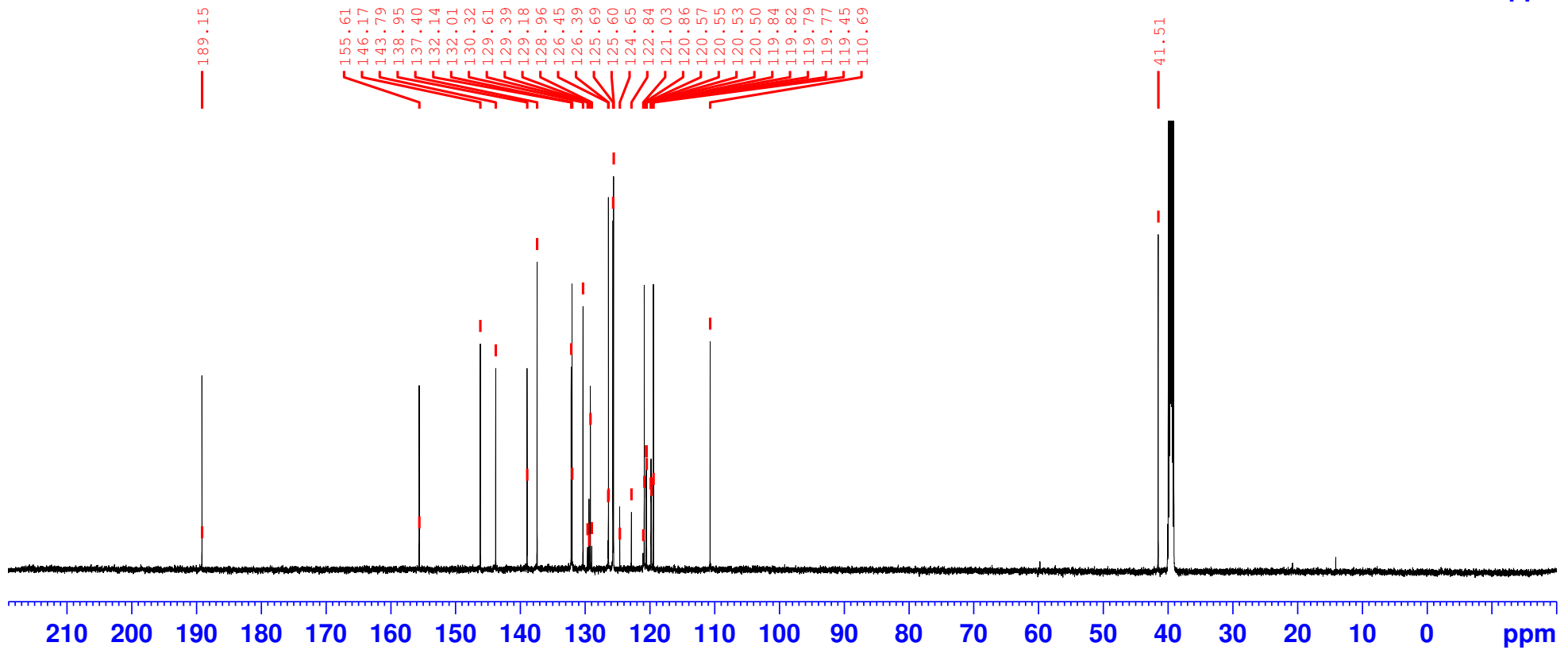
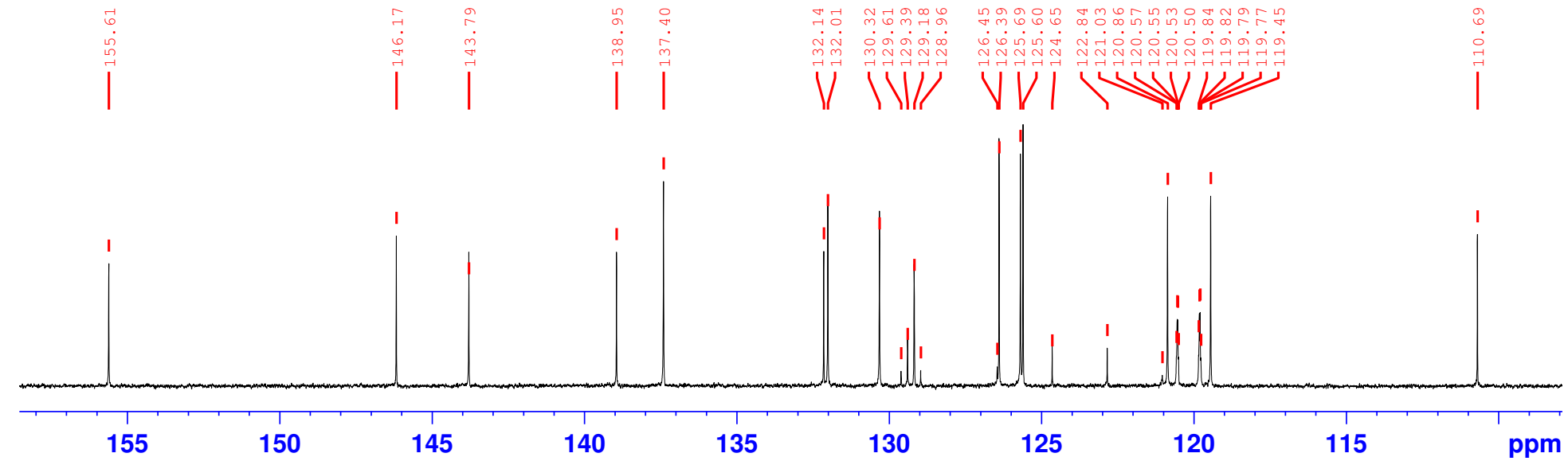
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	14.989	VB	0.0688	23.22619	4.94741	0.0627
6	15.278	BB	0.0772	19.17062	3.40290	0.0517
7	15.718	BV	0.0777	38.66483	7.13433	0.1044
8	16.055	VV	0.1539	267.20959	22.69629	0.7213
9	16.243	VB	0.0720	248.54134	50.43850	0.6709
10	16.708	VB	0.1168	22.43918	2.61044	0.0606
11	17.459	BV R	0.1337	3.57887e4	3704.77710	96.6014
12	17.994	VV E	0.0663	25.06681	5.58914	0.0677
13	18.297	VV E	0.0913	353.53152	54.08081	0.9543
14	18.429	VV E	0.0560	13.77770	3.49556	0.0372
15	18.548	VB E	0.0770	52.10620	9.64934	0.1406
16	19.467	BV	0.0813	15.09106	2.78262	0.0407
17	19.621	VV	0.0936	69.62948	10.20920	0.1879
18	19.733	VB	0.0634	22.03541	5.20063	0.0595

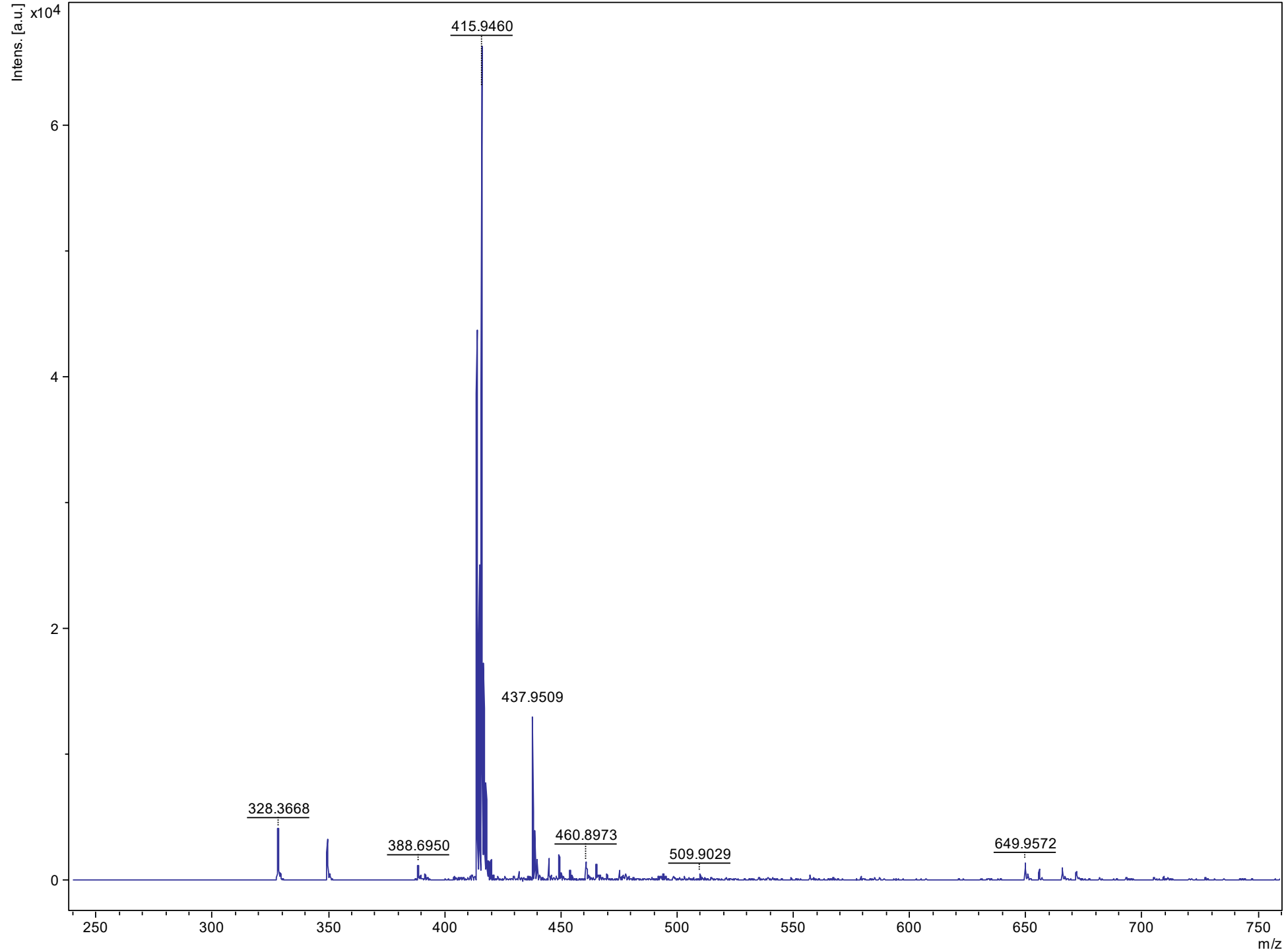
Totals : 3.70478e4 3899.42776

=====
*** End of Report ***









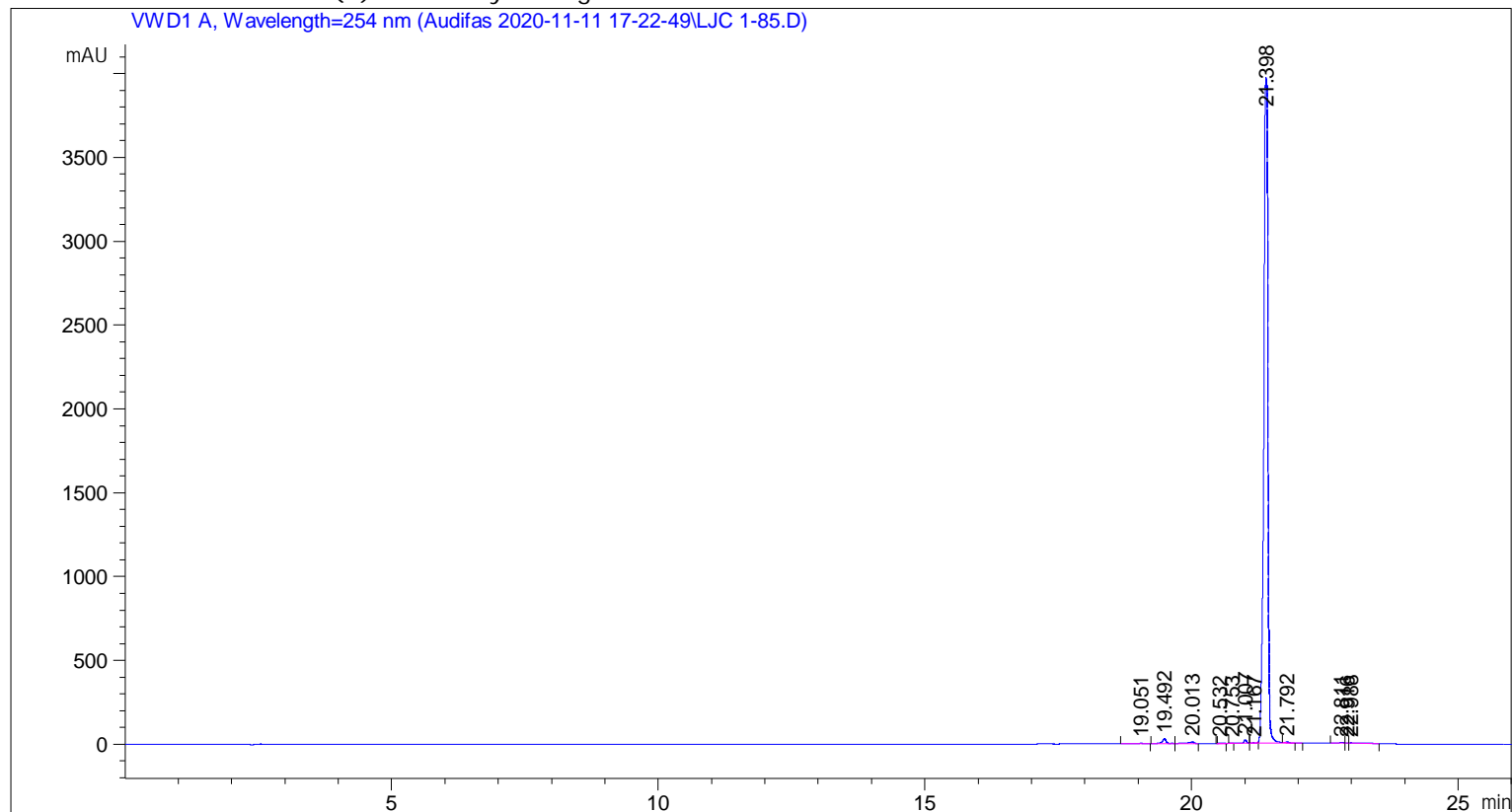
Sample Name: LJC 1-85

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    2
Acq. Instrument : 1220 HPLC                     Location  :    4
Injection Date  : 11/11/2020 5:52:23 PM      Inj       :    1
                                           Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\Audifas 2020-11-11 17-22-49\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 11/11/2020 5:22:52 PM by SYSTEM
Method Info     : Water/MeOH

Sample Info     : LJC 1-85
  
```

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====
  
```

```

Sorted By           :      Signal
Multiplier          :      1.0000
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.051	VB R	0.1591	39.64460	3.03182	0.1827
2	19.492	BV R	0.0751	151.18680	29.10480	0.6968
3	20.013	BB	0.1068	81.95588	10.30119	0.3777
4	20.532	BV E	0.0570	9.14087	2.31754	0.0421

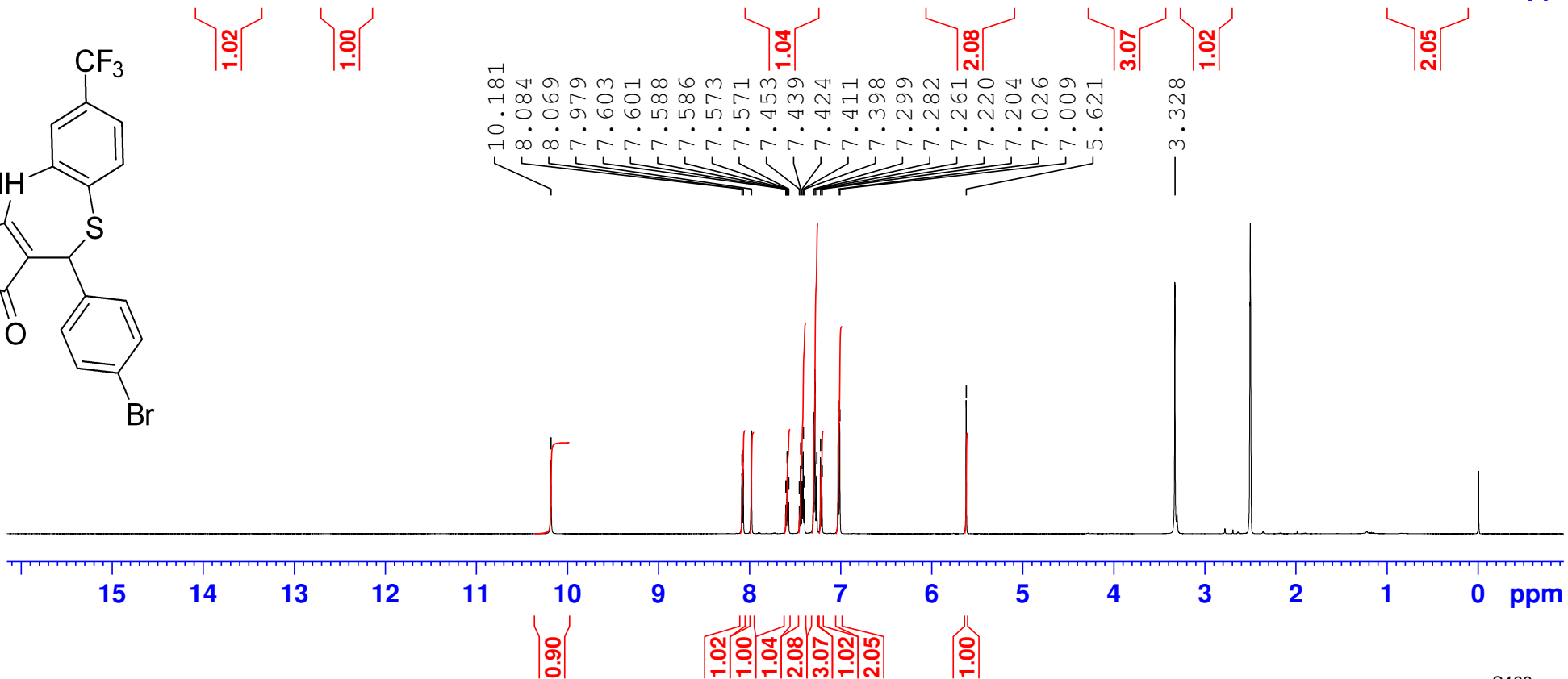
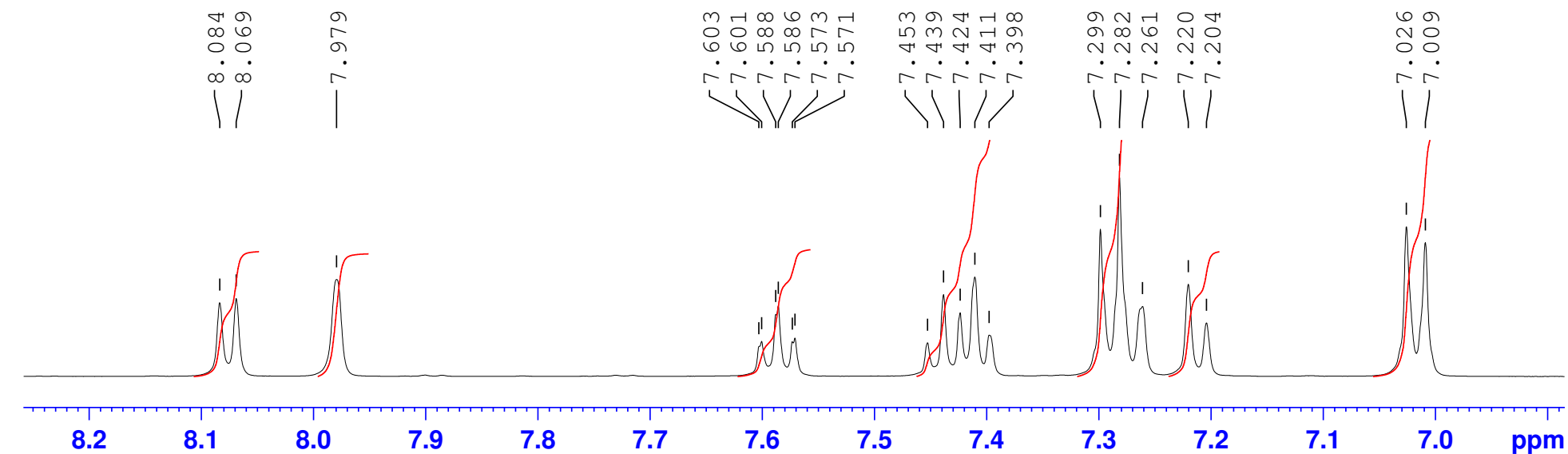
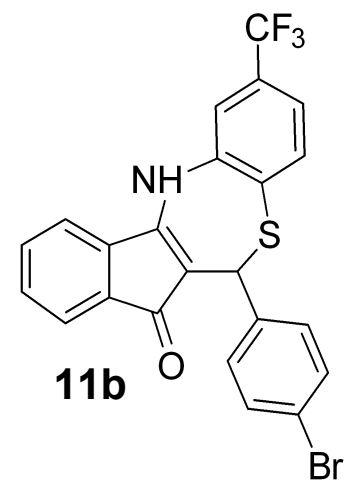
S166

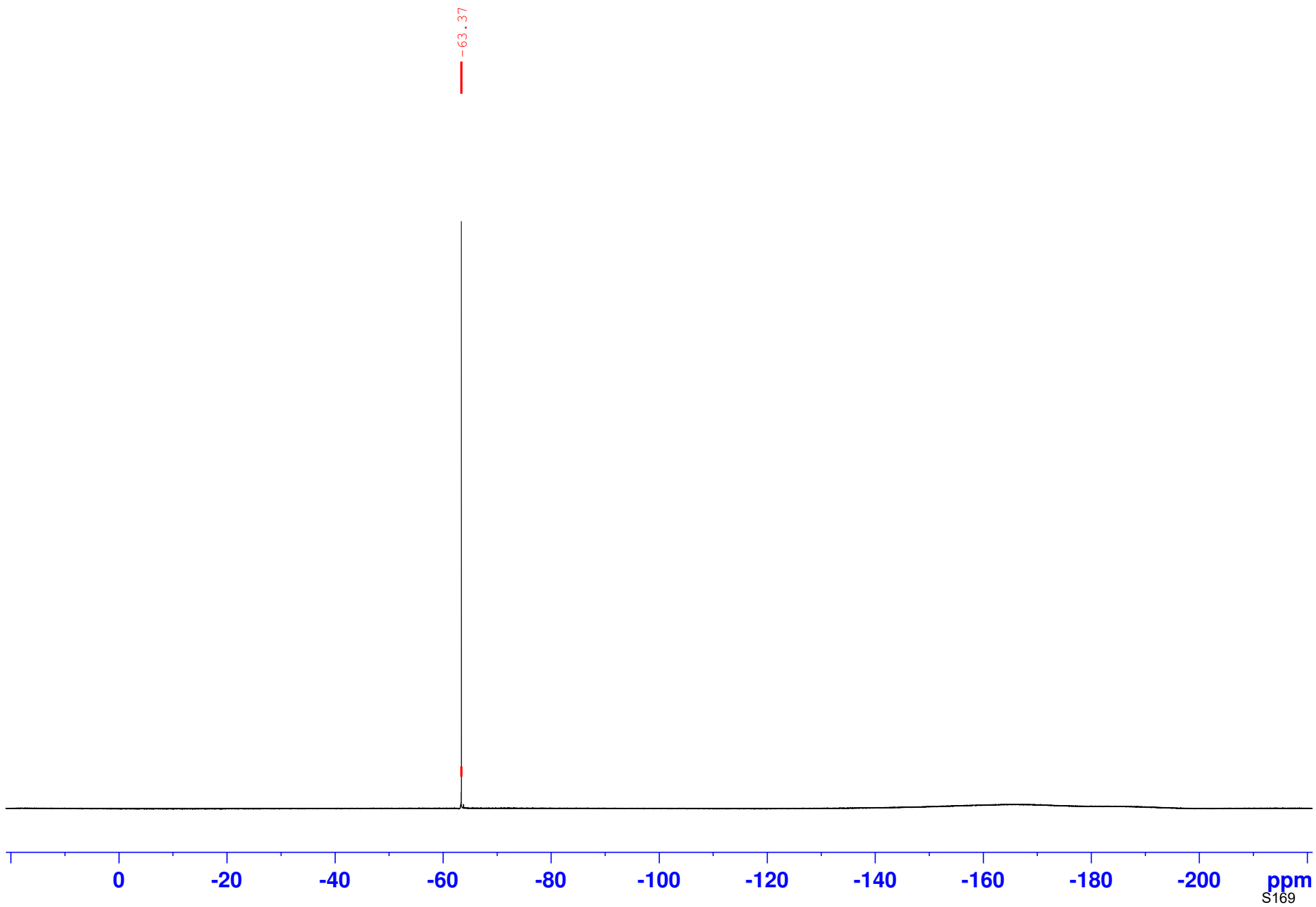
Sample Name: LJC 1-85

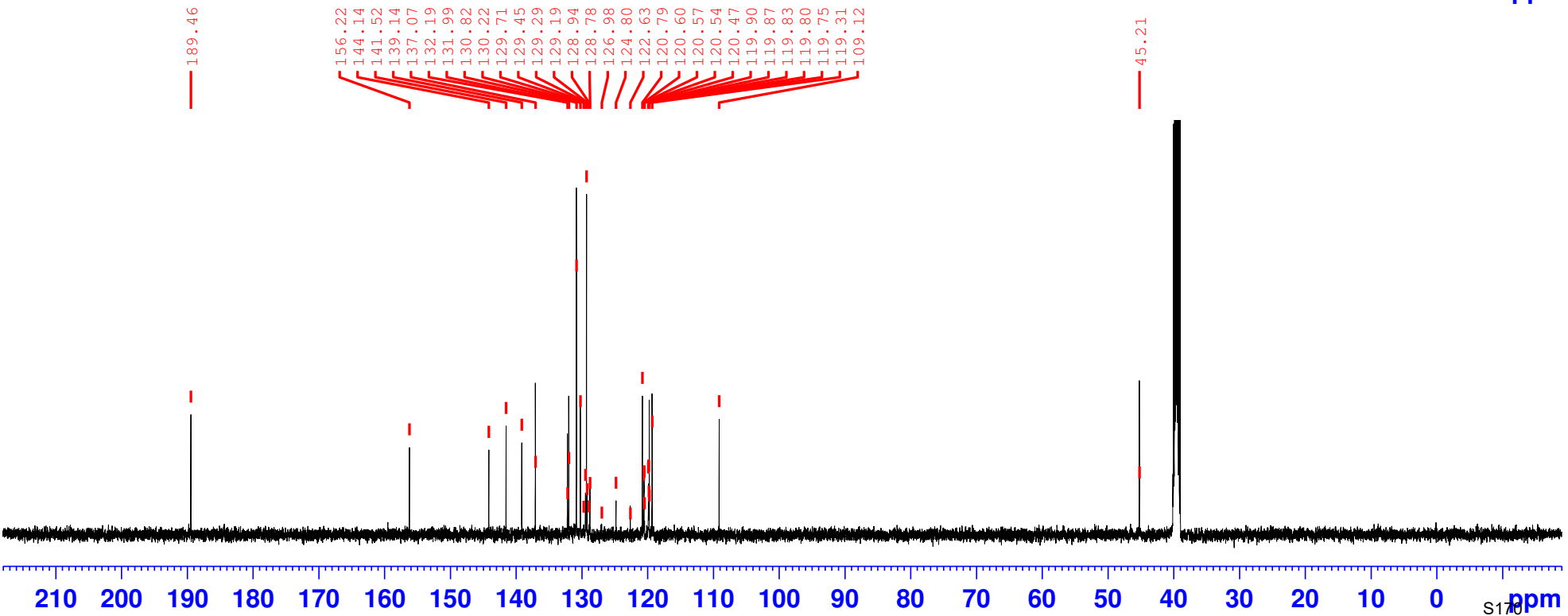
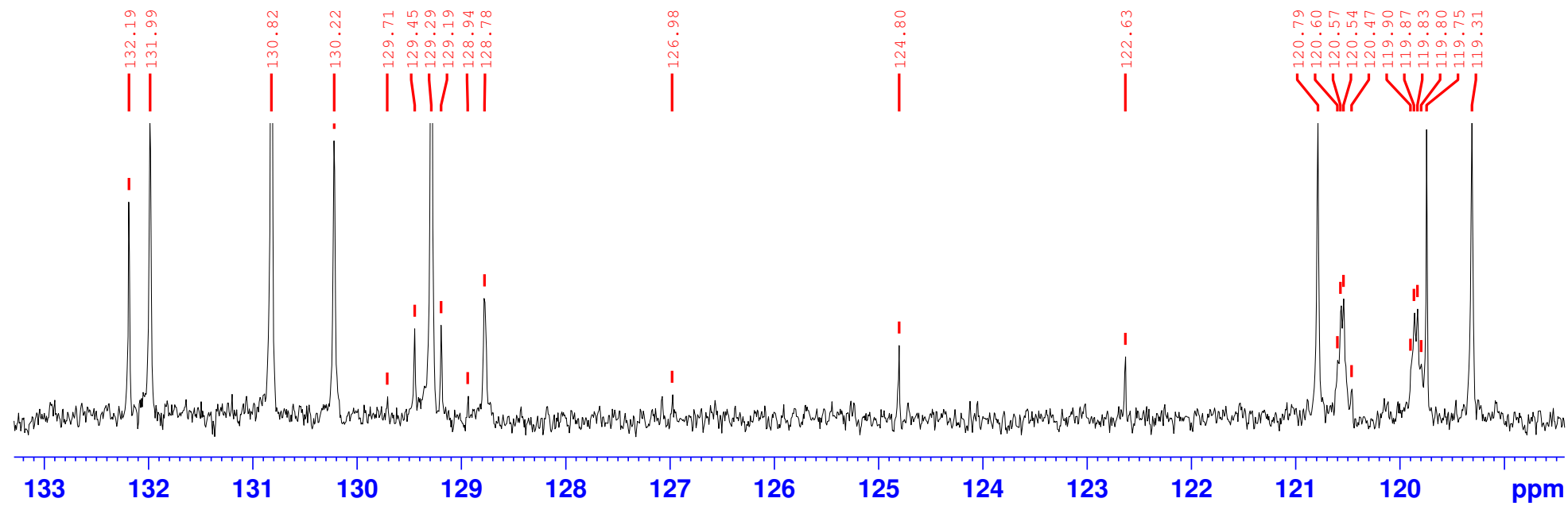
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	20.753	VV E	0.0447	5.68136	1.94046	0.0262
6	21.007	VB R	0.0564	83.93385	21.81769	0.3869
7	21.167	BV E	0.0608	12.68903	2.91231	0.0585
8	21.398	VV R	0.0729	2.11830e4	3962.42065	97.6362
9	21.792	VV E	0.0642	25.06209	5.54760	0.1155
10	22.811	VV R	0.0705	30.99144	6.13338	0.1428
11	22.916	VV	0.0519	8.87932	2.36049	0.0409
12	22.988	VB	0.2403	63.67598	3.17738	0.2935

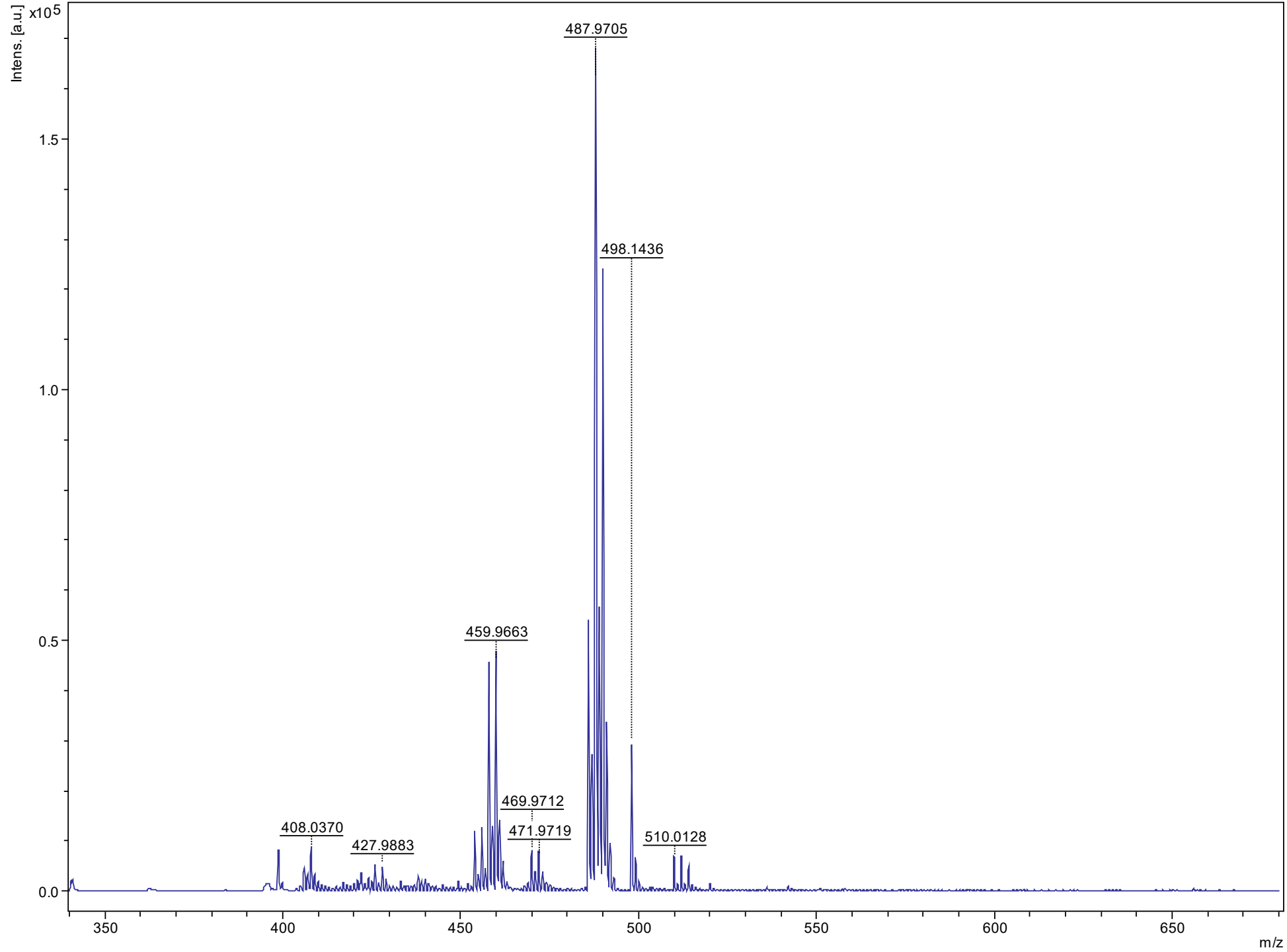
Totals : 2.16958e4 4051.06532

=====
*** End of Report ***









Sample Name: LJC1-77

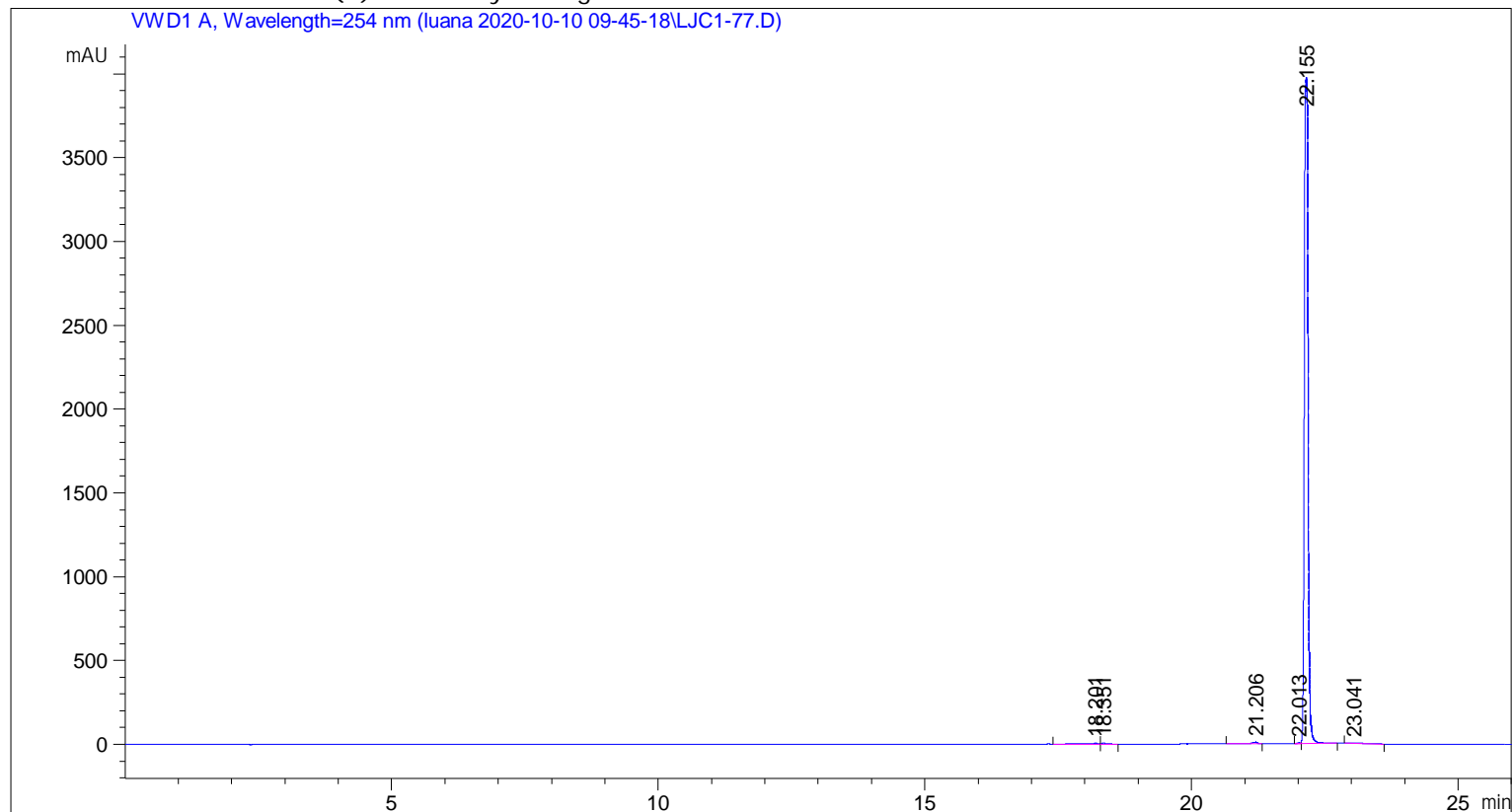
```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    7
Acq. Instrument : 1220 HPLC                   Location  :   15
Injection Date  : 10/10/2020 12:31:07 PM     Inj       :    1
                                           Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-10-10 09-45-18\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 10/10/2020 10:17:41 AM by SYSTEM
Method Info     : Water/MeOH

Sample Info     : LJC1-77

```

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====

```

```

Sorted By           :      Signal
Multiplier          :      1.0000
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

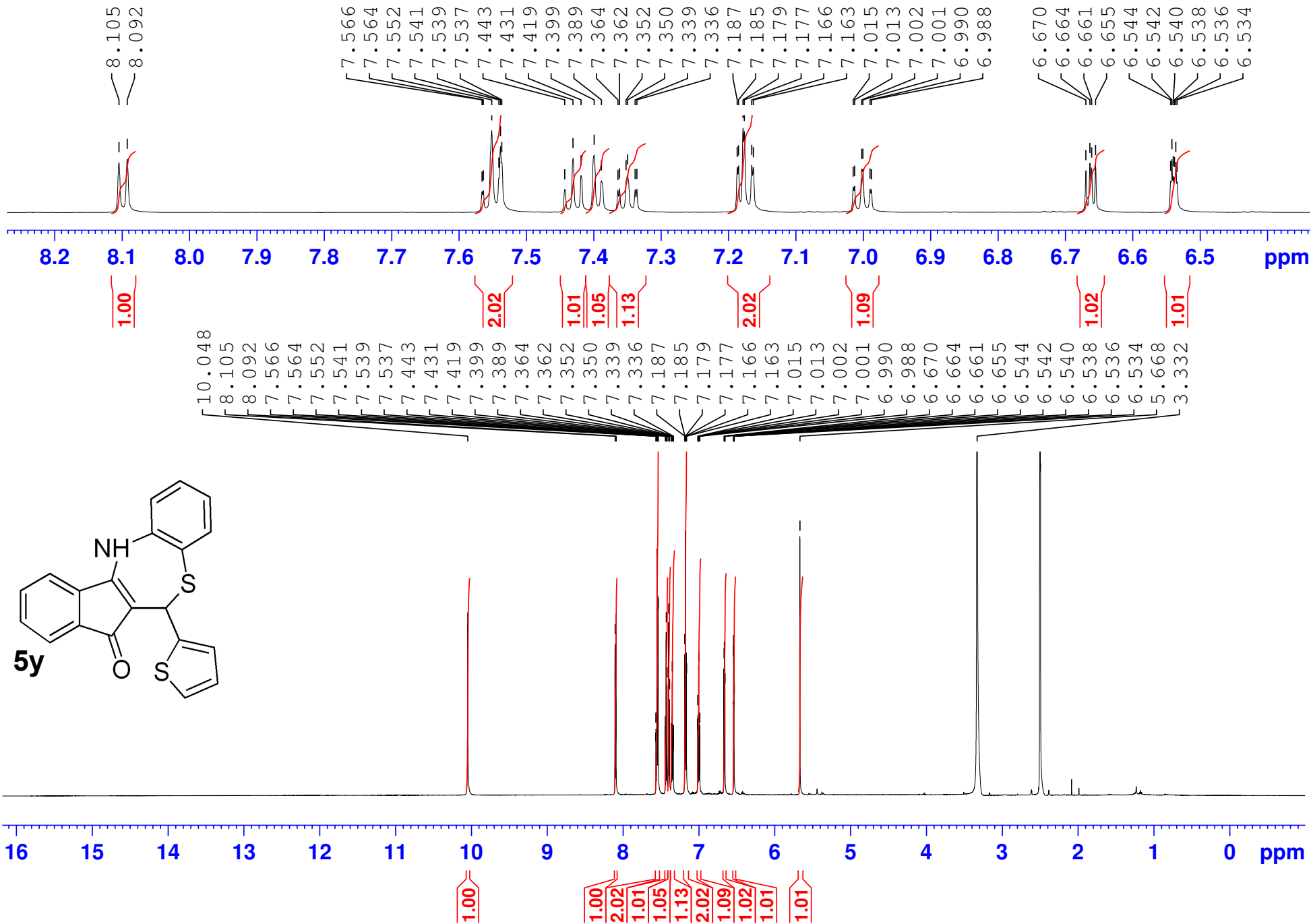
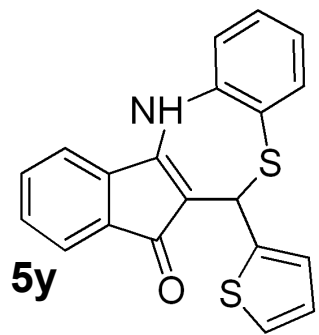
Signal 1: VWD1 A, Wavelength=254 nm

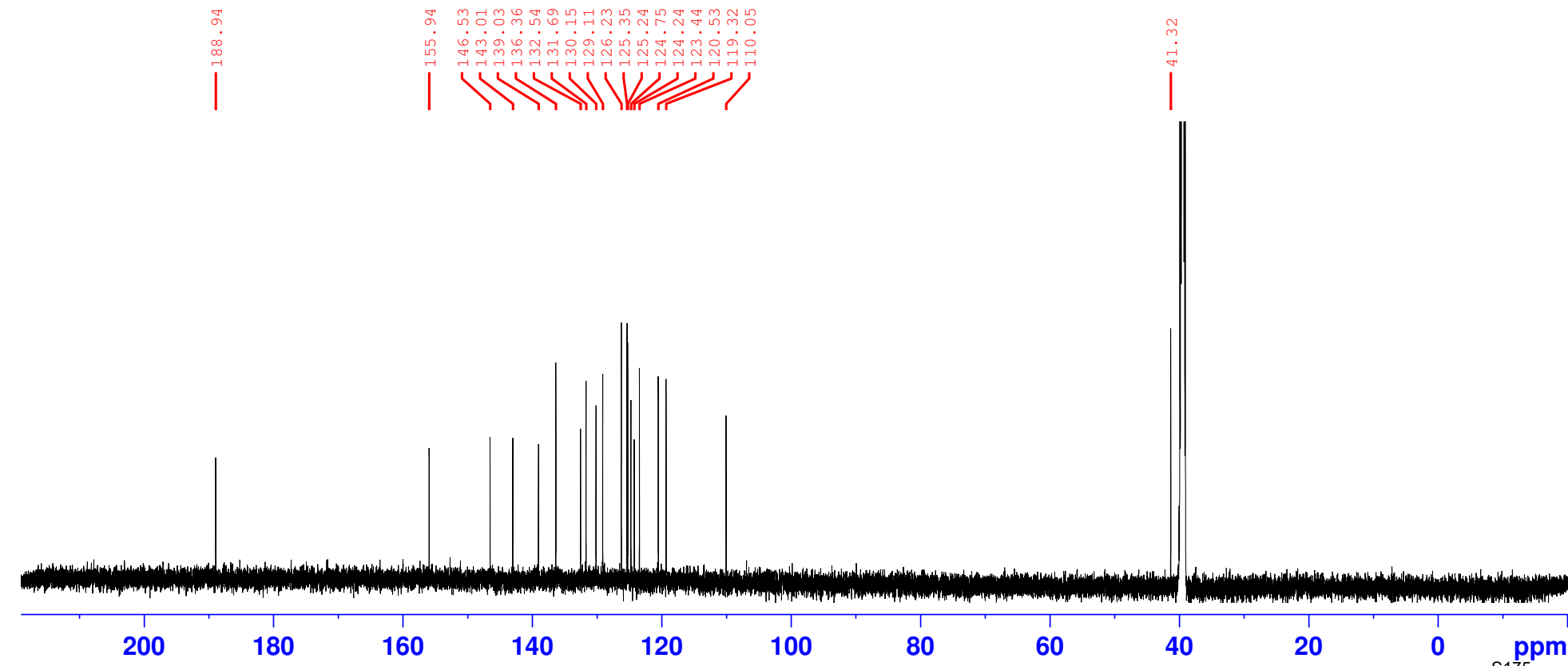
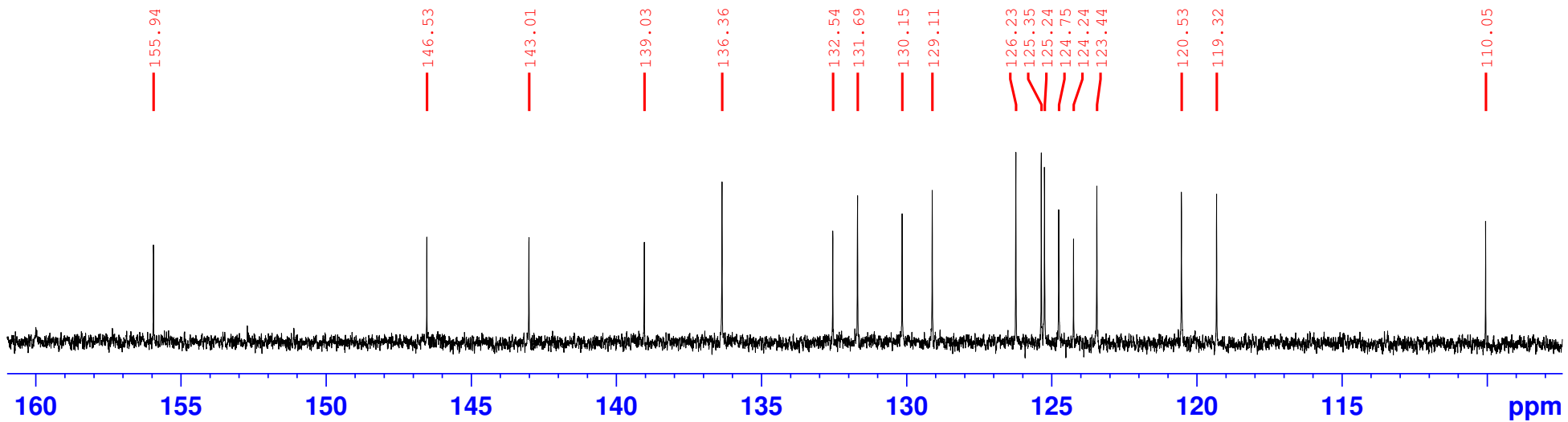
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.201	BV	0.2573	97.64452	4.44441	0.4965
2	18.351	VB	0.1076	40.13965	4.87056	0.2041
3	21.206	VB R	0.1084	84.85110	10.21556	0.4315
4	22.013	BV E	0.0524	20.70164	5.98061	0.1053

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	22.155	VV R	0.0585	1.93762e4	3968.03247	98.5324
6	23.041	VB R	0.1424	45.25863	4.00457	0.2301

Totals : 1.96648e4 3997.54817

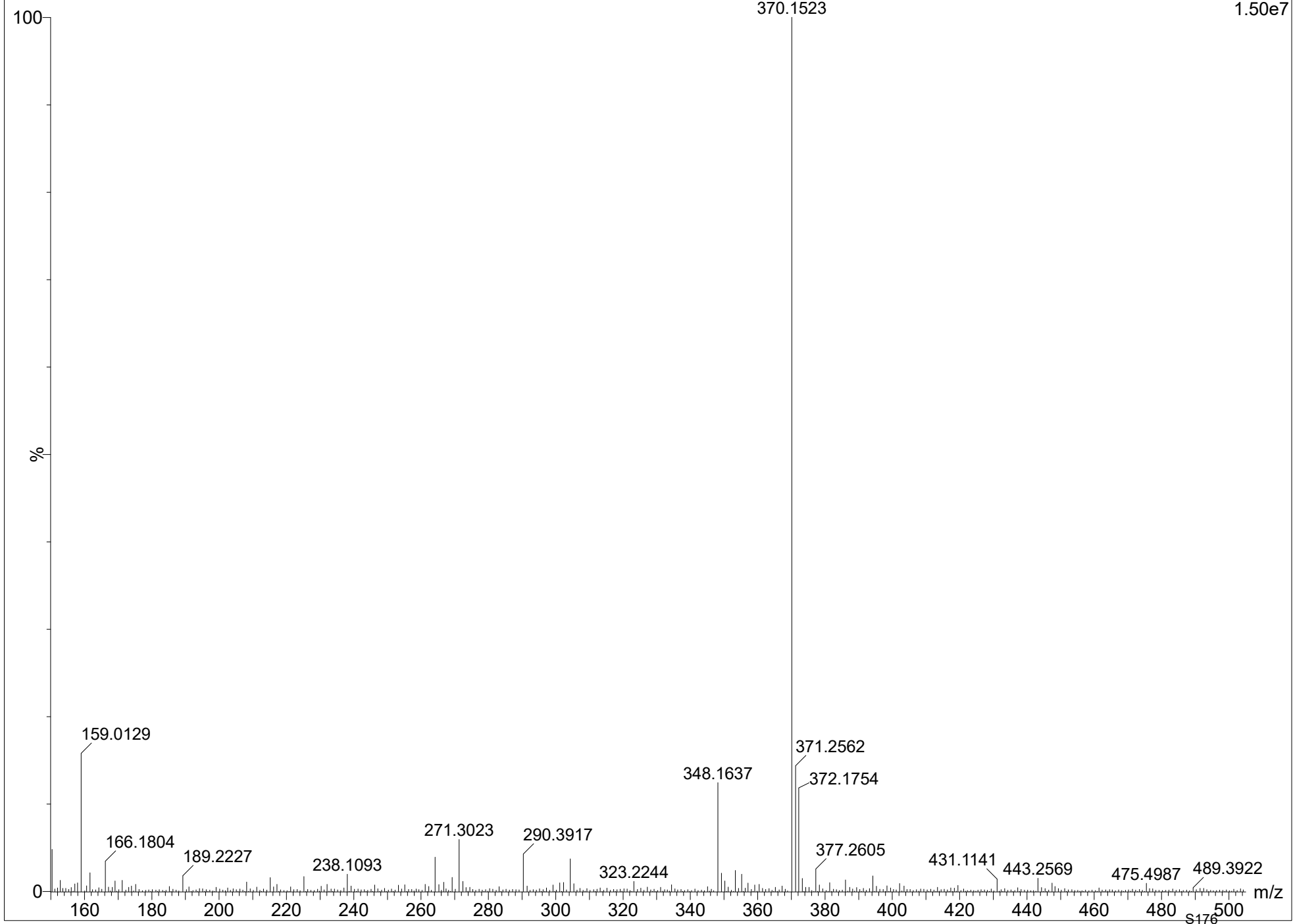
=====
*** End of Report ***





MAS-1-86 83 (1.395) Cm (3:120)

Scan ES+
1.50e7



Sample Name: MAS 1-86

```

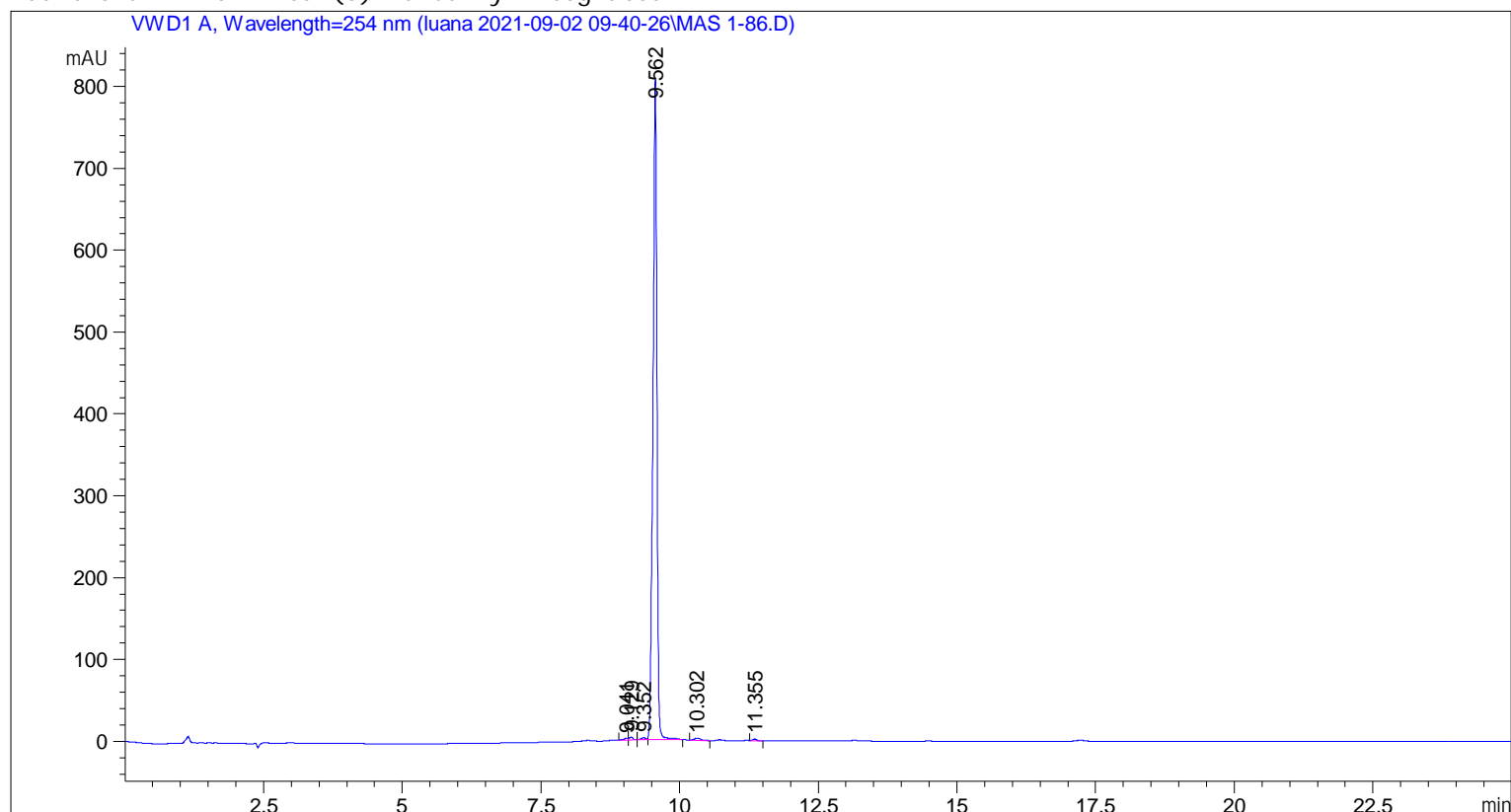
=====
Acq. Operator   : SYSTEM                      Seq. Line :    5
Acq. Instrument : 1220 HPLC                    Location  :   67
Injection Date  : 9/2/2021 11:20:56 AM      Inj       :    1
                                           Inj Volume: 50.000 µl

Acq. Method    : C:\Chem32\1\Data\luana 2021-09-02 09-40-26\Luana_small_molecule.M
Last changed   : 9/2/2021 10:12:00 AM by SYSTEM
Analysis Method: C:\Chem32\1\Data\luana 2021-09-02 09-40-26\Luana_small_molecule.M (Sequence
Method)
Last changed   : 9/2/2021 10:25:25 AM by SYSTEM
Method Info    : MeOH/water

Sample Info    : MAS 1-86

```

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

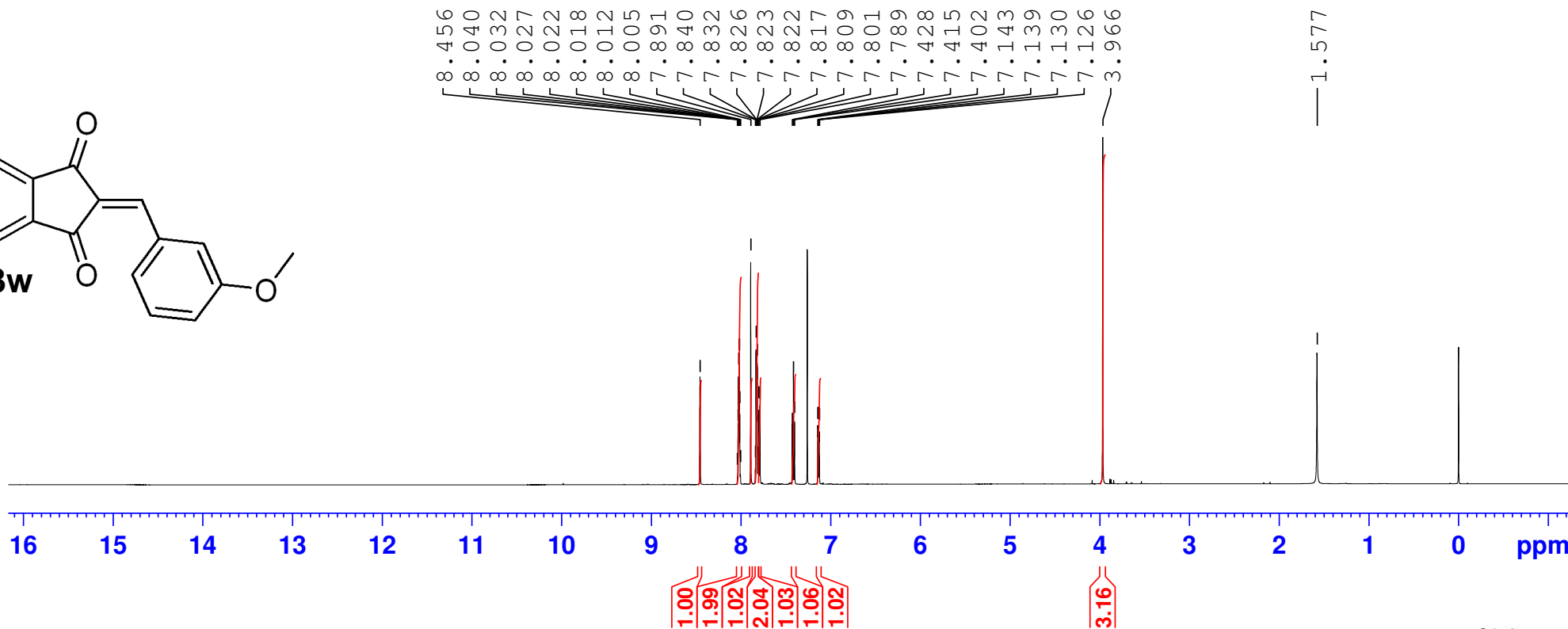
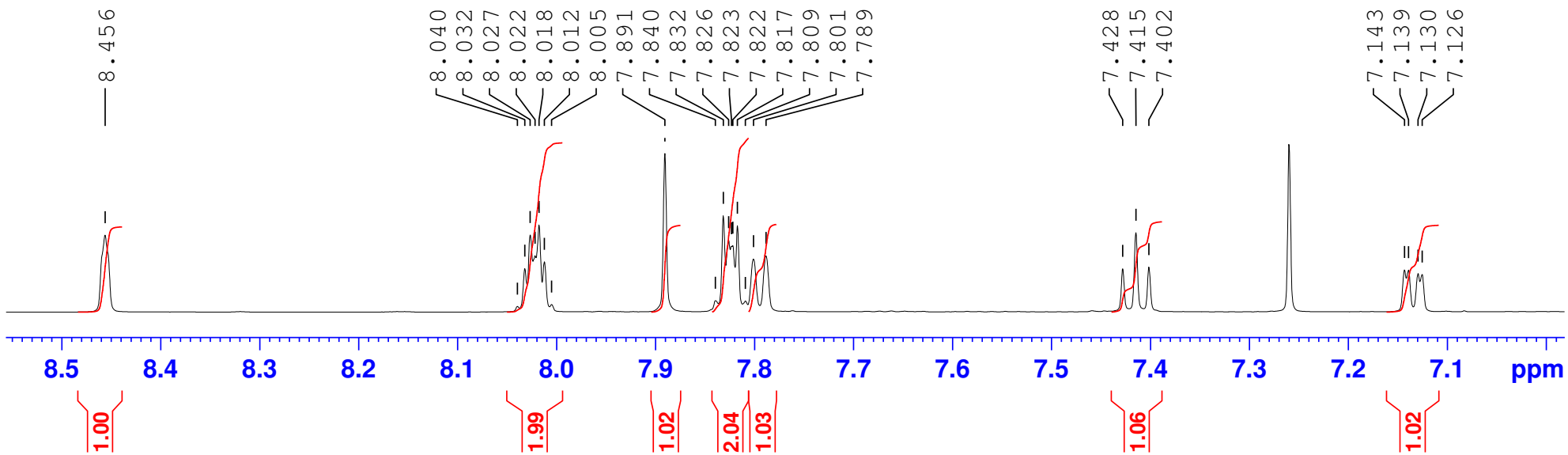
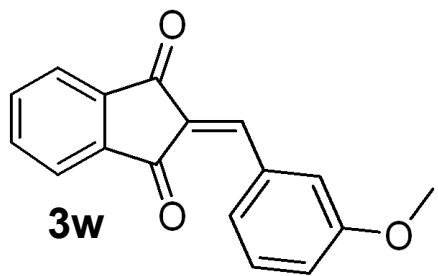
Signal 1: VWD1 A, Wavelength=254 nm

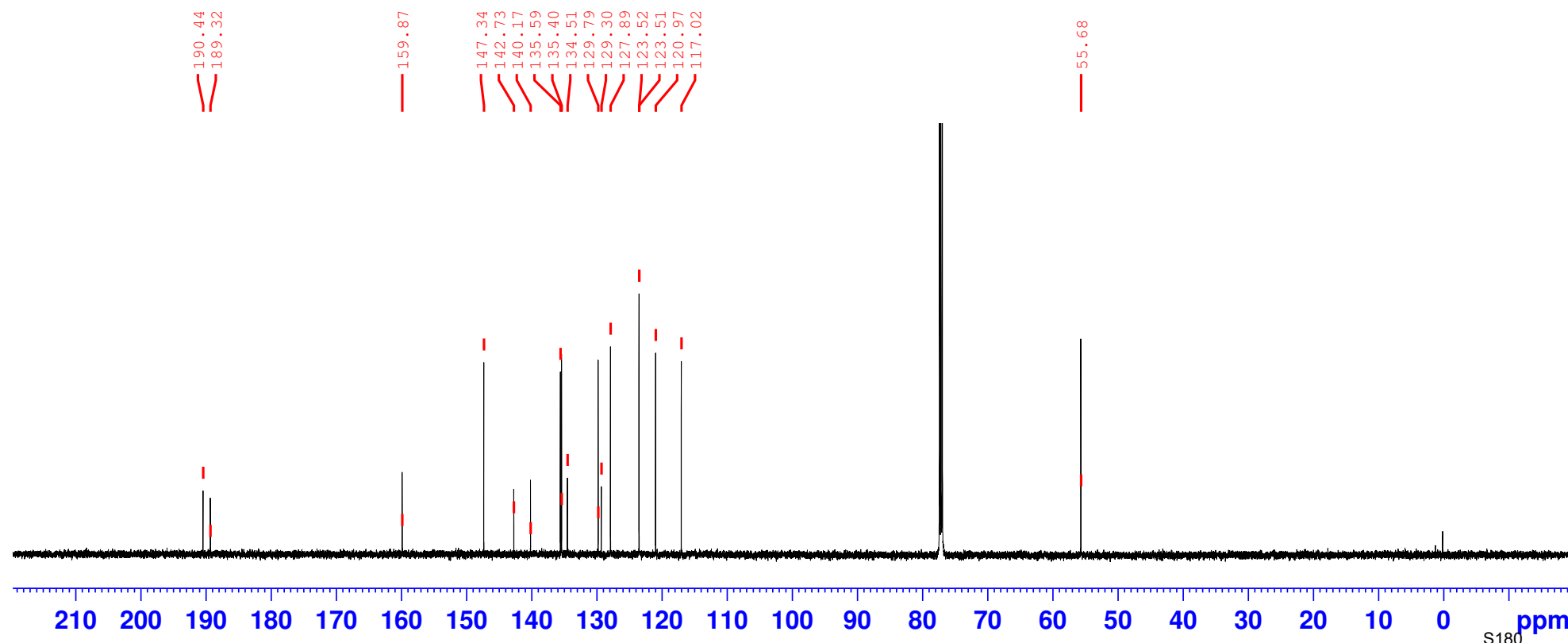
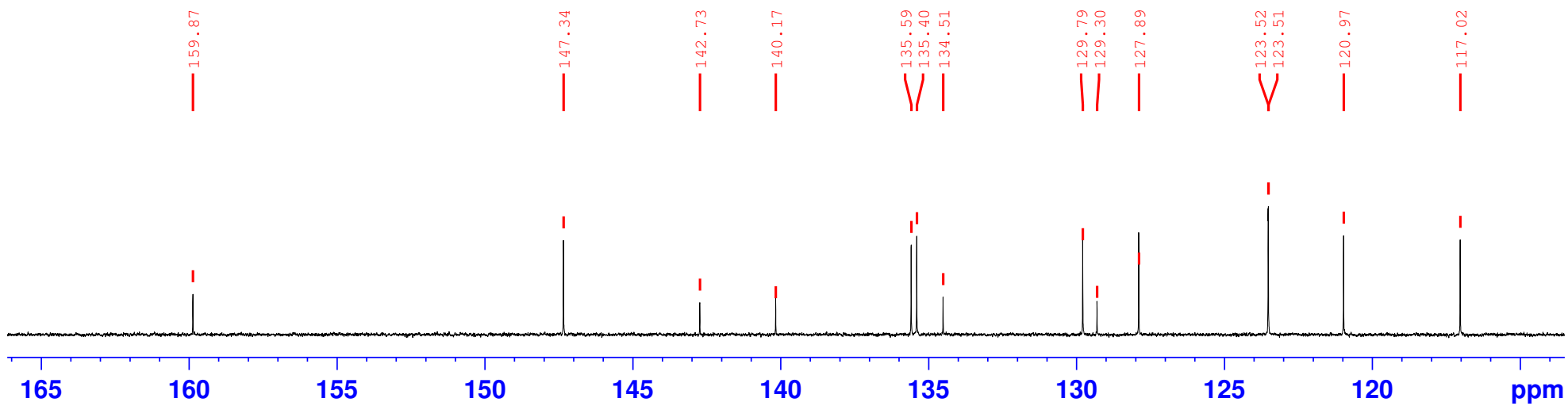
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.041	BV	0.0704	10.51690	2.17390	0.2579
2	9.129	VB	0.0662	14.83191	3.31304	0.3637
3	9.352	BV E	0.0740	13.16839	2.55932	0.3229

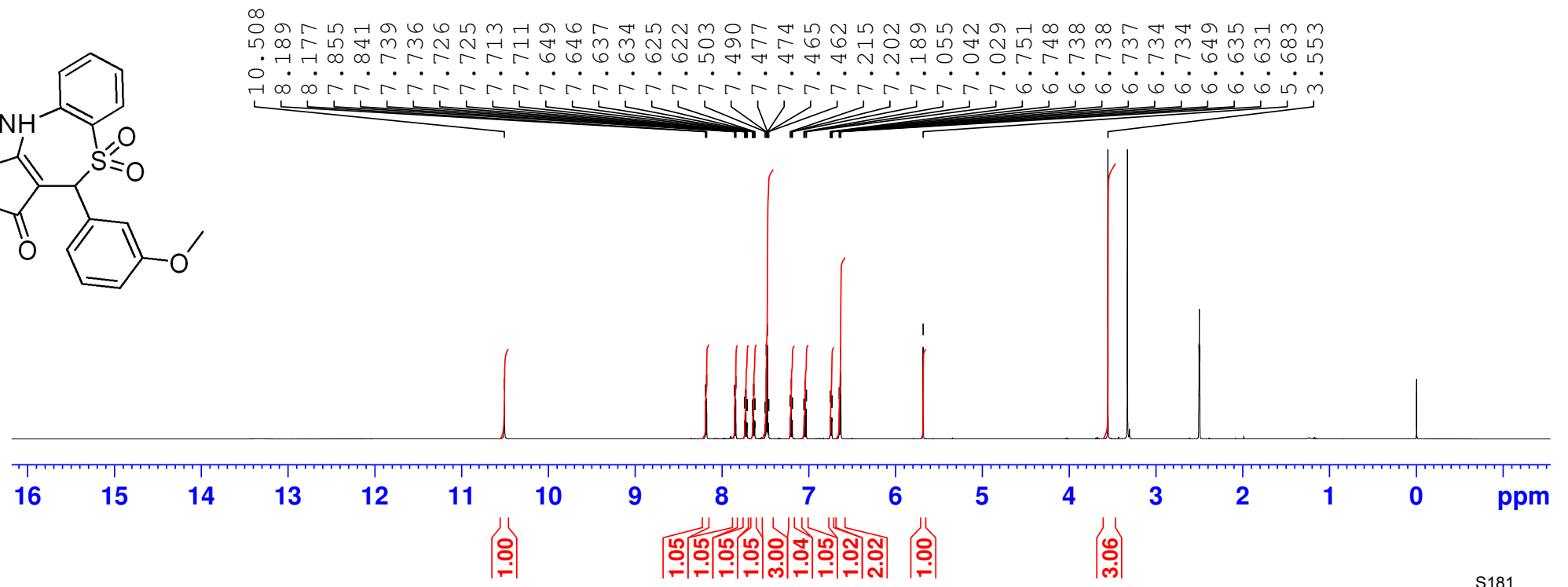
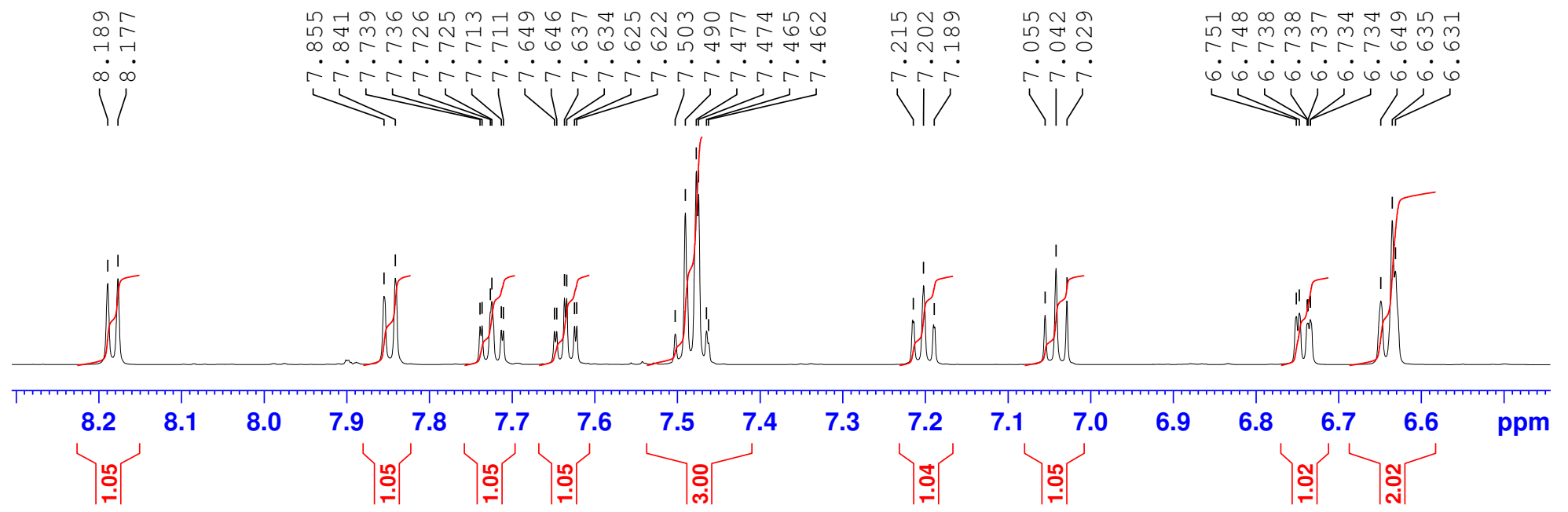
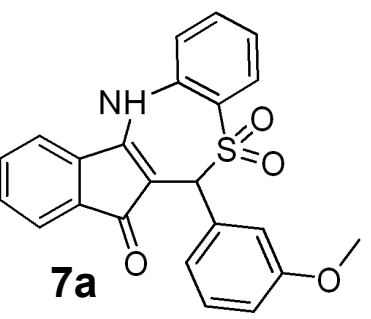
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
4	9.562	VV R	0.0730	4008.14185	806.80585	98.2792
5	10.302	BB	0.1155	20.46943	2.35254	0.5019
6	11.355	VB	0.0780	11.19344	2.17644	0.2745

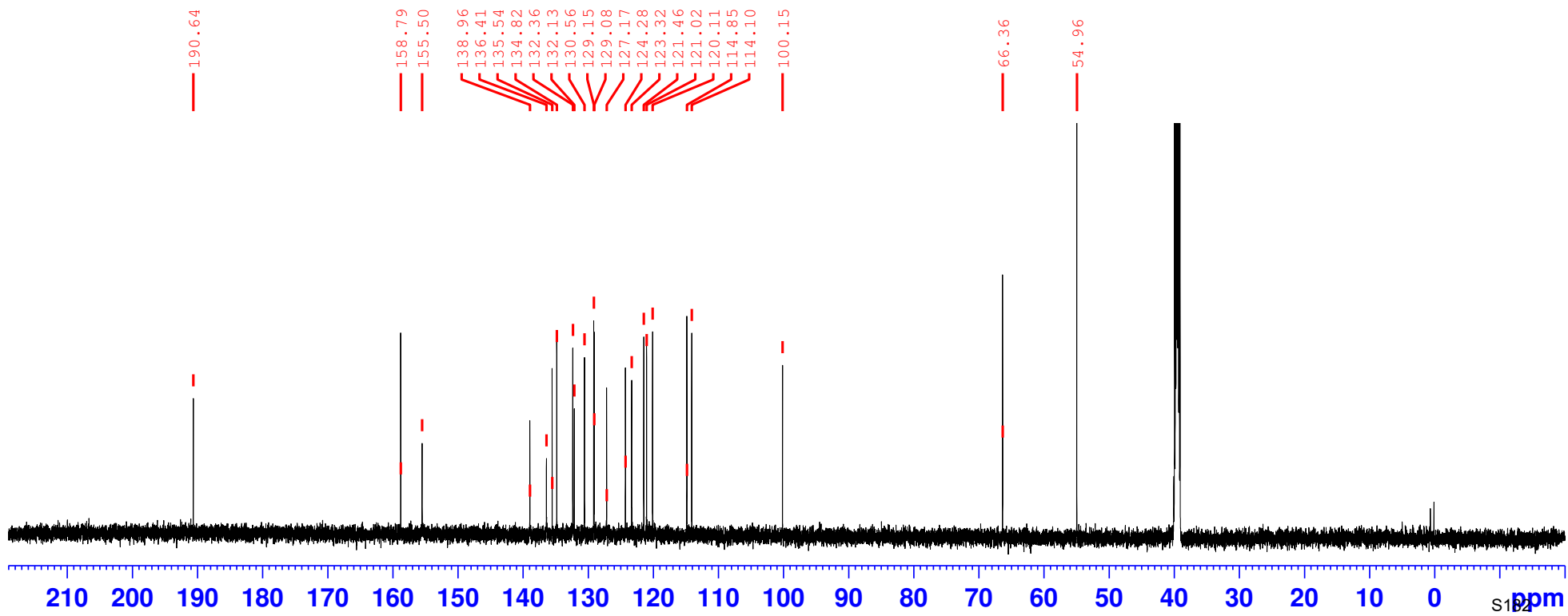
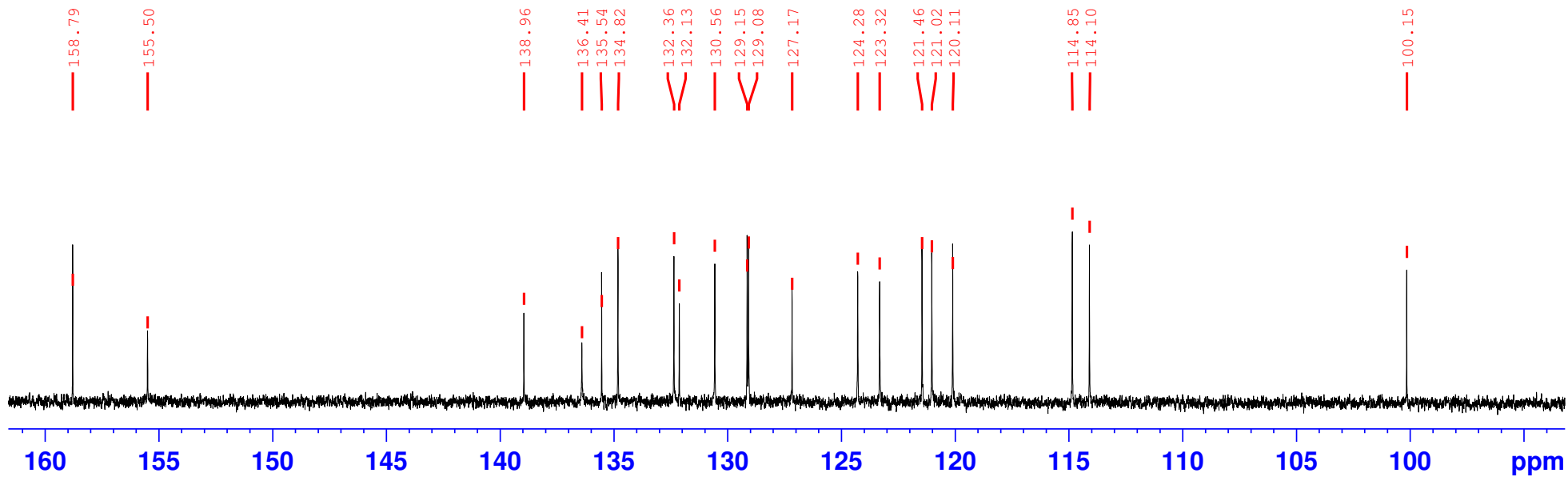
Totals : 4078.32192 819.38109

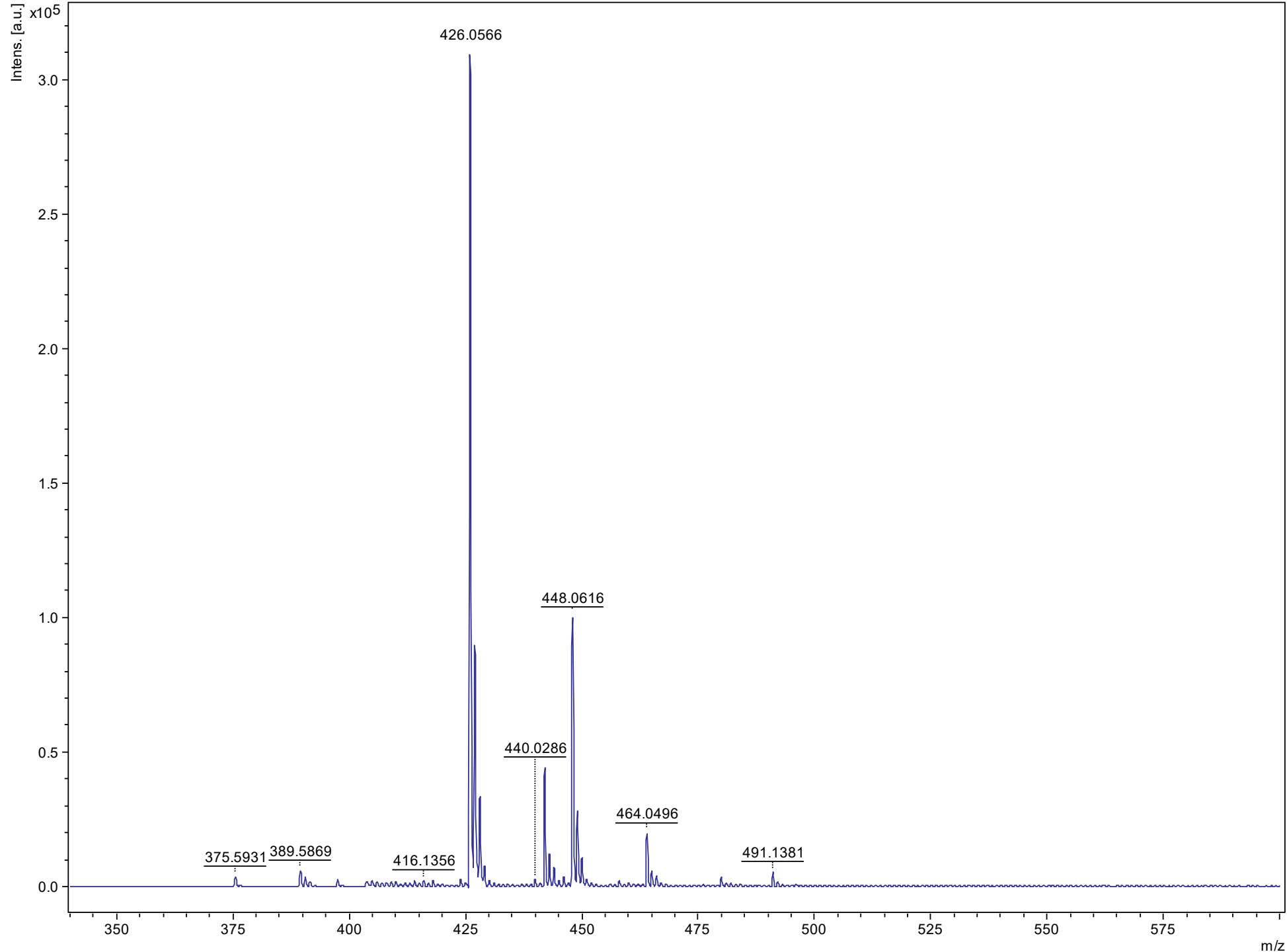
=====
*** End of Report ***











Sample Name: MAS 1-89

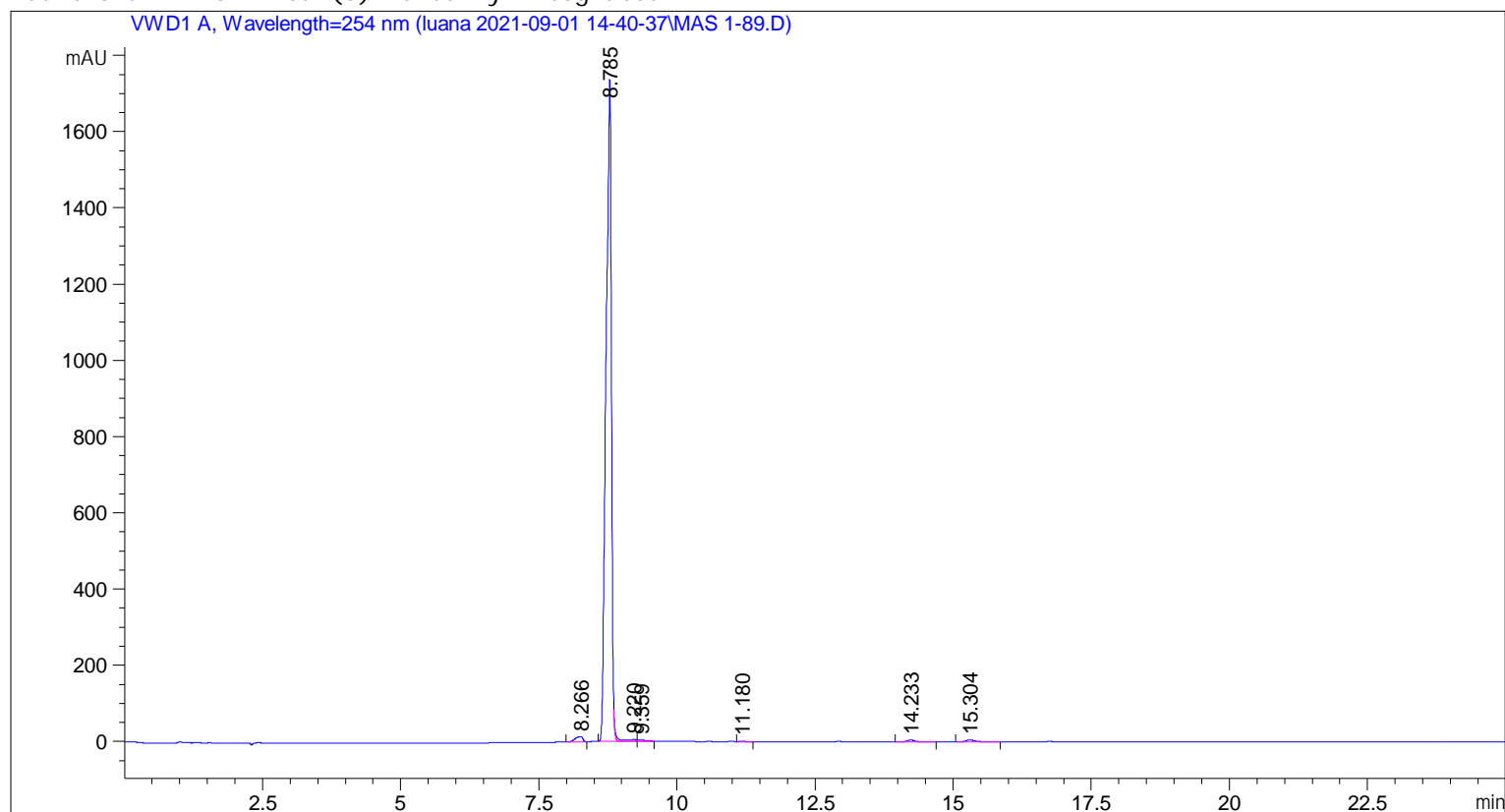
```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    4
Acq. Instrument : 1220 HPLC                   Location  :   64
Injection Date  : 9/1/2021 3:45:56 PM       Inj       :    1
                                           Inj Volume: 50.000 µl

Acq. Method    : C:\Chem32\1\Data\luana 2021-09-01 14-40-37\Luana_small_molecule.M
Last changed   : 9/1/2021 3:22:09 PM by SYSTEM
Analysis Method : C:\Chem32\1\Data\luana 2021-09-01 14-40-37\Luana_small_molecule.M (Sequence
Method)
Last changed   : 9/1/2021 3:44:43 PM by SYSTEM
Method Info    : MeOH/water

Sample Info    : MAS 1-89
  
```

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====
  
```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

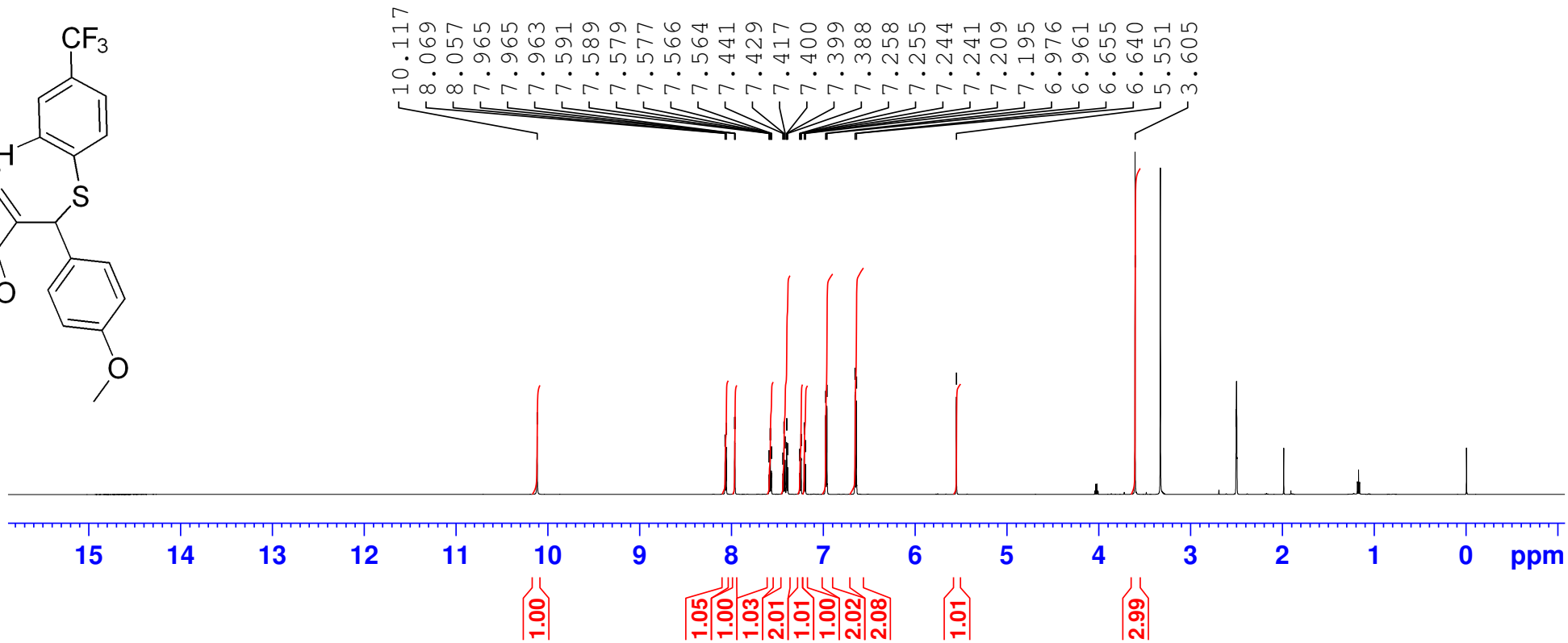
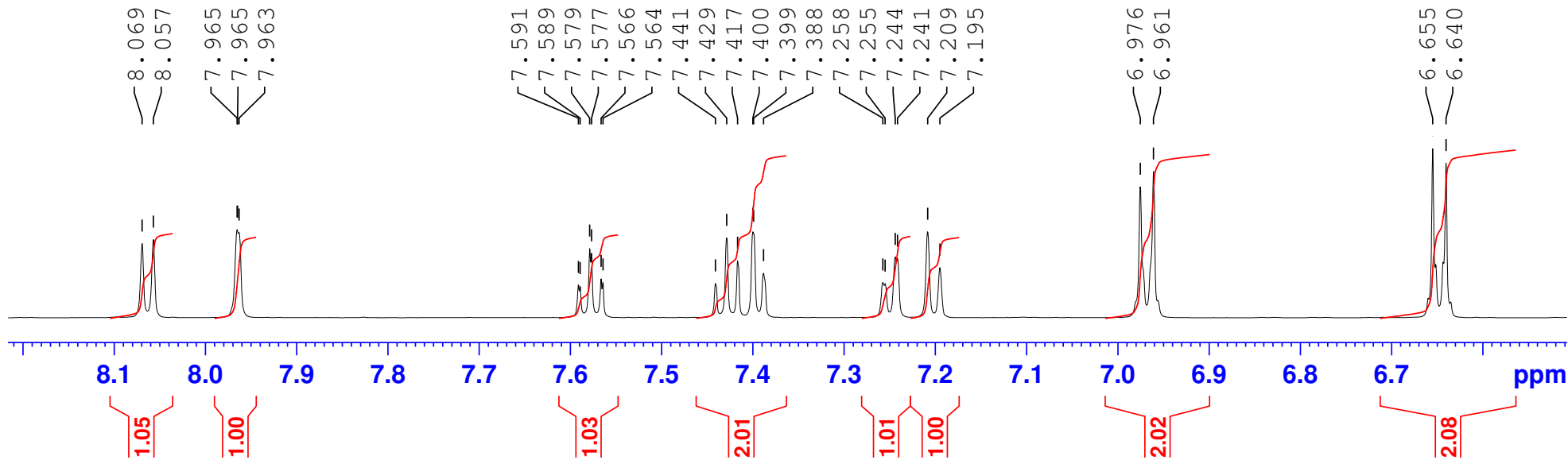
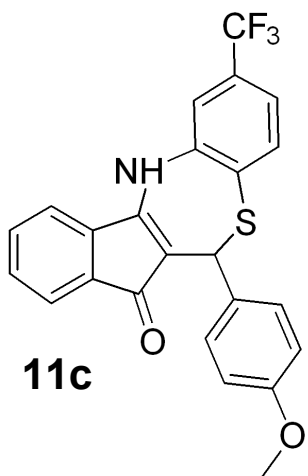
Signal 1: VWD1 A, Wavelength=254 nm

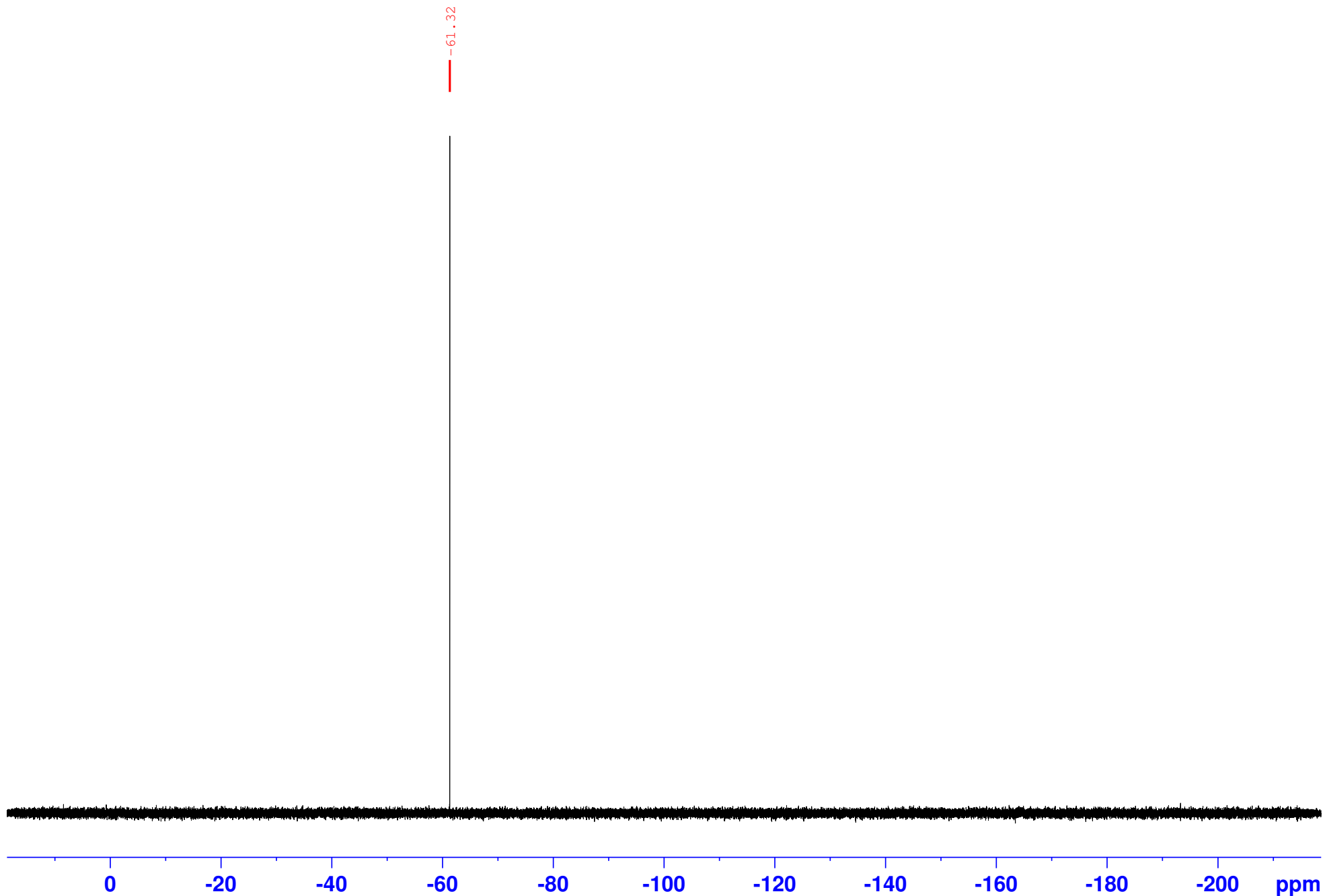
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.266	BB	0.1293	135.62256	13.60912	1.1246
2	8.785	BV R	0.0914	1.16741e4	1736.51917	96.8028
3	9.220	VV E	0.2645	99.85096	4.65096	0.8280

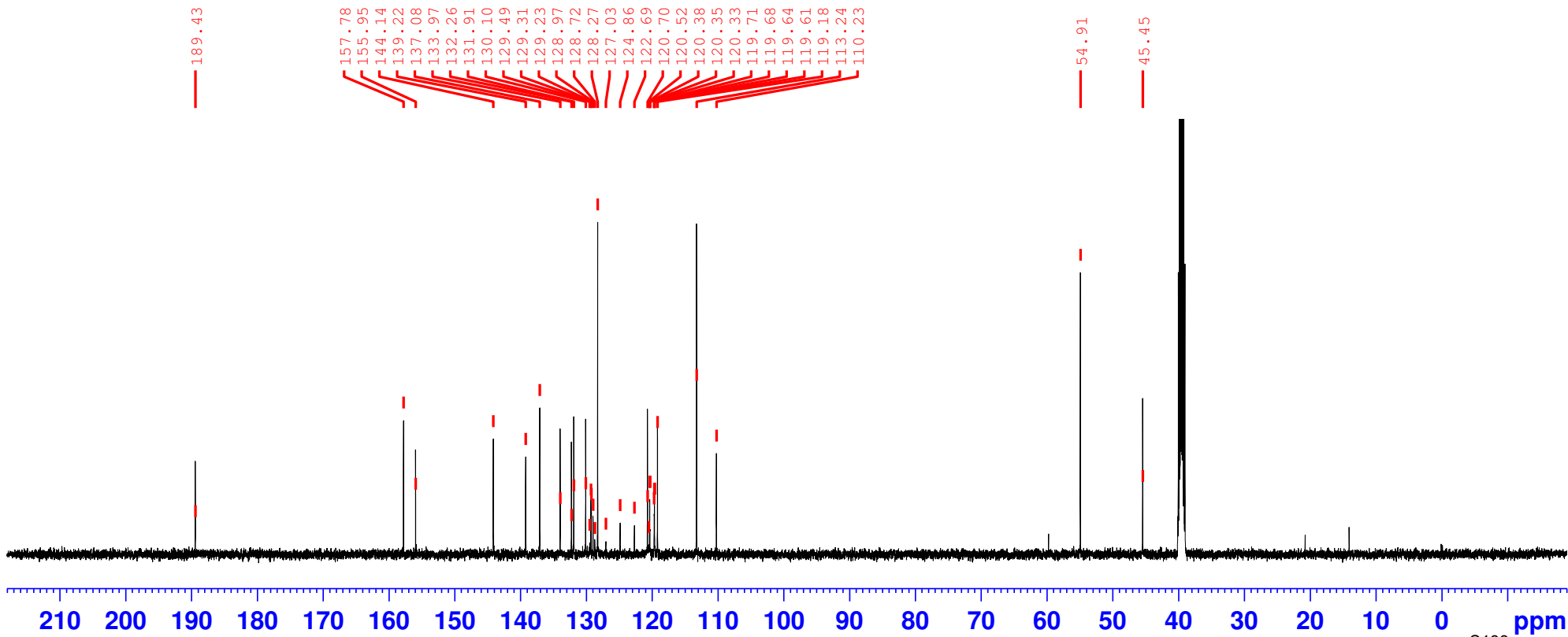
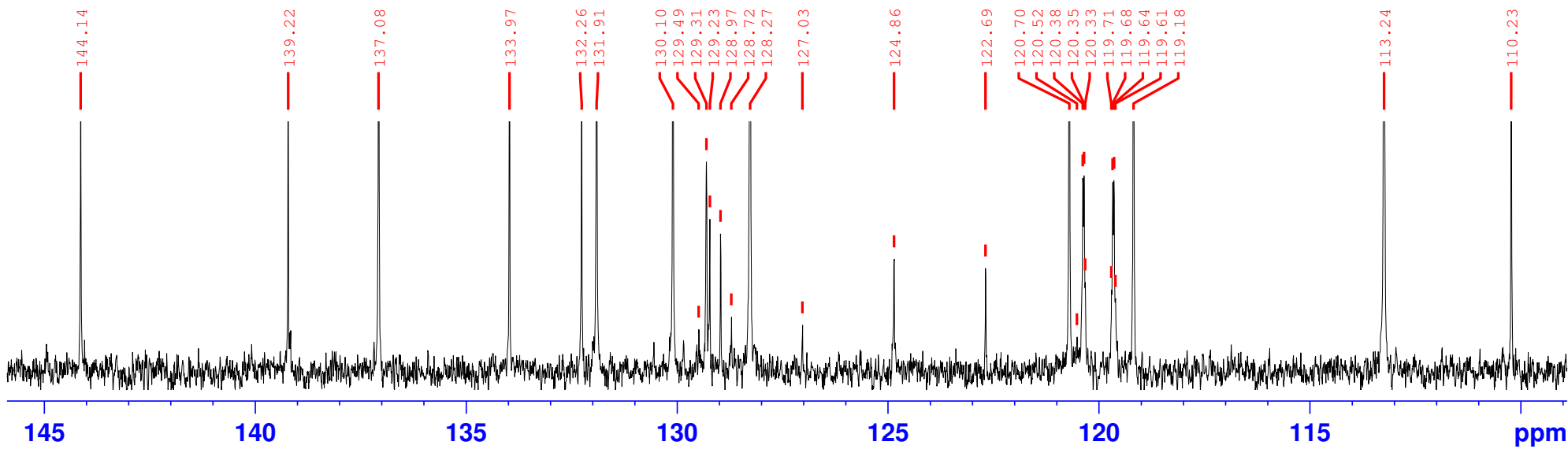
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
4	9.359	VB E	0.1130	30.70151	3.61733	0.2546
5	11.180	VB	0.0873	9.99174	1.73174	0.0829
6	14.233	BB	0.1517	48.99443	4.93881	0.4063
7	15.304	BB	0.1597	60.41753	5.56179	0.5010

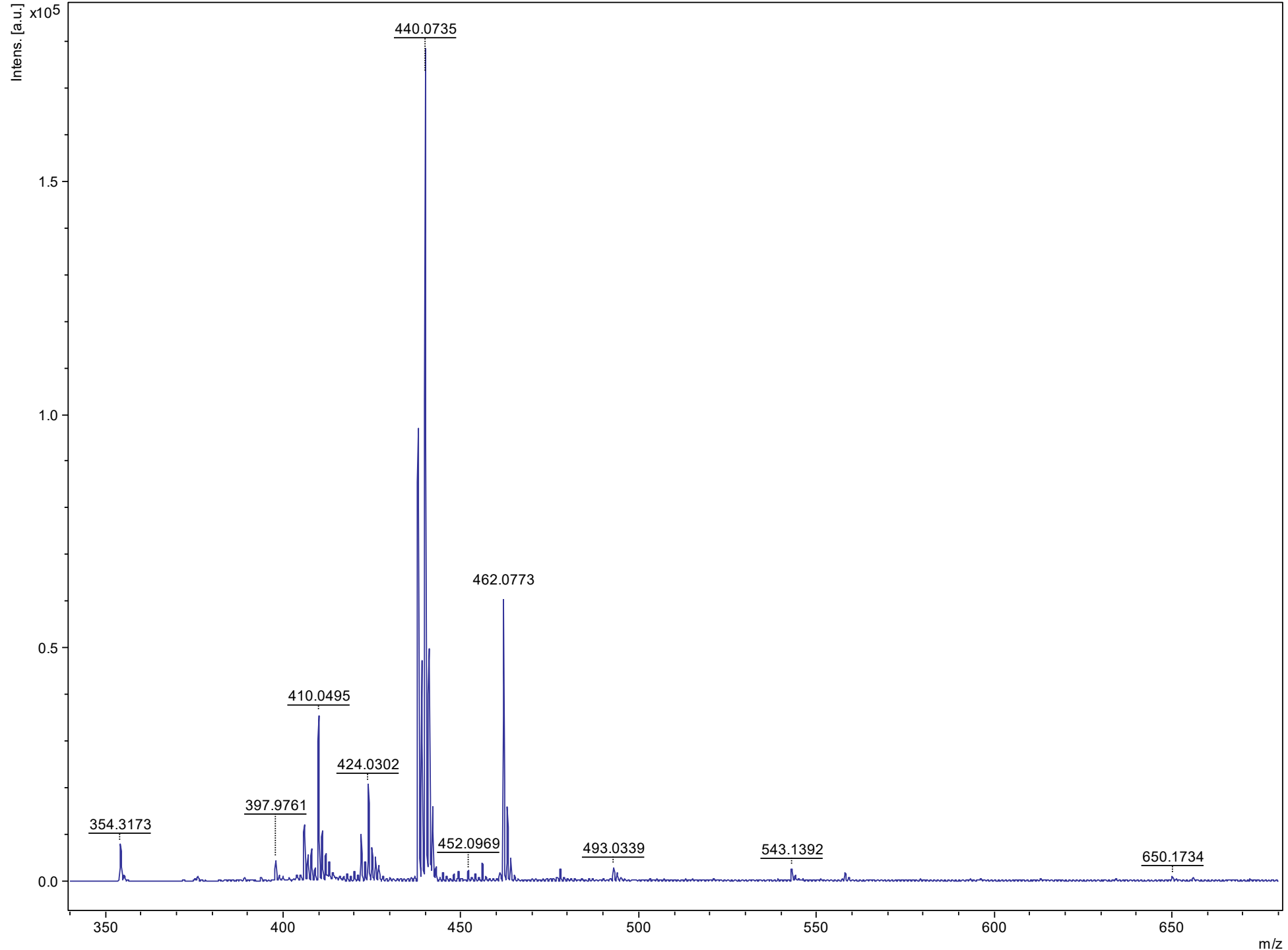
Totals : 1.20597e4 1770.62891

=====
*** End of Report ***









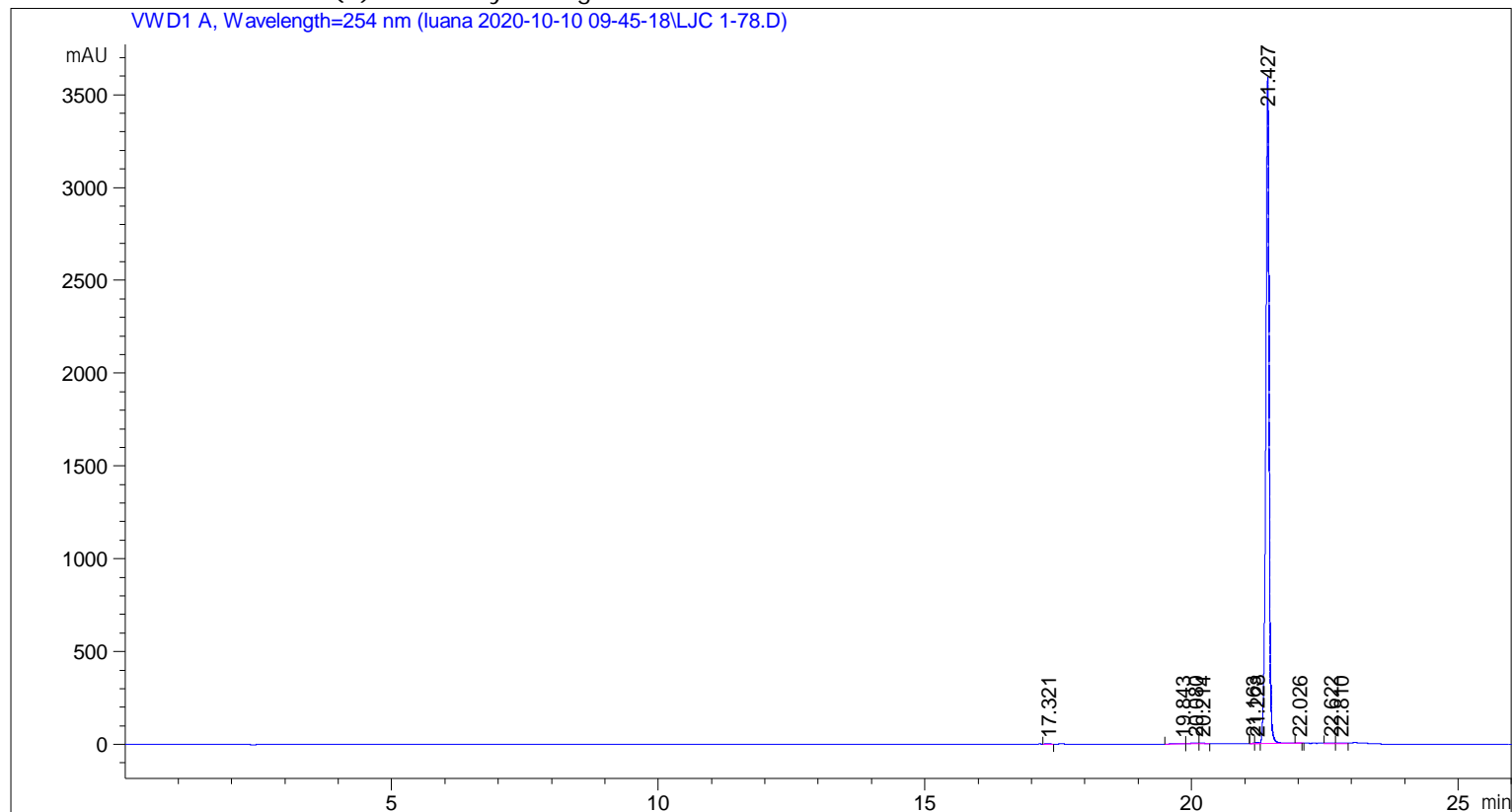
Sample Name: LJC 1-78

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :   14
Acq. Instrument : 1220 HPLC                    Location  :   16
Injection Date  : 10/10/2020 3:44:21 PM      Inj       :    1
                                           Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method         : C:\Chem32\1\Data\luana 2020-10-10 09-45-18\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed   : 10/10/2020 10:17:41 AM by SYSTEM
Method Info    : Water/MeOH

Sample Info    : LJC 1-78
  
```

Additional Info : Peak(s) manually integrated



```

=====
                        Area Percent Report
=====
  
```

```

Sorted By       :      Signal
Multiplier      :      1.0000
Dilution        :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

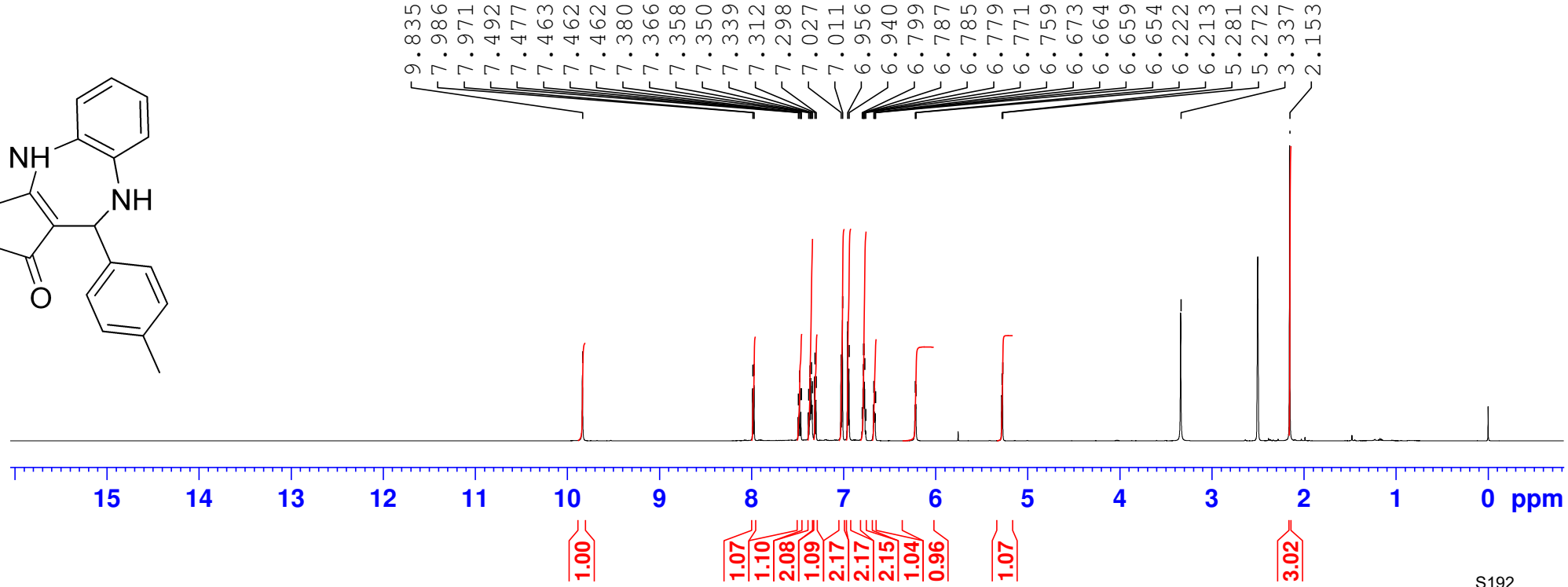
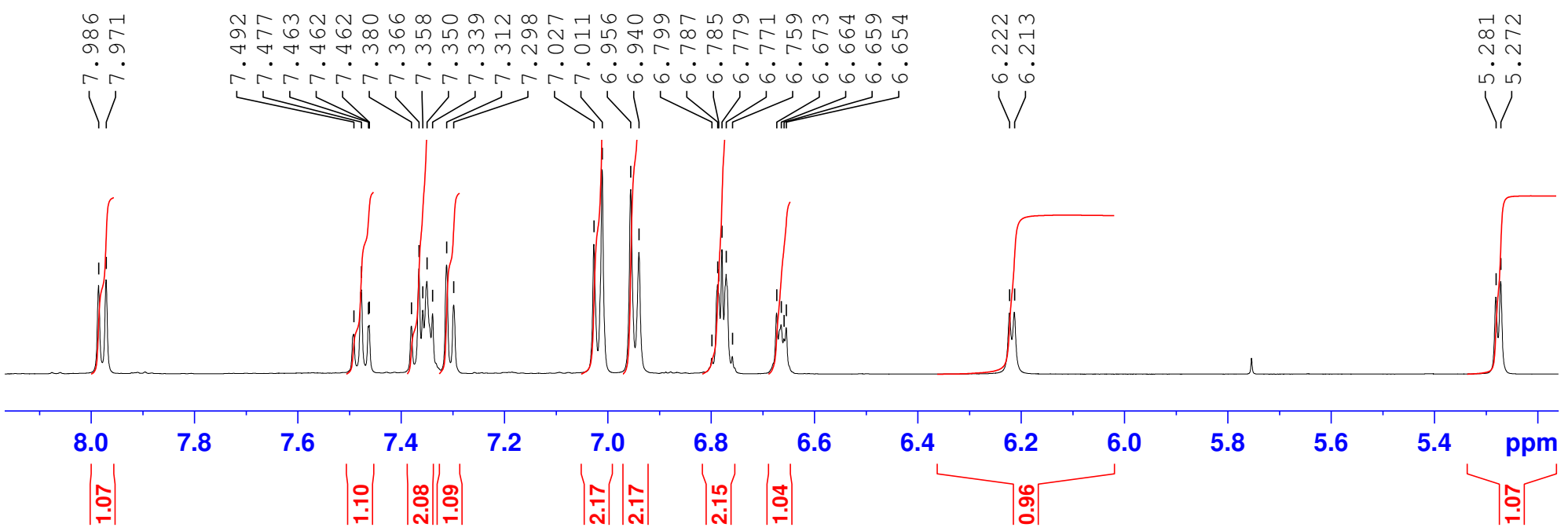
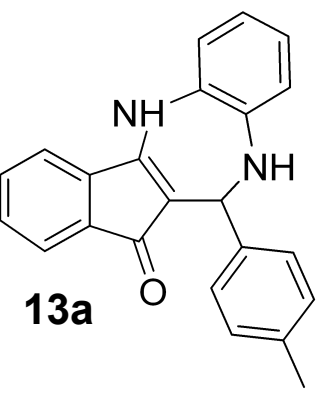
Signal 1: VWD1 A, Wavelength=254 nm

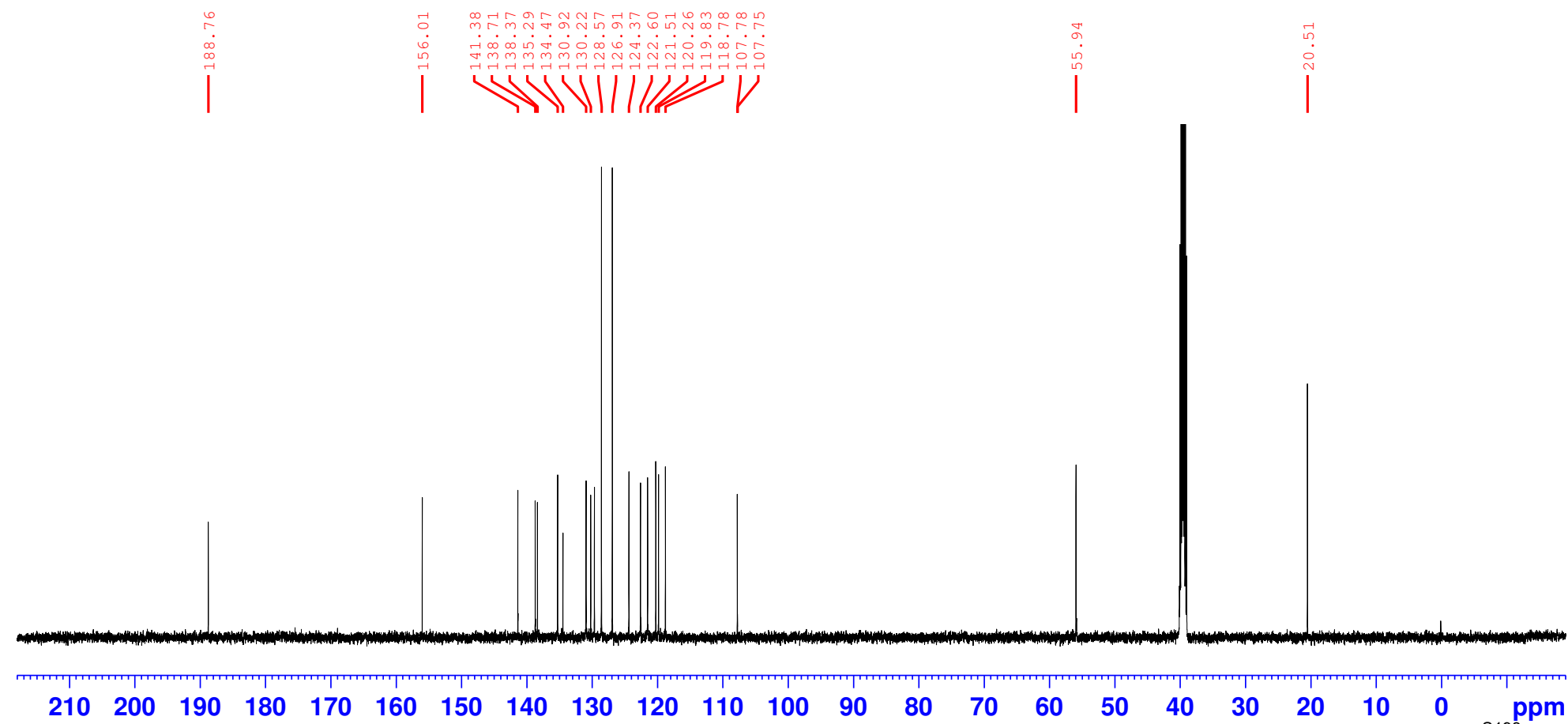
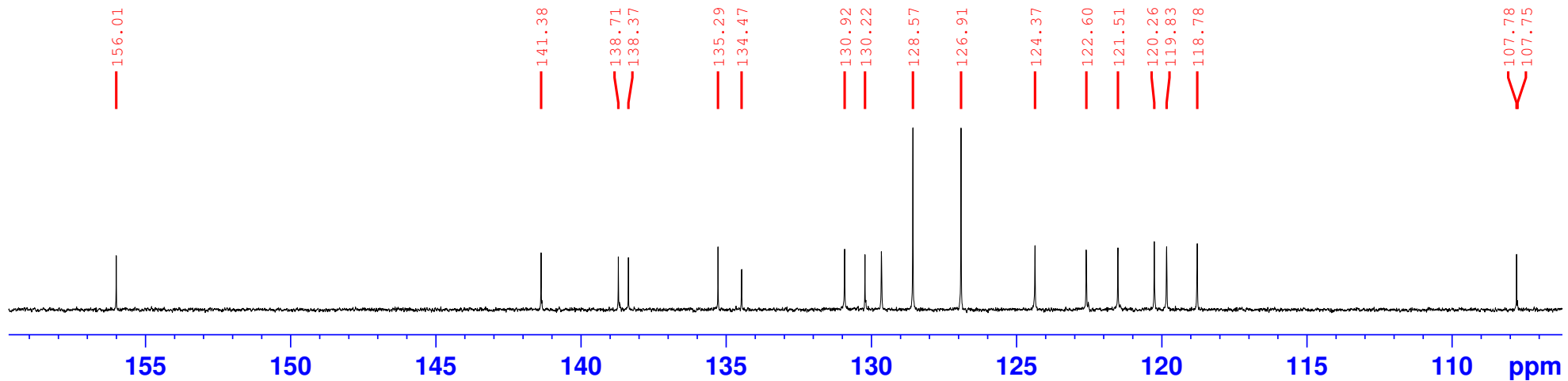
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.321	VV	0.0921	19.61564	2.73871	0.1237
2	19.843	BV	0.1106	26.51312	3.10481	0.1673
3	20.080	VV	0.1316	61.31062	6.05472	0.3868
4	20.214	VB	0.0835	37.57326	6.30641	0.2370

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	21.163	BV E	0.0422	9.25904	3.25664	0.0584
6	21.228	VV E	0.0550	24.77566	6.87709	0.1563
7	21.427	VV R	0.0653	1.56056e4	3583.66895	98.4485
8	22.026	VB E	0.0564	6.26016	1.76614	0.0395
9	22.622	VV	0.1019	19.76054	2.65313	0.1247
10	22.810	VV	0.1606	40.87181	3.07372	0.2578

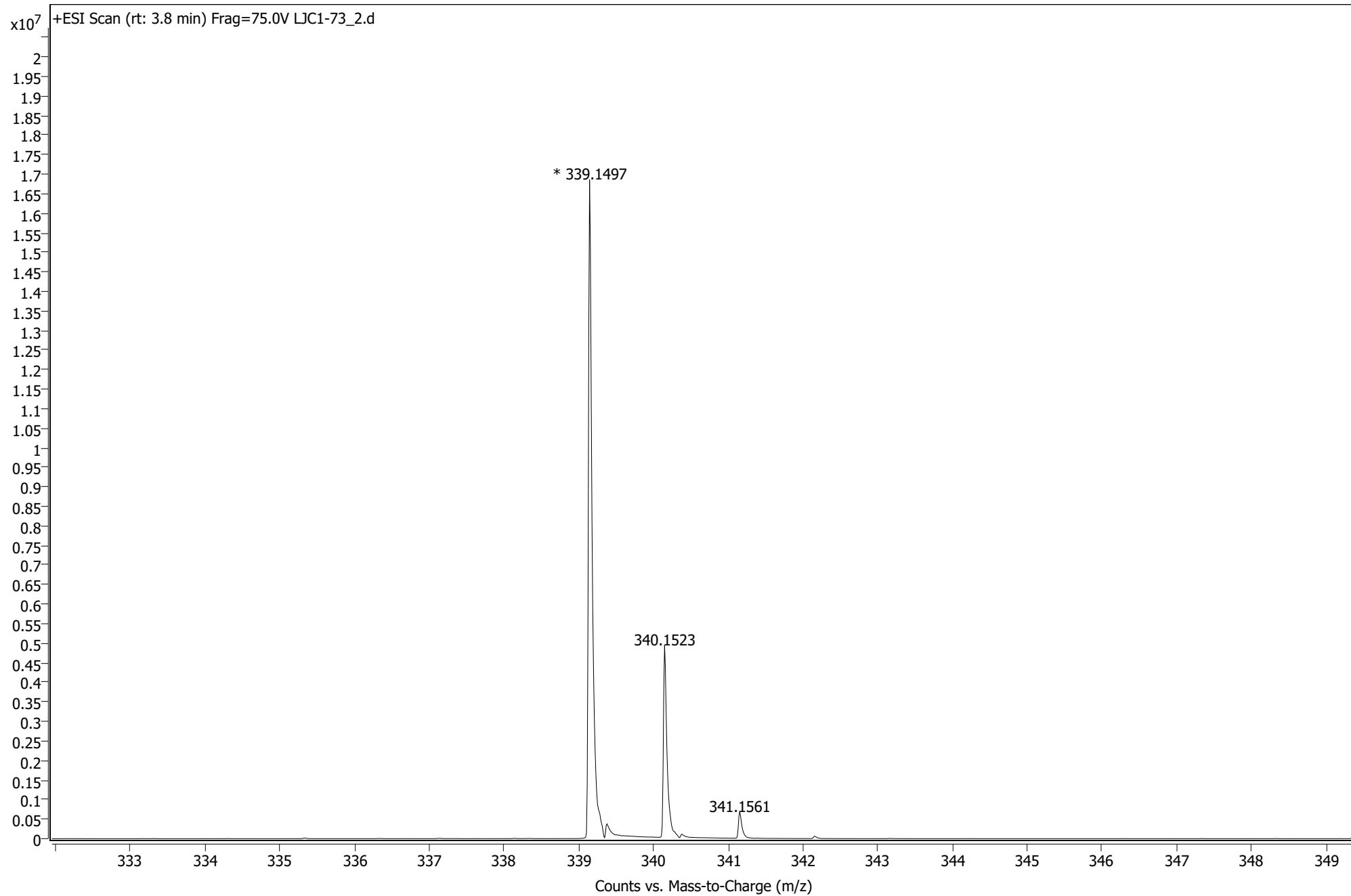
Totals : 1.58515e4 3619.50030

=====
*** End of Report ***





User Spectrum Plot Report



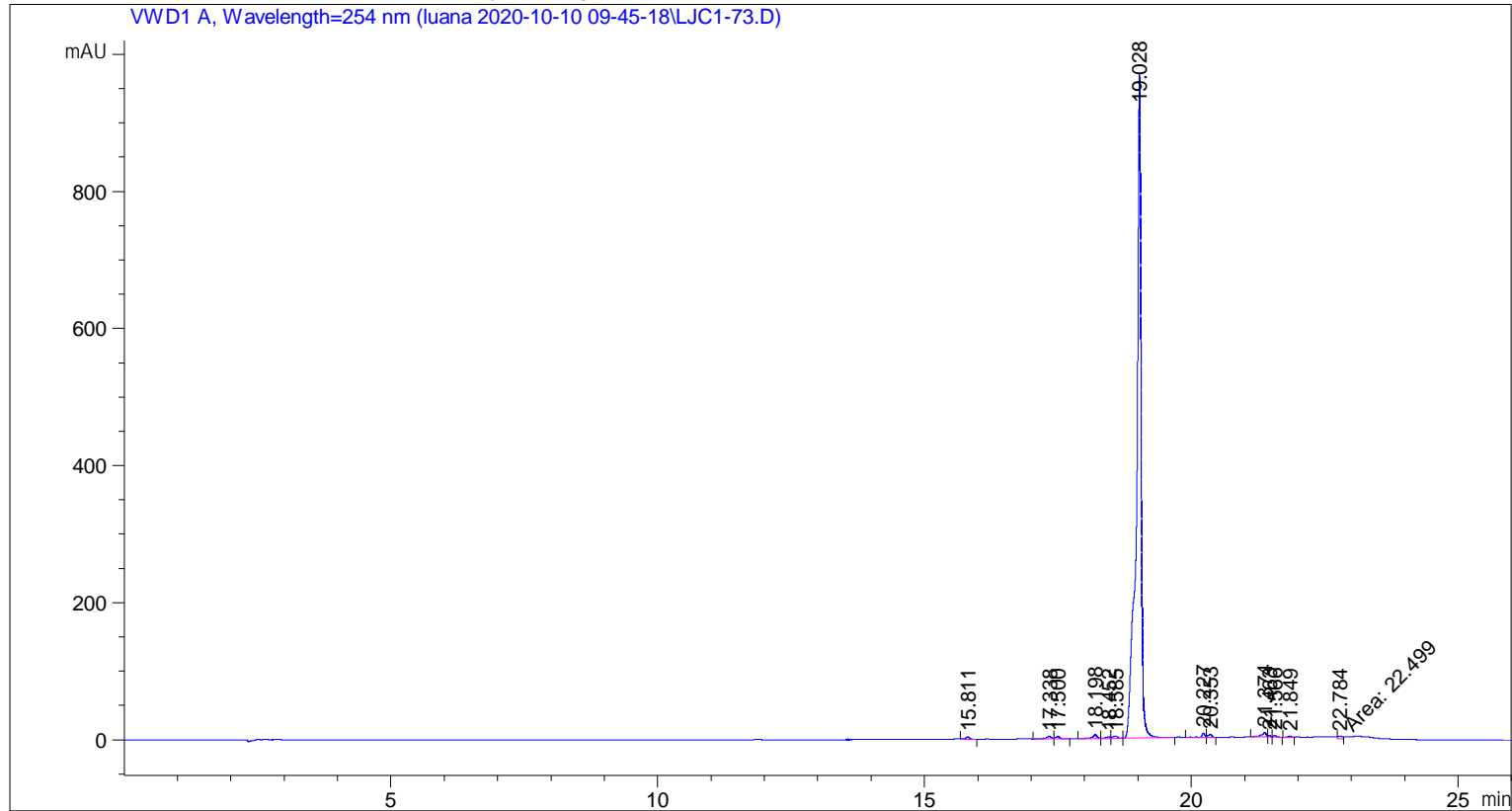
Sample Name: LJC1-73

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    5
Acq. Instrument : 1220 HPLC                   Location  :   13
Injection Date  : 10/10/2020 11:35:41 AM     Inj       :    1
                                           Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-10-10 09-45-18\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 10/10/2020 10:17:41 AM by SYSTEM
Method Info     : Water/MeOH

Sample Info     : LJC1-73
    
```

Additional Info : Peak(s) manually integrated



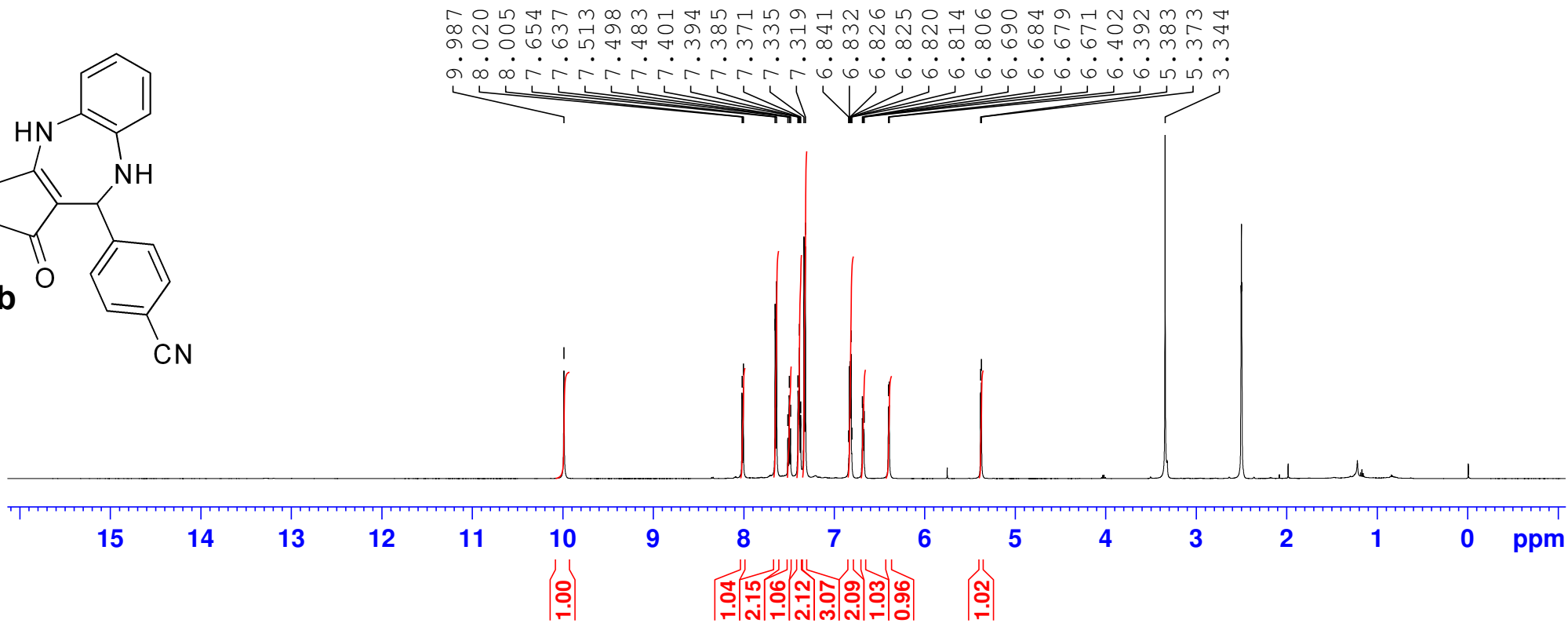
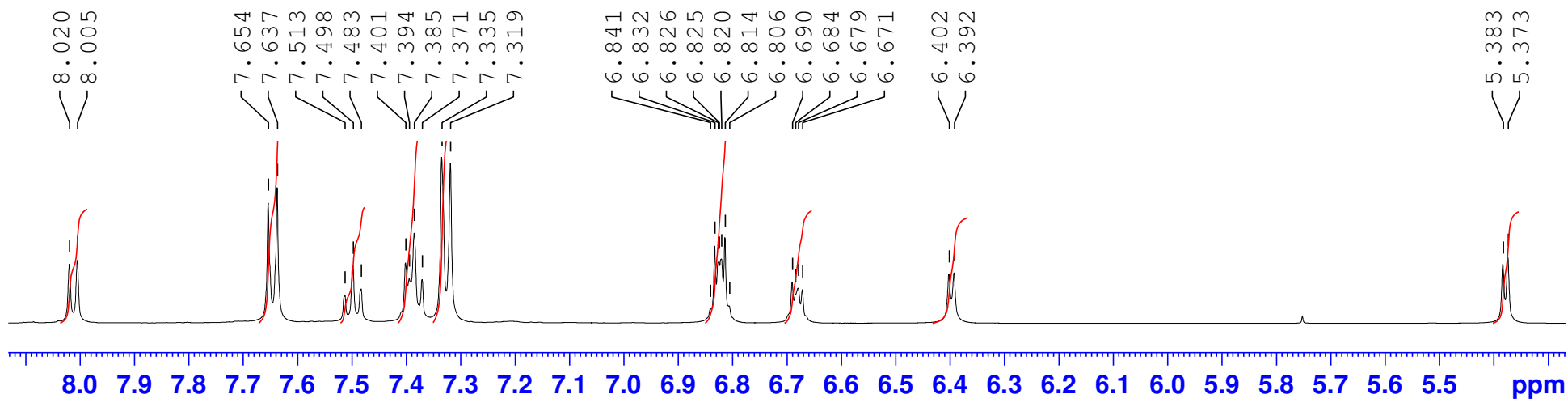
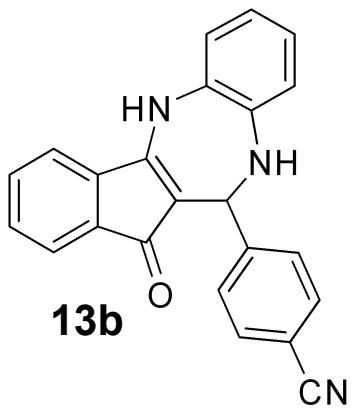
Area Percent Report

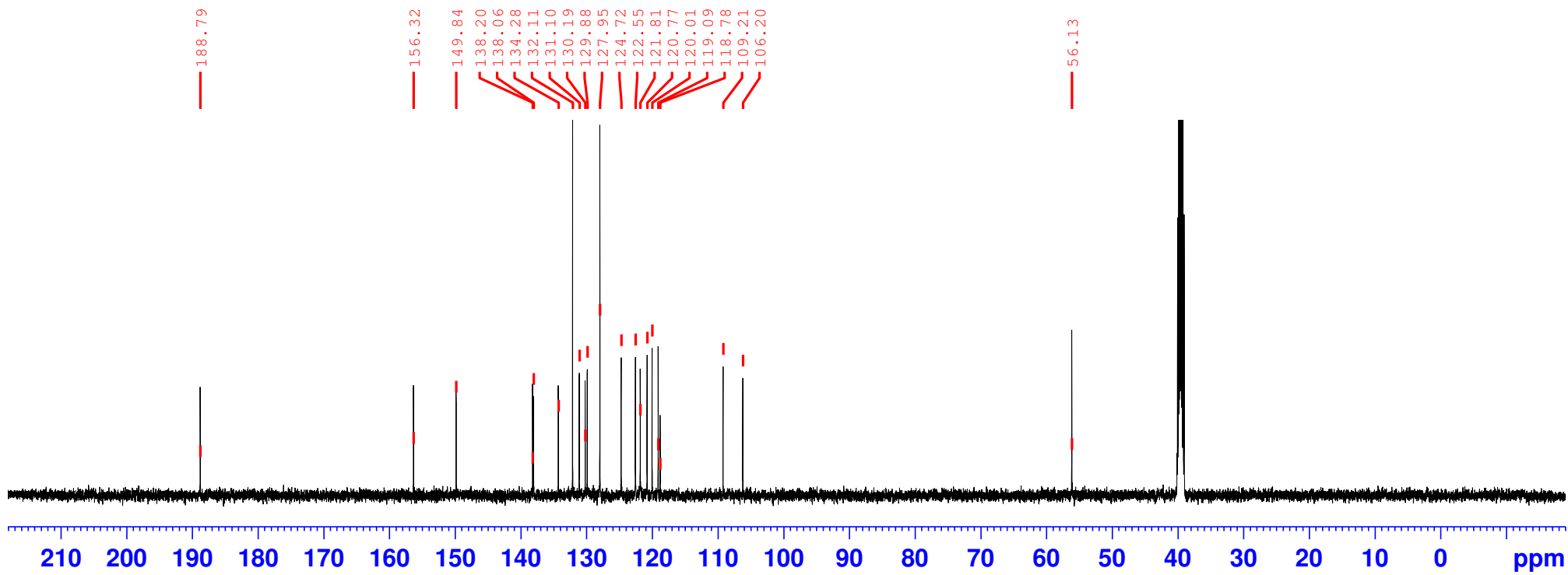
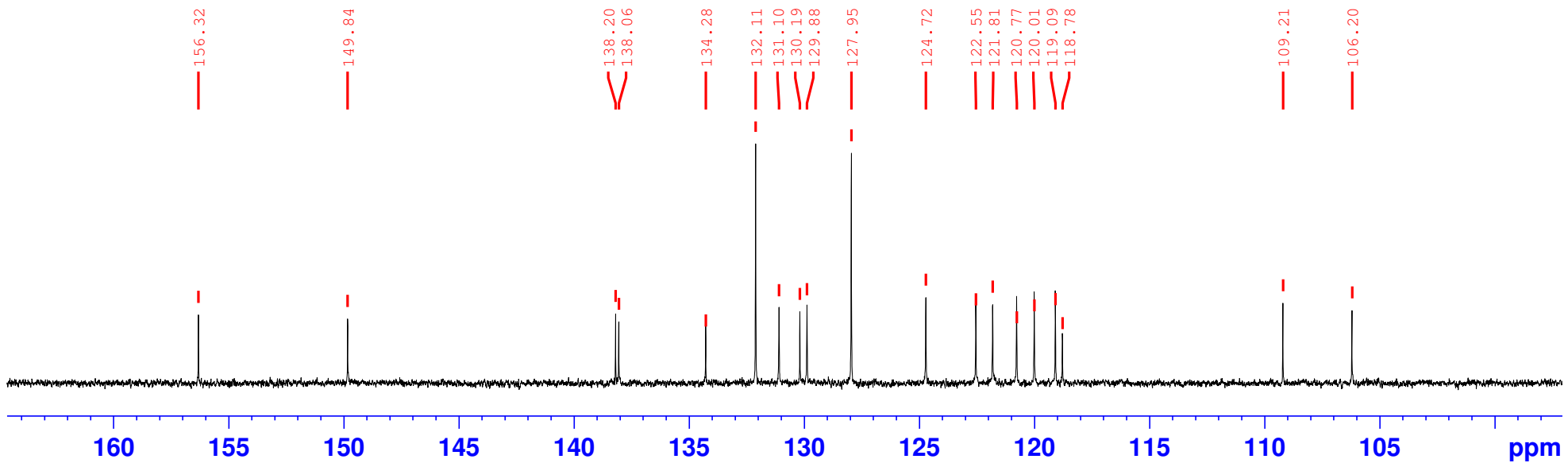
```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

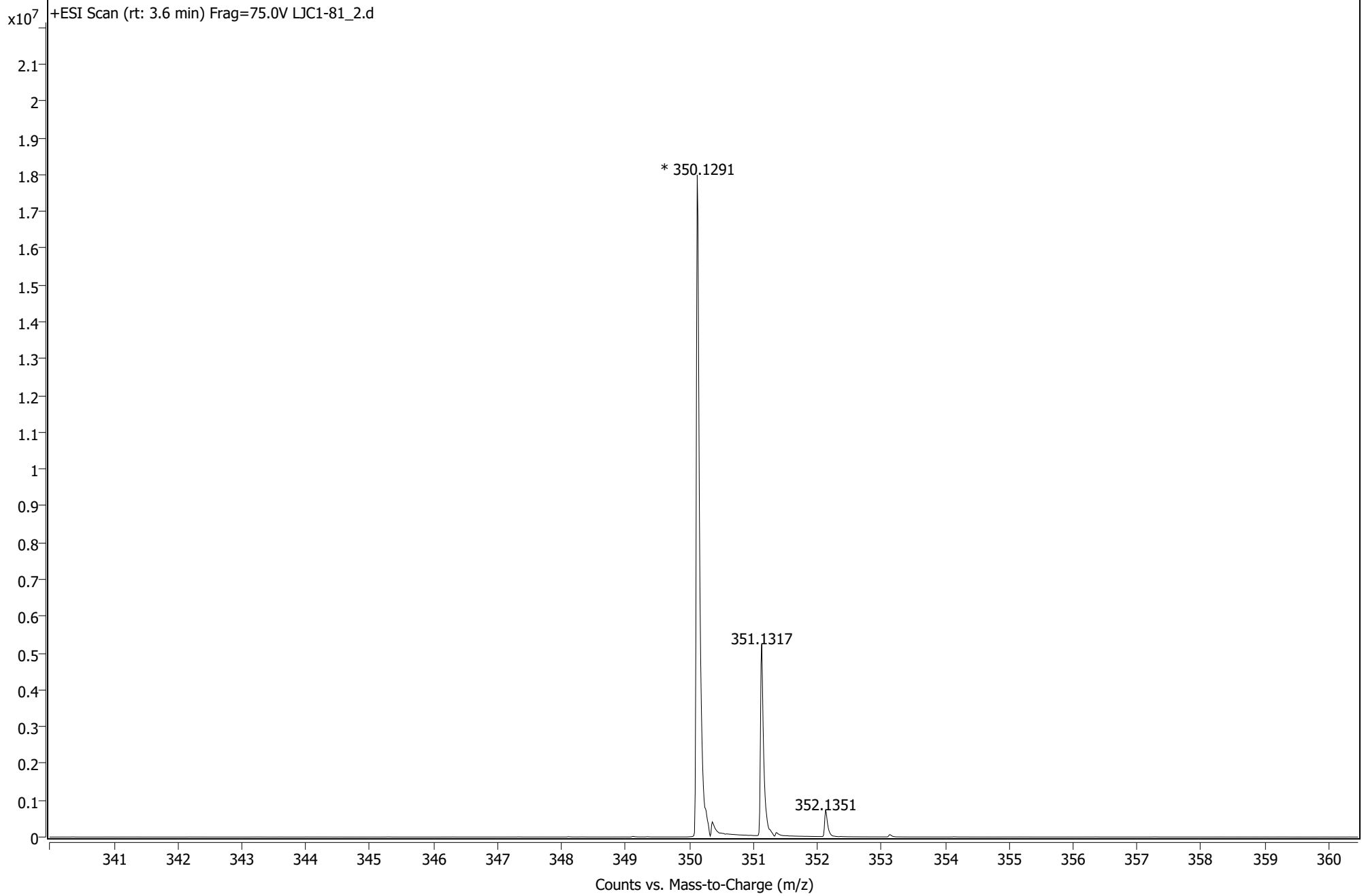
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.811	VB	0.0831	21.59780	3.56684	0.3549
2	17.338	BV	0.0999	31.56418	4.28780	0.5187
3	17.500	VB	0.0738	21.13401	3.92349	0.3473
4	18.198	BV	0.0910	40.75897	6.10017	0.6698





User Spectrum Plot Report



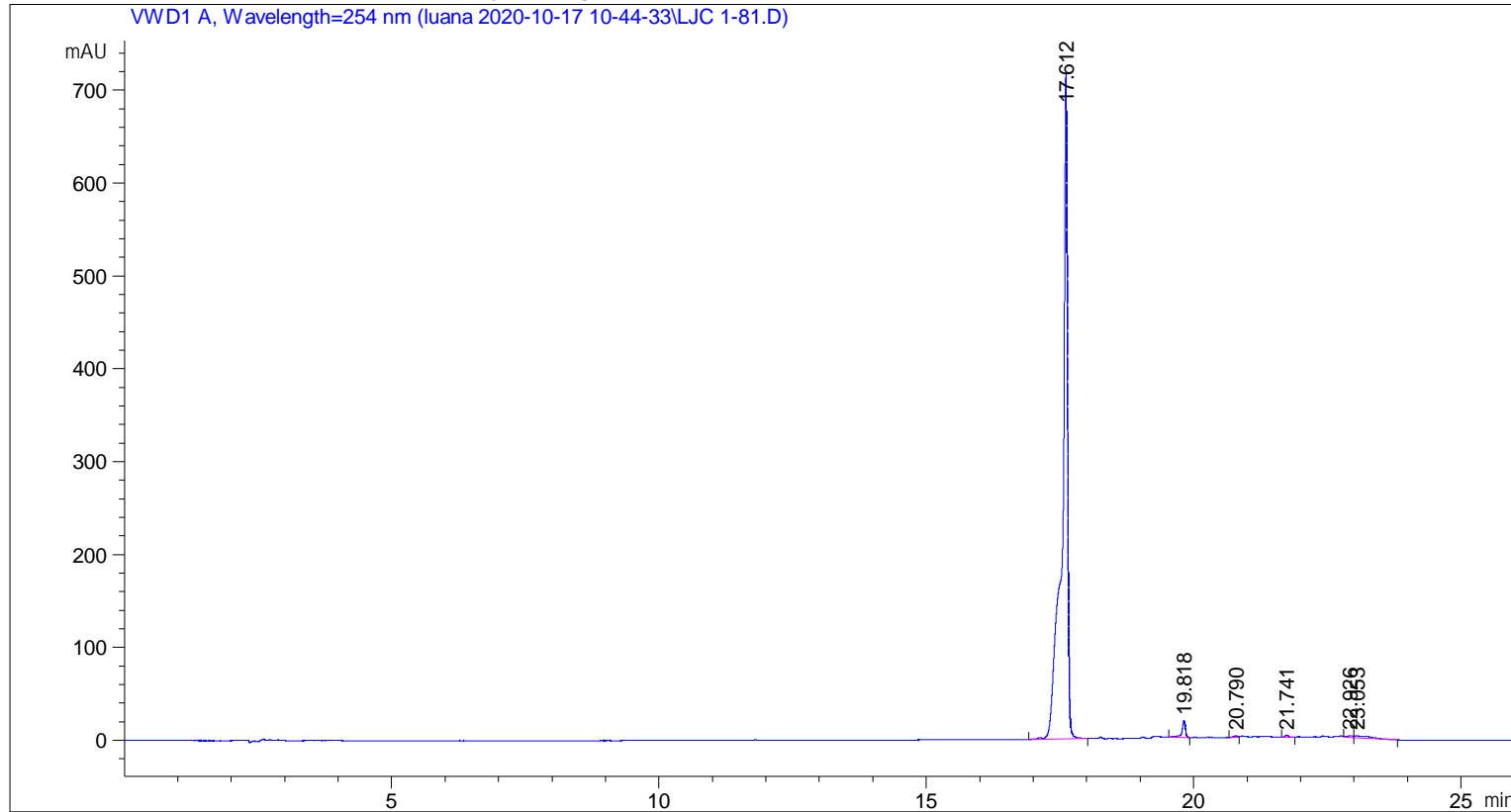
Sample Name: LJC 1-81

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    7
Acq. Instrument : 1220 HPLC                   Location  :   15
Injection Date  : 10/17/2020 1:30:36 PM      Inj       :    1
                                           Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-10-17 10-44-33\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 10/17/2020 11:15:13 AM by SYSTEM
Method Info     : Water/MeOH

Sample Info     : LJC 1-81
    
```

Additional Info : Peak(s) manually integrated



Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

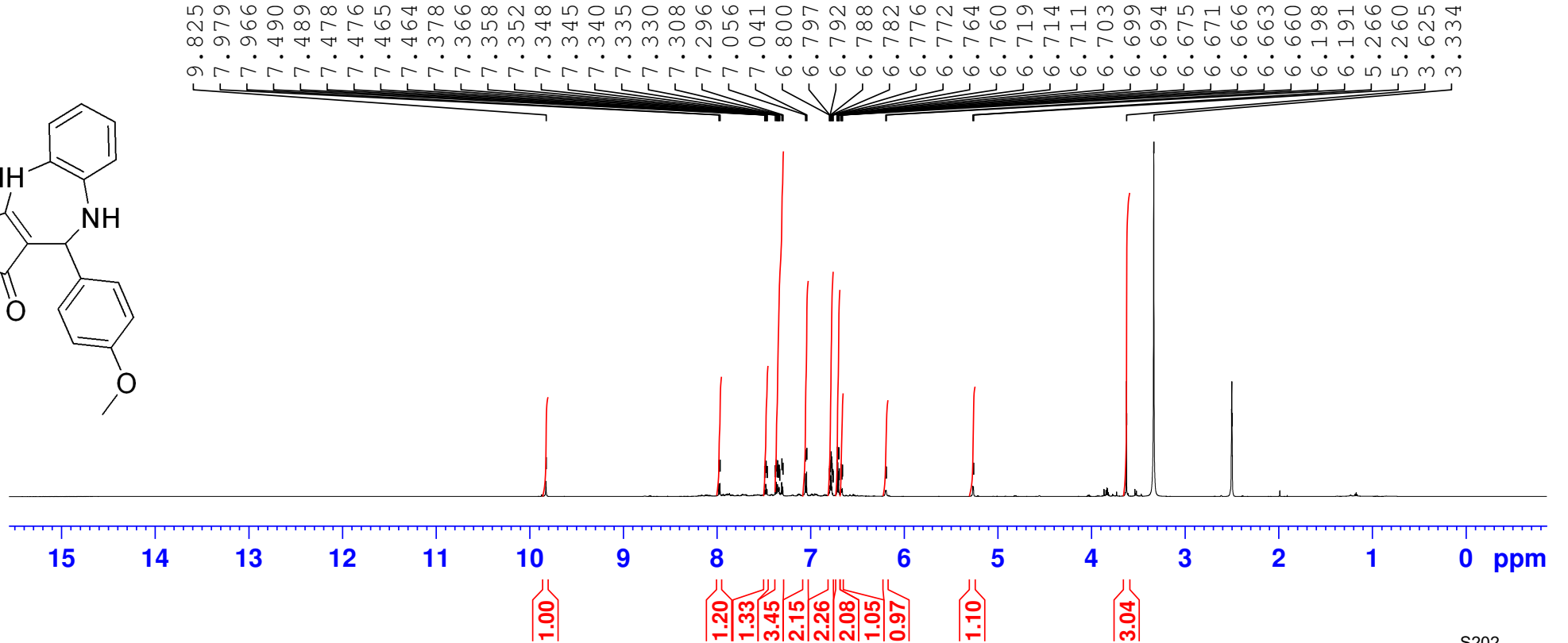
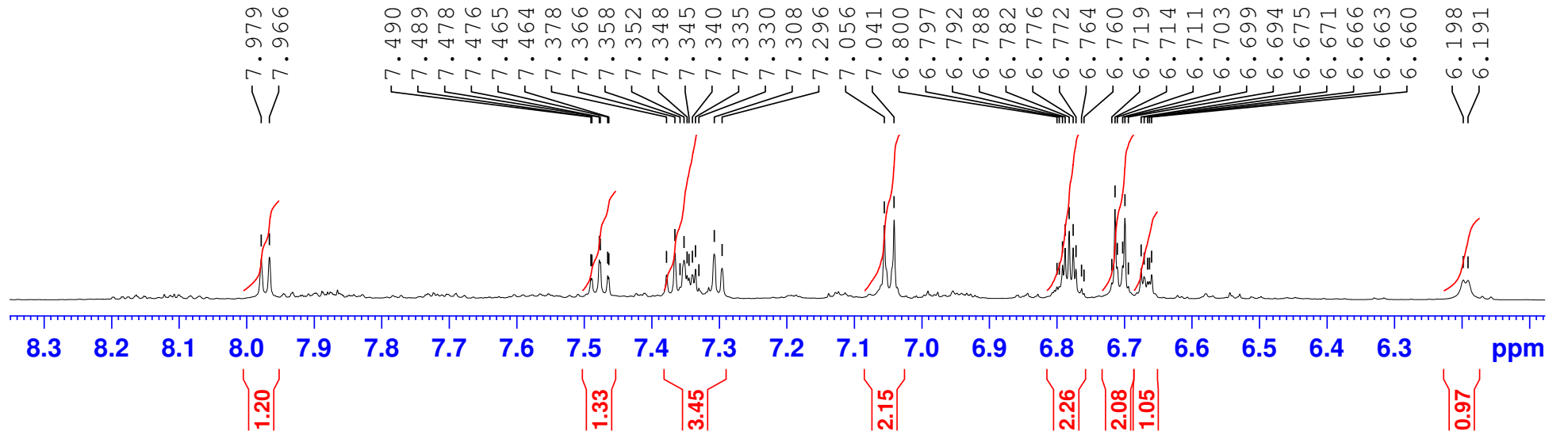
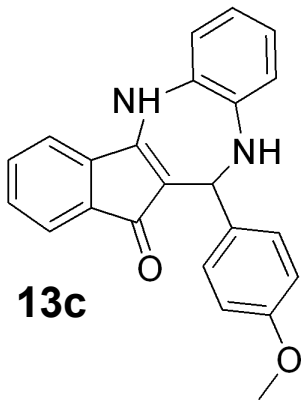
Signal 1: VWD1 A, Wavelength=254 nm

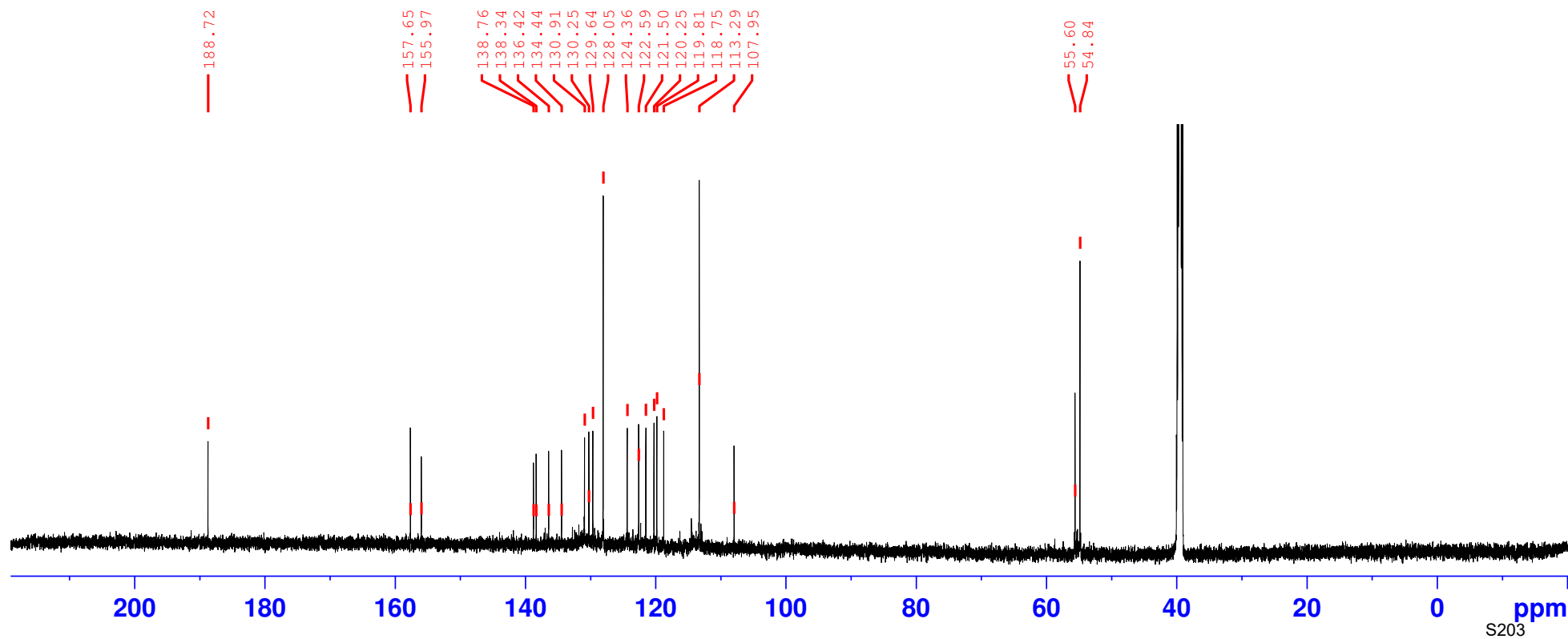
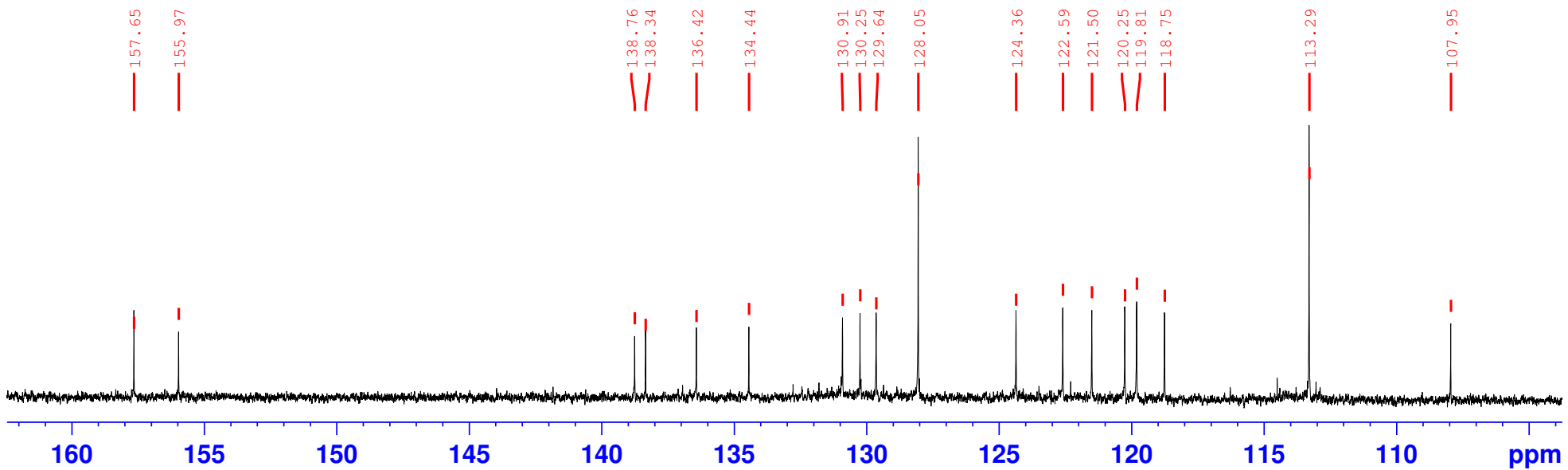
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.612	VV R	0.0932	4860.79980	716.14459	96.5196
2	19.818	VB R	0.0682	85.58815	18.43436	1.6995
3	20.790	BV	0.0759	10.26132	1.85938	0.2038
4	21.741	BV R	0.0662	10.21728	2.30685	0.2029

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	22.926	VV	0.1234	18.14906	1.74426	0.3604
6	23.053	VB	0.2912	51.05789	2.06357	1.0138

Totals : 5036.07350 742.55301

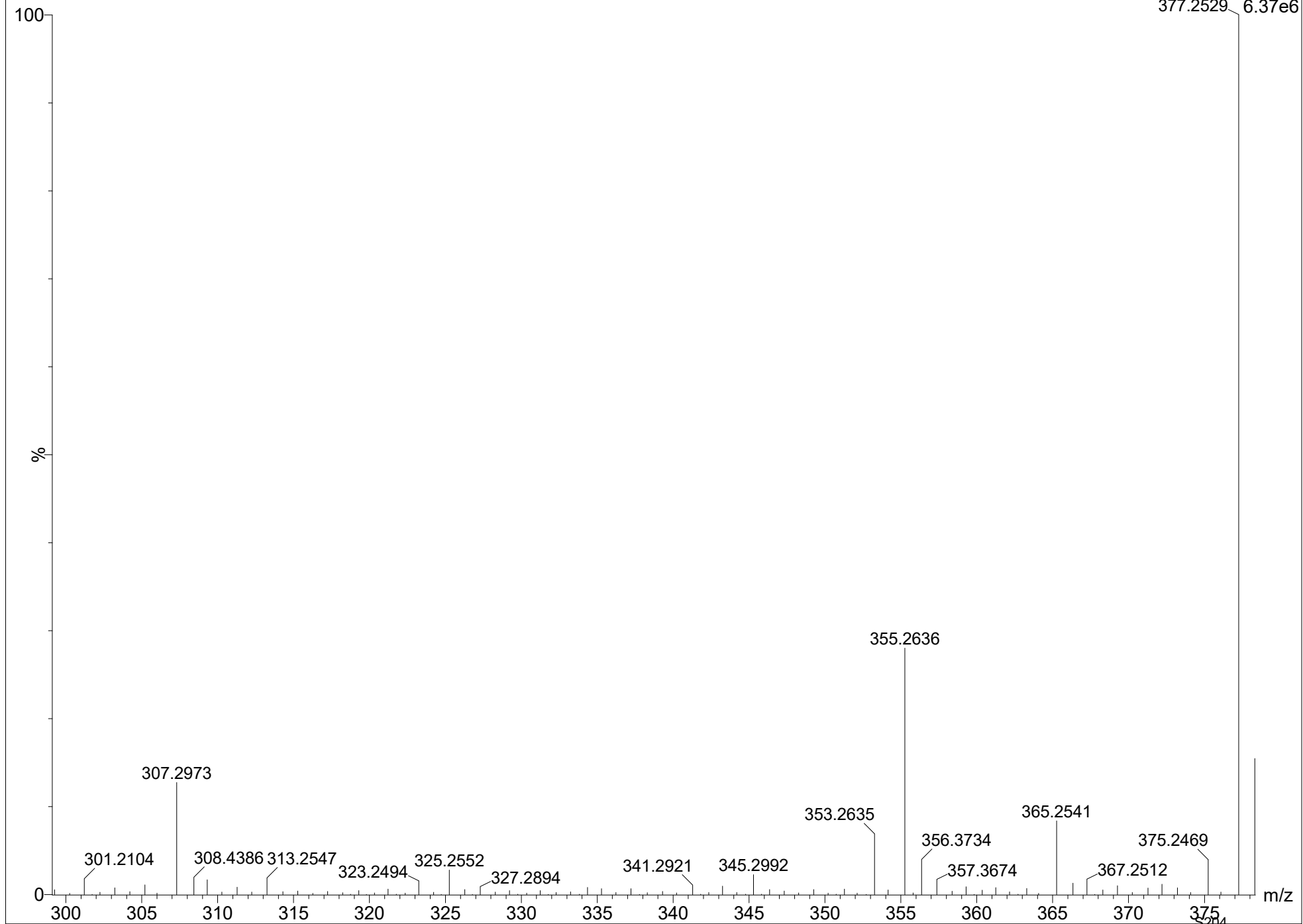
=====
*** End of Report ***





LJC-1-74 45 (0.756) Cm (3:120)

Scan ES+
377.2529 6.37e6



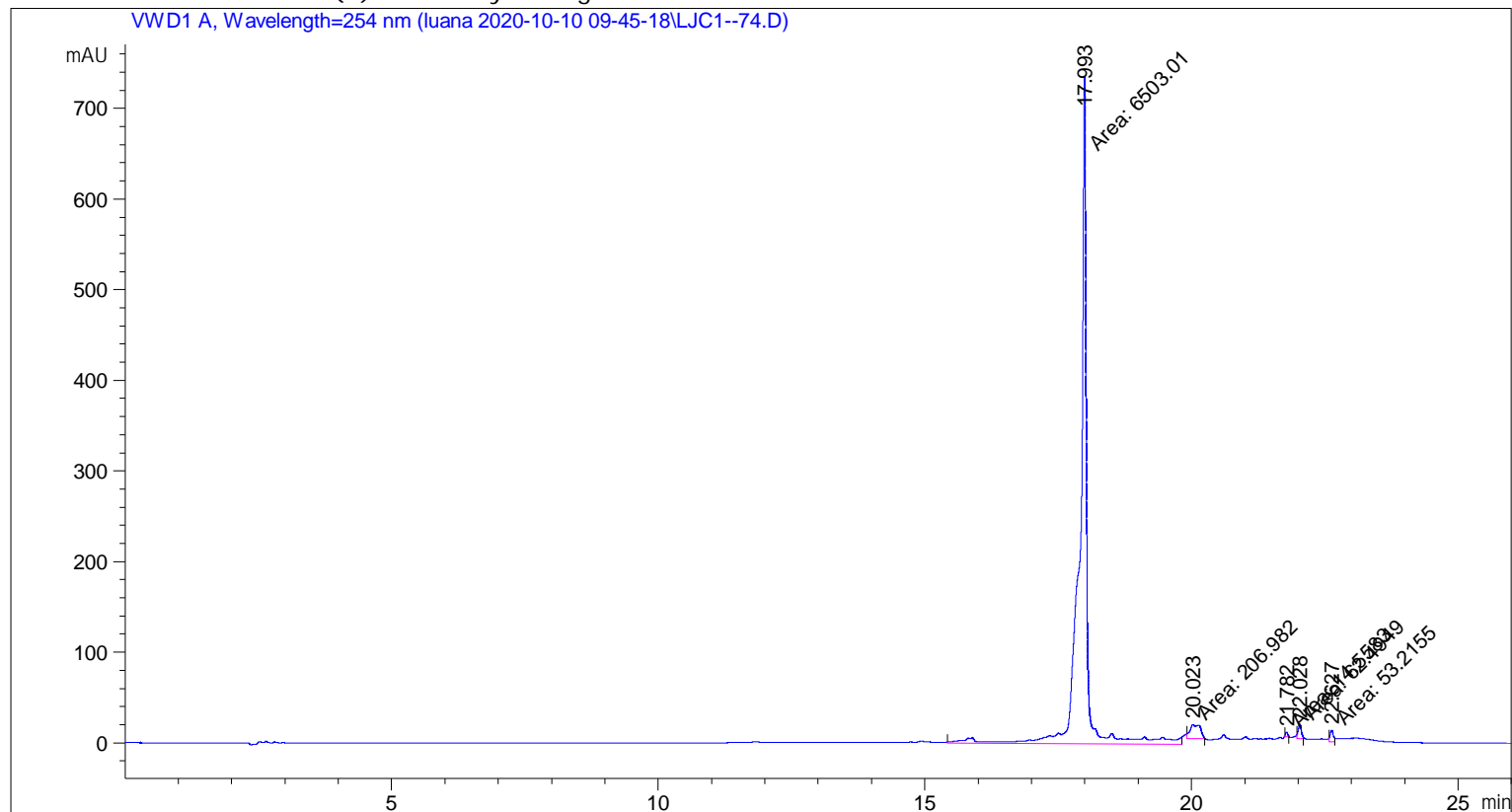
Sample Name: LJC1--74

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    6
Acq. Instrument : 1220 HPLC                    Location  :   14
Injection Date  : 10/10/2020 12:03:24 PM      Inj       :    1
                                           Inj Volume: 30.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2020-10-10 09-45-18\MOHAMED-SMALL MOLECULE.M (
                Sequence Method)
Last changed    : 10/10/2020 10:17:41 AM by SYSTEM
Method Info     : Water/MeOH

Sample Info     : LJC1--74
  
```

Additional Info : Peak(s) manually integrated



```

=====
                          Area Percent Report
=====
  
```

```

Sorted By       :      Signal
Multiplier      :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: VWD1 A, Wavelength=254 nm

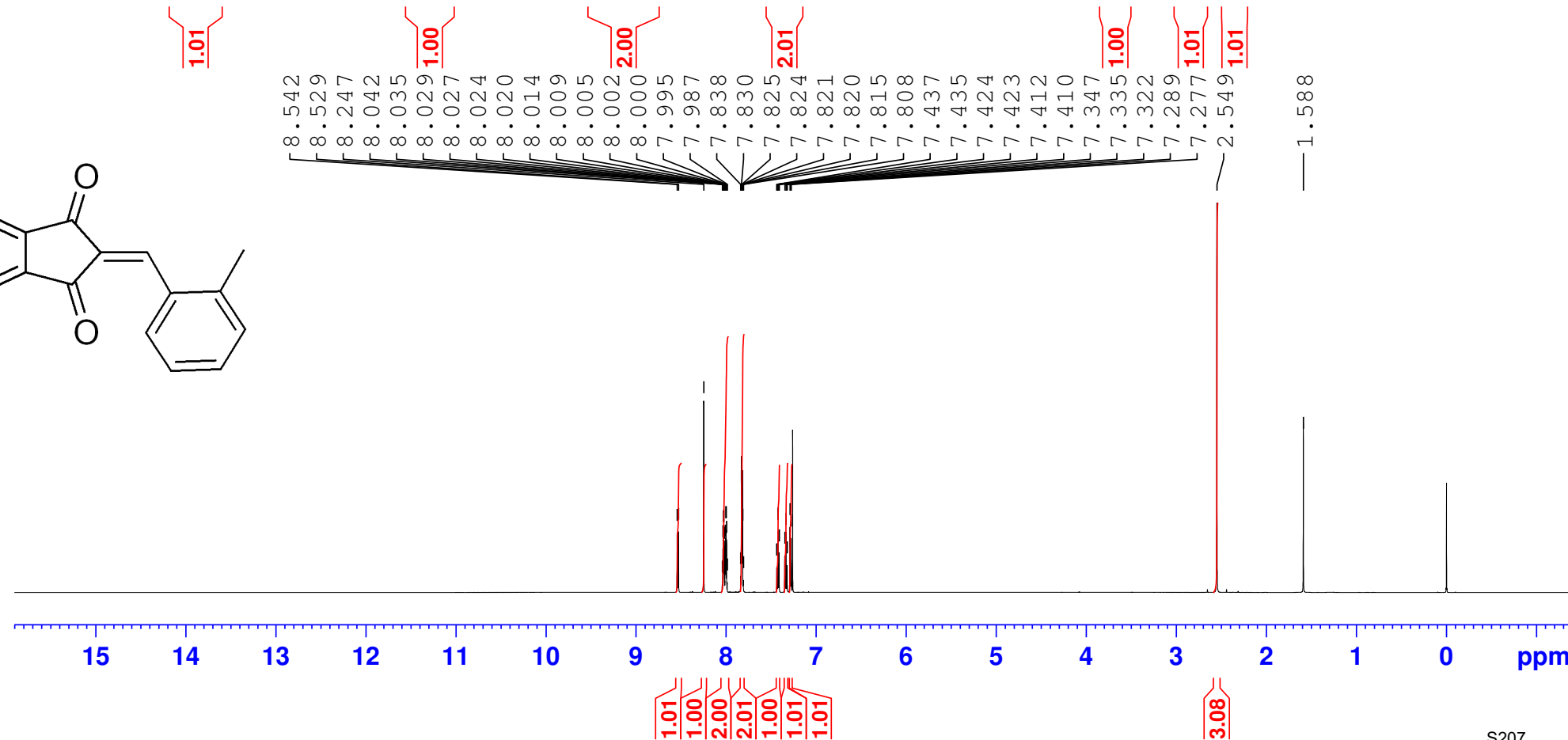
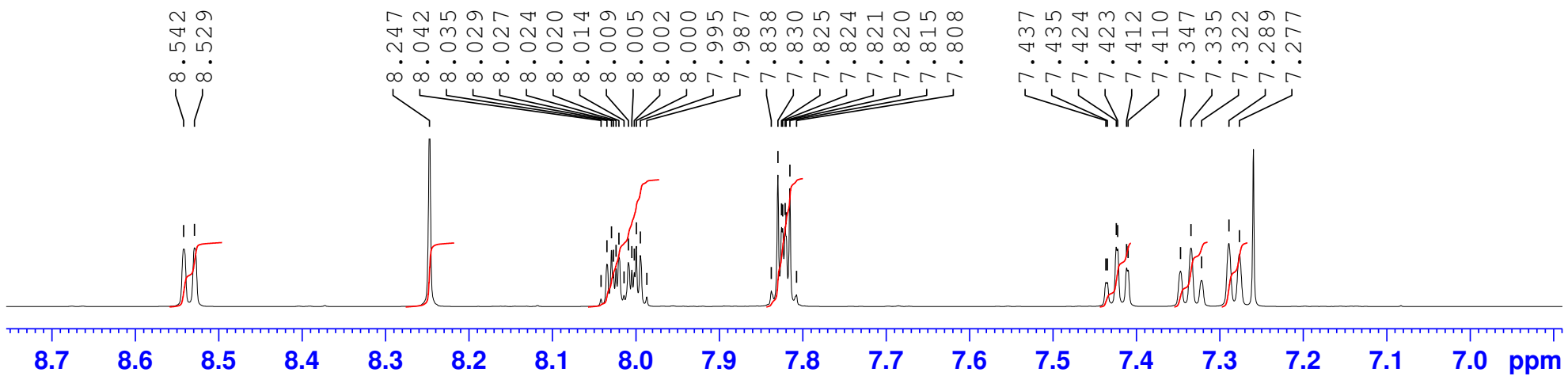
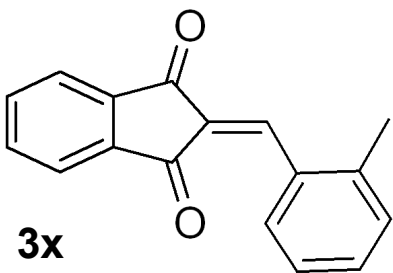
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.993	MM	0.1474	6503.00537	735.39545	95.0696
2	20.023	MM	0.2217	206.98235	15.55880	3.0259
3	21.782	MM	0.0461	14.55834	5.26897	0.2128
4	22.028	MM	0.0655	62.49493	15.89236	0.9136

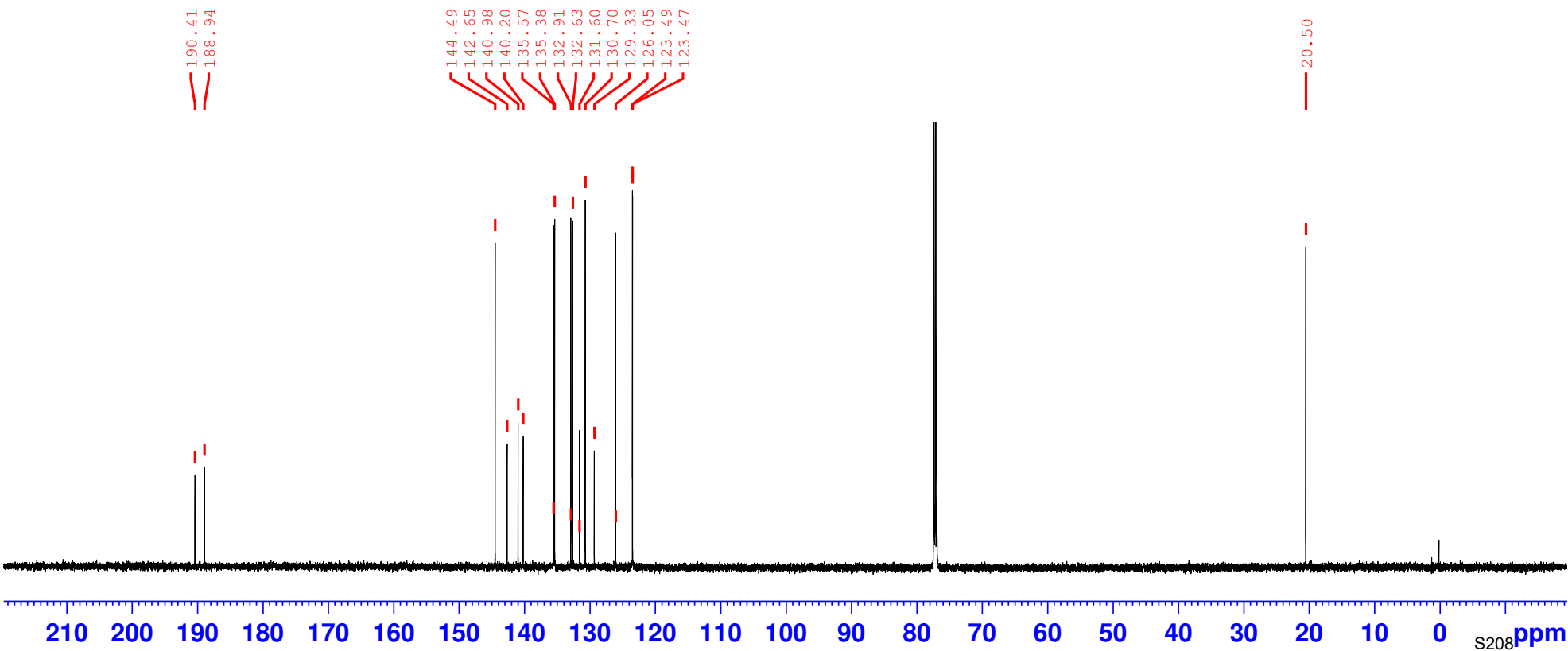
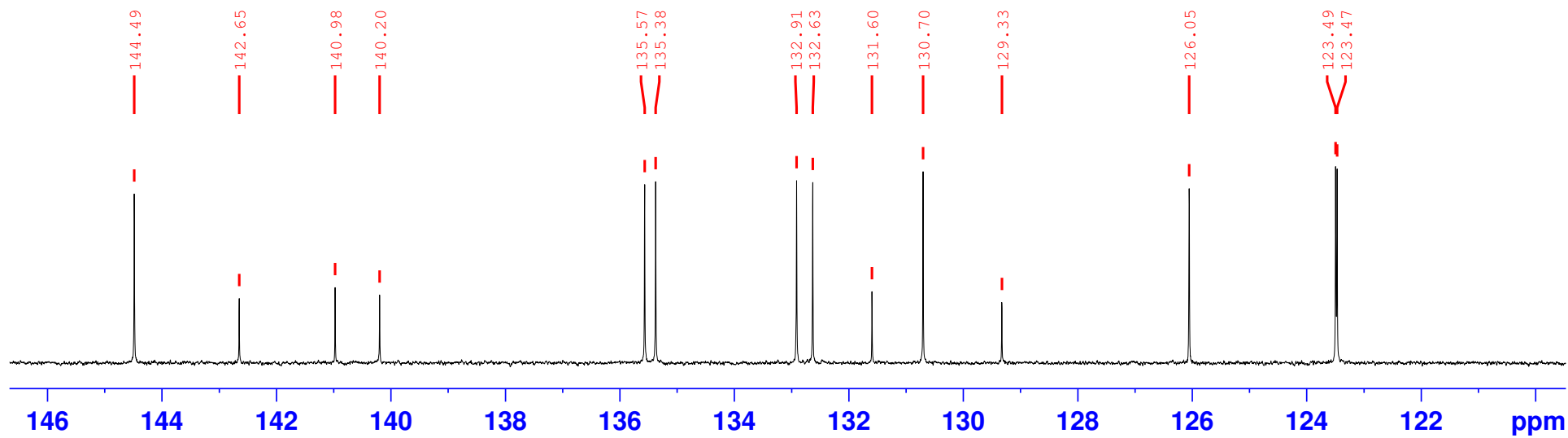
S205

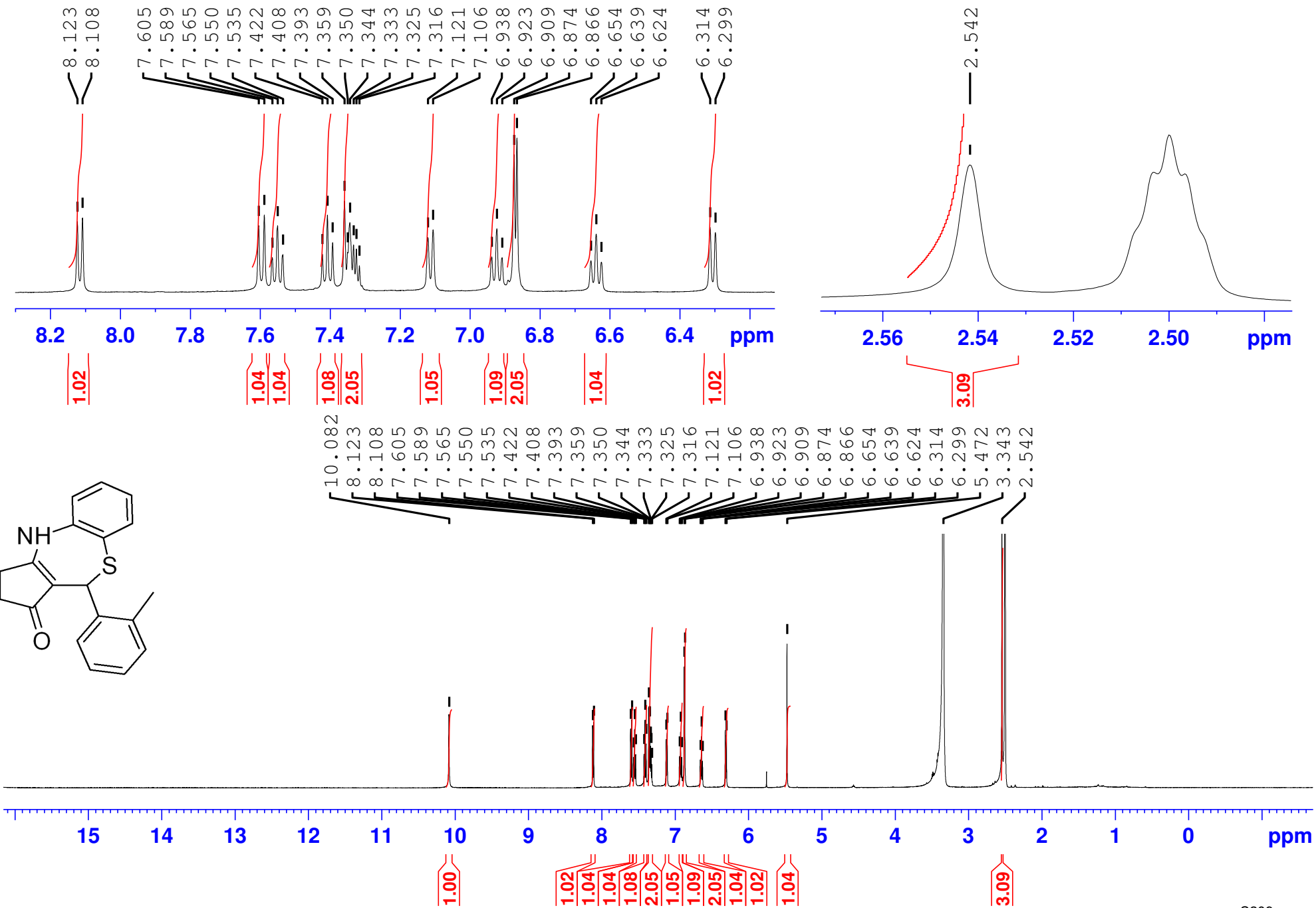
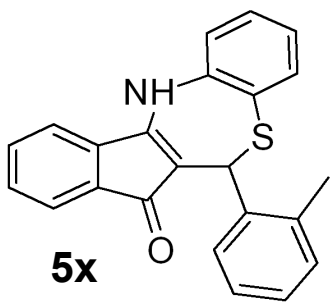
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	22.627	MM	0.0677	53.21552	13.09496	0.7780

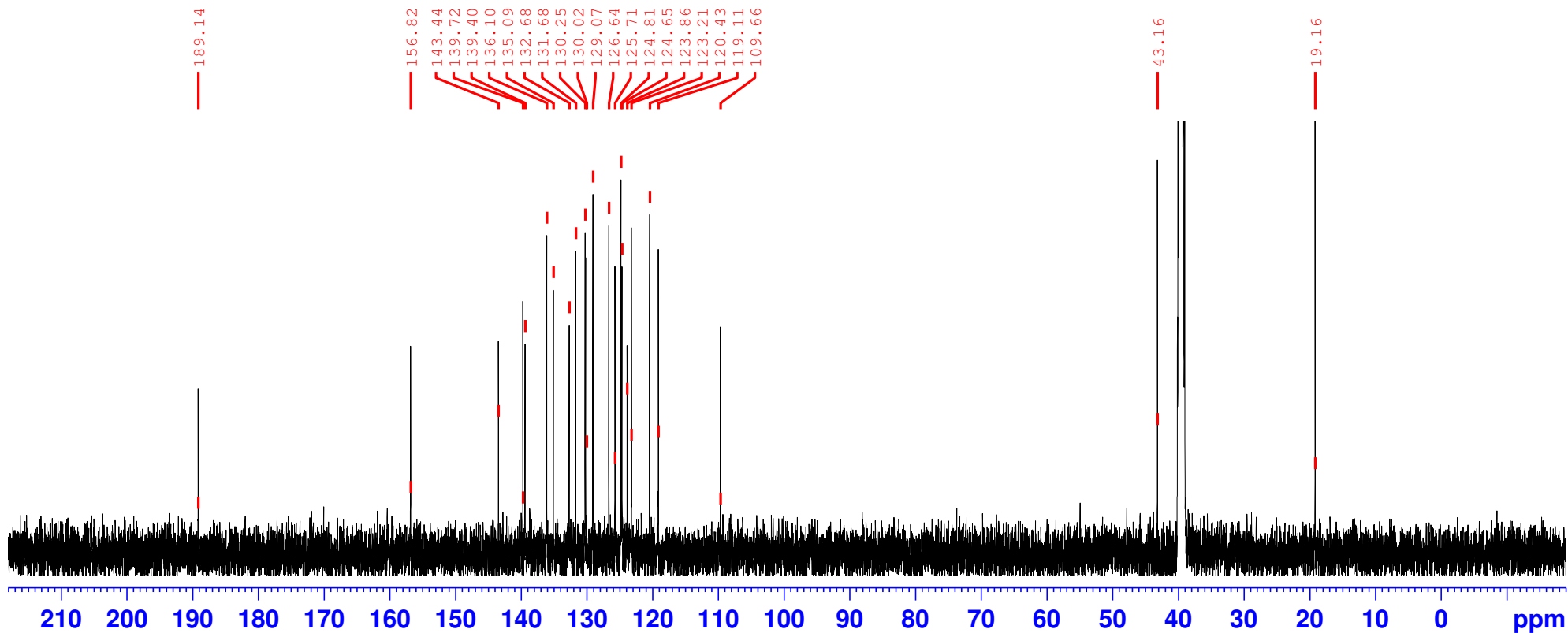
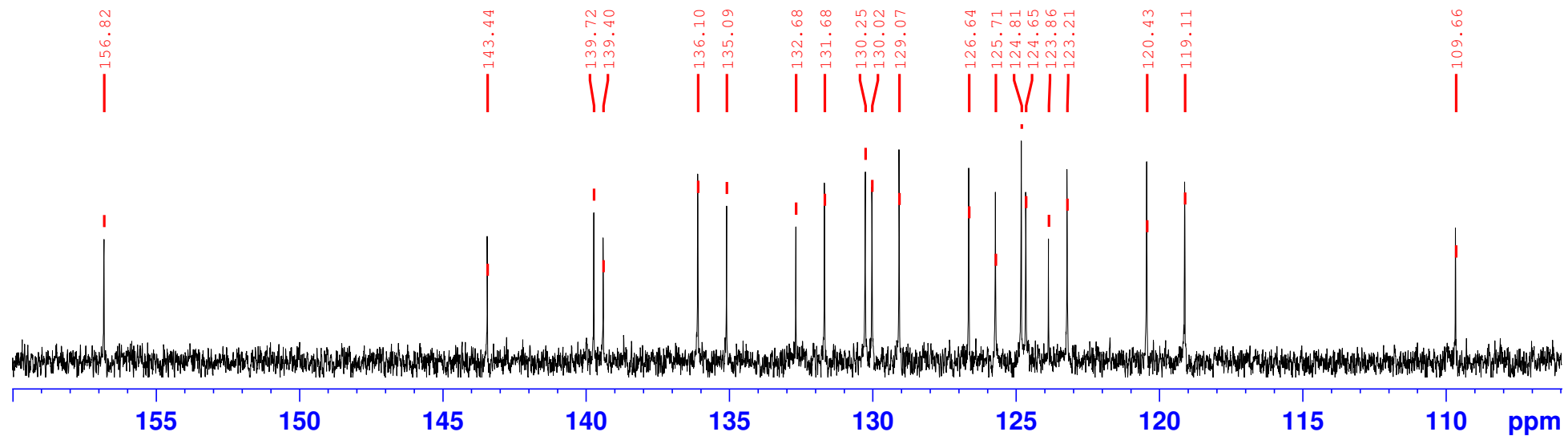
Totals : 6840.25651 785.21053

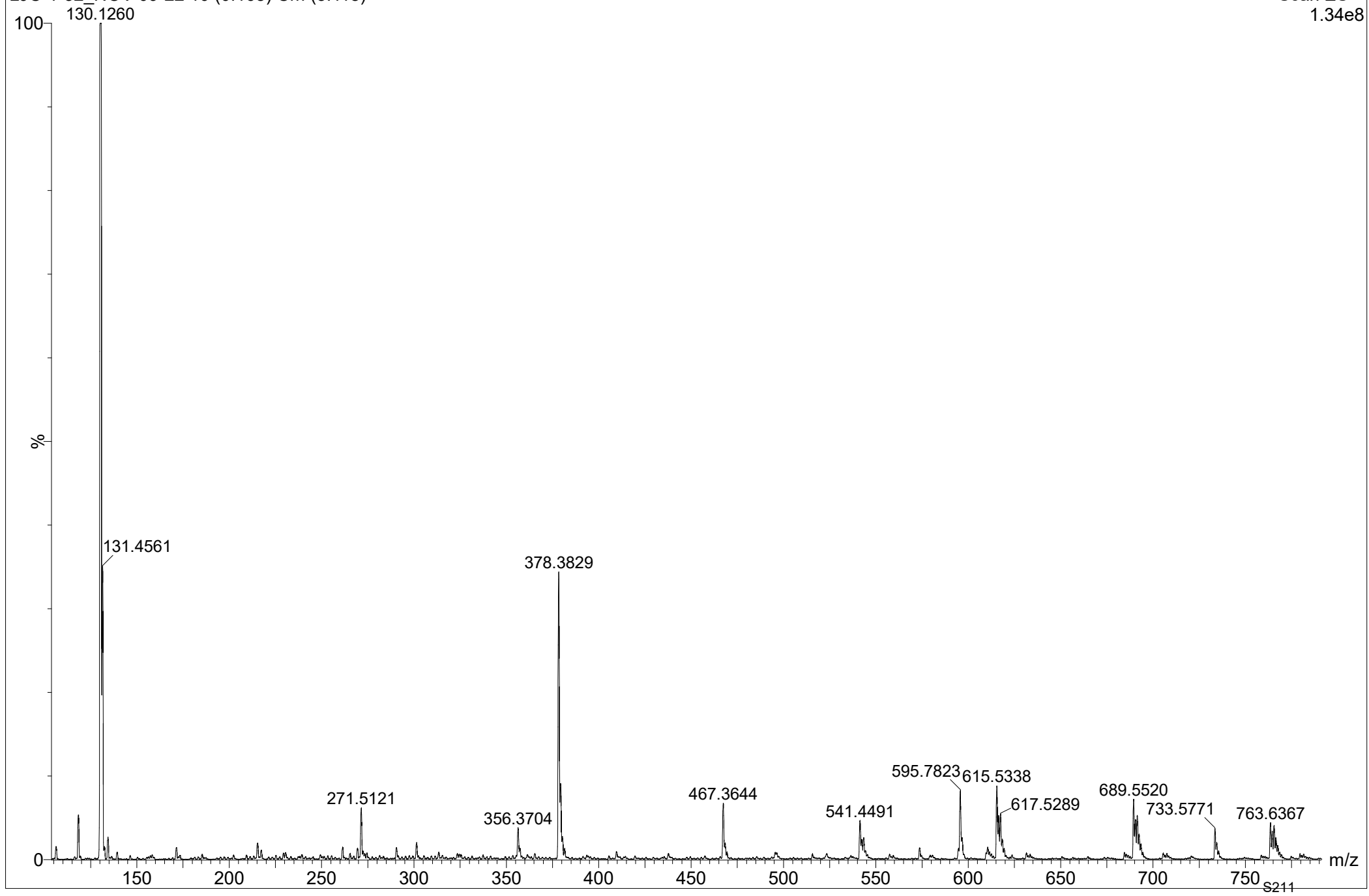
=====
*** End of Report ***









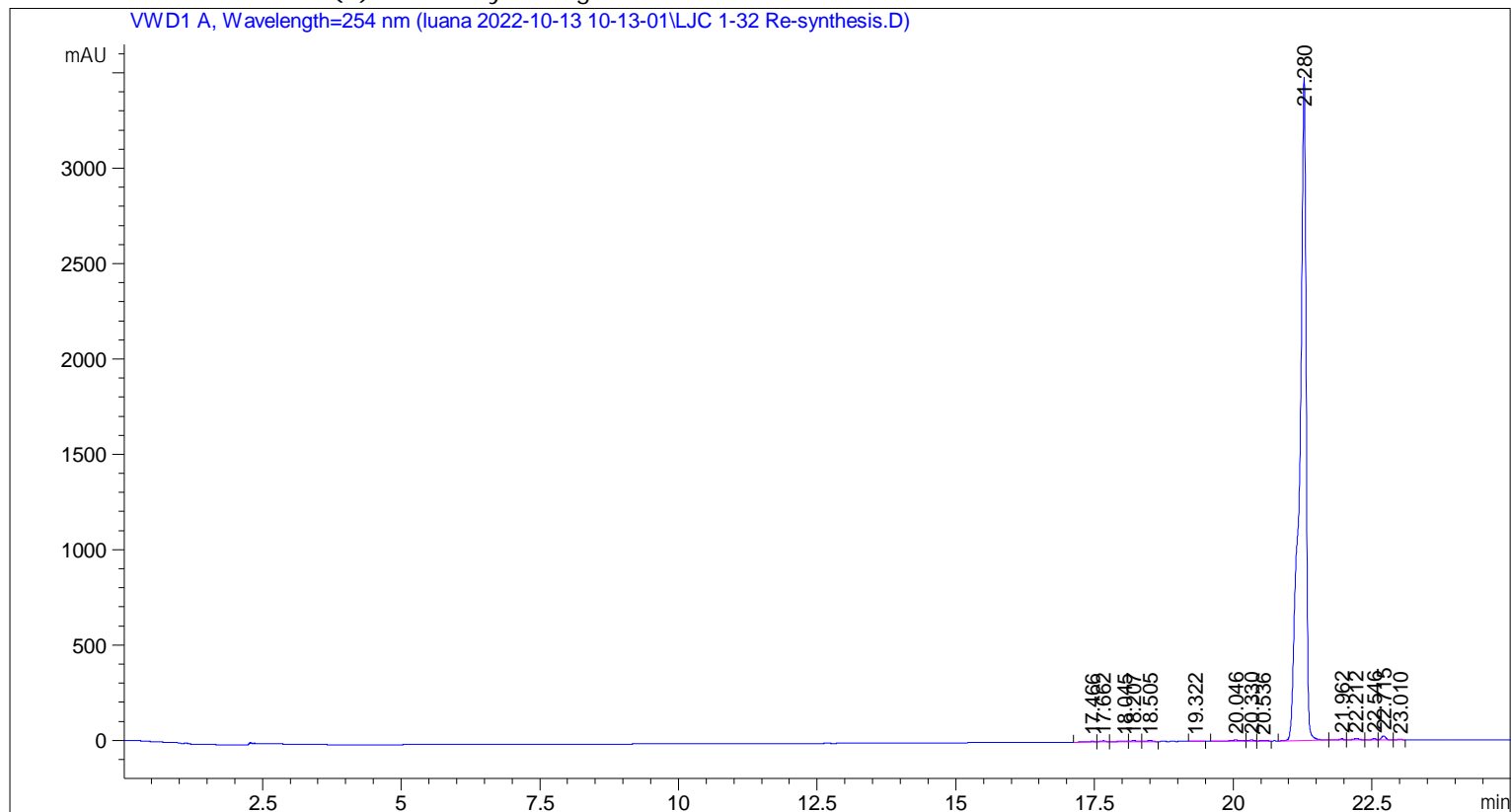


```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    8
Acq. Instrument : 1220 HPLC                    Location  :   87
Injection Date  : 10/13/2022 1:23:21 PM      Inj       :    1
                                           Inj Volume: 70.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2022-10-13 10-13-01\Luana_small_molecule.M (Sequence
                :                               Method)
Last changed    : 10/13/2022 10:13:06 AM by SYSTEM
Method Info     : MeOH/water
  
```

Sample Info : LJC 1-32 Re-synthesis

Additional Info : Peak(s) manually integrated



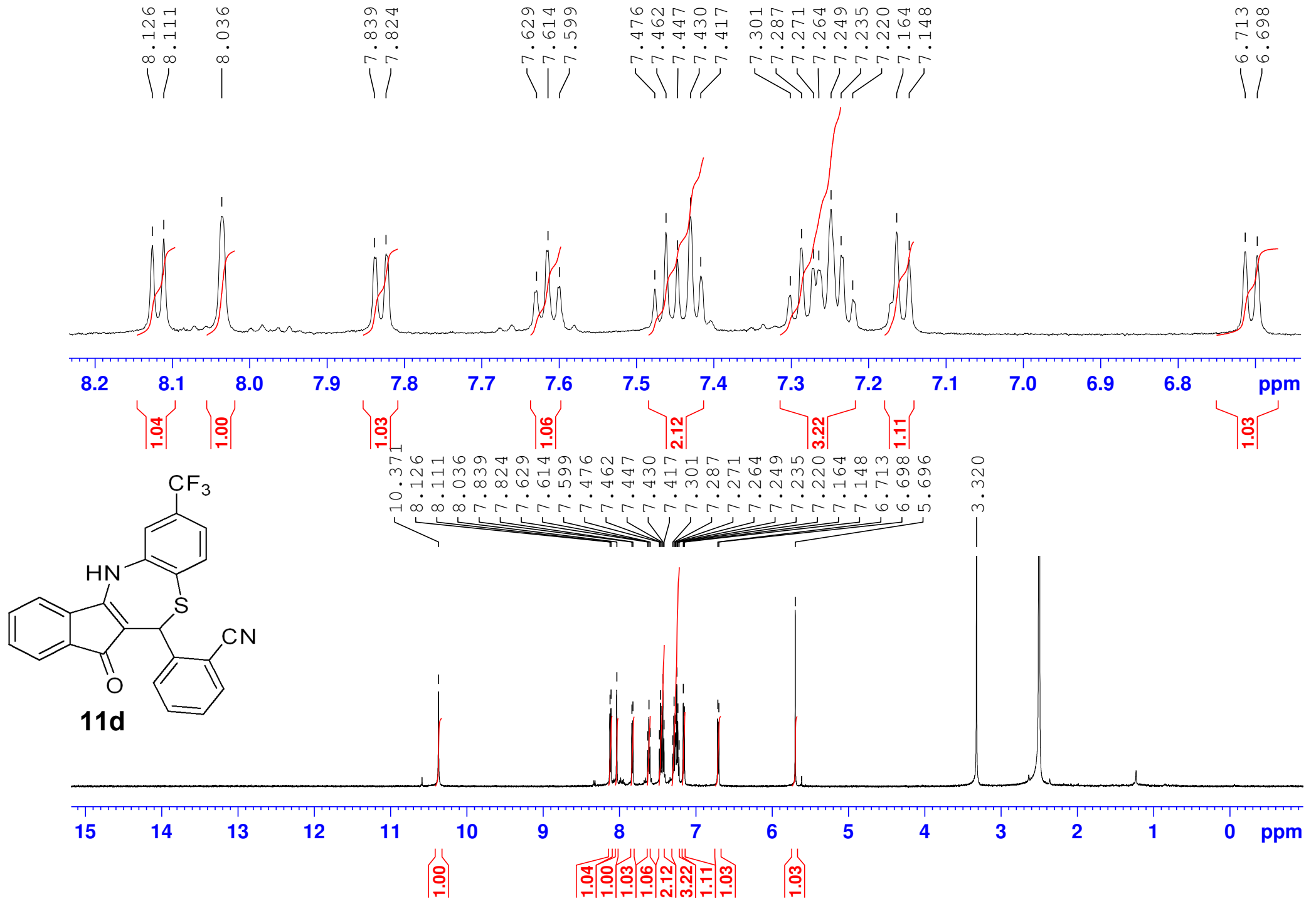
Area Percent Report

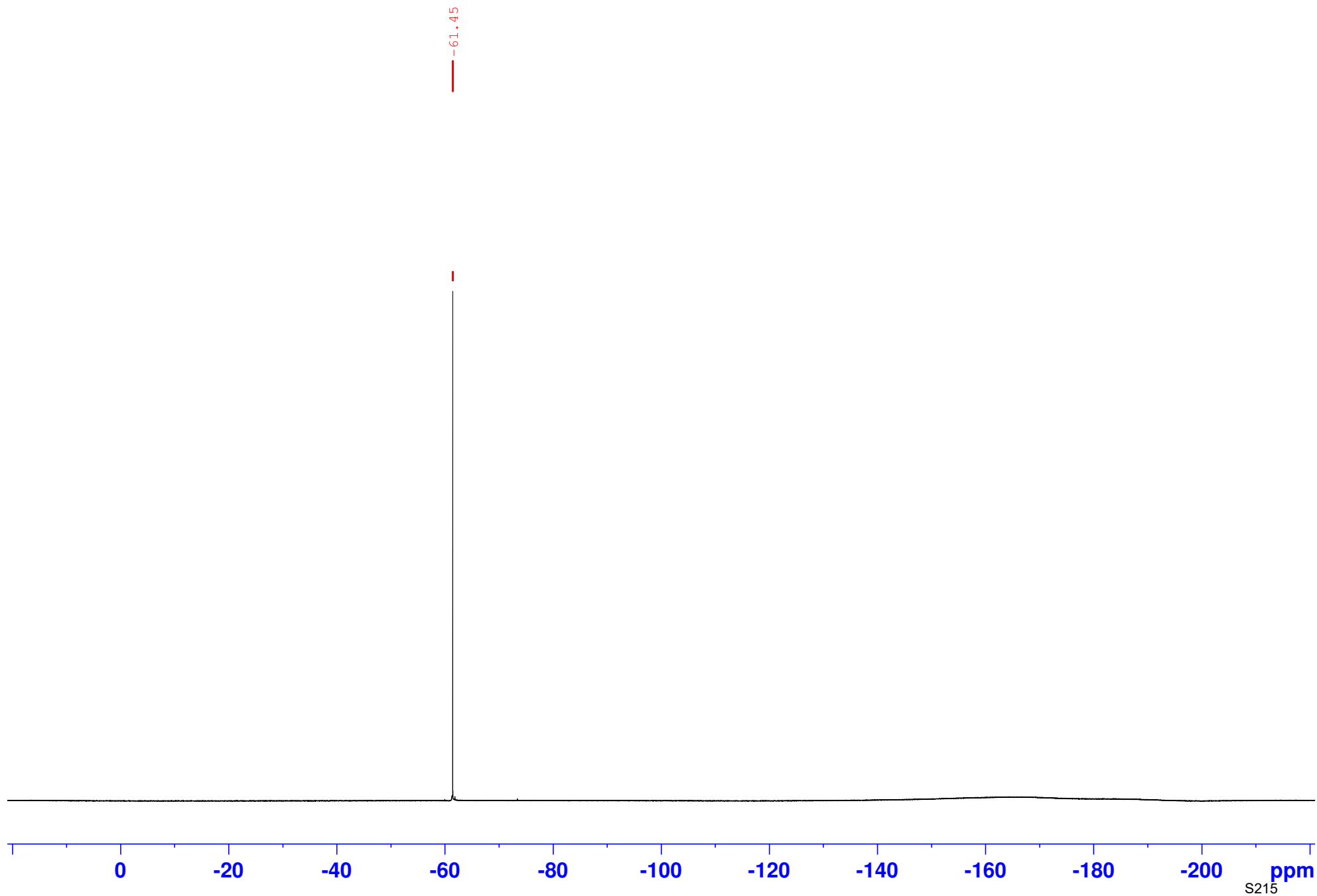
```

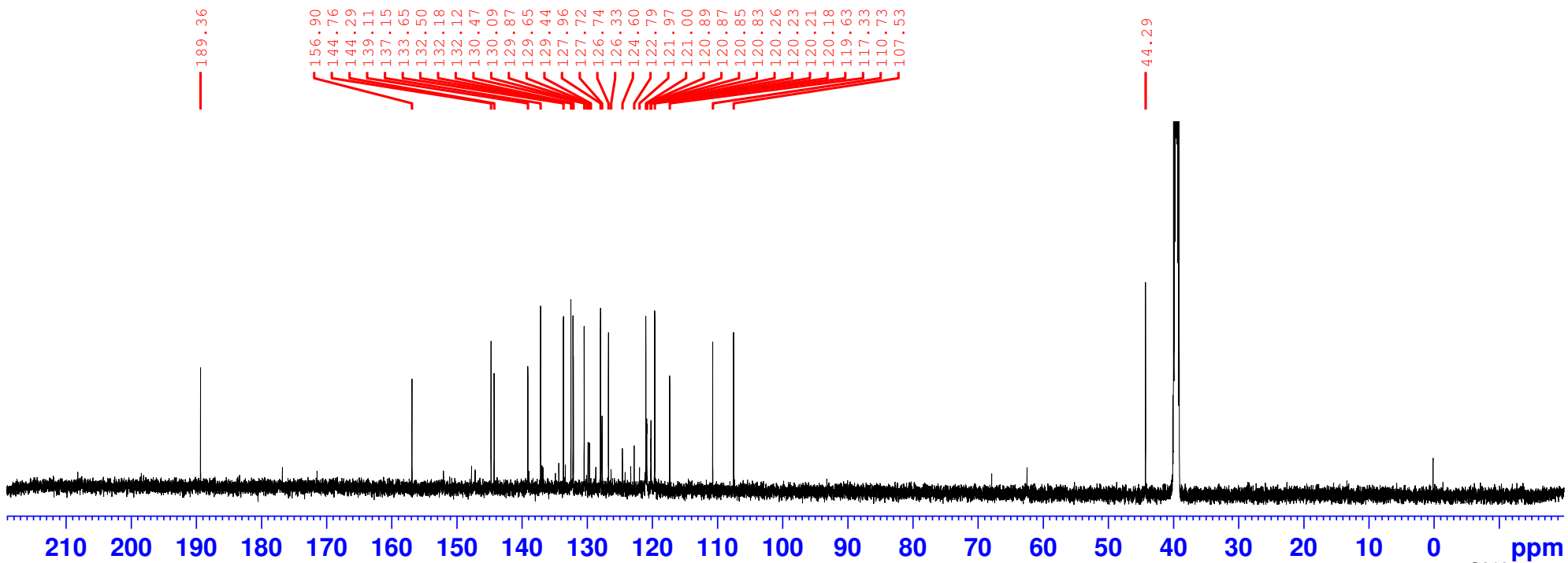
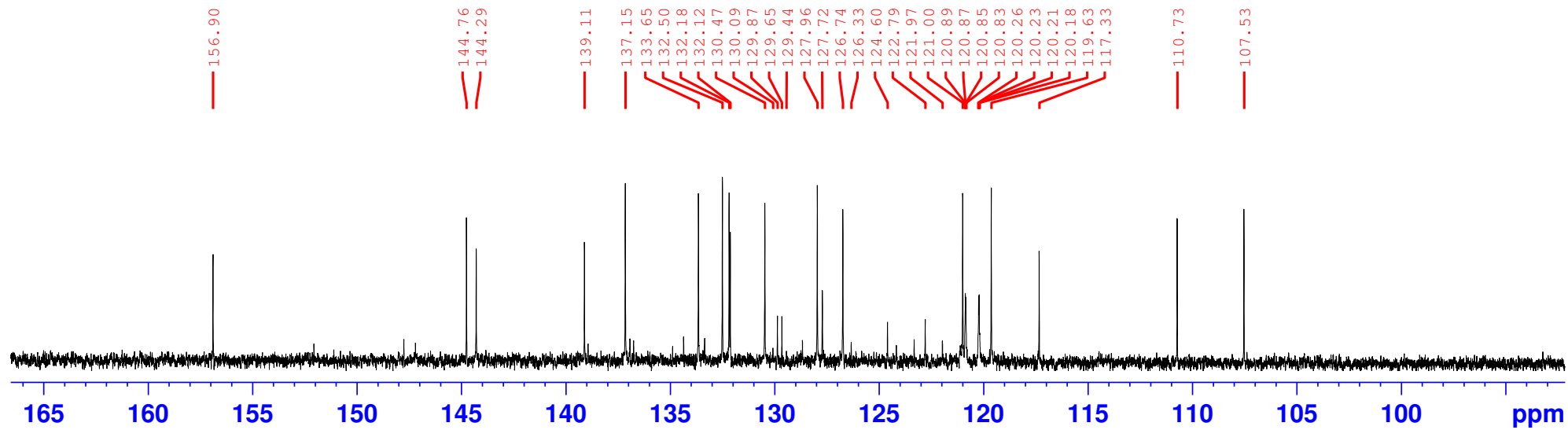
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

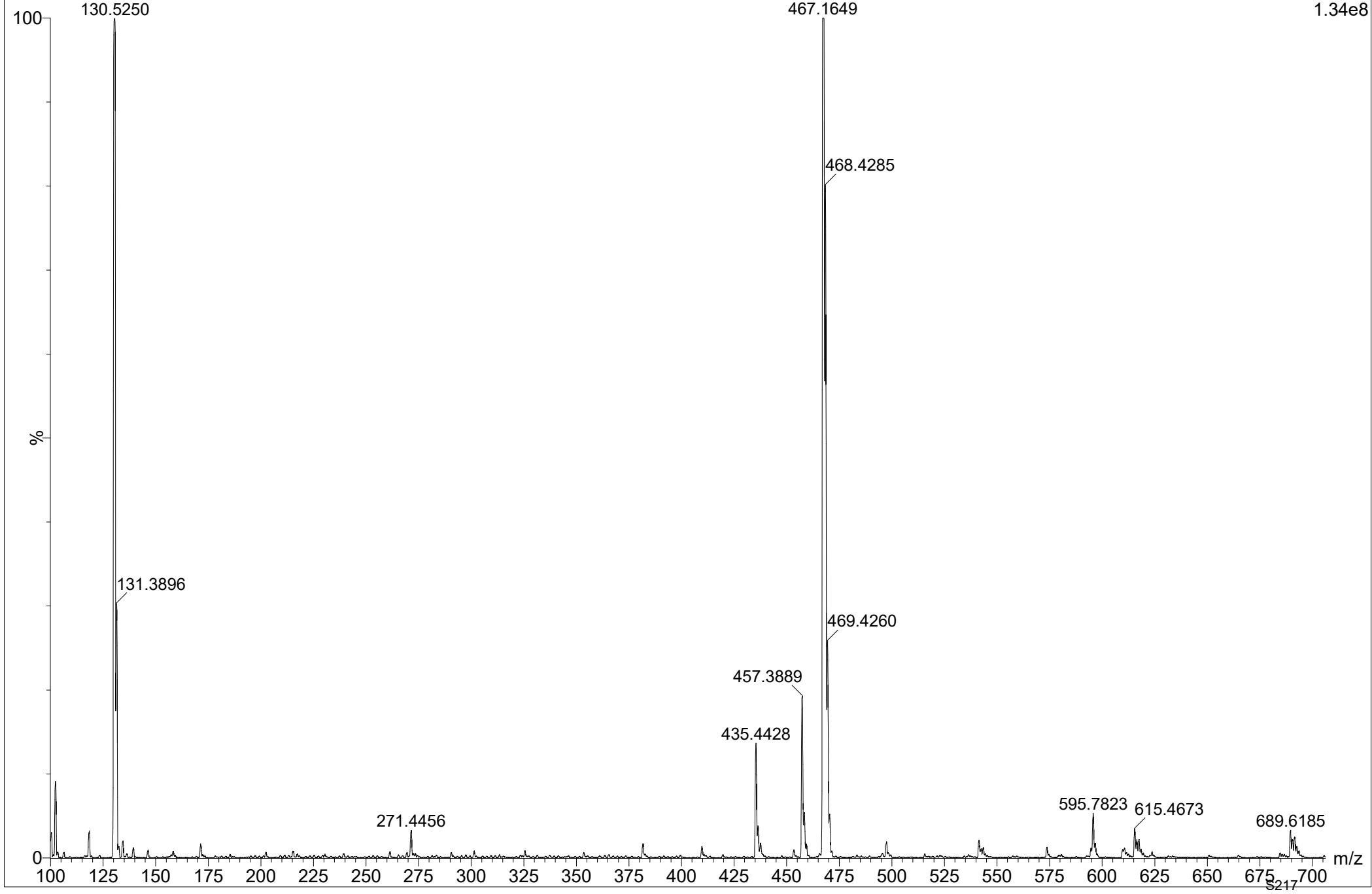
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.466	BV	0.1879	33.52855	2.50929	0.1170
2	17.662	VB	0.0965	34.66453	5.28821	0.1210
3	18.045	BV	0.1315	31.91075	3.36862	0.1114
4	18.207	VV	0.1095	40.12352	5.28878	0.1401









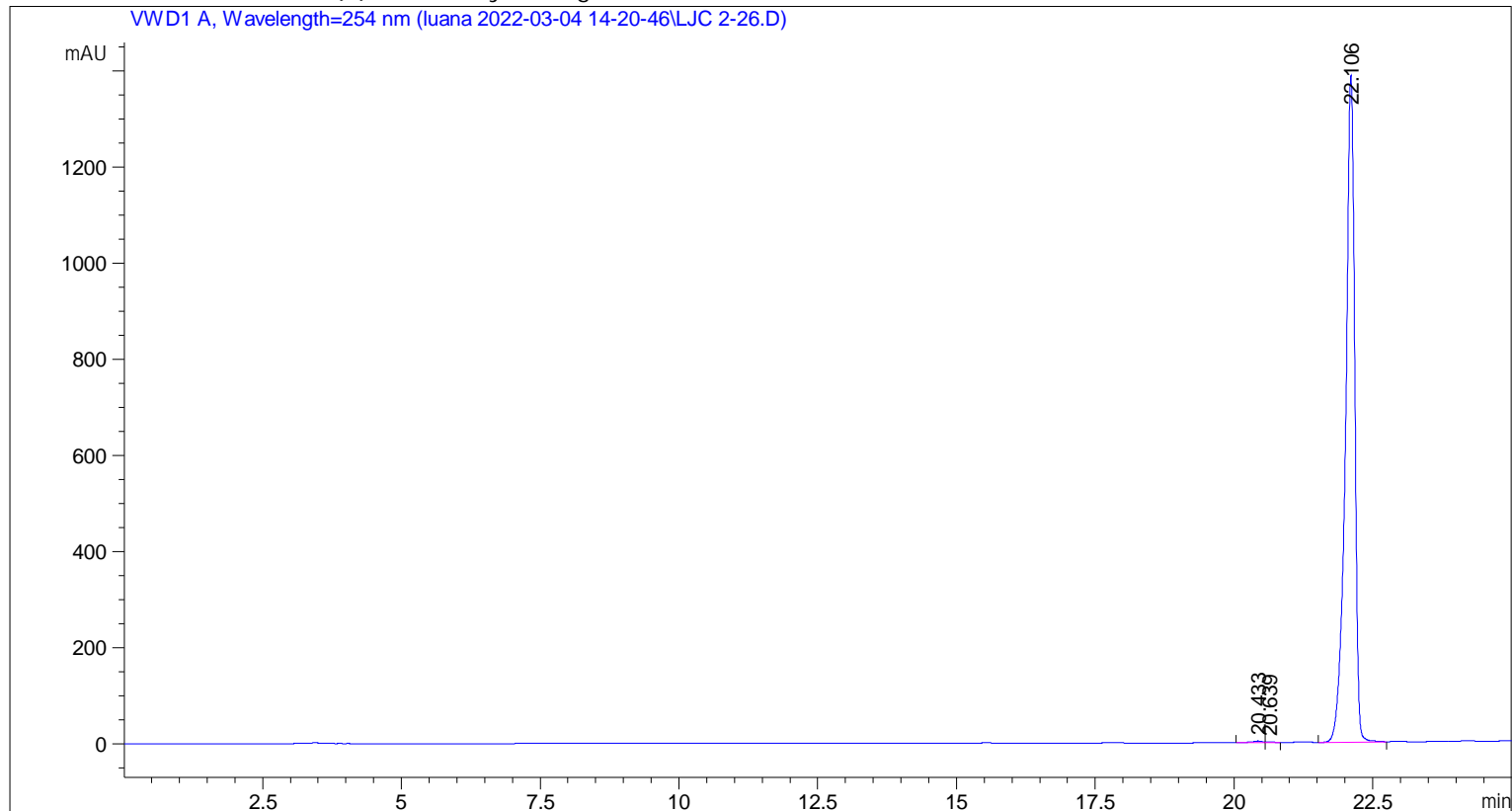
Sample Name: LJC 2-26

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    1
Acq. Instrument : 1220 HPLC                   Location  :   41
Injection Date  : 3/4/2022 2:22:12 PM        Inj       :    1
                                                Inj Volume: 70.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2022-03-04 14-20-46\Luana_small_molecule.M (Sequence
                :                               Method)
Last changed    : 3/4/2022 2:20:50 PM by SYSTEM
Method Info     : MeOH/water

Sample Info     : LJC 2-26
    
```

Additional Info : Peak(s) manually integrated



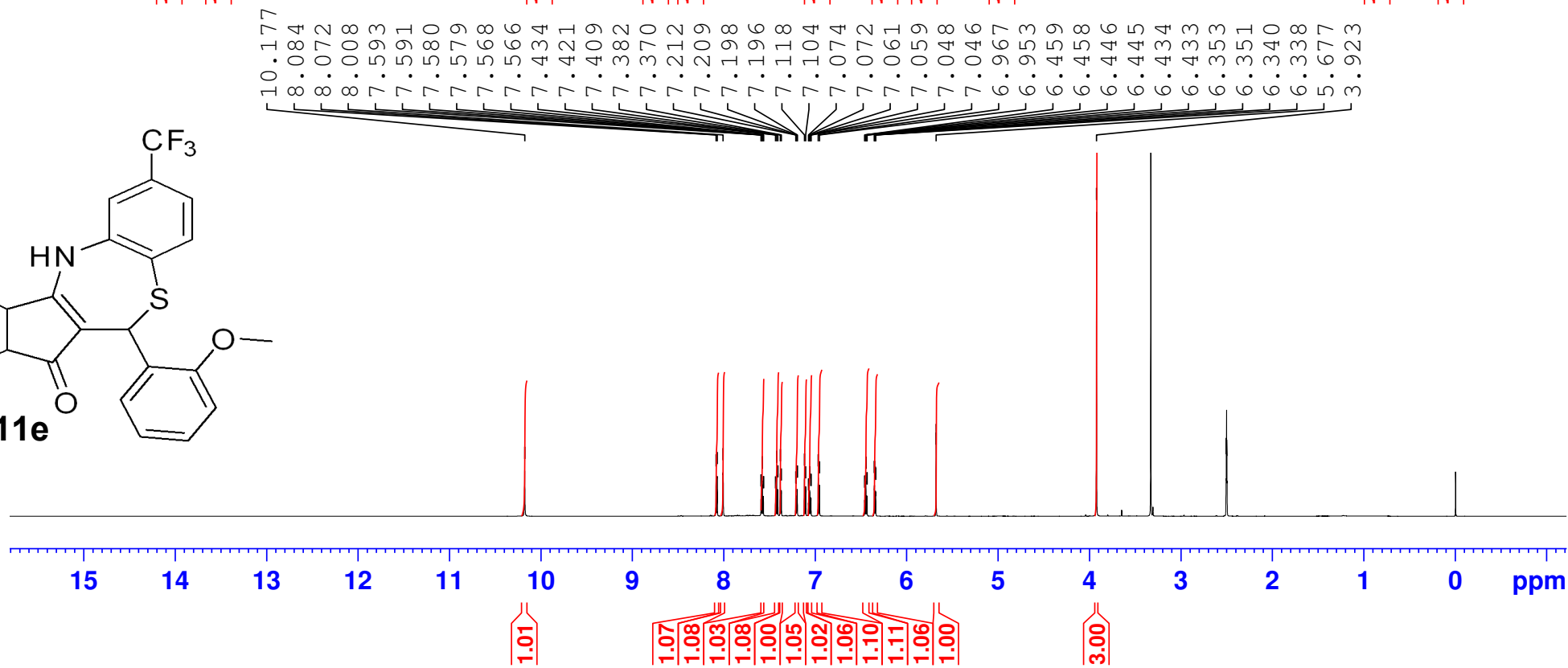
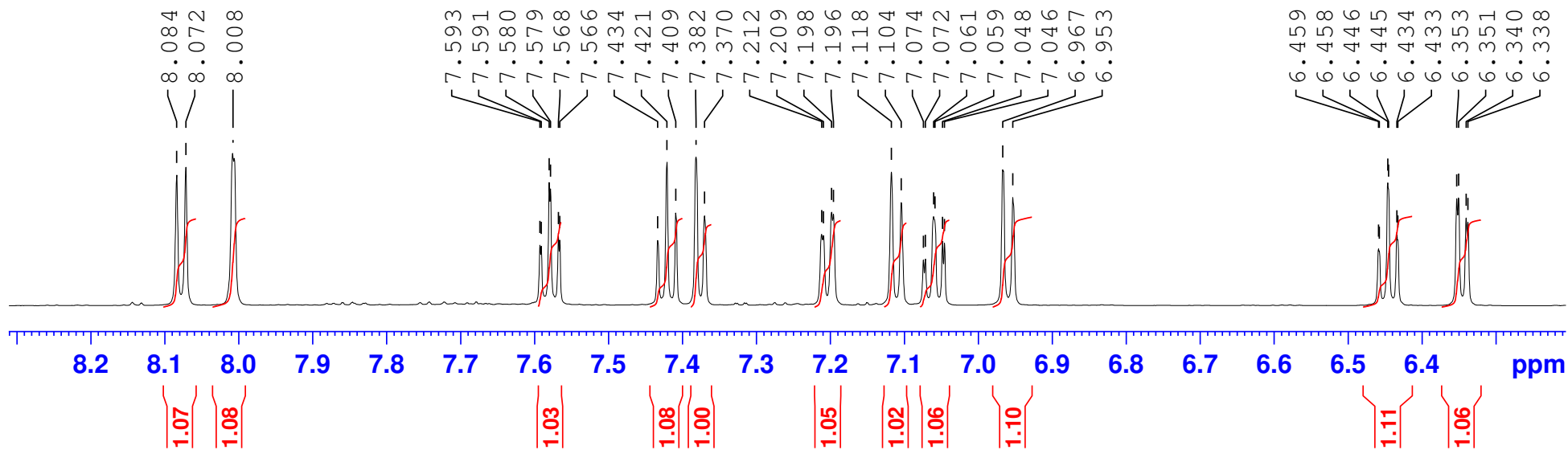
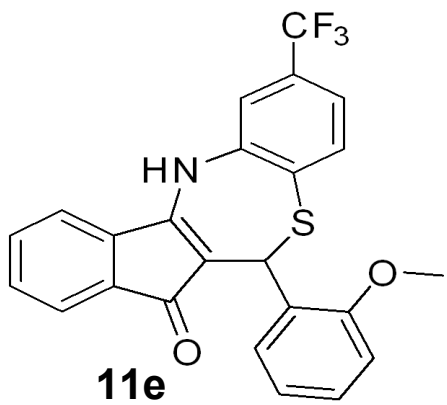
Area Percent Report

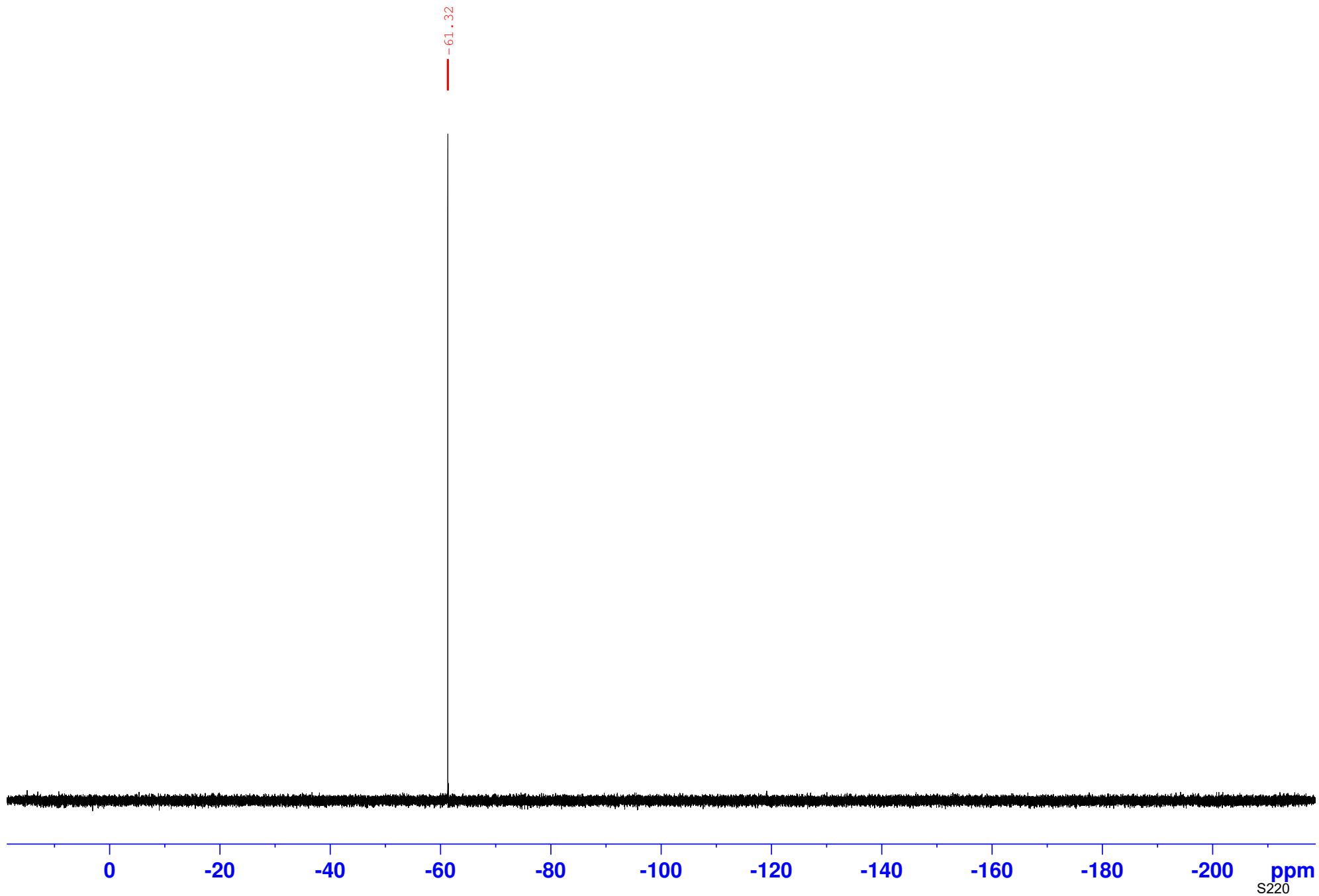
```

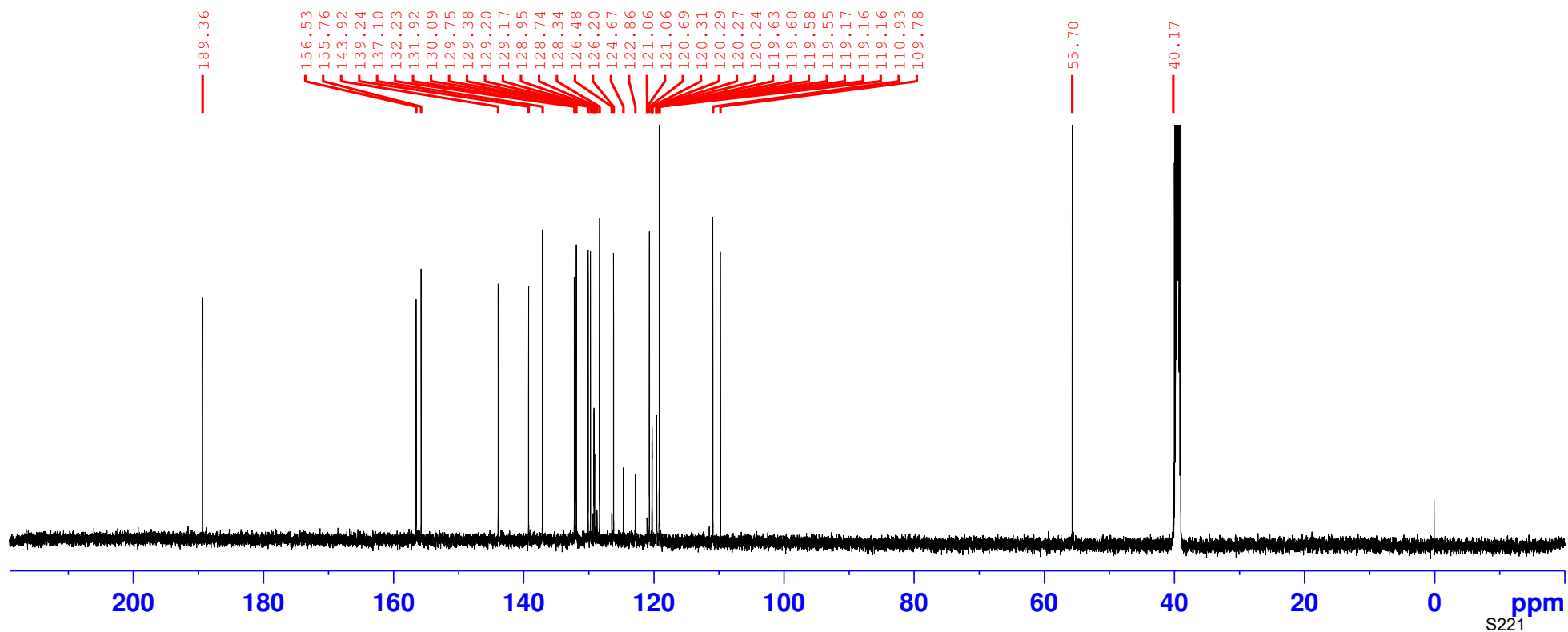
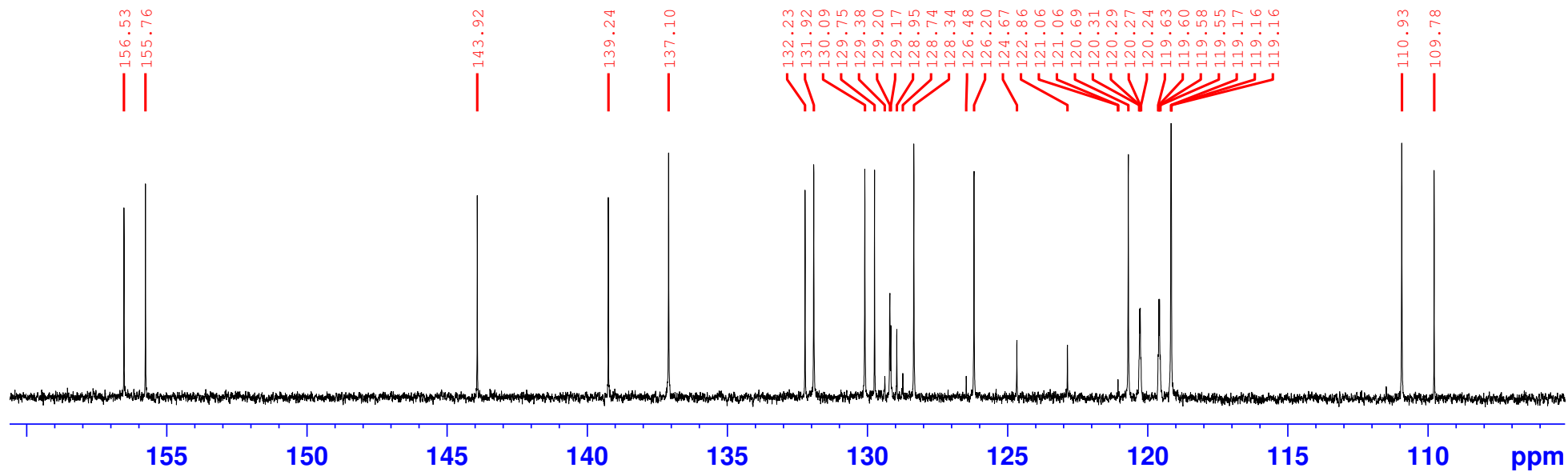
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

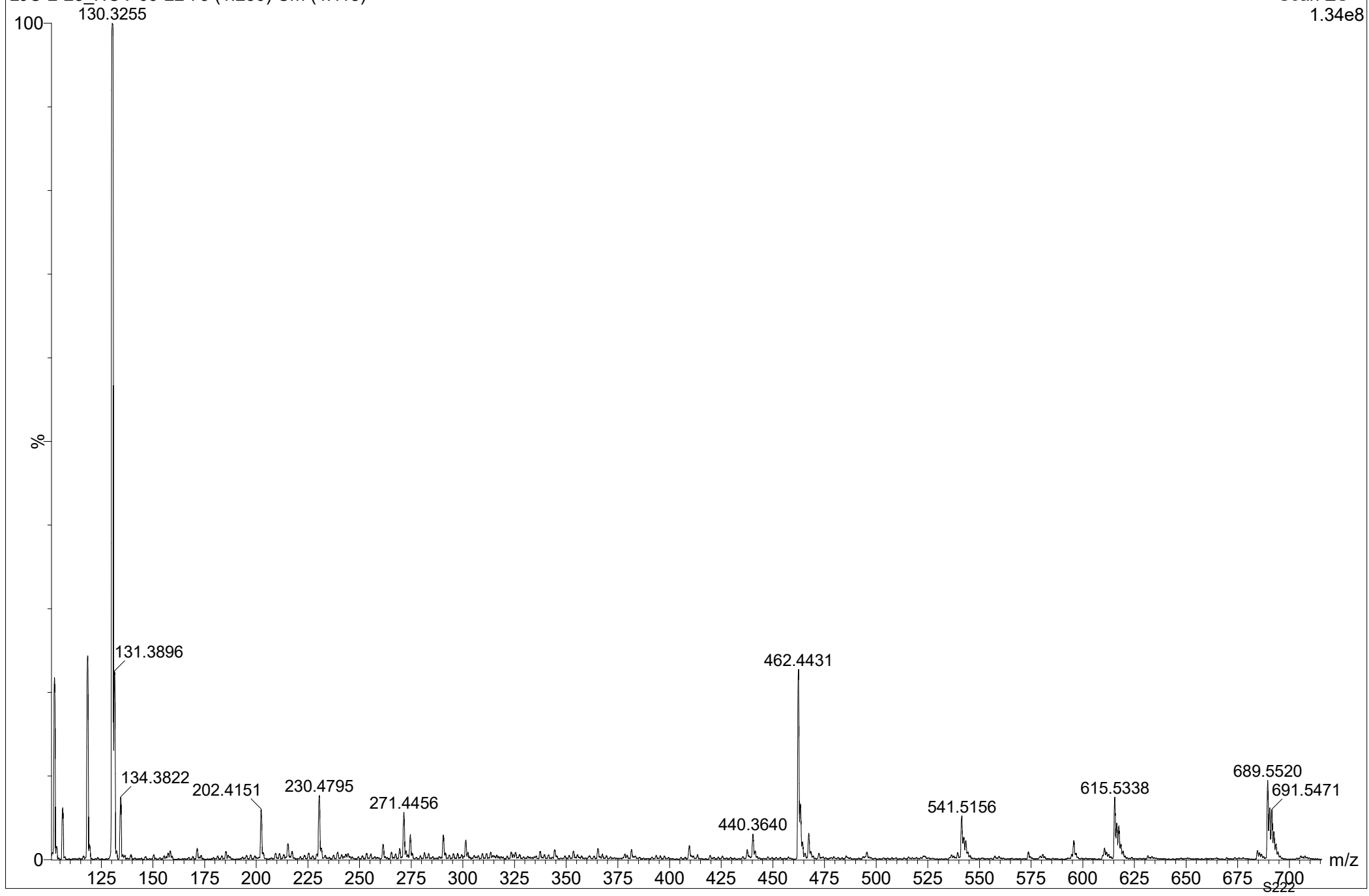
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.433	VV	0.1916	47.67384	3.52861	0.2986
2	20.639	VB	0.1433	17.11752	1.82795	0.1072
3	22.106	BB	0.1727	1.58997e4	1386.95178	99.5942









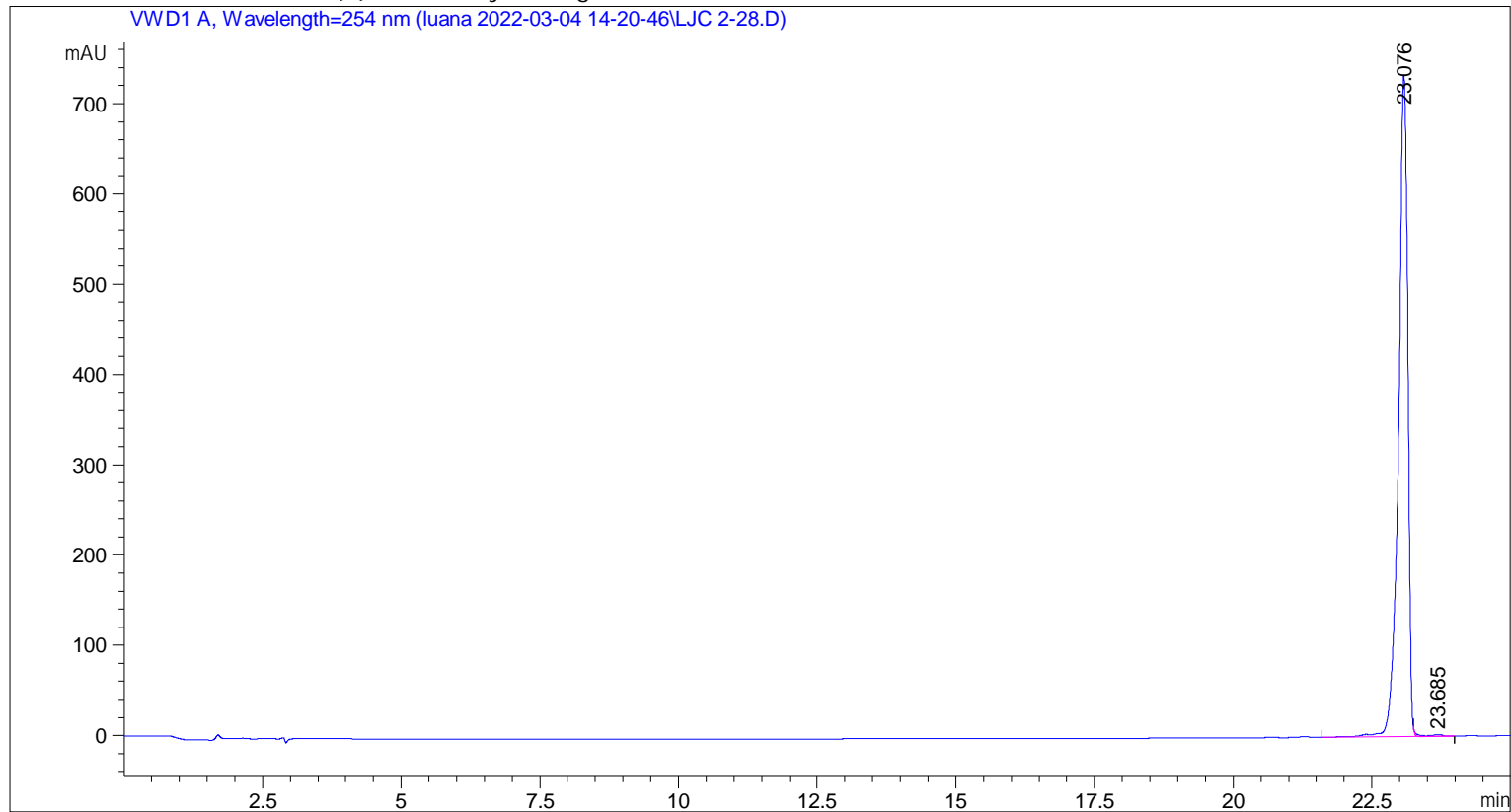
Sample Name: LJC 2-28

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    3
Acq. Instrument : 1220 HPLC                   Location  :   43
Injection Date  : 3/4/2022 3:16:31 PM        Inj       :    1
                                                Inj Volume: 70.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 50.000 µl
Method          : C:\Chem32\1\Data\luana 2022-03-04 14-20-46\Luana_small_molecule.M (Sequence Method)
Last changed    : 3/4/2022 2:20:50 PM by SYSTEM
Method Info     : MeOH/water

Sample Info     : LJC 2-28
    
```

Additional Info : Peak(s) manually integrated



Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.076	VV R	0.1774	8504.40430	732.51331	99.4797
2	23.685	VB E	0.2999	44.47955	2.02823	0.5203

Totals : 8548.88384 734.54154

=====
*** End of Report ***