

Photoelectrocyclization Reactions of Amidonaphthoquinones

Jinya Yin, Michael B. Landward, and Jon D. Rainier*

315 South, 1400 East

Department of Chemistry

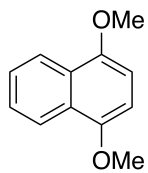
University of Utah

Salt Lake City, UT 84112

email: rainier@chem.utah.edu

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5, ¹H NMR (500 MHz, CDCl₃)

8.308
8.306
8.301
8.300
8.293
8.287
8.282
8.281
7.583
7.581
7.576
7.569
7.563
7.556
7.550
7.260
6.724
3.993

2.01

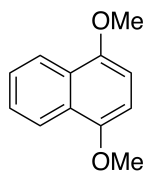
2.01

2.00

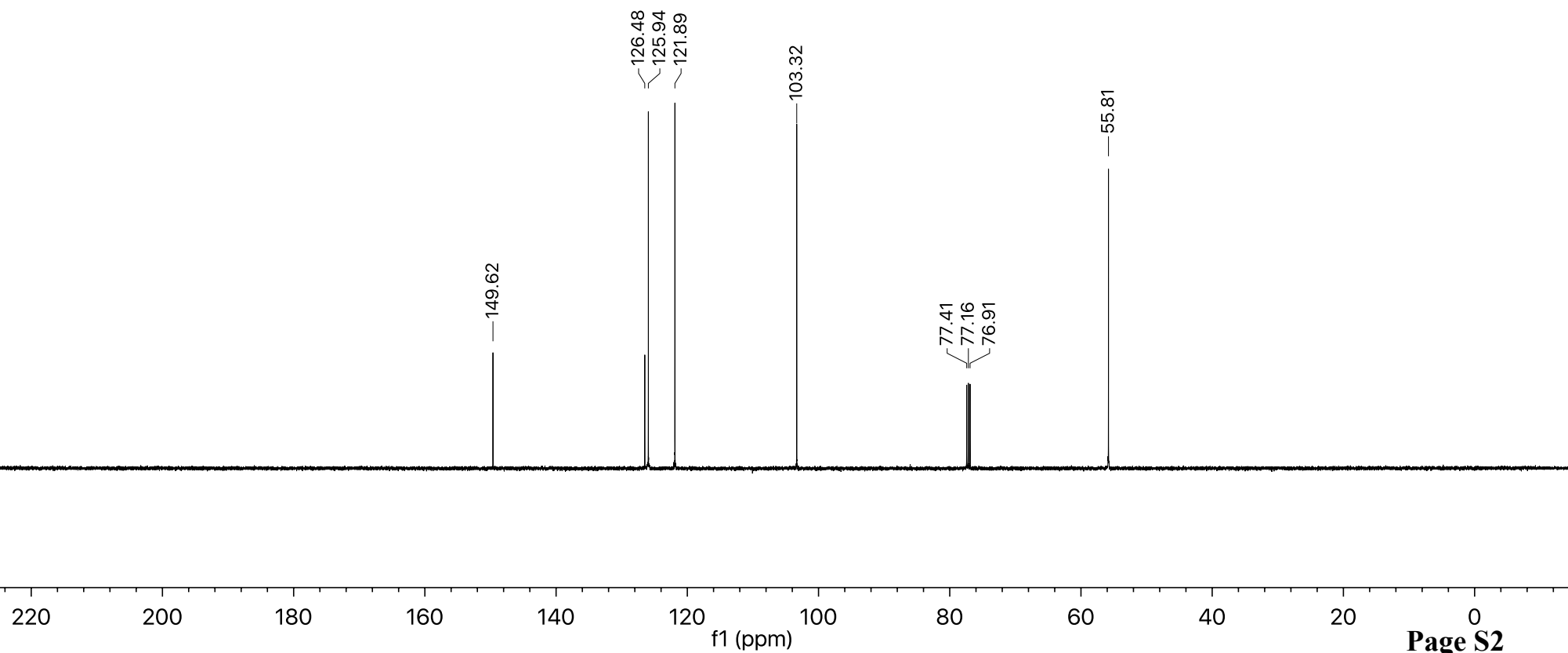
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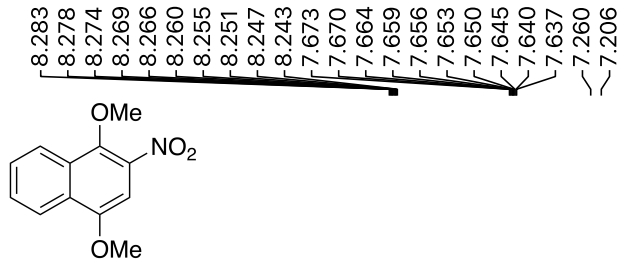
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f1 (ppm)



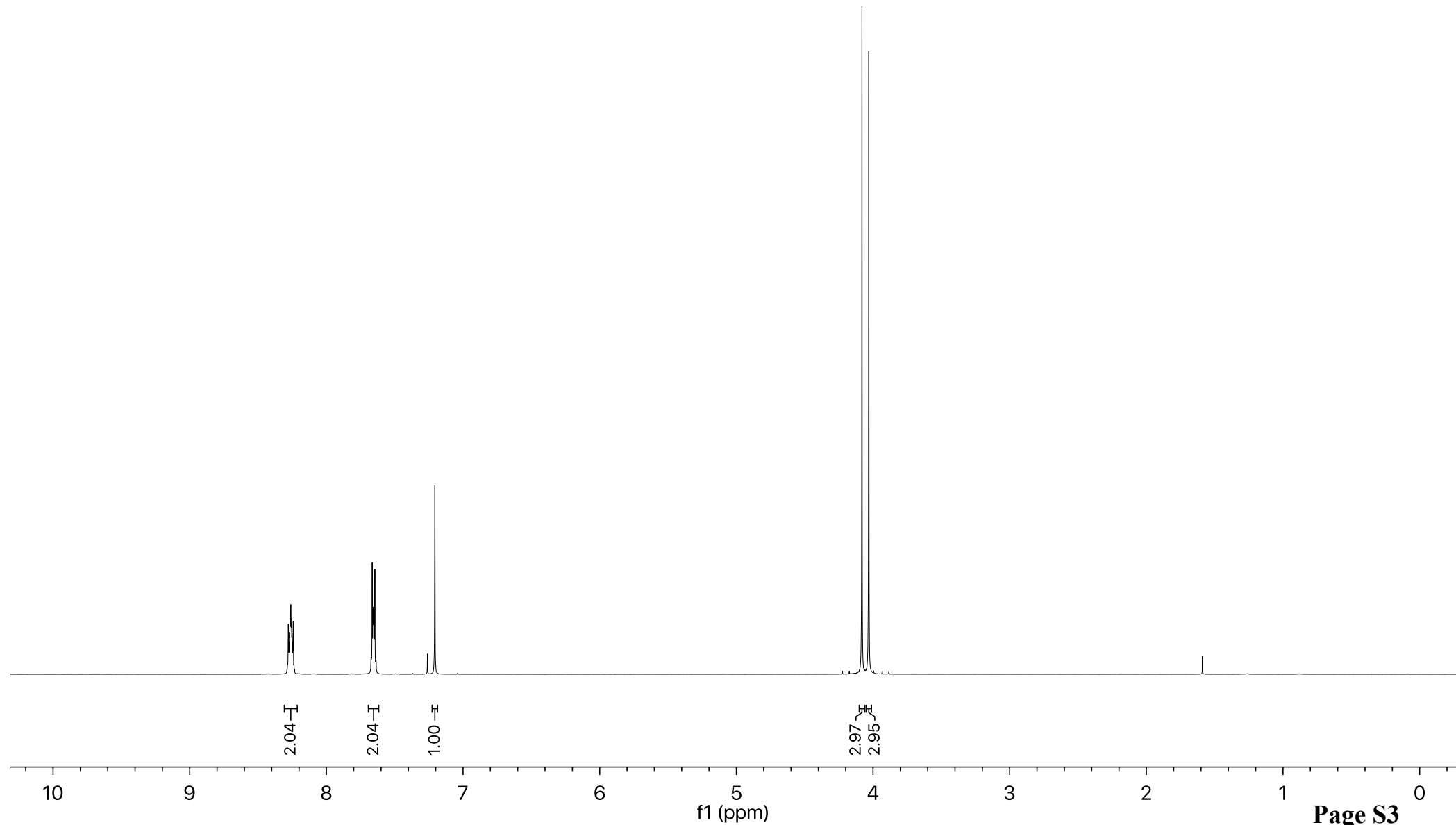
5, ^{13}C NMR (126 MHz, CDCl_3)

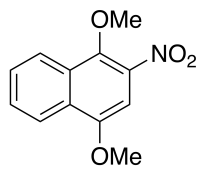




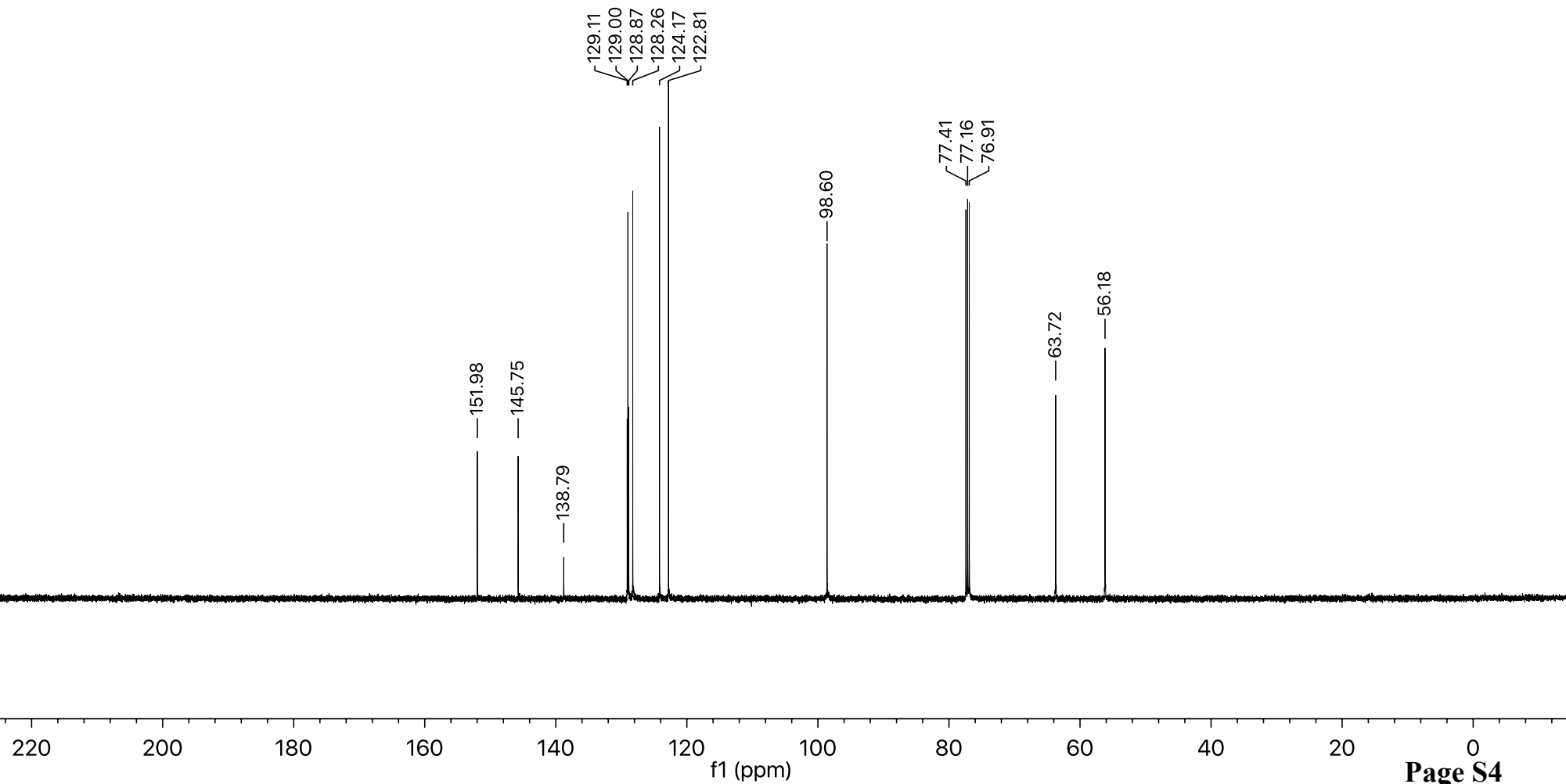
4.081
4.031

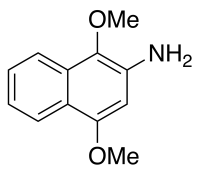
S1, ^1H NMR (500 MHz, CDCl_3)





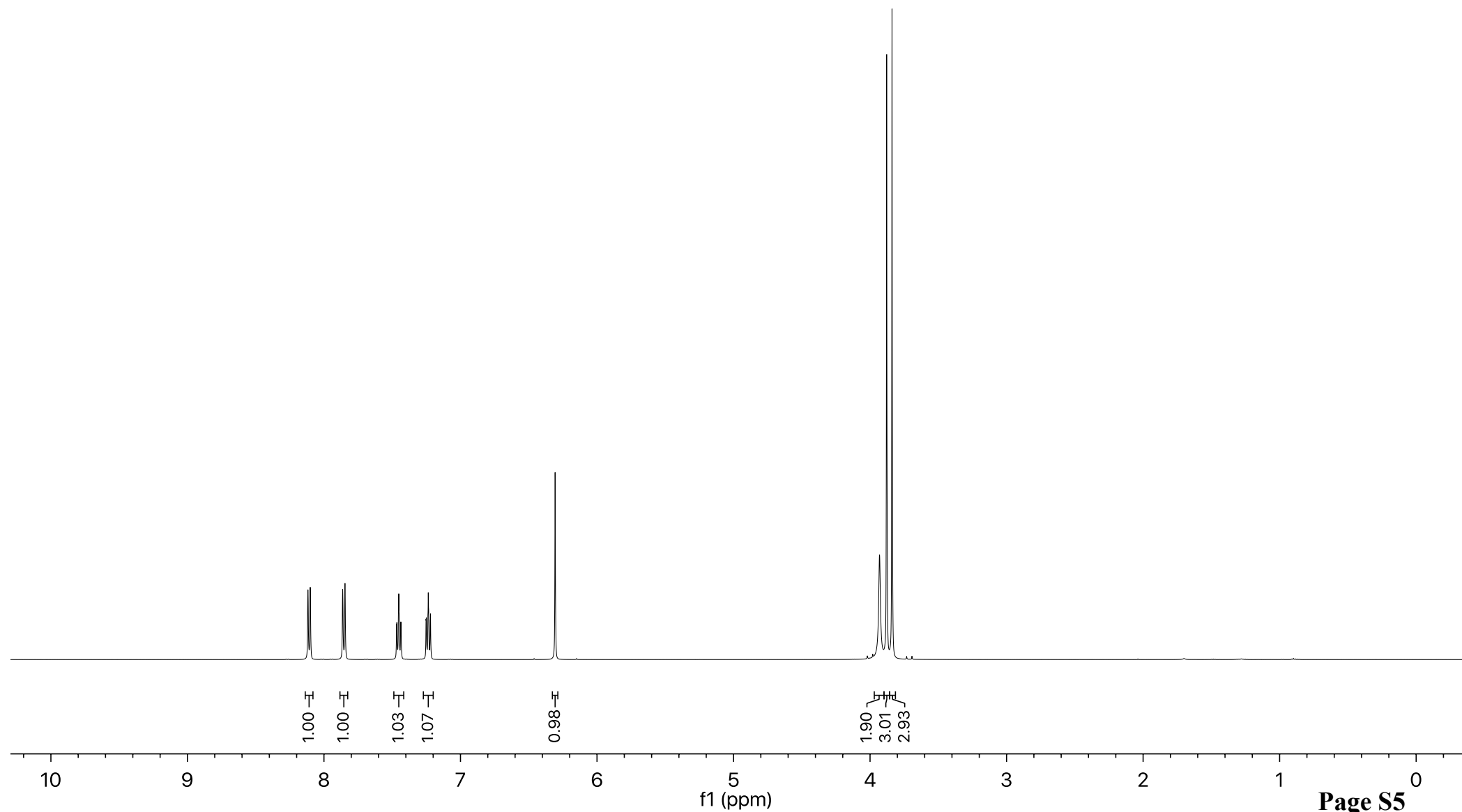
S1, ^{13}C NMR (126 MHz, CDCl_3)

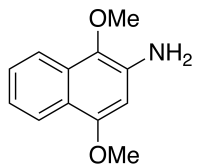




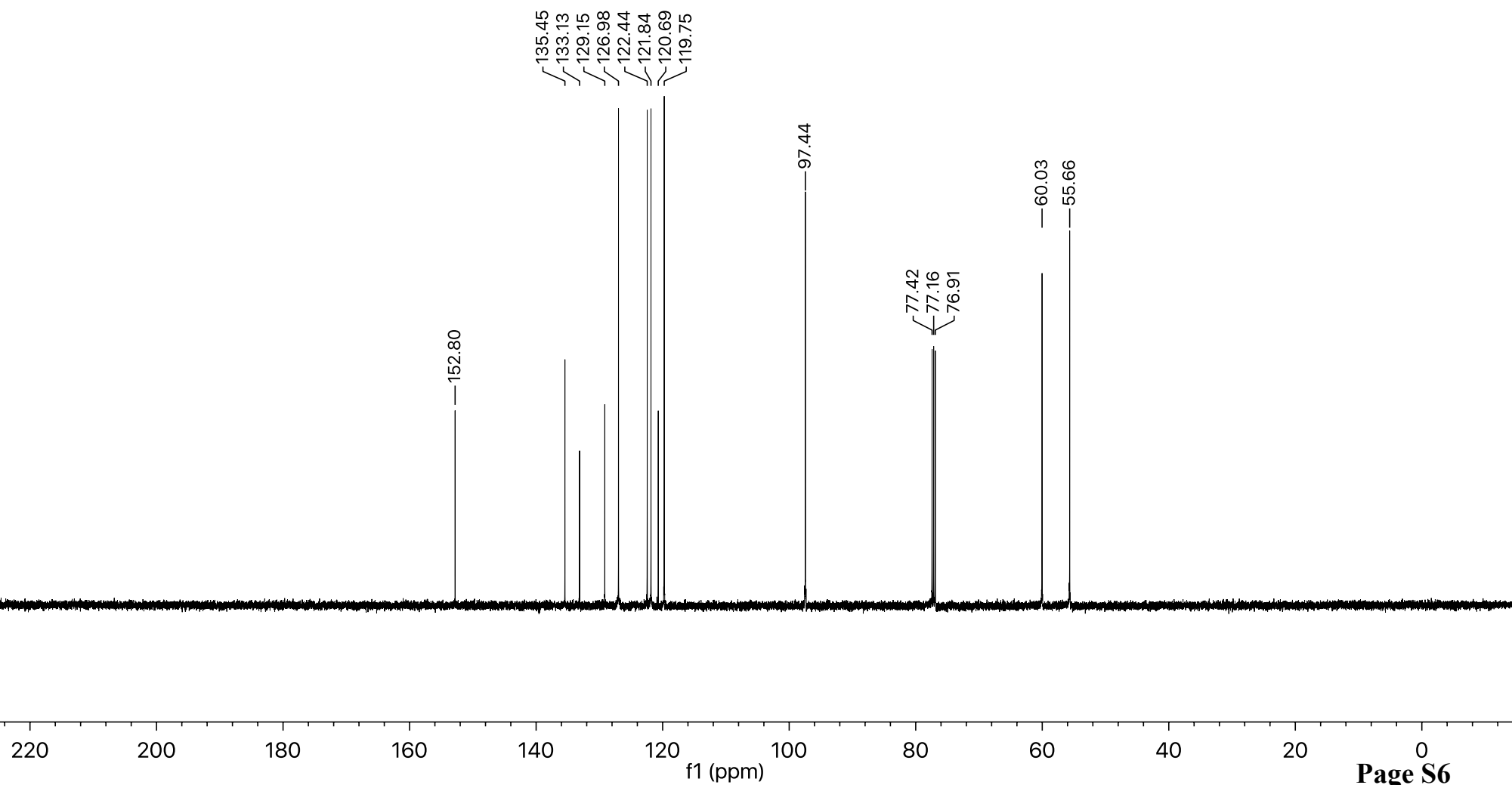
8.117
8.100
7.863
7.846
7.468
7.466
7.452
7.438
7.436
7.252
7.250
7.236
7.220
6.307
3.931
3.878
3.839

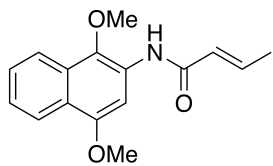
6, ¹H NMR (500 MHz, CDCl₃)





6, ^{13}C NMR (126 MHz, CDCl_3)



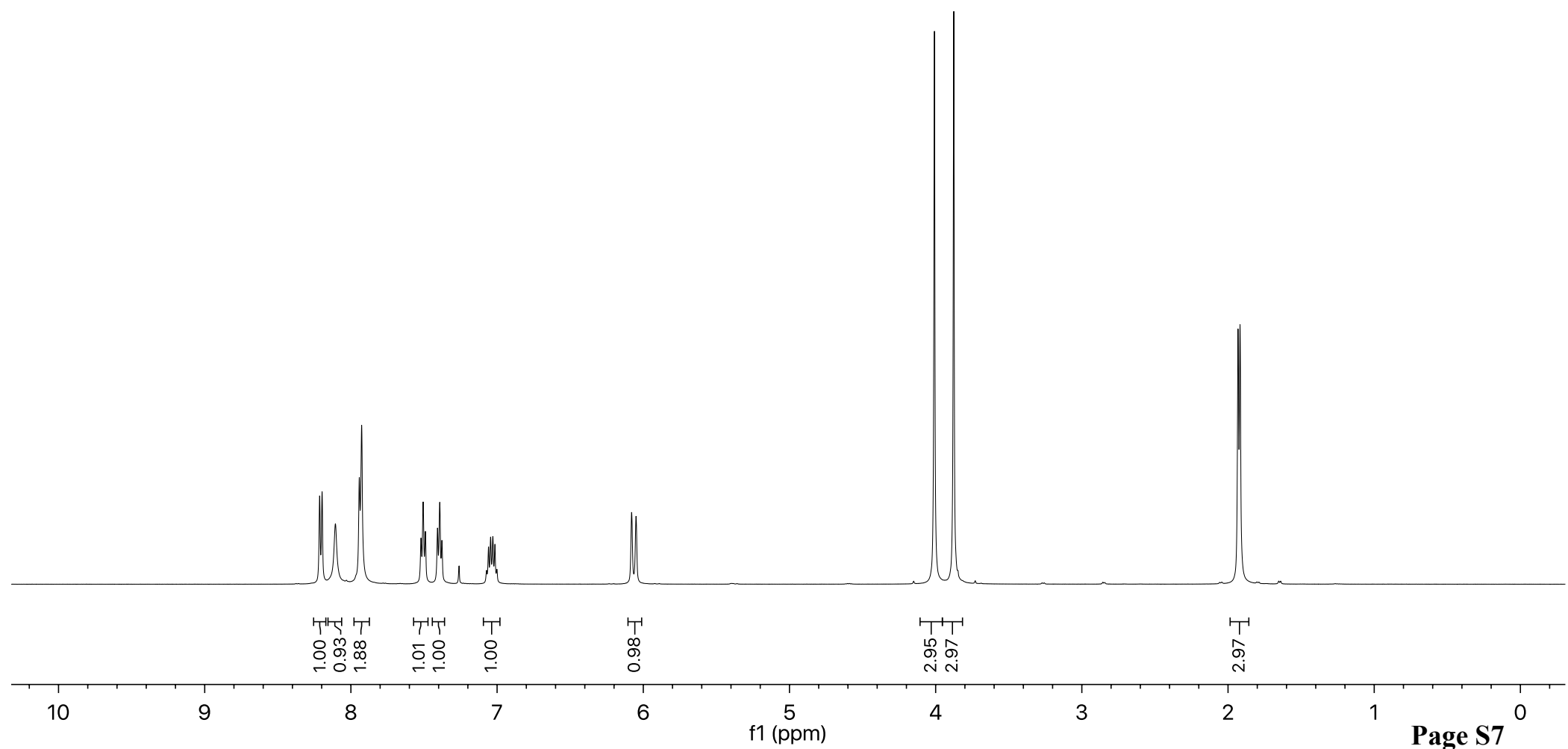


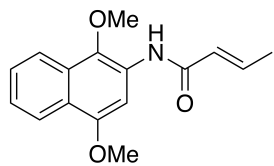
8.214
8.197
8.106
7.942
7.926
7.520
7.506
7.490
7.407
7.392
7.377
7.260
7.072
7.058
7.044
7.029
7.015
7.001
6.080
6.050

4.008
3.876

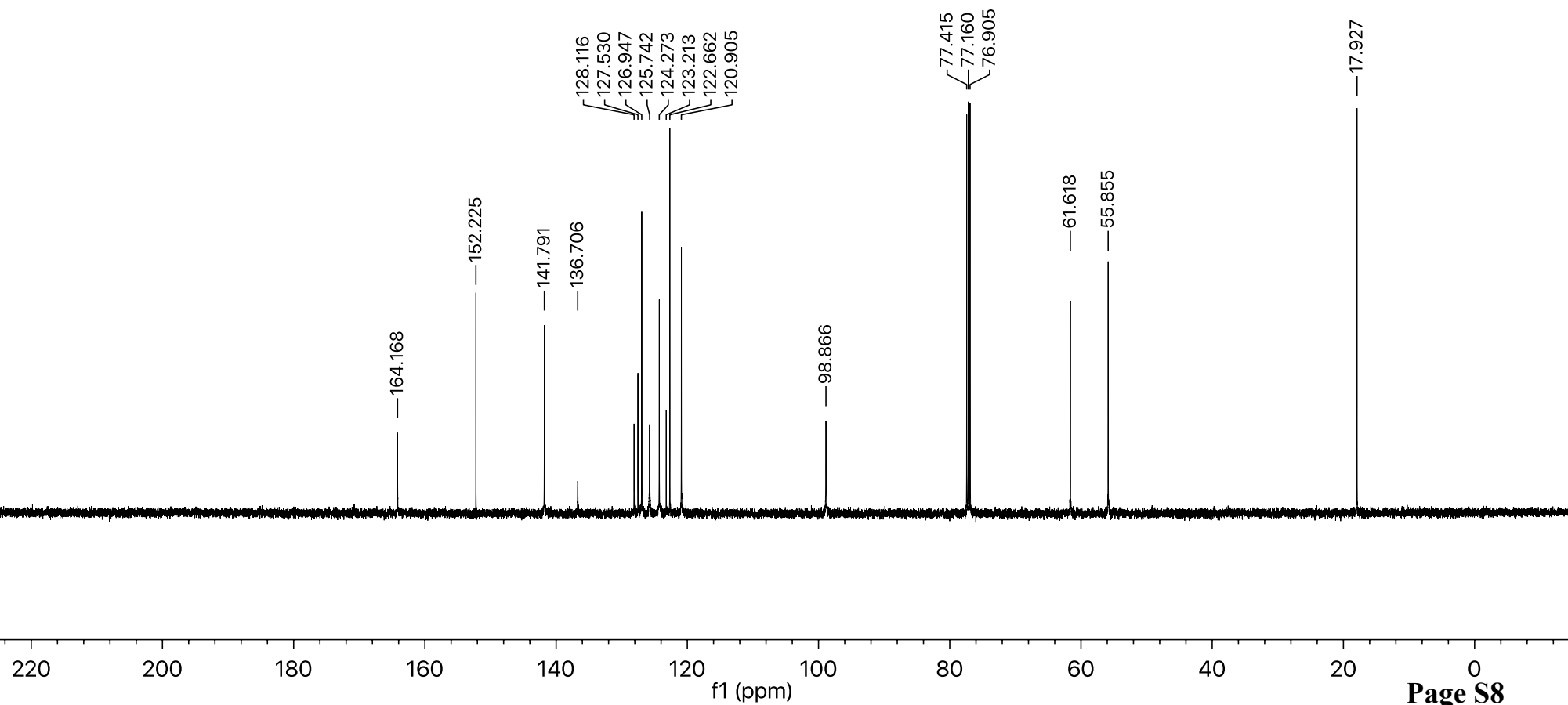
1.932
1.918

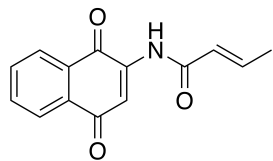
S2, ¹H NMR (500 MHz, CDCl₃)





S2, ^{13}C NMR (126 MHz, CDCl_3)

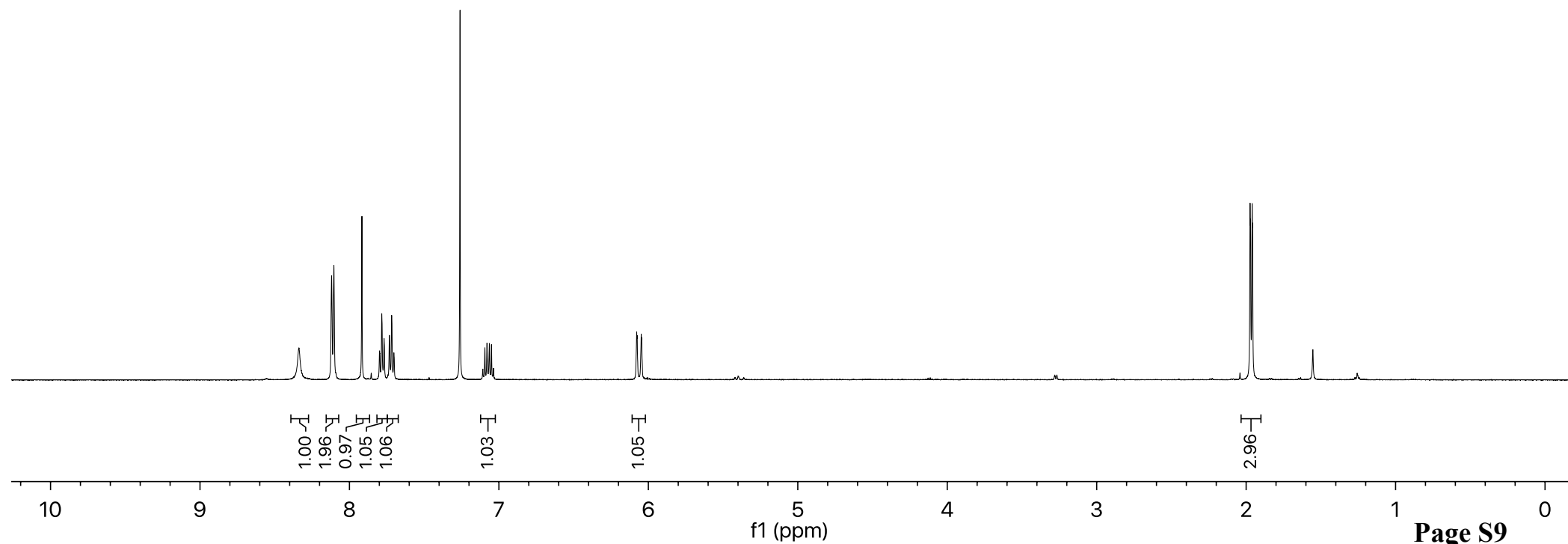


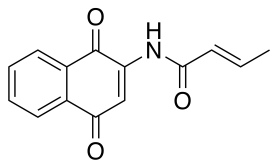


7, ¹H NMR (500 MHz, CDCl₃)

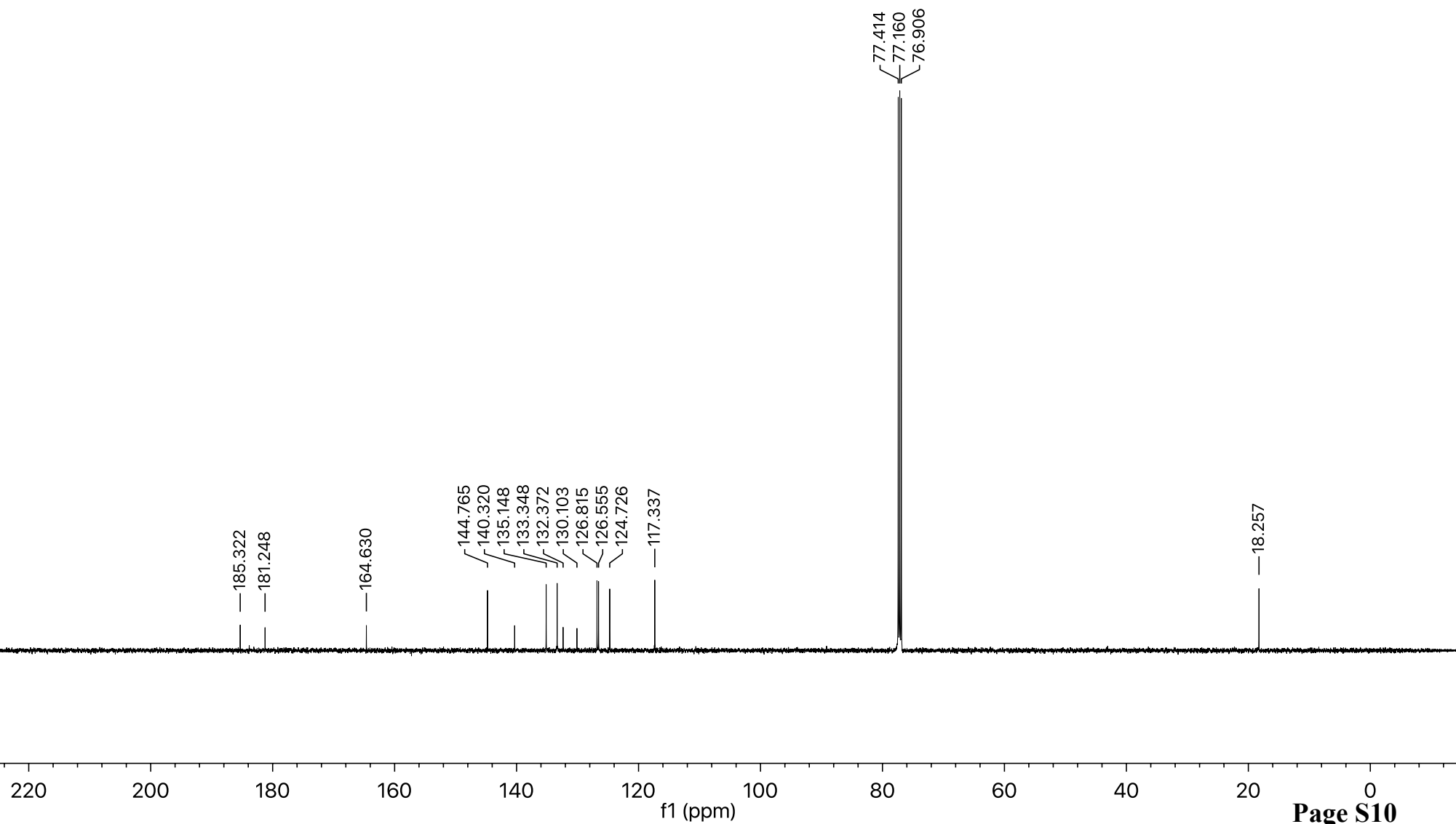
8.338
8.119
8.104
7.917
7.854
7.799
7.784
7.768
7.733
7.718
7.703
7.260
7.107
7.094
7.080
7.063
7.049
7.036
6.078
6.075
6.048
6.045

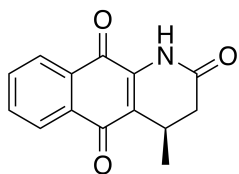
1.974
1.971
1.960
1.957



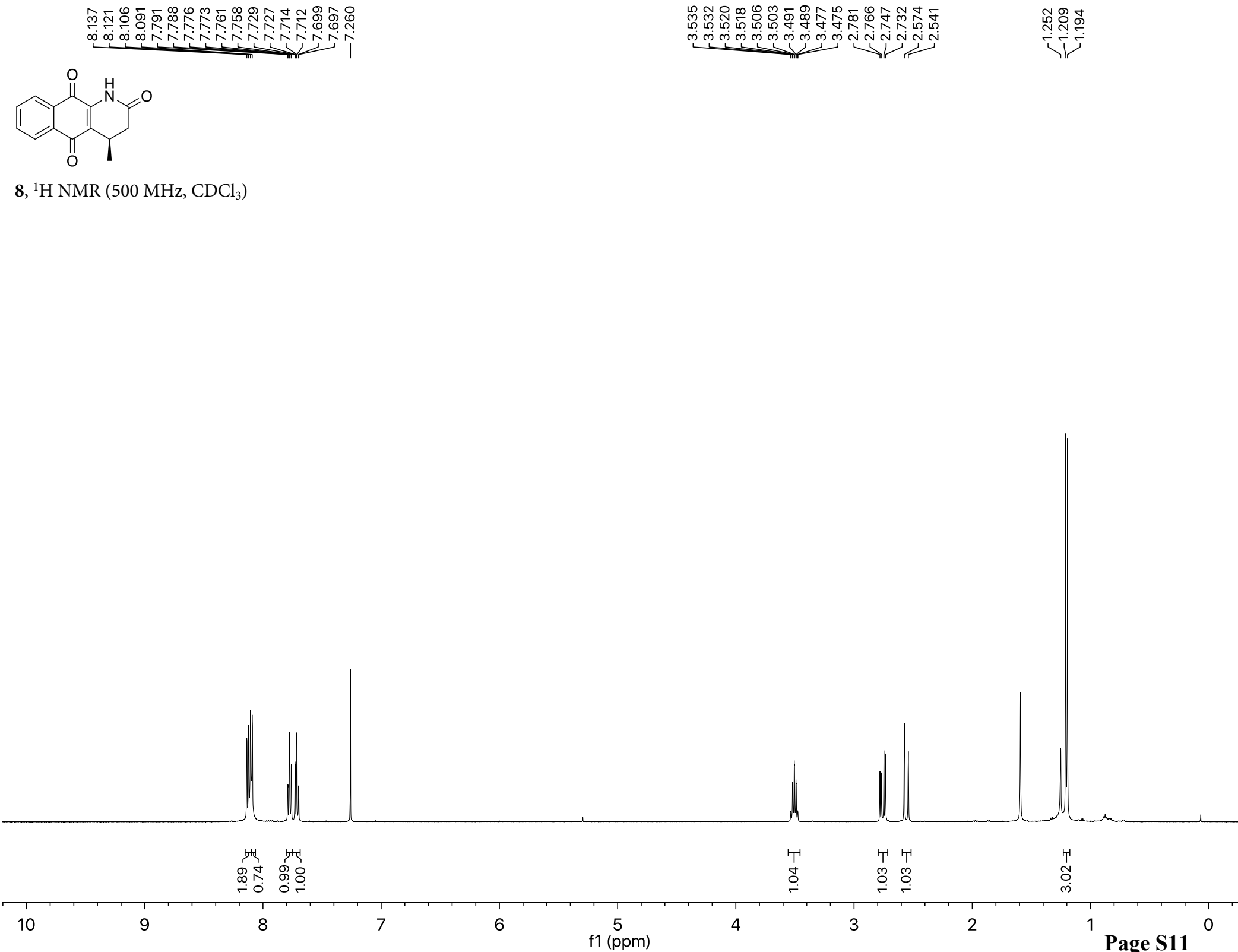


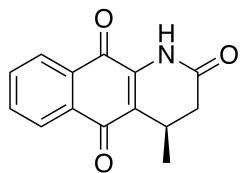
7, ^{13}C NMR (126 MHz, CDCl_3)



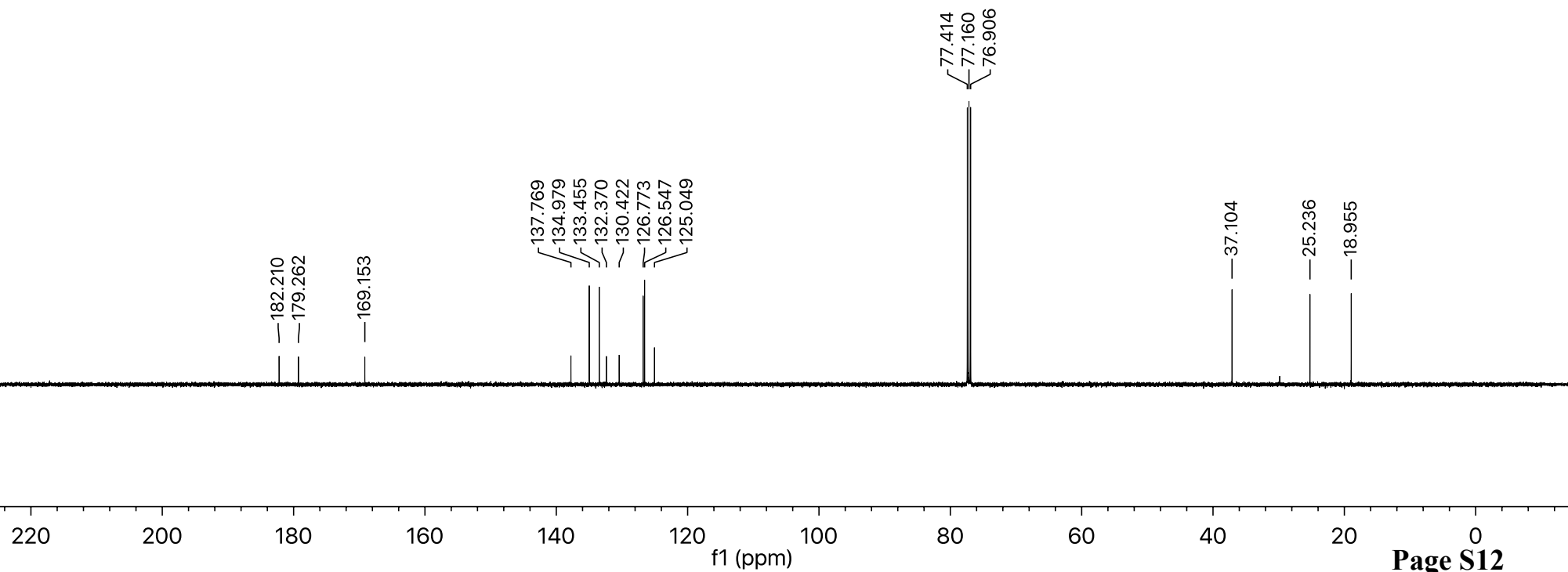


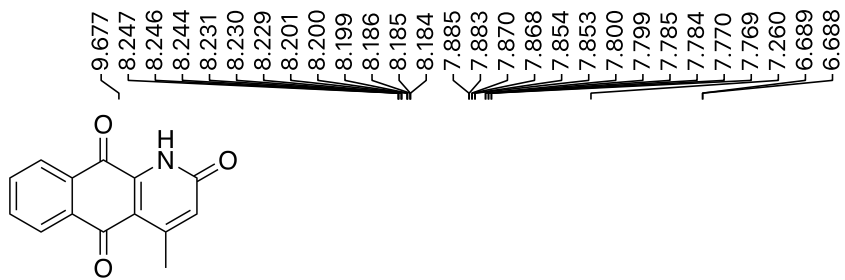
8, ^1H NMR (500 MHz, CDCl_3)



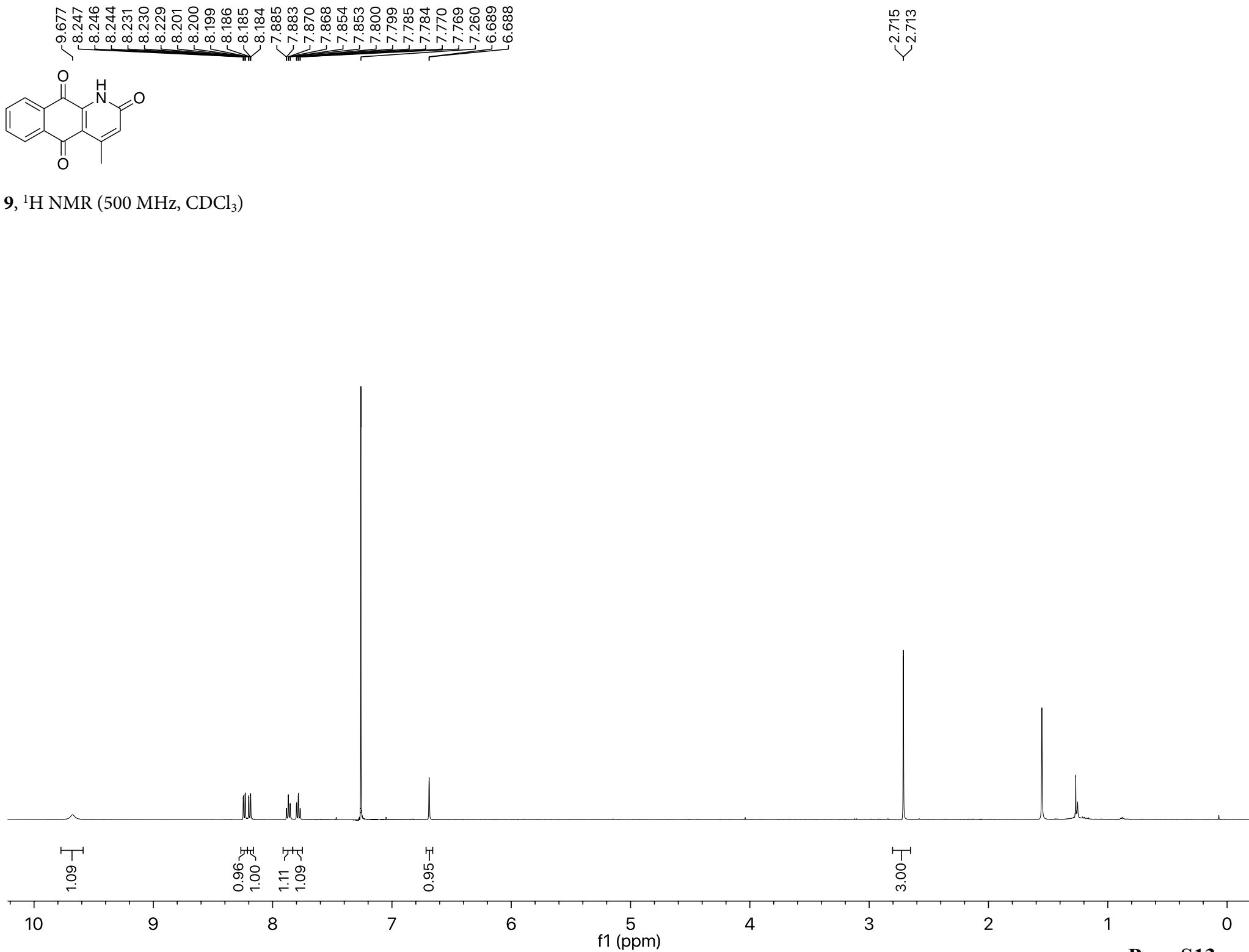


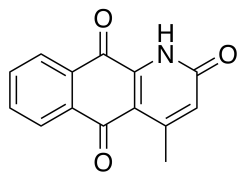
8, ^{13}C NMR (126 MHz, CDCl_3)



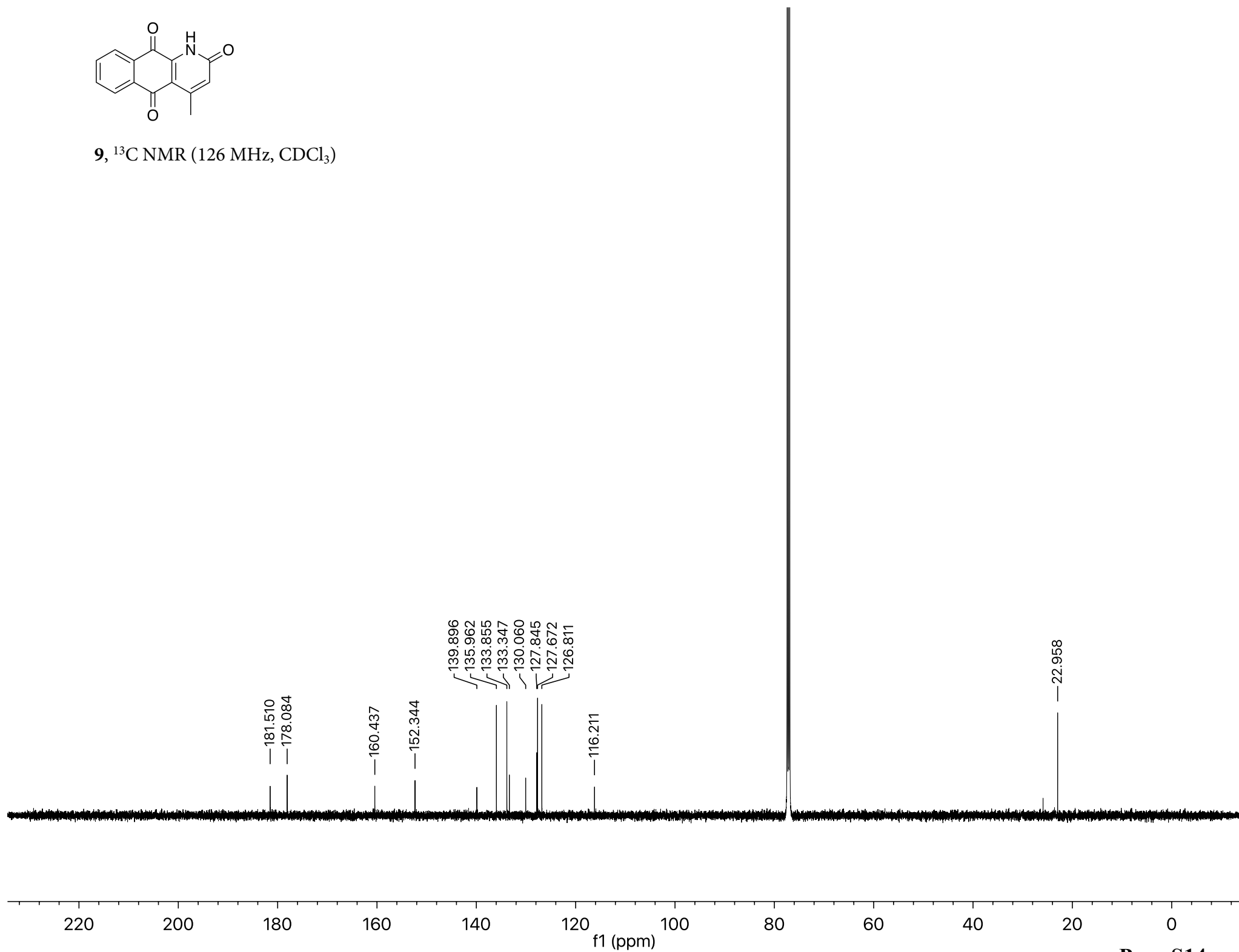


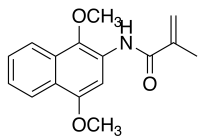
9, ¹H NMR (500 MHz, CDCl₃)





9, ^{13}C NMR (126 MHz, CDCl_3)





S3, ^1H NMR (500 MHz, CDCl_3)

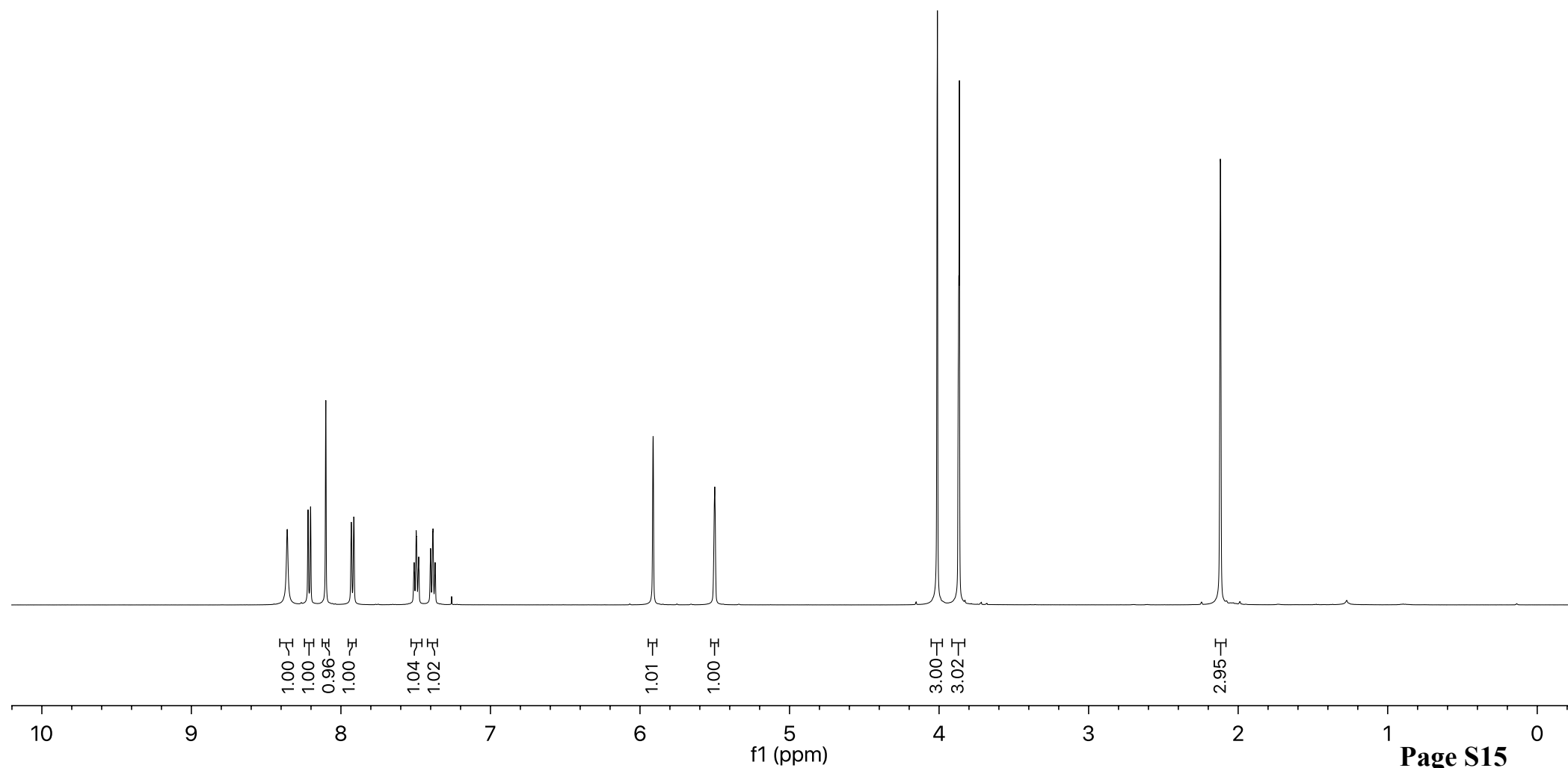
8.359
8.220
8.203
8.101
7.931
7.914
7.510
7.496
7.494
7.480
7.400
7.386
7.384
7.370
7.260

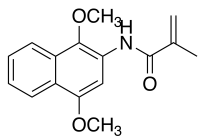
5.912

5.500

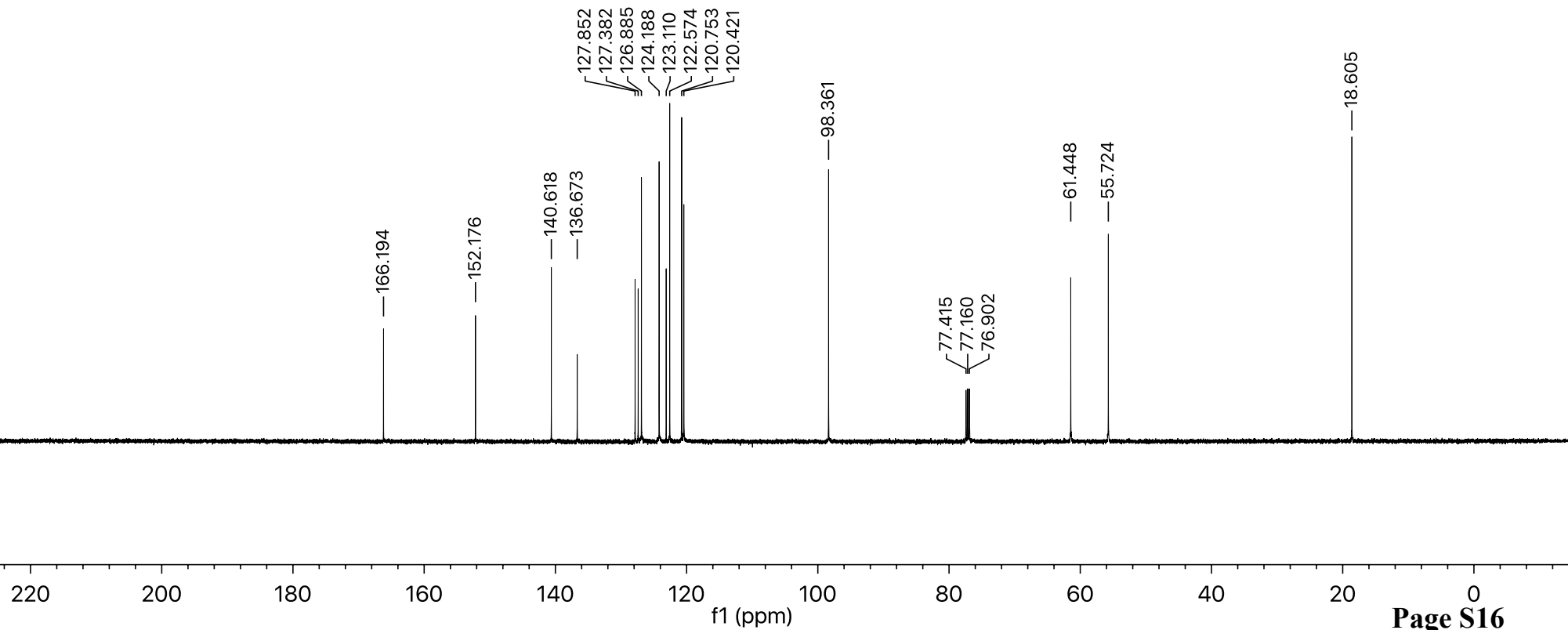
4.011
3.868
3.864

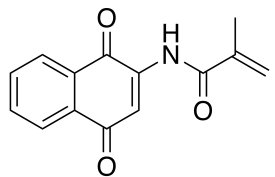
2.119





S3, ^{13}C NMR (126 MHz, CDCl_3)



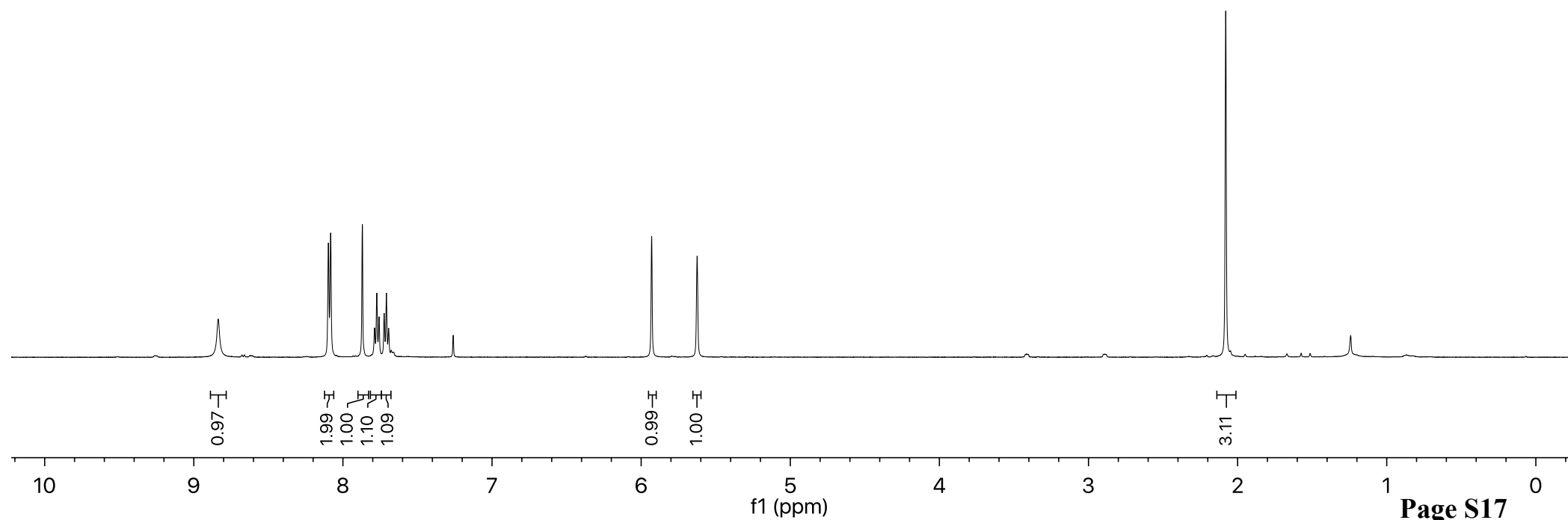


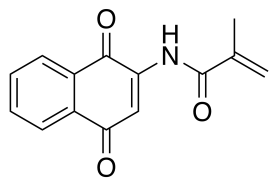
8.837
8.098
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7.870
7.788
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7.758
7.723
7.708
7.693
7.260

5.930
5.625

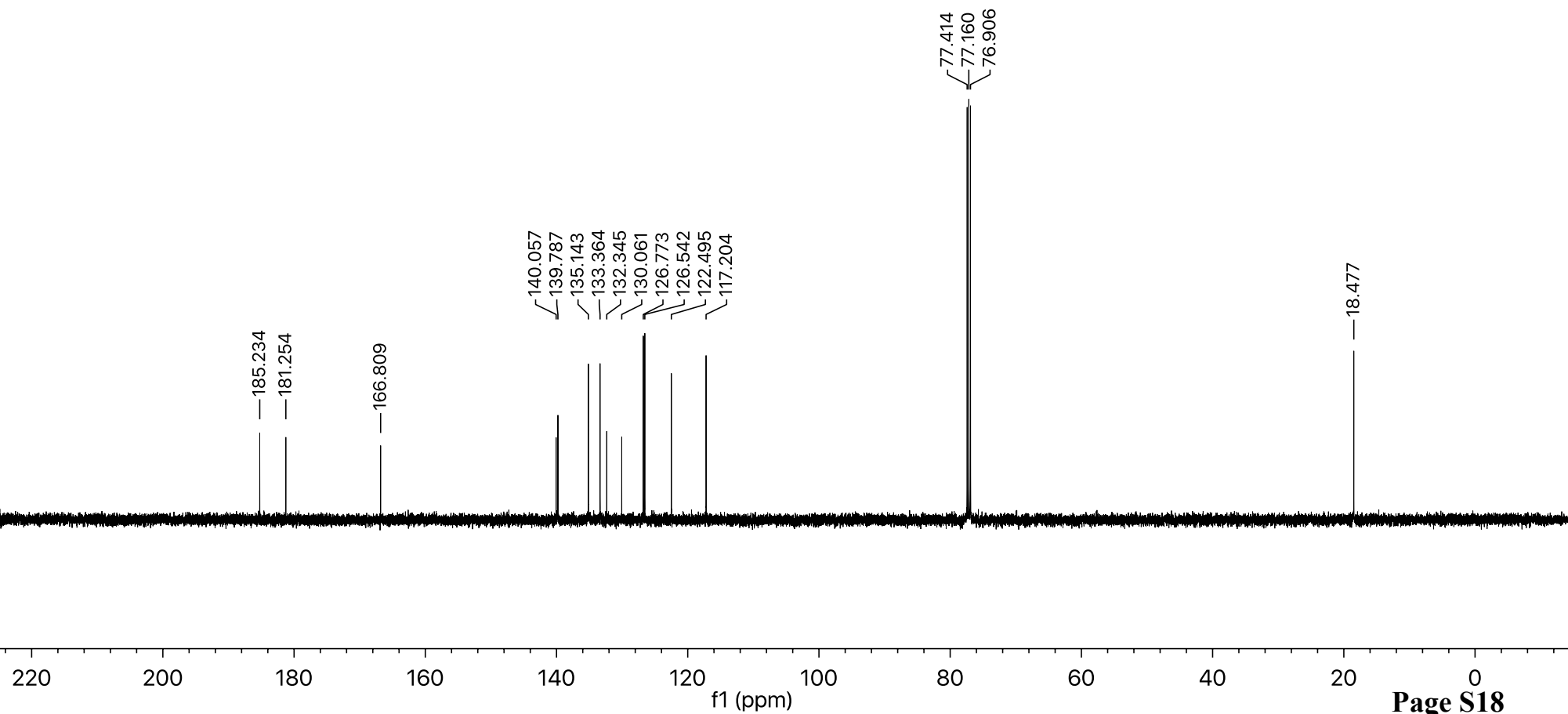
2.080

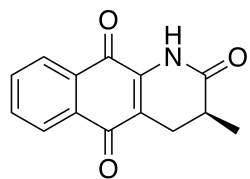
10, ^1H NMR (500 MHz, CDCl_3)



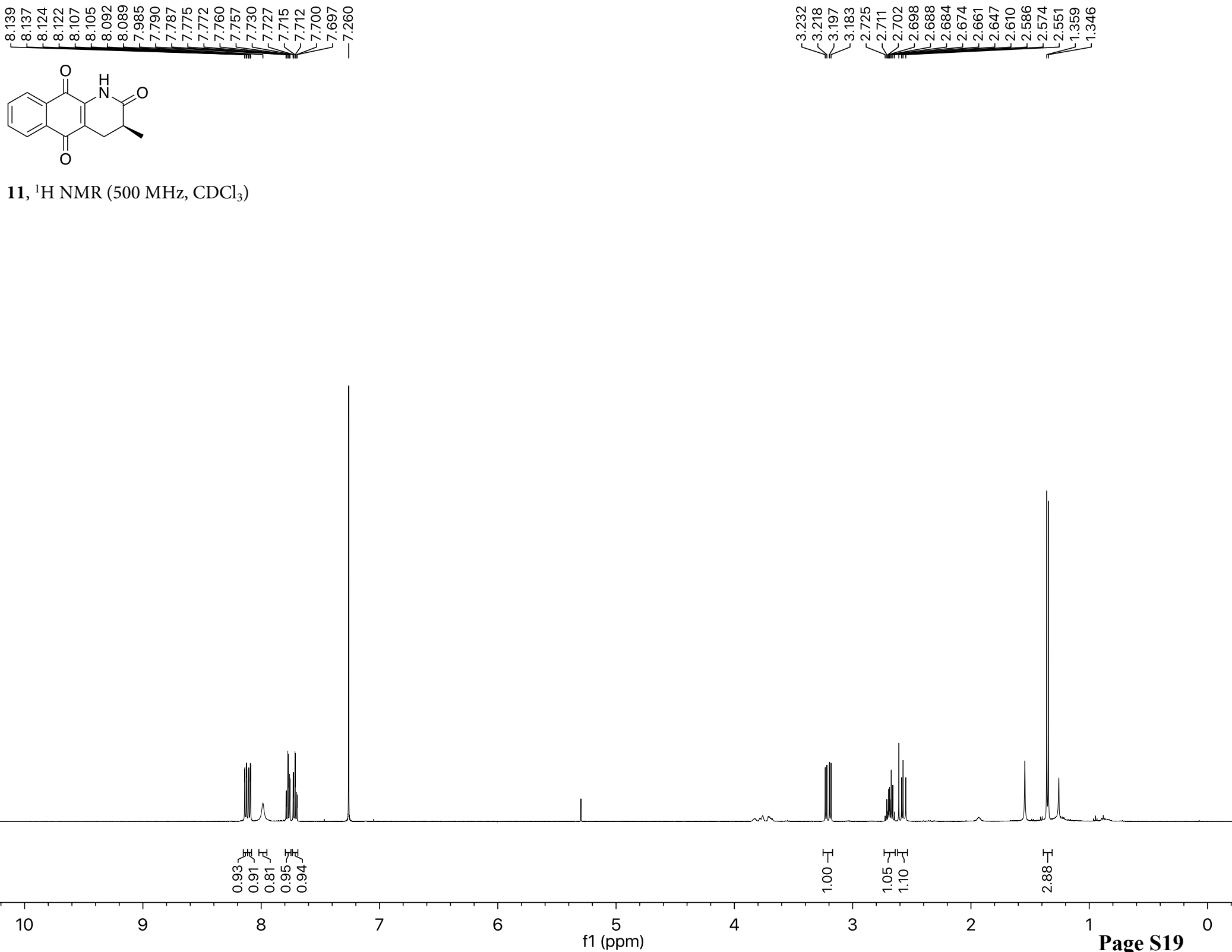


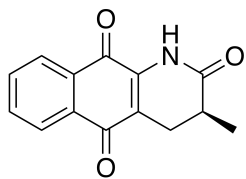
10, ^{13}C NMR (126 MHz, CDCl_3)



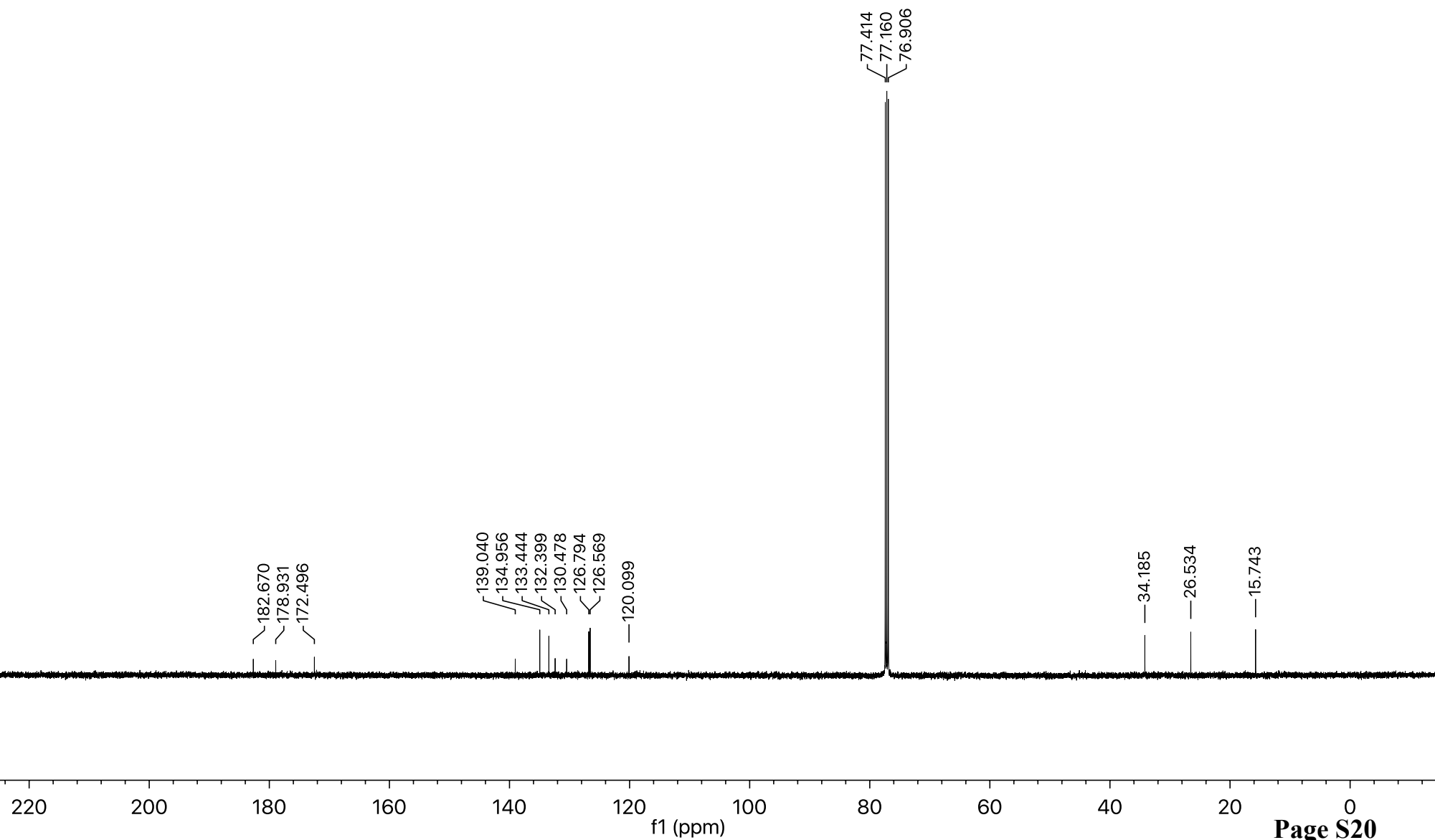


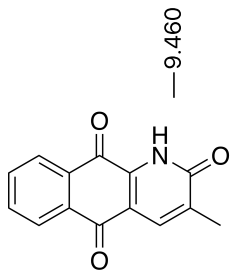
11, ^1H NMR (500 MHz, CDCl_3)





11, ^{13}C NMR (126 MHz, CDCl_3)



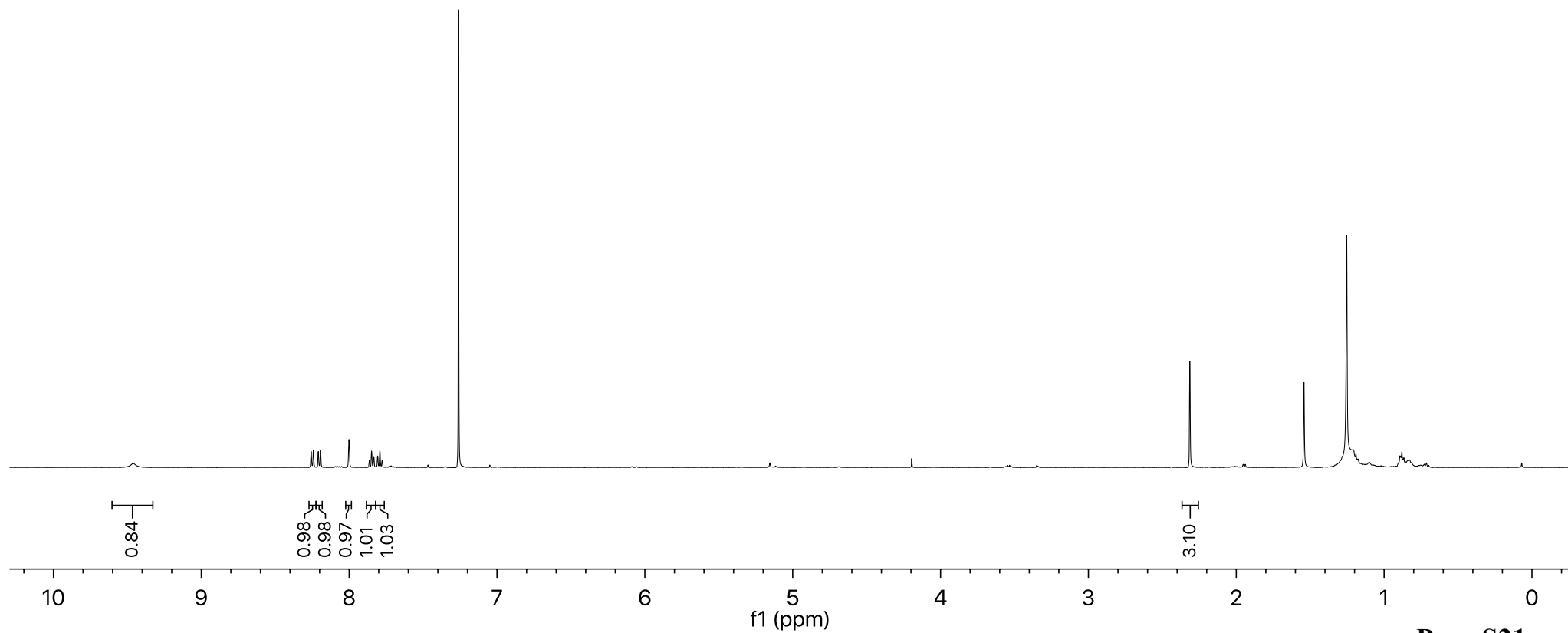


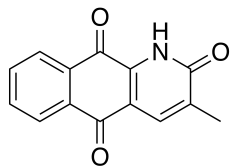
—9.460

8.257
8.242
8.209
8.194
8.001
7.863
7.849
7.834
7.807
7.792
7.778
—7.260

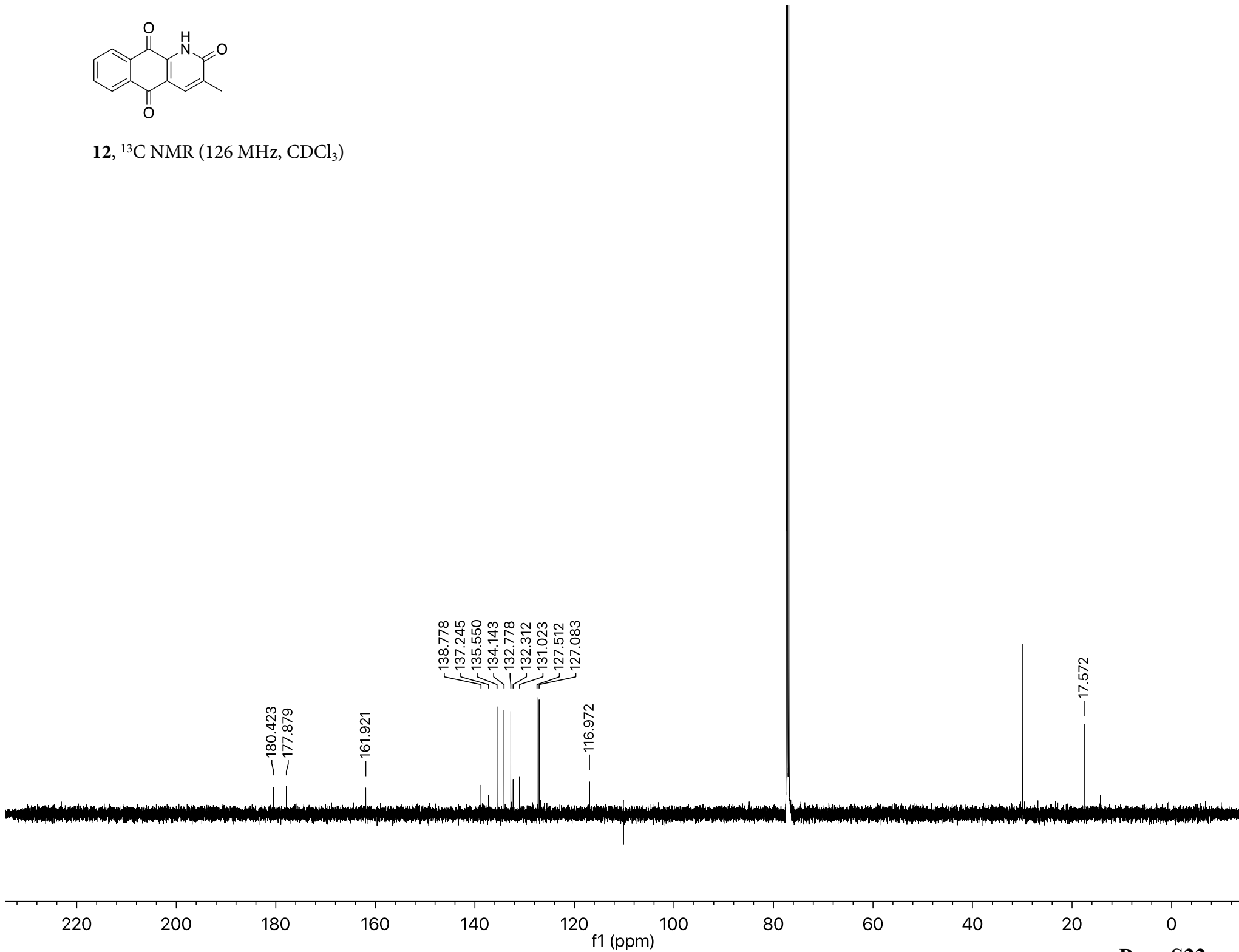
—2.314

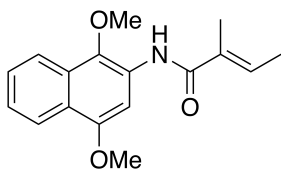
12, ^1H NMR (500 MHz, CDCl_3)





12, ^{13}C NMR (126 MHz, CDCl_3)



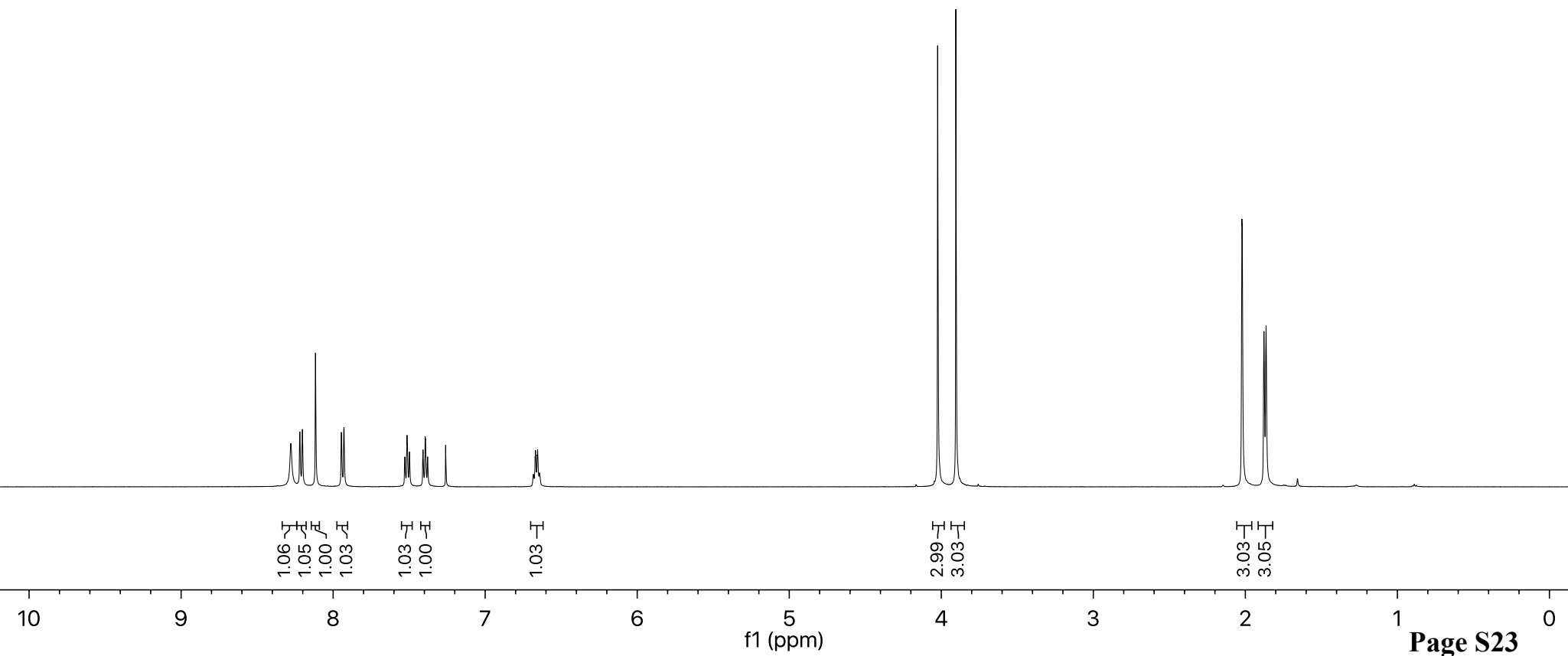


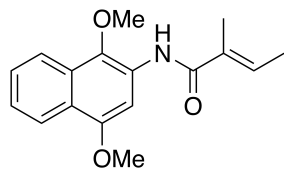
8.278
8.219
8.202
8.116
7.946
7.929
7.528
7.514
7.498
7.409
7.394
7.392
7.378
7.260
6.683
6.672
6.669
6.658
6.655
6.641

4.024

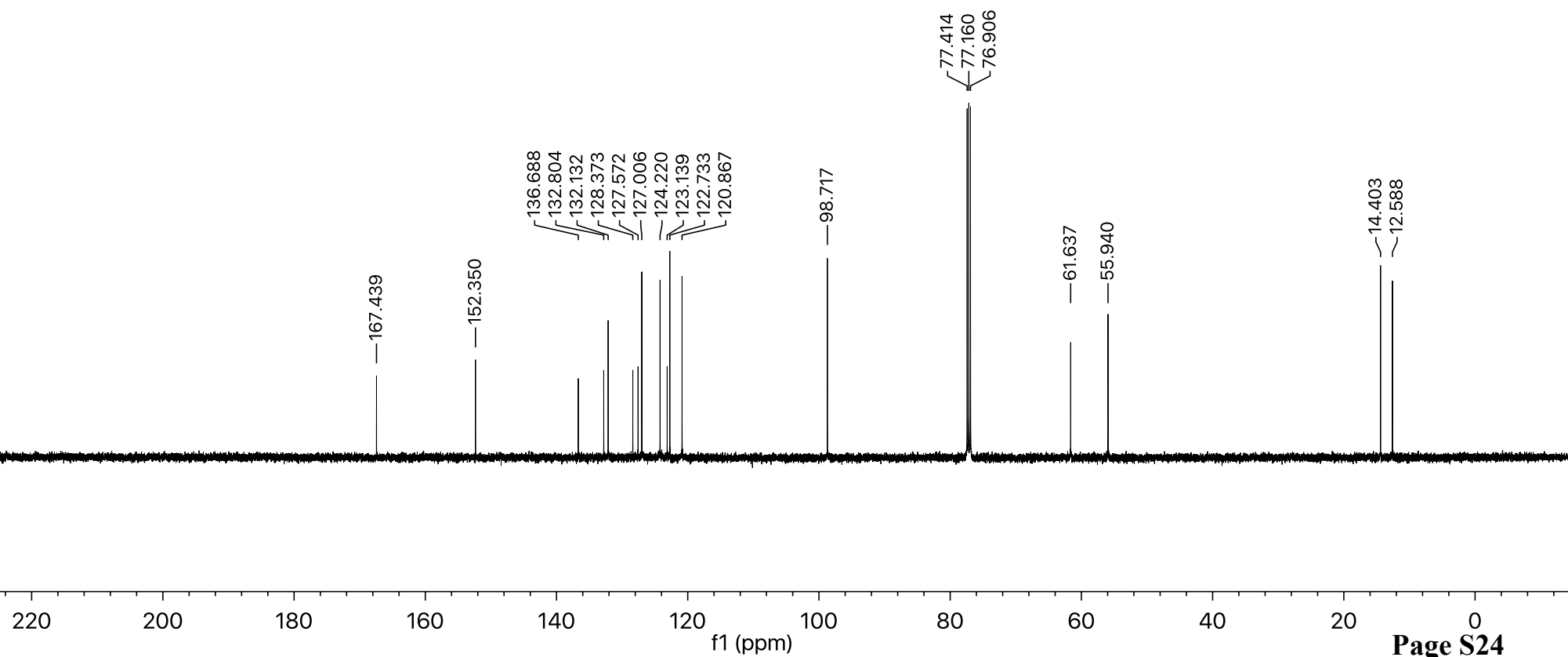
2.022
2.021
1.877
1.864

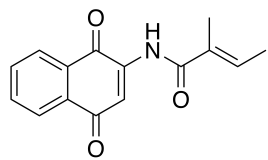
S4, ¹H NMR (500 MHz, CDCl₃)





S4, ^{13}C NMR (126 MHz, CDCl_3)

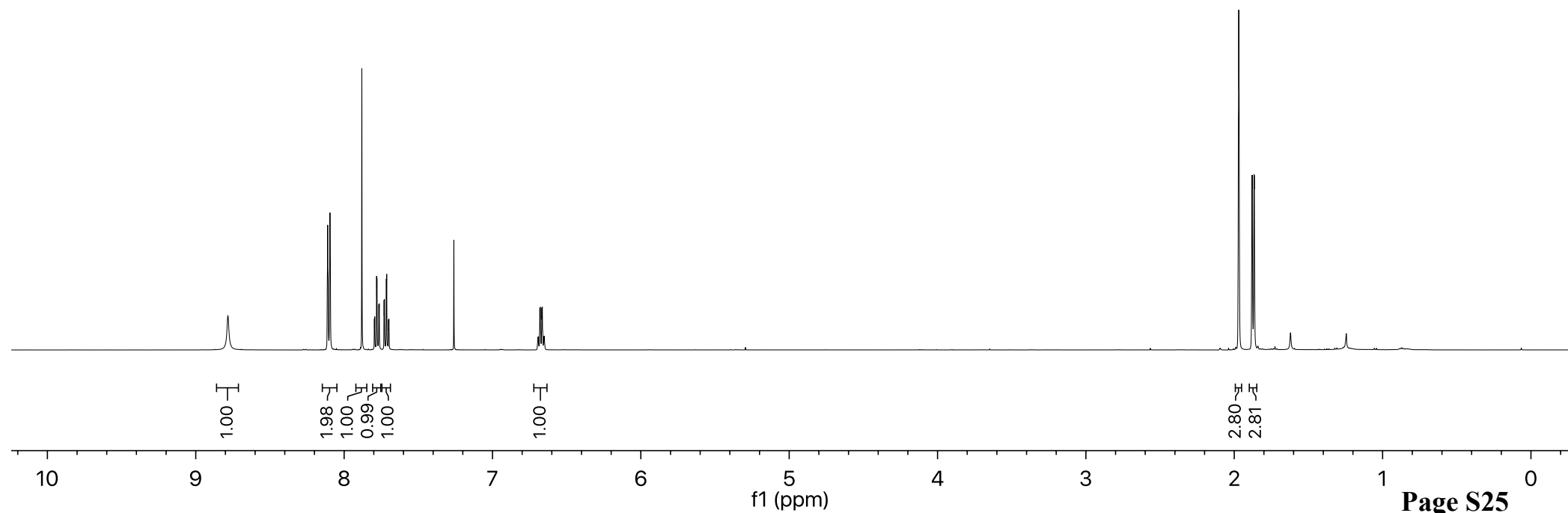


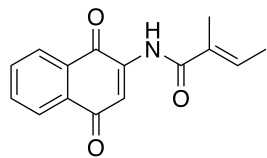


8.783
8.111
8.095
7.881
7.796
7.793
7.781
7.778
7.766
7.763
7.731
7.728
7.715
7.713
7.701
7.698
7.260
6.694
6.692
6.681
6.678
6.667
6.664
6.653
6.650

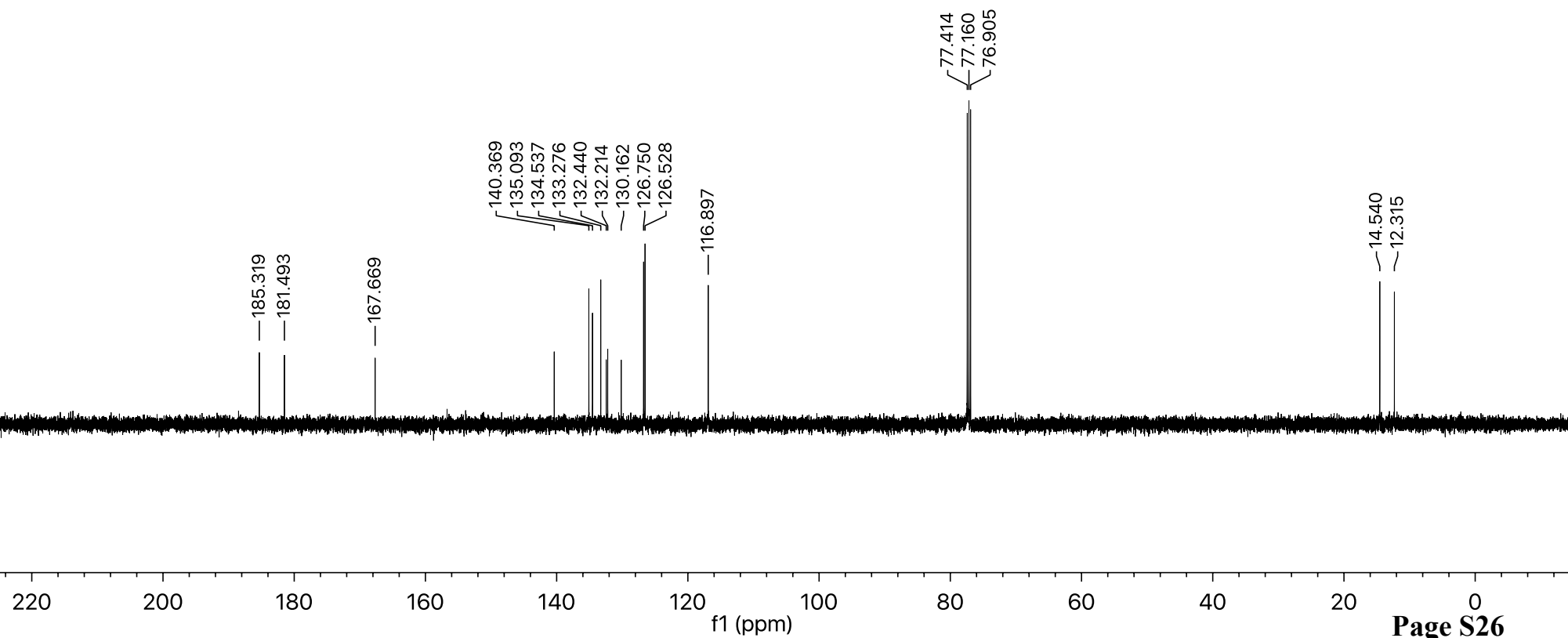
1.970
1.968
1.881
1.879
1.867
1.865

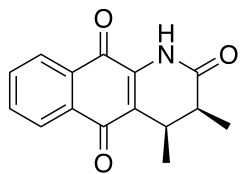
13, ¹H NMR (500 MHz, CDCl₃)





13, ^{13}C NMR (126 MHz, CDCl_3)





14, ¹H NMR (500 MHz, CDCl₃)

8.126
8.111
8.089
8.074
8.015
7.779
7.777
7.764
7.749
7.716
7.714
7.701
7.686
7.260

3.393
3.379
3.366
3.352
3.338
2.806
2.792
2.779
2.765
2.752

1.322
1.308
1.055
1.041

0.99
0.96
0.88
1.03
1.02

1.00

1.00

2.99

2.90

10

9

8

7

6

5

4

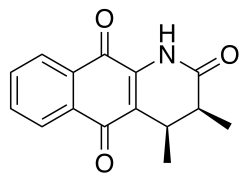
3

2

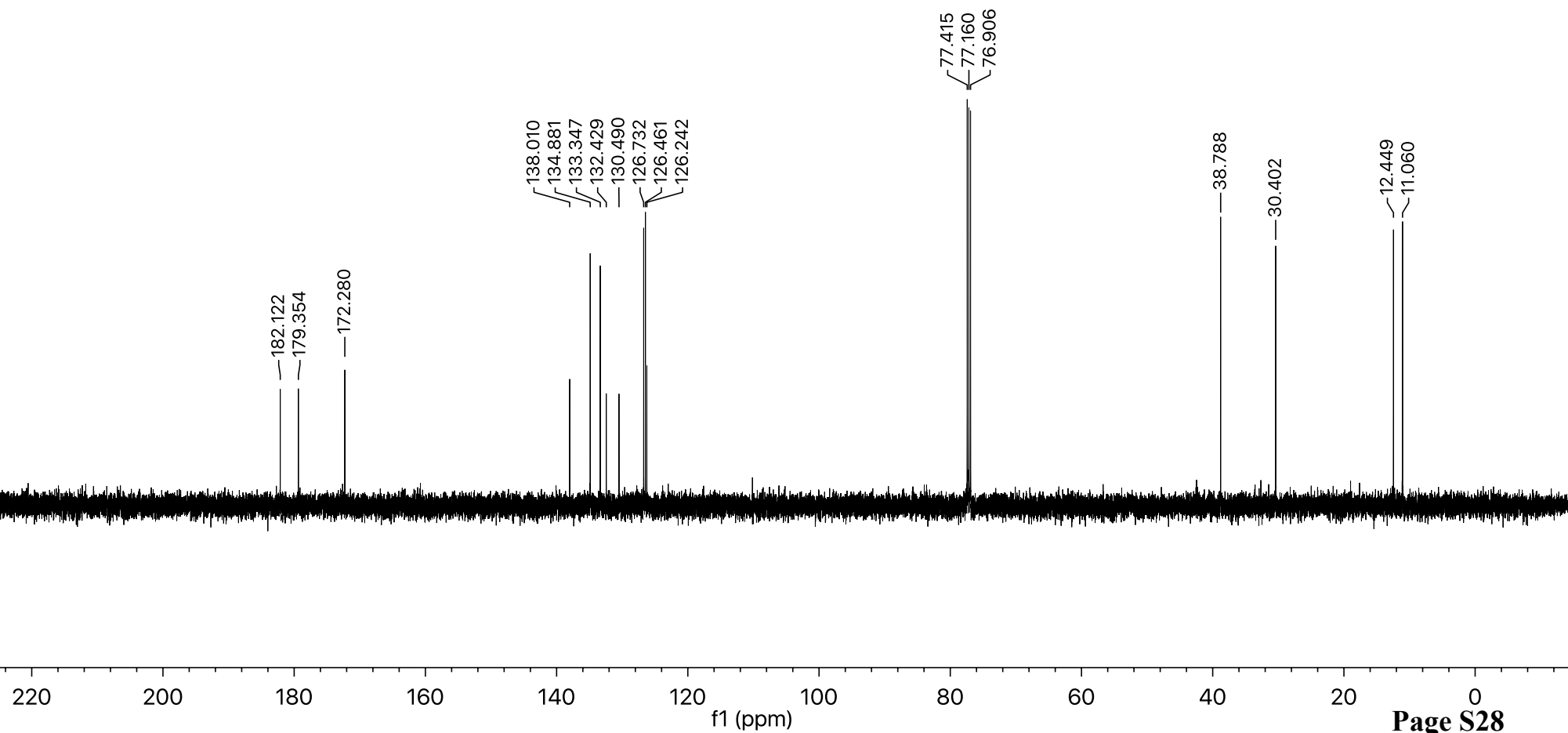
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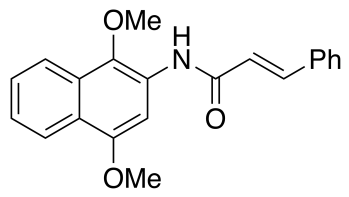
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f1 (ppm)

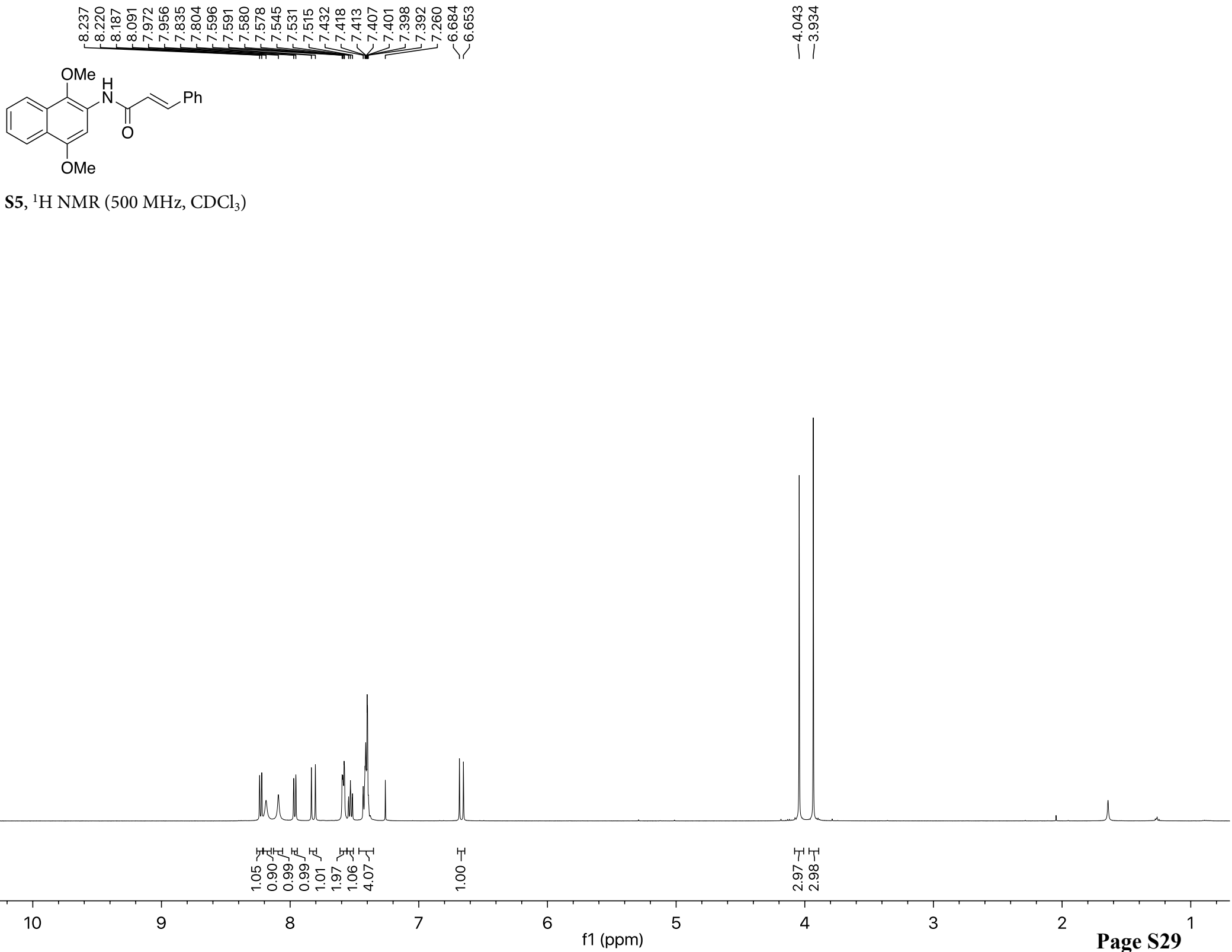


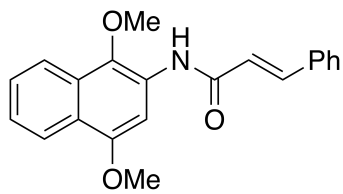
14, ^{13}C NMR (126 MHz, CDCl_3)



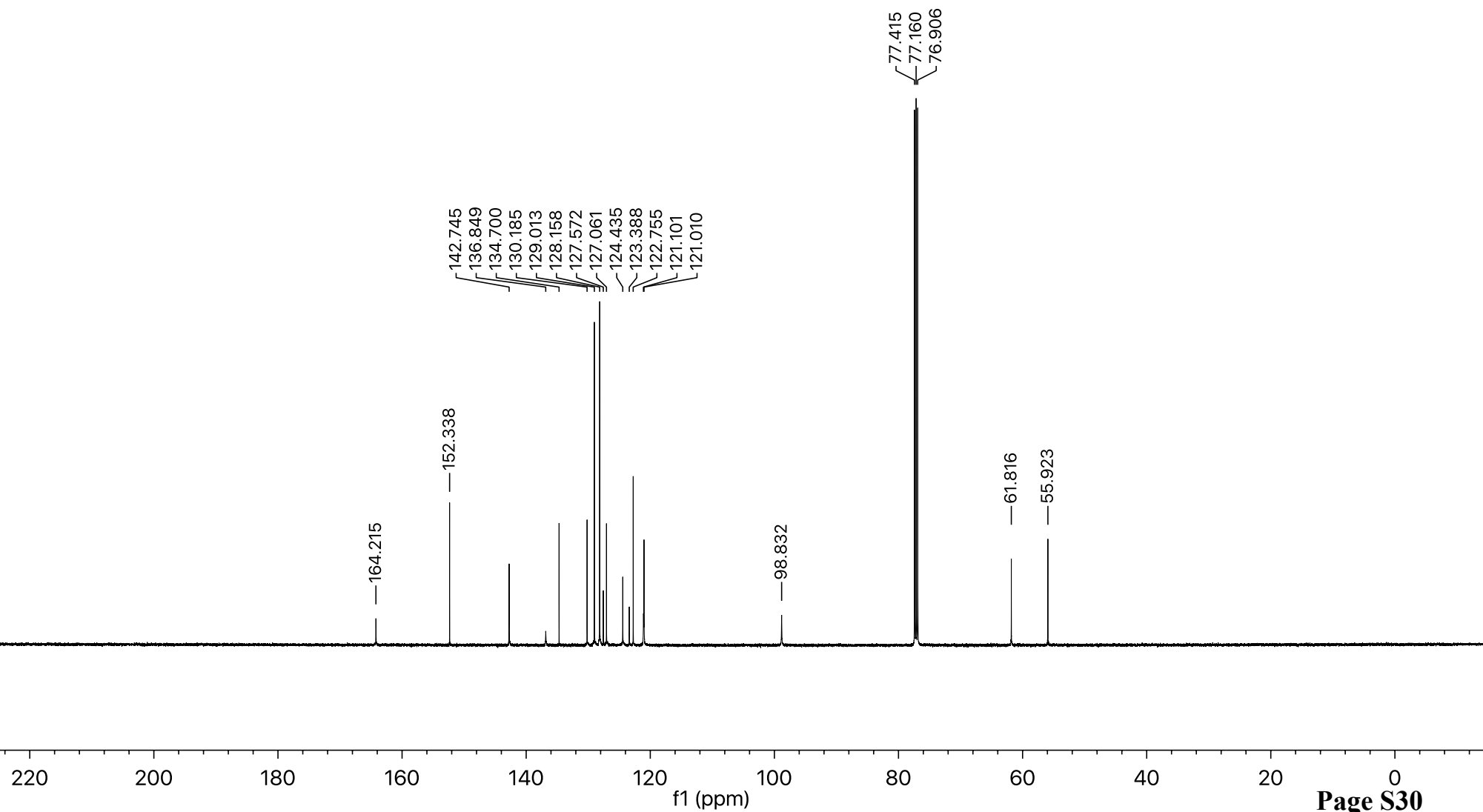


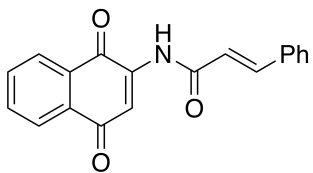
S5, ¹H NMR (500 MHz, CDCl₃)



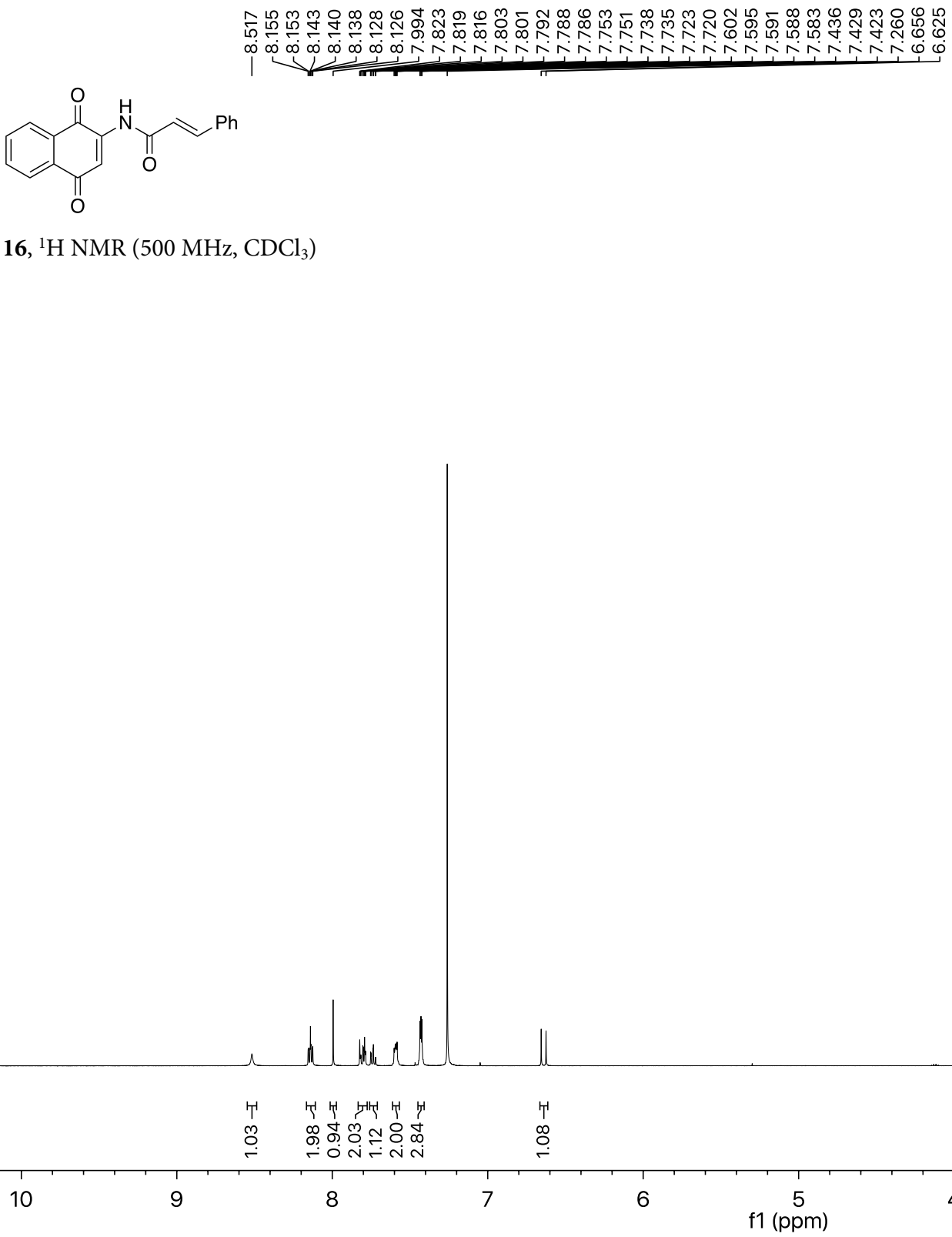


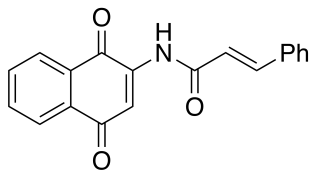
S5, ^{13}C NMR (126 MHz, CDCl_3)



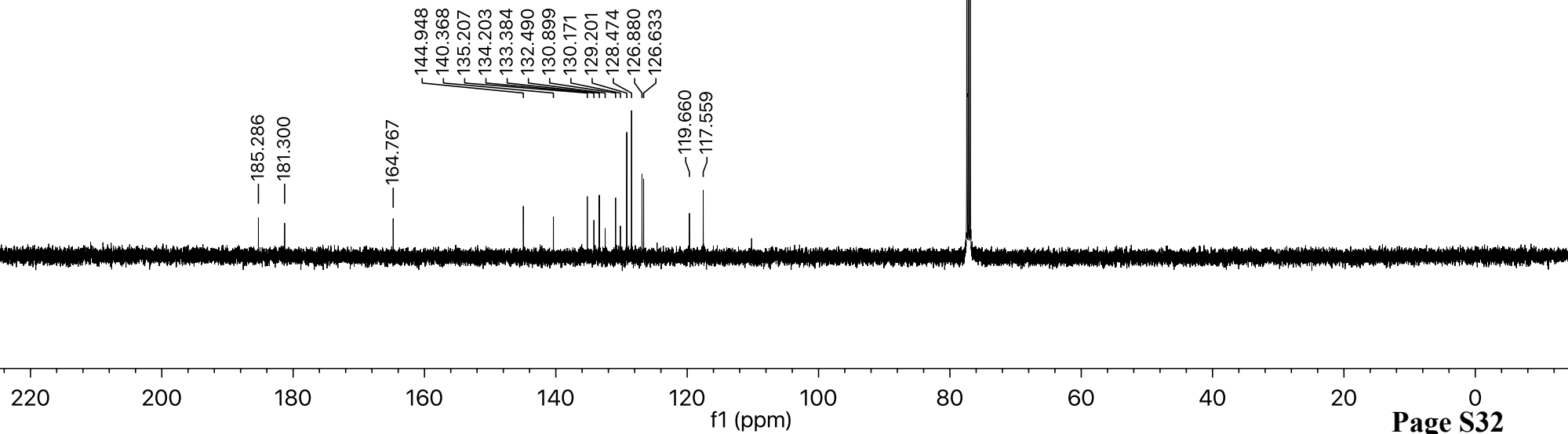


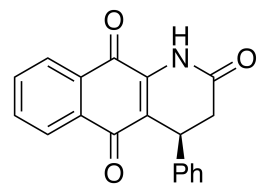
16, ¹H NMR (500 MHz, CDCl₃)





16, ^{13}C NMR (126 MHz, CDCl_3)



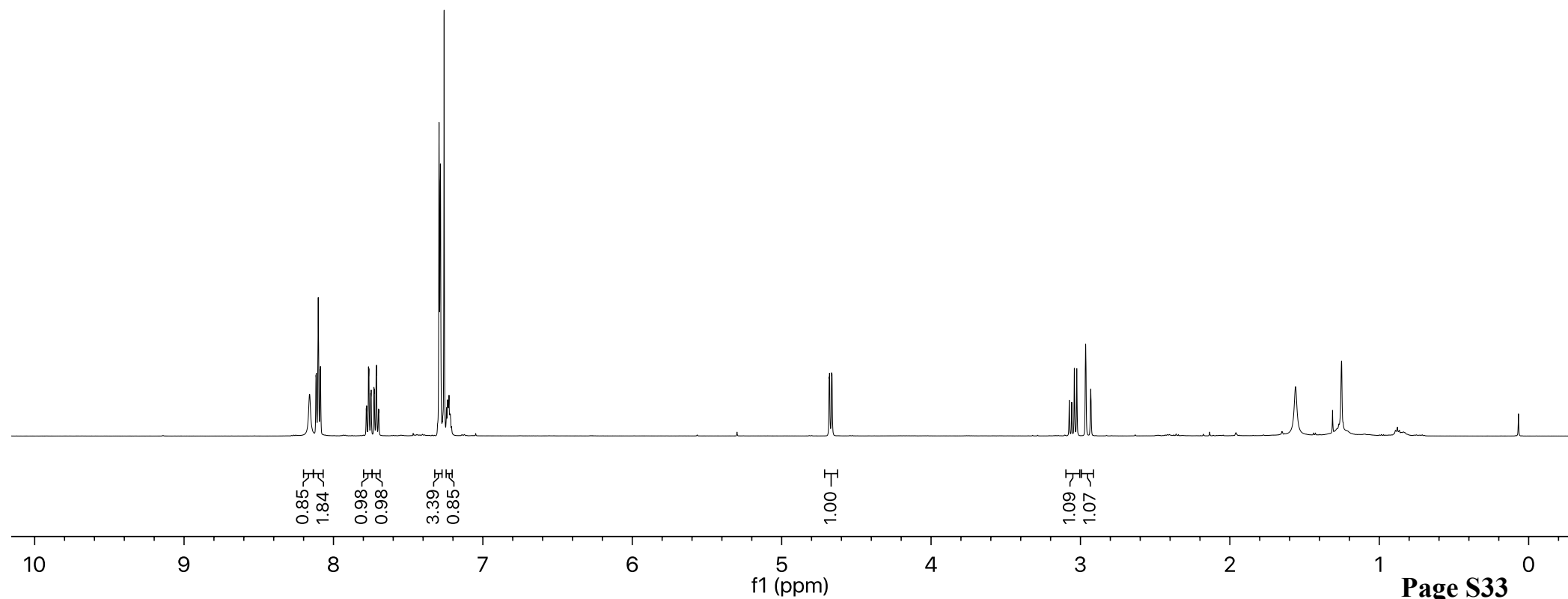


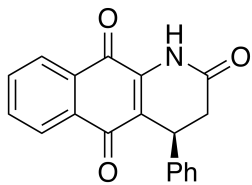
17, ¹H NMR (500 MHz, CDCl₃)

8.160
8.117
8.115
8.102
8.089
8.087
7.781
7.778
7.766
7.763
7.751
7.748
7.729
7.727
7.714
7.712
7.699
7.697
7.293
7.284
7.272
7.260
7.244
7.237
7.226
7.218
7.209

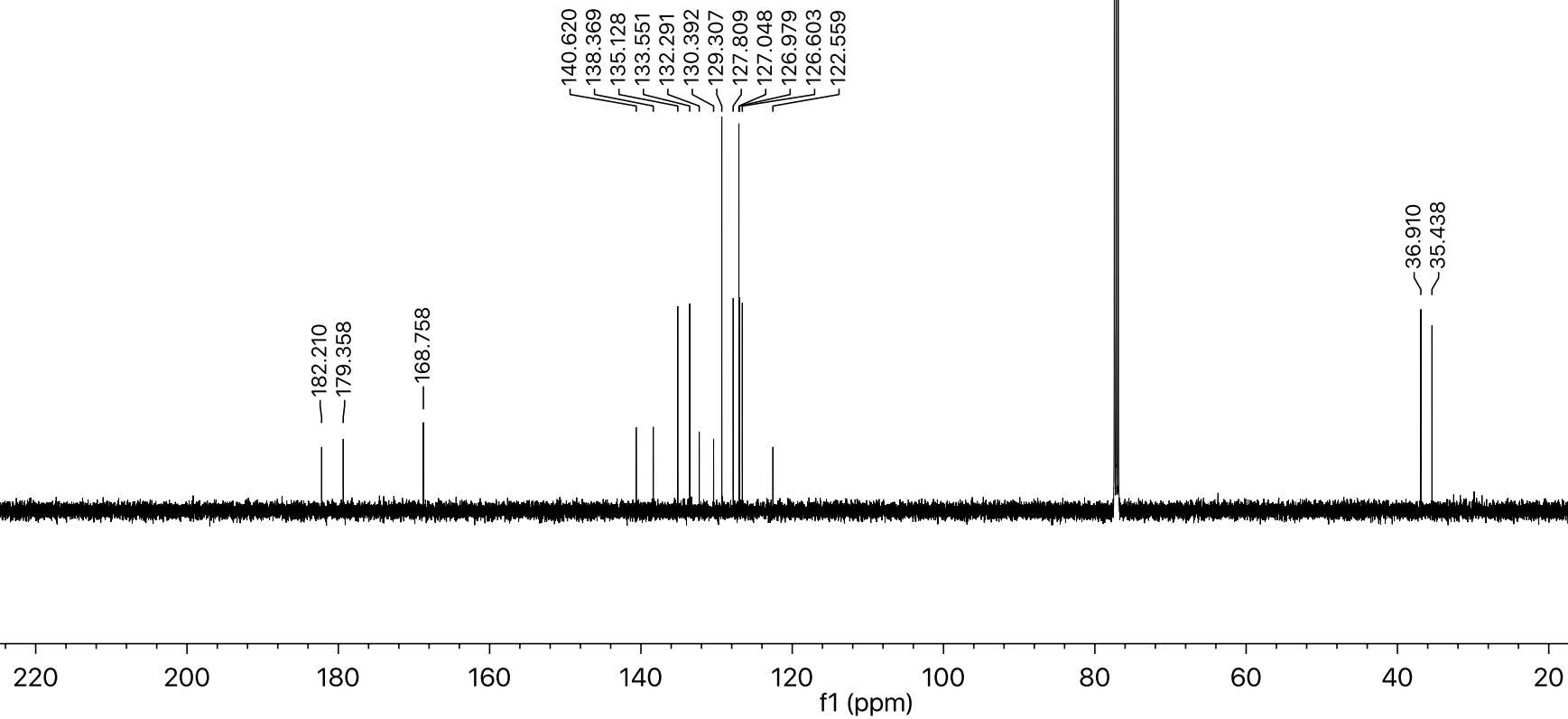
4.682
4.680
4.665
4.663

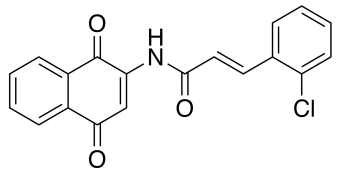
3.075
3.059
3.041
3.024
2.965
2.931





17, ^{13}C NMR (126 MHz, CDCl_3)

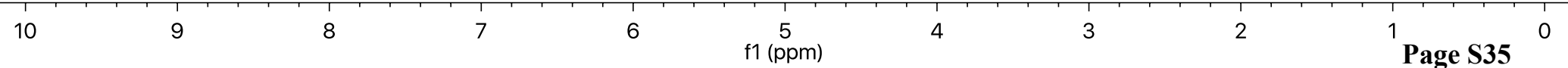


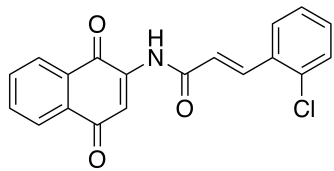


19, ¹H NMR (500 MHz, CDCl₃)

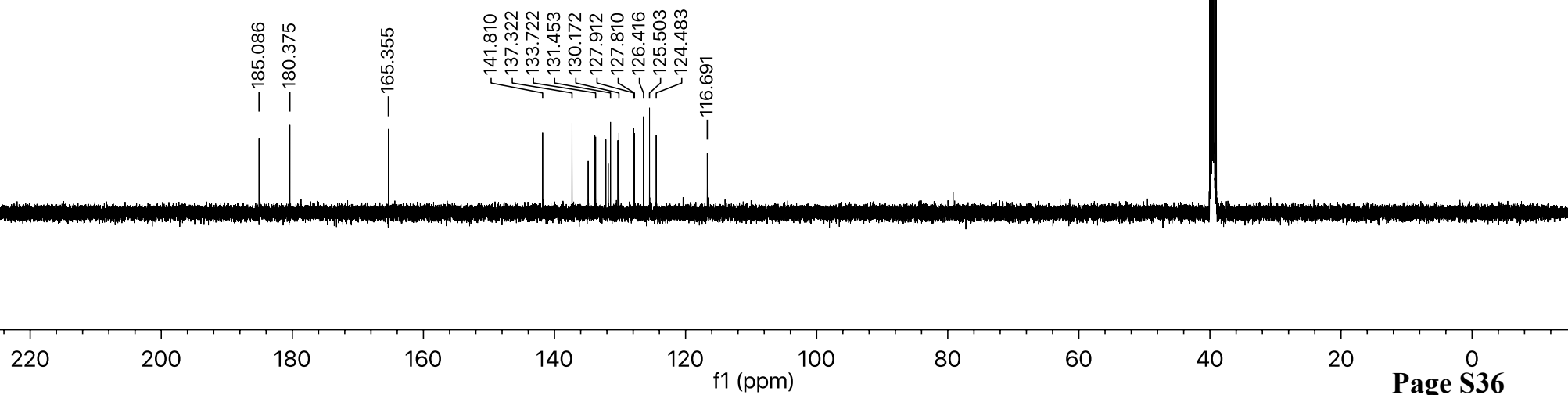
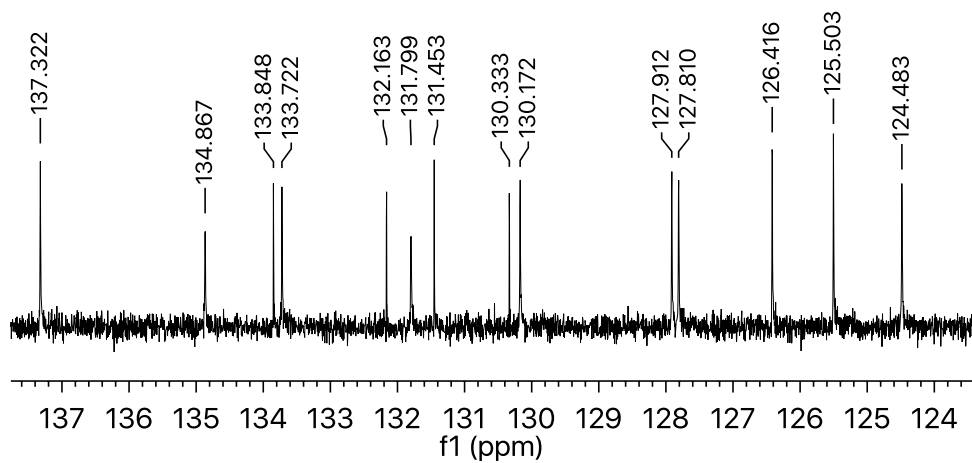
8.556
8.213
8.182
8.152
8.145
8.142
8.139
8.136
8.128
7.998
7.821
7.818
7.806
7.803
7.791
7.788
7.755
7.753
7.740
7.738
7.725
7.723
7.676
7.673
7.662
7.658
7.466
7.463
7.450
7.448
7.368
7.366
7.354
7.351
7.339
7.335
7.320
7.319
7.307
7.304
7.259
6.664
6.633

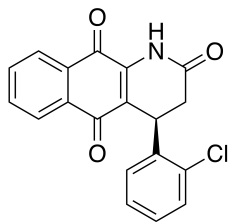
1.10
1.00
1.85
0.89
1.07
1.07
1.00
0.97
2.05
1.05





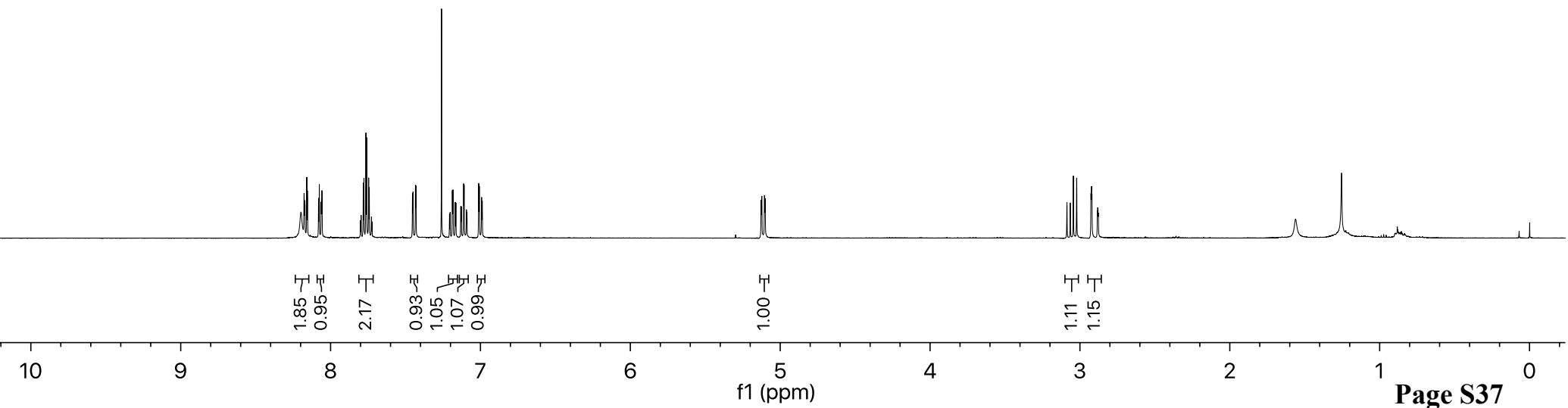
19, ^{13}C NMR (126 MHz, DMSO- d_6)

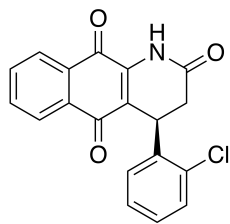




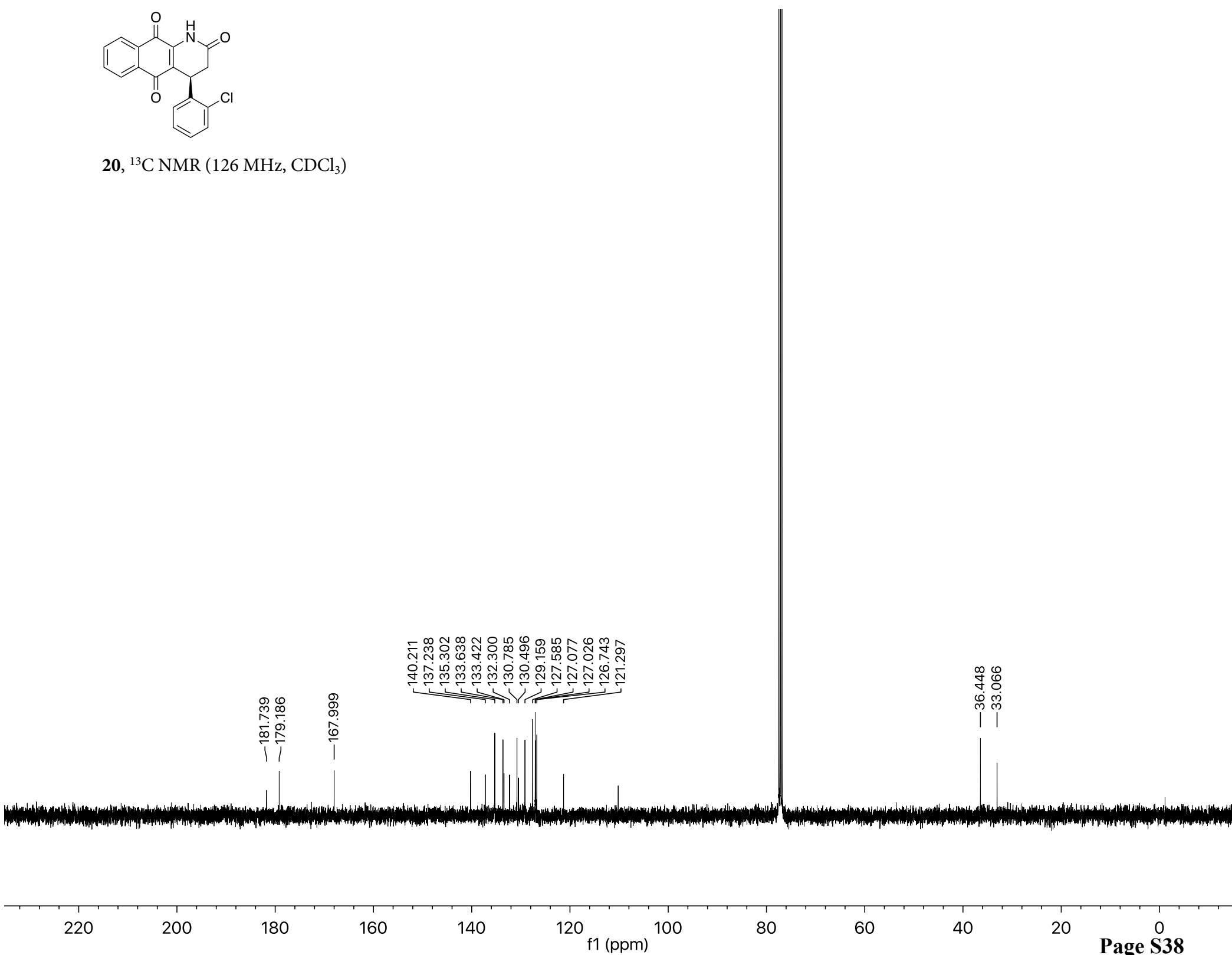
20, ¹H NMR (400 MHz, CDCl₃)

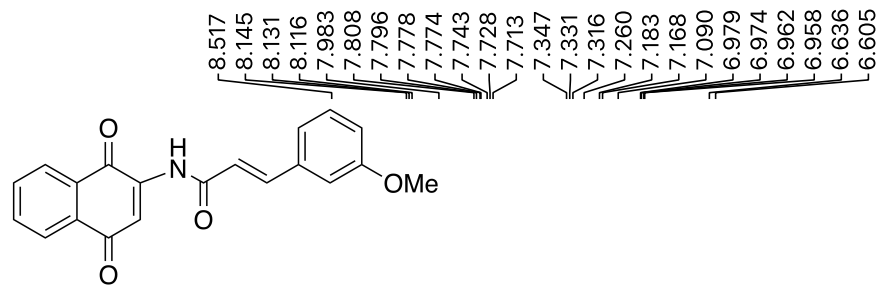
8.198
8.177
8.173
8.171
8.159
8.155
8.080
8.075
8.063
8.060
8.058
7.800
7.796
7.782
7.778
7.764
7.759
7.746
7.742
7.727
7.723
7.753
7.450
7.434
7.430
7.260
7.206
7.202
7.188
7.183
7.168
7.164
7.131
7.128
7.112
7.109
7.093
7.090
7.012
7.007
6.992
6.988
5.127
5.123
5.105
5.100
3.087
3.064
3.044
3.022
2.926
2.924
2.922
2.920
2.884
2.881
2.879
2.877



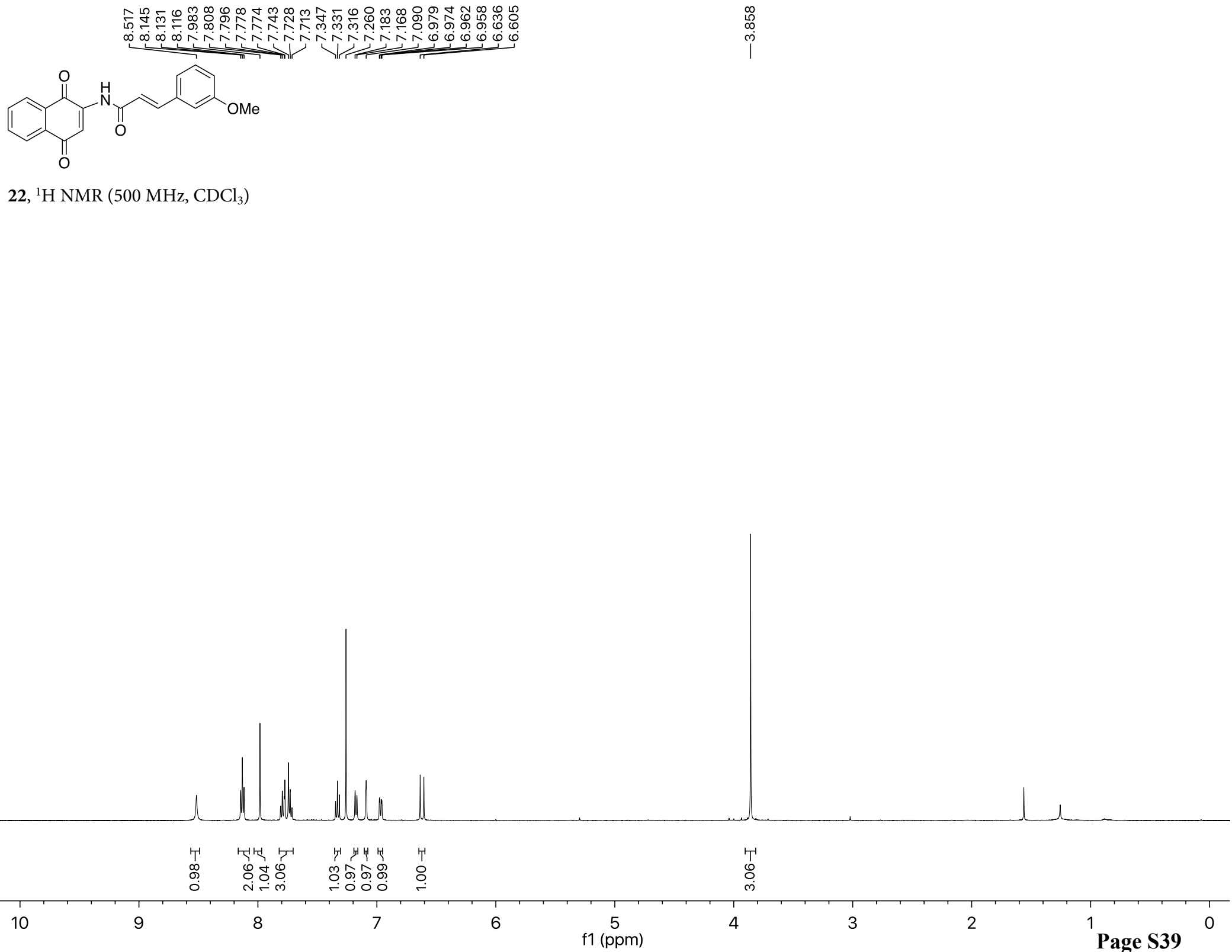


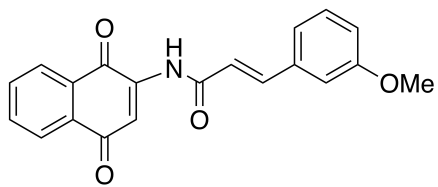
20, ^{13}C NMR (126 MHz, CDCl_3)



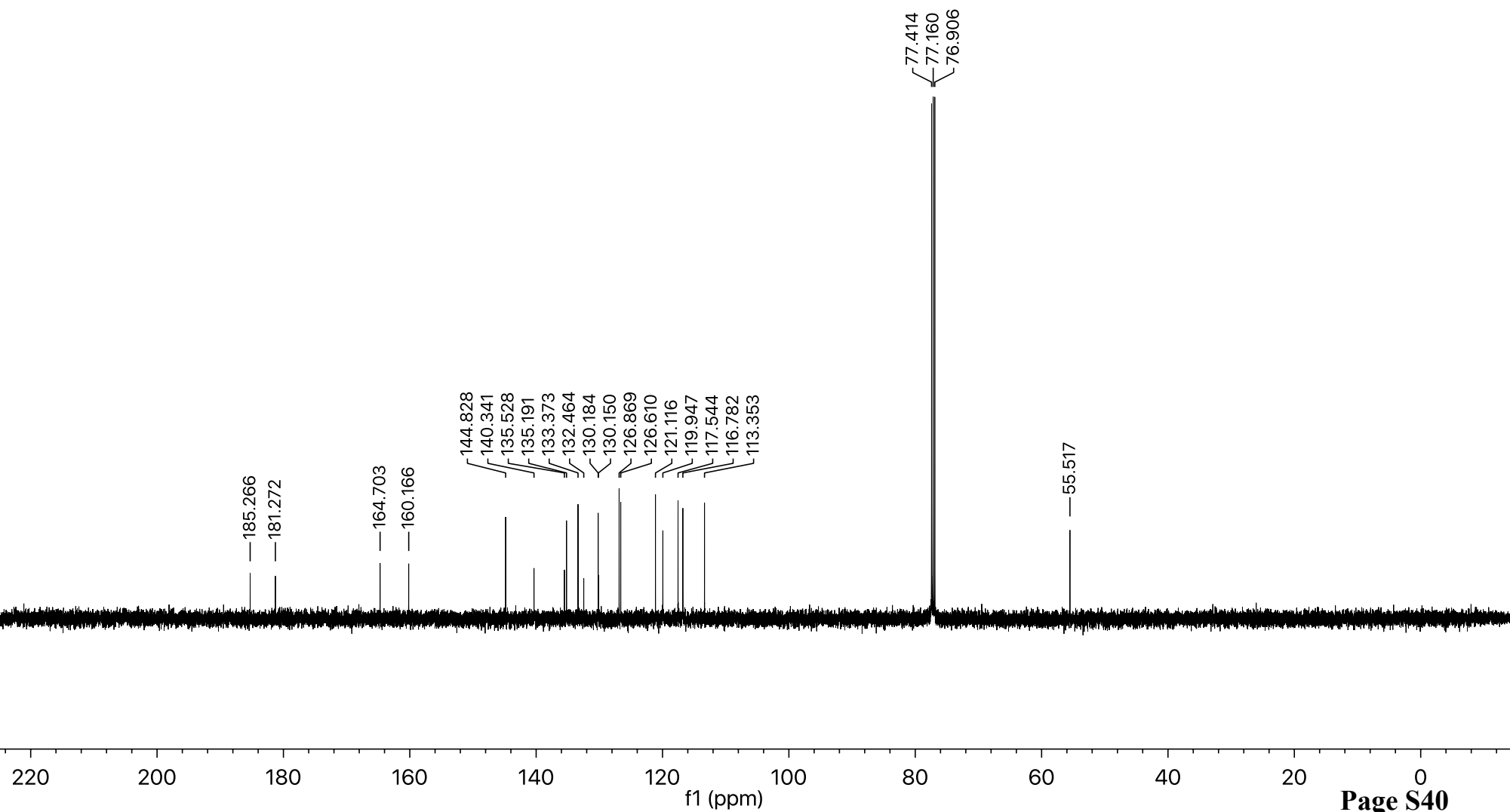


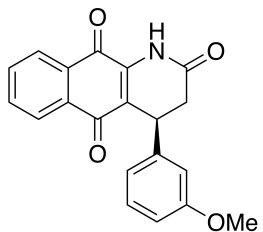
22, ¹H NMR (500 MHz, CDCl₃)





22, ^{13}C NMR (126 MHz, CDCl_3)





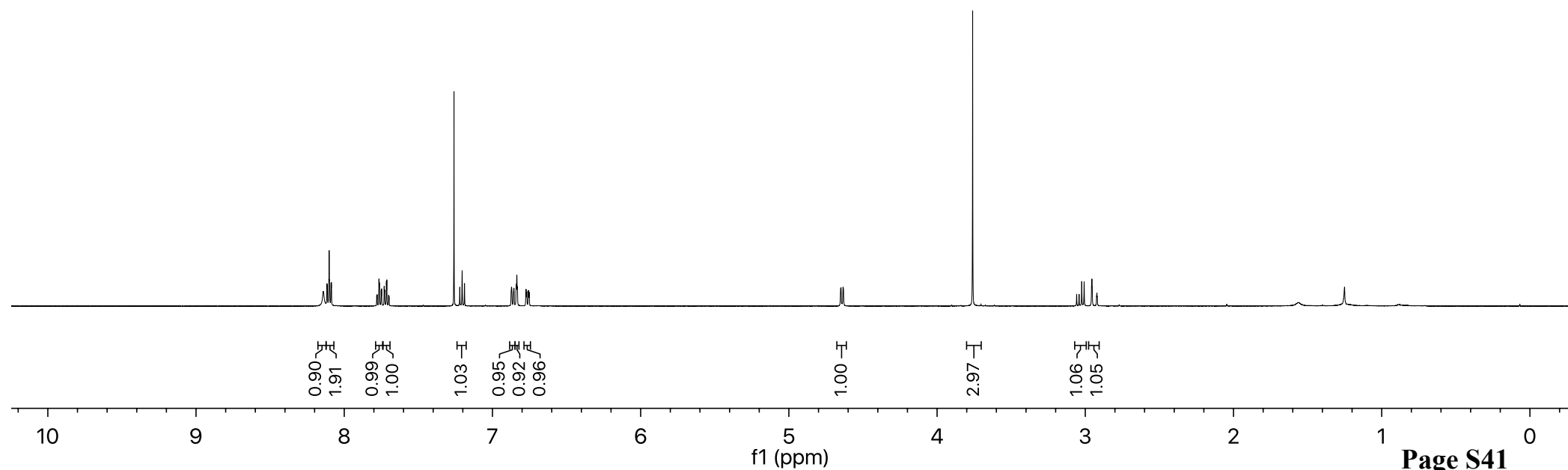
23, ¹H NMR (500 MHz, CDCl₃)

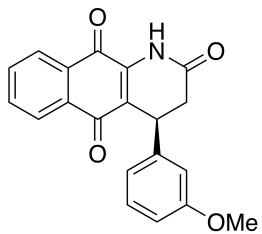
8.141
8.117
8.115
8.102
8.089
8.087
7.781
7.778
7.766
7.763
7.751
7.748
7.731
7.727
7.716
7.713
7.700
7.698
7.260
7.220
7.205
7.189
6.872
6.856
6.840
6.835
6.832
6.773
6.769
6.758
6.753

4.648
4.634

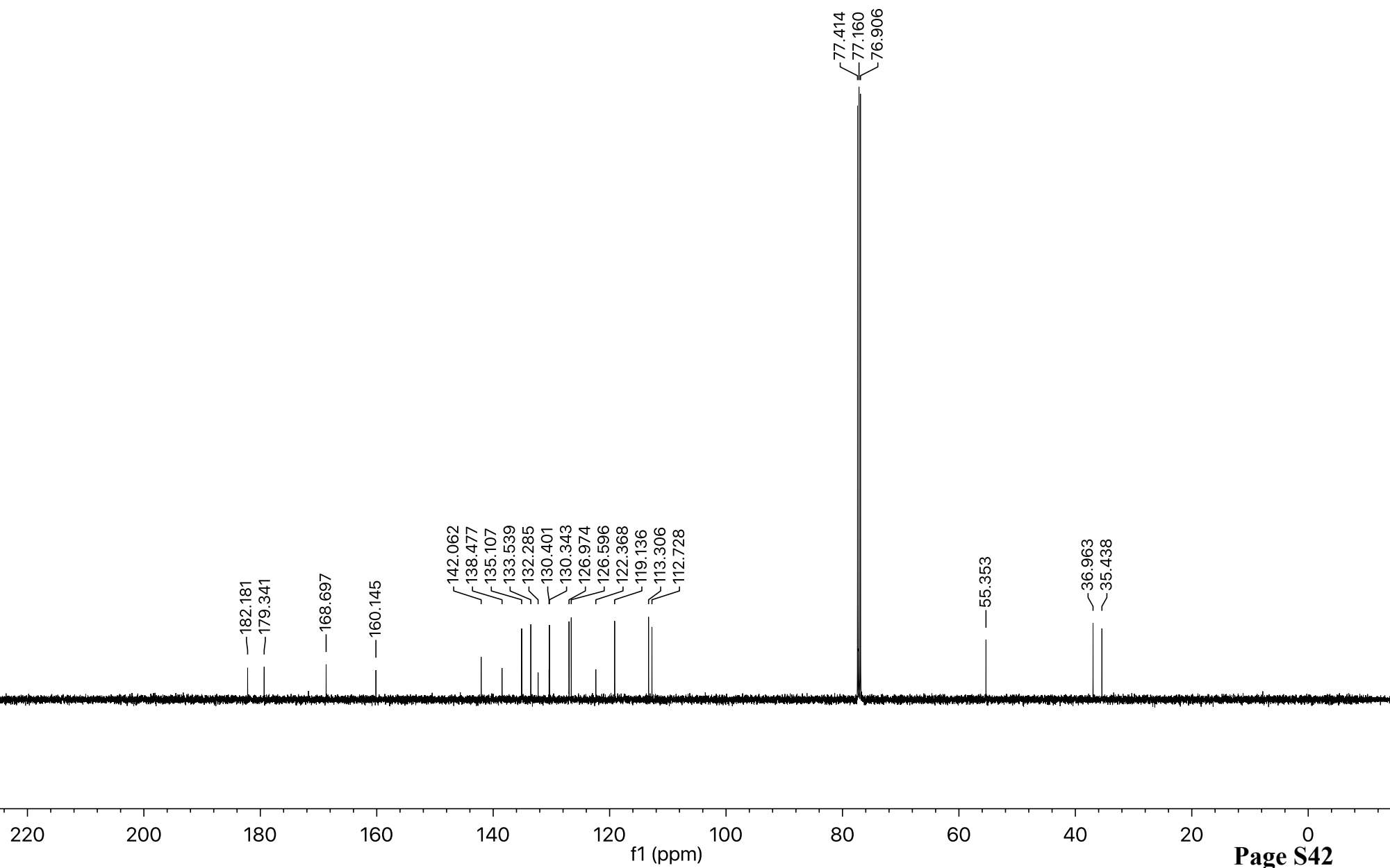
3.760

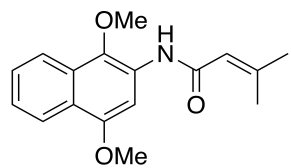
3.058
3.042
3.024
3.008
2.955
2.922





23, ^{13}C NMR (126 MHz, CDCl_3)





8.216
8.199
8.124
7.941
7.924
7.836
7.518
7.504
7.502
7.488
7.400
7.386
7.384
7.370
7.262
7.260

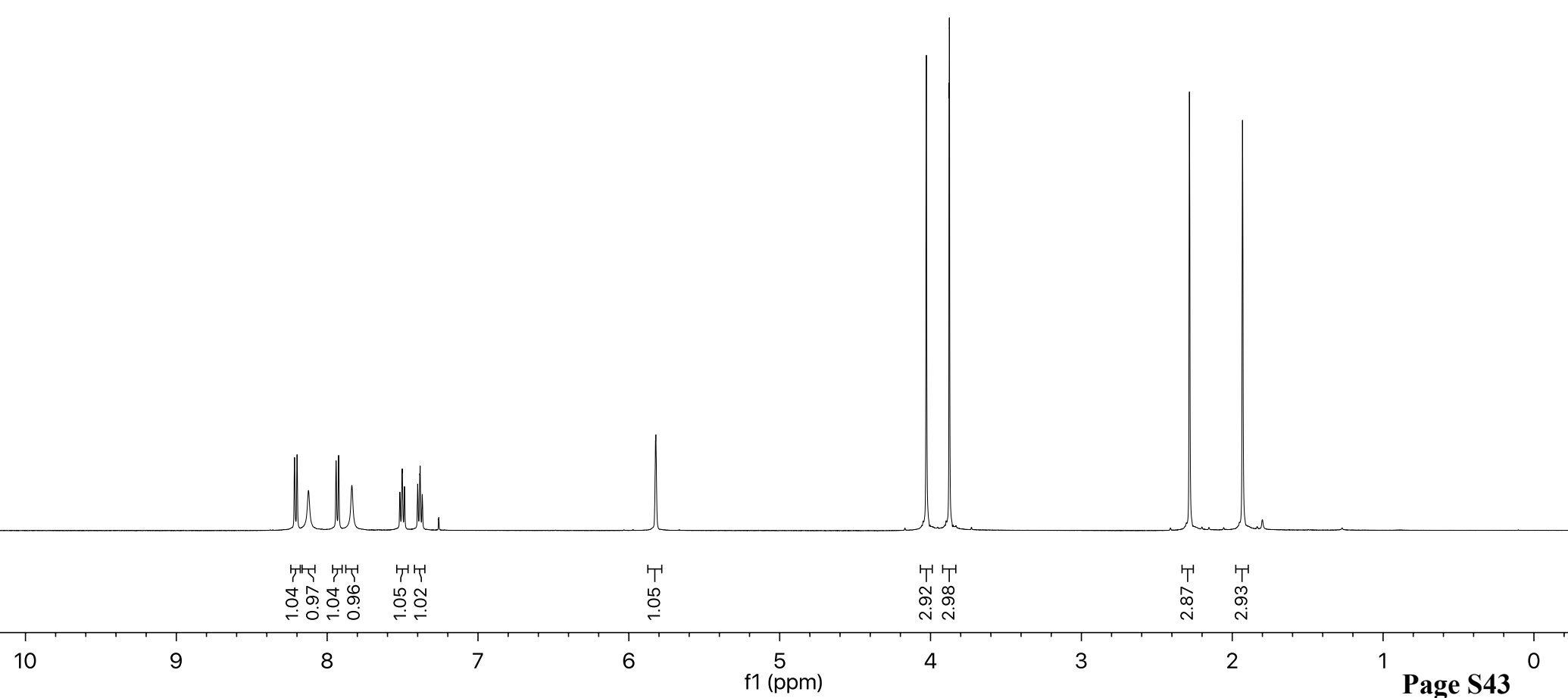
5.823
5.821

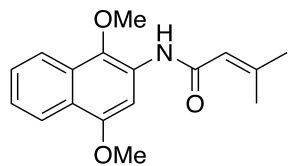
4.028
3.877
3.876

2.284

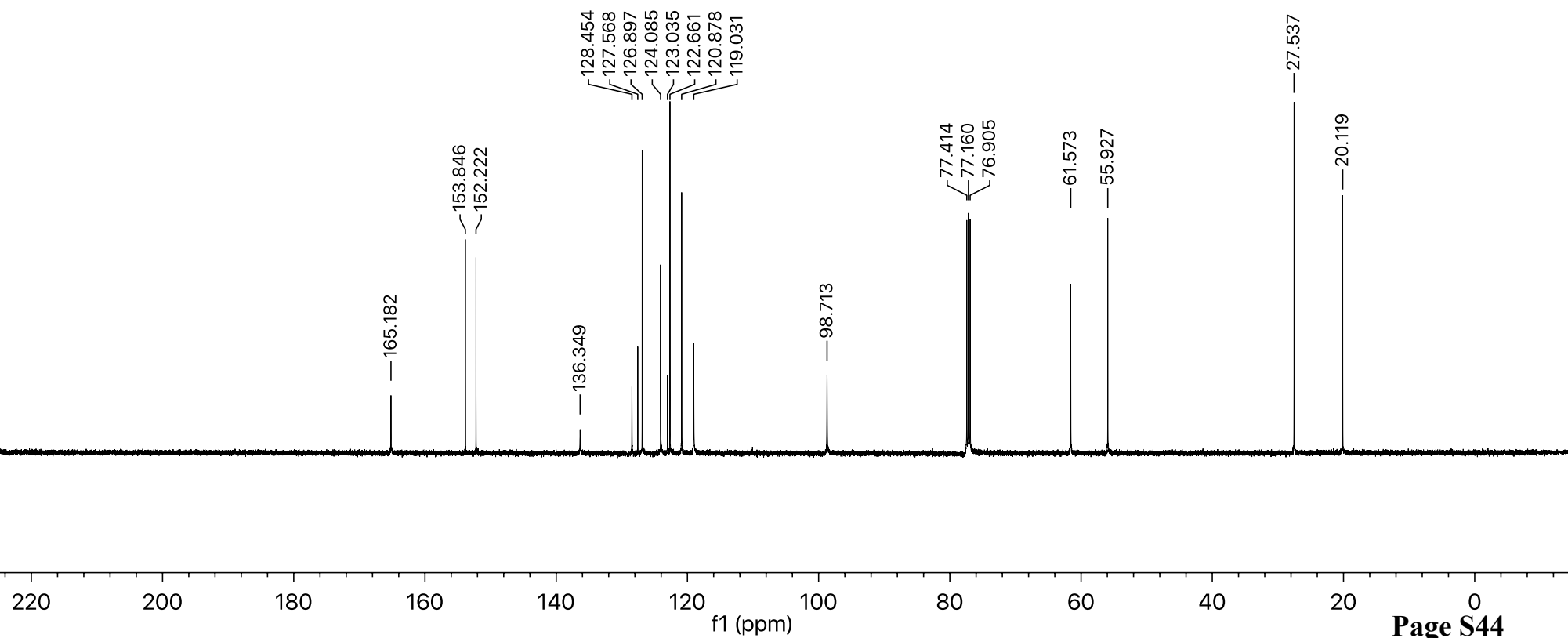
1.932

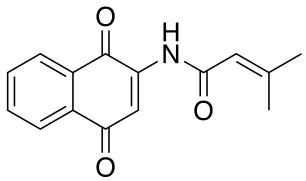
S6, ¹H NMR (500 MHz, CDCl₃)





S6, ^{13}C NMR (126 MHz, CDCl_3)





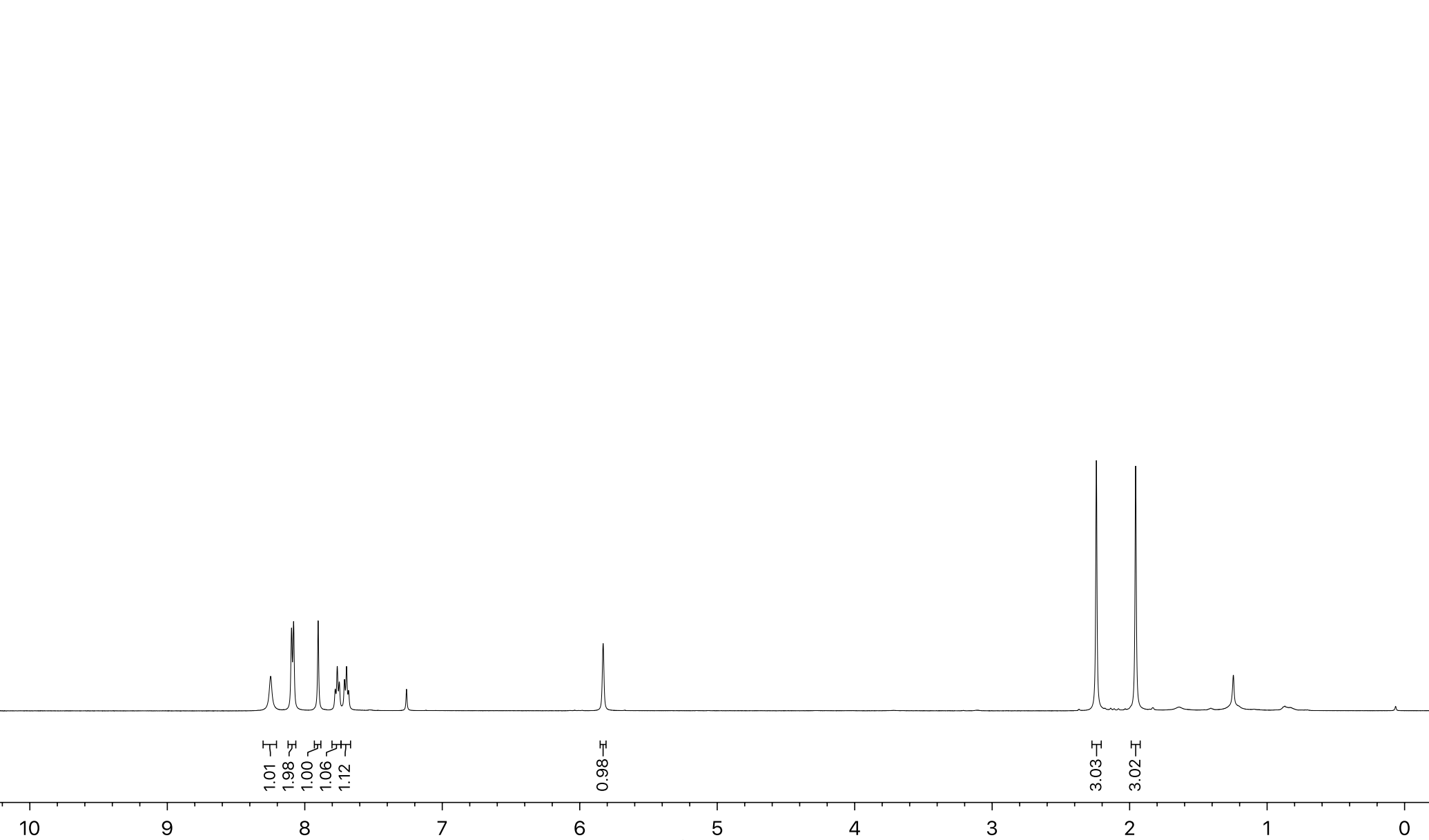
8.249
8.096
8.081
7.903
7.778
7.764
7.749
7.711
7.696
7.681
7.260

5.830

2.242

1.956

29, ¹H NMR (500 MHz, CDCl₃)

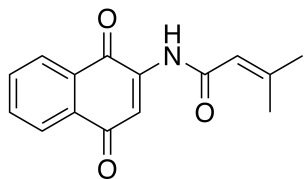


1.01
1.98
1.00
1.06
1.12

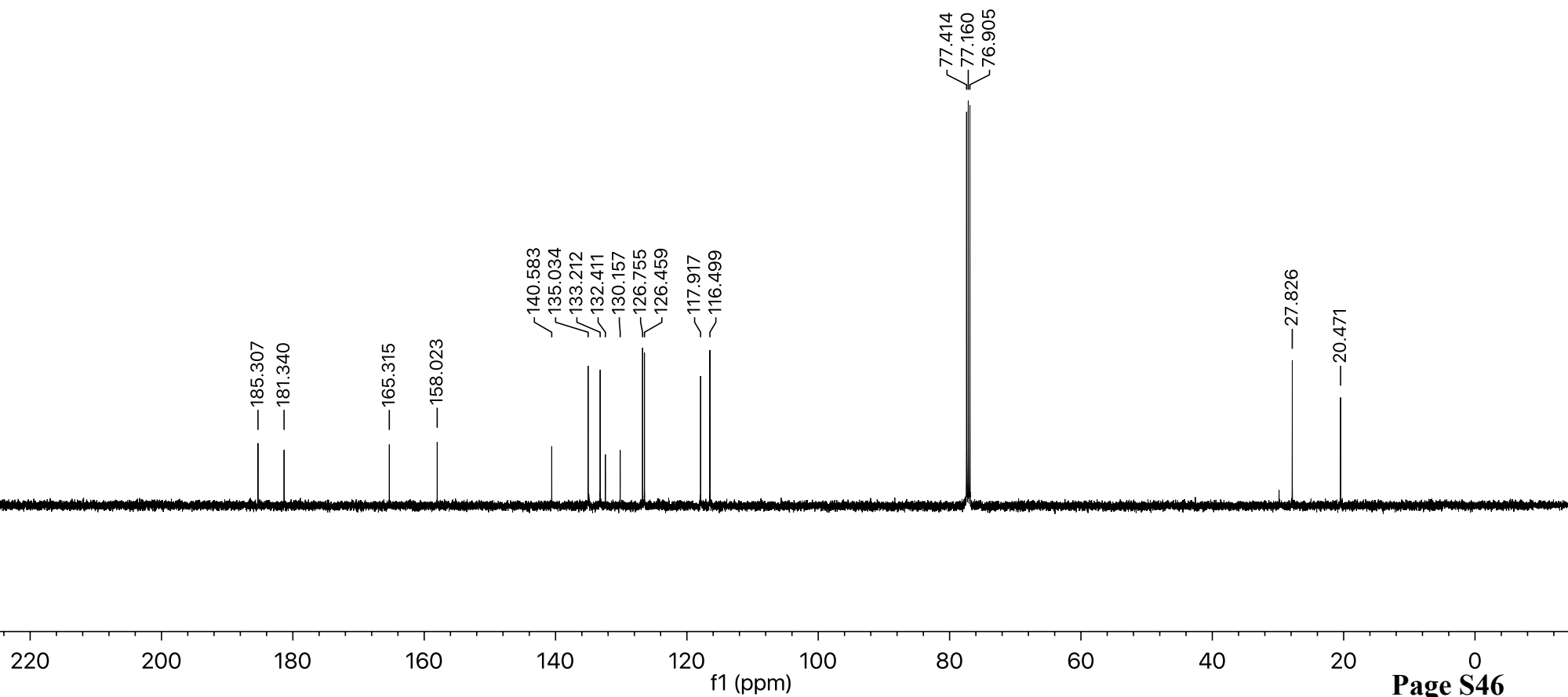
0.98

3.03

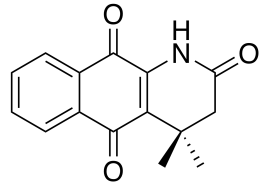
3.02



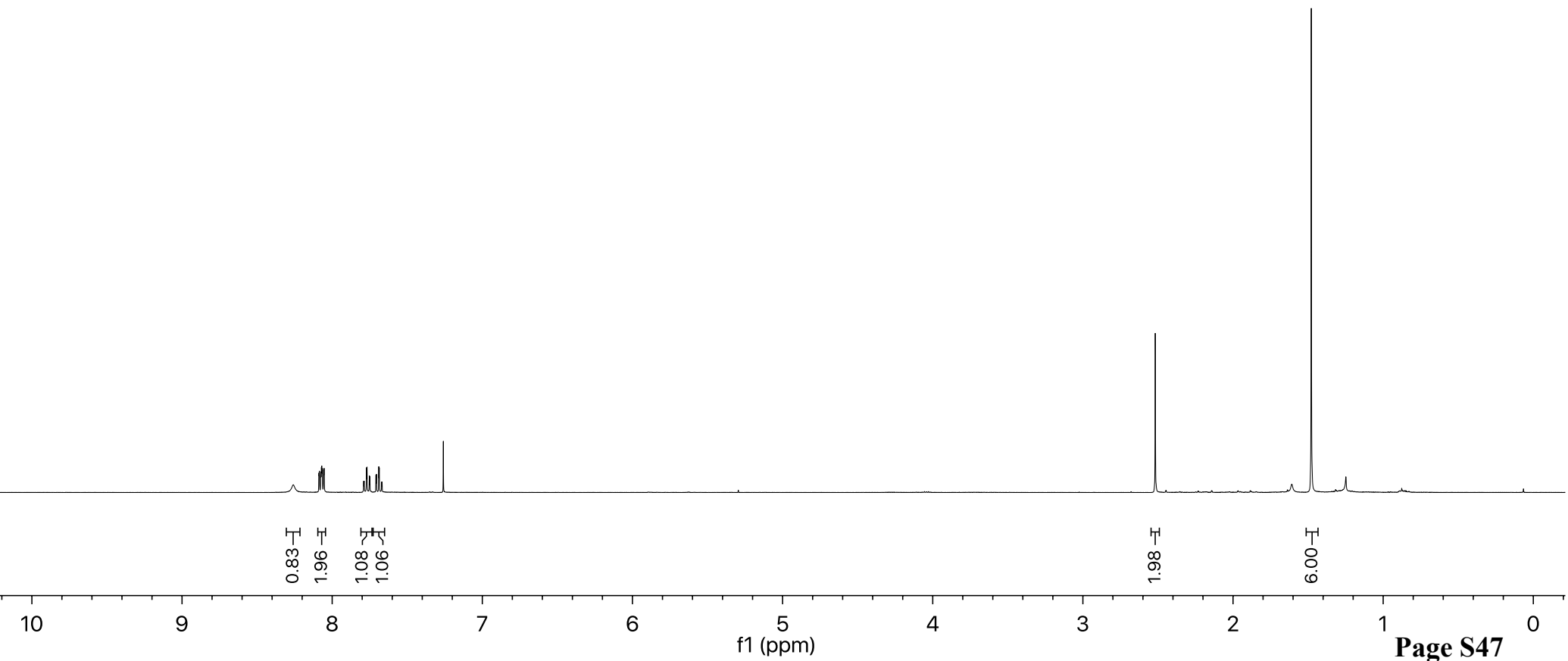
29, ^{13}C NMR (126 MHz, CDCl_3)

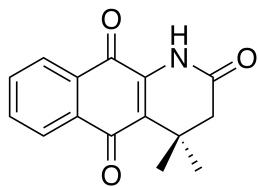


8.258
8.088
8.085
8.076
8.072
8.069
8.066
8.057
8.054
7.790
7.787
7.771
7.768
7.752
7.749
7.708
7.705
7.689
7.686
7.670
7.667
7.260

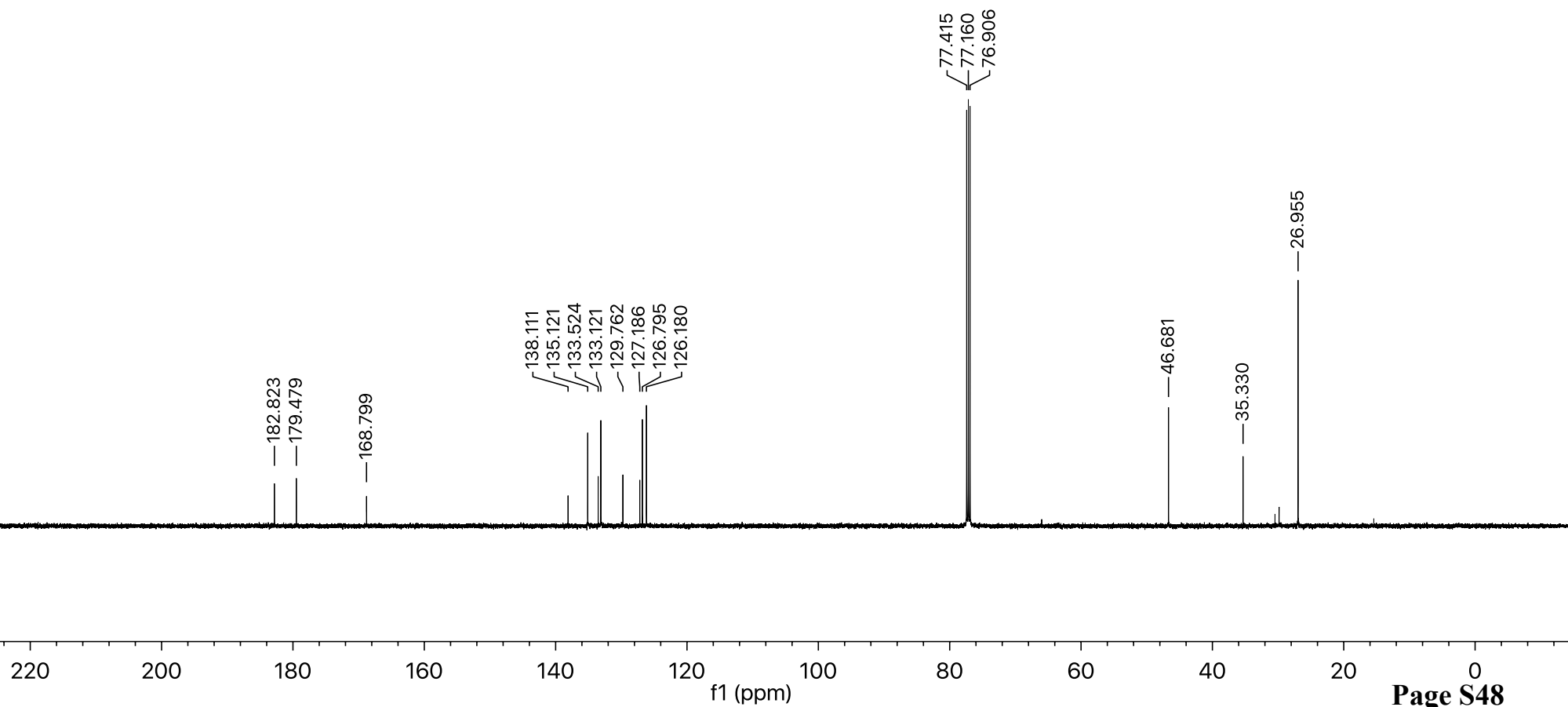


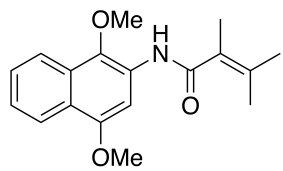
30, ^1H NMR (500 MHz, CDCl_3)





30, ^{13}C NMR (126 MHz, CDCl_3)



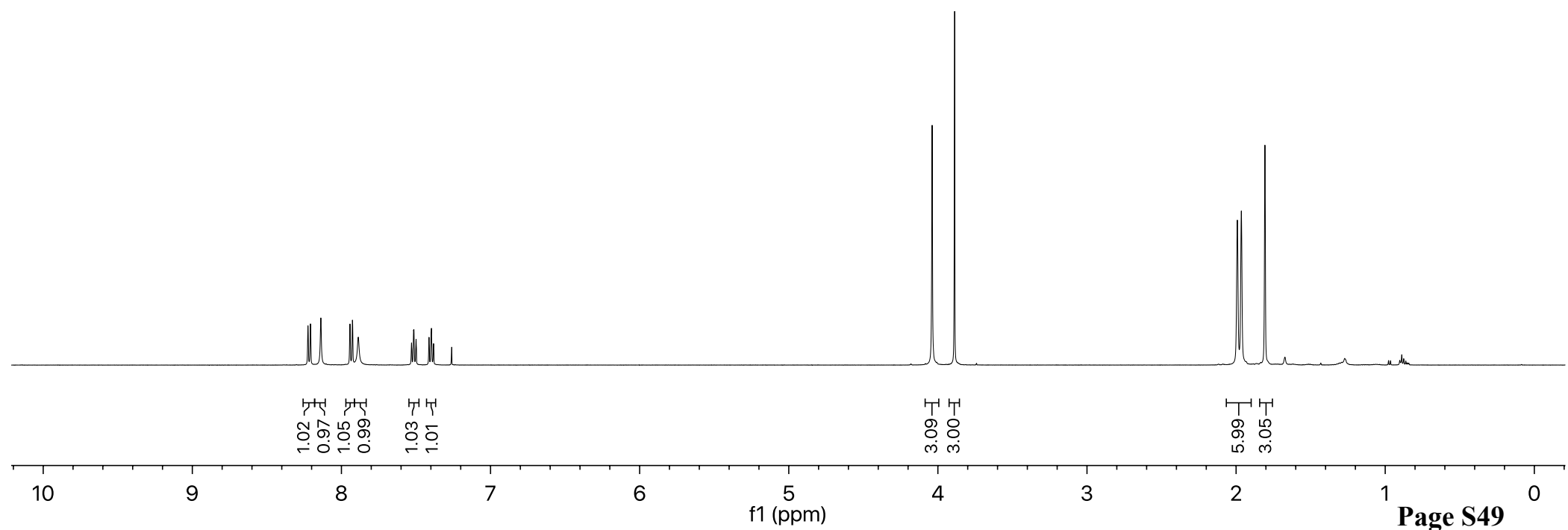


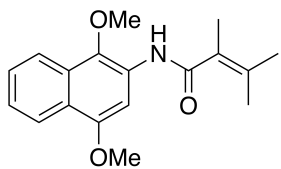
8.224
8.208
8.138
7.943
7.926
7.887
7.530
7.516
7.514
7.499
7.412
7.396
7.382
7.260

4.038
3.888

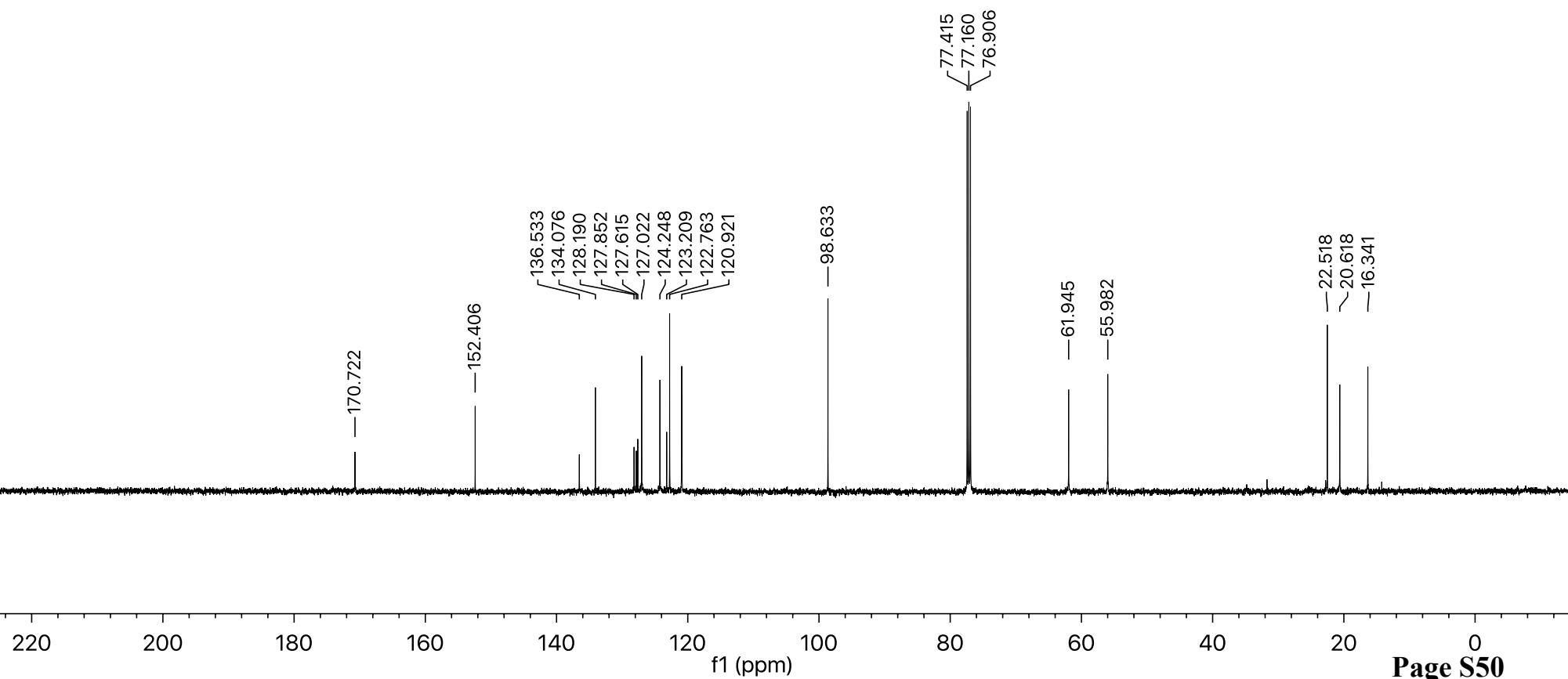
1.992
1.965
1.807

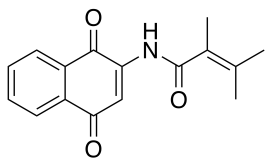
S7, ¹H NMR (500 MHz, CDCl₃)





S7, ^{13}C NMR (126 MHz, CDCl_3)





31, ^1H NMR (500 MHz, CDCl_3)

8.391
8.108
8.106
8.104
8.103
8.094
8.092
8.090
8.089
7.908
7.795
7.792
7.780
7.777
7.765
7.762
7.729
7.726
7.714
7.711
7.698
7.696
7.260

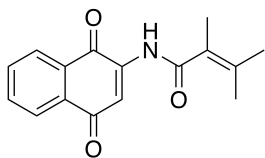
1.940
1.937
1.935
1.920
1.918
1.915
1.805
1.804

0.96
1.00
1.07
0.98
1.08
1.10

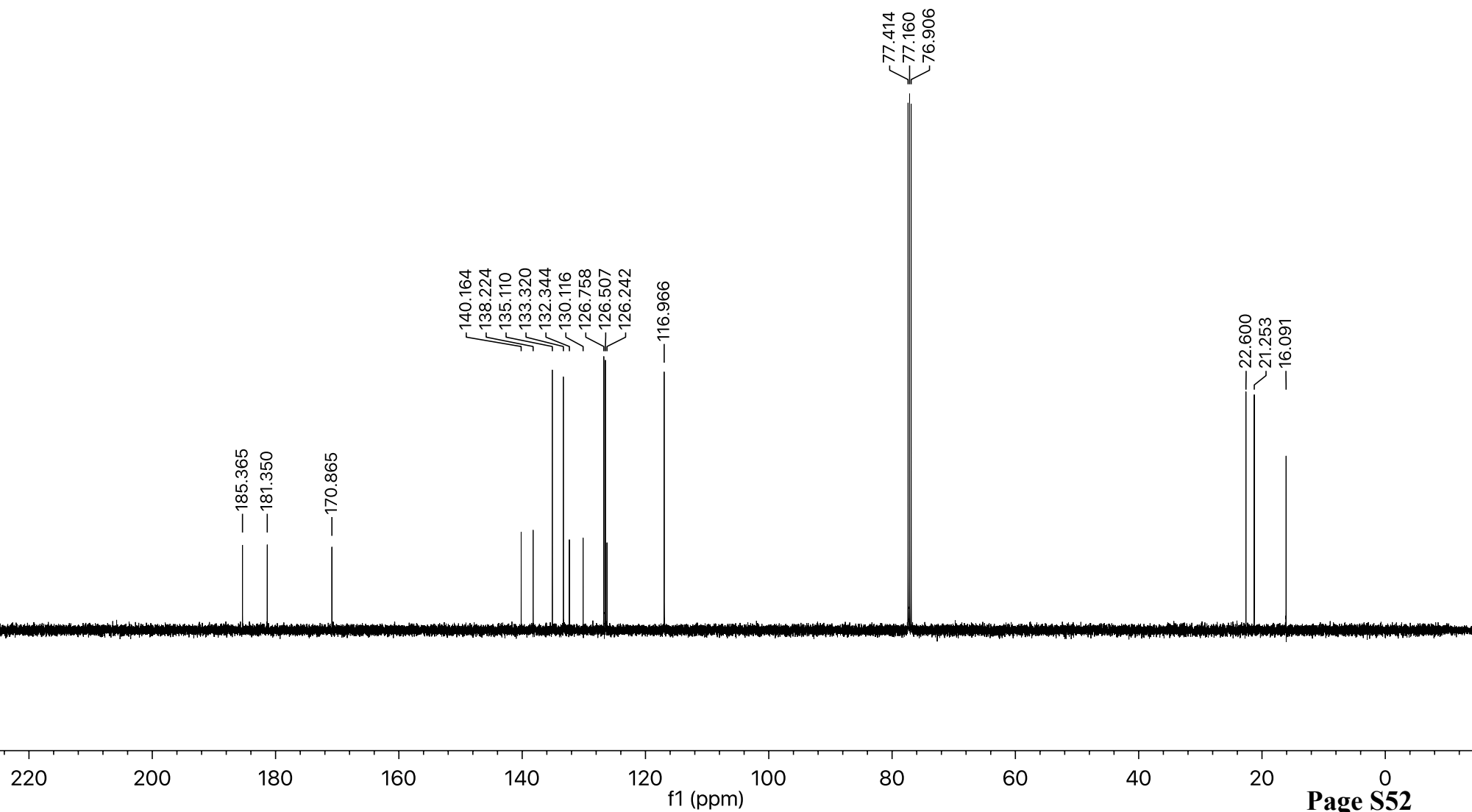
3.11
3.05
3.04

10 9 8 7 6 5 4 3 2 1 0

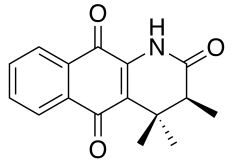
f1 (ppm)



31, ^{13}C NMR (126 MHz, CDCl_3)

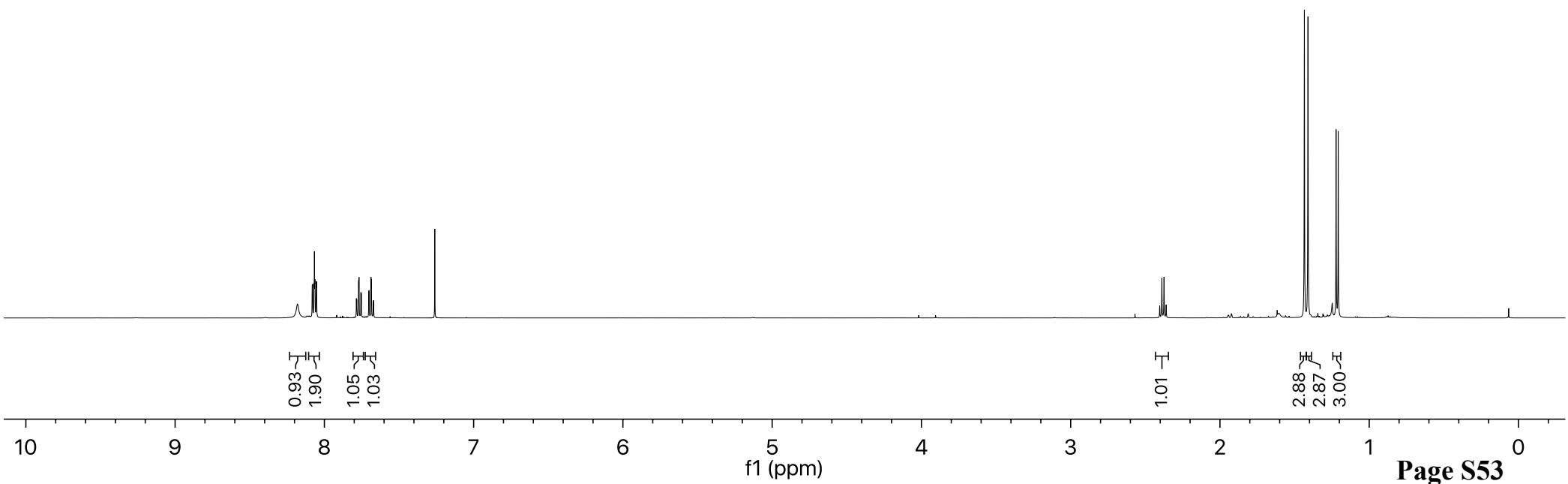


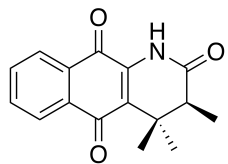
8.180
8.081
8.079
8.070
8.067
8.064
8.055
8.052
7.786
7.783
7.770
7.768
7.755
7.753
7.703
7.700
7.688
7.685
7.672
7.670
7.260



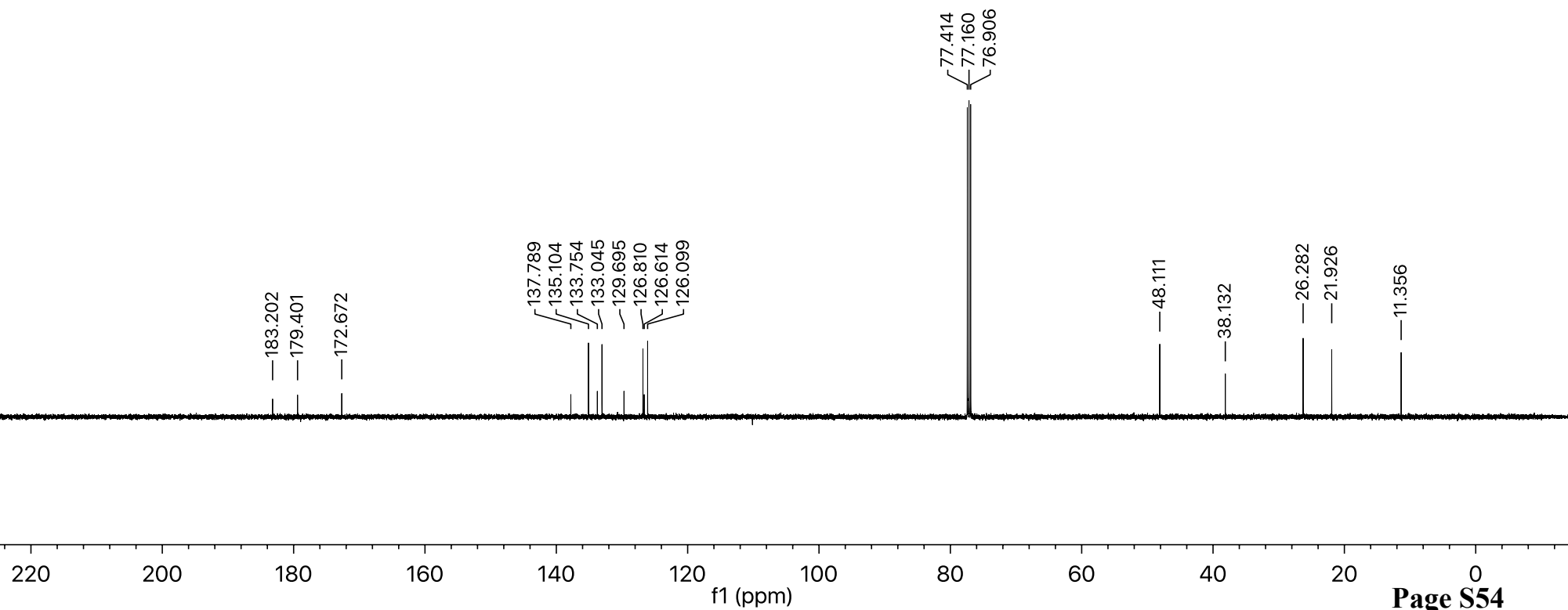
32, ¹H NMR (500 MHz, CDCl₃)

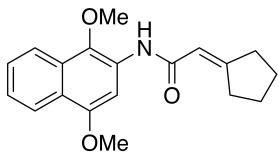
2.404
2.389
2.375
2.360
1.434
1.410
1.222
1.208





32, ^{13}C NMR (126 MHz, CDCl_3)





S8, ¹H NMR (500 MHz, CDCl₃)

8.209
8.188
8.146
7.935
7.914
7.830
7.524
7.521
7.507
7.504
7.486
7.483
7.400
7.397
7.380
7.362
7.359
7.260
5.984
5.979
5.974

4.032
3.883

2.962
2.944
2.926
2.529
2.512
2.494
1.841
1.824
1.806
1.789
1.772
1.734
1.717
1.700
1.683
1.666

1.02
0.86
1.01
0.83

0.99
0.97

0.97

3.00
2.95

1.98

1.98

1.99
2.02

10

9

8

7

6

5

f1 (ppm)

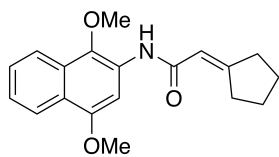
4

3

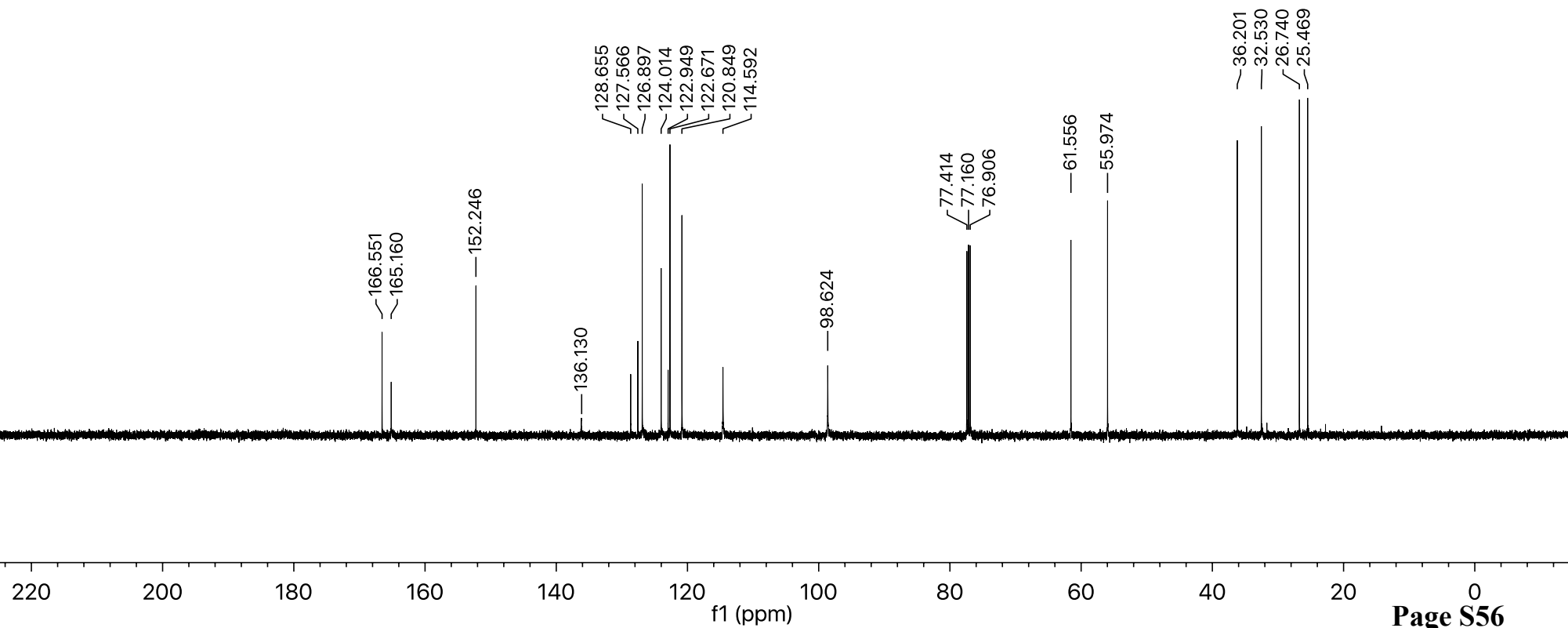
2

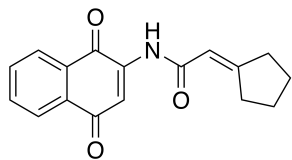
1

0



S8, ^{13}C NMR (126 MHz, CDCl_3)



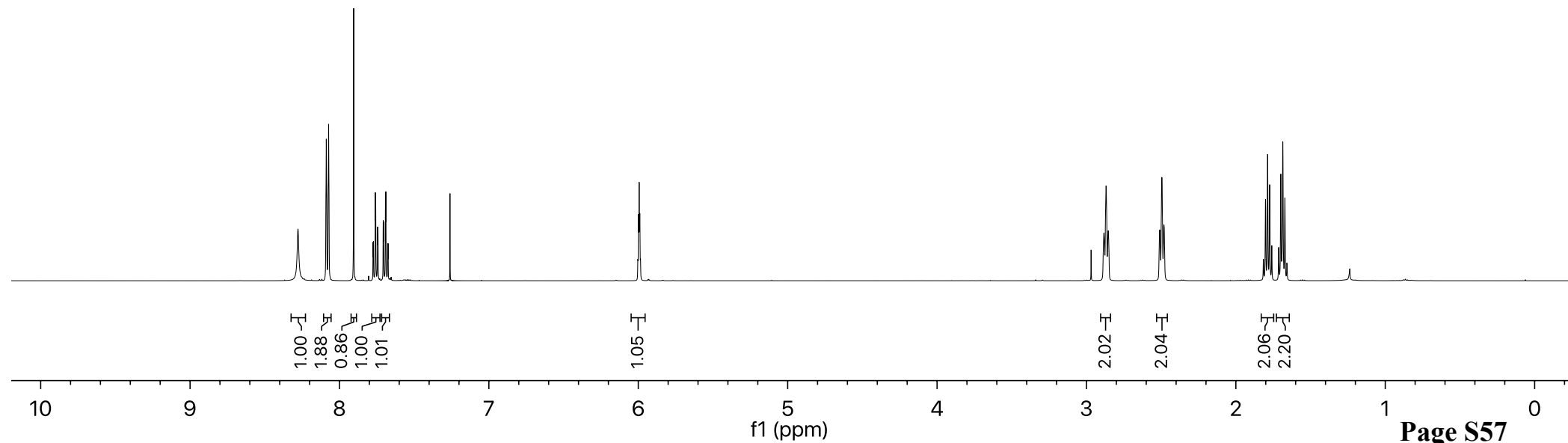


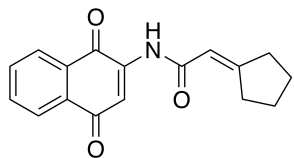
33, ^1H NMR (500 MHz, CDCl_3)

8.278
8.088
8.073
7.905
7.775
7.772
7.760
7.758
7.745
7.742
7.707
7.705
7.692
7.690
7.677
7.675
7.260

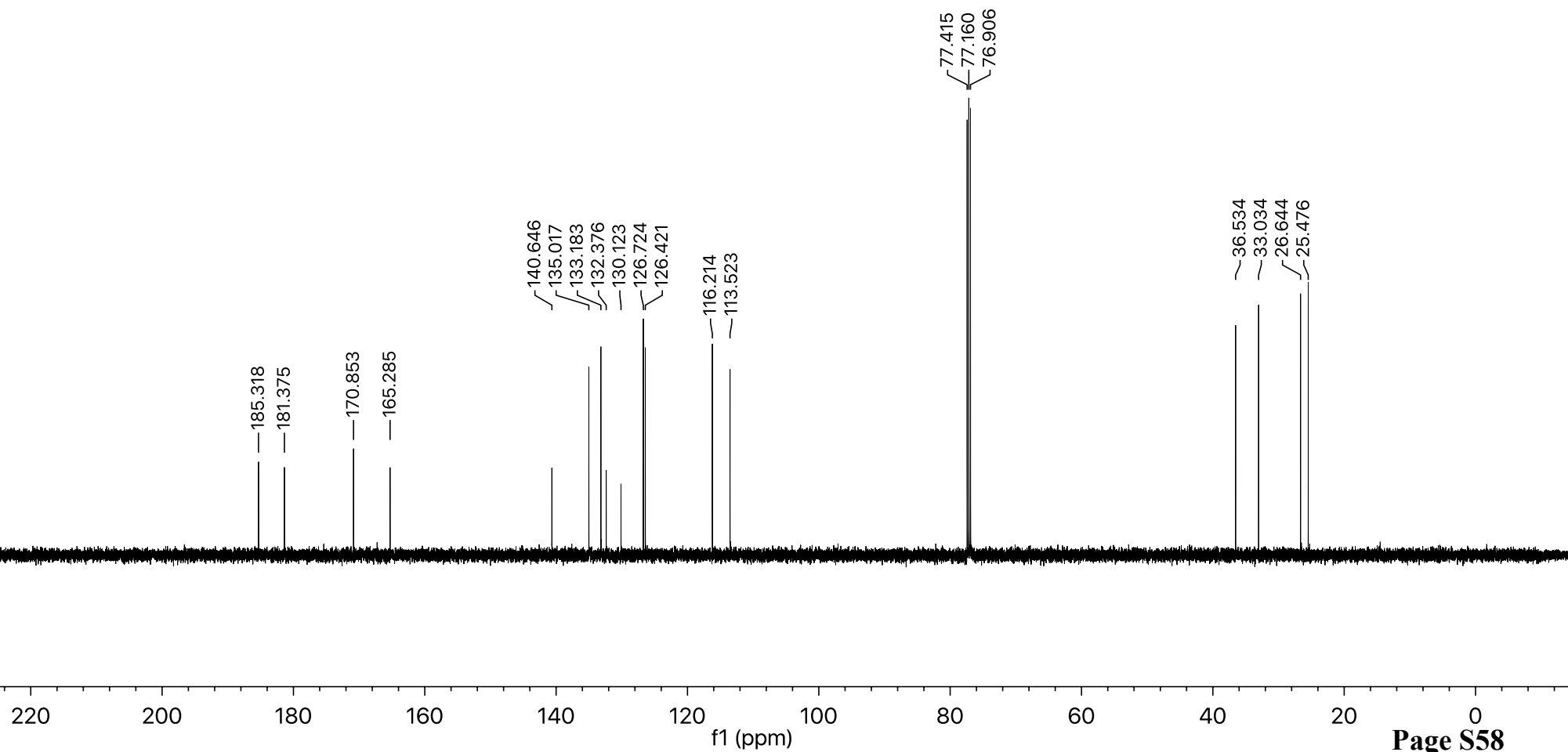
6.003
5.998
5.994
5.990
5.985

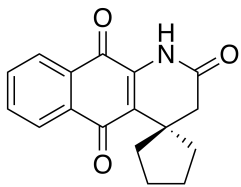
2.883
2.869
2.854
2.509
2.496
2.482
1.815
1.801
1.787
1.774
1.760
1.713
1.699
1.686
1.672
1.659





33, ^{13}C NMR (126 MHz, CDCl_3)





34, ¹H NMR (500 MHz, CDCl₃)

8.211
8.074
8.058
7.782
7.767
7.752
7.750
7.705
7.689
7.674
7.260

2.574
2.329
2.314
2.302
2.289
2.275
2.031
2.016
2.005
2.000
1.987
1.974
1.806
1.798
1.790
1.777
1.768
1.758
1.631
1.619
1.607
1.594
1.582

0.96
1.94

1.10
1.02

1.94

1.99

1.98

2.00

2.59

10

9

8

7

6

5

4

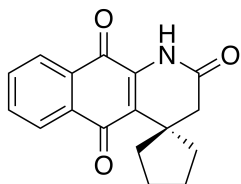
3

2

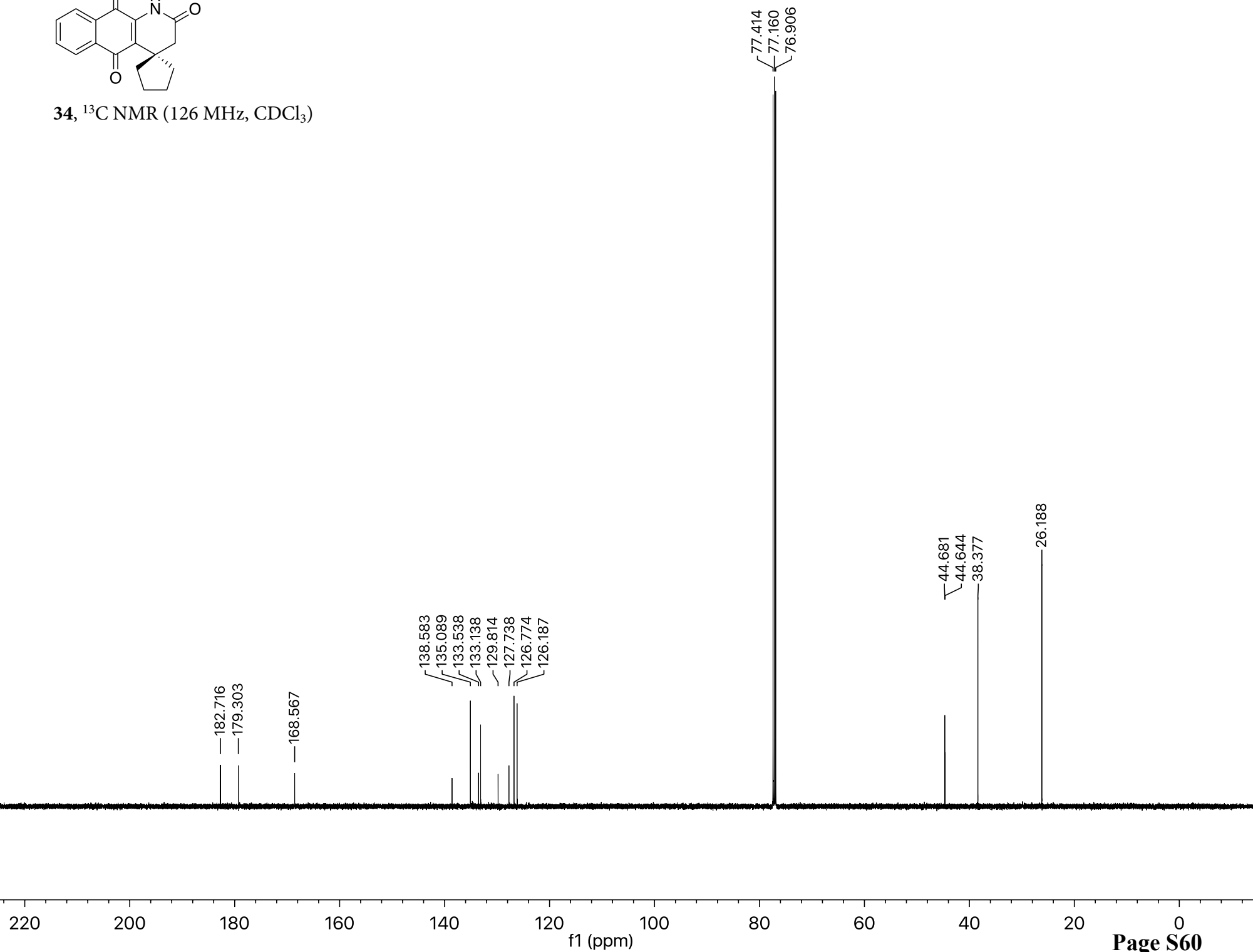
1

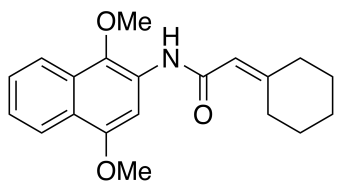
0

f1 (ppm)



34, ^{13}C NMR (126 MHz, CDCl_3)





8.210
8.193
8.148
7.938
7.921
7.860
7.522
7.507
7.491
7.400
7.386
7.370
7.260

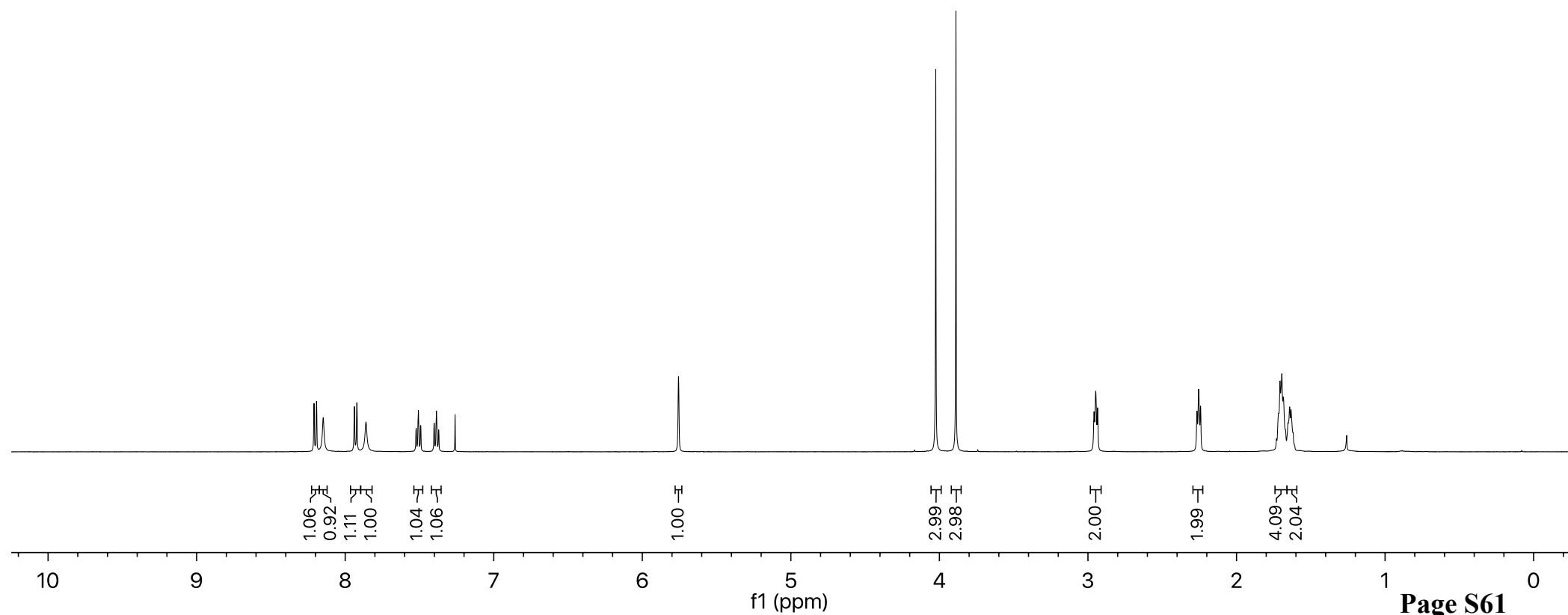
5.756

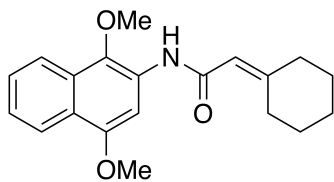
4.025
3.889

2.959
2.948
2.935

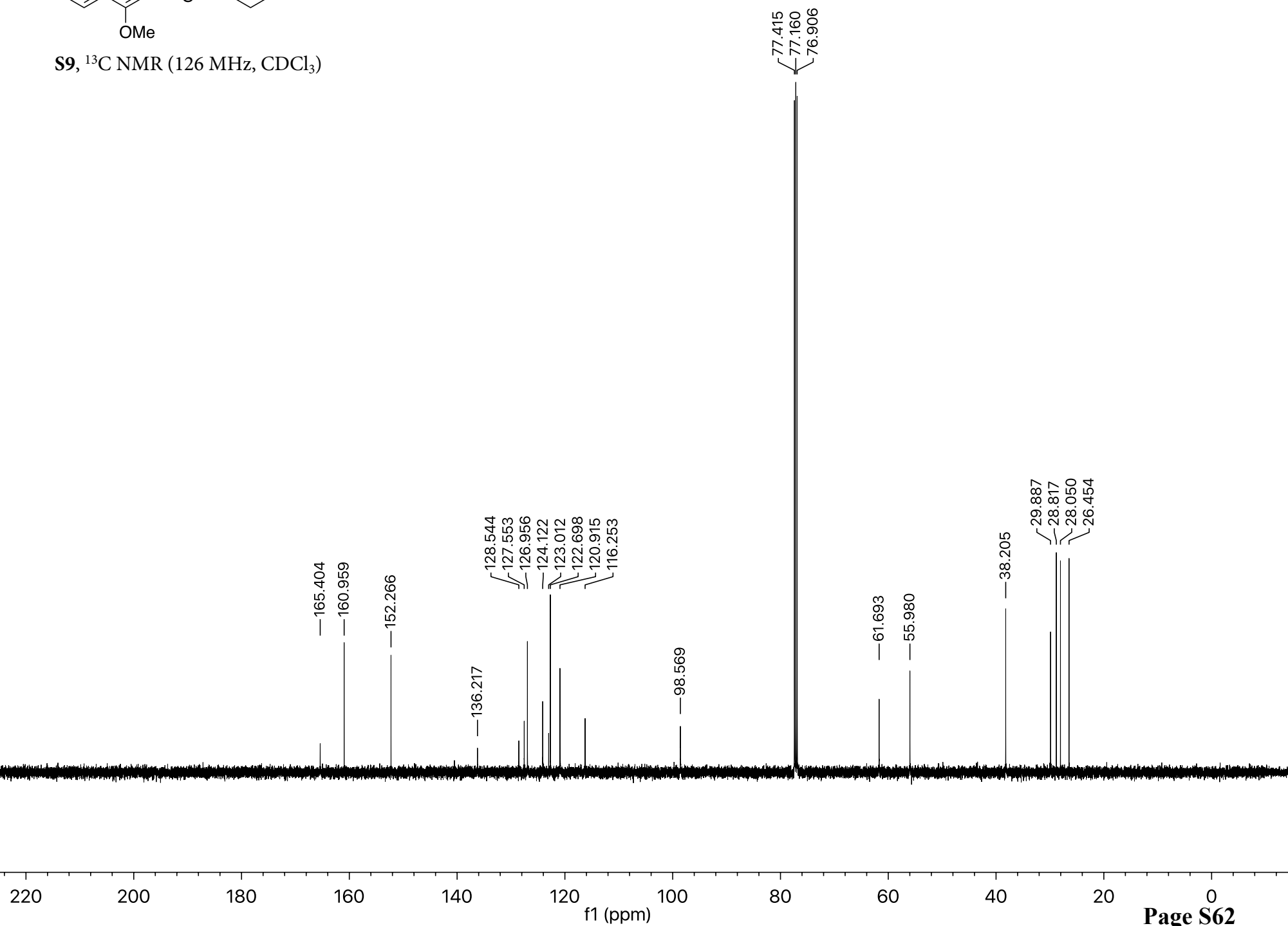
2.266
2.255
2.242
1.731
1.716
1.707
1.695
1.685
1.653
1.642
1.633
1.619

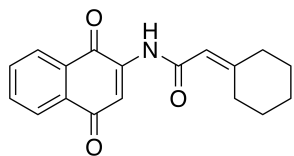
S9, ¹H NMR (500 MHz, CDCl₃)





S9, ^{13}C NMR (126 MHz, CDCl_3)





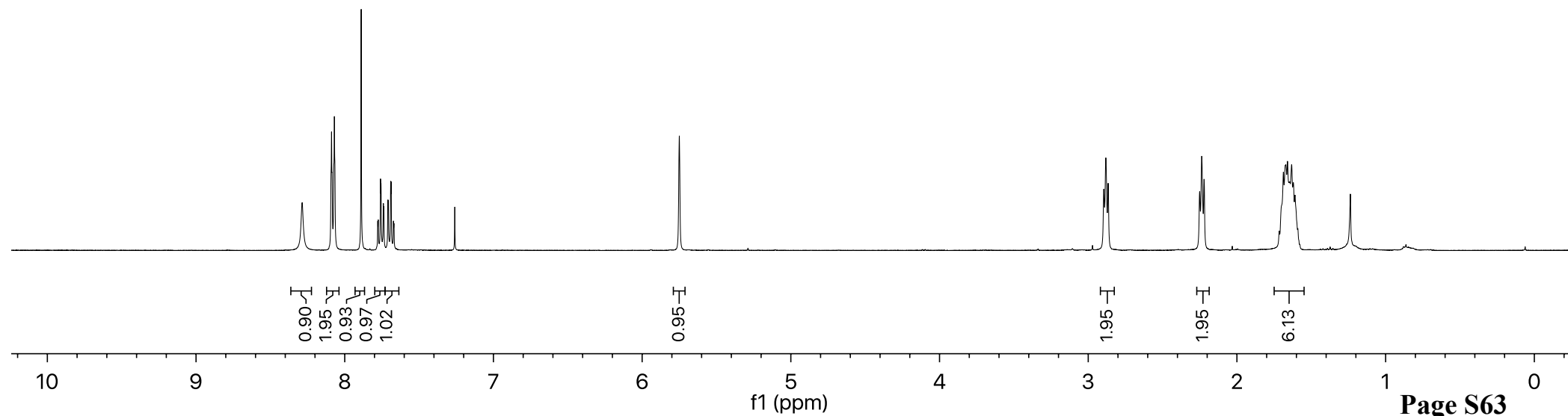
35, ¹H NMR (500 MHz, CDCl₃)

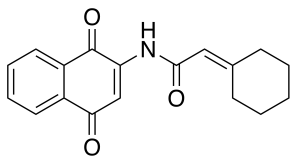
8.286
8.089
8.070
7.889
7.778
7.775
7.759
7.756
7.740
7.737
7.710
7.707
7.691
7.688
7.672
7.669
7.260

5.750

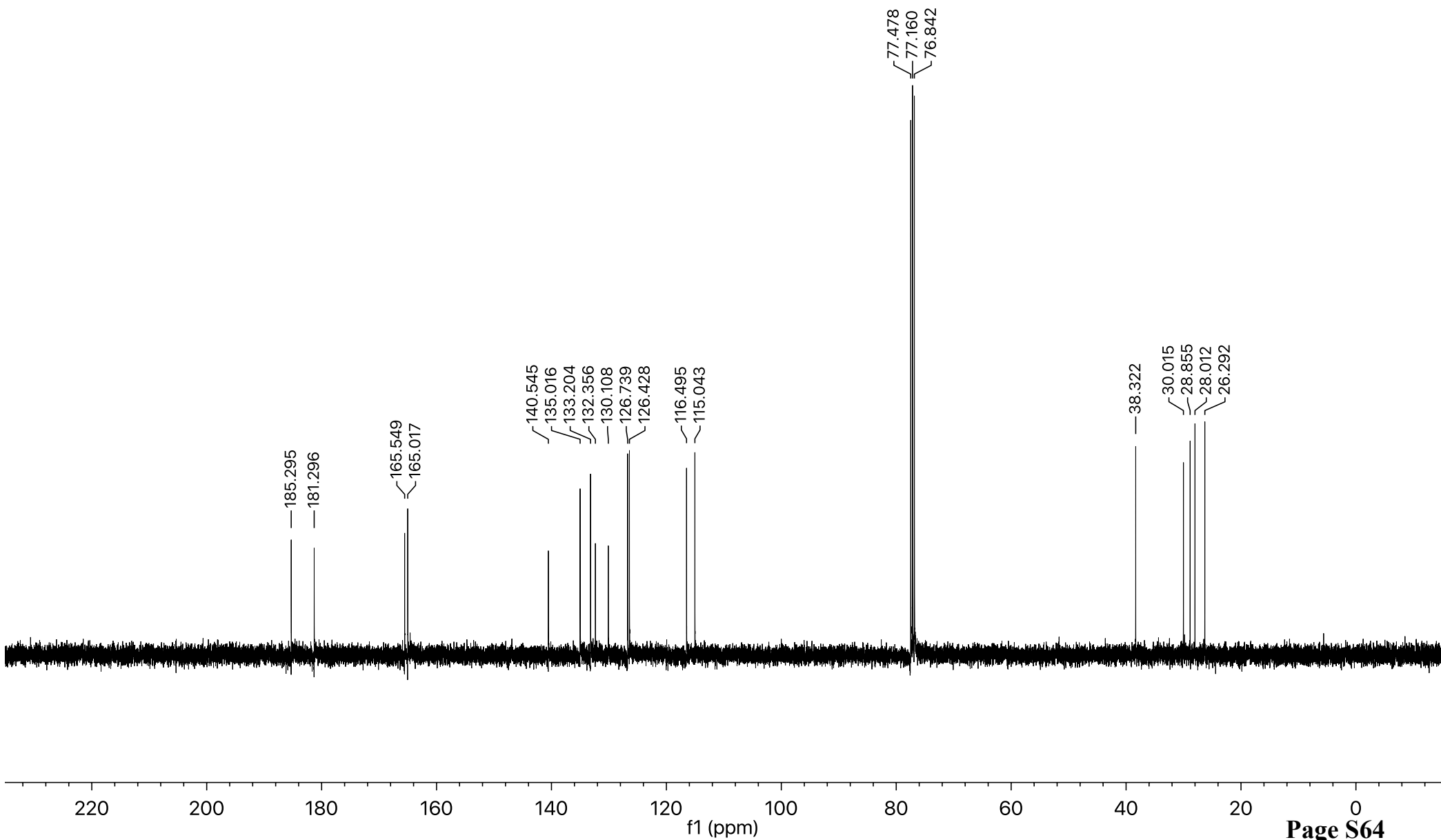
2.895
2.882
2.866

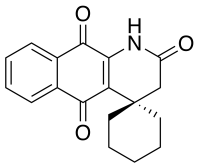
2.250
2.237
2.221
1.715
1.688
1.671
1.660
1.645
1.632
1.621
1.610
1.591



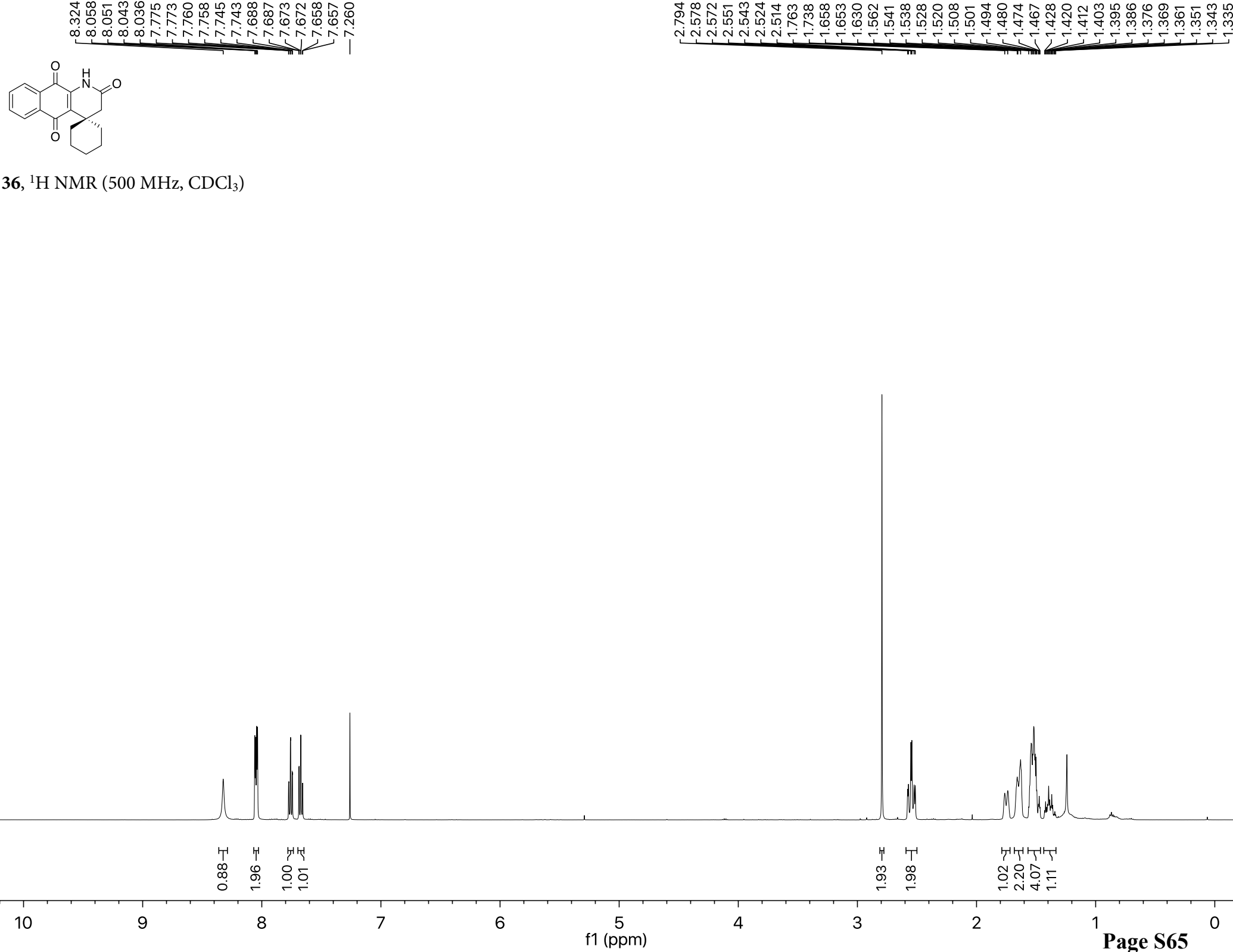


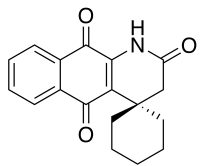
35, ^{13}C NMR (126 MHz, CDCl_3)



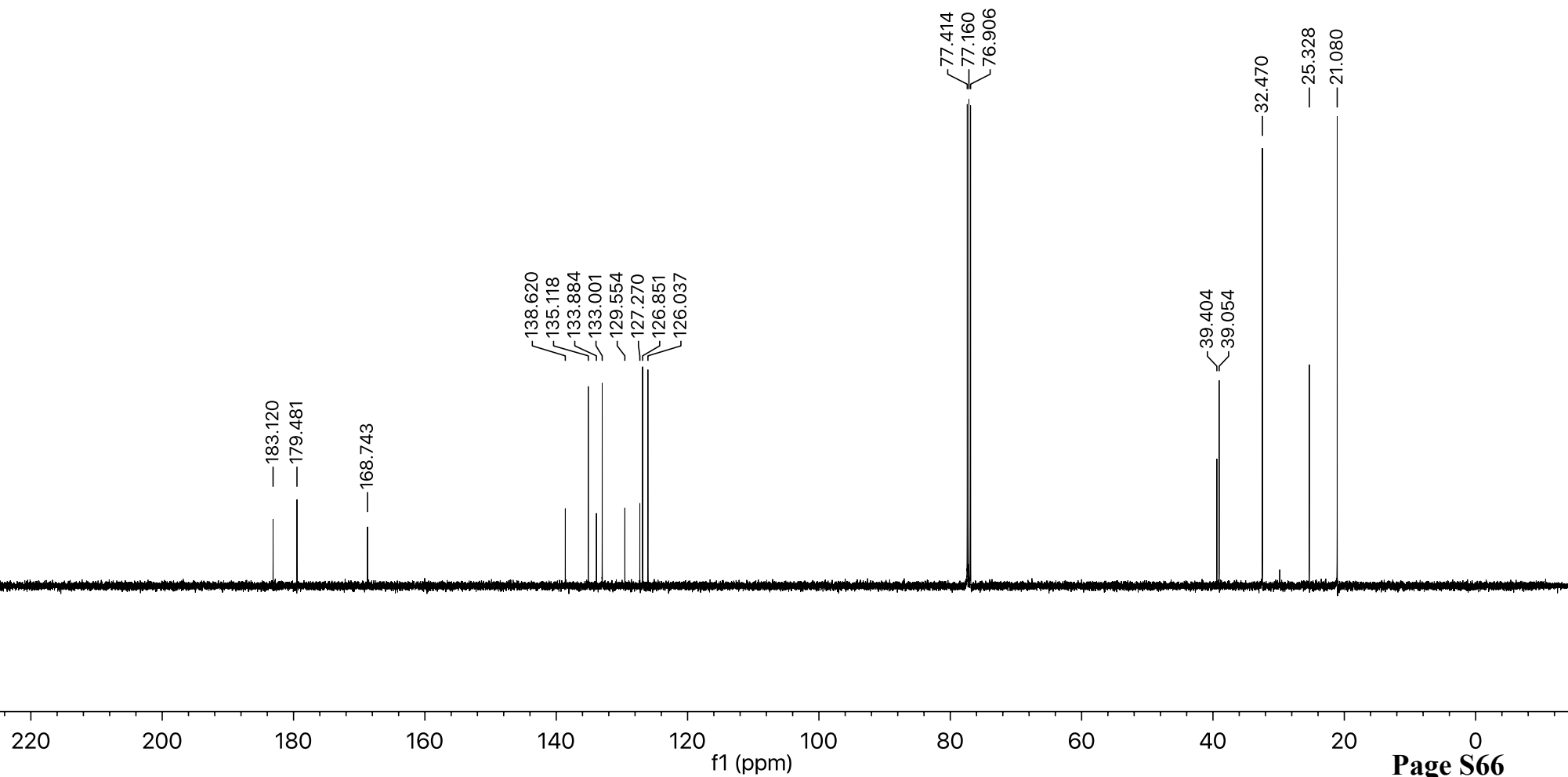


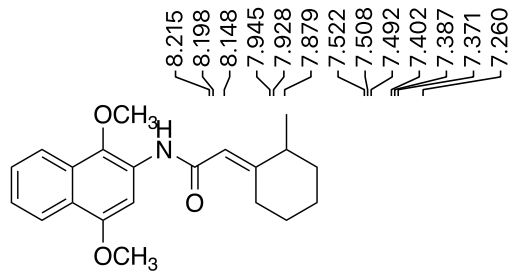
36, ¹H NMR (500 MHz, CDCl₃)



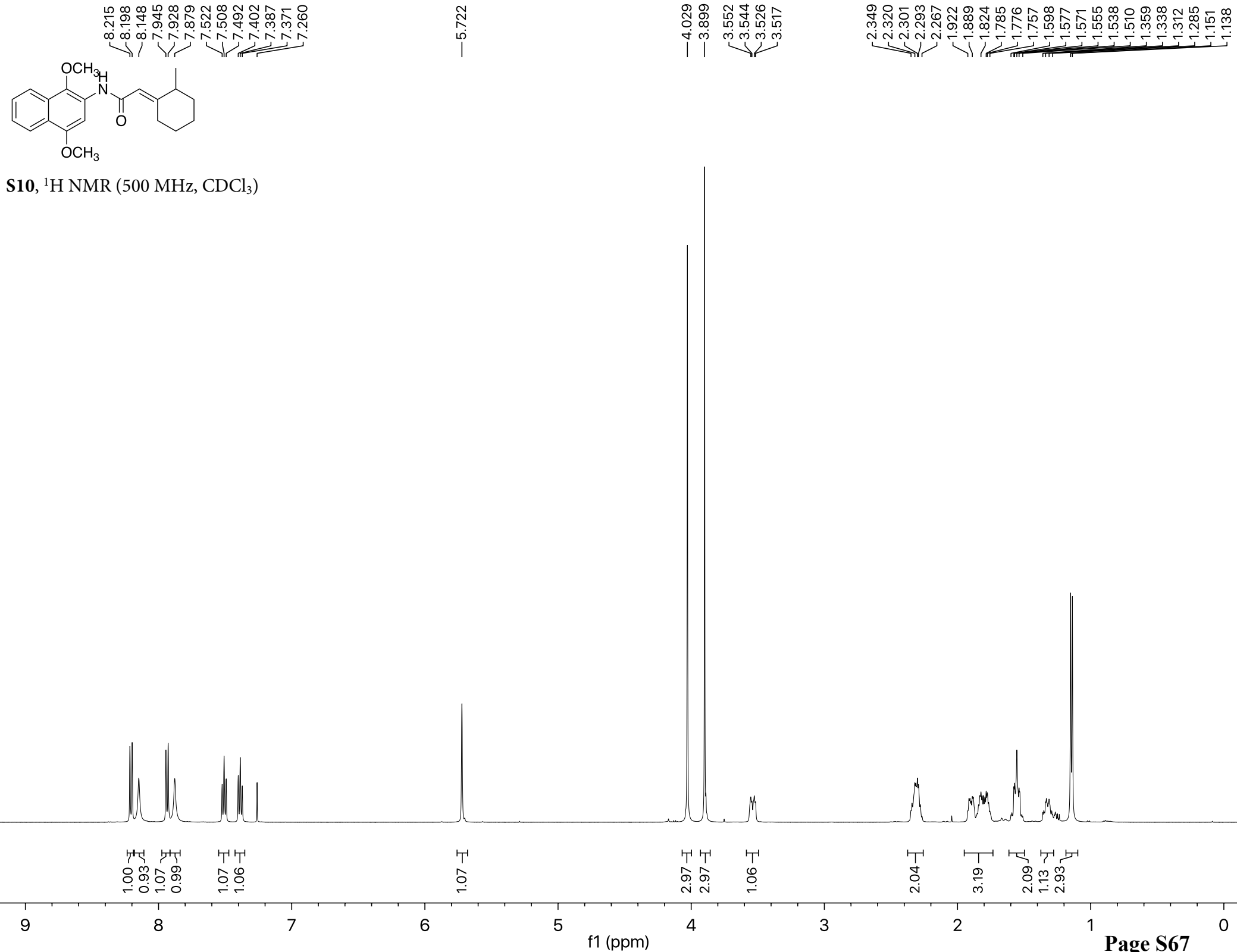


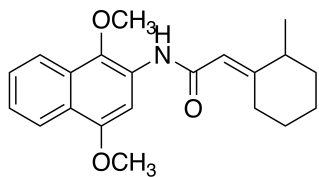
36, ^{13}C NMR (126 MHz, CDCl_3)



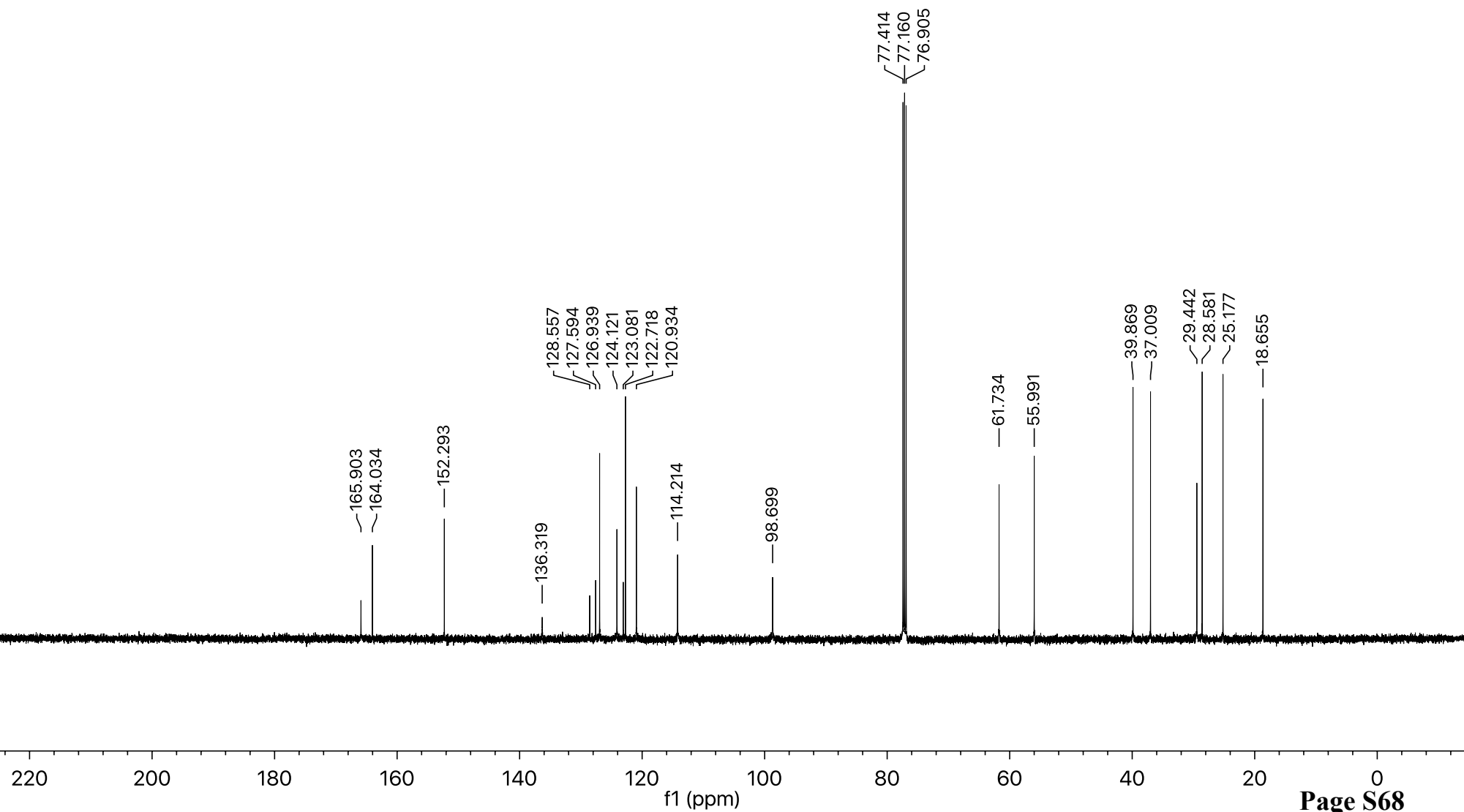


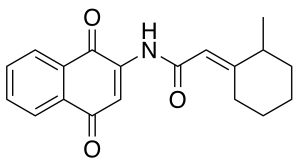
S10, ^1H NMR (500 MHz, CDCl_3)



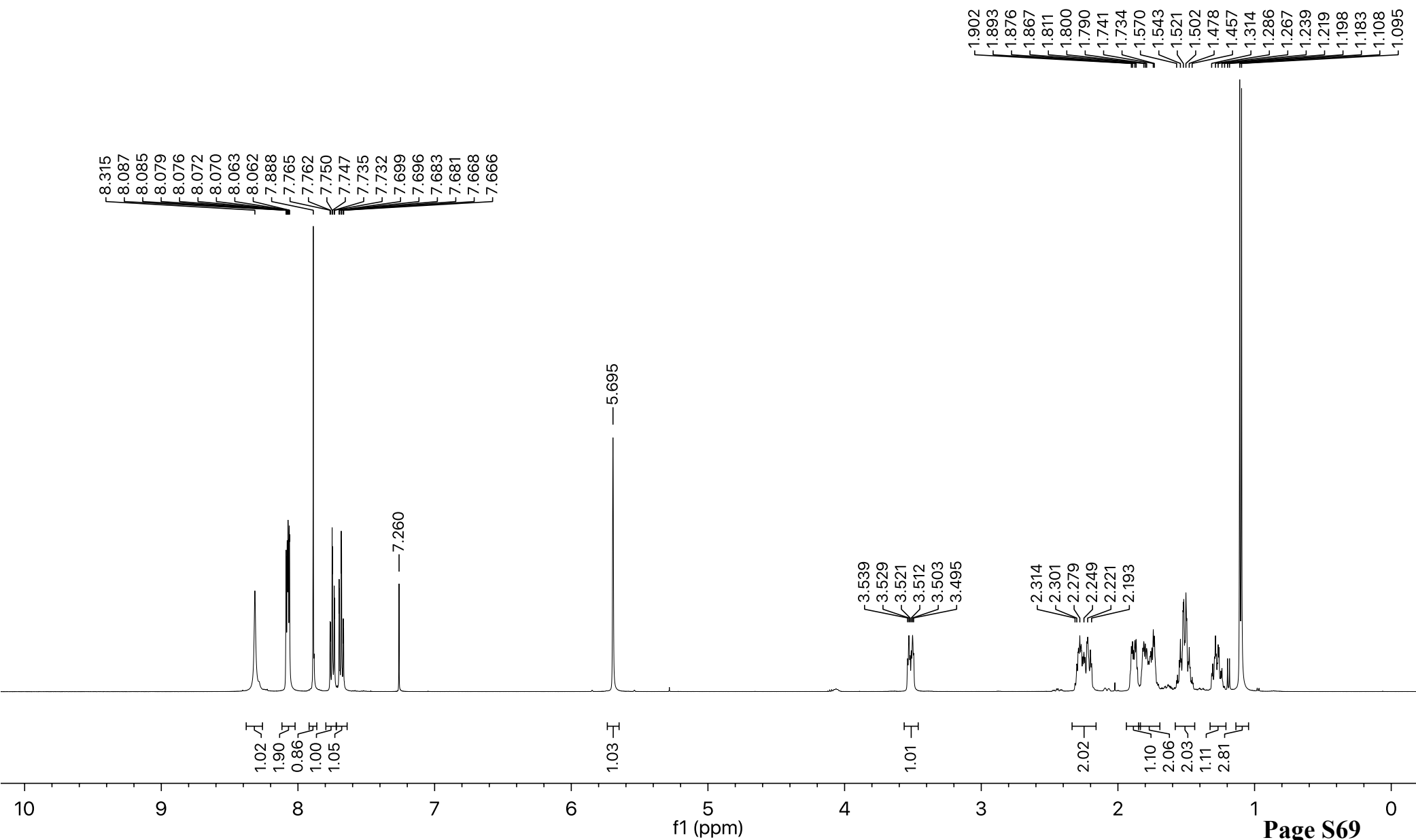


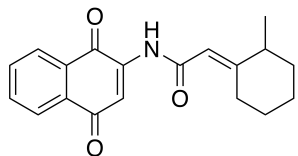
S10, ^{13}C NMR (126 MHz, CDCl_3)



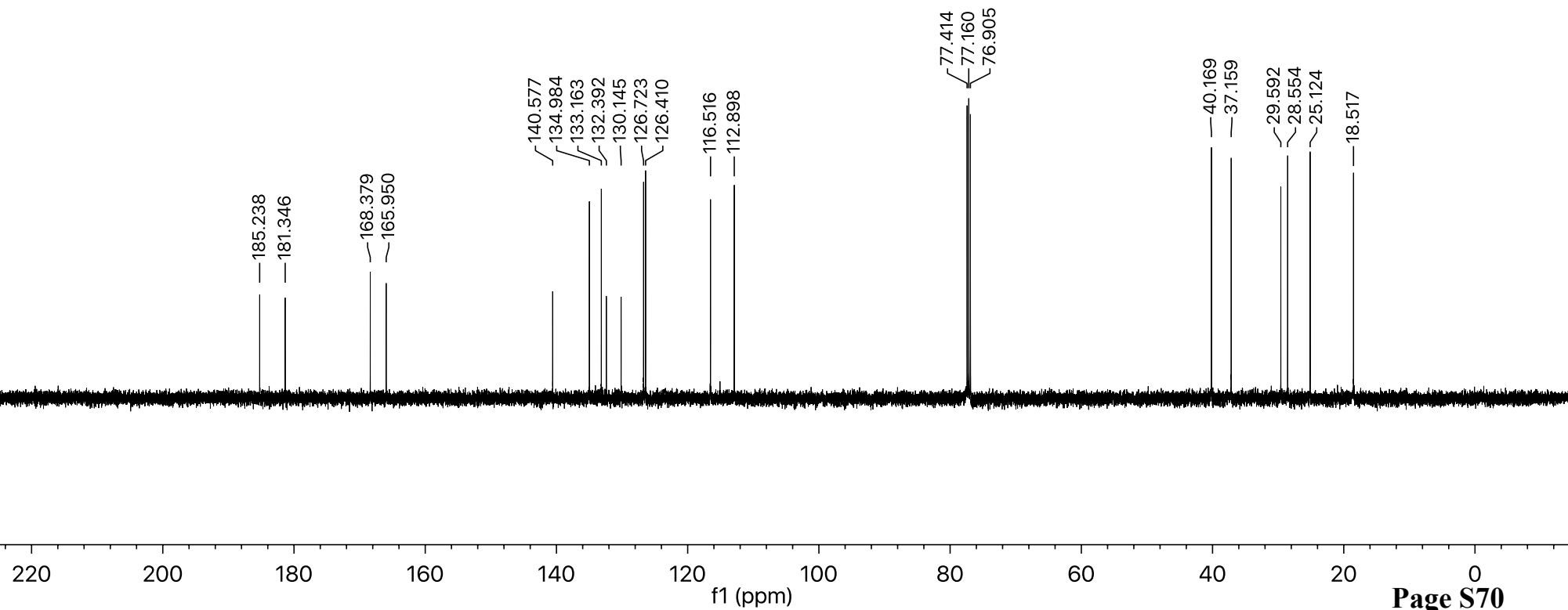


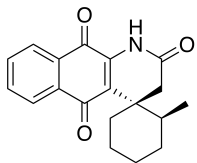
37, ^1H NMR (500 MHz, CDCl_3)



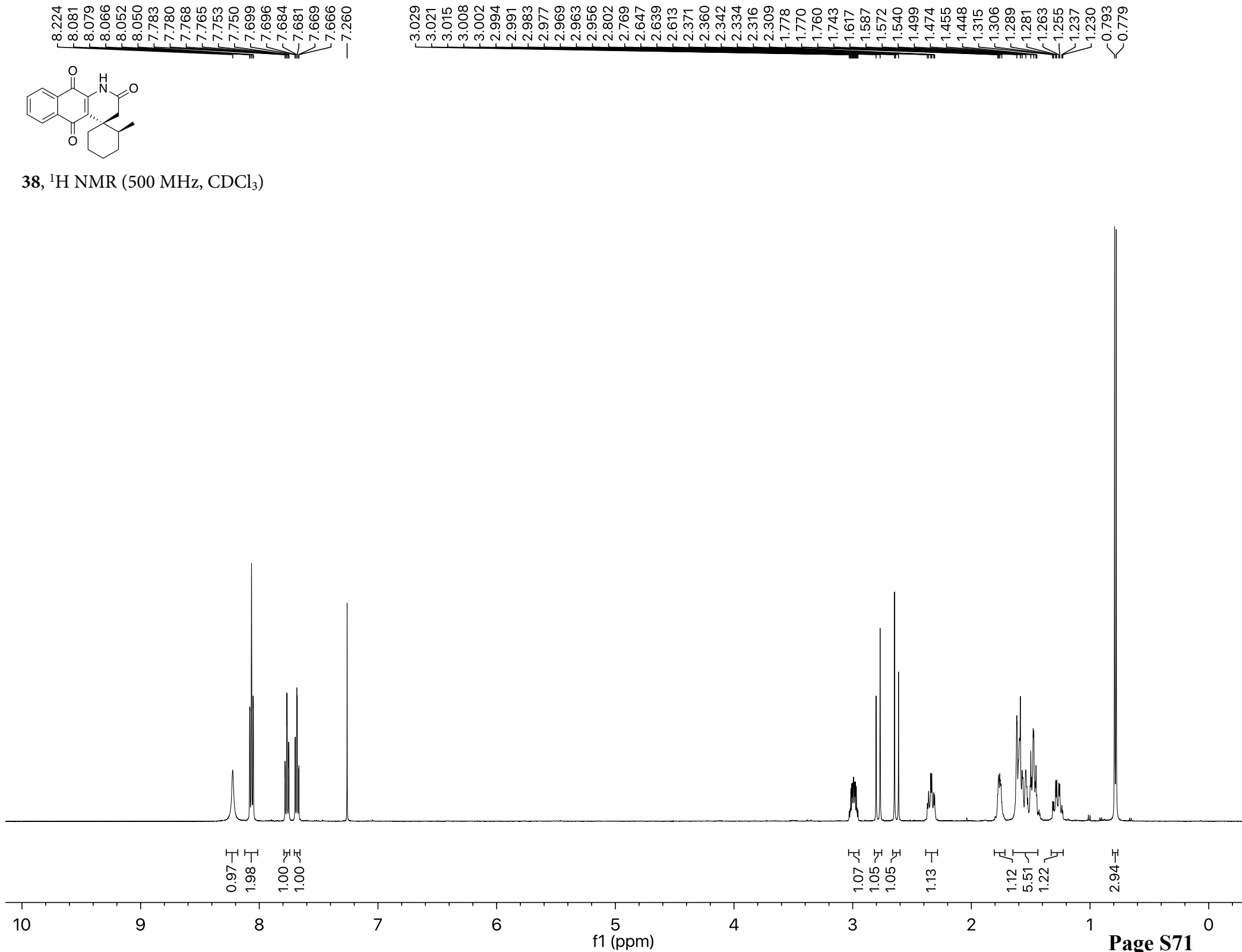


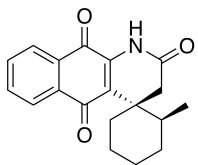
37, ^{13}C NMR (126 MHz, CDCl_3)



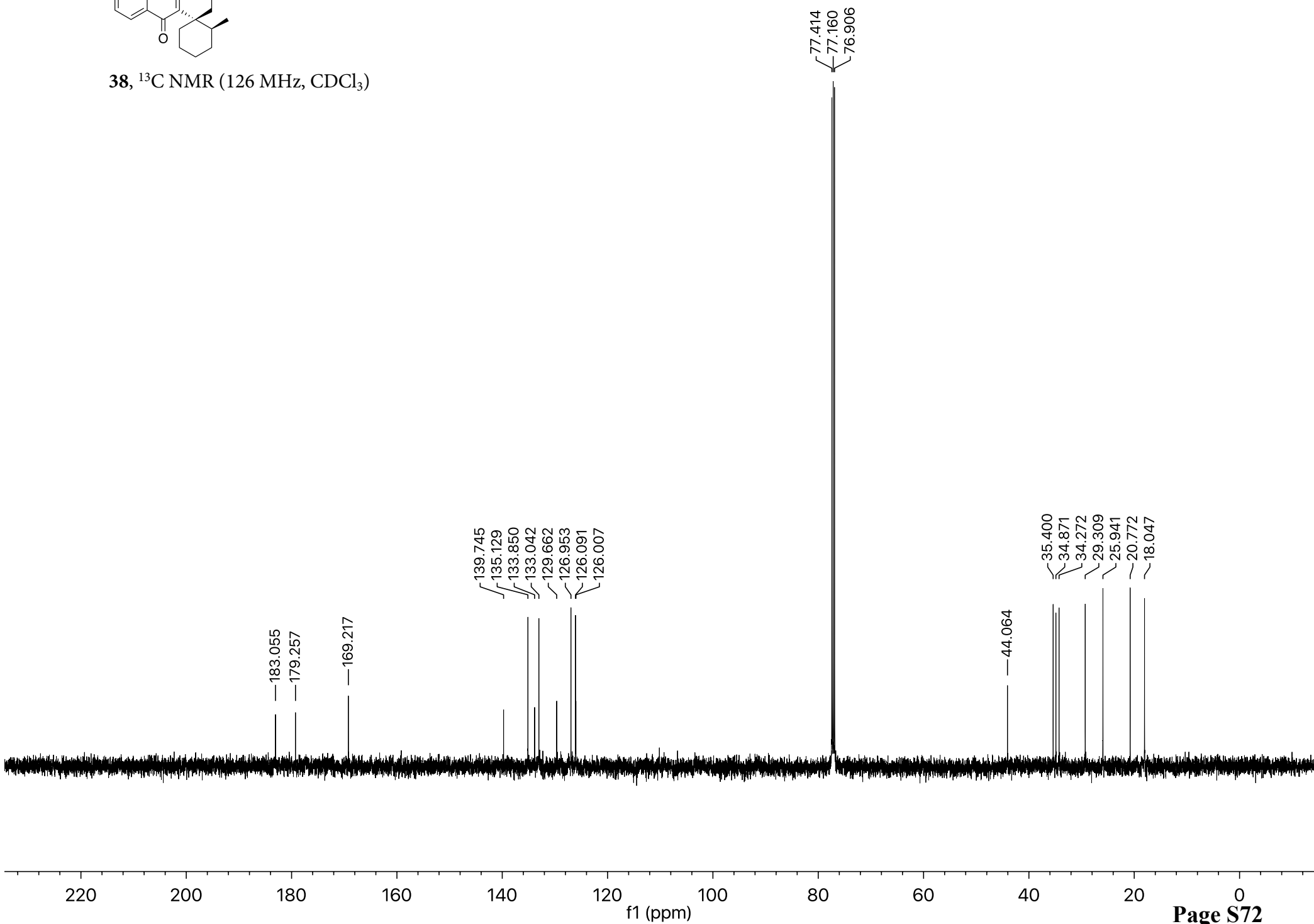


38, ¹H NMR (500 MHz, CDCl₃)

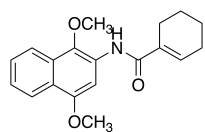




38, ^{13}C NMR (126 MHz, CDCl_3)



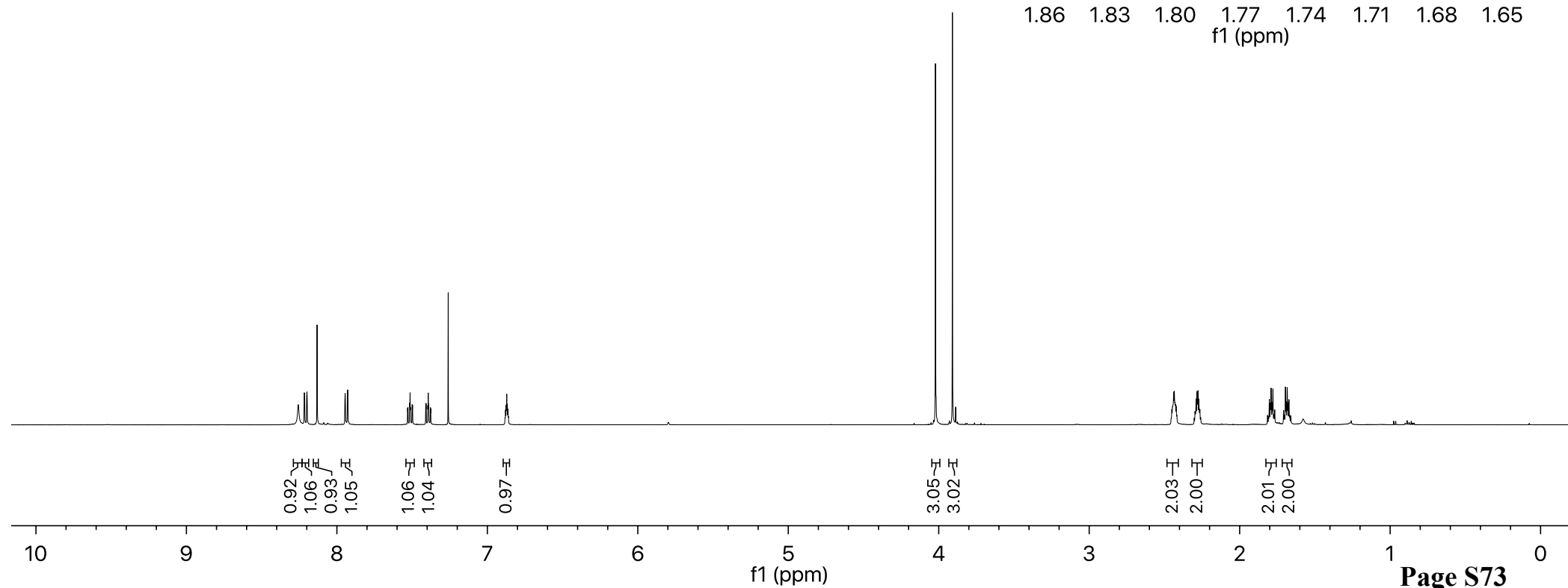
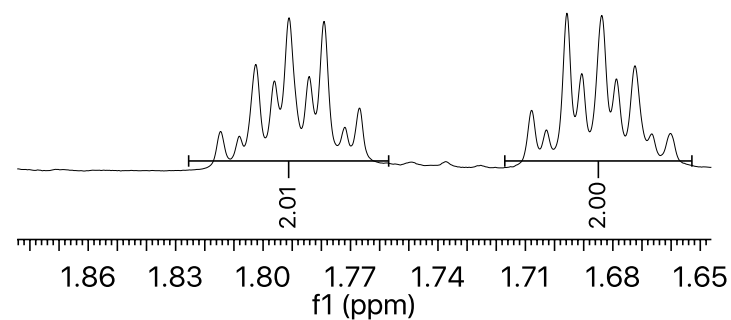
8.257
8.216
8.199
8.132
7.945
7.928
7.530
7.528
7.516
7.514
7.511
7.499
7.497
7.409
7.407
7.396
7.393
7.390
7.379
7.376
7.260
6.882
6.879
6.875
6.871
6.867
6.863
6.860

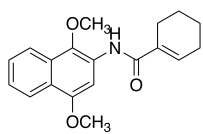


S11, ¹H NMR (500 MHz, CDCl₃)

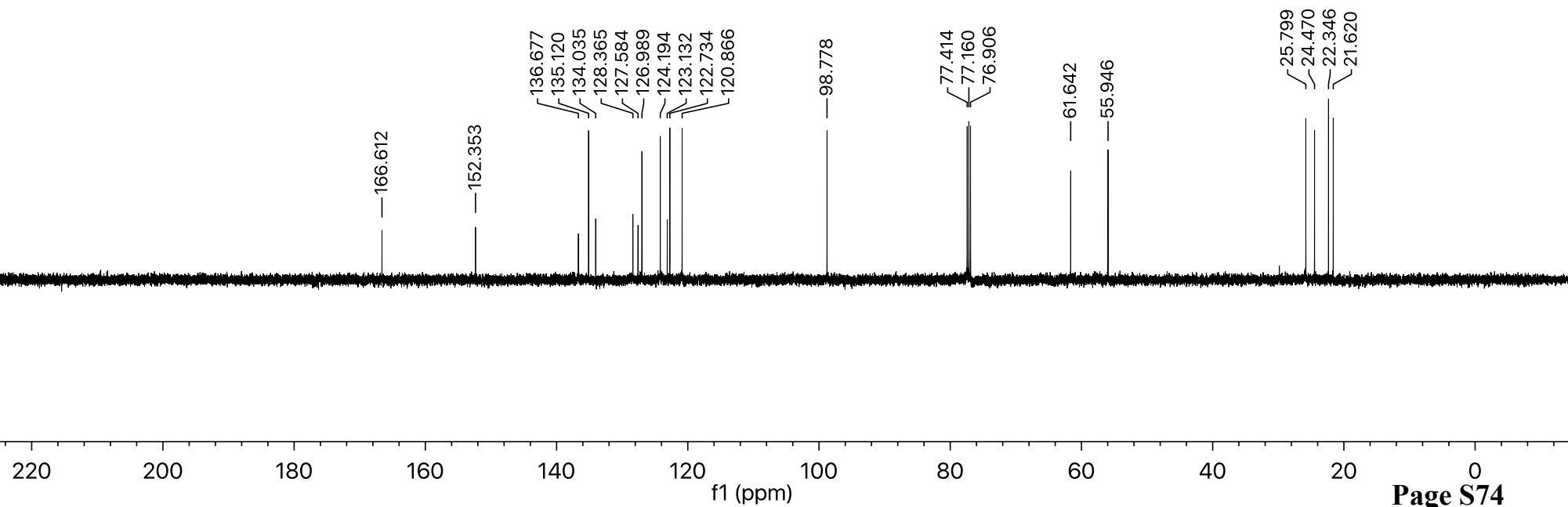
4.022
3.909
2.451
2.447
2.438
2.434
2.430
2.426
2.422
2.417
2.302
2.297
2.289
2.284
2.277
2.272
2.264
2.259

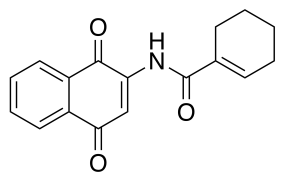
1.815
1.808
1.803
1.796
1.791
1.784
1.779
1.772
1.767
1.708
1.703
1.696
1.691
1.684
1.679
1.672
1.667
1.660





S11, ^{13}C NMR (126 MHz, CDCl_3)

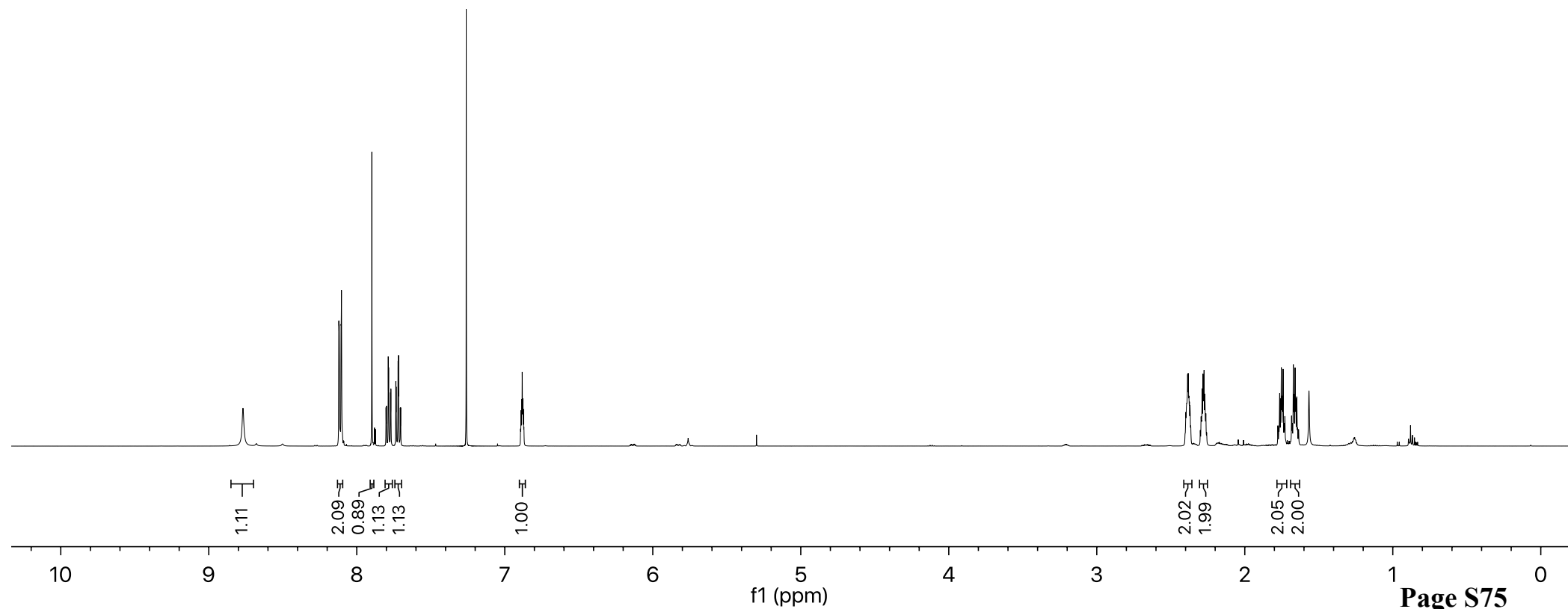


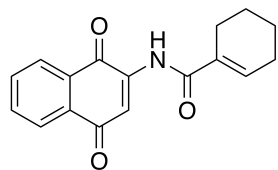


39, ^1H NMR (500 MHz, CDCl_3)

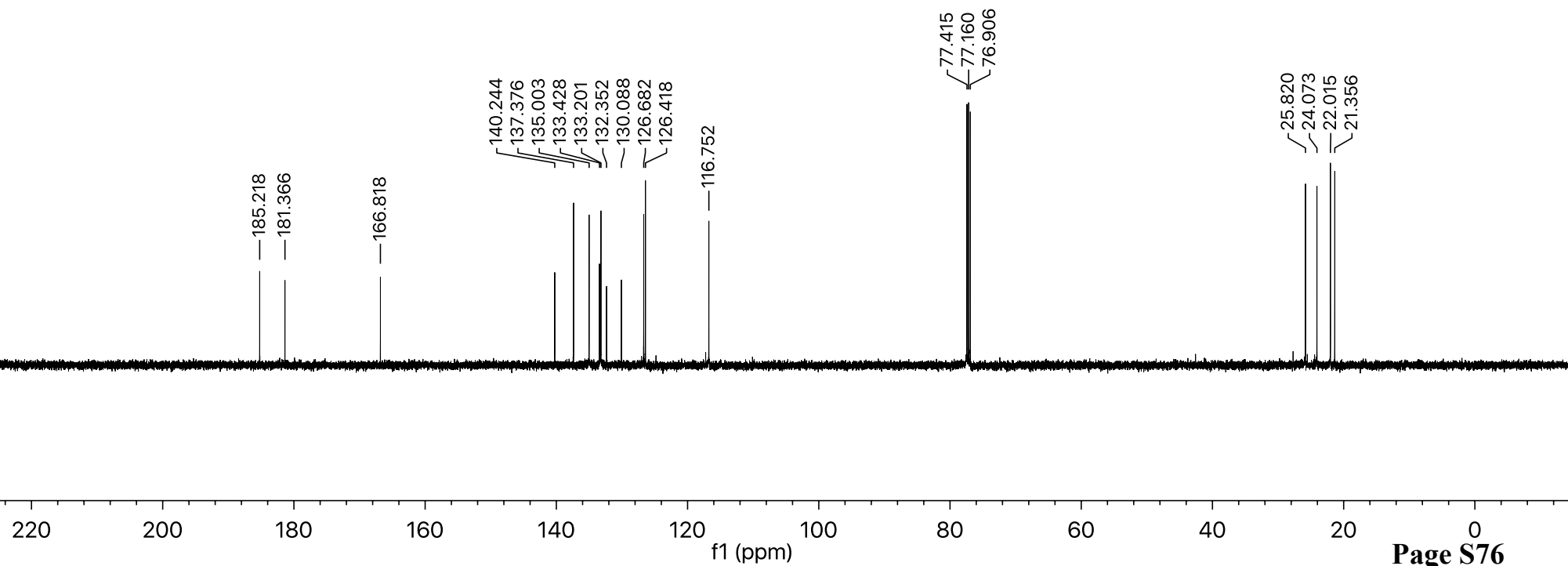
8.769
8.121
8.120
8.119
8.106
8.103
7.898
7.802
7.799
7.787
7.785
7.772
7.769
7.736
7.734
7.721
7.718
7.706
7.703
7.260
6.893
6.890
6.886
6.882
6.879
6.874
6.871

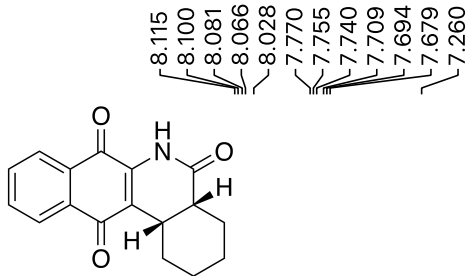
2.398
2.386
2.382
2.365
2.301
2.288
2.283
2.275
2.270
2.263
2.258
1.776
1.764
1.753
1.741
1.729
1.684
1.672
1.667
1.660
1.649
1.637
1.566





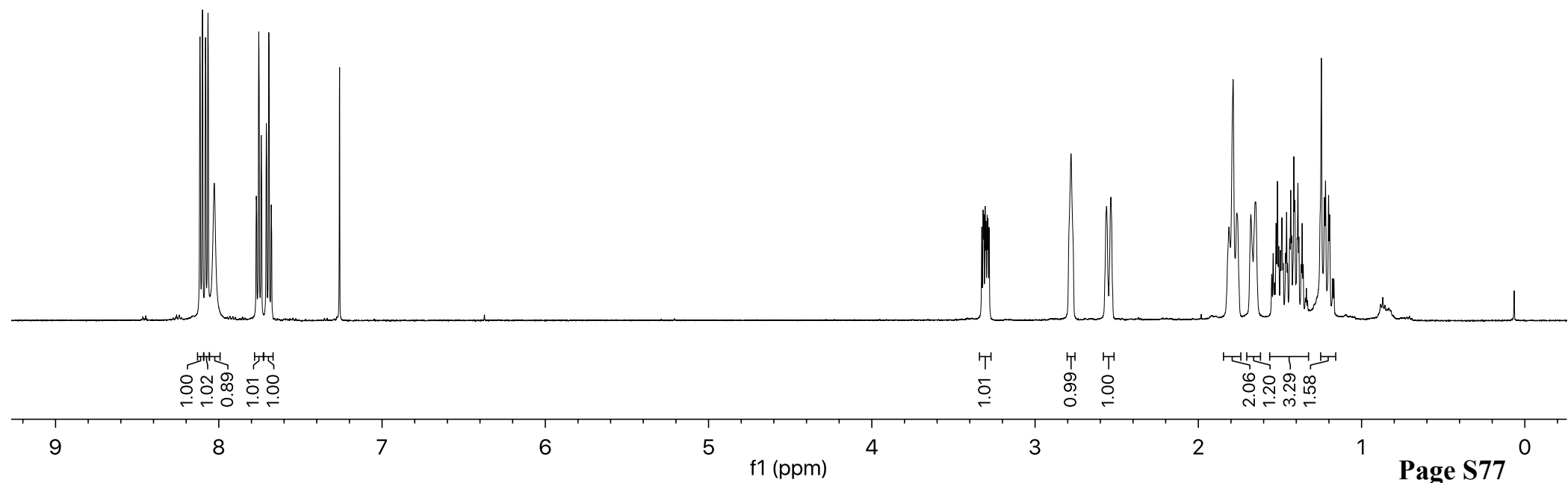
39, ^{13}C NMR (126 MHz, CDCl_3)

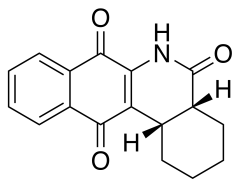




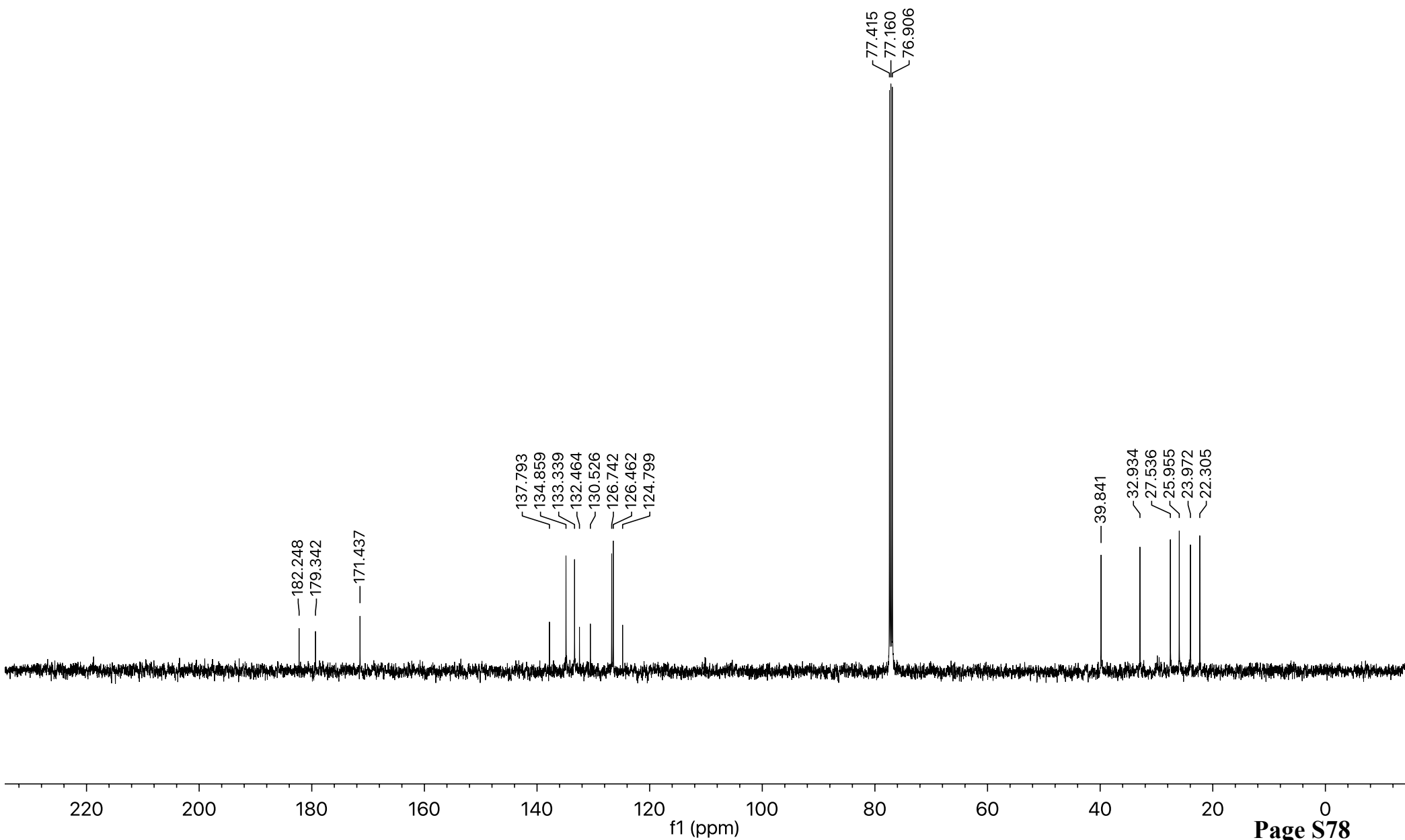
40, ^1H NMR (500 MHz, CDCl_3)

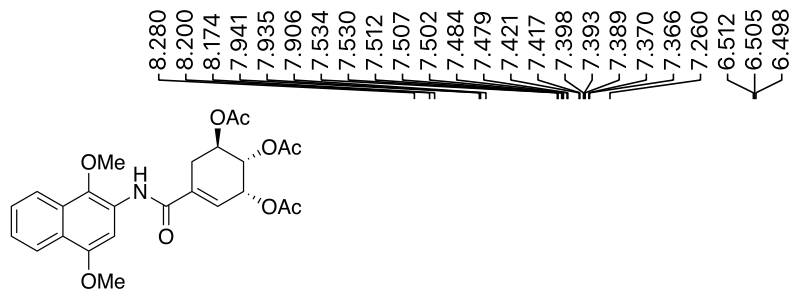
3.326
3.318
3.314
3.306
3.301
3.293
3.288
3.281
2.780
2.562
2.535
1.812
1.764
1.679
1.652
1.550
1.542
1.515
1.488
1.459
1.434
1.415
1.390
1.364
1.338
1.331
1.246
1.227
1.221
1.202
1.196
1.177
1.170



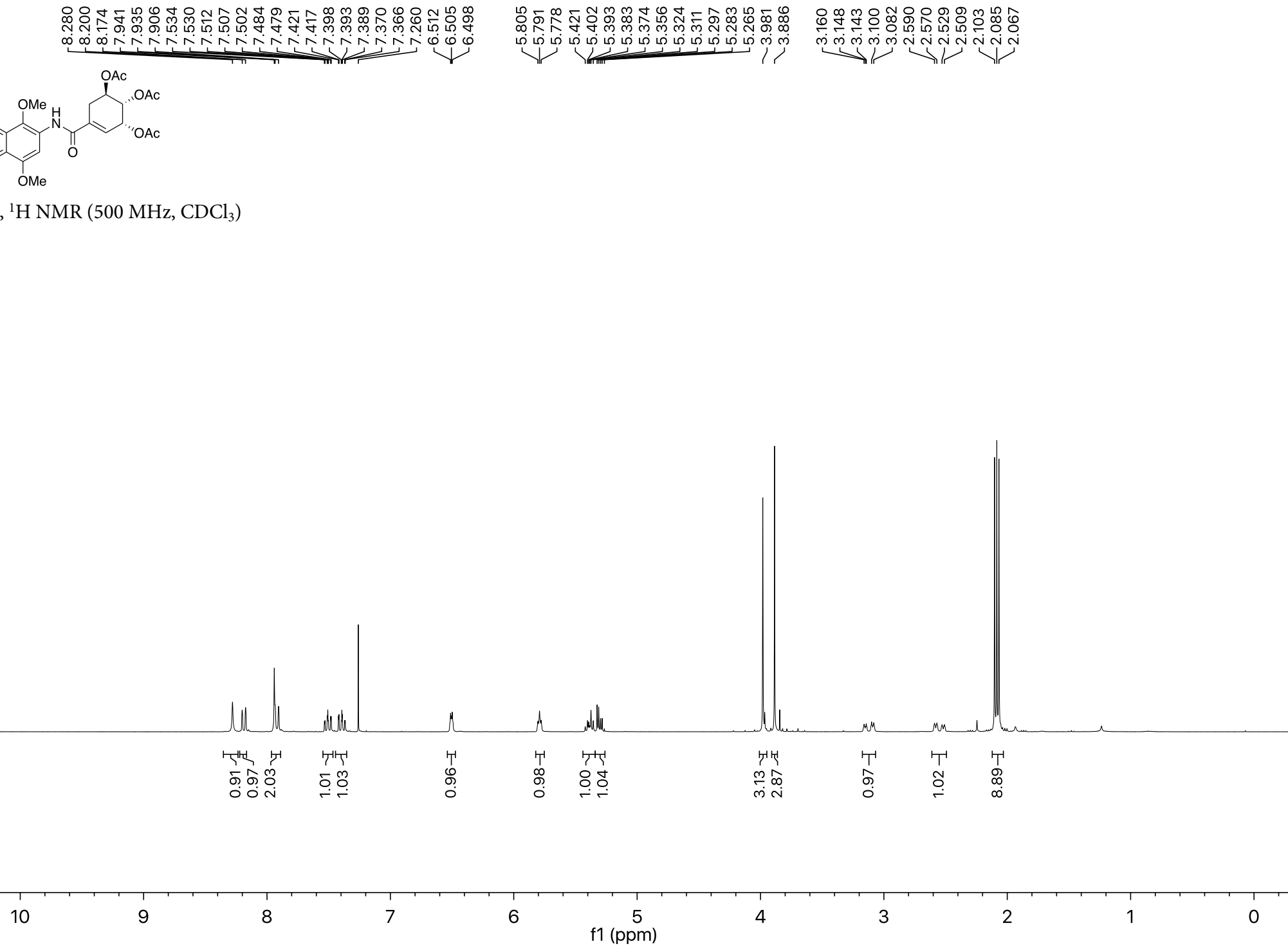


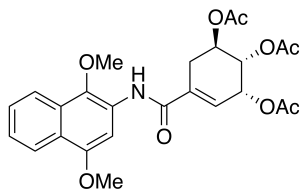
40, ^{13}C NMR (126 MHz, CDCl_3)



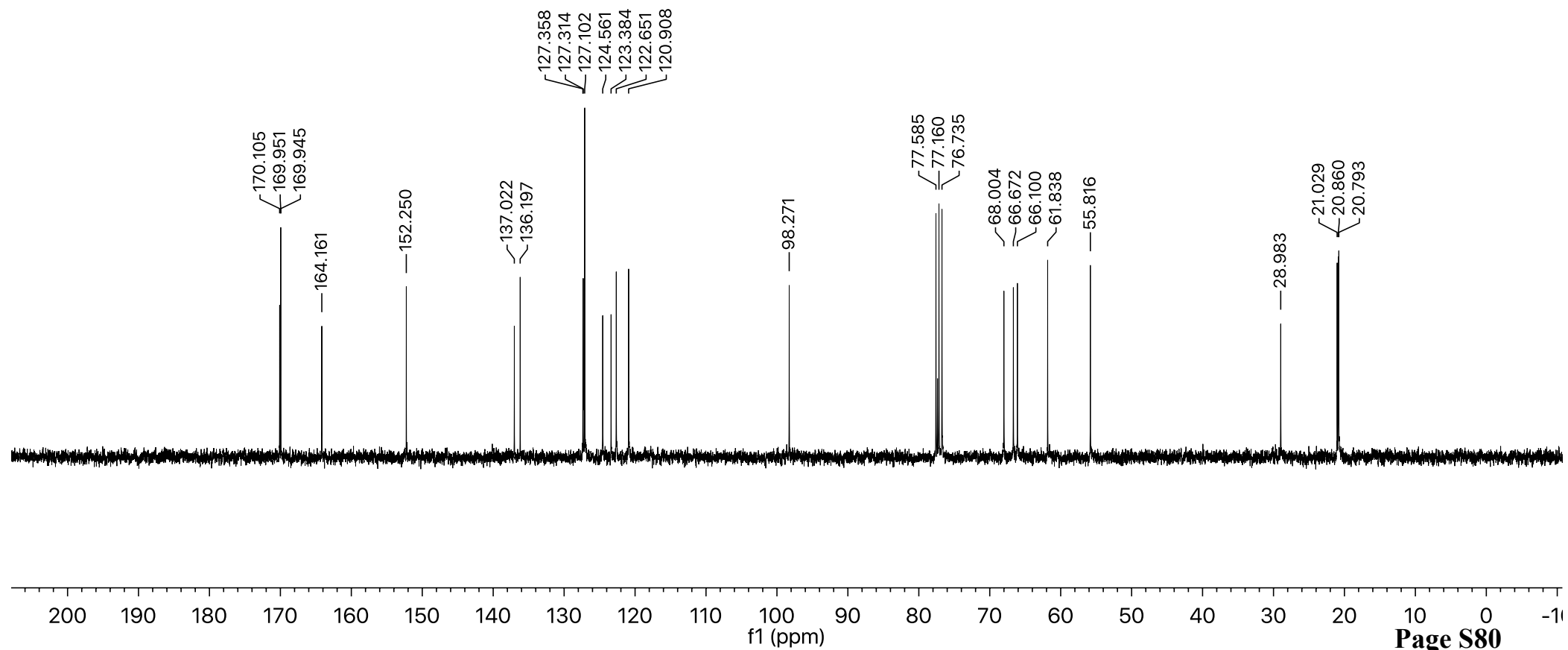


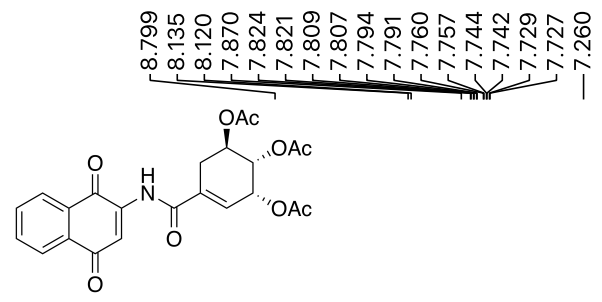
S12, ^1H NMR (500 MHz, CDCl_3)



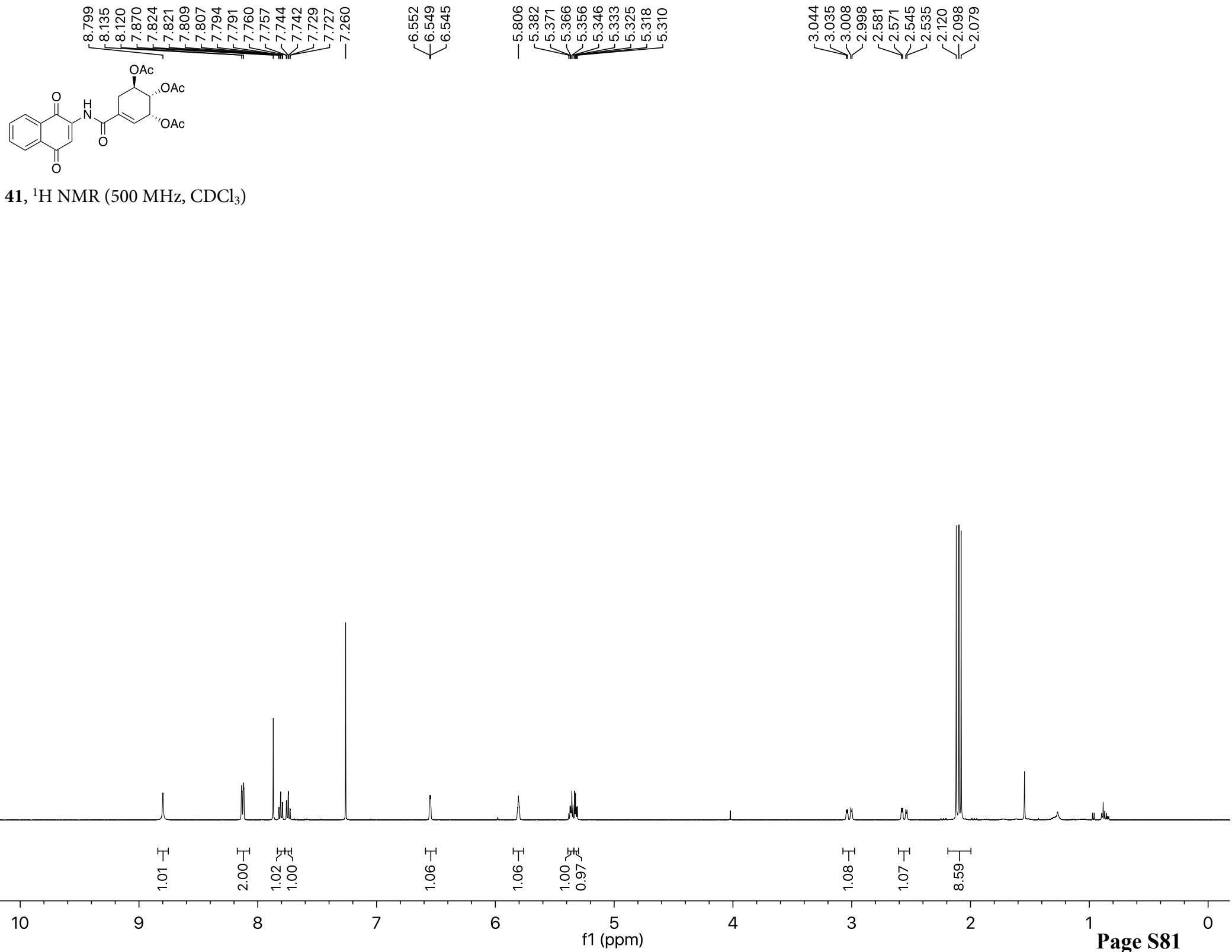


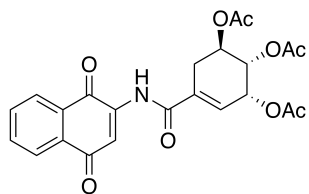
S12, ^{13}C NMR (126 MHz, CDCl_3)



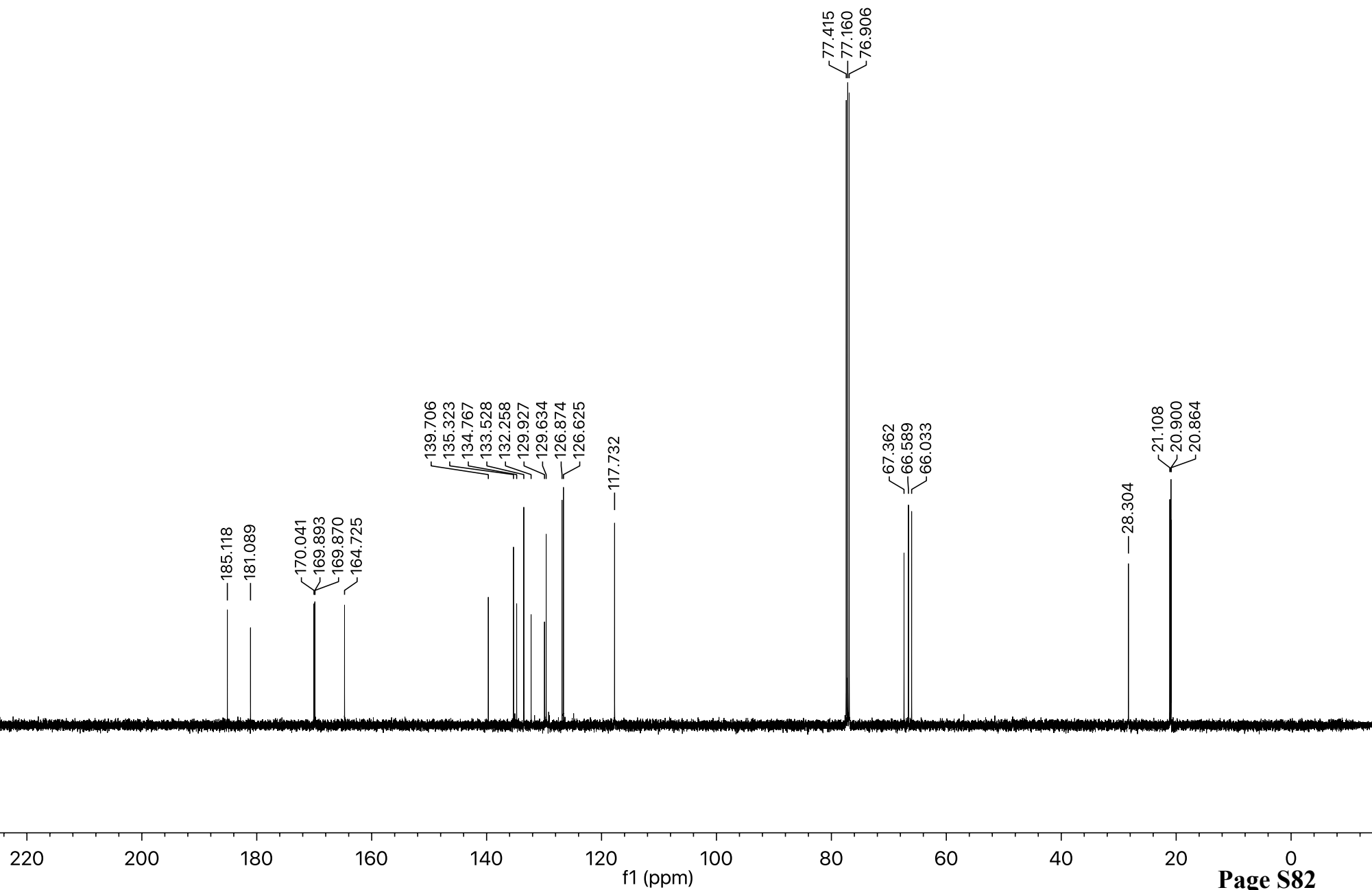


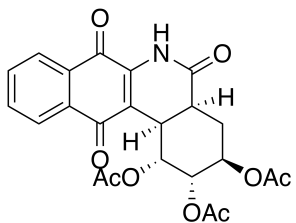
41, ¹H NMR (500 MHz, CDCl₃)





41, ^{13}C NMR (126 MHz, CDCl_3)





42, ^1H NMR (500 MHz, CDCl_3)

8.158
8.116
8.115
8.100
8.099
7.800
7.786
7.770
7.747
7.731
7.717
7.261
7.260

5.356
5.350
5.333
5.327
5.280
5.272
5.266
5.039
5.034
5.027
5.020

4.020
4.007
3.997
3.983

2.947
2.917
2.911
2.898
2.886
2.225
2.224
2.049
2.048
2.020
2.014
2.008
2.002
1.990
1.984
1.978
1.972
1.970
1.807
1.806

0.92
1.91

1.05
1.07

1.05
1.00
1.00

1.06

2.08

3.03
2.98
1.22
2.99

10

9

8

7

6

f1 (ppm)

5

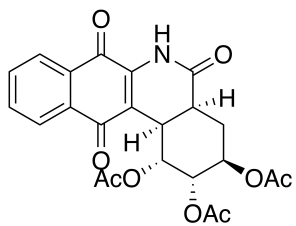
4

3

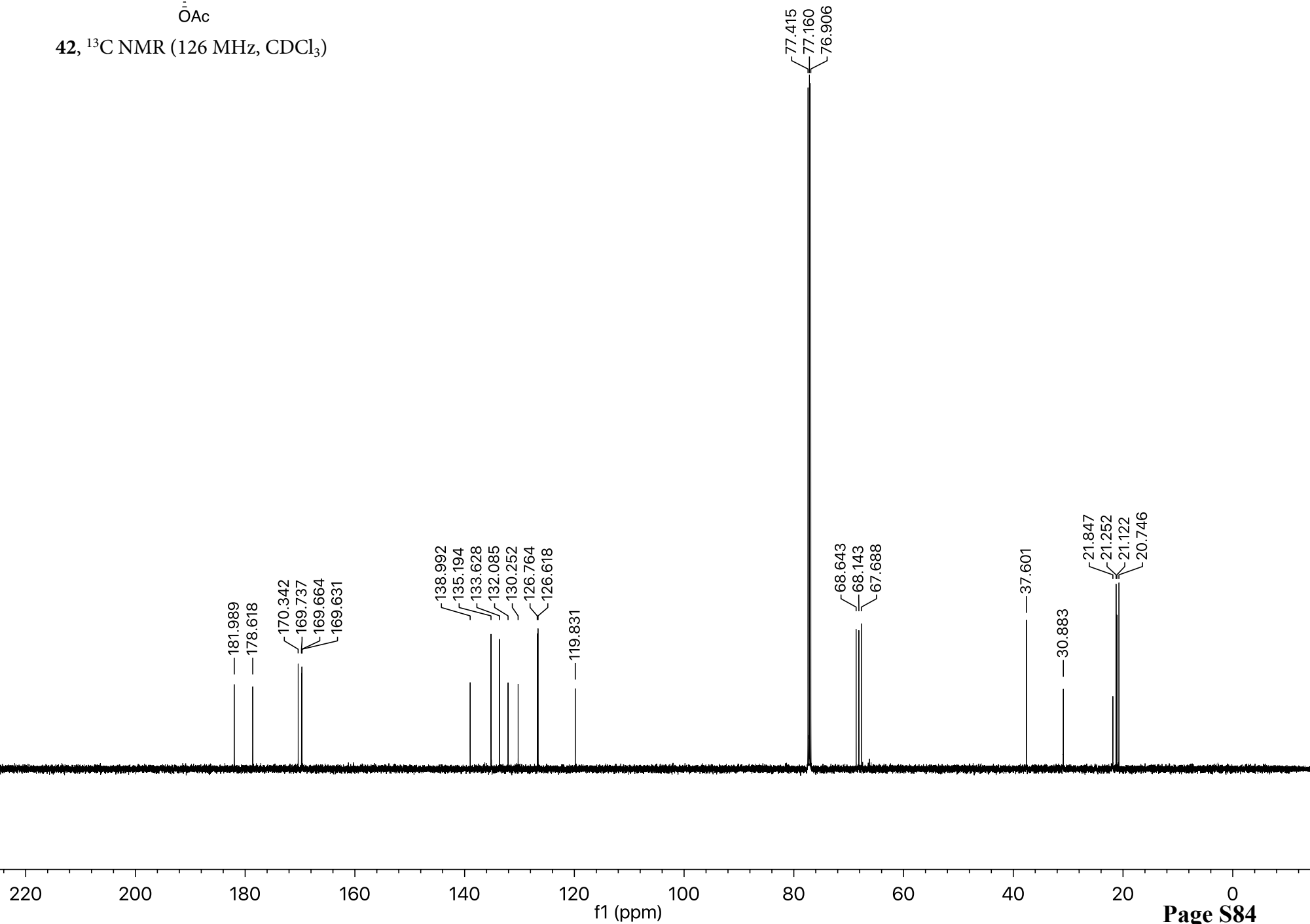
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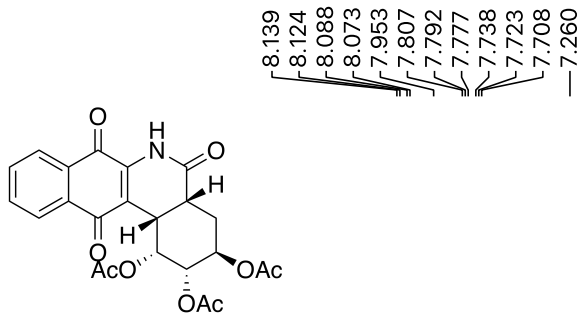
1

0



42, ^{13}C NMR (126 MHz, CDCl_3)



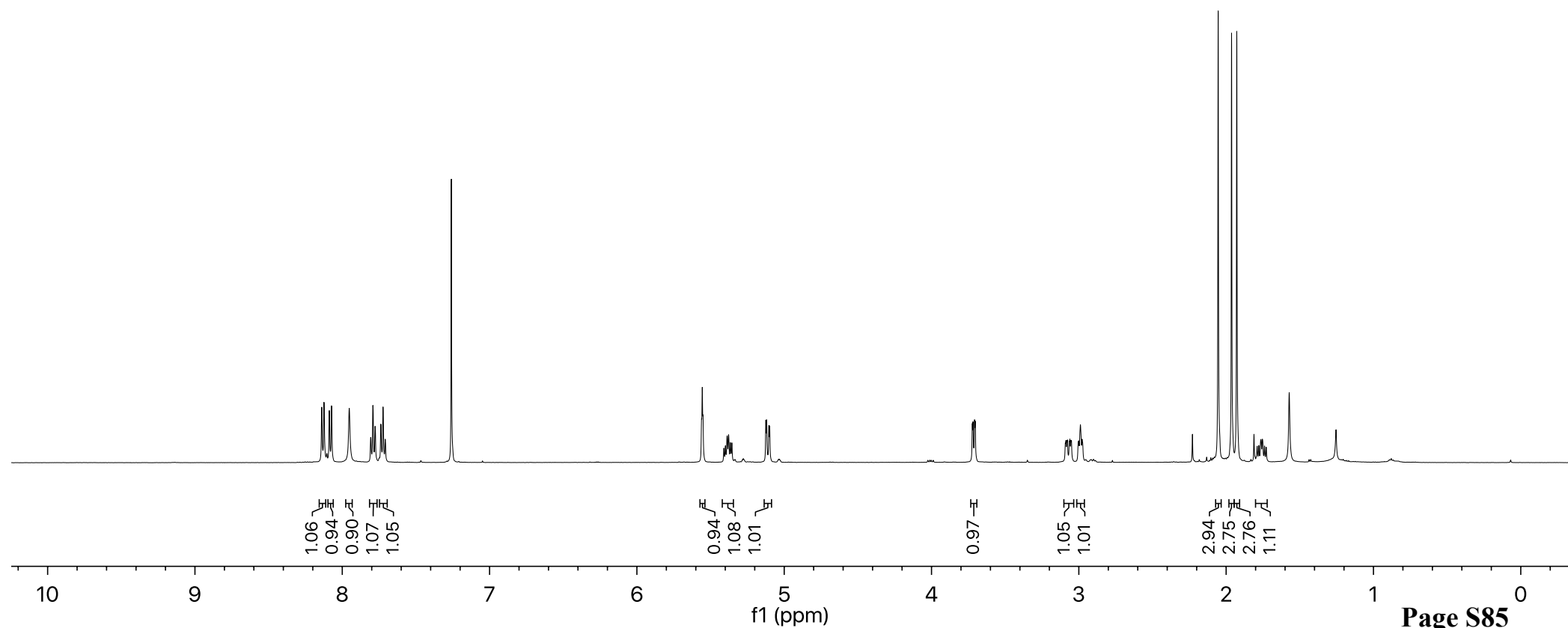


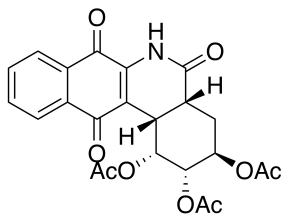
43, ^1H NMR (500 MHz, CDCl_3)

8.139
8.124
8.088
8.073
7.953
7.807
7.792
7.777
7.738
7.723
7.708
7.260

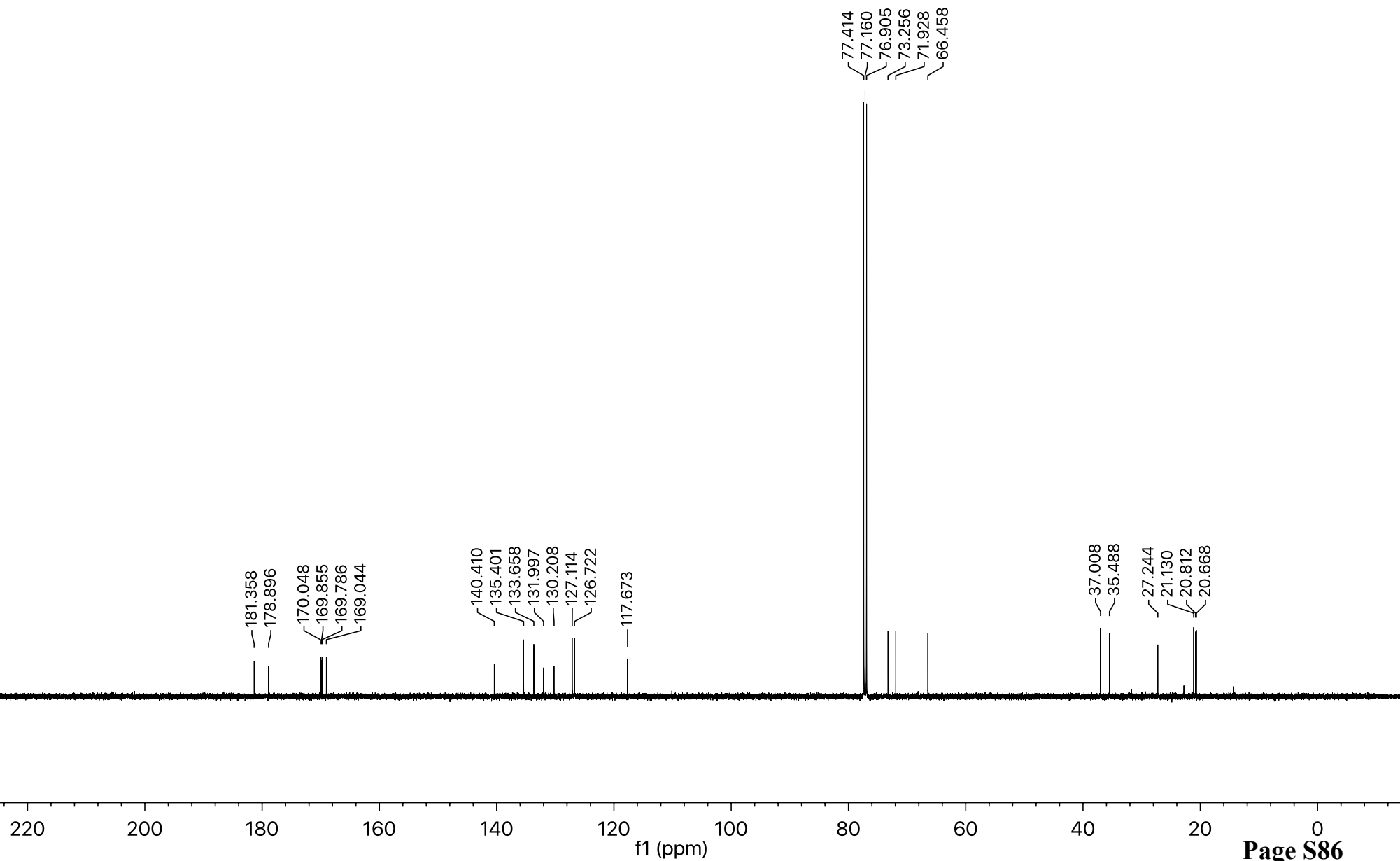
5.561
5.556
5.551
5.409
5.399
5.387
5.378
5.366
5.355
5.125
5.119
5.104
5.099

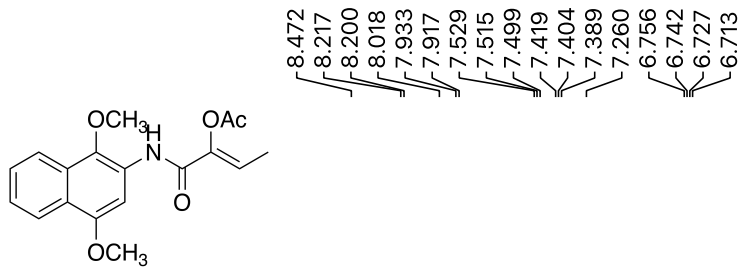
3.723
3.718
3.708
3.703
3.091
3.088
3.081
3.077
3.064
3.061
3.054
3.050
3.001
2.989
2.978
2.054
1.963
1.928
1.790
1.778
1.764
1.754
1.739
1.728



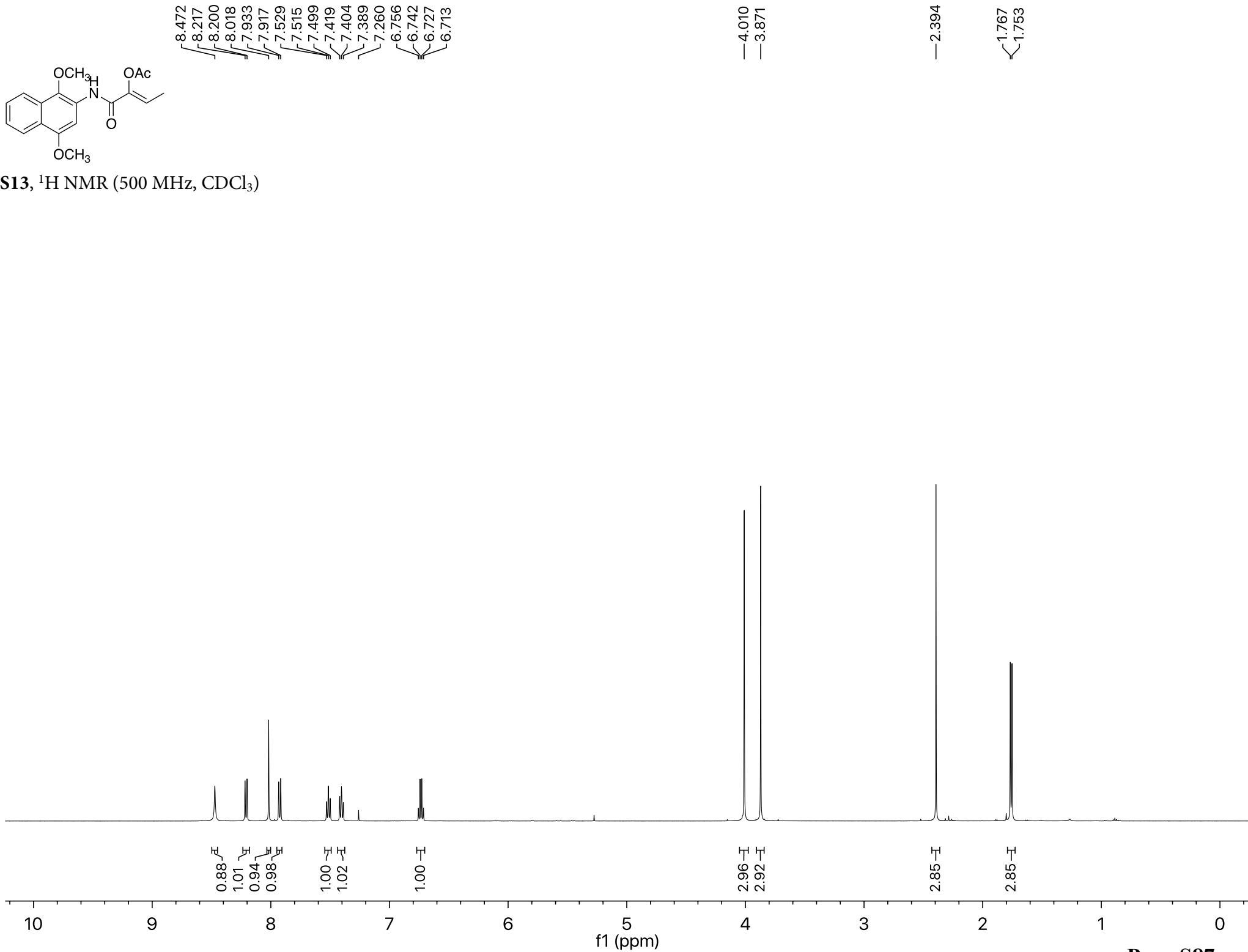


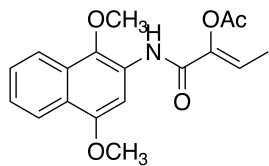
43, ^{13}C NMR (126 MHz, CDCl_3)



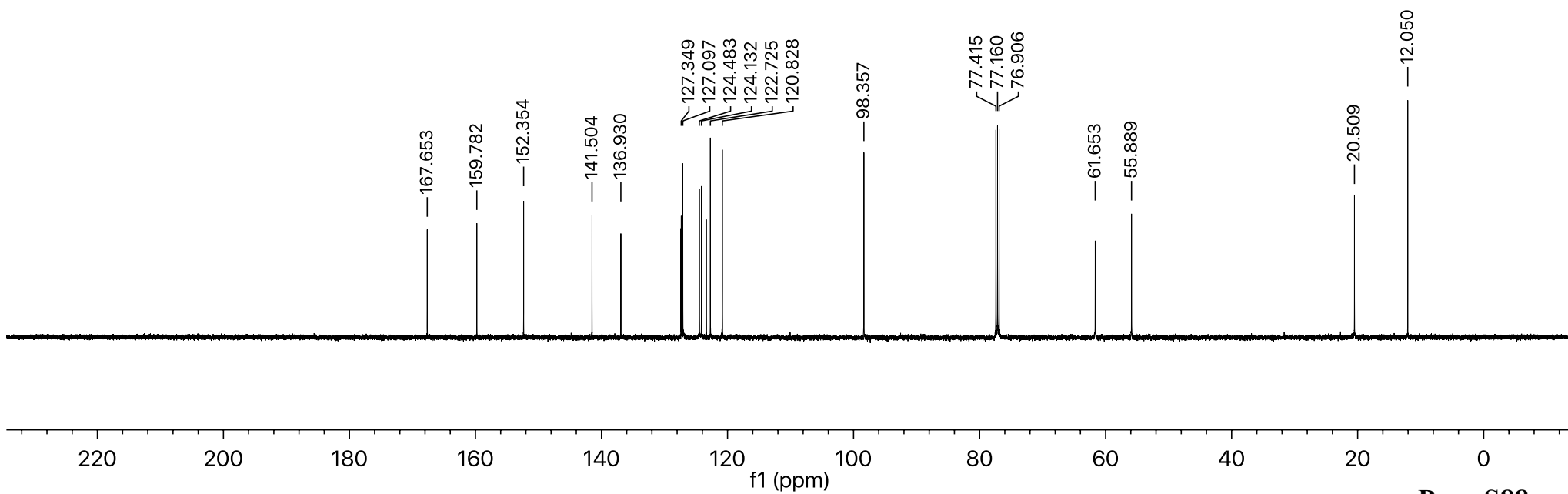
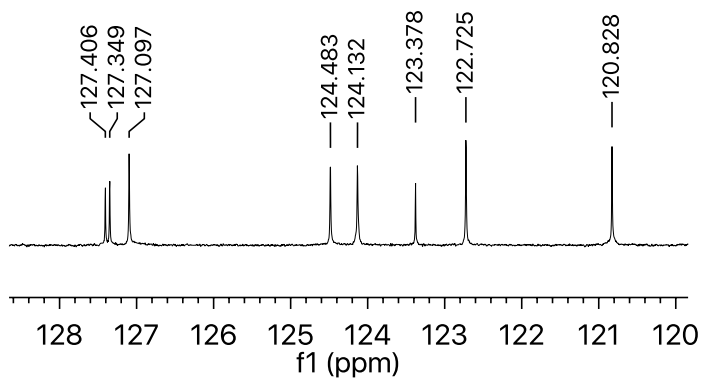


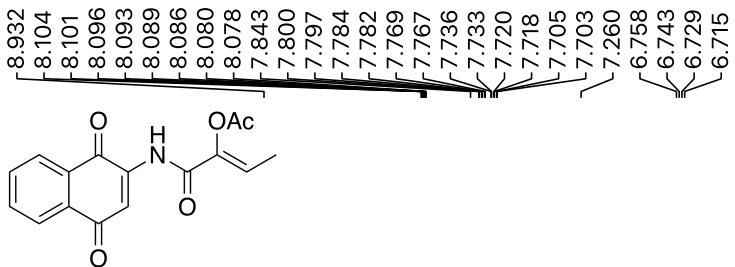
S13, ^1H NMR (500 MHz, CDCl_3)



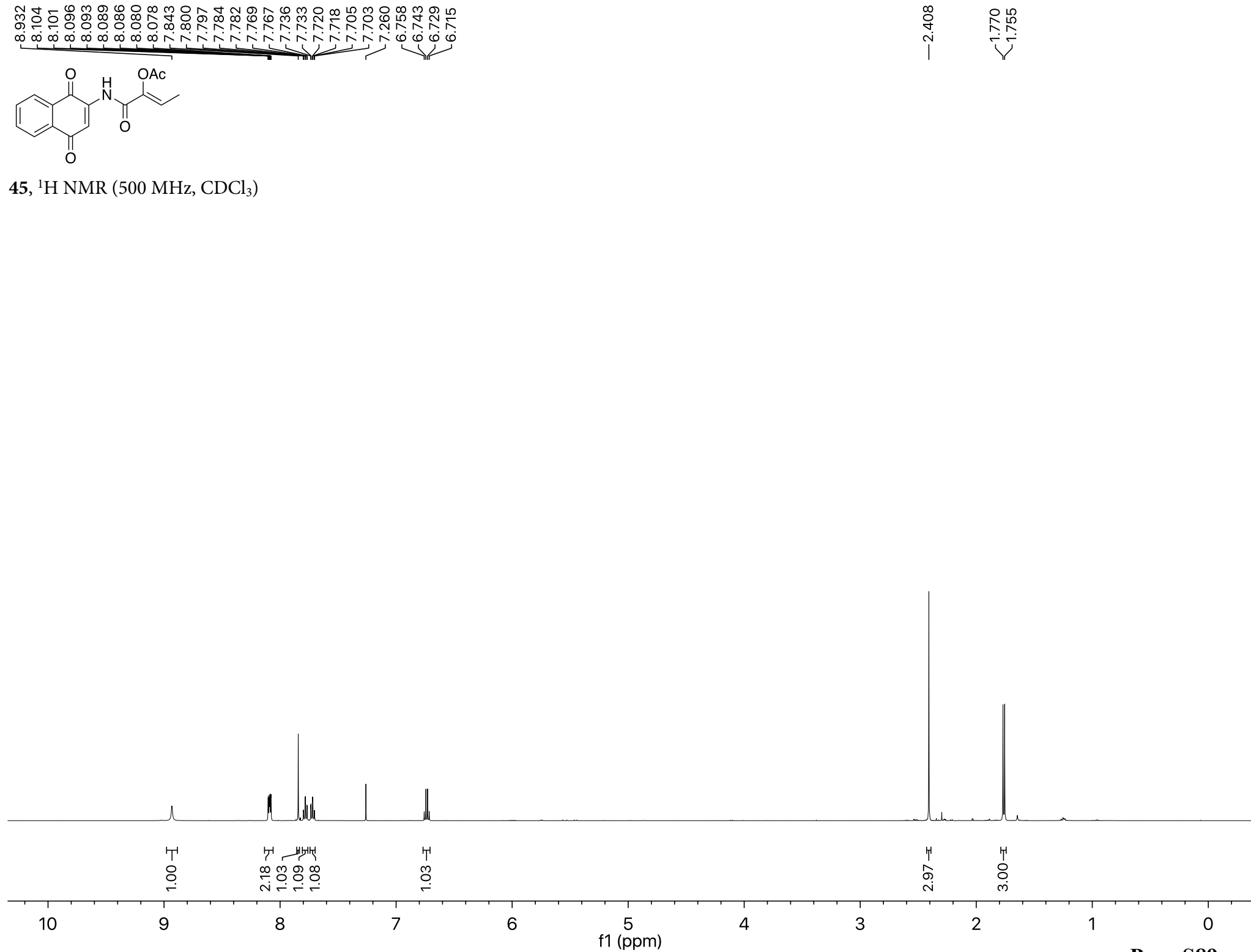


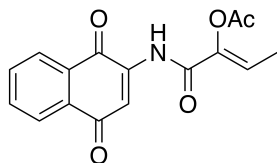
S13, ^{13}C NMR (126 MHz, CDCl_3)



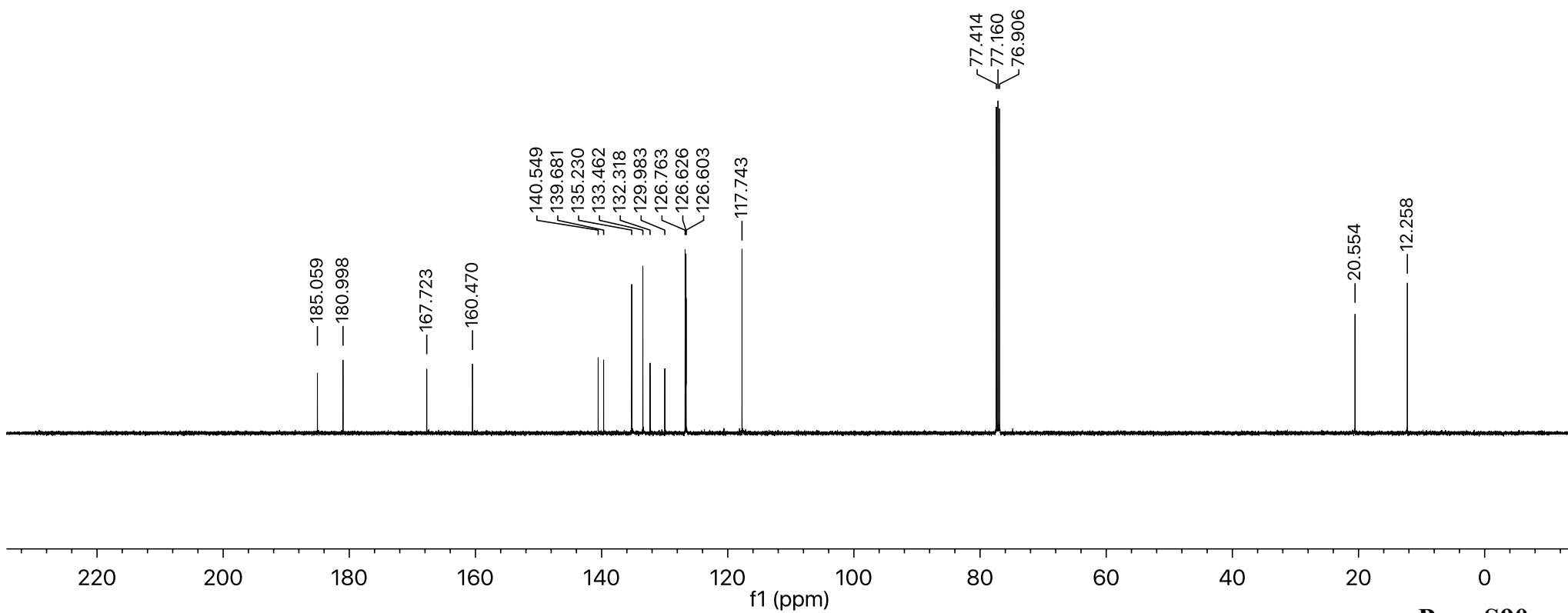


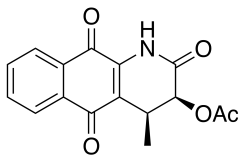
45, ^1H NMR (500 MHz, CDCl_3)



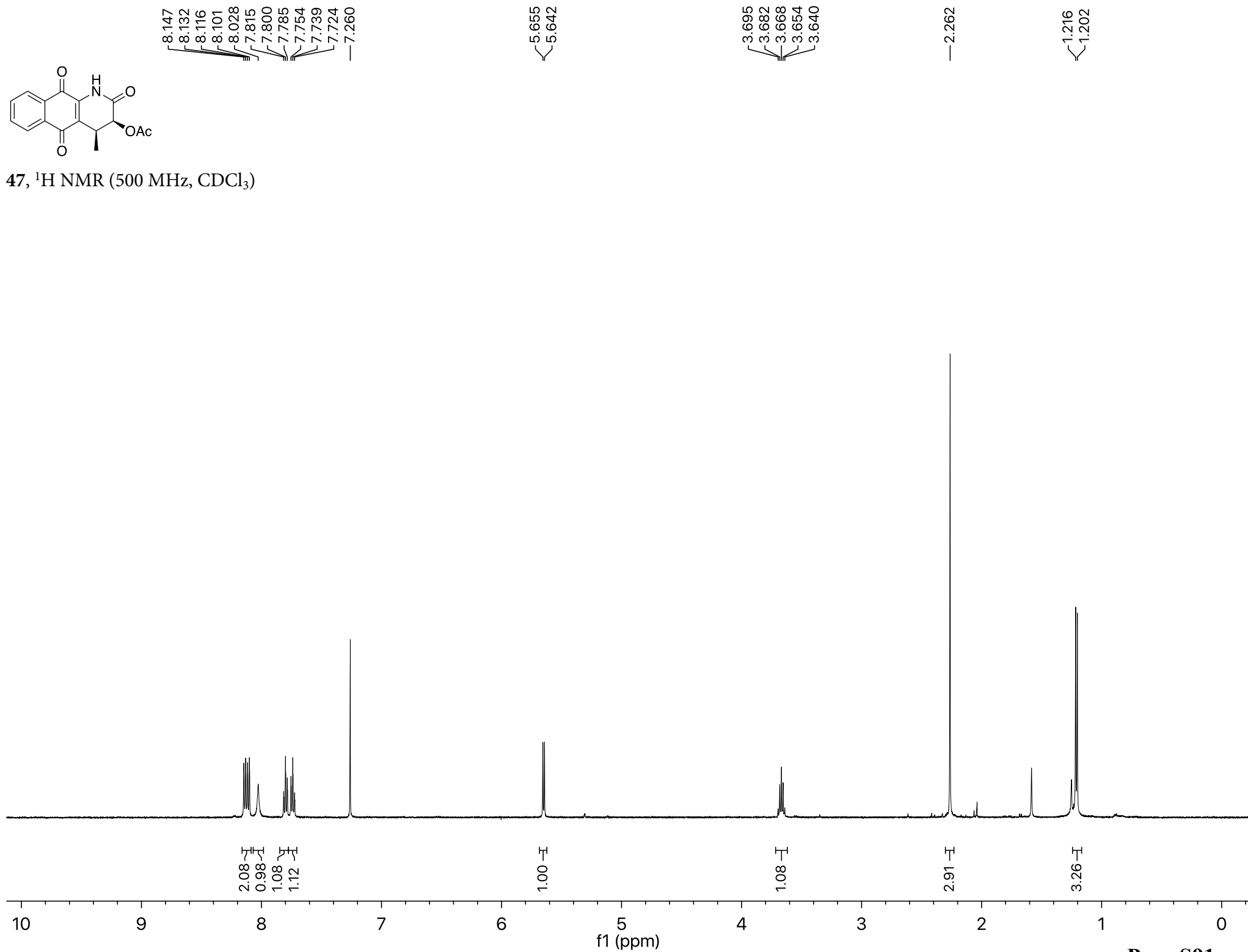


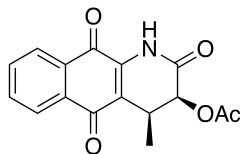
45, ^{13}C NMR (126 MHz, CDCl_3)



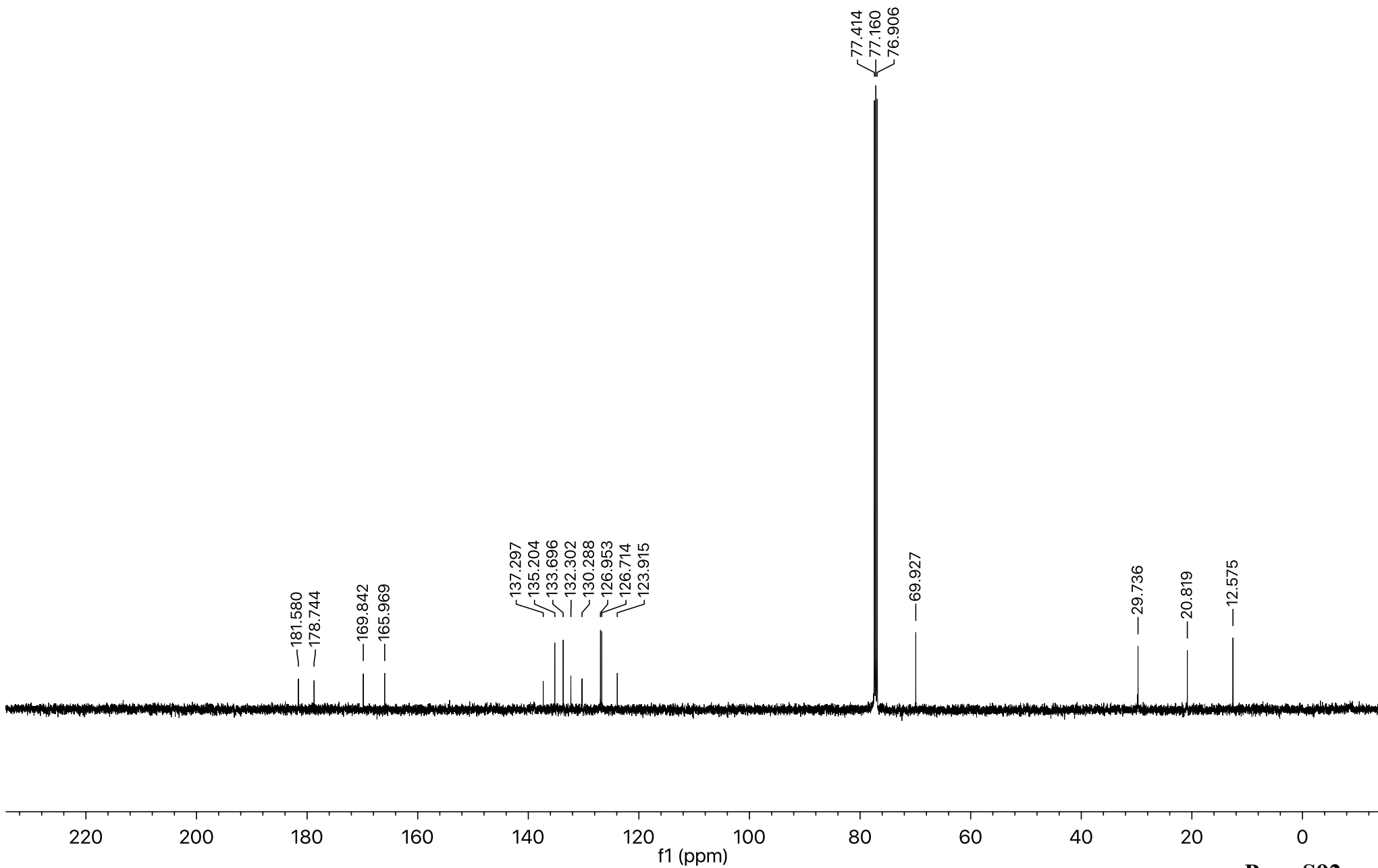


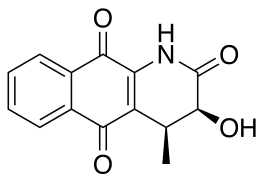
47, ^1H NMR (500 MHz, CDCl_3)



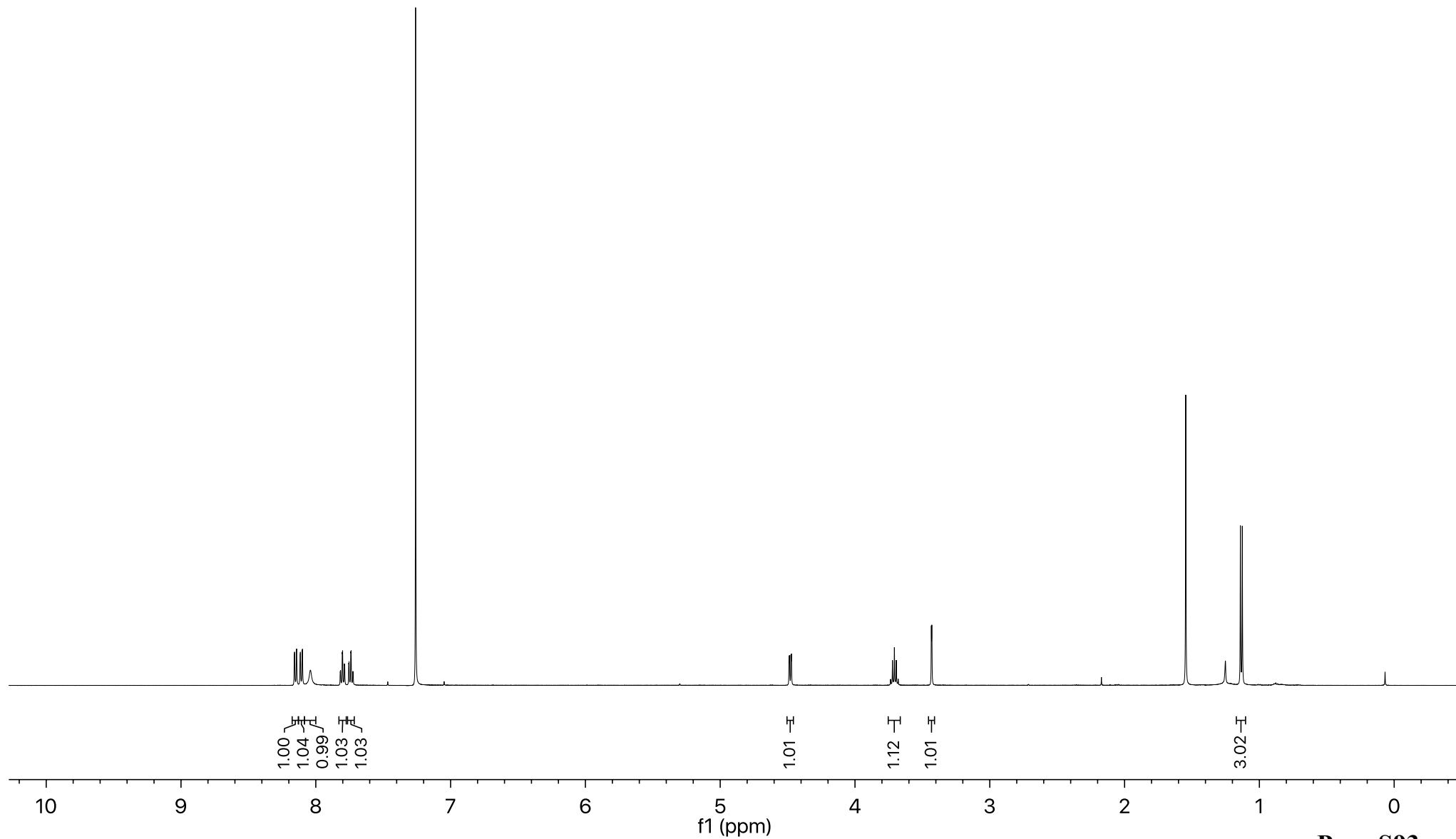


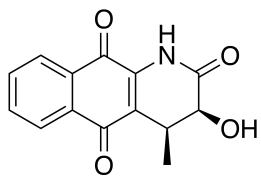
47, ^{13}C NMR (126 MHz, CDCl_3)



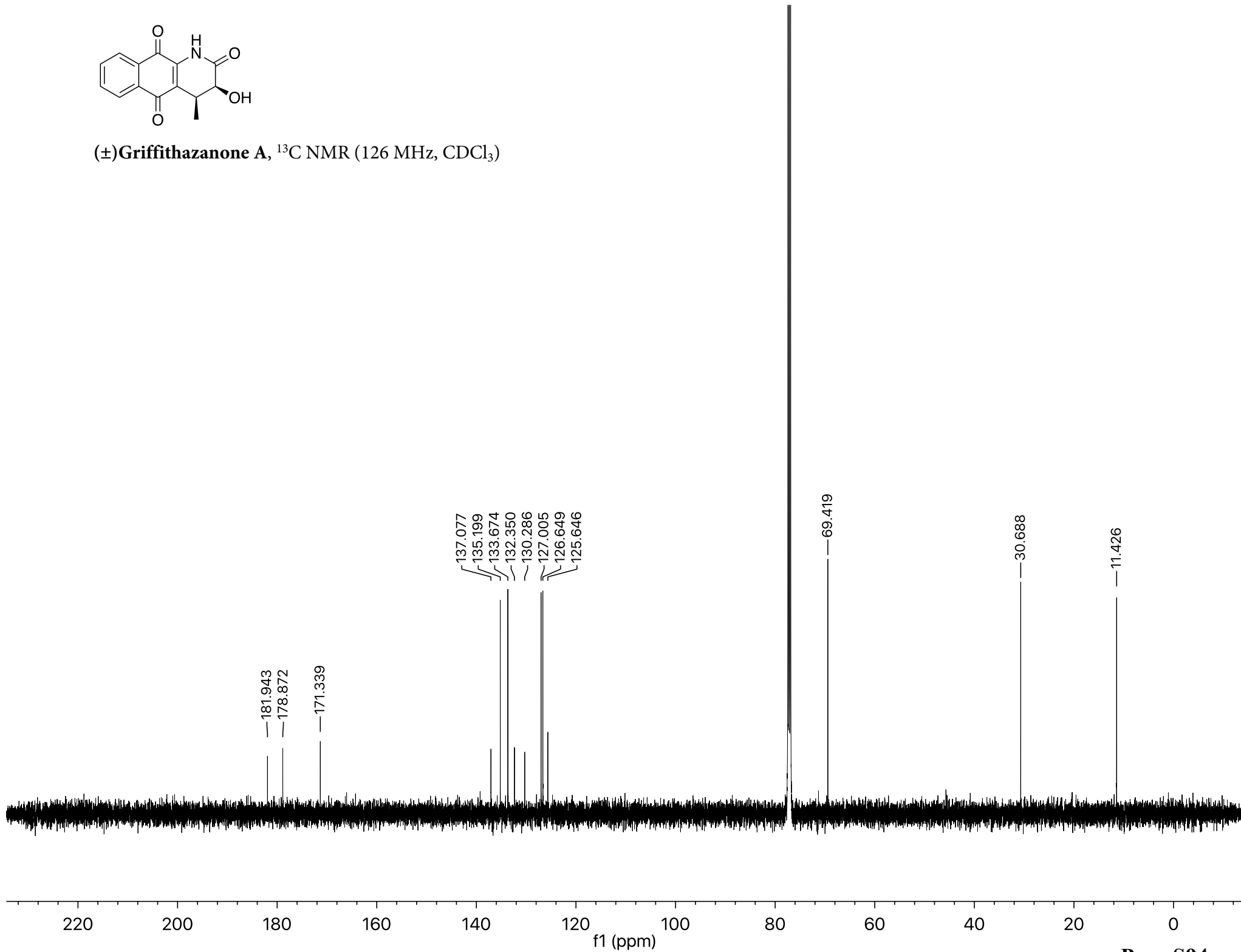


(±)Griffithazanone A, ¹H NMR (500 MHz, CDCl₃)





(±)Griffithazanone A, ^{13}C NMR (126 MHz, CDCl_3)



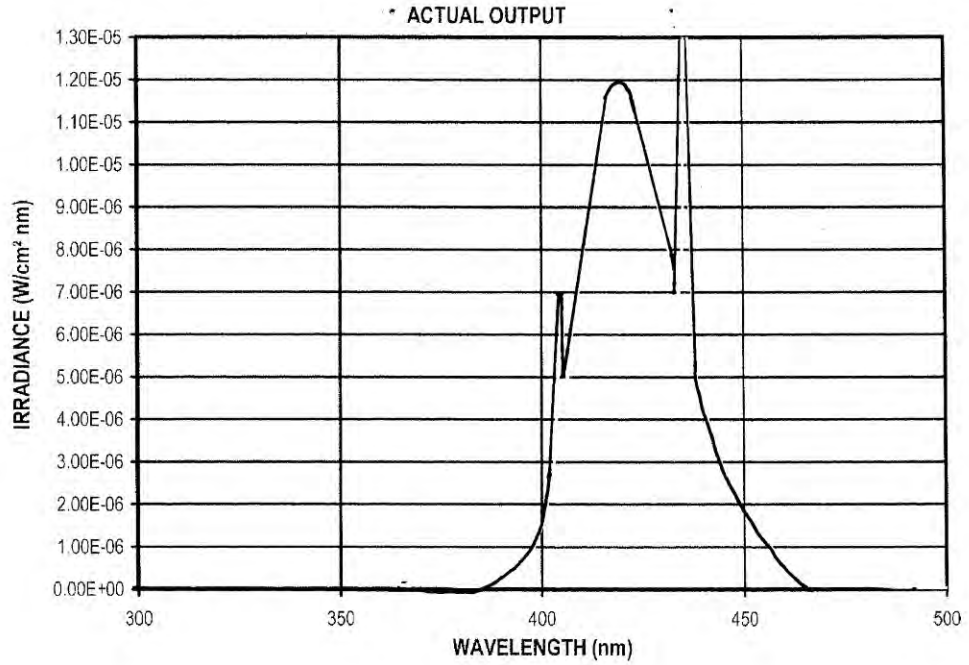


Fig S1: spectral distribution and intensity of the light source RPR-4190A.

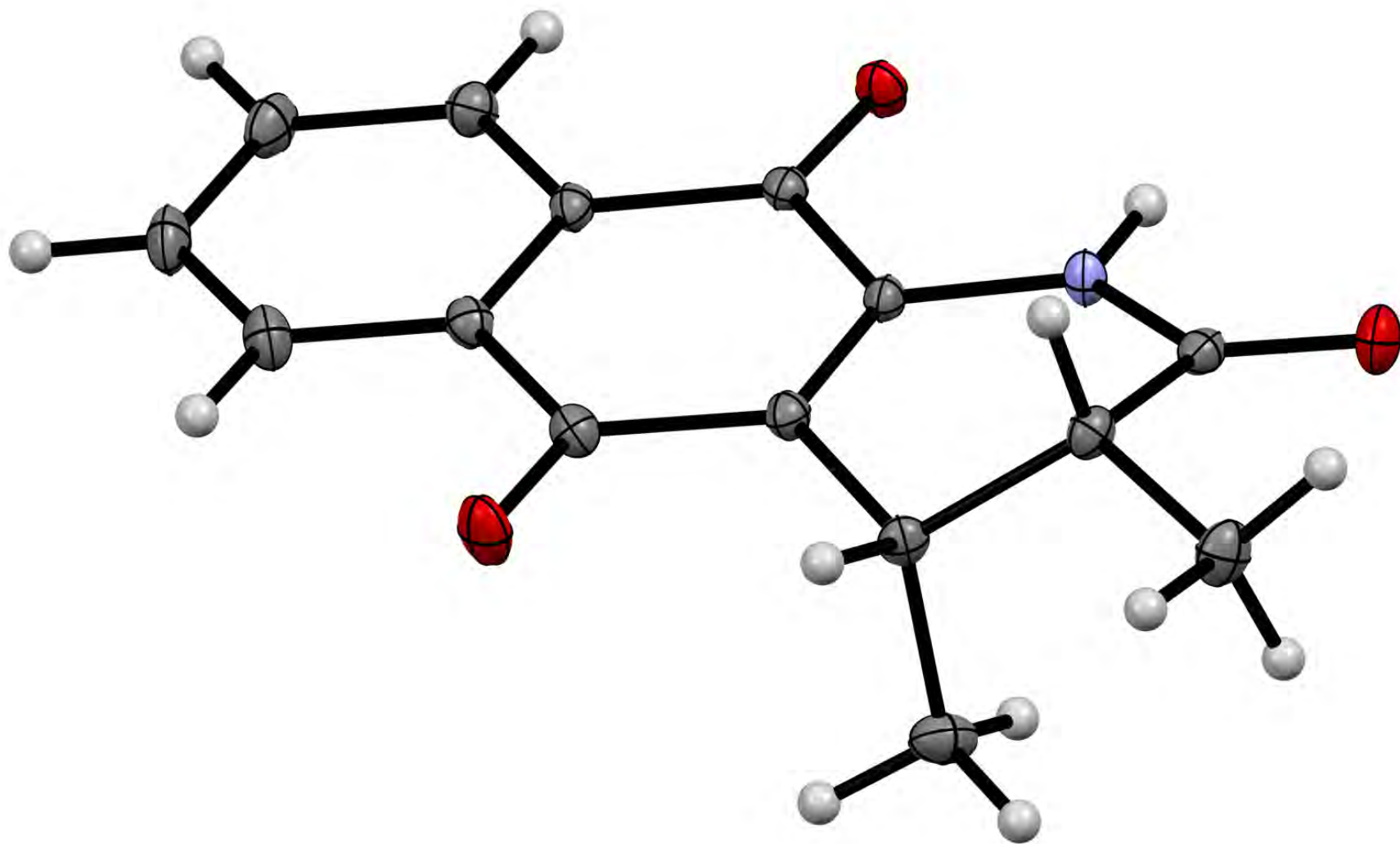


Figure S2: Crystal structure of **14**. The ellipsoid contour percent probability of 50% was used for the caption of this image.

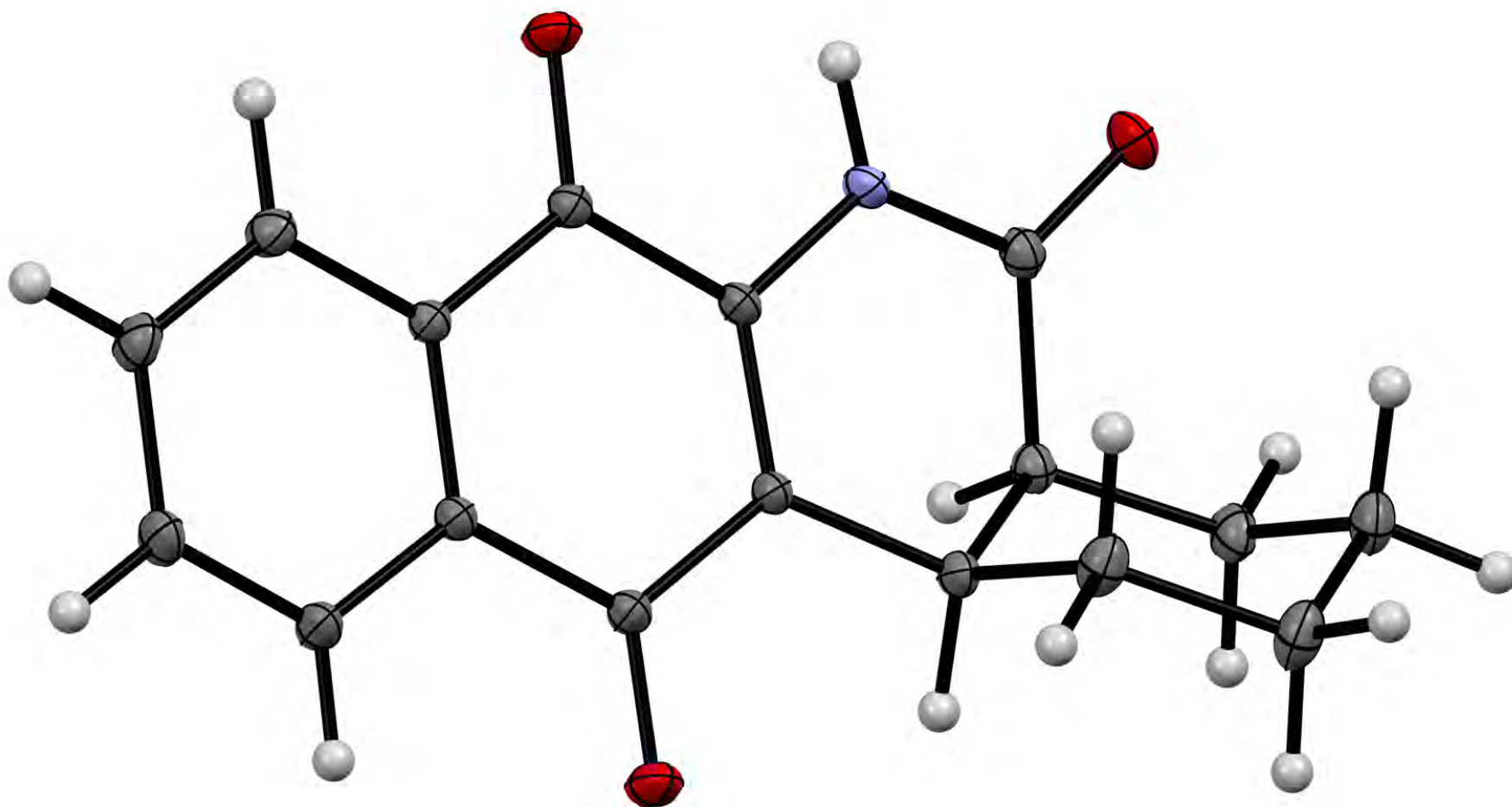


Figure S3: Crystal structure of **40**. The ellipsoid contour percent probability of 50% was used for the caption of this image.

XRD sample preparation of compound 14. Compound **14** (5 mg) was dissolved in MeOH (2 mL) in a 5 mL scintillation vial. On the top of the resulting solution was carefully added hexanes (2 mL) so that there were 2 layers. The uncapped scintillation vial was placed in the center of a larger chamber filled with hexanes (about 10 mL). The outer chamber was capped. 6 months later all of the solvents had escaped and the resulting crystal was subjected to X-ray diffraction.

XRD sample preparation of compound 40. Compound **40** (5 mg) was dissolved in CHCl₃ (~ 0.2 mL) in a 5 mL scintillation vial. On the top of the resulting solution was carefully added hexanes (2 mL) so that there were 2 layers. The uncapped scintillation vial was placed in the center of a larger chamber filled with hexanes (about 10 mL). The outer chamber was capped. 6 months later all of the solvents had escaped and the resulting crystal was subjected to X-ray diffraction.

Crystal Structure Determination. Single-crystal X-ray diffraction data was collected on a Nonius Kappa diffractometer equipped with Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$) and a BRUKER APEXII CCD. The APEX31 software suite was used to manage data collection, reduction (SAINT V8.38A¹), absorption correction by the Multi-scan method (SADABS²), structure determination via direct methods (SHLEX³) and model refinement (SHELXL⁴). All data were collected at 103(2) K. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms, with the exception of those bound to nitrogen, were refined with their positions ideally constrained to their carriers. Hydrogen bonded with nitrogen were refined isotropically with restrained bond lengths. The crystal structures were deposited to the CCDC with deposition numbers 1967034 (**14**) and 1967030 (**40**).

References:

1. APEX3. Ver. 2017.3-0. Bruker AXS Inc., Madison, Wisconsin, USA, 2017.
2. L. Krause, R. Herbst-Irmer, G. M. Sheldrick and D. Stalke, *J. Appl. Cryst.* 2015, 48, 3-10.
3. G. M. Sheldrick, *Acta Cryst. A* 2015, 71, 3-8.5.
4. G. M. Sheldrick, *Acta Cryst. C* 2015, 71, 3-8.6.

Table S1: Summary of XRD Parameter of compound **14** and **40**

Compound number	14	40
CCDC	1967034	1967030
Moiety Formula	C ₁₅ H ₁₃ NO ₃	C ₁₇ H ₁₅ NO ₃
UNIT Formula	C ₁₅ H ₁₃ NO ₃	C ₁₇ H ₁₅ NO ₃
UNIT Mw	255.26	281.30
Space group	P 1 21/c 1	P 1 21/n 1
Unit cell		
a (Å)	5.1388(3)	10.6981(13)
b (Å)	19.7529(12)	5.3875(6)
c (Å)	11.7294(8)	22.901(3)
α (°)	90.000	90.000
β (°)	100.519(2)	100.847(3)
γ (°)	90.000	90.000
Volume (Å ³)	1170.60(13)	1296.3(3)
Z	4	4
Reflections		
Total	15099	15921
Unique	3425	5152
Resolution (Å)	0.71	0.64
Completeness (%)	99.8	99.7
R _{int} (%)	3.54	2.06
R _{sig} (%)	3.02	2.48
Structure Refinement		
R1 (%)	4.15	4.16
wR2 (%)	11.3	12.1
GOF	1.031	1.031