Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Synthesis and Characterization of various 5'-Dye-labeled Ribonucleosides for Sensor Application

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^{1}H NMR and ^{13}C NMR spectra of compounds **3-8, 18-24, 26, 27, 29, 30.**

Figure S1. Illustration of competition test between a red coloured nucleoside immobilized on a dipstick and urinary uridine homologue.

Figure S2. Absorbance spectra for 5'-tagged-nucleosides: **4, 5, 6, 8, 19, 21, 23, 27** and **30**

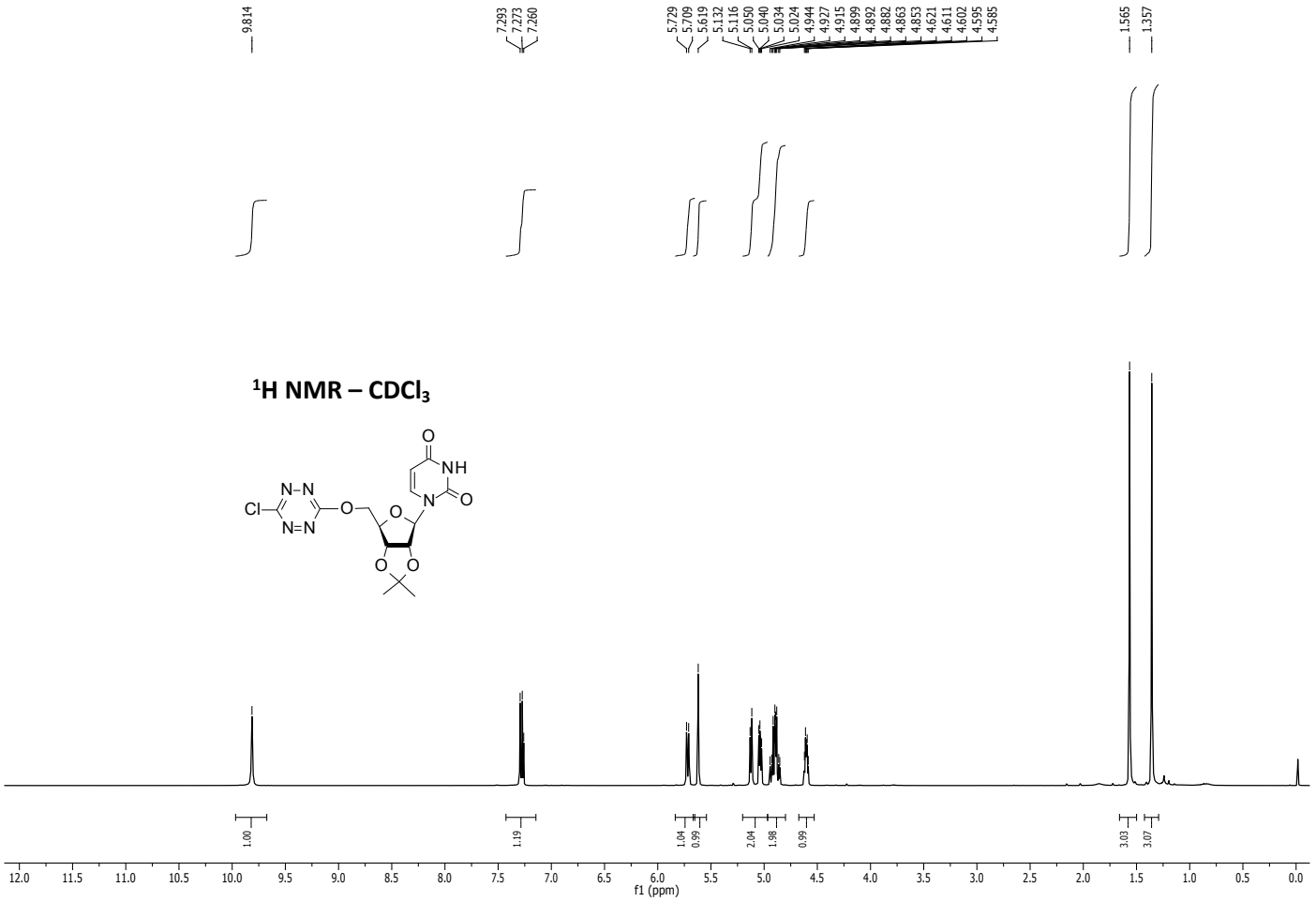
Figure S3. Fluorescence spectra for 5'-tagged-nucleosides: **4**, **8**, **19**, **21**, **30**

Figure S4. Picture of the solutions prepared for the UV measurements of **20** at various dilutions

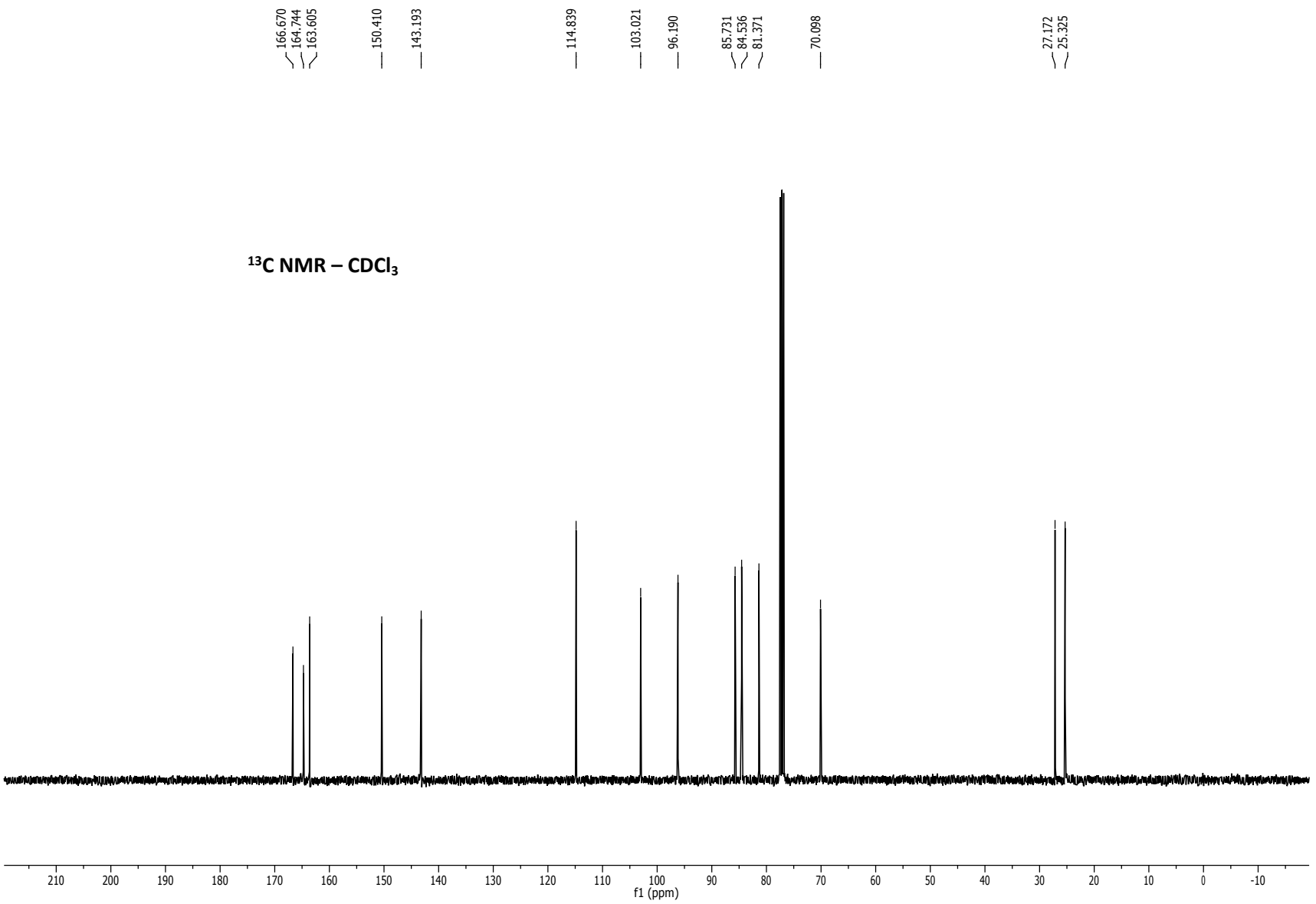
Figure S5. Picture of the solutions prepared for the UV measurements of **22** at various dilutions

Figure S6. Picture of the solutions prepared for the UV measurements of **26** at various dilutions

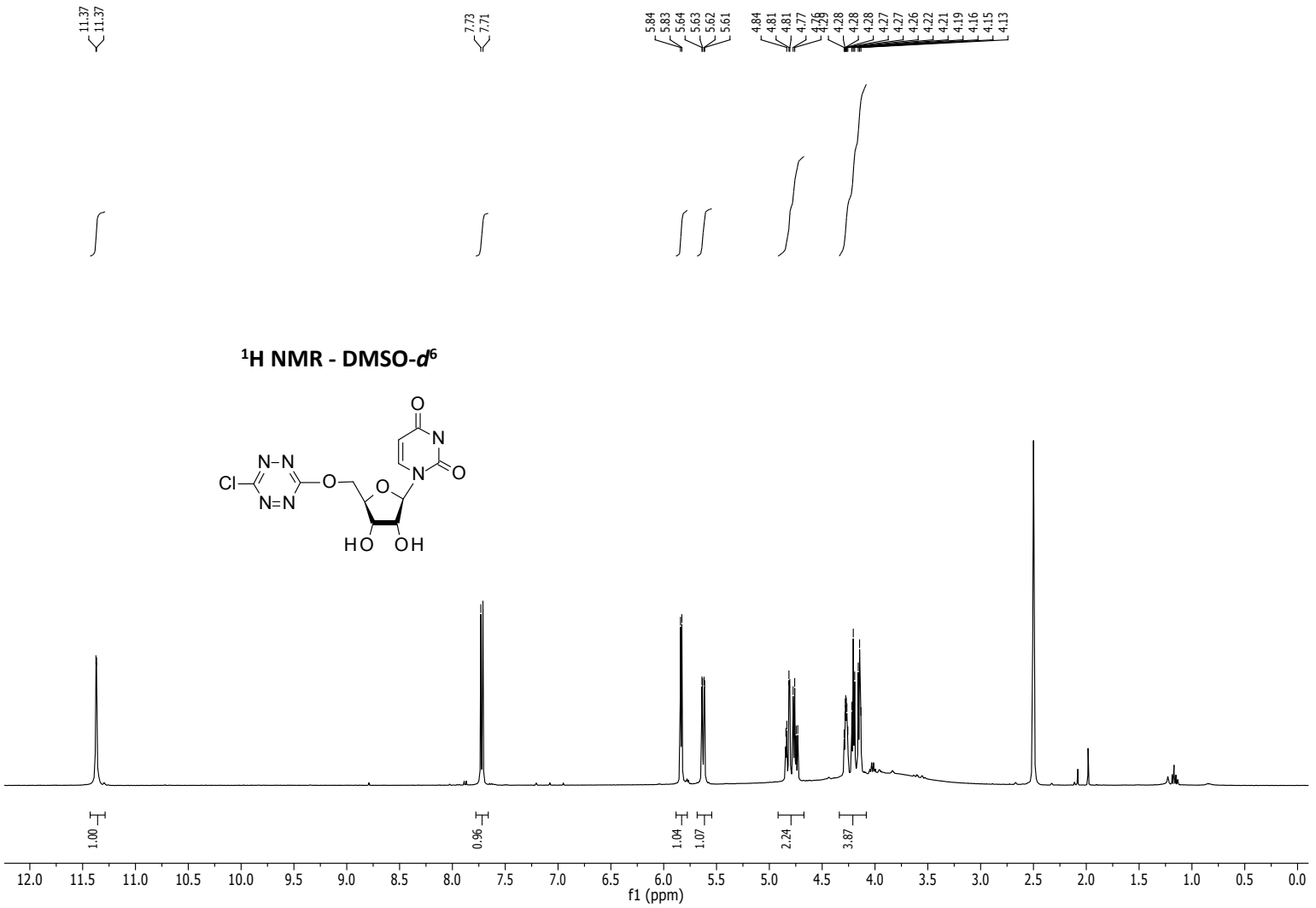
^{1}H NMR and ^{13}C NMR spectra of **compound 3**

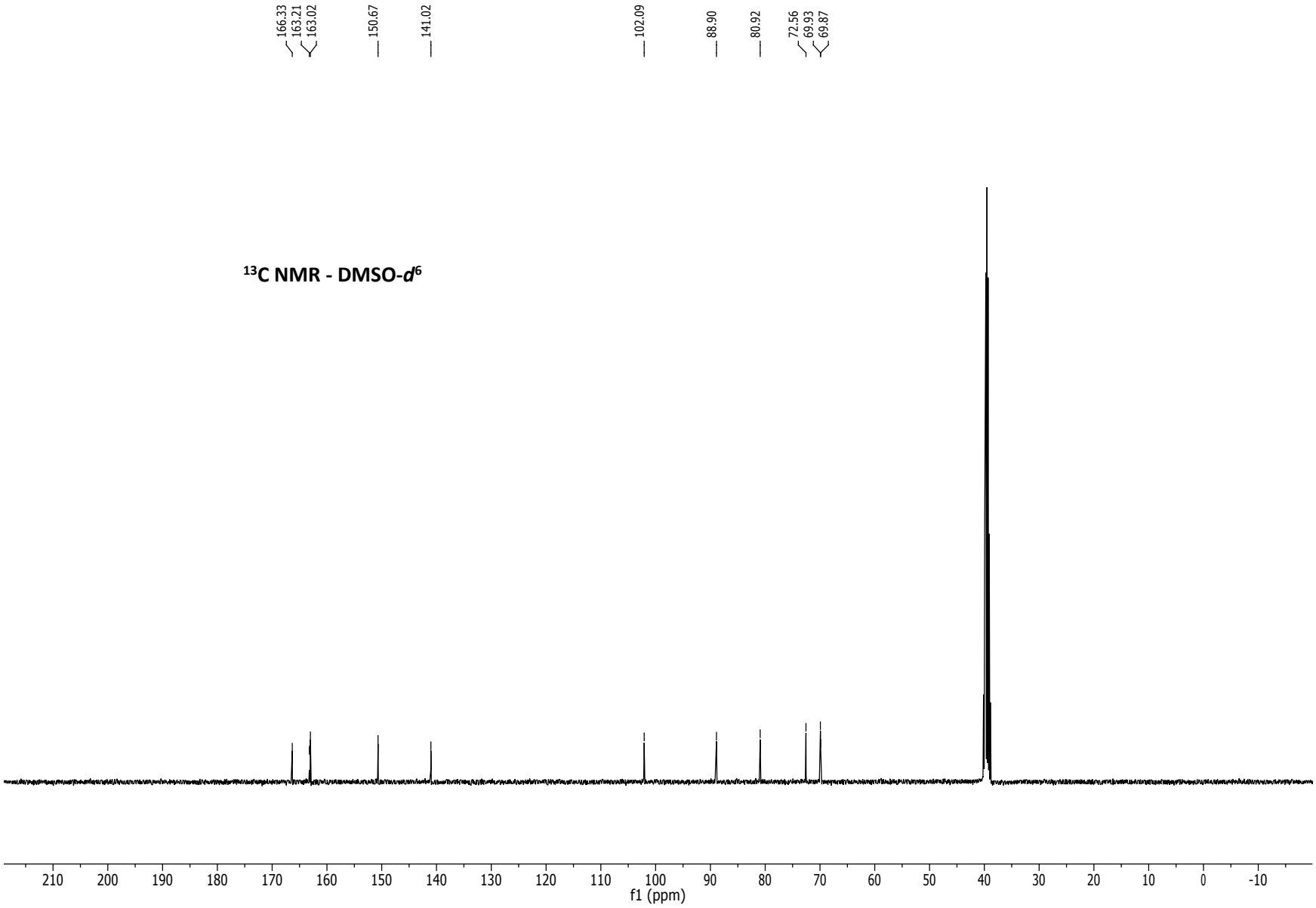


^{13}C NMR – $CDCl_3$

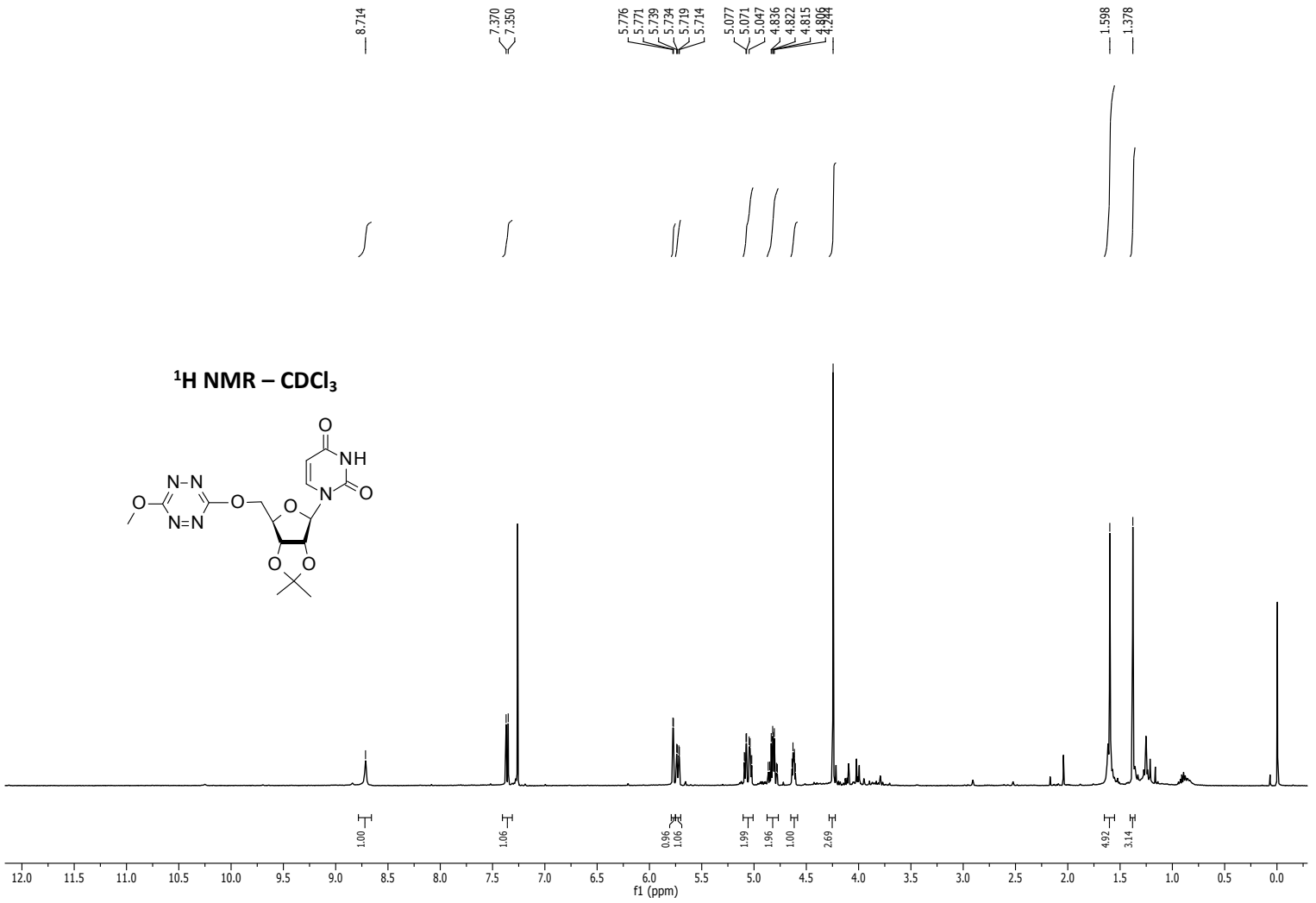


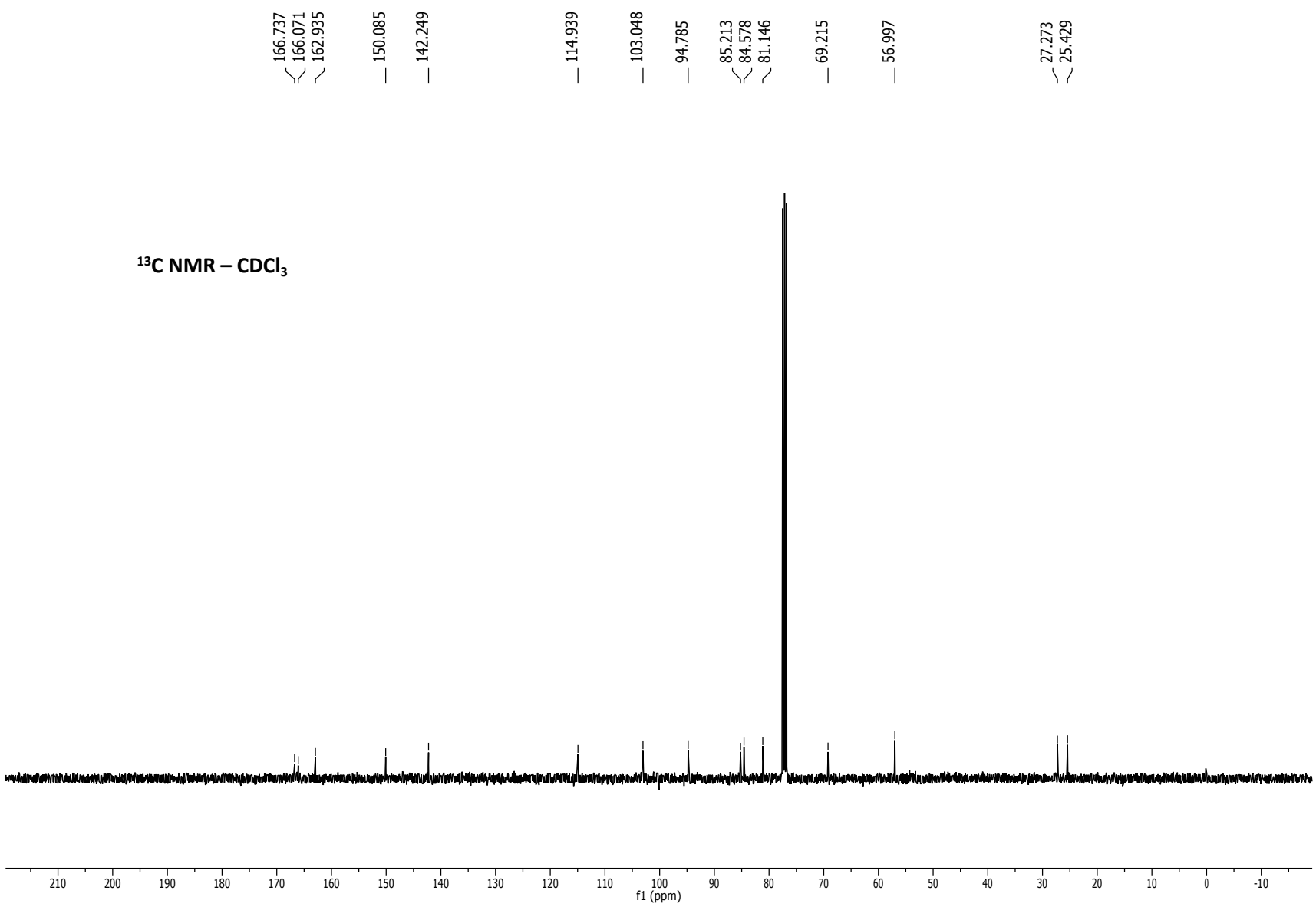
^{1}H NMR and ^{13}C NMR spectra of **compound 4**



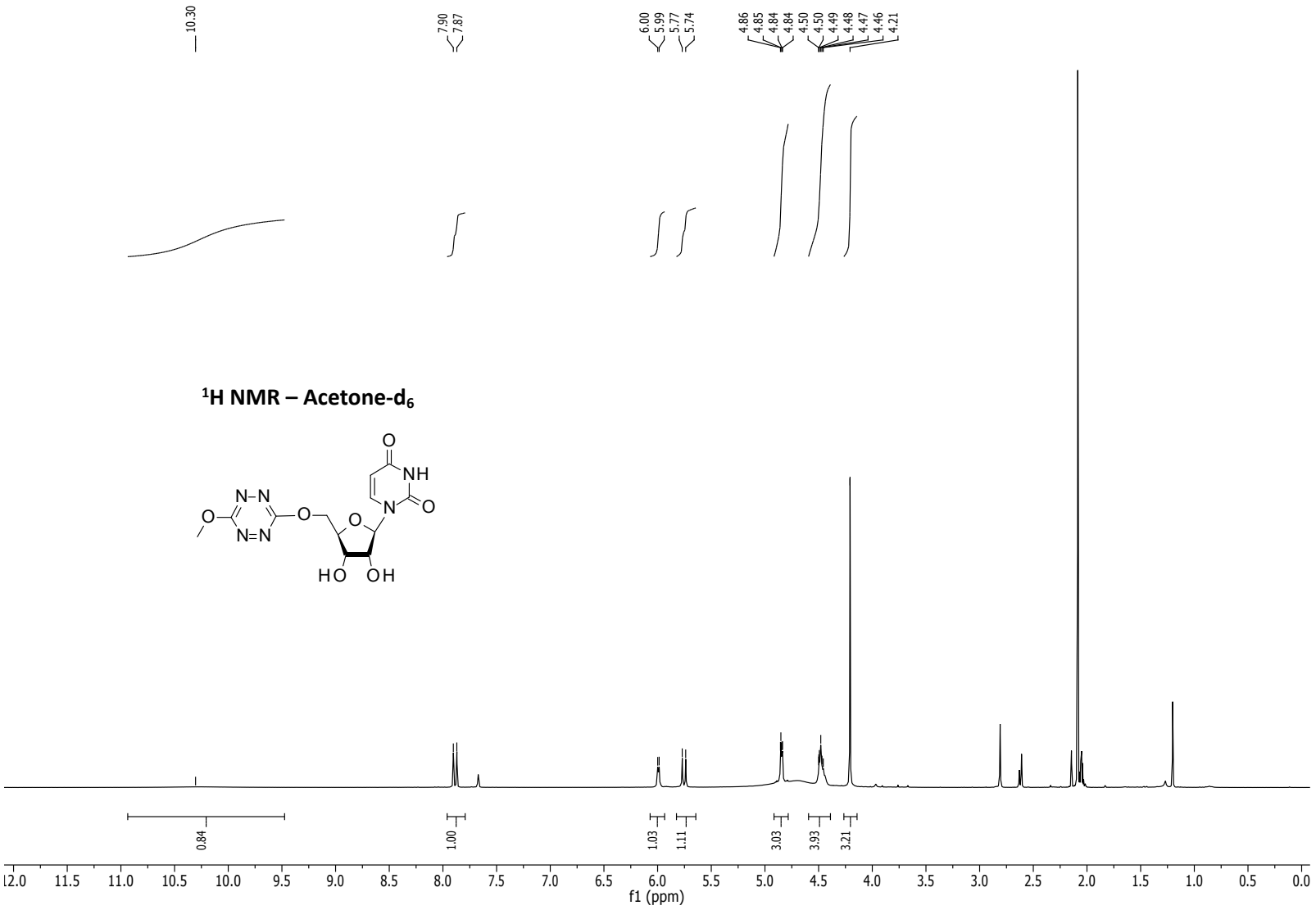

166.33
163.21
163.02
150.67
141.02
102.09
88.90
80.92
72.56
69.93
69.87
^{13}C NMR - DMSO-*d*^{6}
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

^{1}H NMR and ^{13}C NMR spectra of **compound 7**

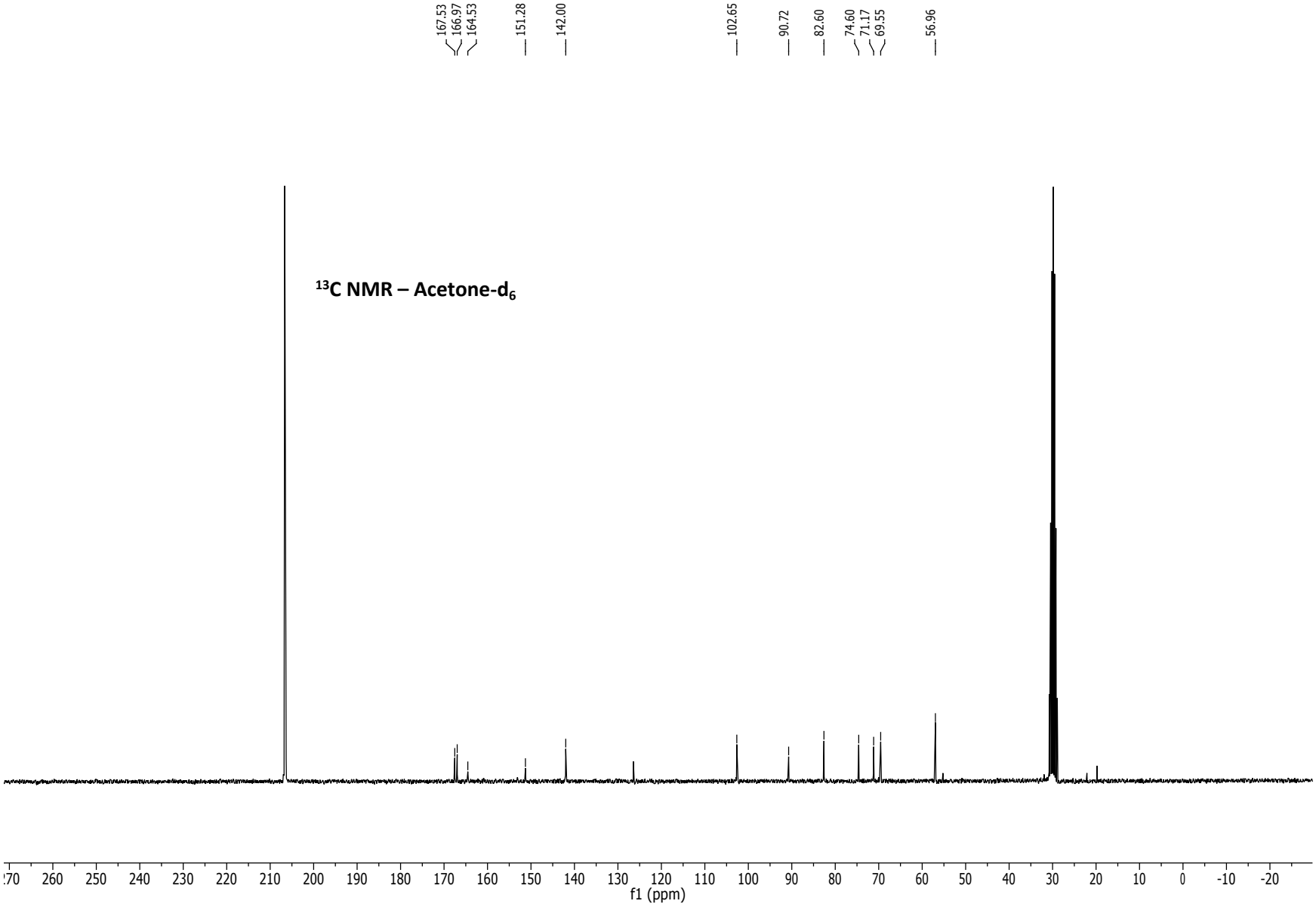



166.737
166.071
162.935
150.085
142.249
114.939
103.048
94.785
85.213
84.578
81.146
69.215
56.997
27.273
25.429
^{13}C NMR – $CDCl_3$
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

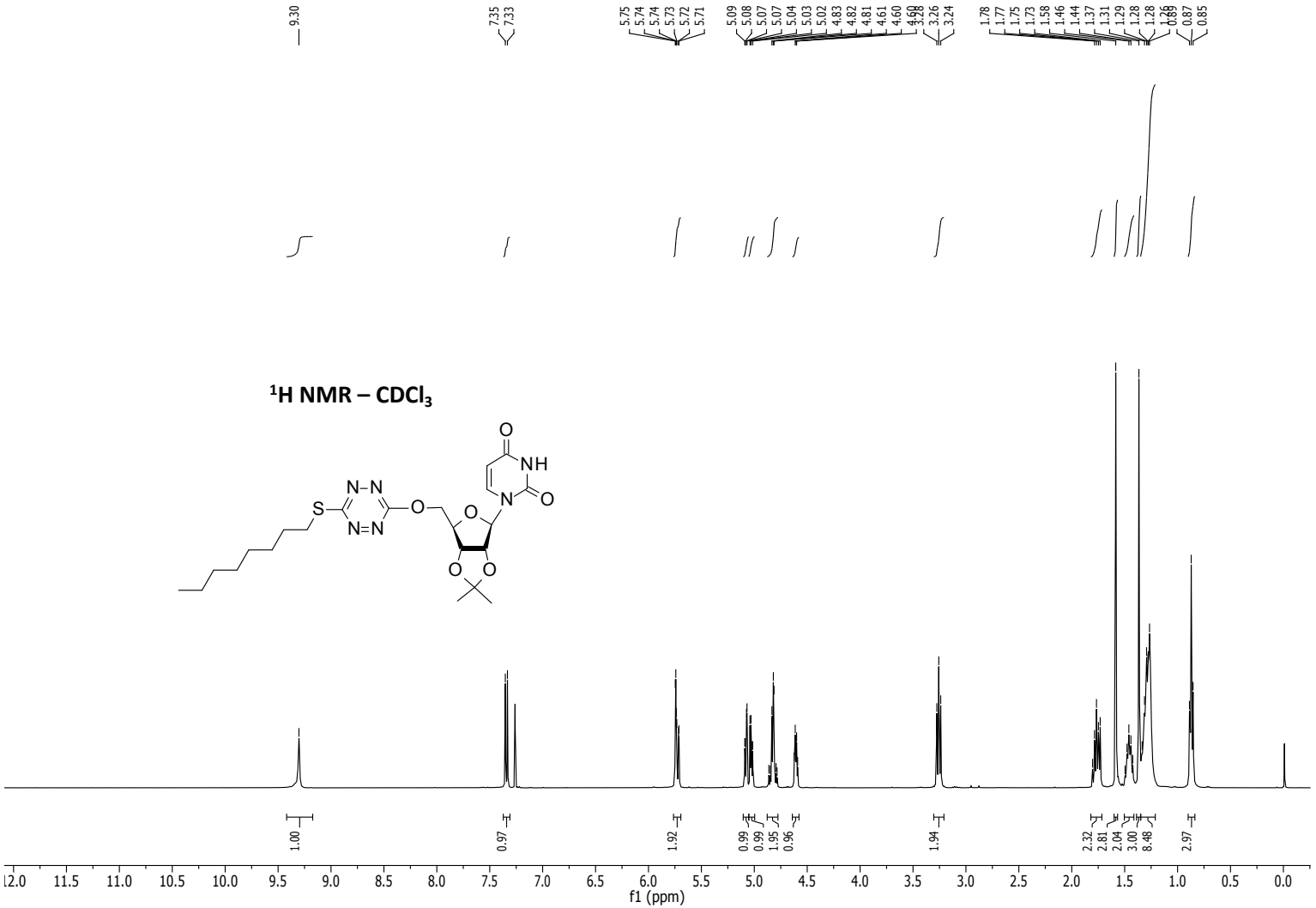
^{1}H NMR and ^{13}C NMR spectra of **compound 8**

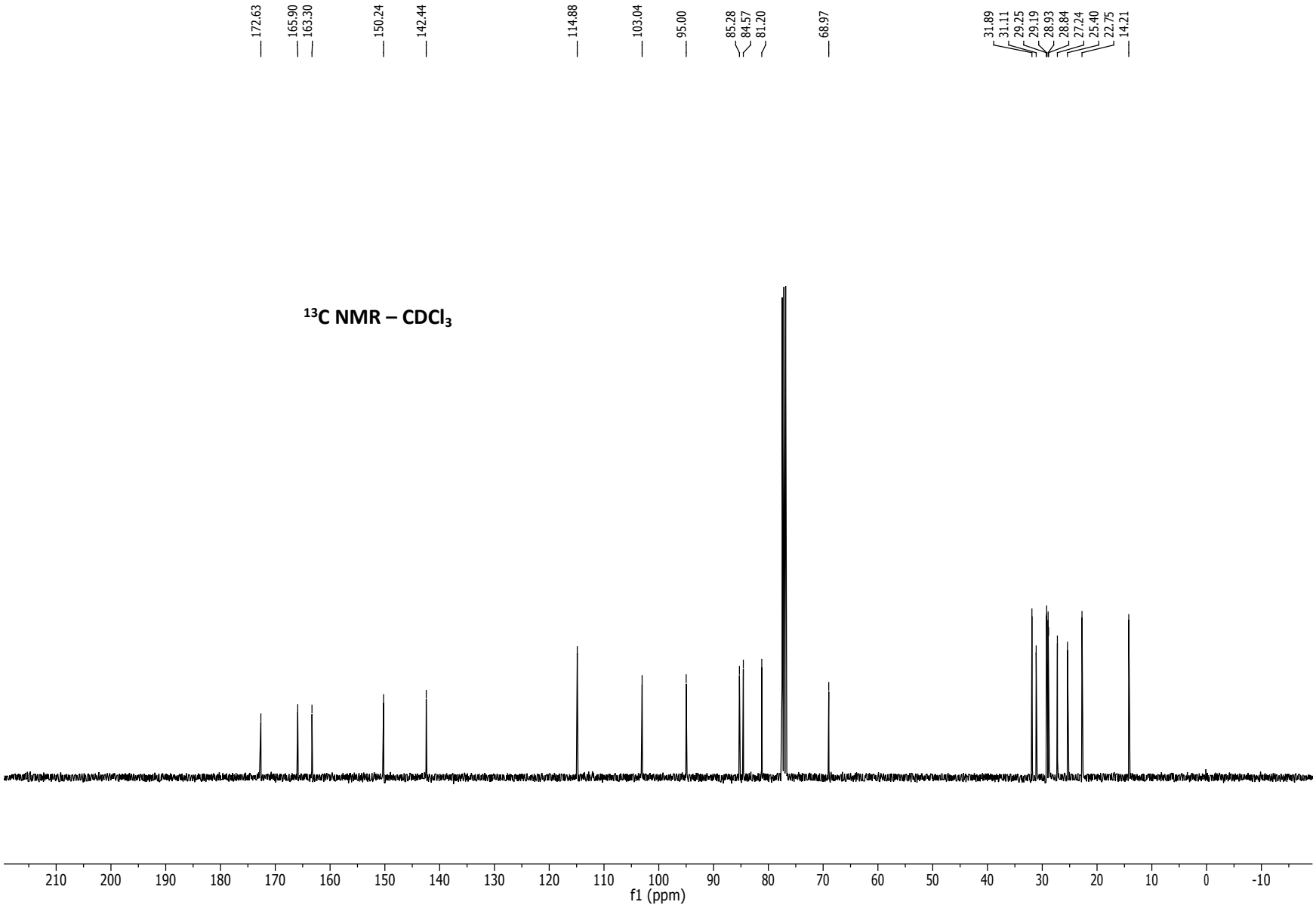


^{1}H NMR – Acetone-d_6

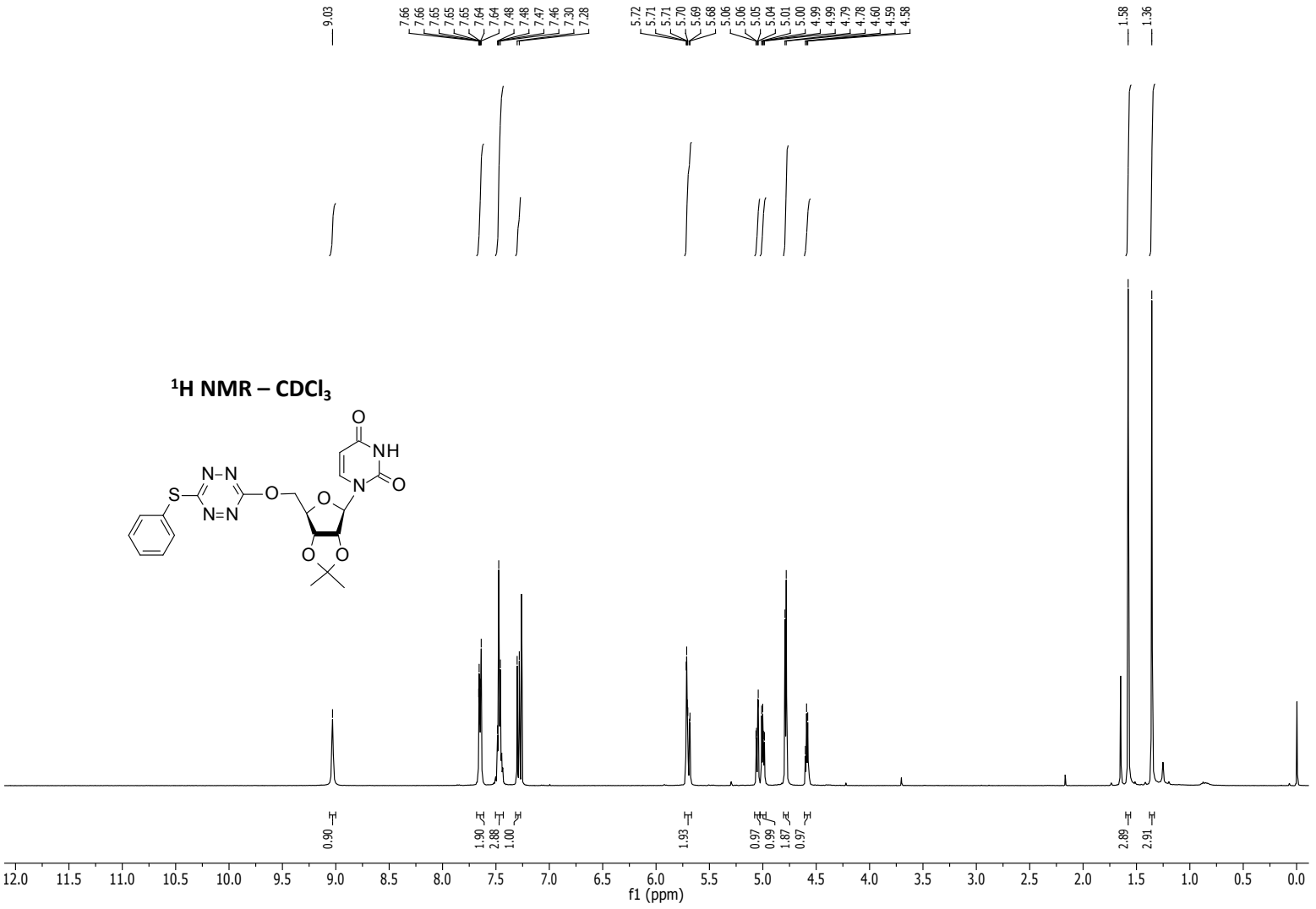

167.53
166.97
164.53
151.28
142.00
102.65
90.72
82.60
74.60
71.17
69.55
56.96
^{13}C NMR – Acetone-d$_6$
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

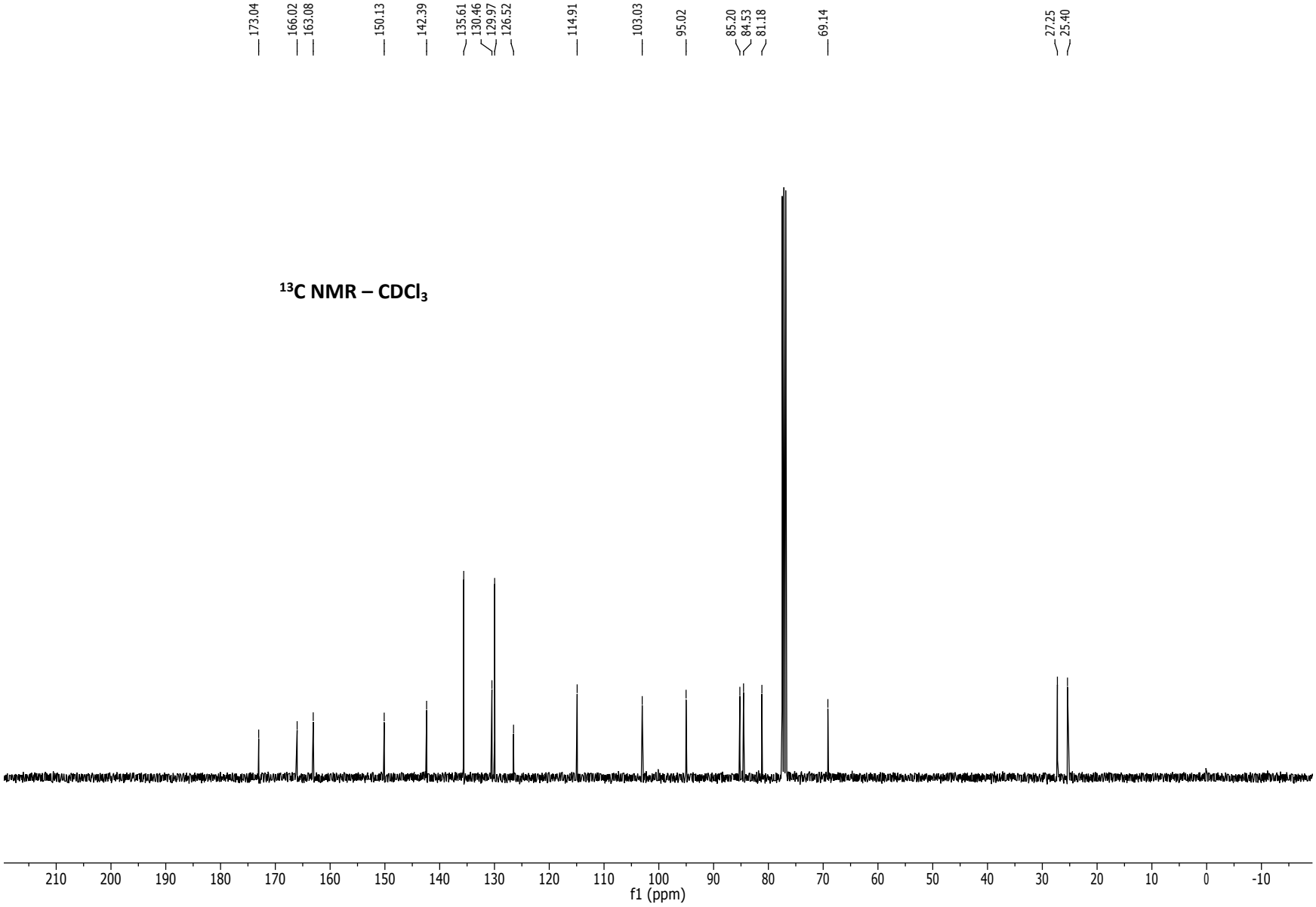
^{1}H NMR and ^{13}C NMR spectra of **compound 5**



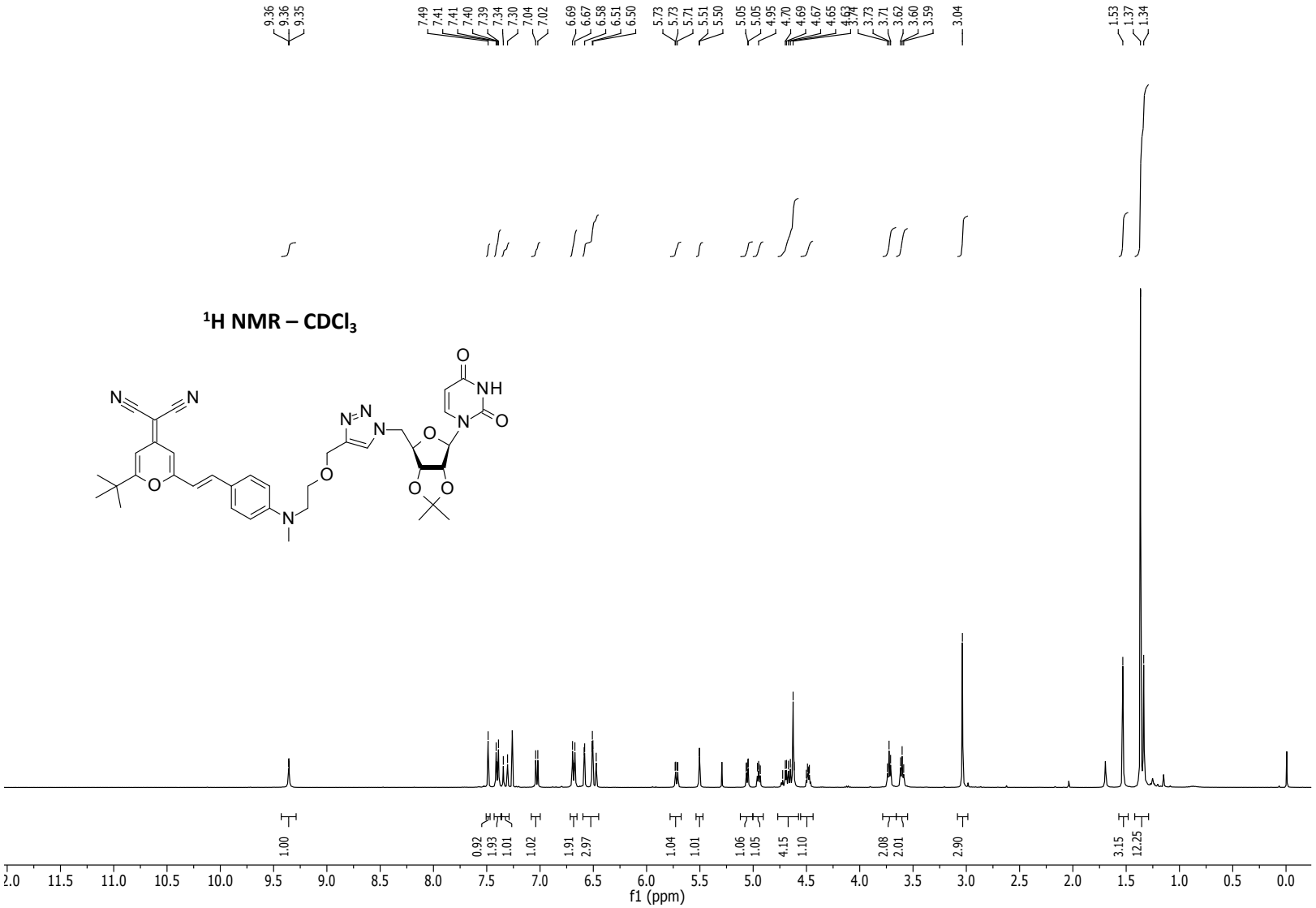

172.63
165.90
163.30
150.24
142.44
114.88
103.04
95.00
85.28
84.57
81.20
68.97
31.89
31.11
29.25
29.19
28.93
28.84
27.24
25.40
22.75
14.21
13C NMR – CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

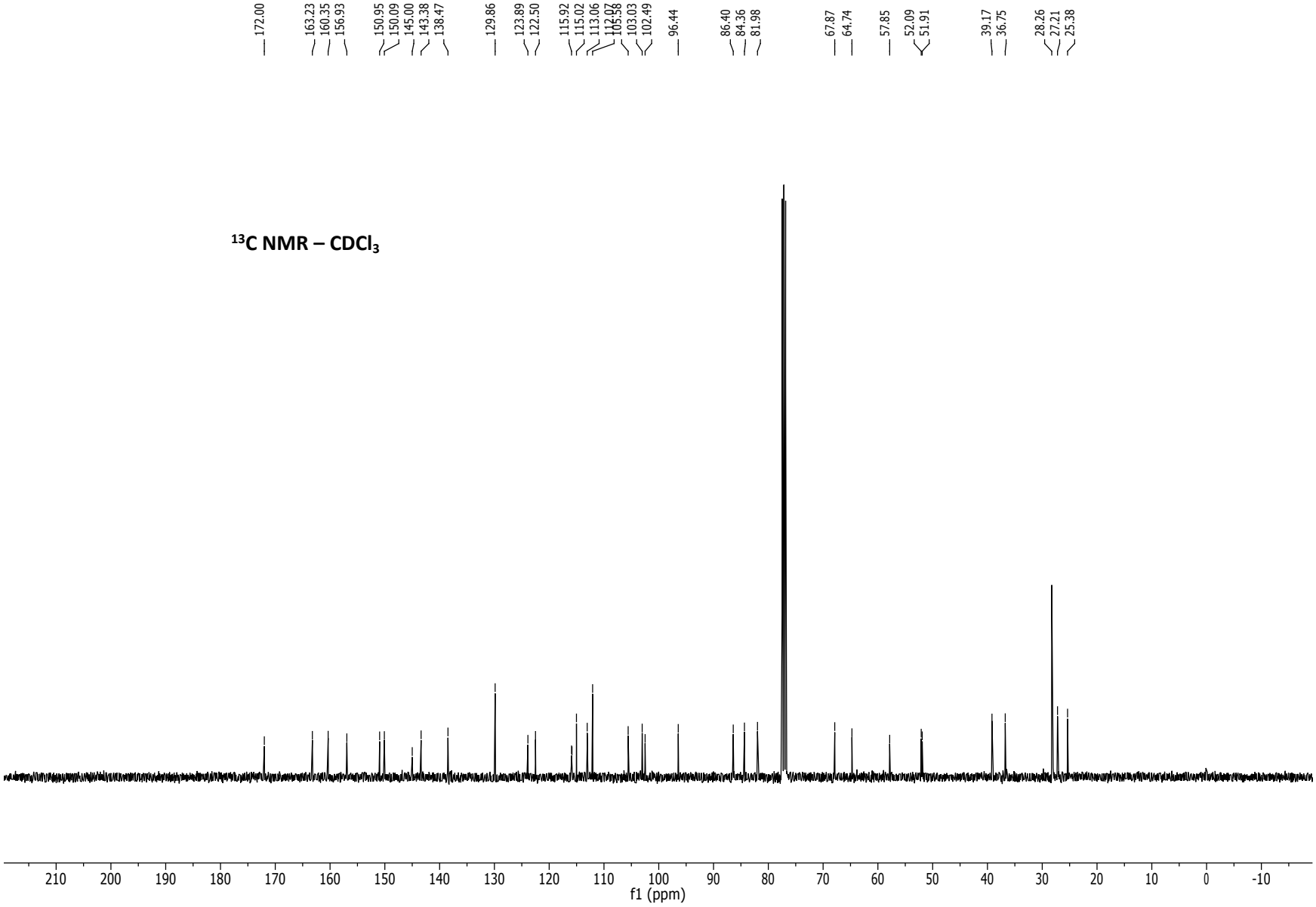
^{1}H NMR and ^{13}C NMR spectra of **compound 6**



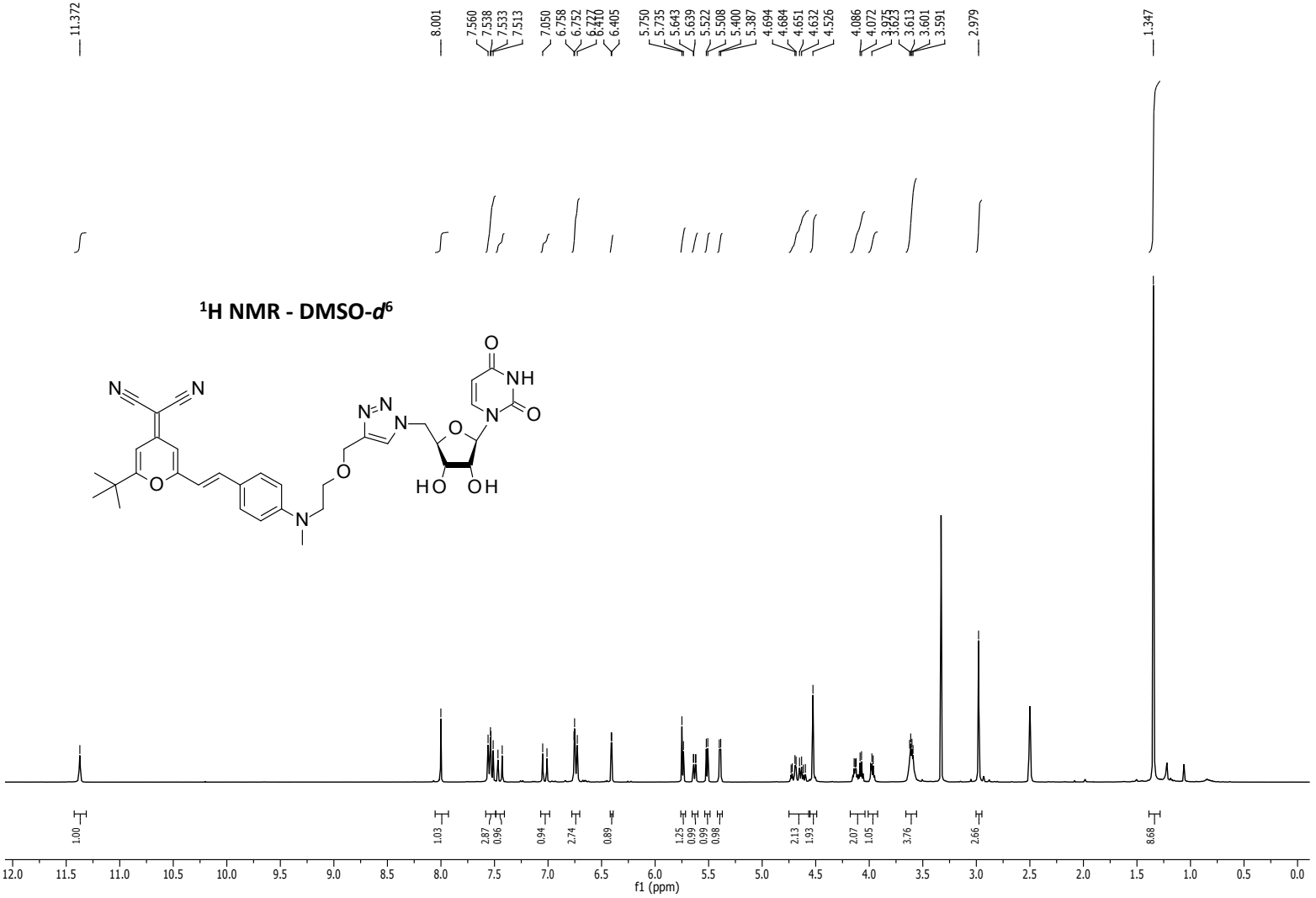

173.04
166.02
163.08
150.13
142.39
135.61
130.46
129.97
126.52
114.91
103.03
95.02
85.20
84.53
81.18
69.14
27.25
25.40
^{13}C NMR – CDCl$_3$
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

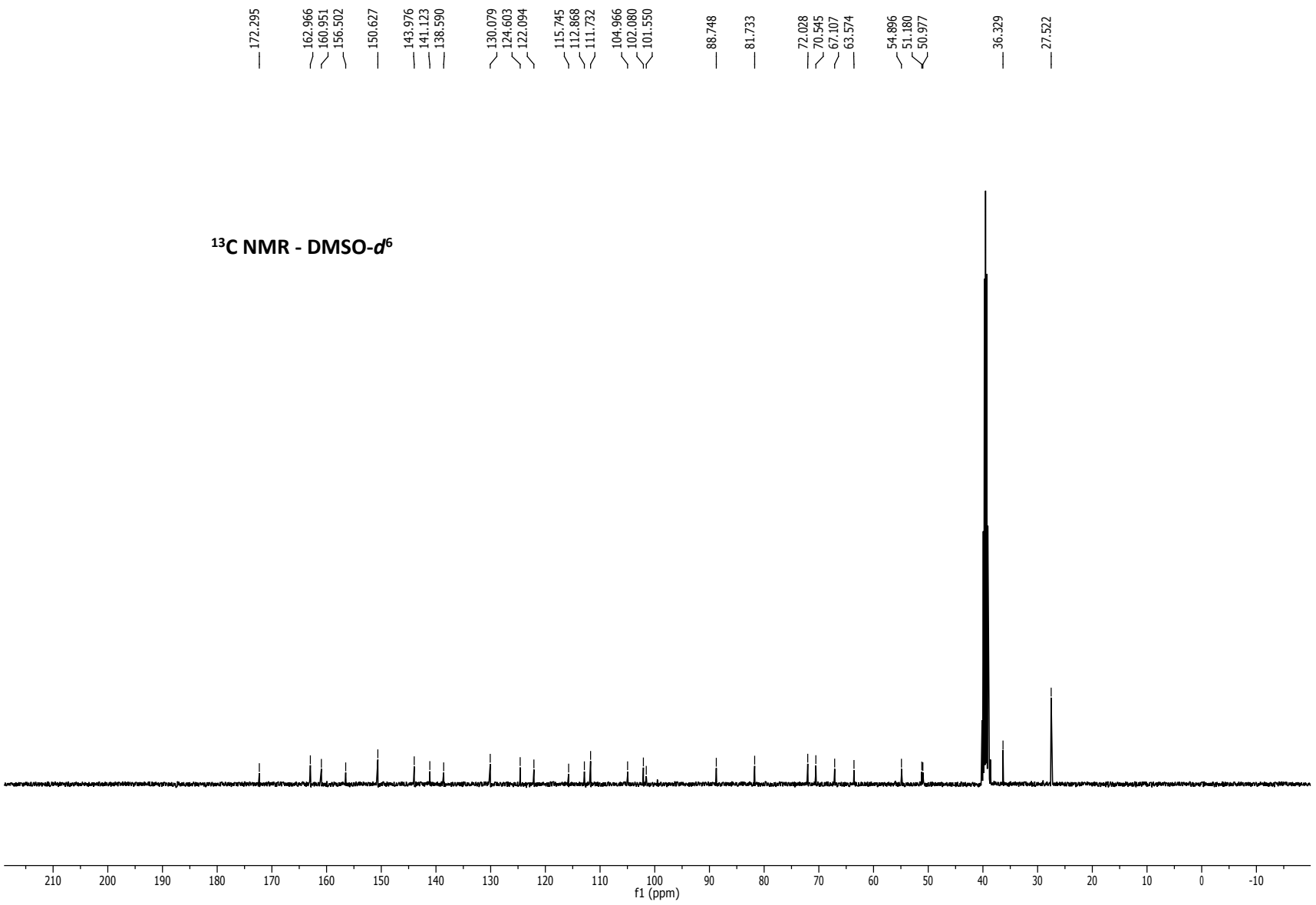
^{1}H NMR and ^{13}C NMR spectra of **compound 18**



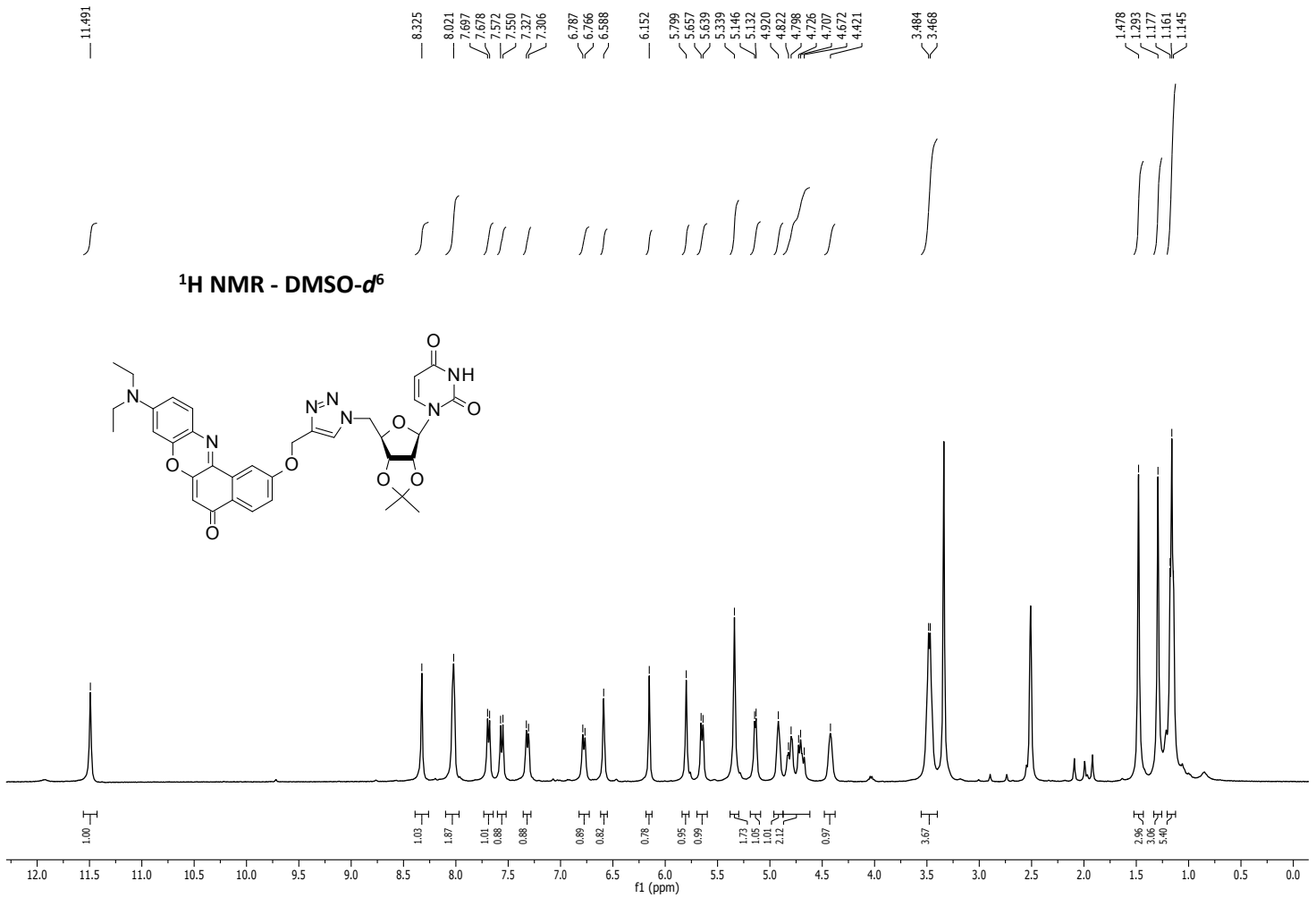

172.00
163.23
160.35
156.93
150.95
150.09
145.00
143.38
138.47
129.86
123.89
122.50
115.92
115.02
113.06
112.07
105.58
103.03
102.49
96.44
86.40
84.36
81.98
67.87
64.74
57.85
52.09
51.91
39.17
36.75
28.26
27.21
25.38
^{13}C NMR – $CDCl_3$
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

^{1}H NMR and ^{13}C NMR spectra of **compound 19**



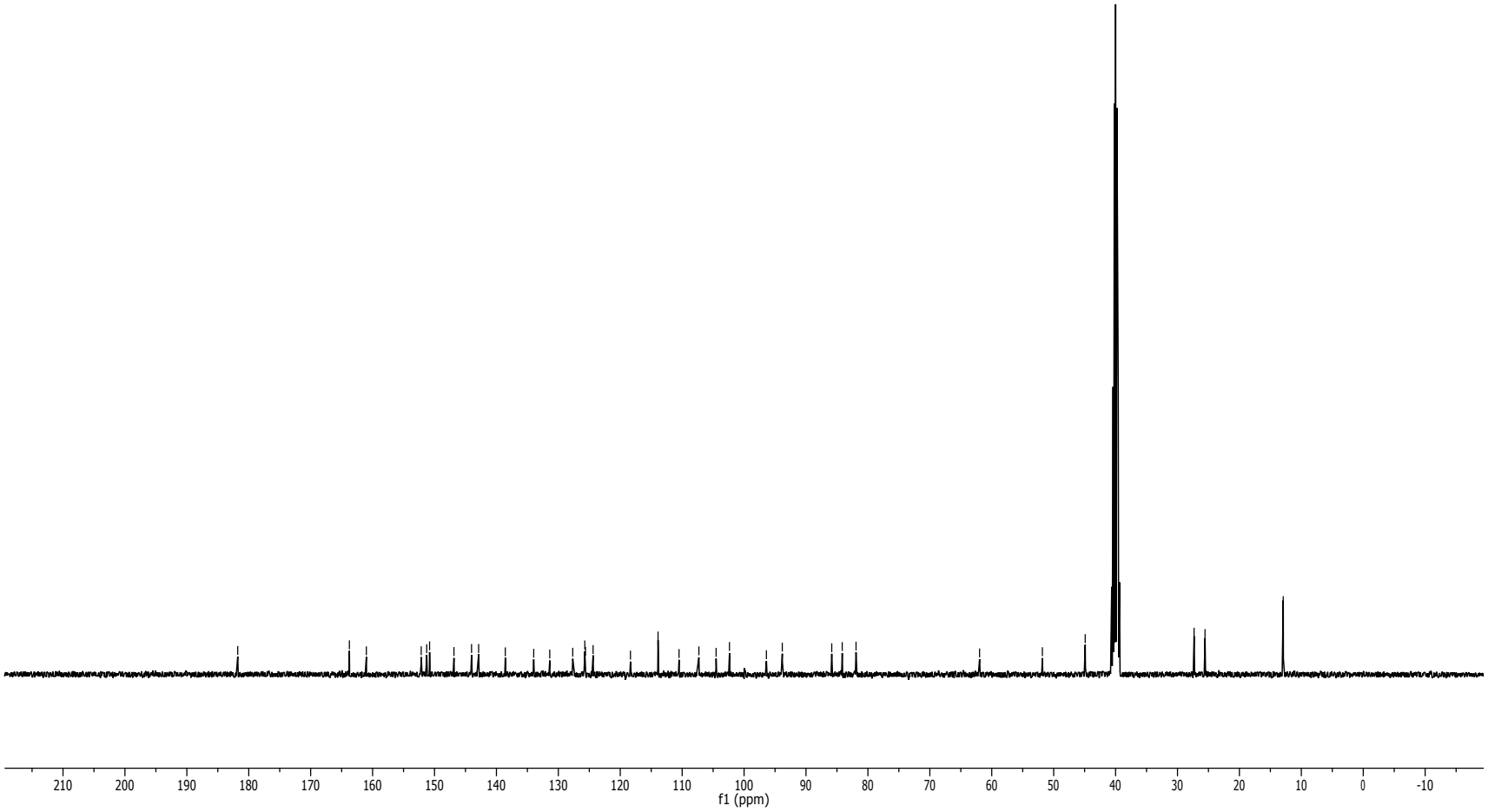

172.295
162.966
160.951
156.502
150.627
143.976
141.123
138.590
130.079
124.603
122.094
115.745
112.868
111.732
104.966
102.080
101.550
88.748
81.733
72.028
70.545
67.107
63.574
54.896
51.180
50.977
36.329
27.522
13C NMR - DMSO-d6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

^{1}H NMR and ^{13}C NMR spectra of **compound 20**

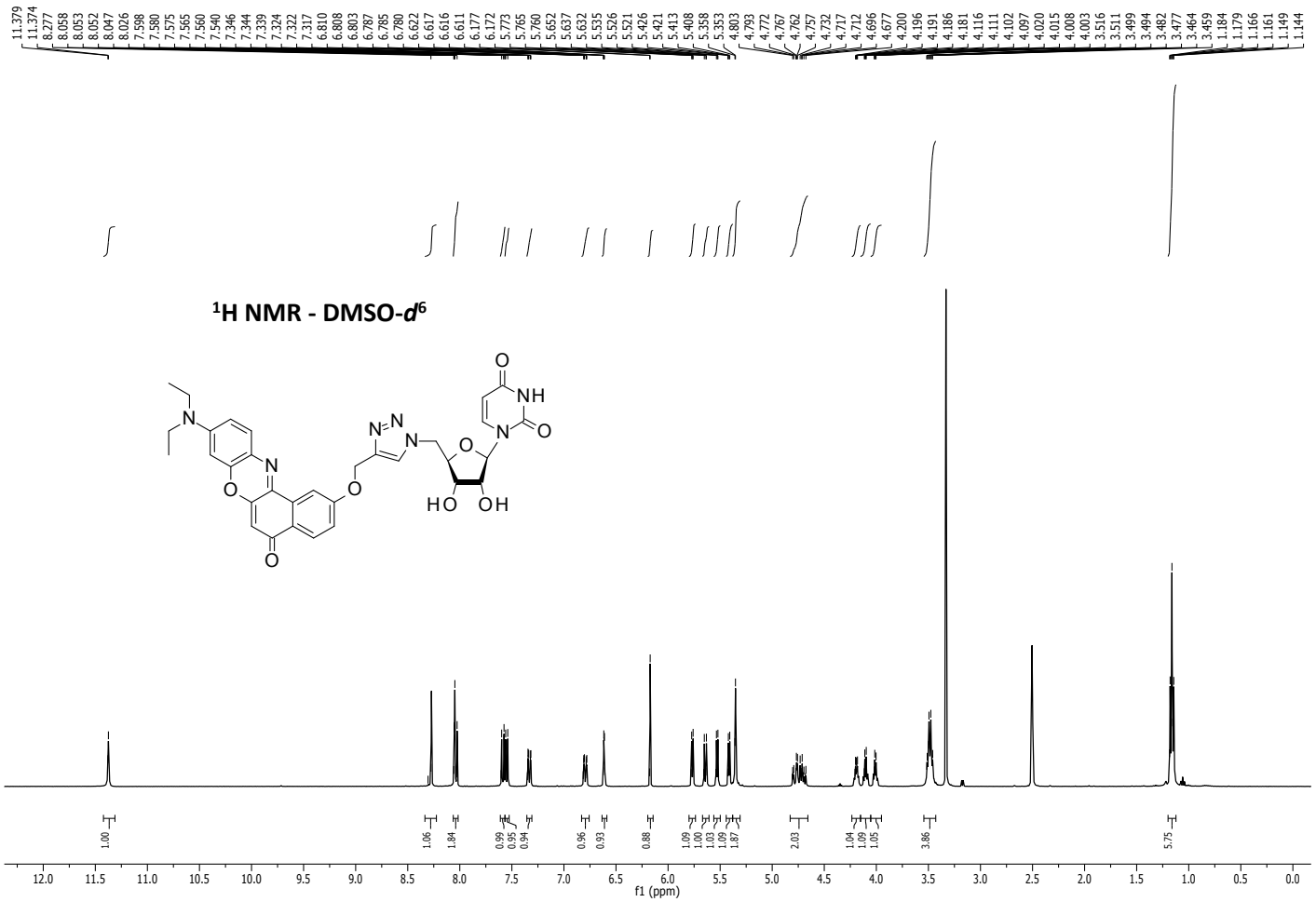


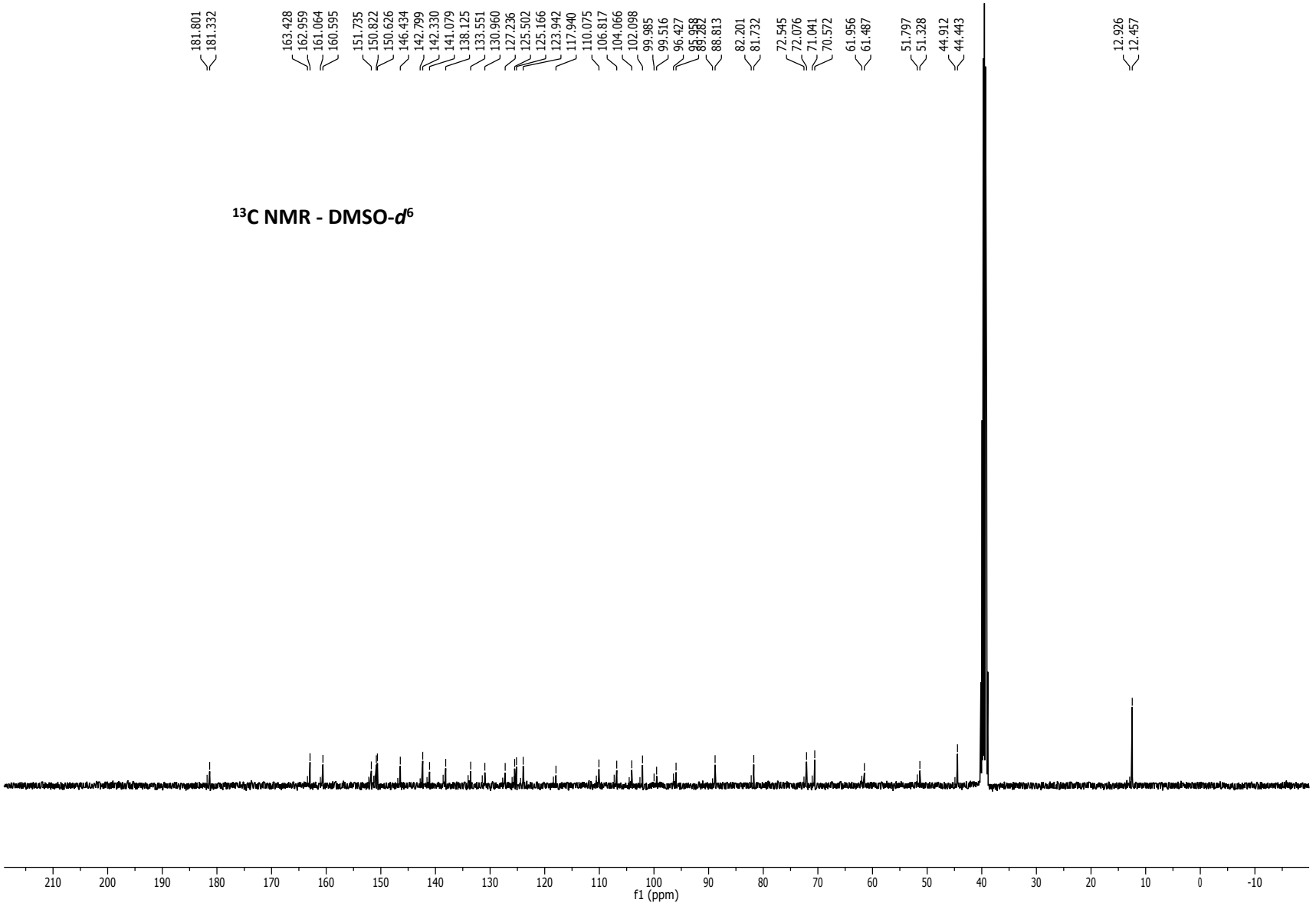
181.779
163.748
161.007
152.147
151.257
150.795
146.858
144.018
142.872
138.568
133.977
131.390
127.673
125.727
125.613
124.388
118.351
113.896
110.506
107.300
104.520
102.360
96.395
93.830
85.842
84.148
81.919
61.966
51.821
44.906
27.320
25.555
12.924

^{13}C NMR - DMSO-*d*^{6}



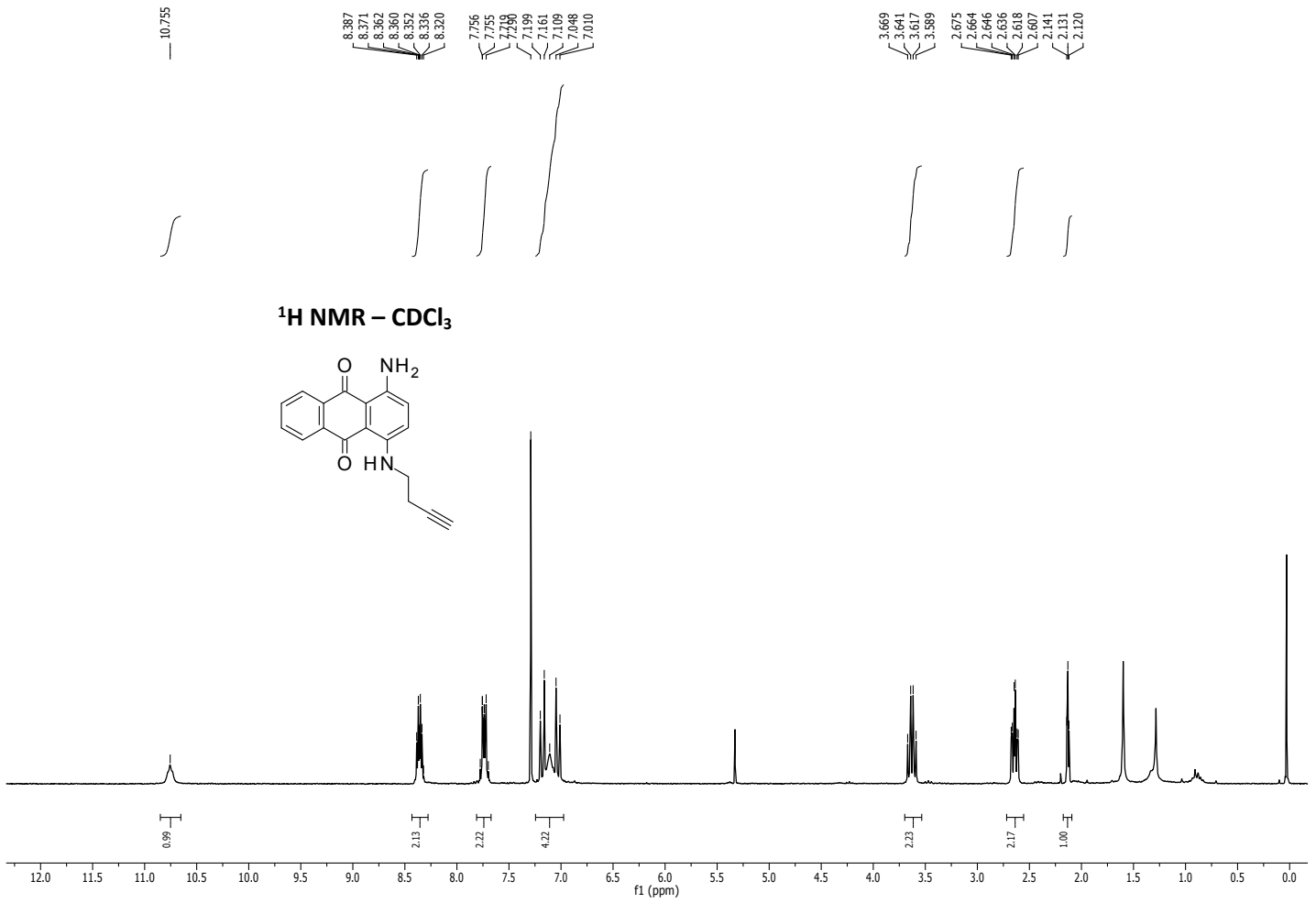
^{1}H NMR and ^{13}C NMR spectra of **compound 20**



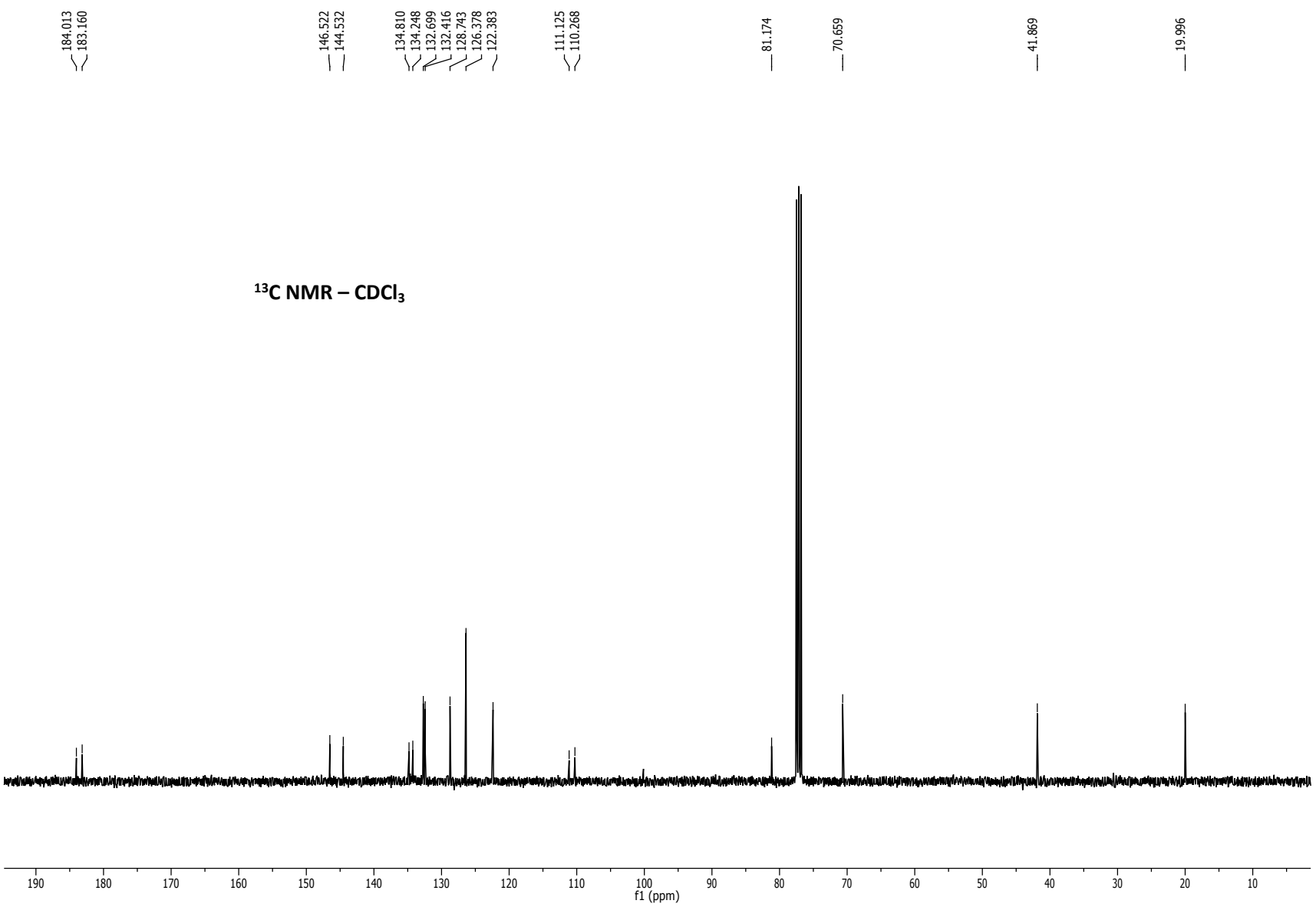


^{13}C NMR - DMSO-*d*^{6}

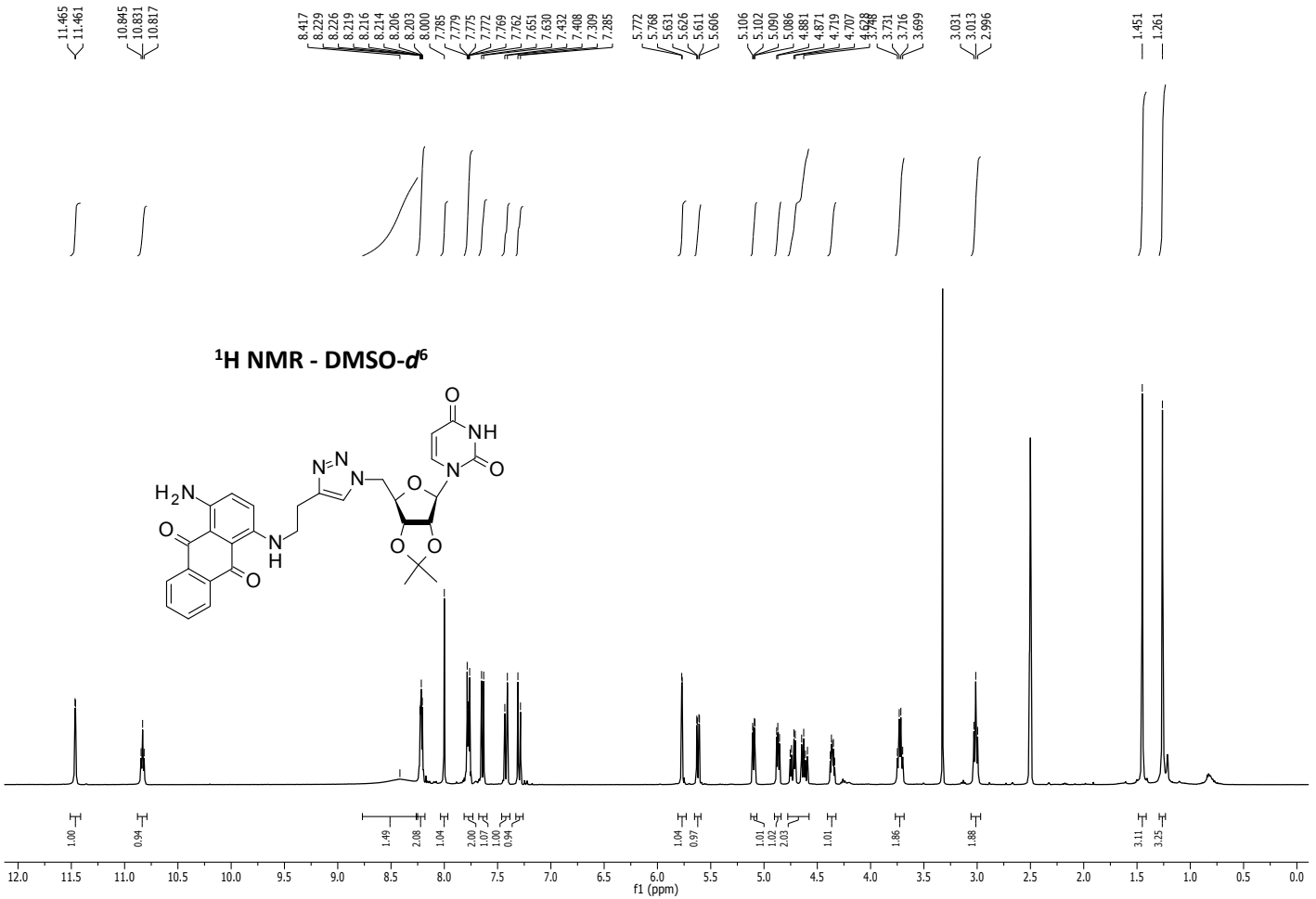
^{1}H NMR and ^{13}C NMR spectra of **compound 16**



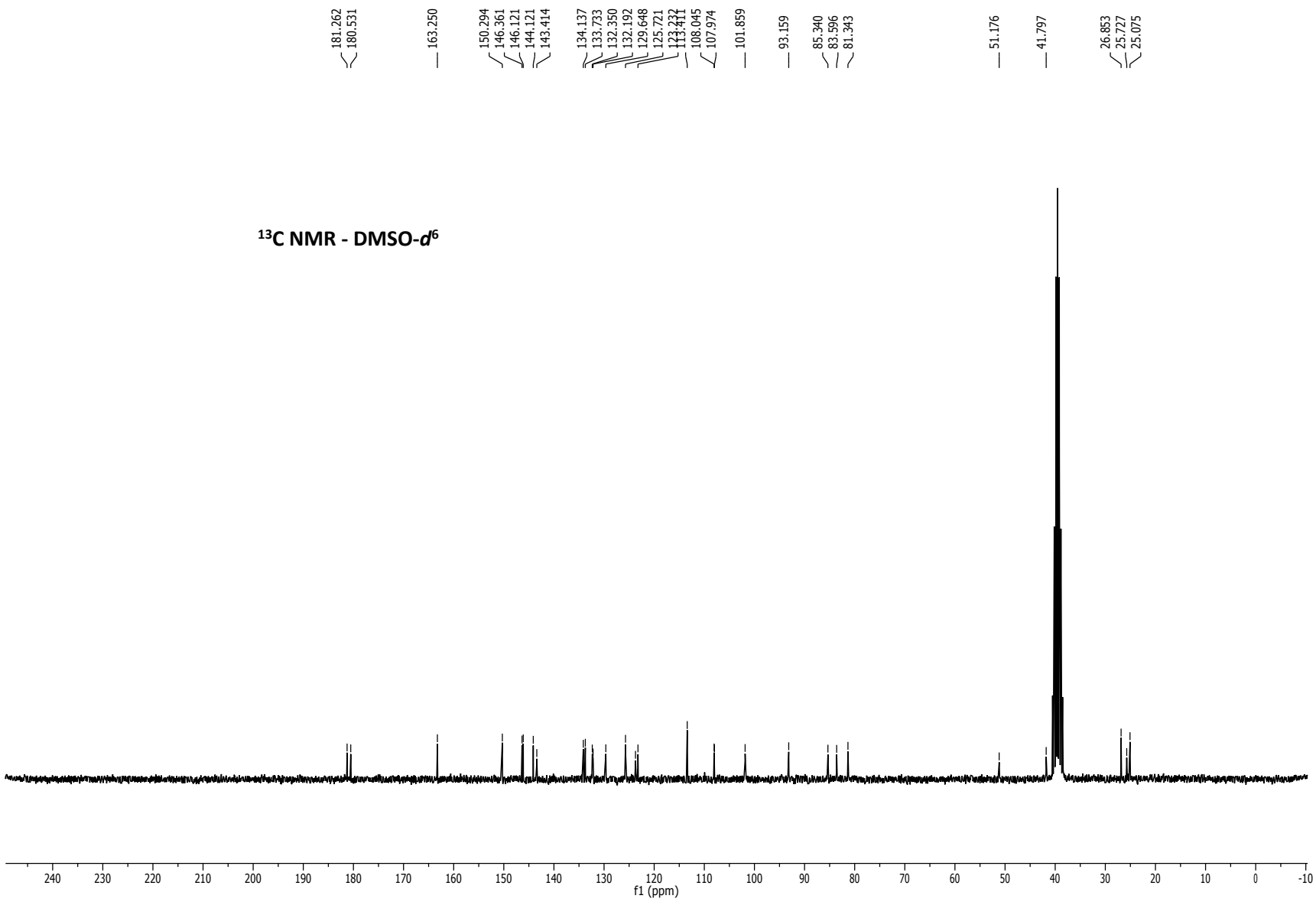
^{1}H NMR – $CDCl_3$


184.013
183.160
146.522
144.532
134.810
134.248
132.699
132.416
128.743
126.378
122.383
111.125
110.268
81.174
70.659
41.869
19.996
^{13}C NMR – $CDCl_3$
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

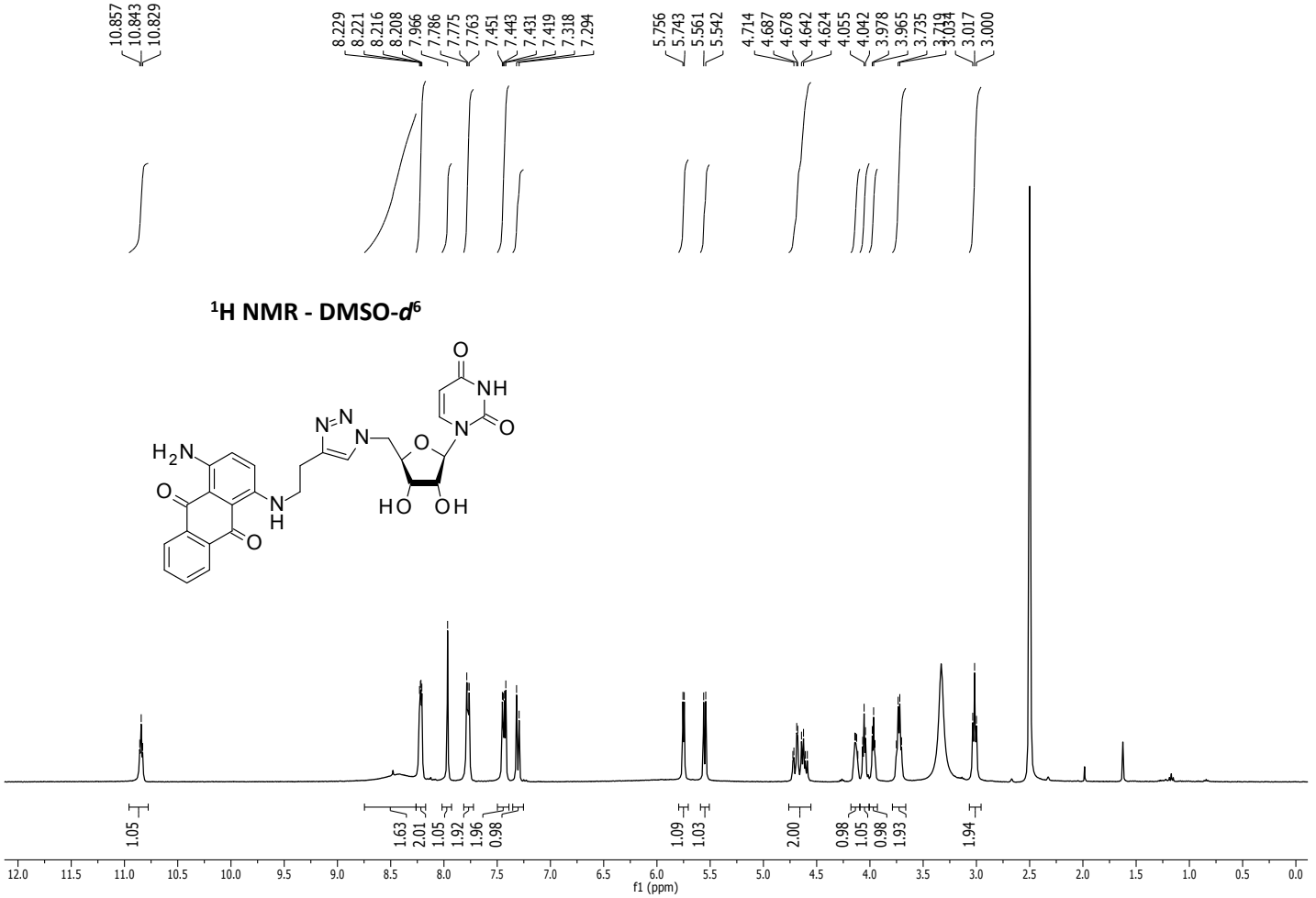
^{1}H NMR and ^{13}C NMR spectra of **compound 22**

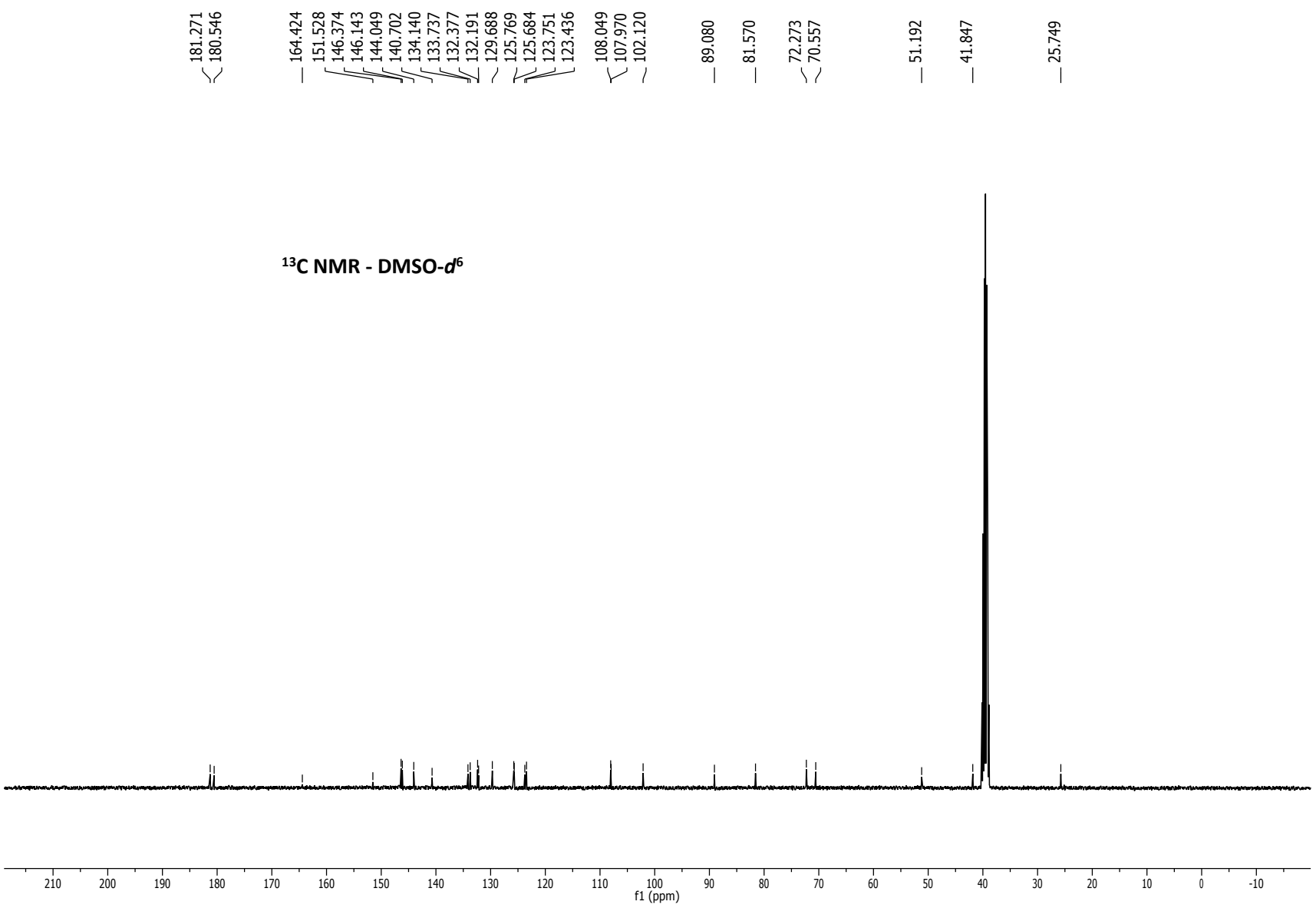


^{13}C NMR - DMSO-*d*^{6}

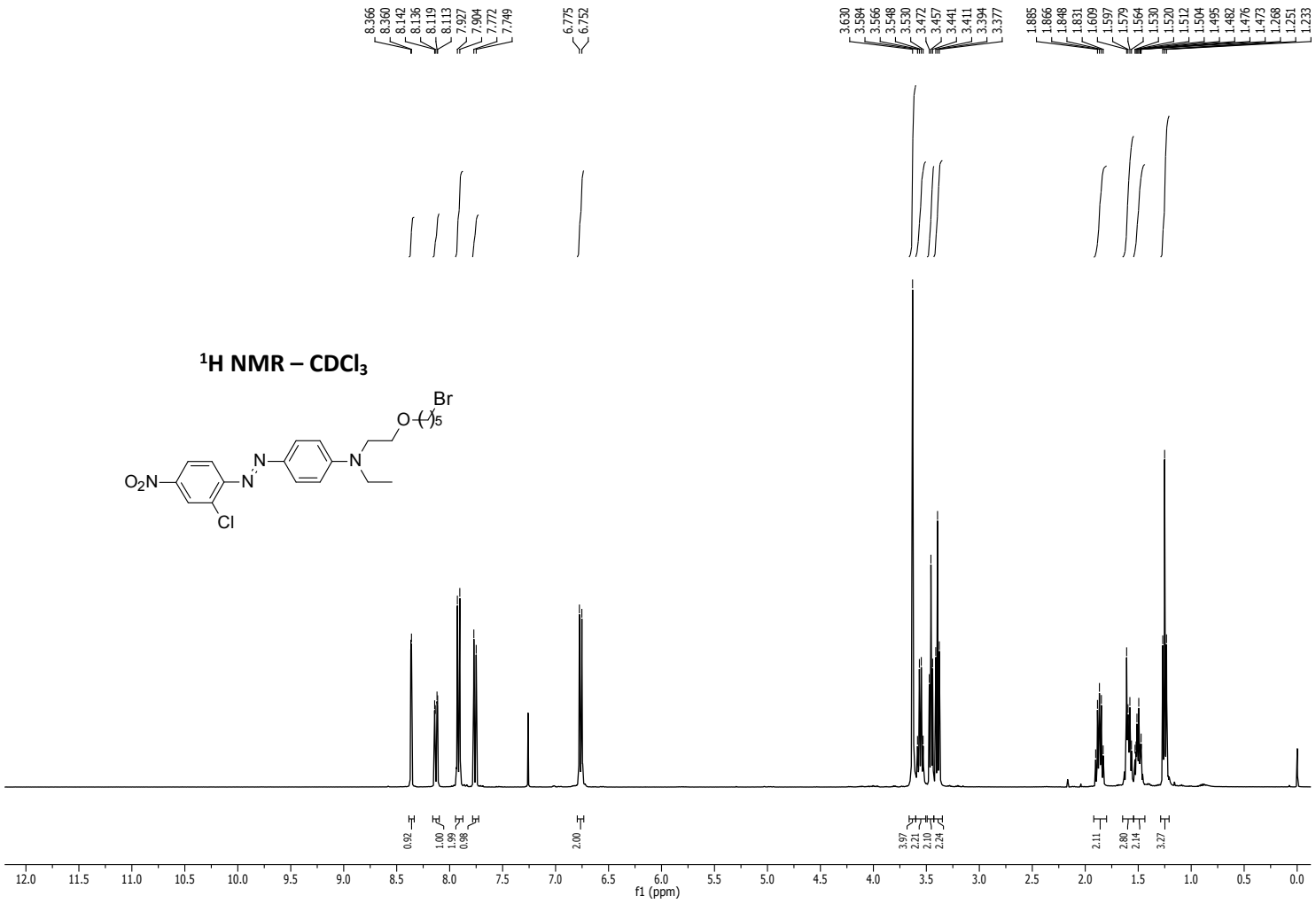


^{1}H NMR and ^{13}C NMR spectra of **compound 23**

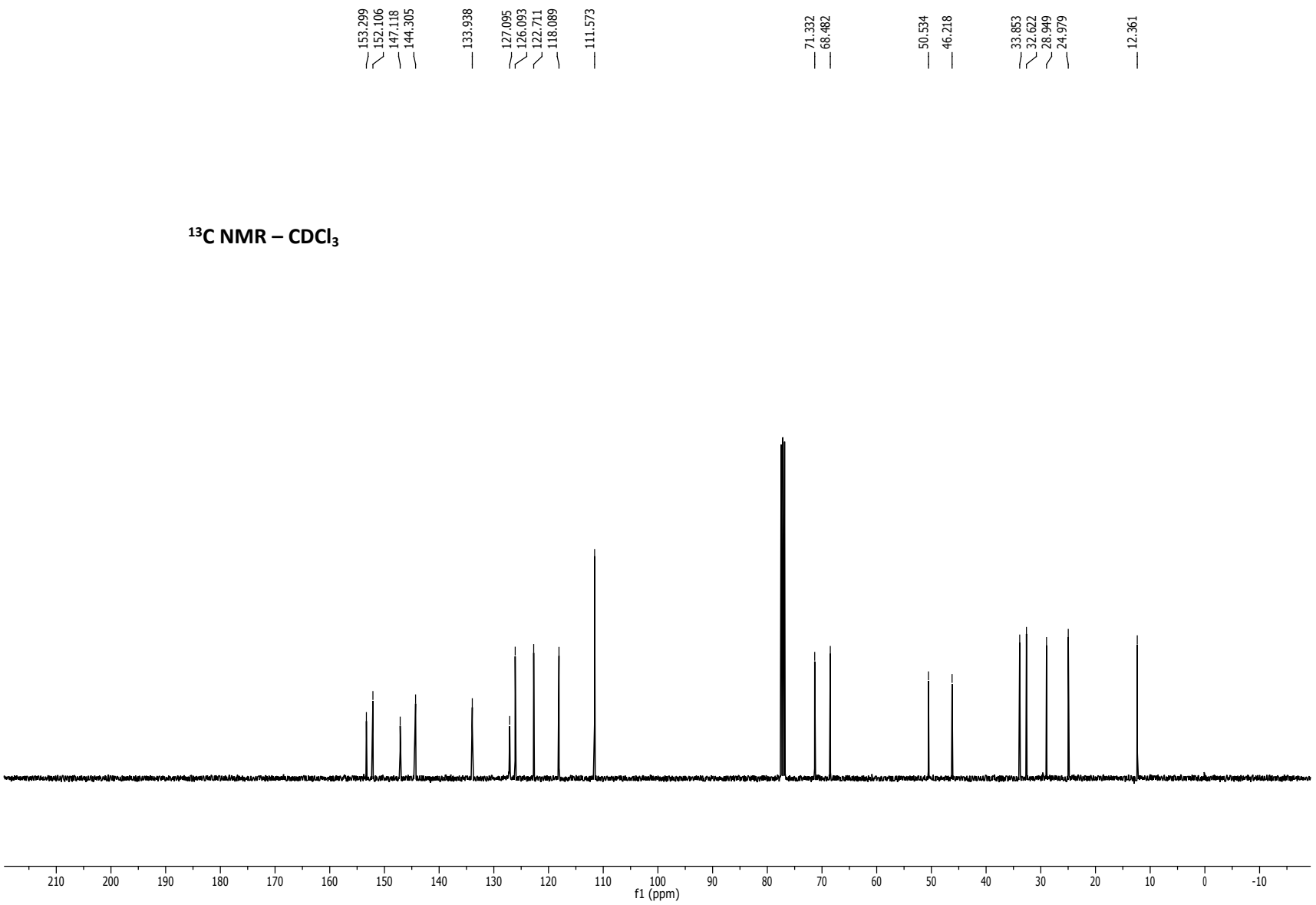



181.271
180.546
164.424
151.528
146.374
146.143
144.049
140.702
134.140
133.737
132.377
132.191
129.688
125.769
125.684
123.751
123.436
108.049
107.970
102.120
89.080
81.570
72.273
70.557
51.192
41.847
25.749
^{13}C NMR - DMSO-*d*^{6}
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

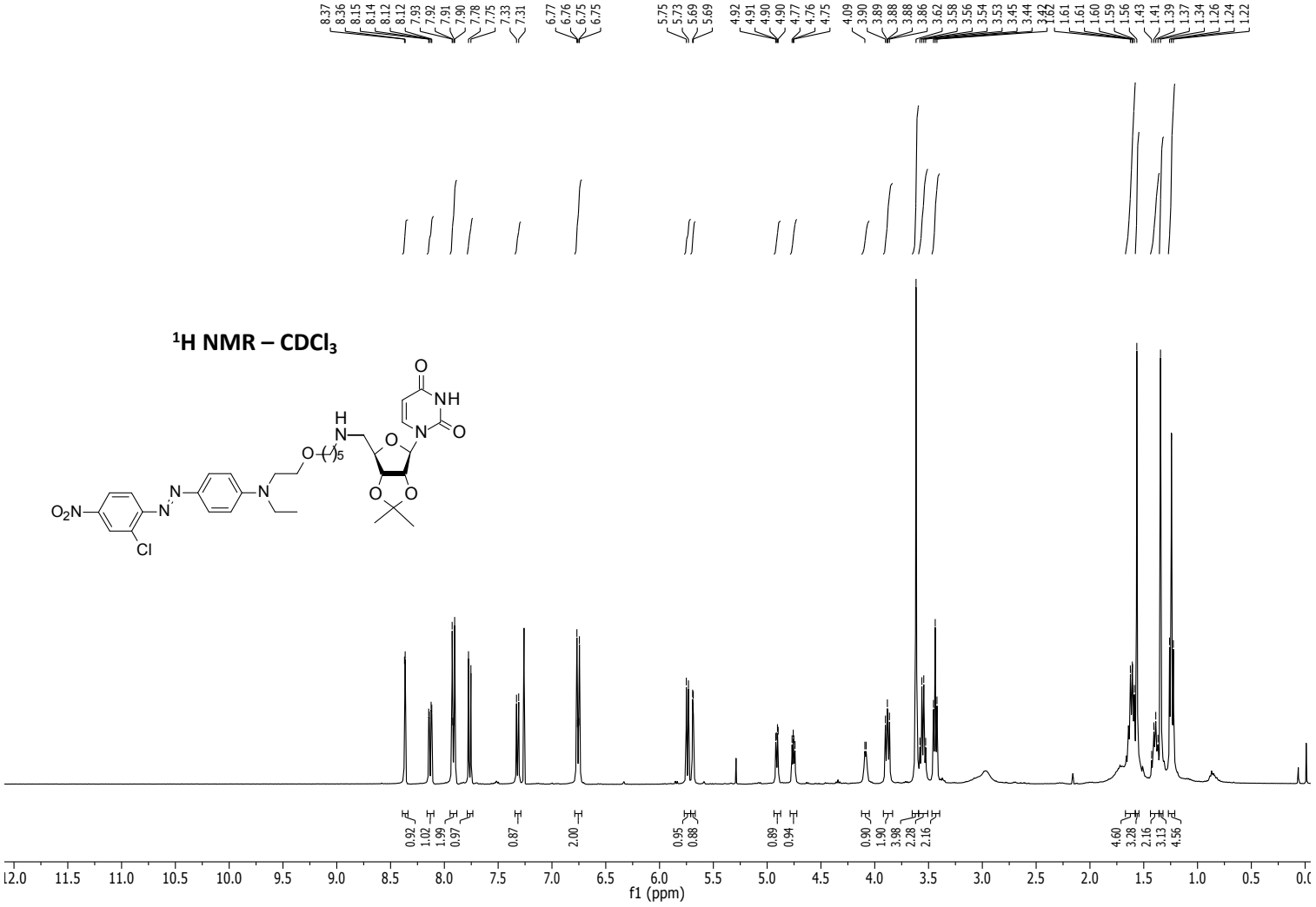
^{1}H NMR and ^{13}C NMR spectra of **compound 24**



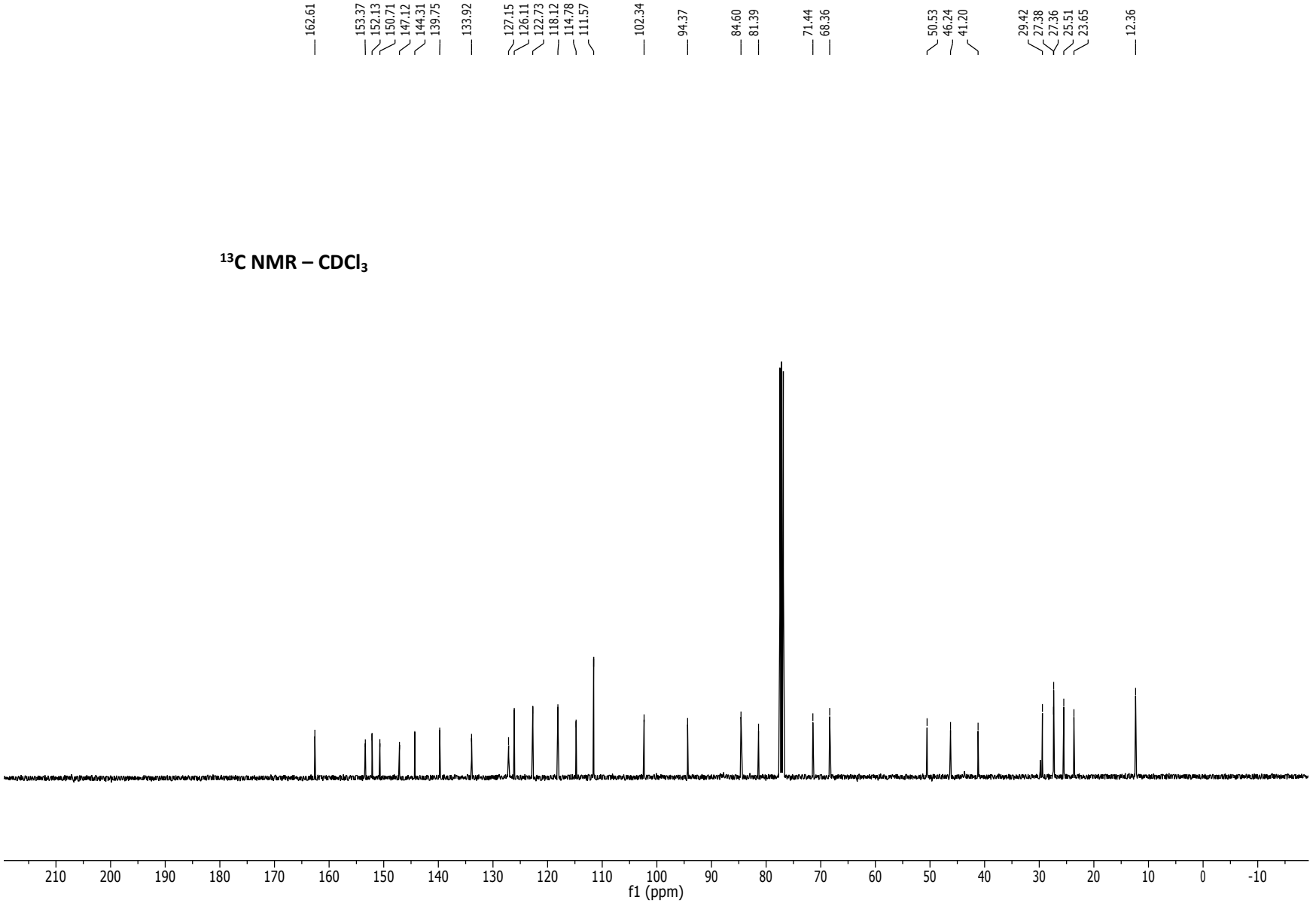
^{13}C NMR – $CDCl_3$



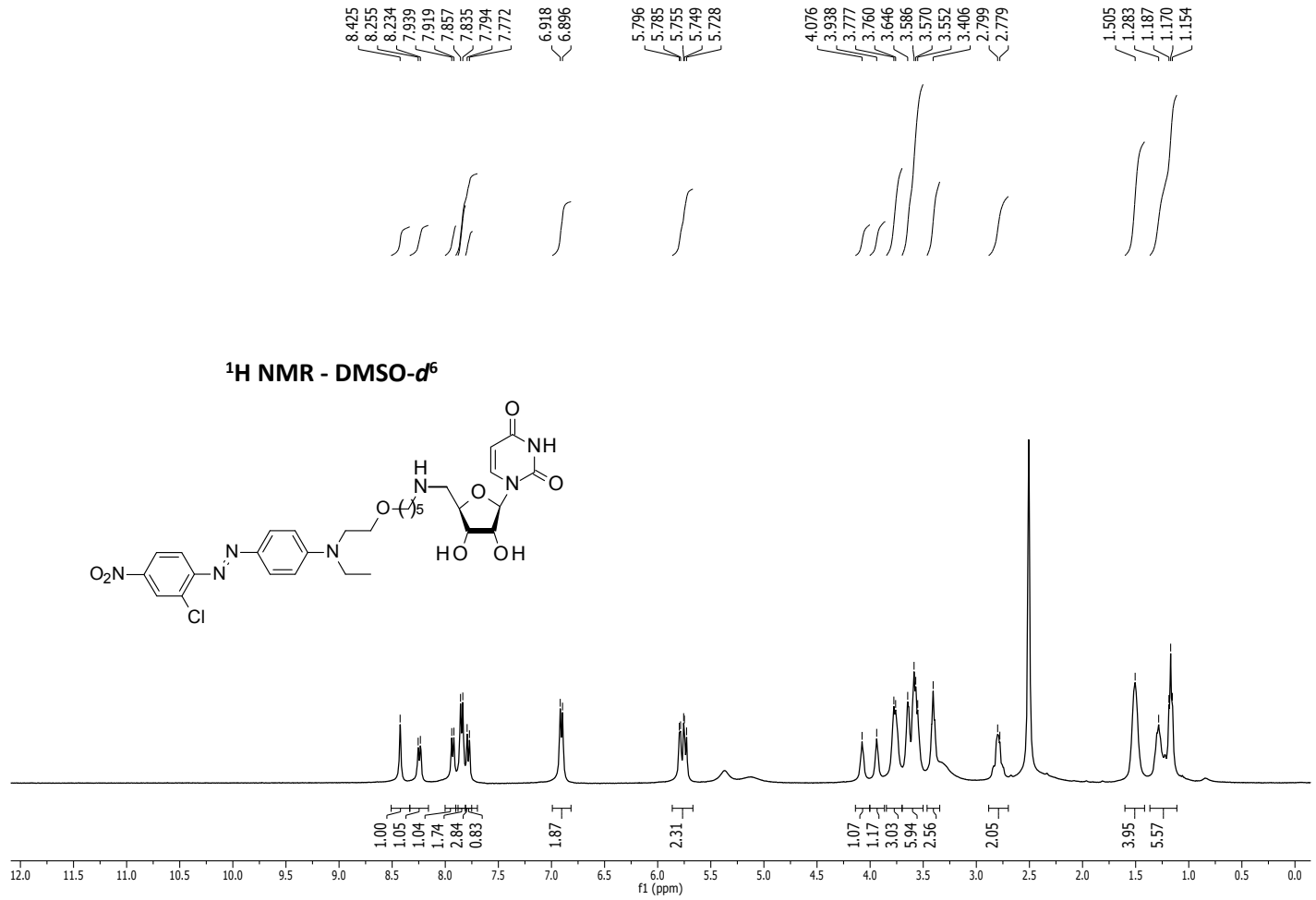
^{1}H NMR and ^{13}C NMR spectra of **compound 26**

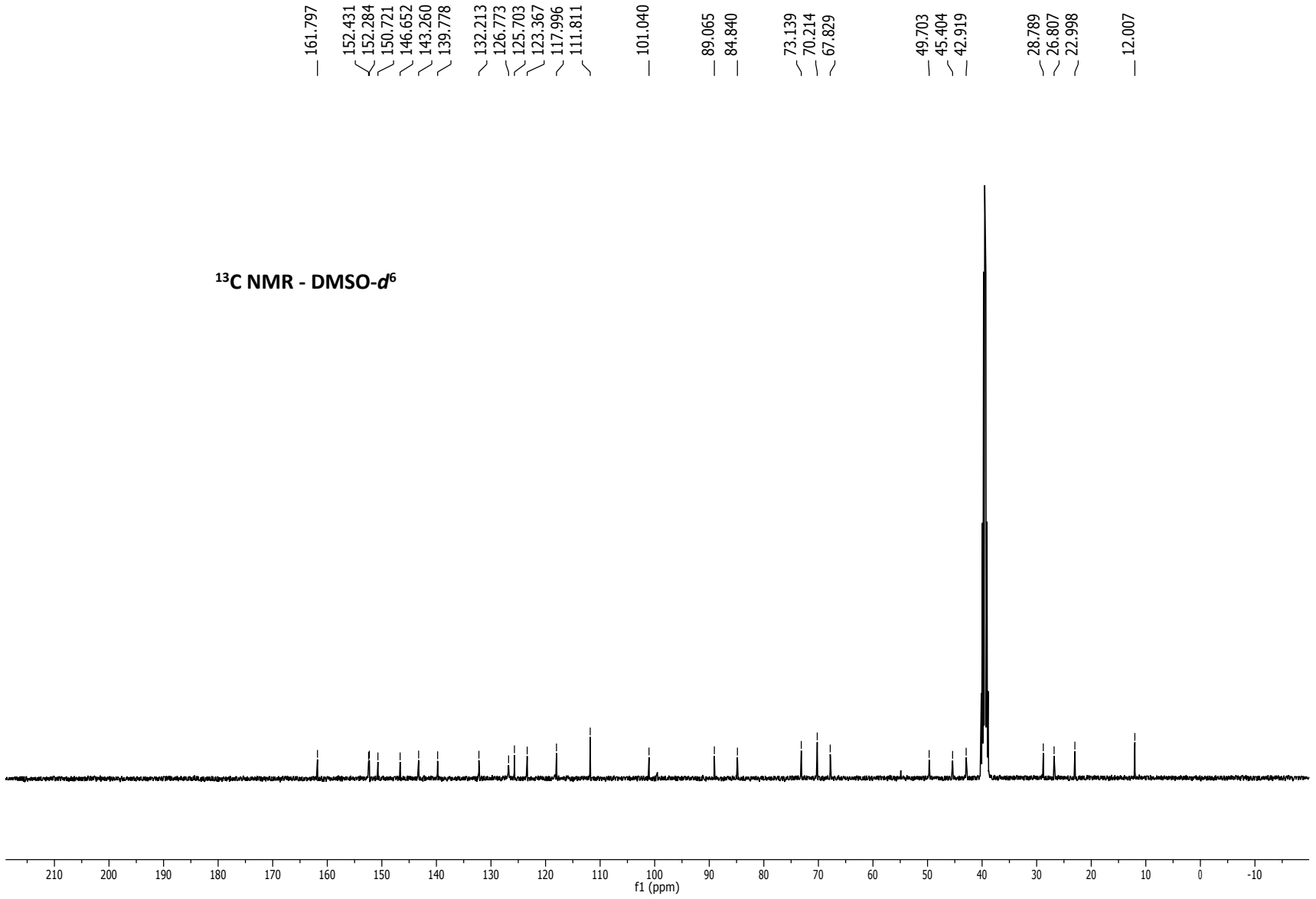


^{13}C NMR – $CDCl_3$

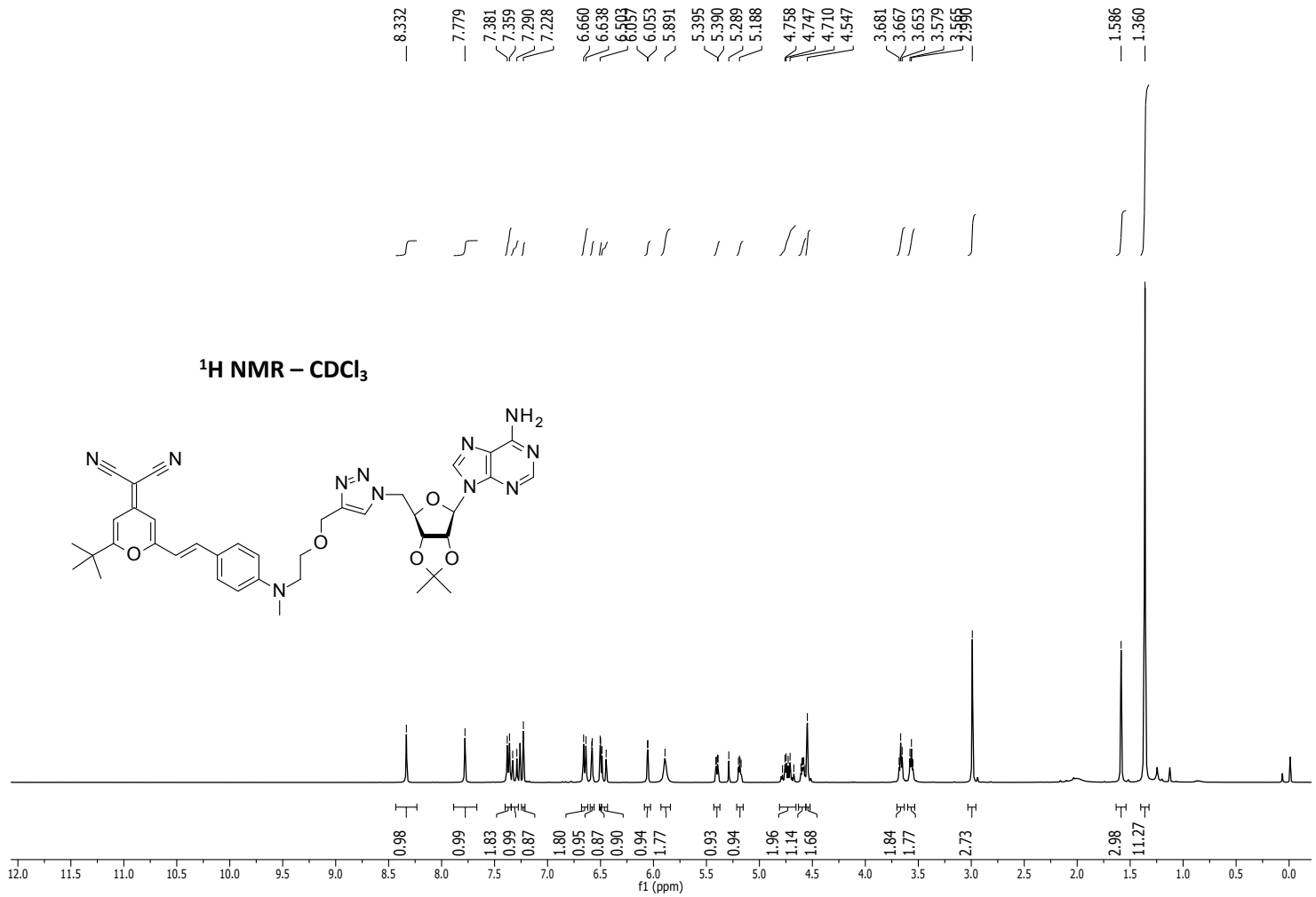


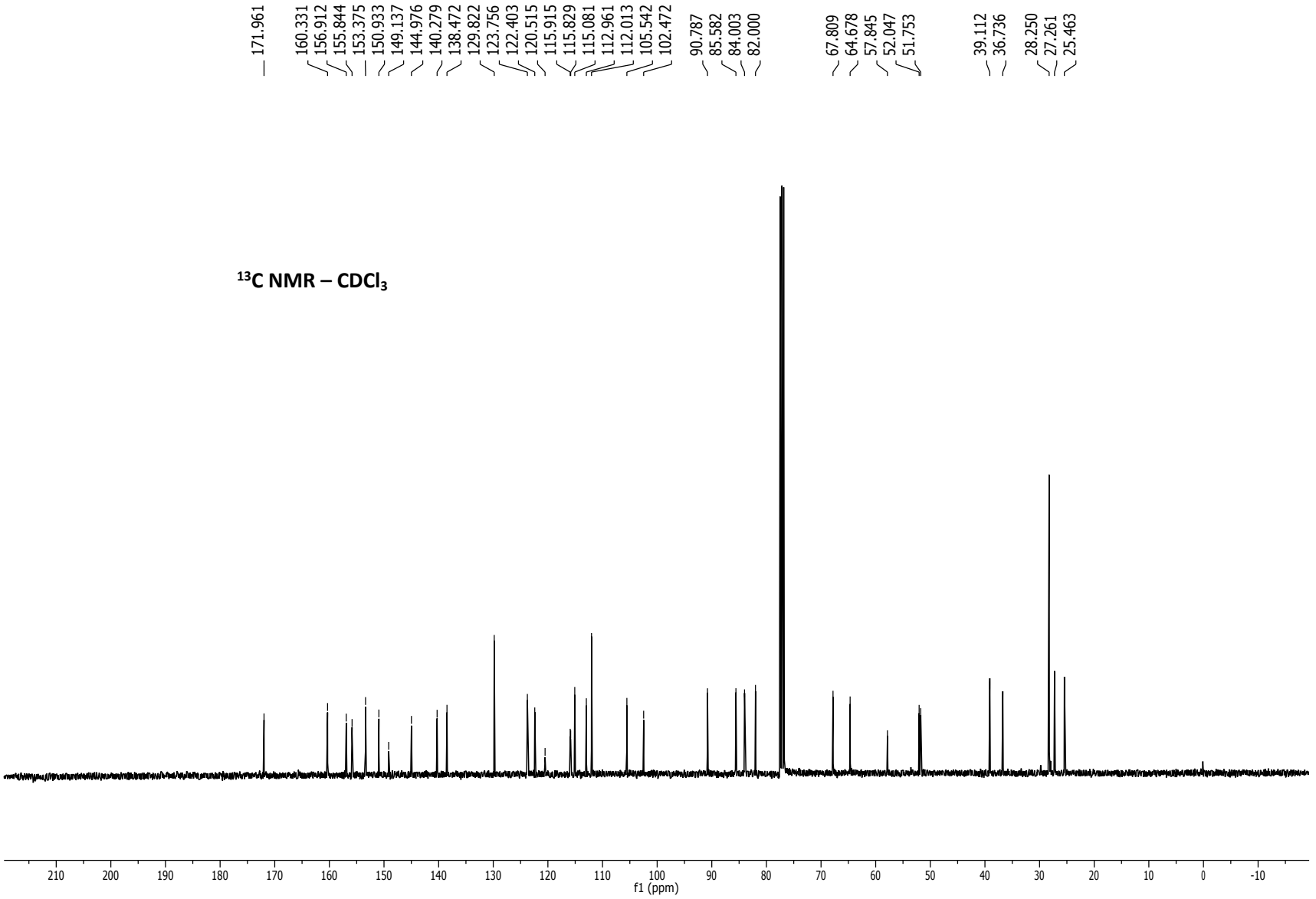
^{1}H NMR and ^{13}C NMR spectra of **compound 27**



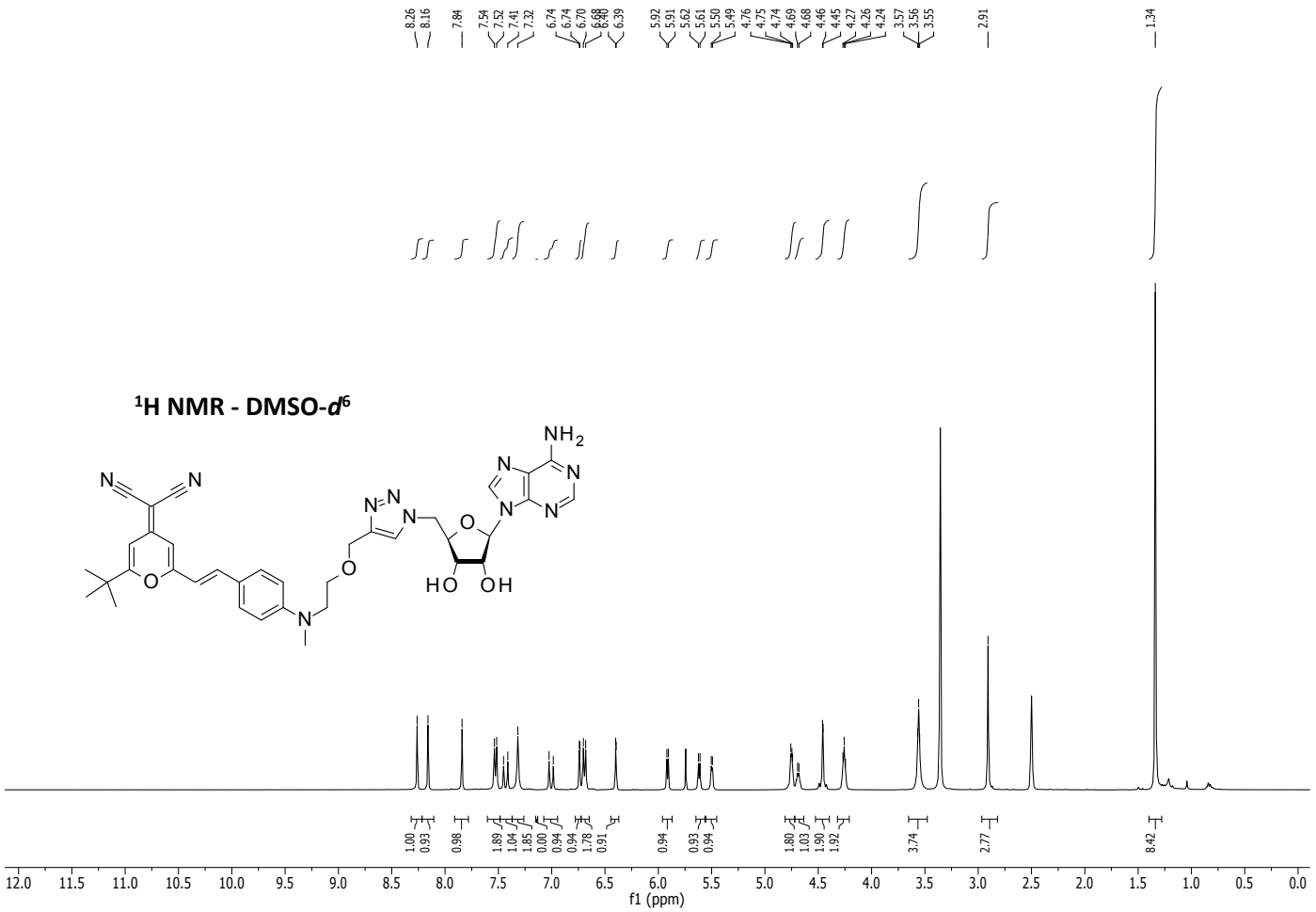

161.797
152.431
152.284
150.721
146.652
143.260
139.778
132.213
126.773
125.703
123.367
117.996
111.811
101.040
89.065
84.840
73.139
70.214
67.829
49.703
45.404
42.919
28.789
26.807
22.998
12.007
13C NMR - DMSO-d6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

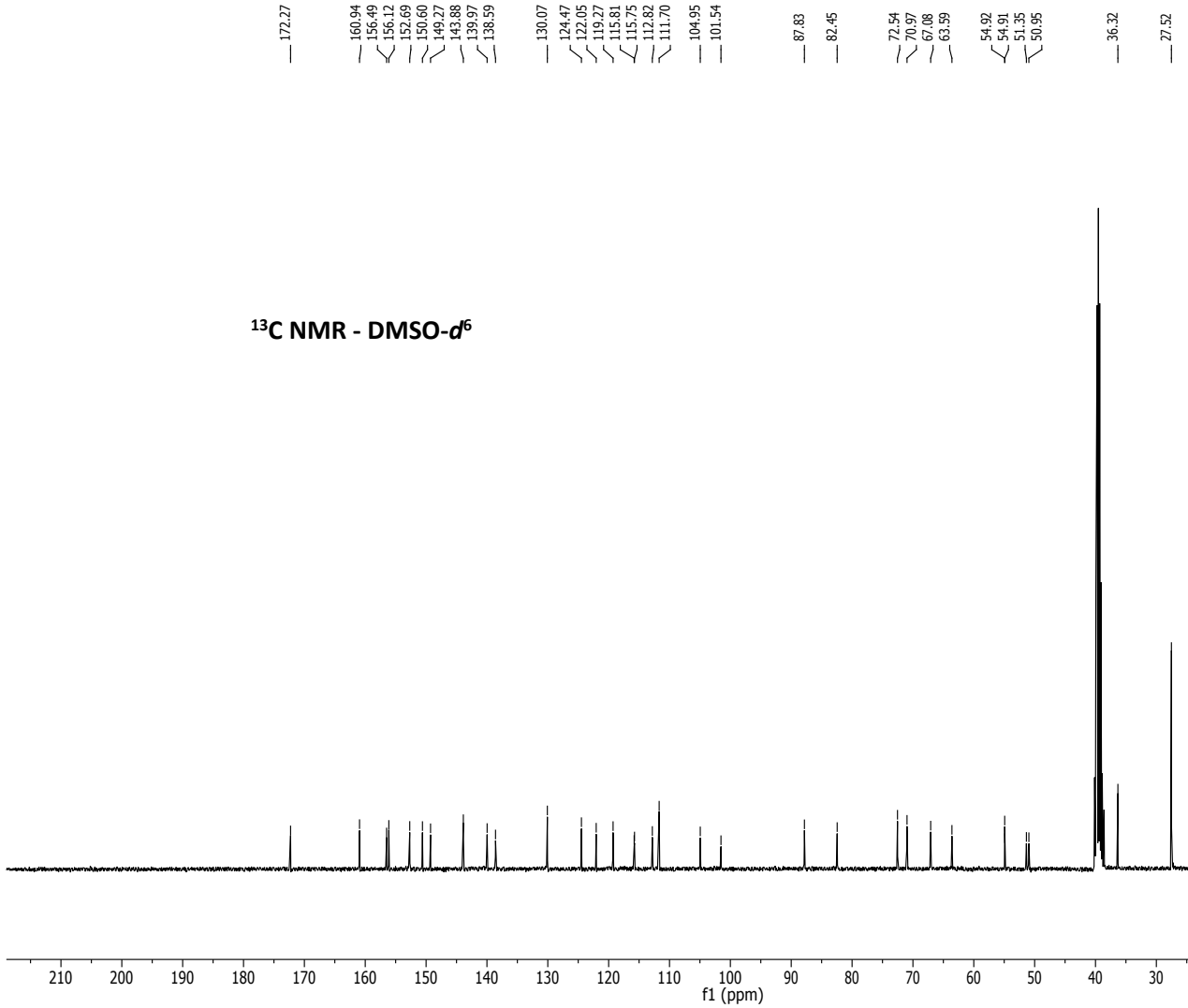
^{1}H NMR and ^{13}C NMR spectra of **compound 29**




171.961
160.331
156.912
155.844
153.375
150.933
149.137
144.976
140.279
138.472
129.822
123.756
122.403
120.515
115.915
115.829
115.081
112.961
112.013
105.542
102.472
90.787
85.582
84.003
82.000
67.809
64.678
57.845
52.047
51.753
39.112
36.736
28.250
27.261
25.463
^{13}C NMR – $CDCl_3$
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

^{1}H NMR and ^{13}C NMR spectra of **compound 30**





^{13}C NMR - DMSO-*d*^{6}

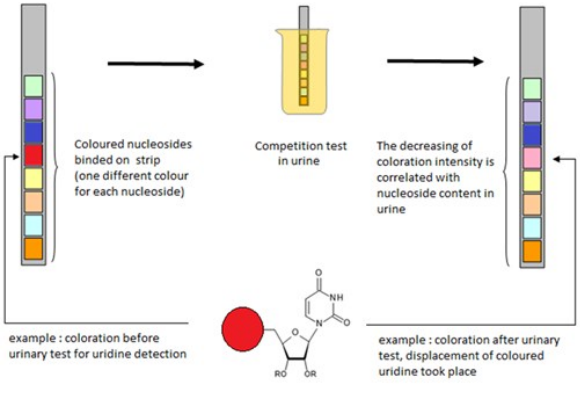


Figure S1. Illustration of competition test between a red coloured nucleoside immobilized on a dipstick and urinary uridine homologue. The test strip is immersed to the urine, and the red coloration located on a small square field decreased according the concentration of urinary nucleoside. The resulting colour of the field would indicate normal or abnormal level of biomarker.

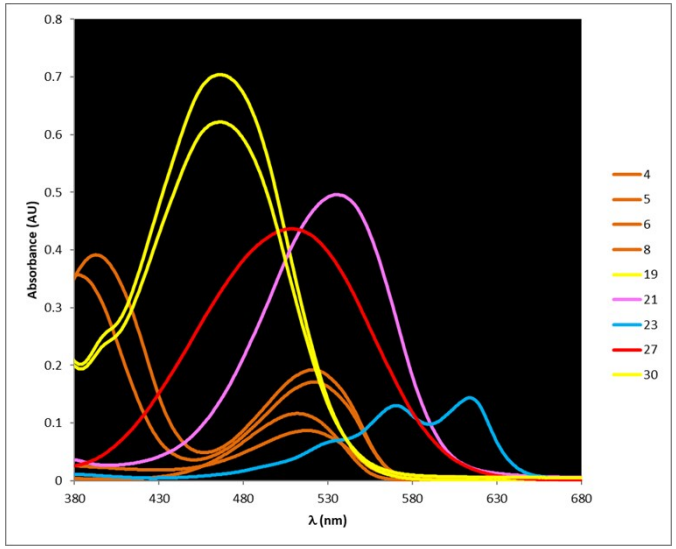


Figure S2. Absorbance spectra for 5′-tagged-nucleosides: **4, 5, 6, 8, 19, 21, 23, 27** and **30** in CH_3CN (except **23** in MeOH), at 400 µM for tetrazine substituted nucleosides and at 20 µM for others.

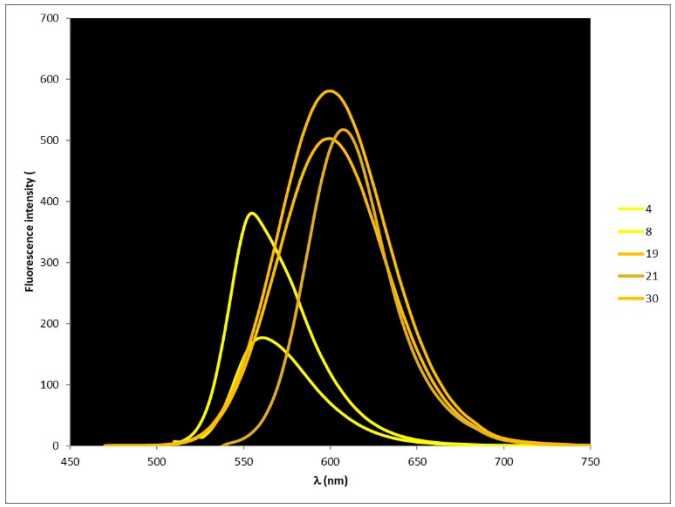


Figure S3. Fluorescence spectra for 5'-tagged-nucleosides: **4**, **8**, **19**, **21**, **30** in CH_3CN (except **23** in MeOH), at 200 µM for tetrazine substituted nucleosides and at 2 µM for others.

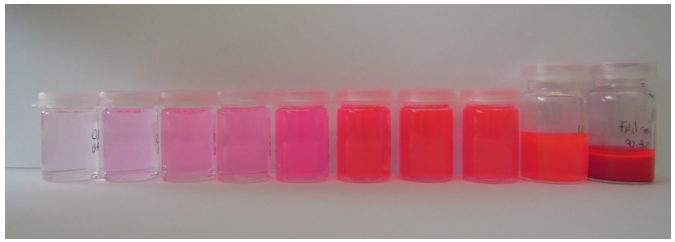


Figure S4. Picture of the solutions prepared for the UV measurements of **20** (from left to right: 2 µM, 5 µM, 8 µM, 10 µM, 20 µM, 40 µM, 60 µM, 80 µM, 0.1 mM and 1.47 mM in ACN)

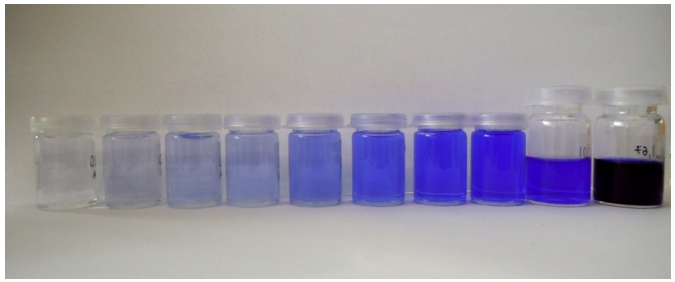


Figure S5. (up) Picture of the solutions prepared for the UV measurements of **22** (from left to right: 2 µM, 5 µM, 8 µM, 10 µM, 20 µM, 40 µM, 60 µM, 80 µM, 0.1 mM and 1.67 mM in ACN); (down) Picture of **22** in ACN at 0.1 mM.

Figure S6. (up) Picture of the solutions prepared for the UV measurements of **26** (from left to right: 2 µM, 5 µM, 8 µM, 10 µM, 20 µM, 40 µM, 60 µM, 80 µM, 0.1 mM and 1.43 mM in ACN); (down) Picture of **26** in ACN at 0.1 mM.