Supporting Information

tert-Butyl Nitrite-Induced Radical Nitrile Oxidation Cycloaddition: Synthesis of Isoxazole/Isoxazoline-Fused Benzo 6/7/8-membered Oxacyclic Ketones

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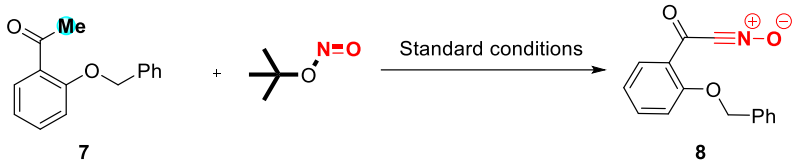
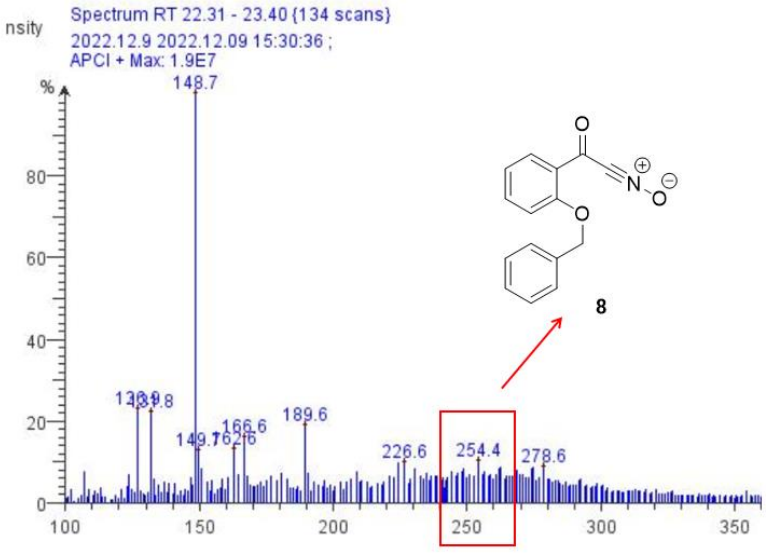
1. Evidence in support of the hypothetic mechanism

To gain further insight into the reaction mechanism, some control experiments were performed as illustrated in **Scheme S1**. To address the possible reaction intermediate, 1-(2-(benzyloxy)phenyl)ethan-1-one (**7**) was reacted under the standard conditions for 20 mins, nitrile oxides (**8**) could be detected by MS (APCI) (Schemes S1 and S2).



7 8

Scheme S1. Control experiment of **7** with TBN.



Scheme S2. The MS(APCI) results for the reaction of **7** was reacted under the standard conditions for 20 mins.

2. X-ray crystal structure and crystallographic data

The purified compound **2a** is dissolved in chloroform and petroleum ether, and placed in a dark cabinet to slowly evaporate. After several days, a white bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart APEX CCD area detector diffra ctometer at 296(2) K.

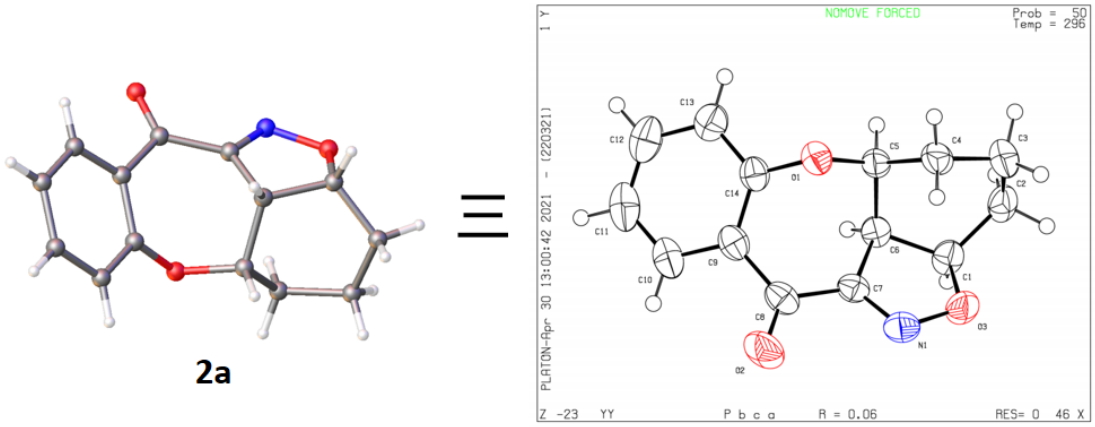


Figure S1. X-ray crystal structure of compound **2a** (displacement ellipsoids are drawn at the 50% probability level).

Table S1. Crystal data and structure refinement for compound **2a**

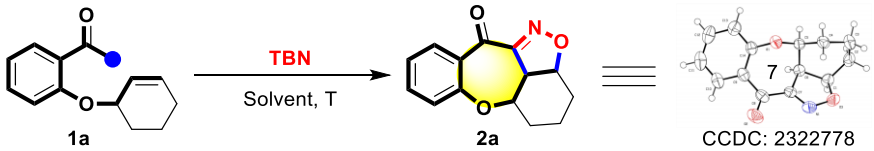
Identification code	CCDC: 2322778
Empirical formula	$C_{14}H_{13}NO_3$
Formula weight	243.09
Temperature/K	296 (2)
Crystal system	monoclinic
Space group	C2/c
a/Å	10.959 (6)
b/Å	10.915 (7)
c/Å	19.007 (11)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2274 (2)
Z	8
ρ_{calc}g/cm^3	1.421
μ/mm^{-1}	0.101
F(000)	1024.0

3. Experimental Procedures

3.1 Optimization of reaction conditions for the synthesis of ethyl 9-oxo-3,3a-dihydro-9*H*-chromeno[3,2-*c*]isoxazole-3-carboxylate

To evaluate our proposed assumption, **1a** was selected as the starting material for the optimization of the reaction conditions (**Table S2**). We initiated our investigation by performing the reaction of **1a** with TBN. At first, several different solvents were selected to optimize the reaction. The results showed that only when DMSO was used as solvent to participate in the reaction, the target product was generated. To our delight, DMSO as the solvent at 80 °C for 10 h led to a 95% yield (Table S2, entry 7). Subsequently, different temperature were screened for further increasing the reaction conversion. When the temperature was screened below 80 °C, the yield was significantly reduced (entries 8-10). As a further investigation, we screened the effect of reaction time for this annulation reaction (entries 11-13). After a series of screening, it was found that this reaction is best achieved using **1a** (0.2 mmol), TBN (0.8 mmol) at 80 °C for 10 h (entry 7).

Table S2. Optimization of the reaction conditions for **2a**[a].



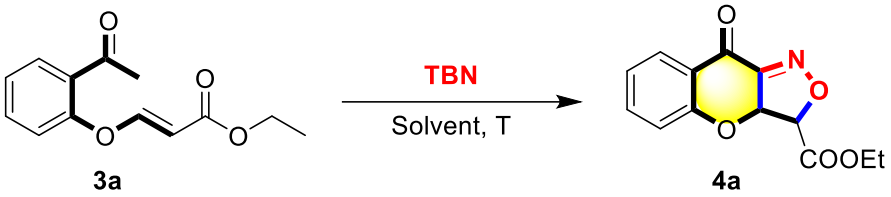
Entry	Solvent	T (°C)	*t*-BuONO	Yield[b] (%)
1	DMSO	80	3.0 equiv	82
2	Toluene	80	3.0 equiv	N.P.
3	Dioxane	80	3.0 equiv	N.P.
4	DEC	80	3.0 equiv	N.P.
5	MeCN	80	3.0 equiv	N.P.
6	DMSO	80	2.0 equiv	78
7	**DMSO**	**80**	**4.0 equiv**	**95**
8	DMSO	70	4.0 equiv	83
9	DMSO	60	4.0 equiv	79
10	DMSO	50	4.0 equiv	73
11[c]	DMSO	80	4.0 equiv	78
12[d]	DMSO	80	4.0 equiv	85
13[e]	DMSO	80	4.0 equiv	88

[a] Reaction conditions: **1a** (0.2 mmol) and TBN (0.8 mmol) were heated in DMSO (2

mL) at 80 ºC for 10 h. [b] Isolated yields. [c] 6 h. [d] 8 h. [e] 12 h.

3.2 Optimization of reaction conditions for the synthesis of ethyl 9-oxo-3,3a-dihydro-9*H*-chromeno[3,2-*c*]isoxazole-3-carboxylate

Table S3. Optimization of the reaction conditions for **4a**[a].



3a **4a**

entry	solvent	T (°C)	*t*-BuONO	Yield[b](%)
1	DMSO	100	4.0 equiv.	50
2	DMSO	100	5.0 equiv.	63
3	DMSO	100	6.0 equiv.	65
4	DMSO	100	7.0 equiv.	76
5	DMSO	90	7.0 equiv.	82
6	**DMSO**	**80**	**7.0 equiv.**	**95**
7	DMSO	70	7.0 equiv.	87
8[c]	DMSO	80	7.0 equiv.	83
9[d]	DMSO	80	7.0 equiv.	86
10[e]	DMSO	80	7.0 equiv.	89

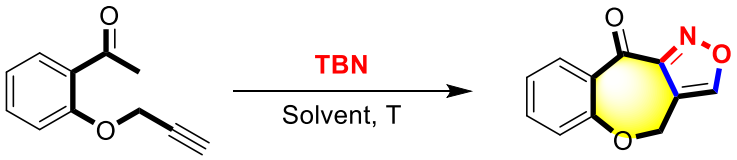
[a] Reaction conditions: **1a** (0.2 mmol) and TBN (1.4 mmol) were heated in DMSO (2 mL) at 80 °C for 10 h. [b] Isolated yields.[c] 6 h. [d] 8 h. [e]12 h.

We initiated our investigation by performing the reaction of ethyl (*E*)-3-(2-acetylphenoxy)acrylate **3a** with TBN. To our delight, DMSO as the solvent at 80 °C for 10 h led to 50% yield (Table S3, entry 1). Firstly, we optimized the equivalent of TBN in the reaction, and the results showed that increasing the amount of TBN can significantly improve the yield. When TBN reached 7 equiv, the yield of **4a** reached 76%. (Table S3, entry 2-4). To further improve the reactivity, different temperature were screened for further increasing the reaction conversion. When the reaction temperature is 80°C , the yield can reach a maximum of 95% (Table S3, entry 5-7). As a further investigation, we screened the effect of reaction time for this

annulation reaction (Table S3, entries 8-10).After a series of screening, it was found that this reaction is best achieved using **1a** (0.2 mmol), TBN (0.8 mmol) at 80 ºC for 10 h (entry 6).

3.3 Optimization of reaction conditions for the synthesis of ethyl 4*H*,10*H*-benzo[6,7]oxepino[4,3-*c*]isoxazol-10-one

Table S4. Optimization of the reaction conditions for **6a**[a].



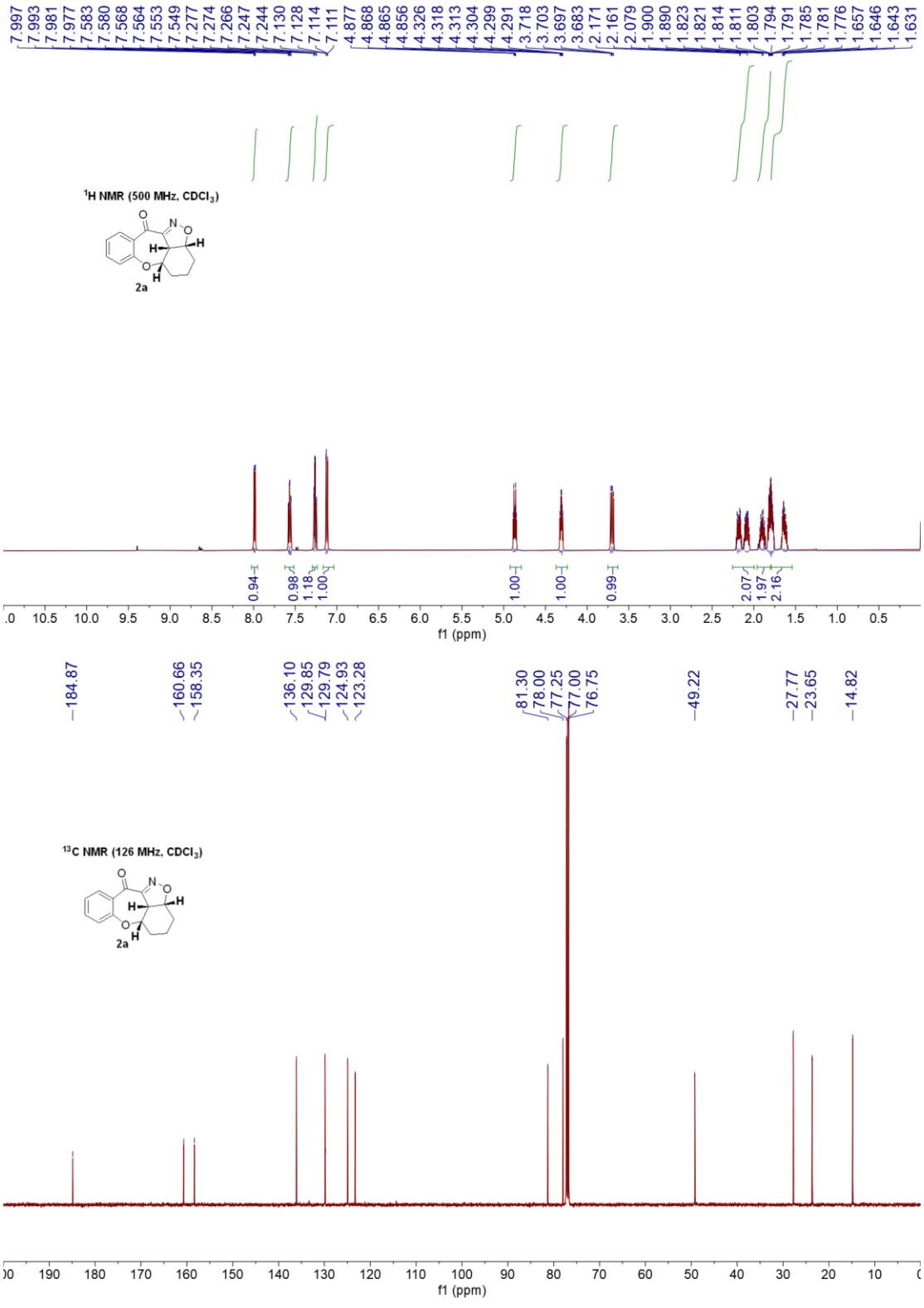
5a **6a**

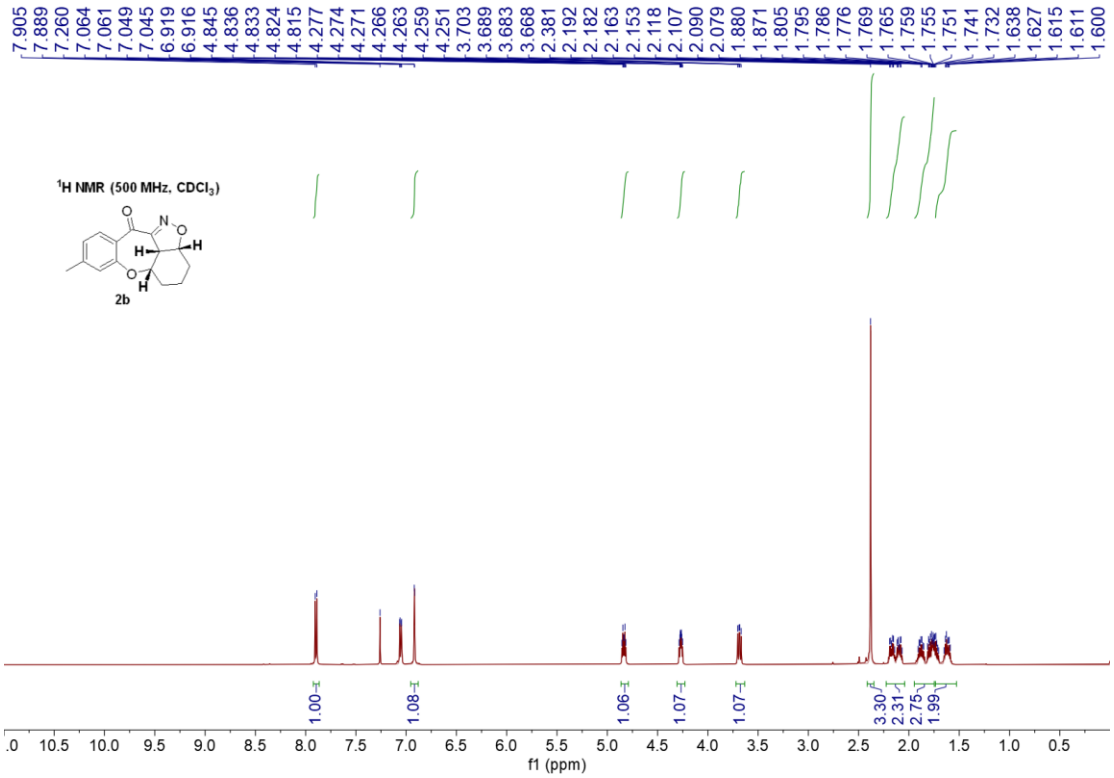
entry	solvent	*T* (°C)	*t*-BuONO	Yield[b](%)
1	DMSO	80	2.0 equiv.	63
2	DMSO	80	3.0 equiv.	70
3	DMSO	80	4.0 equiv.	74
4	**DMSO**	**80**	**5.0 equiv.**	**82**
5	DMSO	90	5.0 equiv.	77
6	DMSO	100	5.0 equiv.	72
7[c]	DMSO	80	5.0 equiv.	68
8[d]	DMSO	80	5.0 equiv.	75
9[e]	DMSO	80	5.0 equiv.	76

[a] Reaction conditions: **1a** (0.2 mmol) and TBN (1.0 mmol) were heated in DMSO (2 mL) at 80 °C for 10 h. [b] Isolated yields. [c]6 h. [d] 8 h. [e] 12 h.

We used 1-(2-(prop-2-yn-1-yloxy)phenyl)ethan-1-one **5a** as the starting material to react with TBN in DMSO. Fortunately, the reaction achieved a yield of 63% at 80 ºC for 10 h. (Table S4, entry 1). Firstly, we optimized the equivalent of TBN in the reaction, and the results showed that increasing the amount of TBN can significantly improve the yield. When TBN reached 5 equiv, the yield of **6a** reached 82%. (Table S4, entry 2-4). As a further investigation, we screened the effect of reaction temperature and reaction time for this annulation reaction (Table S4, entries 5-9). After a series of screening, it was found that this reaction is best achieved using **1a** (0.2 mmol), TBN (0.8 mmol) at 80 ºC for 10 h (entry 4).

4. Copy of 1H and 13C NMR Spectra of Products

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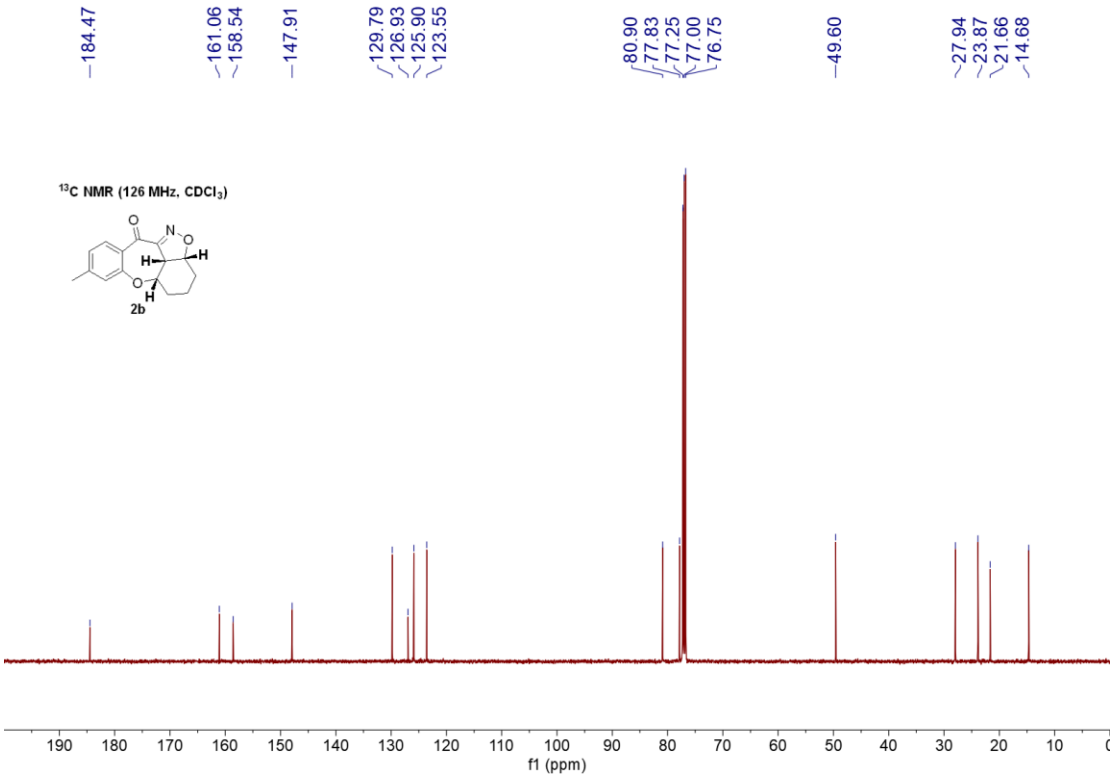
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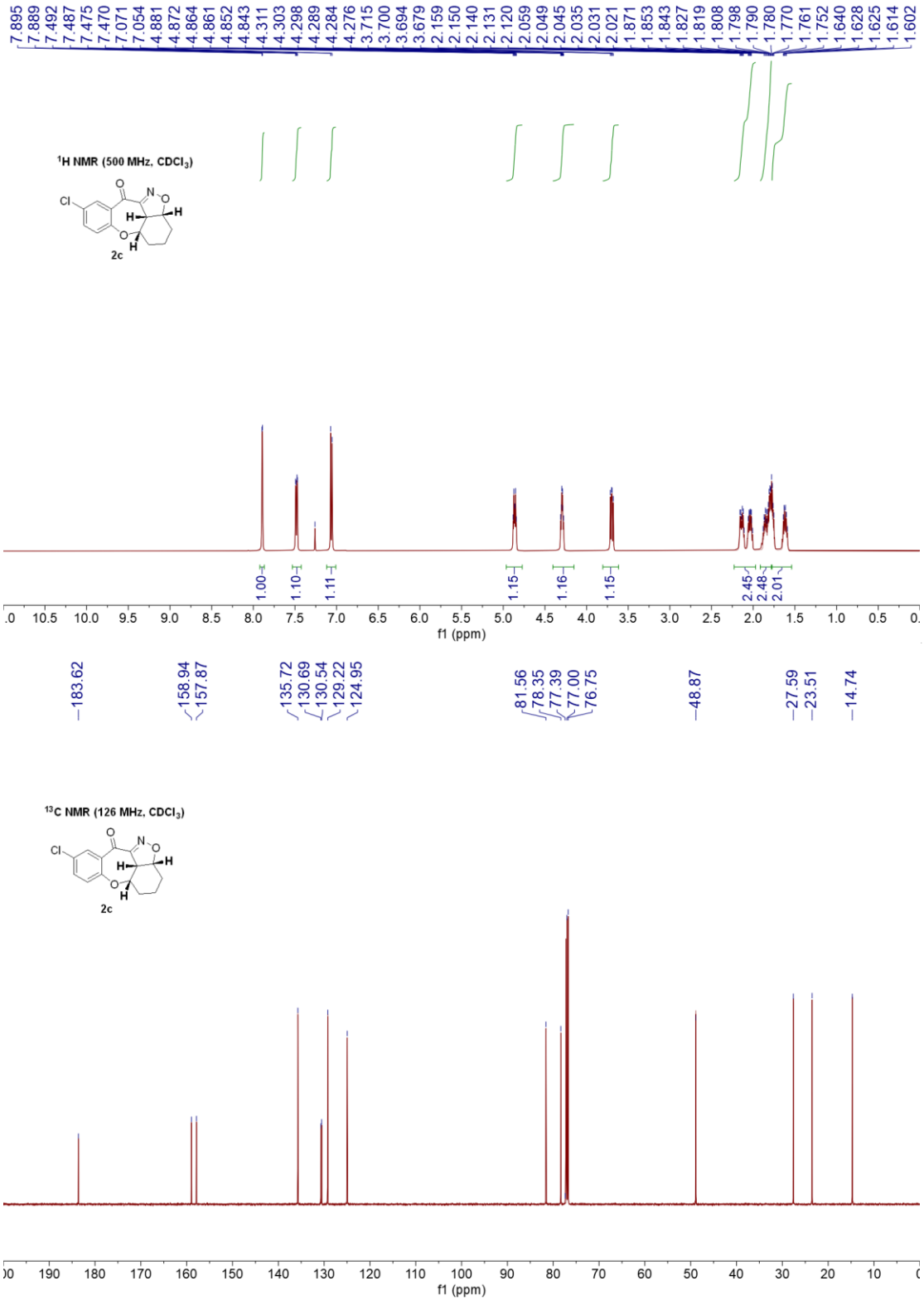
2b
f1 (ppm)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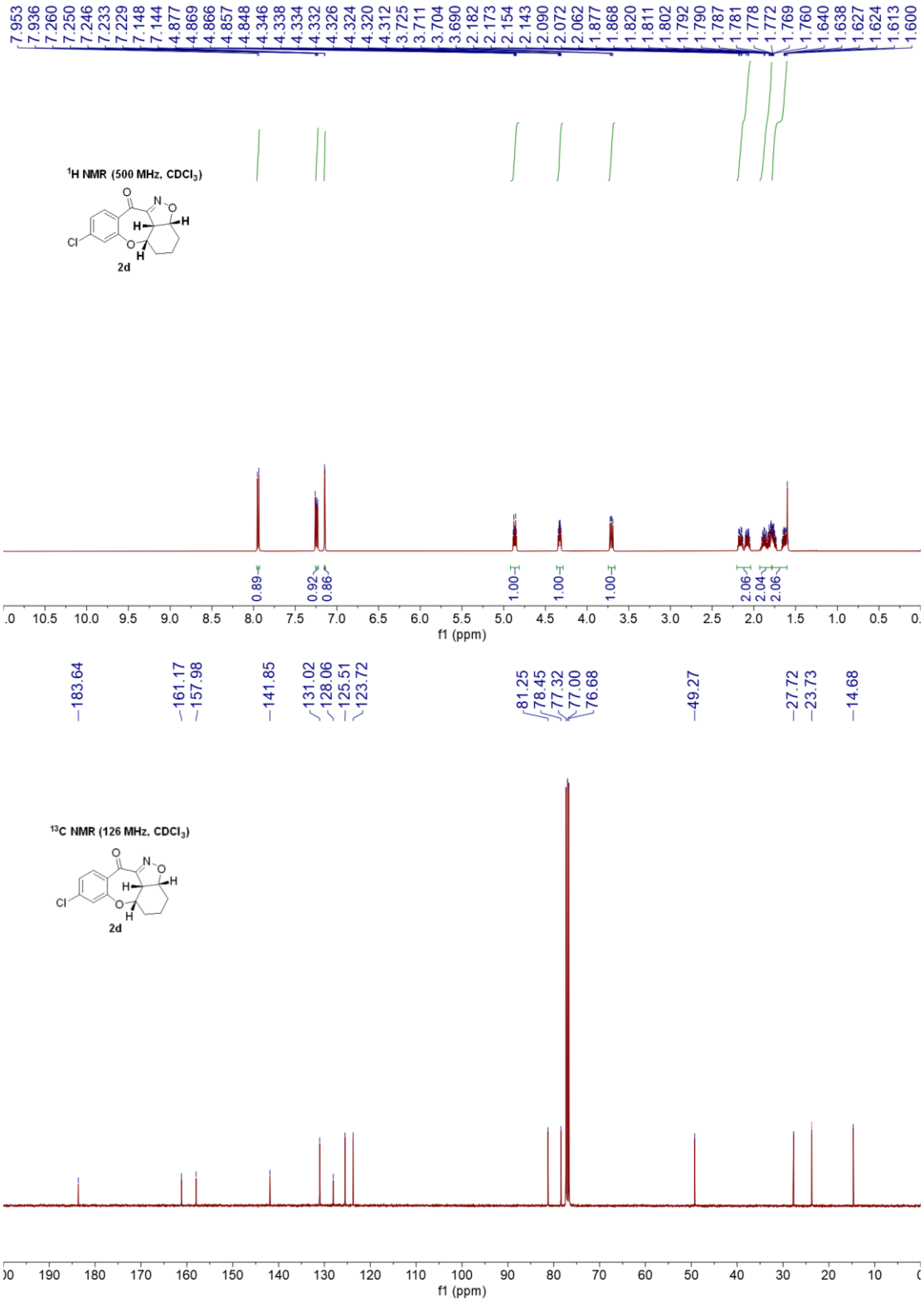
f1 (ppm)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1.624
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1.00
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2.06
f1 (ppm)
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2d
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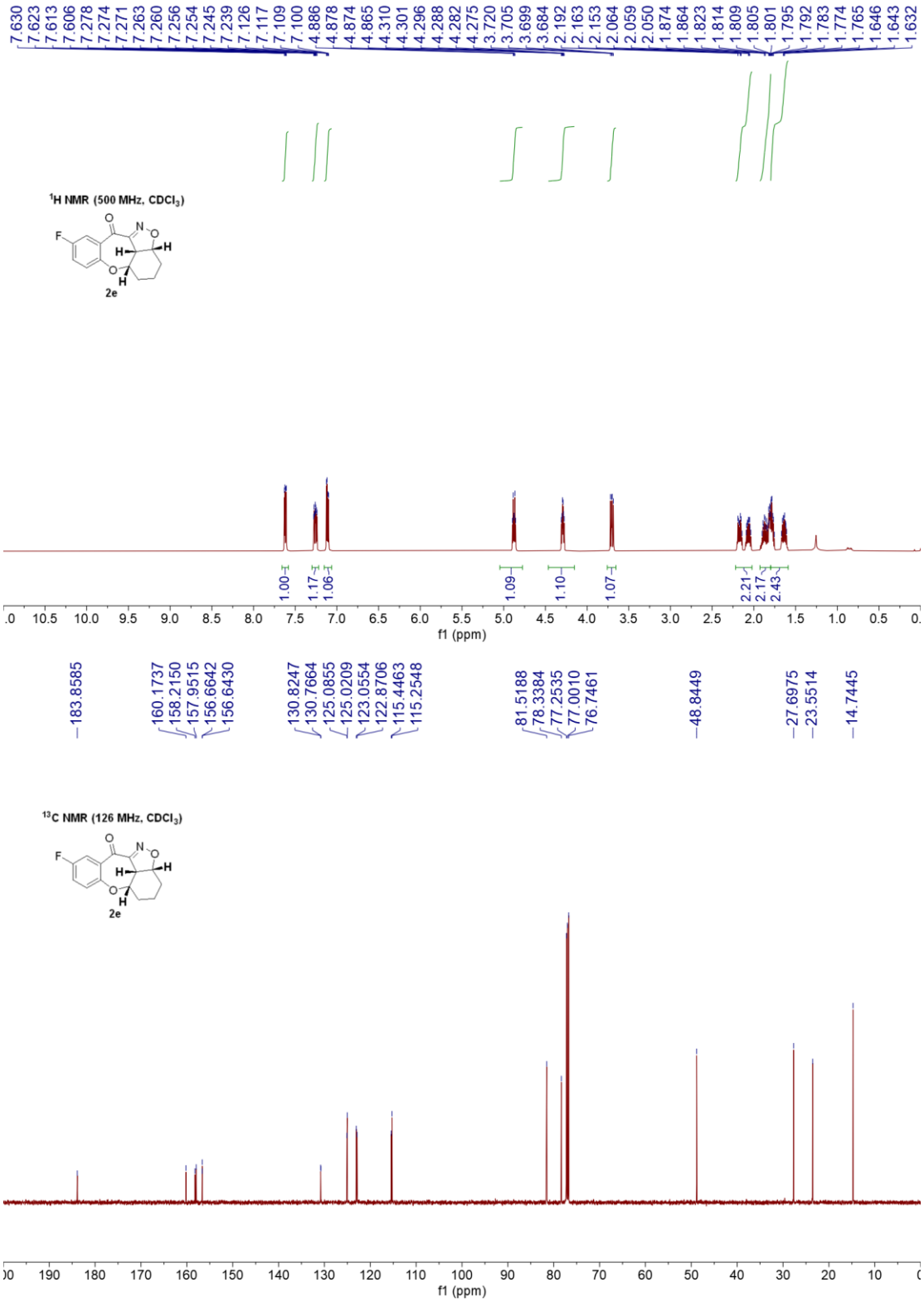
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1.07
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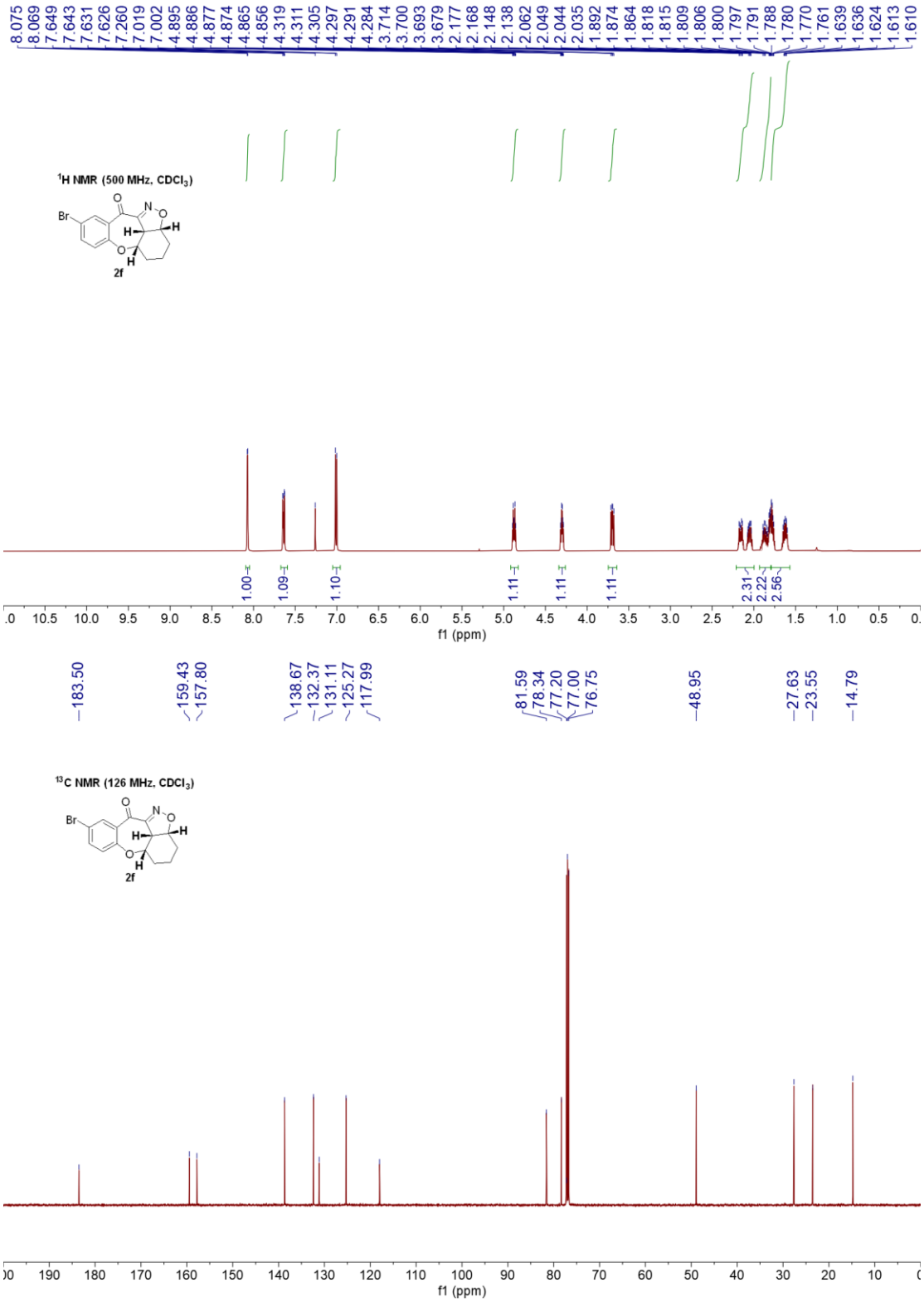
f1 (ppm)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1.11
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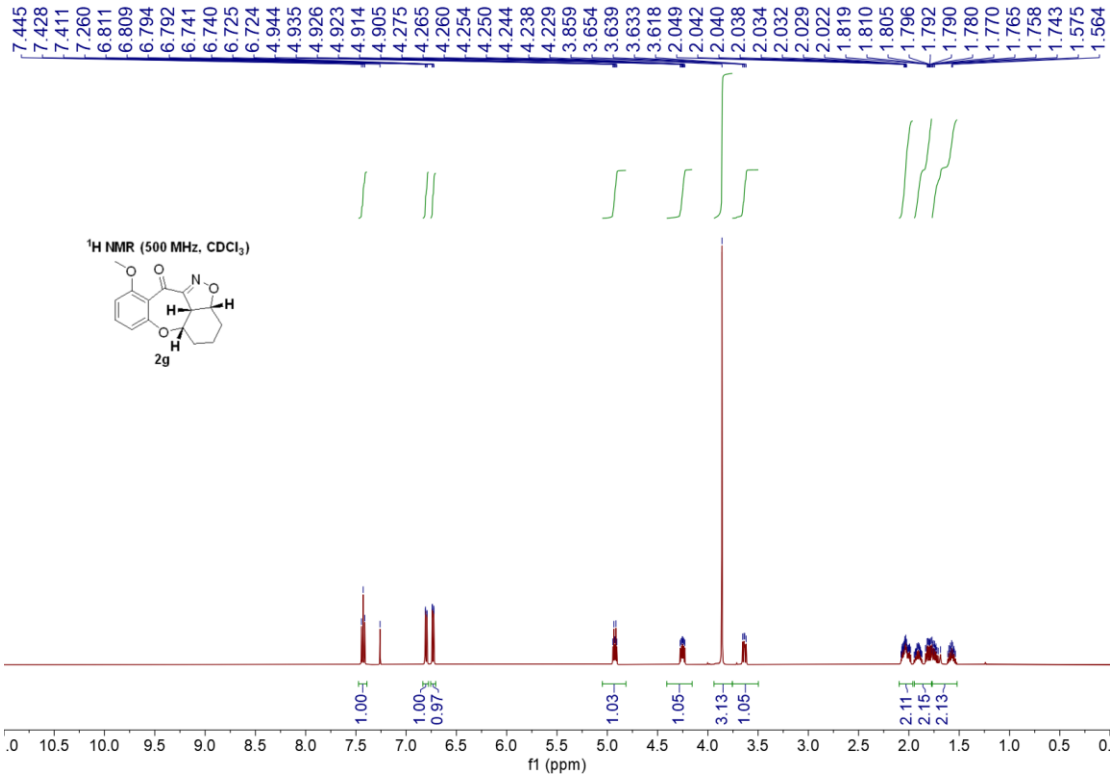
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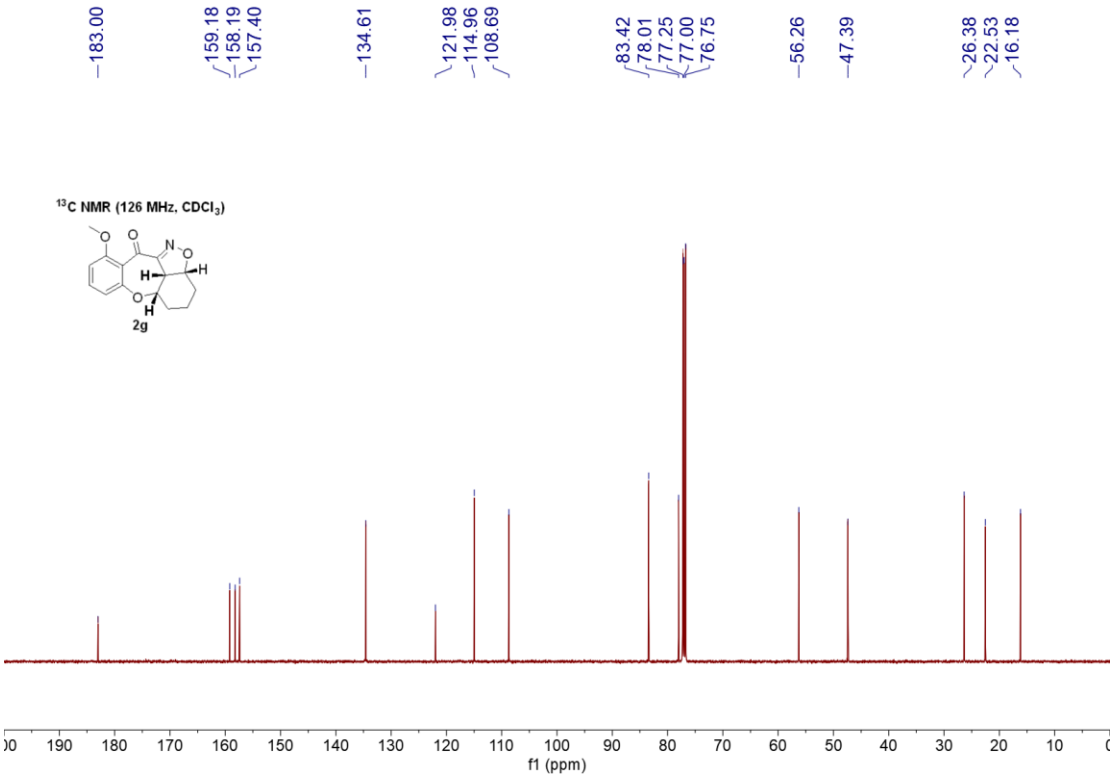
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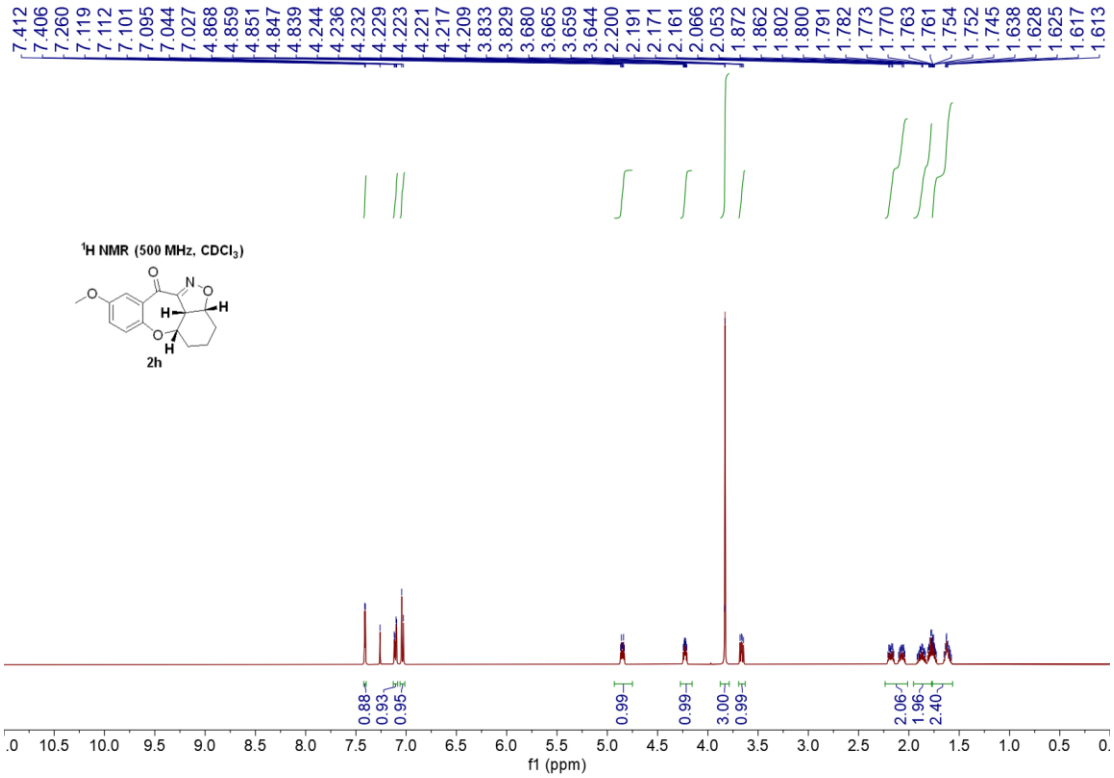
f1 (ppm)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3.644
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2.191
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1.625
1.617
1.613
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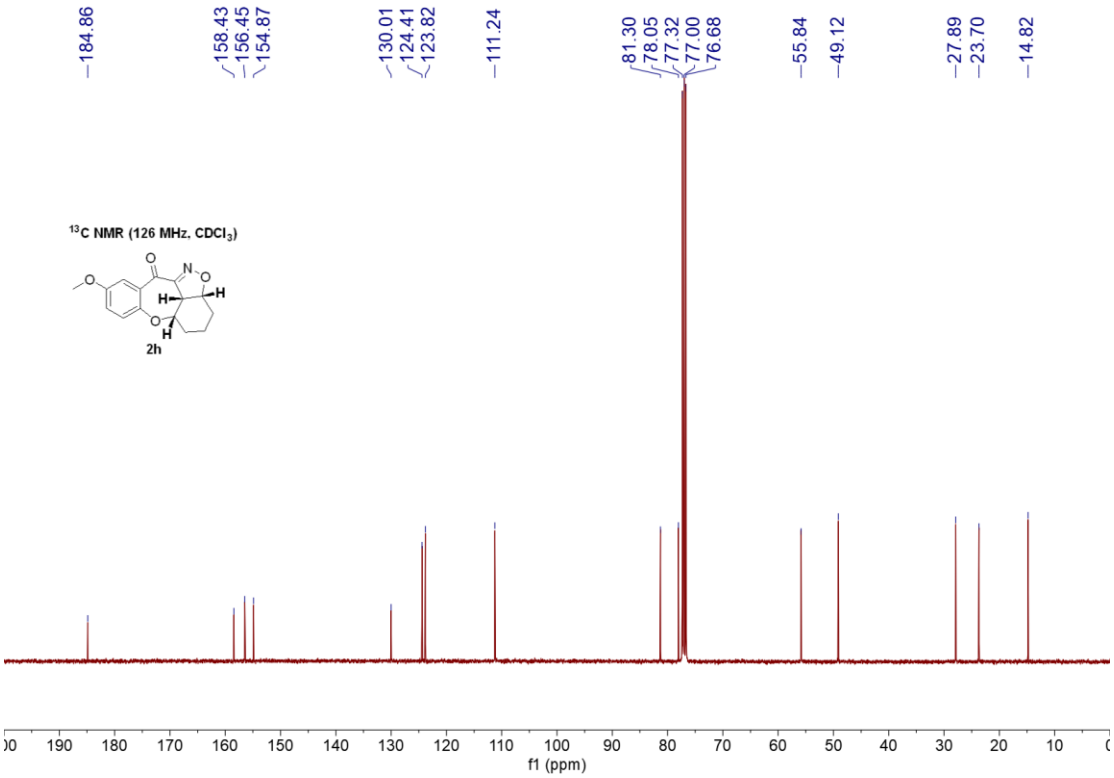
f1 (ppm)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27.89
23.70
14.82
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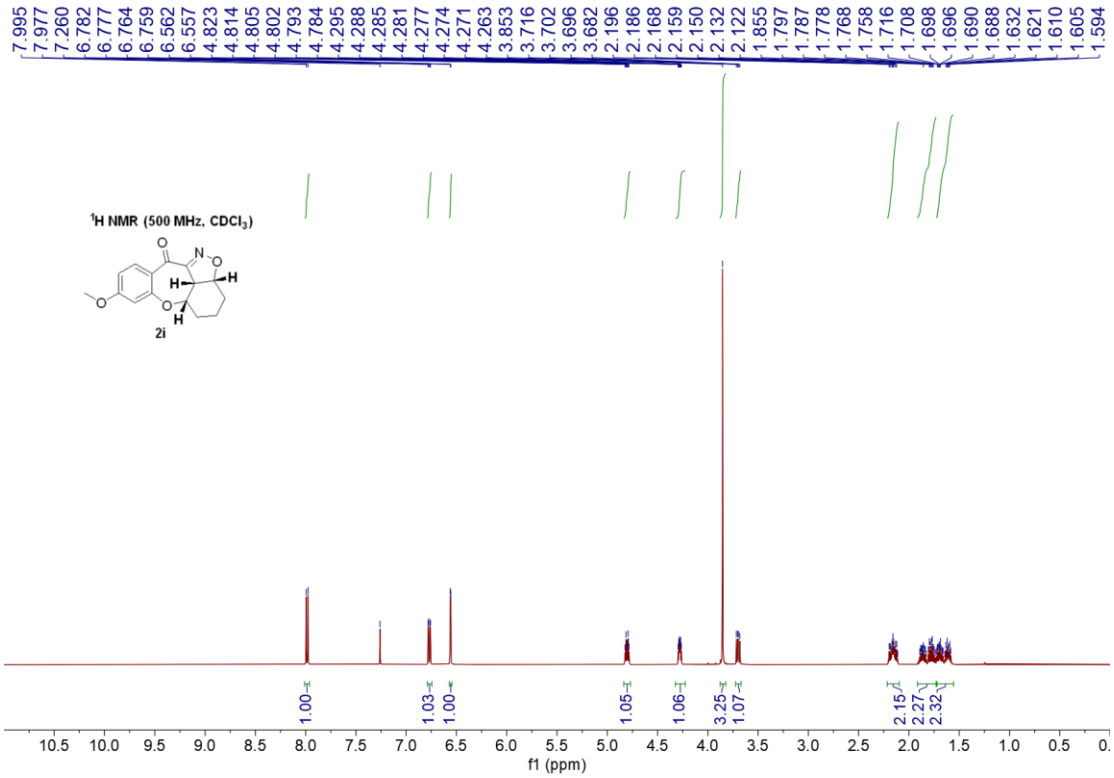
2h
f1 (ppm)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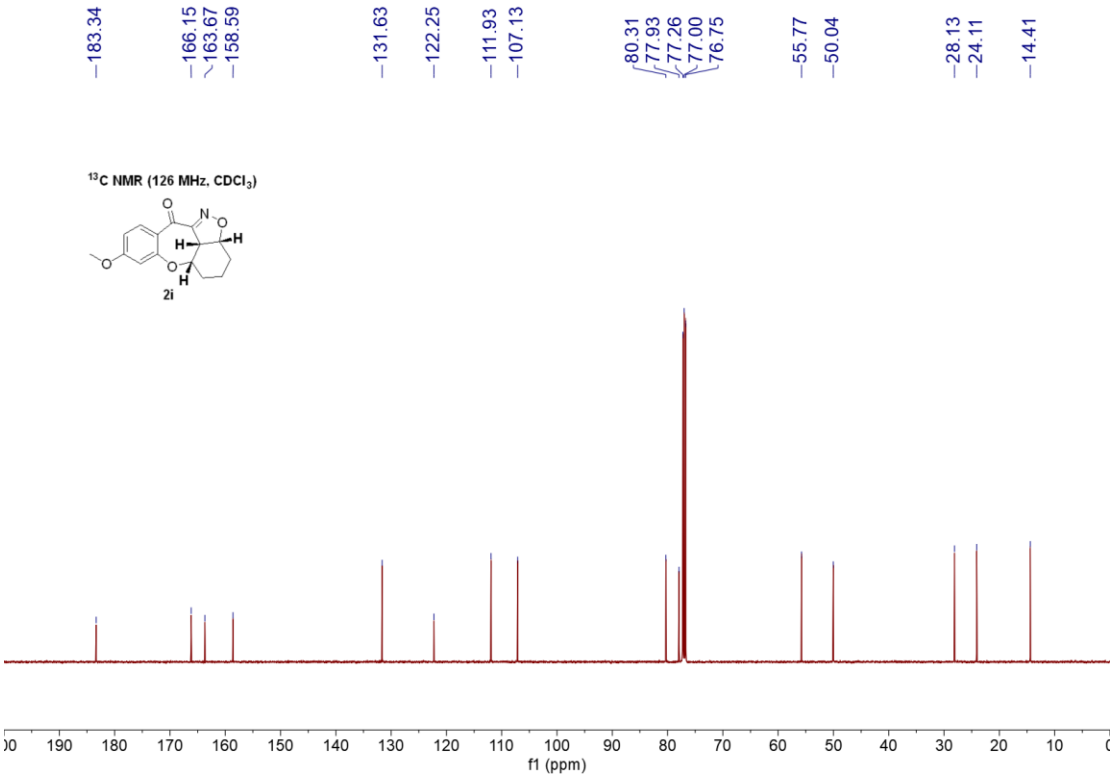
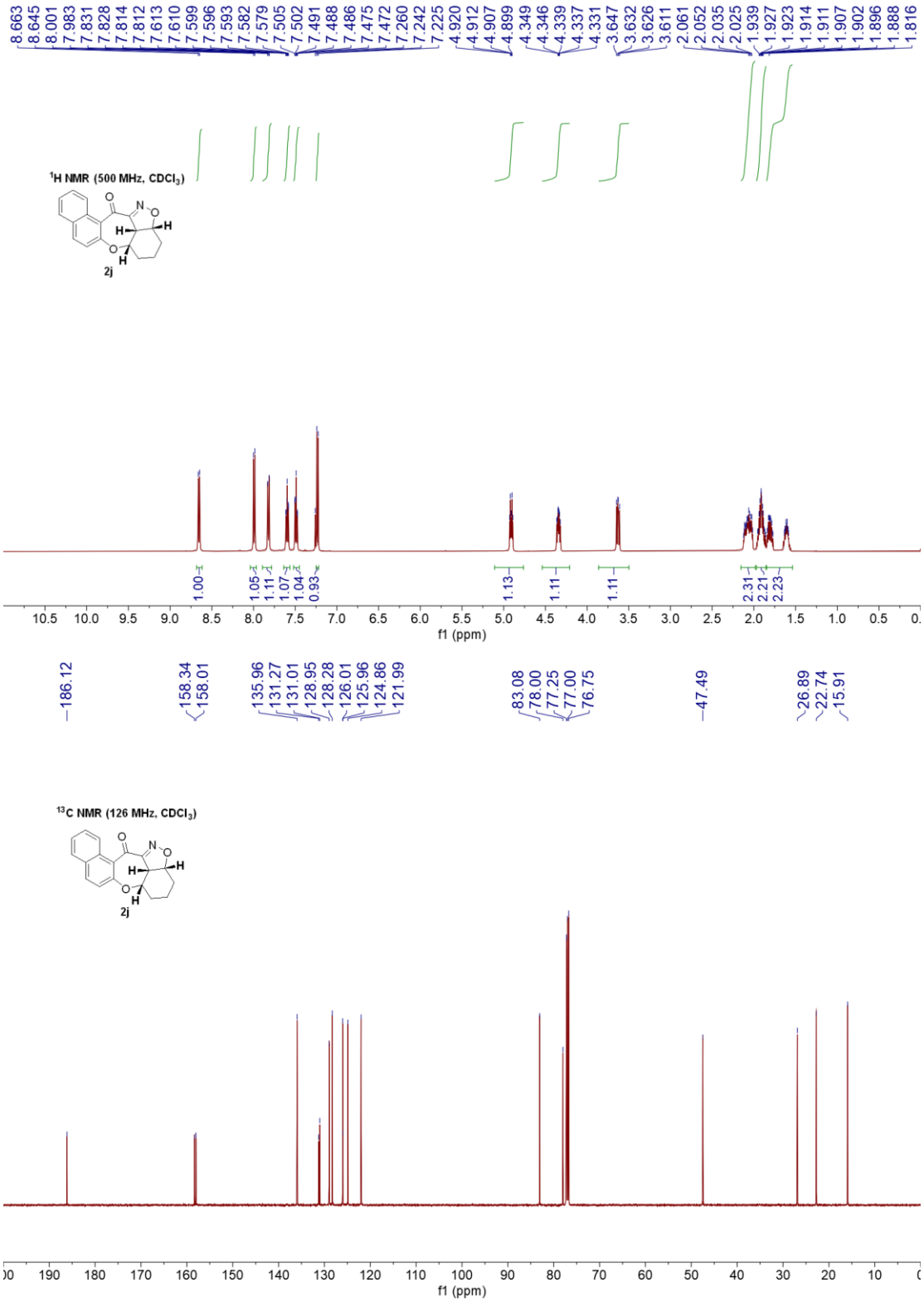
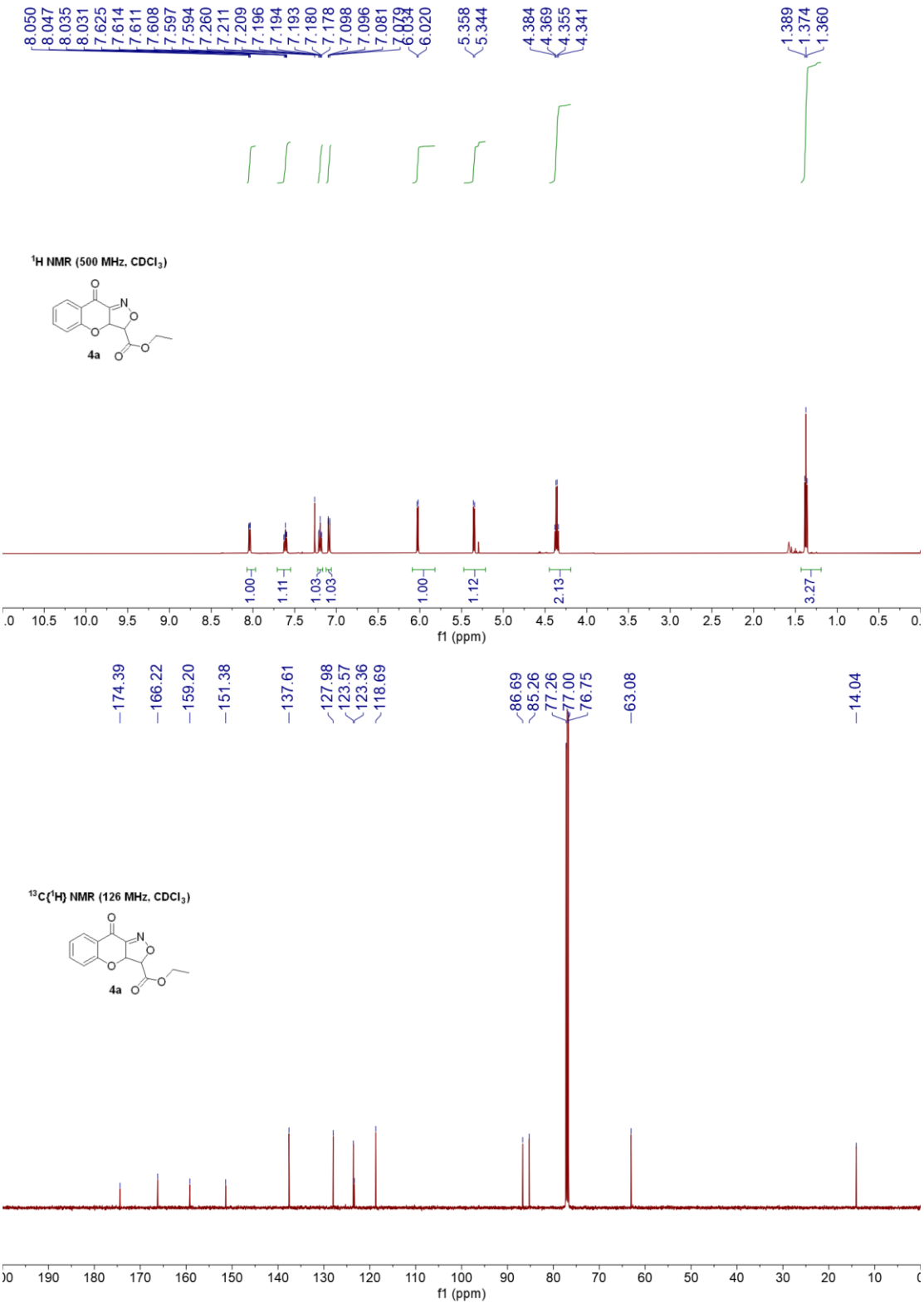
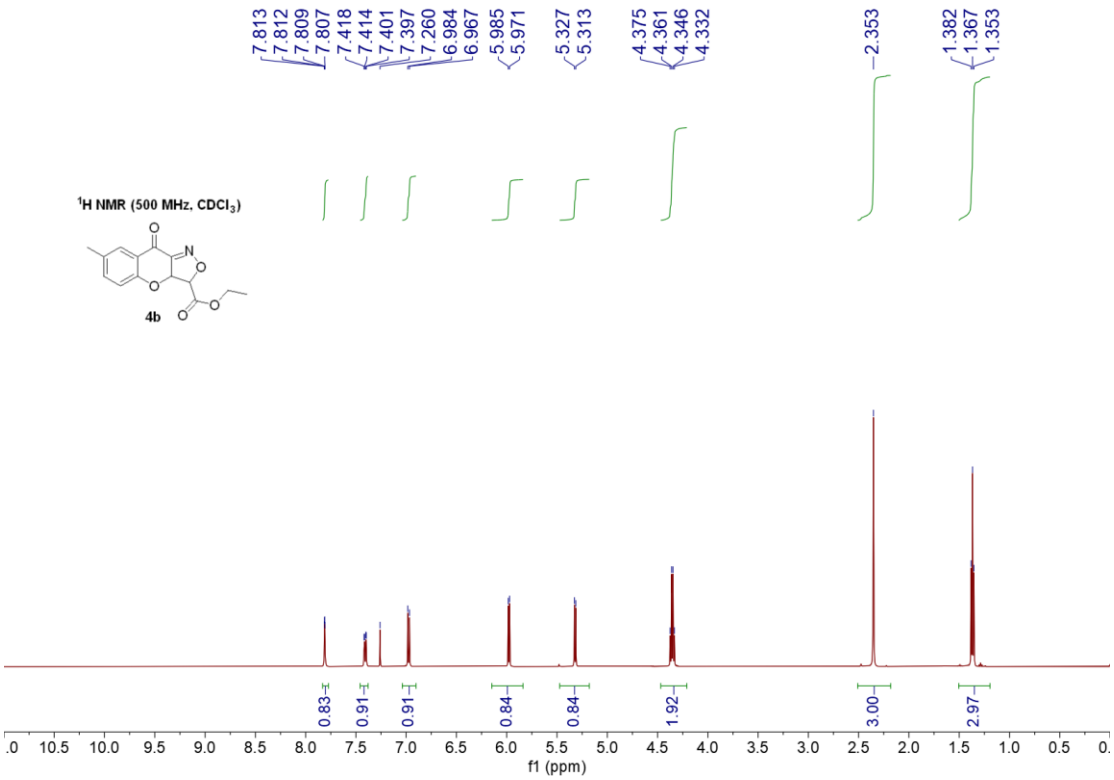
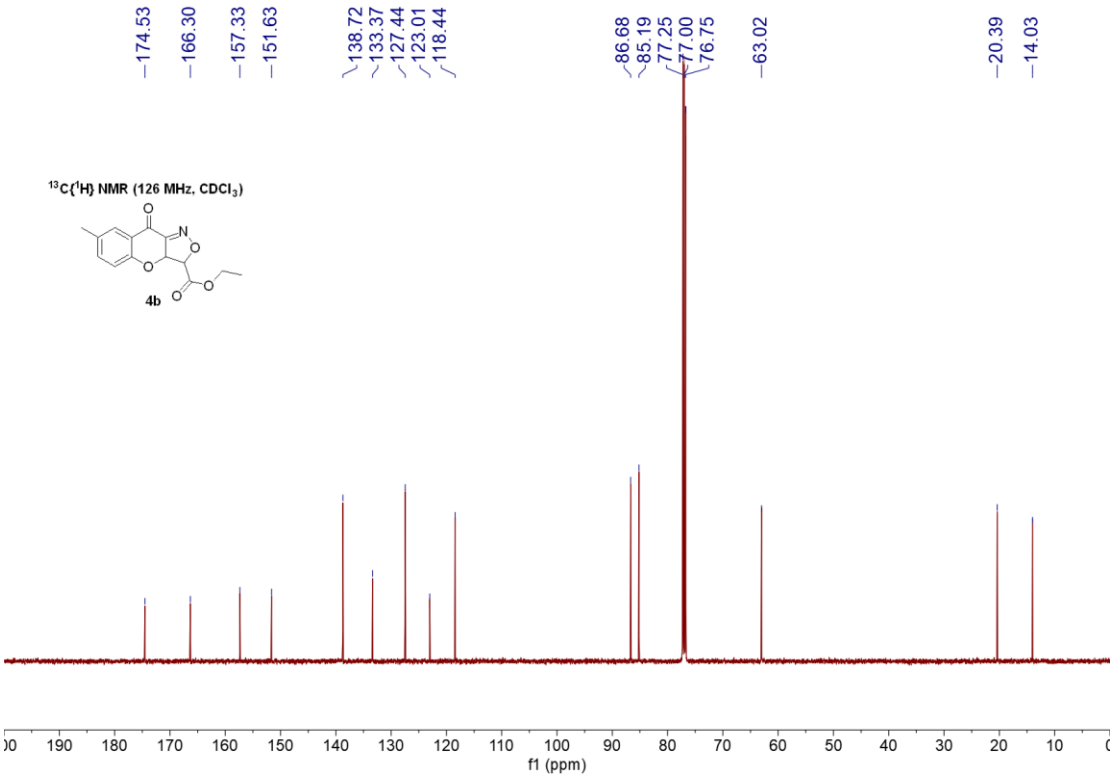
7.977
7.260
6.782
6.777
6.764
6.759
6.562
6.557
4.823
4.814
4.805
4.802
4.793
4.784
4.295
4.288
4.285
4.281
4.277
4.274
4.271
4.263
3.853
3.716
3.702
3.696
3.682
2.196
2.186
2.168
2.159
2.150
2.132
2.122
1.855
1.797
1.787
1.778
1.768
1.758
1.716
1.708
1.698
1.696
1.690
1.688
1.632
1.621
1.610
1.605
1.594
1H NMR (500 MHz, CDCl3)
2i
1.00
1.03
1.00
1.05
1.06
3.25
1.07
2.15
2.27
2.32
f1 (ppm)

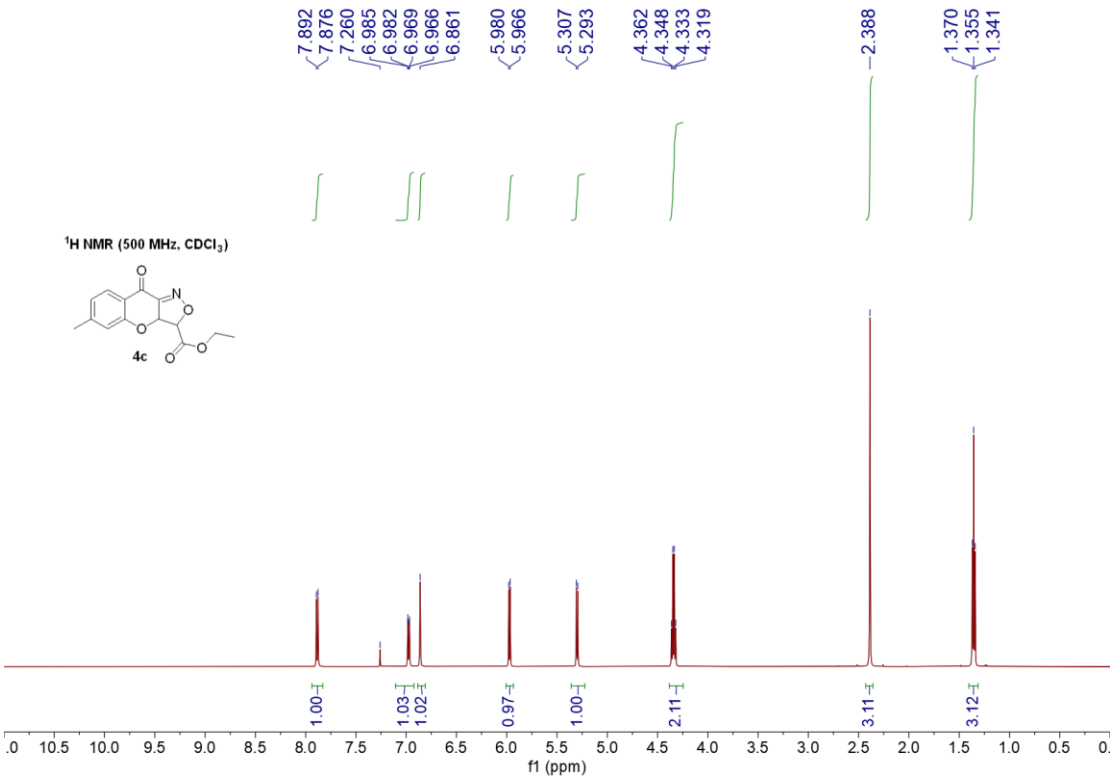

183.34
166.15
163.67
158.59
131.63
122.25
111.93
107.13
80.31
77.93
77.26
77.00
76.75
55.77
50.04
28.13
24.11
14.41
13C NMR (126 MHz, CDCl3)
2i
f1 (ppm)

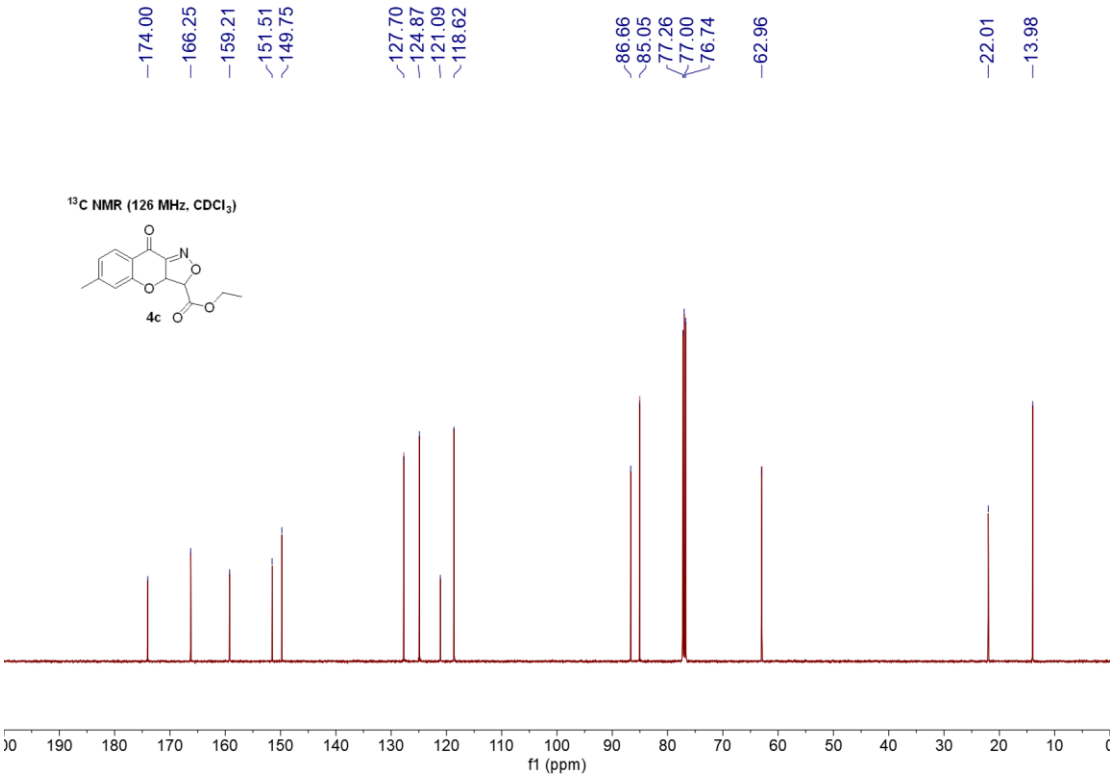

8.663
8.645
8.001
7.983
7.831
7.828
7.814
7.812
7.613
7.610
7.599
7.596
7.593
7.582
7.579
7.505
7.502
7.491
7.488
7.486
7.475
7.472
7.260
7.242
7.225
4.920
4.912
4.907
4.899
4.349
4.346
4.339
4.337
4.331
3.647
3.632
3.626
3.611
2.061
2.052
2.035
2.025
1.939
1.927
1.923
1.914
1.911
1.907
1.902
1.896
1.888
1.816
1H NMR (500 MHz, CDCl3)
2j
1.00
1.05
1.11
1.07
1.04
0.93
1.13
1.11
1.11
2.31
2.21
2.23
f1 (ppm)
186.12
158.34
158.01
135.96
131.27
131.01
128.95
128.28
126.01
125.96
124.86
121.99
83.08
78.00
77.25
77.00
76.75
47.49
26.89
22.74
15.91
13C NMR (126 MHz, CDCl3)
2j
f1 (ppm)

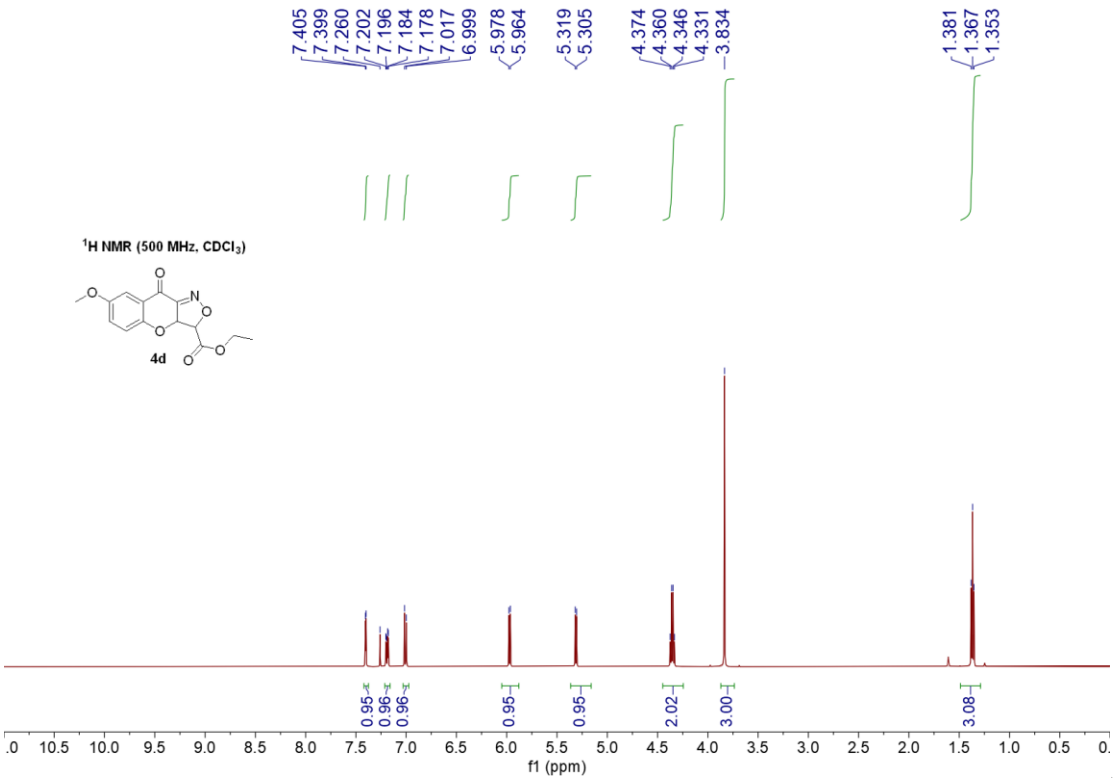

8.050
8.047
8.035
8.031
7.625
7.614
7.611
7.608
7.597
7.594
7.260
7.211
7.209
7.196
7.194
7.193
7.180
7.178
7.098
7.096
7.081
6.020
5.358
5.344
4.384
4.369
4.355
4.341
1.389
1.374
1.360
1H NMR (500 MHz, CDCl3)
4a
1.00
1.11
1.03
1.03
1.00
1.12
2.13
3.27
f1 (ppm)
174.39
166.22
159.20
151.38
137.61
127.98
123.57
123.36
118.69
86.69
85.26
77.26
77.00
76.75
63.08
14.04
13C{1H} NMR (126 MHz, CDCl3)
4a
f1 (ppm)

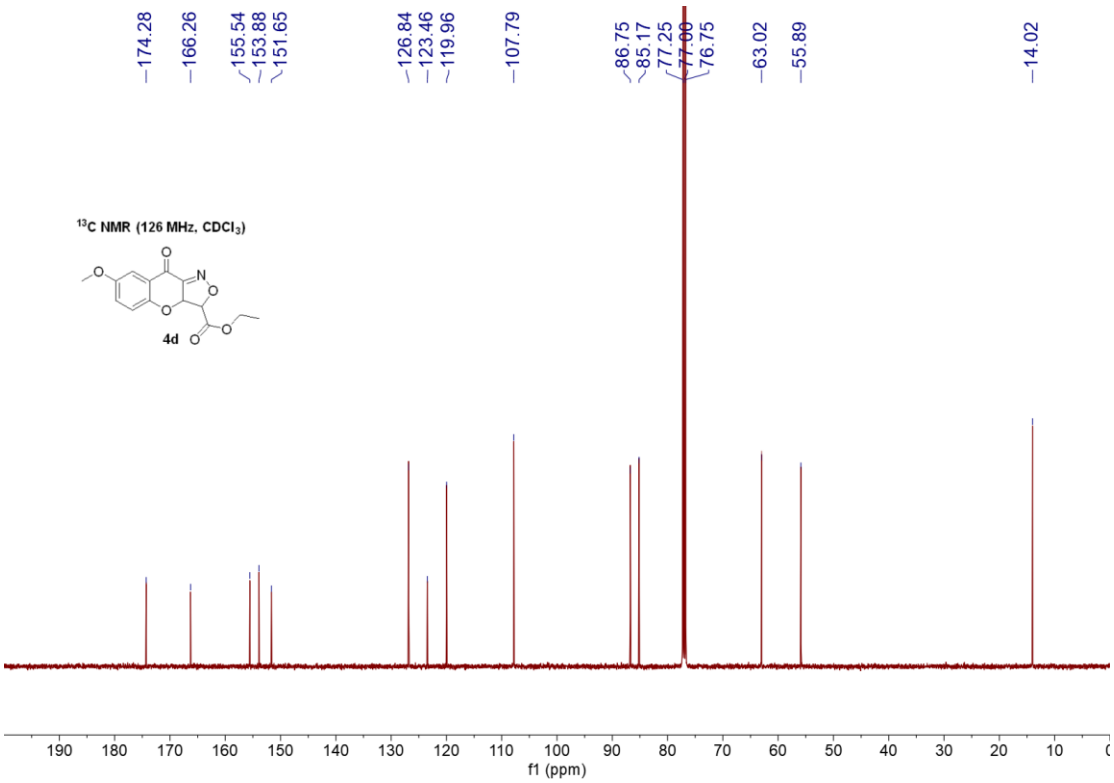

7.813
7.812
7.809
7.807
7.418
7.414
7.401
7.397
7.260
6.984
6.967
5.985
5.971
5.327
5.313
4.375
4.361
4.346
4.332
2.353
1.382
1.367
1.353
^{1}H NMR (500 MHz, CDCl$_3$)
4b
0.83
0.91
0.91
0.84
0.84
1.92
3.00
2.97
f1 (ppm)

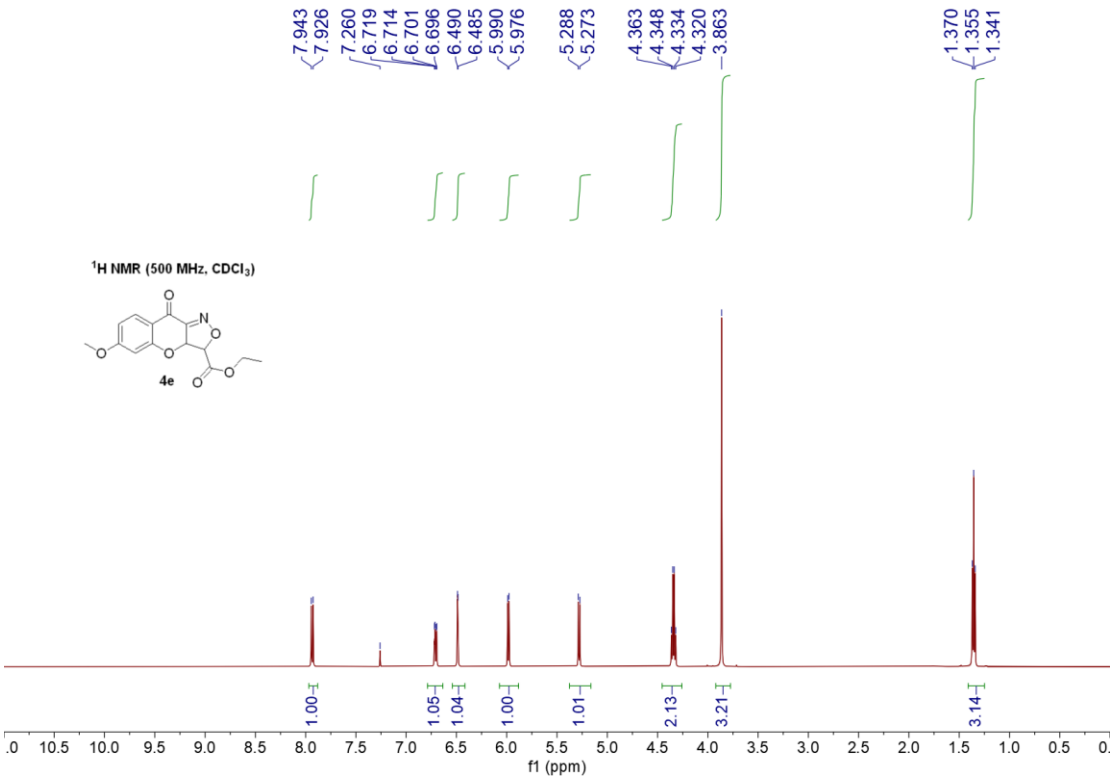

174.53
166.30
157.33
151.63
138.72
133.37
127.44
123.01
118.44
86.68
85.19
77.25
77.00
76.75
63.02
20.39
14.03
^{13}C{^{1}H} NMR (126 MHz, CDCl$_3$)
4b
f1 (ppm)

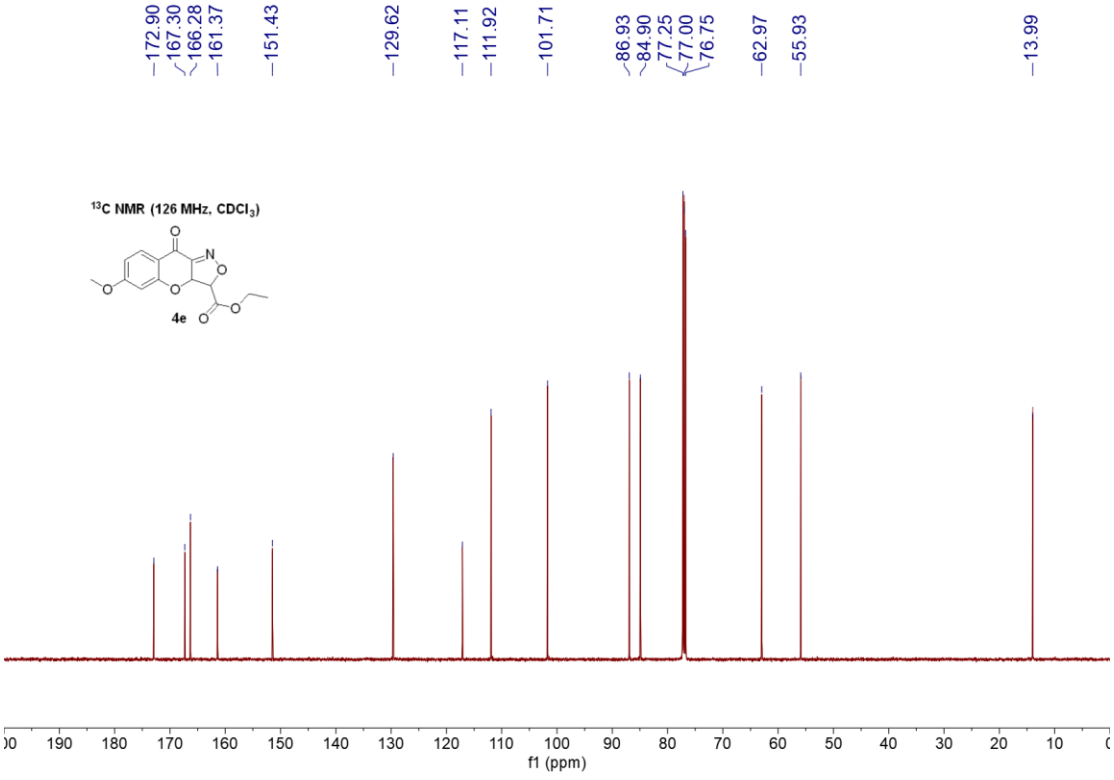

7.892
7.876
7.260
6.985
6.982
6.969
6.966
6.861
5.980
5.966
5.307
5.293
4.362
4.348
4.333
4.319
2.388
1.370
1.355
1.341
1H NMR (500 MHz, CDCl3)
4c
1.00
1.03
1.02
0.97
1.00
2.11
3.11
3.12
f1 (ppm)

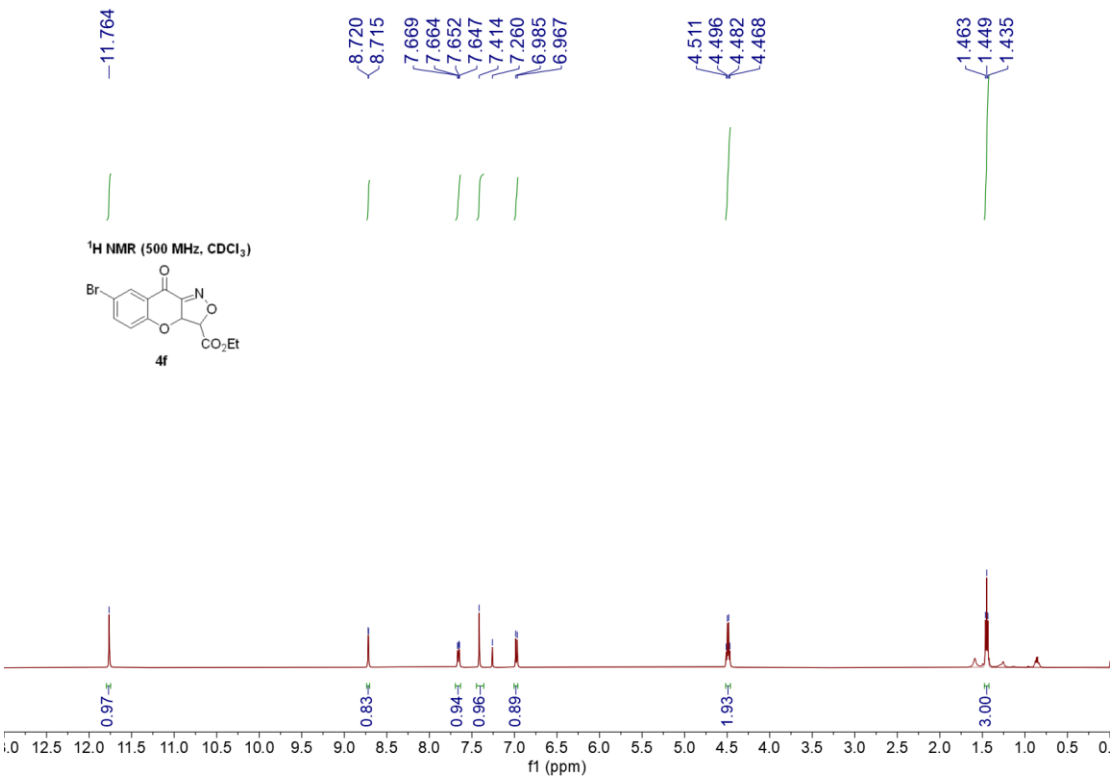

174.00
166.25
159.21
151.51
149.75
127.70
124.87
121.09
118.62
86.66
85.05
77.26
77.00
76.74
62.96
22.01
13.98
13C NMR (126 MHz, CDCl3)
4c
f1 (ppm)

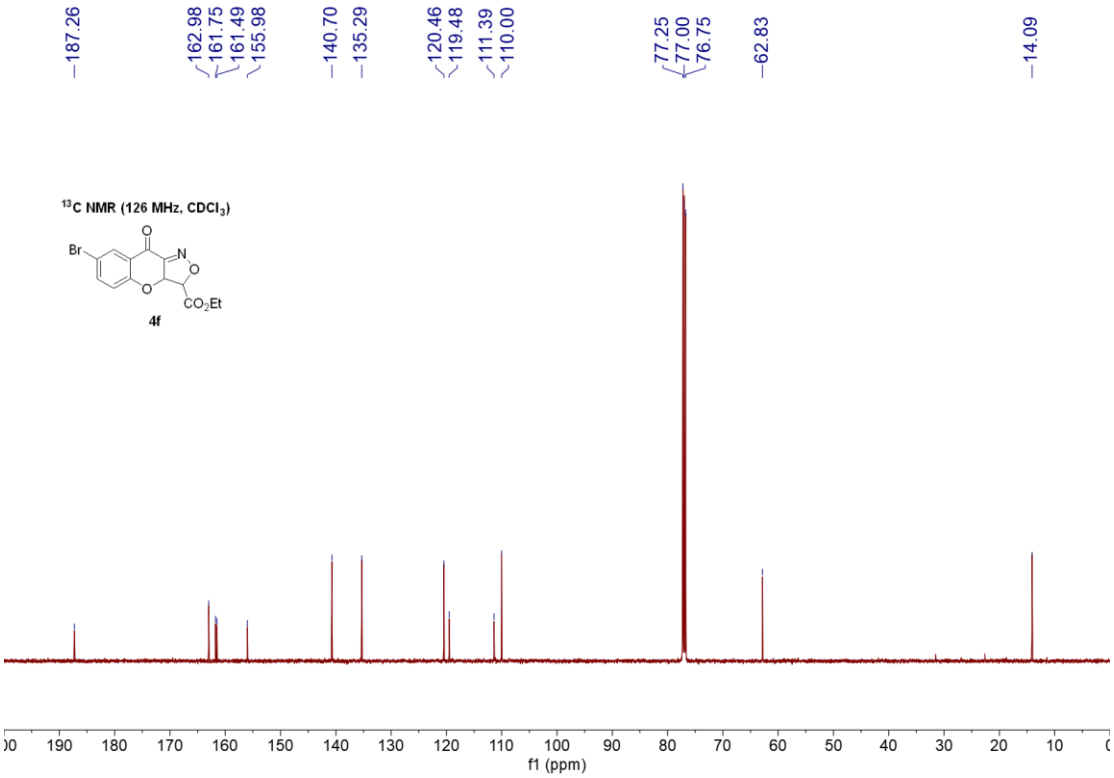

7.405
7.399
7.260
7.202
7.196
7.184
7.178
7.017
6.999
5.978
5.964
5.319
5.305
4.374
4.360
4.346
4.331
3.834
1.381
1.367
1.353
^{1}H NMR (500 MHz, CDCl$_3$)
4d
0.95
0.96
0.96
0.95
0.95
2.02
3.00
3.08
f1 (ppm)

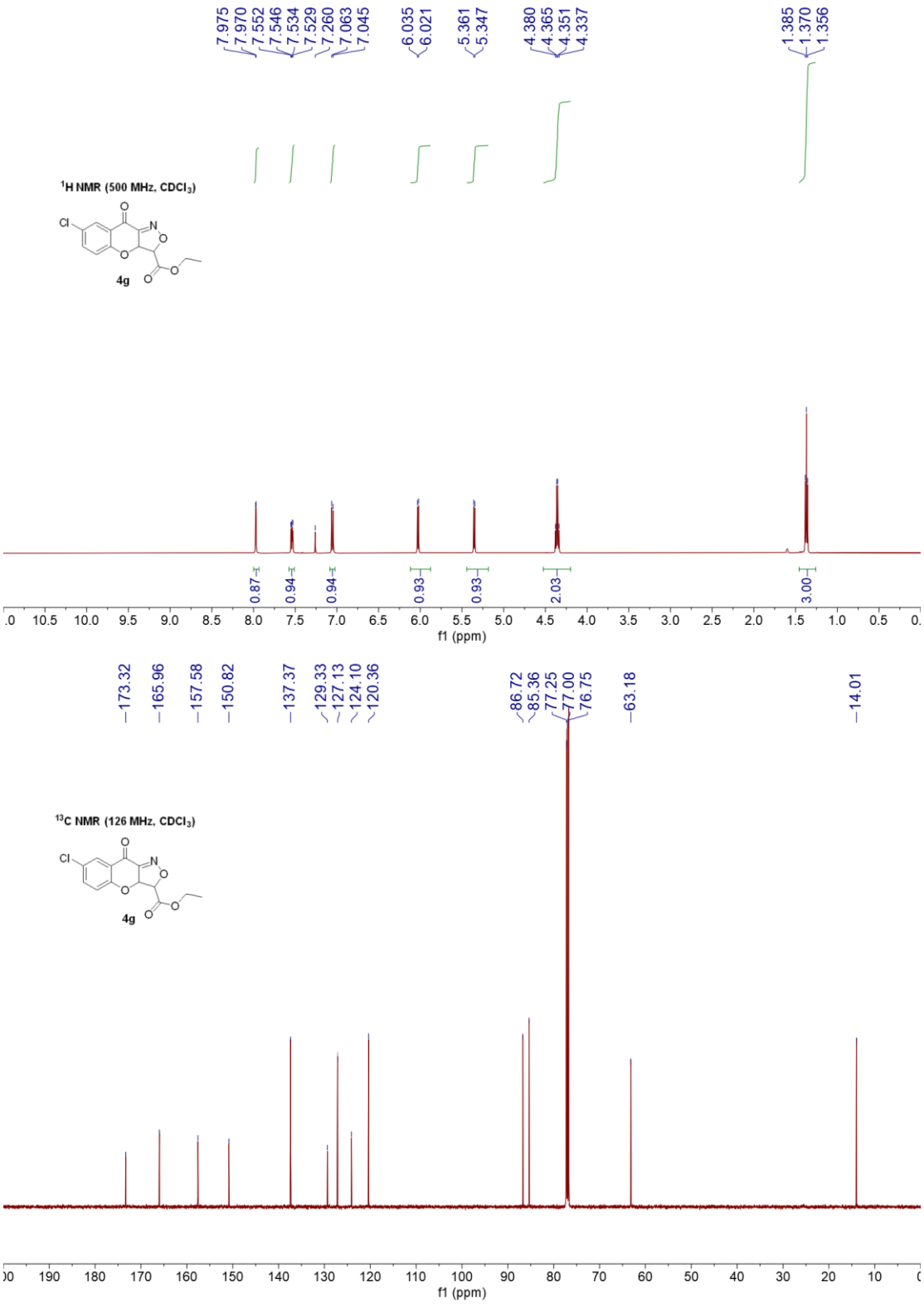

174.28
166.26
155.54
153.88
151.65
126.84
123.46
119.96
107.79
86.75
85.17
77.25
77.00
76.75
63.02
55.89
14.02
^{13}C NMR (126 MHz, CDCl$_3$)
4d
f1 (ppm)

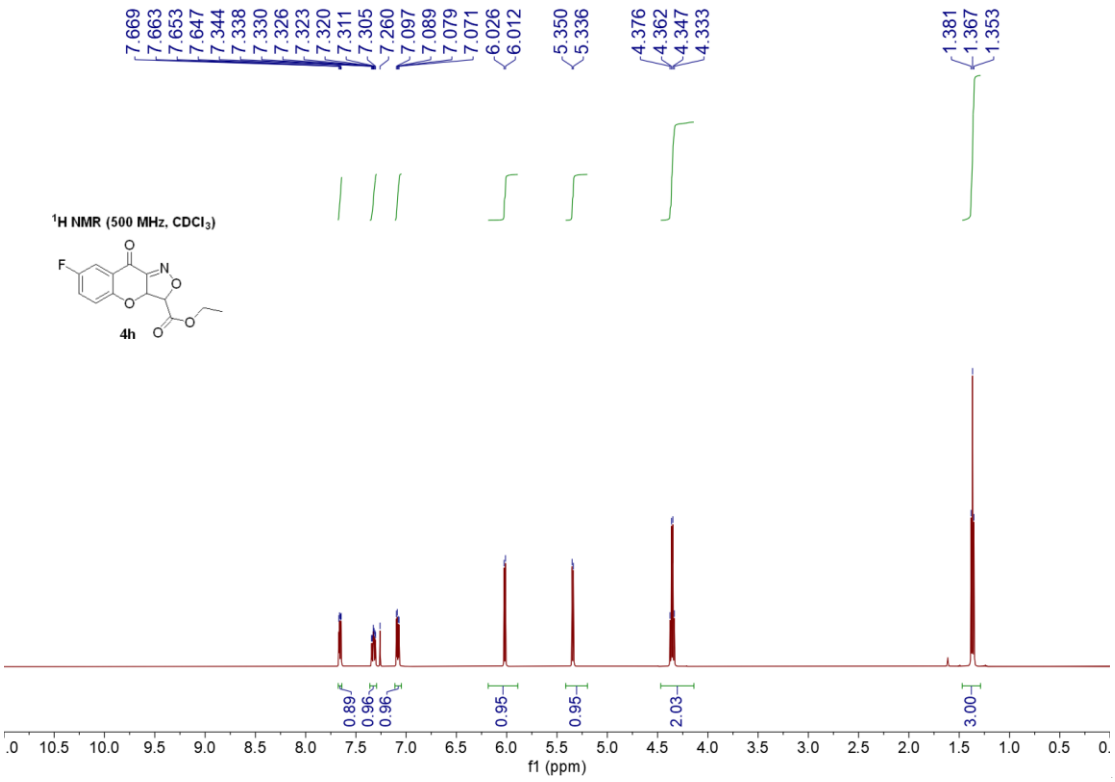

7.943
7.926
7.260
6.719
6.714
6.701
6.696
6.490
6.485
5.990
5.976
5.288
5.273
4.363
4.348
4.334
4.320
3.863
1.370
1.355
1.341
^{1}H NMR (500 MHz, CDCl$_3$)
4e
1.00
1.05
1.04
1.00
1.01
2.13
3.21
3.14
f1 (ppm)

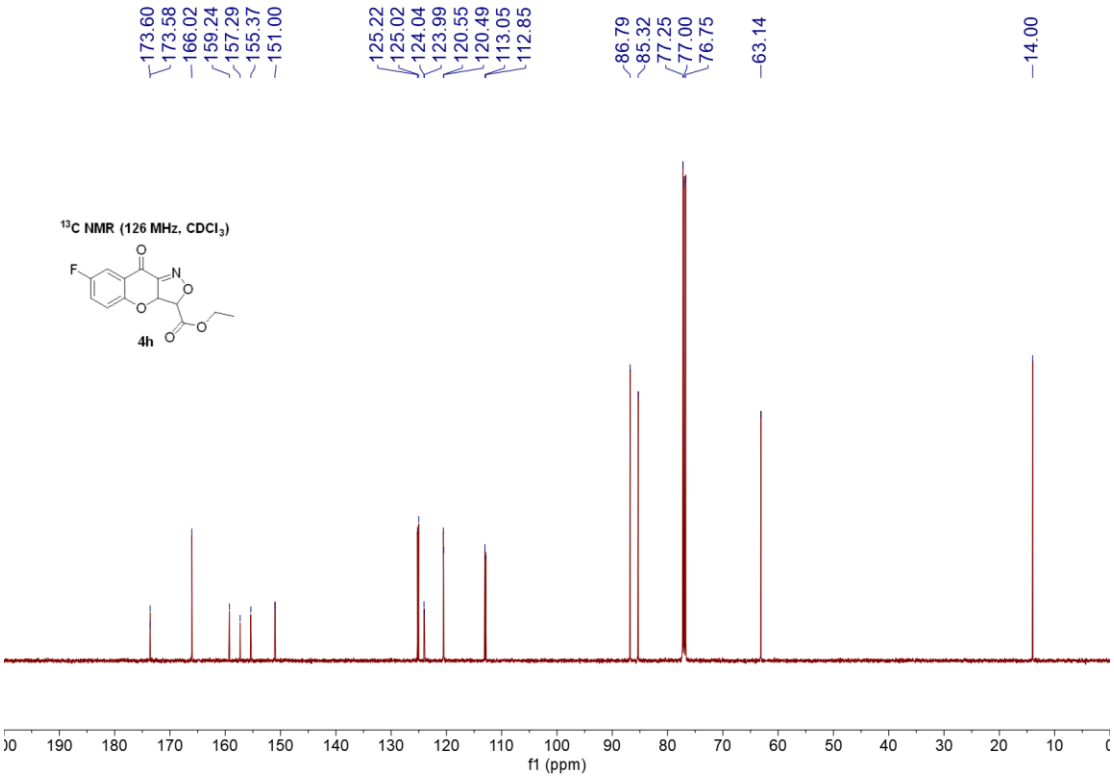

172.90
167.30
166.28
161.37
151.43
129.62
117.11
111.92
101.71
86.93
84.90
77.25
77.00
76.75
62.97
55.93
13.99
^{13}C NMR (126 MHz, CDCl$_3$)
4e
f1 (ppm)

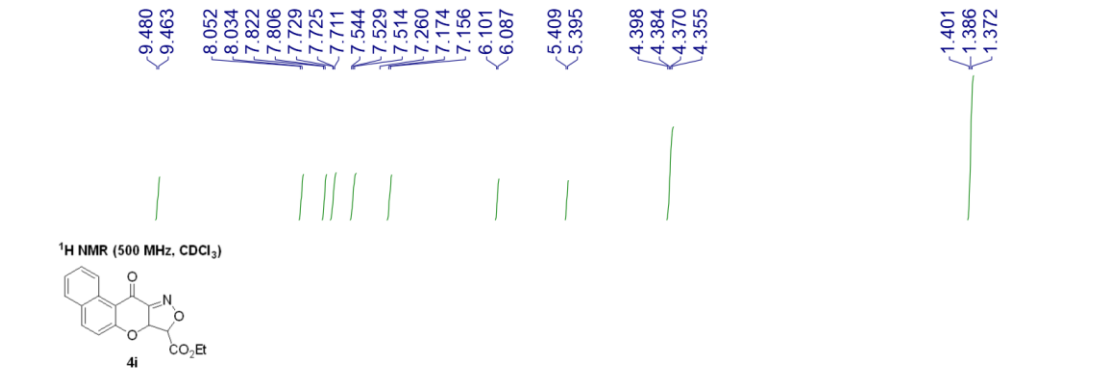

11.764
8.720
8.715
7.669
7.664
7.652
7.647
7.414
7.260
6.985
6.967
4.511
4.496
4.482
4.468
1.463
1.449
1.435
^{1}H NMR (500 MHz, CDCl$_3$)
Br
O
N
O
O
CO$_2$Et
4f
0.97
0.83
0.94
0.96
0.89
1.93
3.00
f1 (ppm)

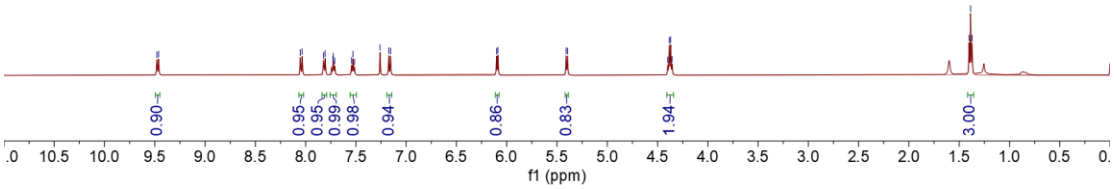

187.26
162.98
161.75
161.49
155.98
140.70
135.29
120.46
119.48
111.39
110.00
77.25
77.00
76.75
62.83
14.09
^{13}C NMR (126 MHz, CDCl$_3$)
Br
O
N
O
O
CO$_2$Et
4f
f1 (ppm)

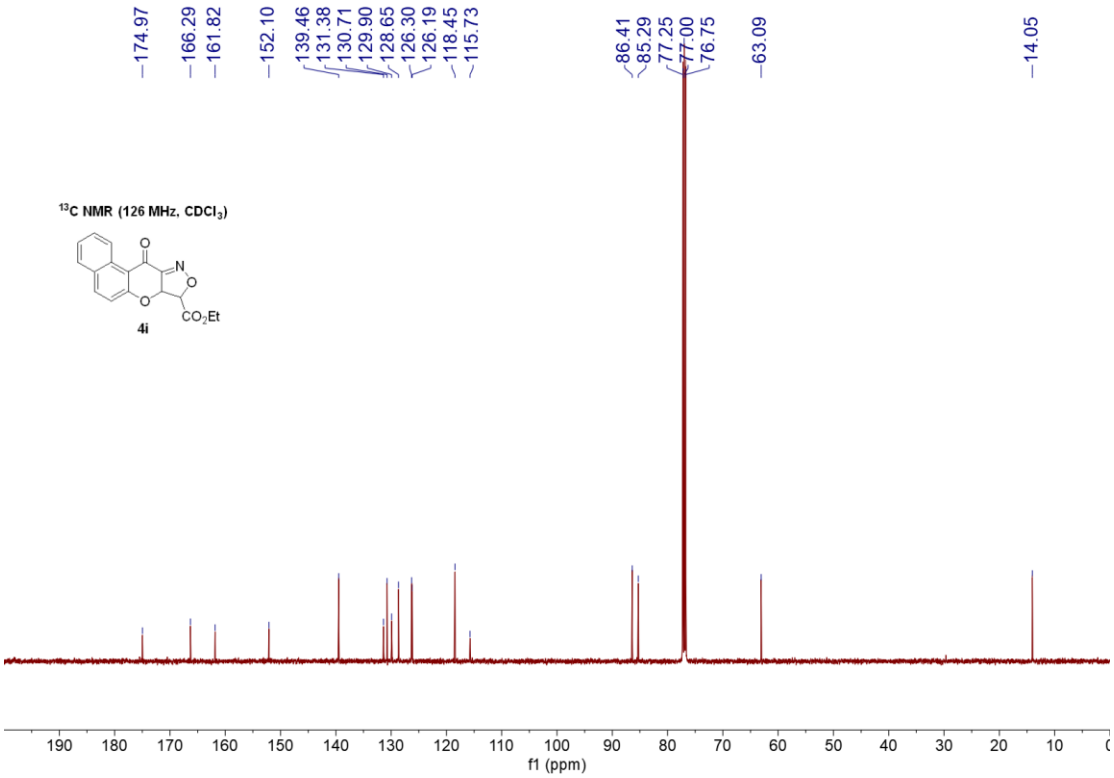

7.975
7.970
7.552
7.546
7.534
7.529
7.260
7.063
7.045
6.035
6.021
5.361
5.347
4.380
4.365
4.351
4.337
1.385
1.370
1.356
^{1}H NMR (500 MHz, CDCl$_3$)
4g
0.87
0.94
0.94
0.93
0.93
2.03
3.00
f1 (ppm)
173.32
165.96
157.58
150.82
137.37
129.33
127.13
124.10
120.36
86.72
85.36
77.25
77.00
76.75
63.18
14.01
^{13}C NMR (126 MHz, CDCl$_3$)
4g
f1 (ppm)

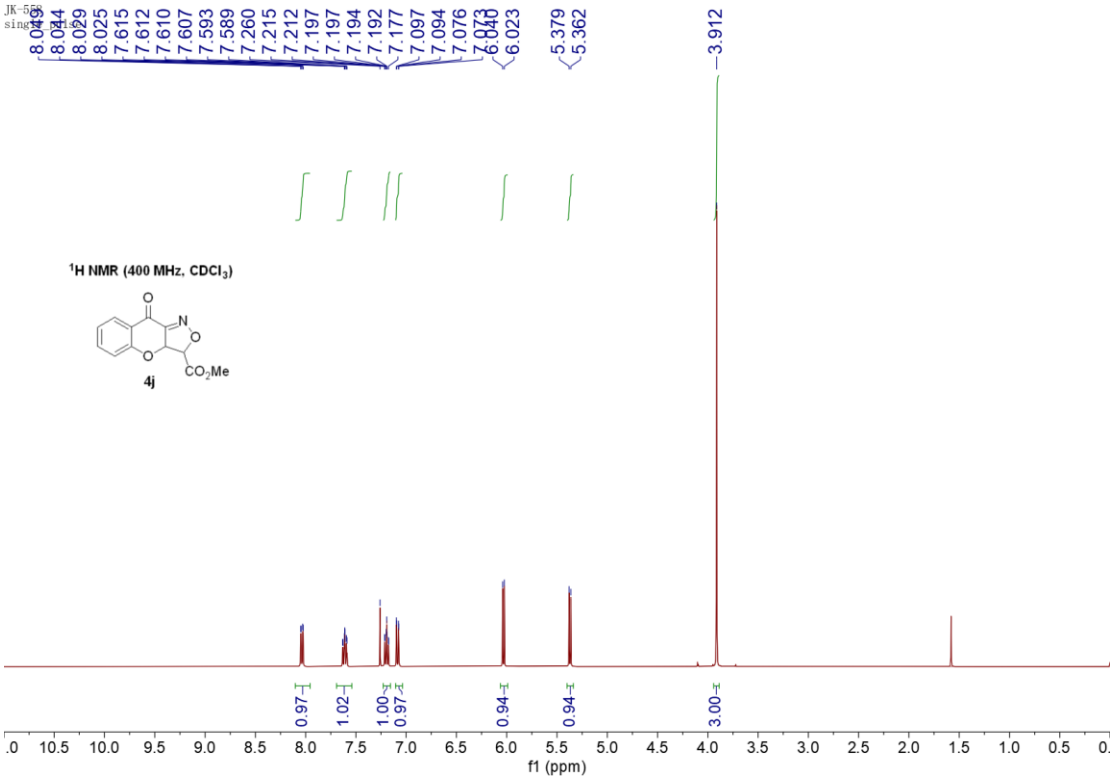

7.669
7.663
7.653
7.647
7.344
7.338
7.330
7.326
7.323
7.320
7.311
7.305
7.260
7.097
7.089
7.079
7.071
6.026
6.012
5.350
5.336
4.376
4.362
4.347
4.333
1.381
1.367
1.353
^{1}H NMR (500 MHz, CDCl$_3$)
4h
0.89
0.96
0.96
0.95
0.95
2.03
3.00
f1 (ppm)


173.60
173.58
166.02
159.24
157.29
155.37
151.00
125.22
125.02
124.04
123.99
120.55
120.49
113.05
112.85
86.79
85.32
77.25
77.00
76.75
63.14
14.00
^{13}C NMR (126 MHz, CDCl$_3$)
4h
f1 (ppm)


9.480
9.463
8.052
8.034
7.822
7.806
7.729
7.725
7.711
7.544
7.529
7.514
7.260
7.174
7.156
6.101
6.087
5.409
5.395
4.398
4.384
4.370
4.355
1.401
1.386
1.372
^{1}H NMR (500 MHz, CDCl$_3$)
CO$_2$Et
4i


0.90
0.95
0.95
0.99
0.98
0.94
0.86
0.83
1.94
3.00
f1 (ppm)

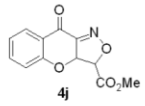

174.97
166.29
161.82
152.10
139.46
131.38
130.71
129.90
128.65
126.30
126.19
118.45
115.73
86.41
85.29
77.25
77.00
76.75
63.09
14.05
^{13}C NMR (126 MHz, CDCl$_3$)
CO$_2$Et
4i
f1 (ppm)



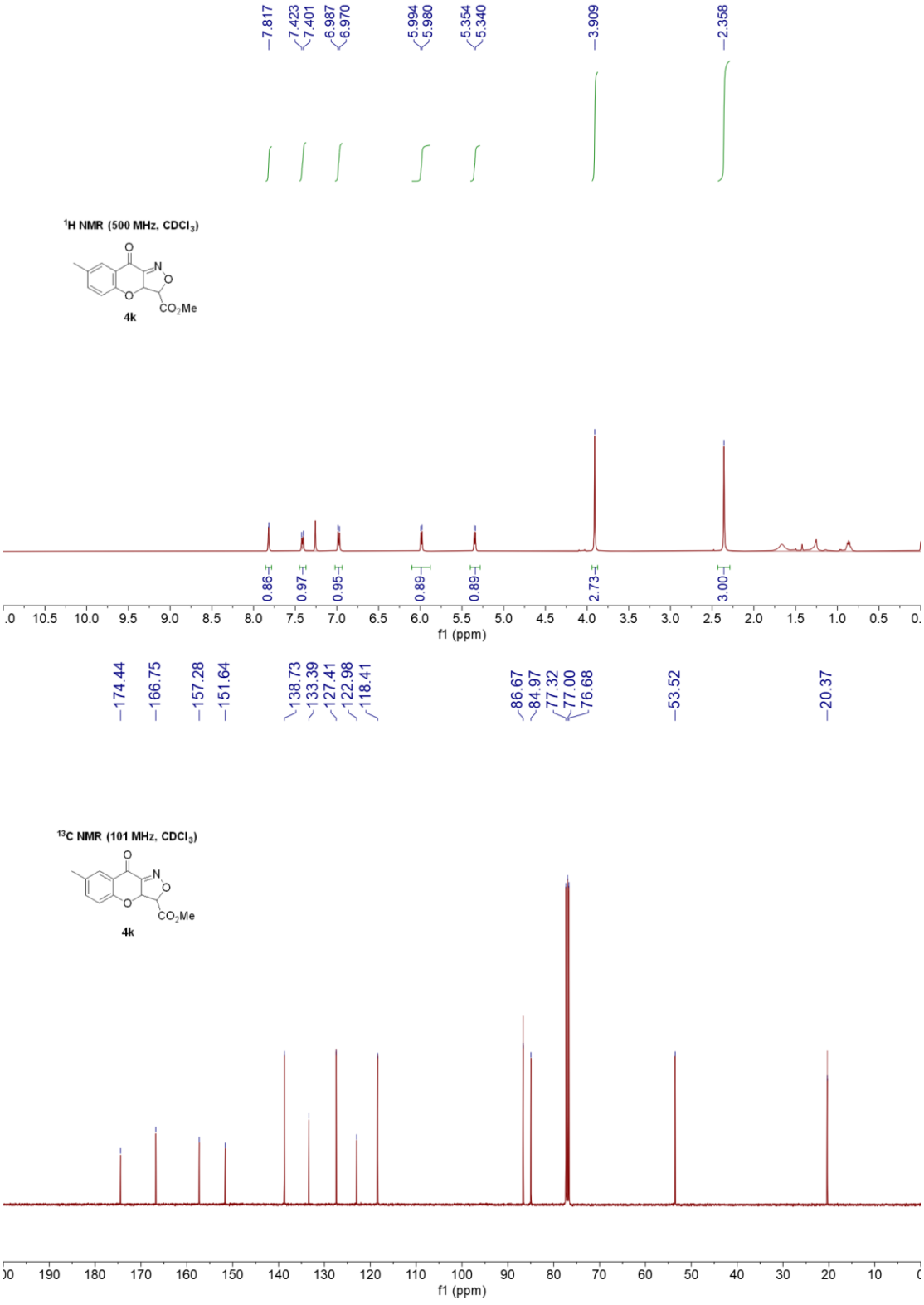
^{1}H NMR (400 MHz, $CDCl_3$)

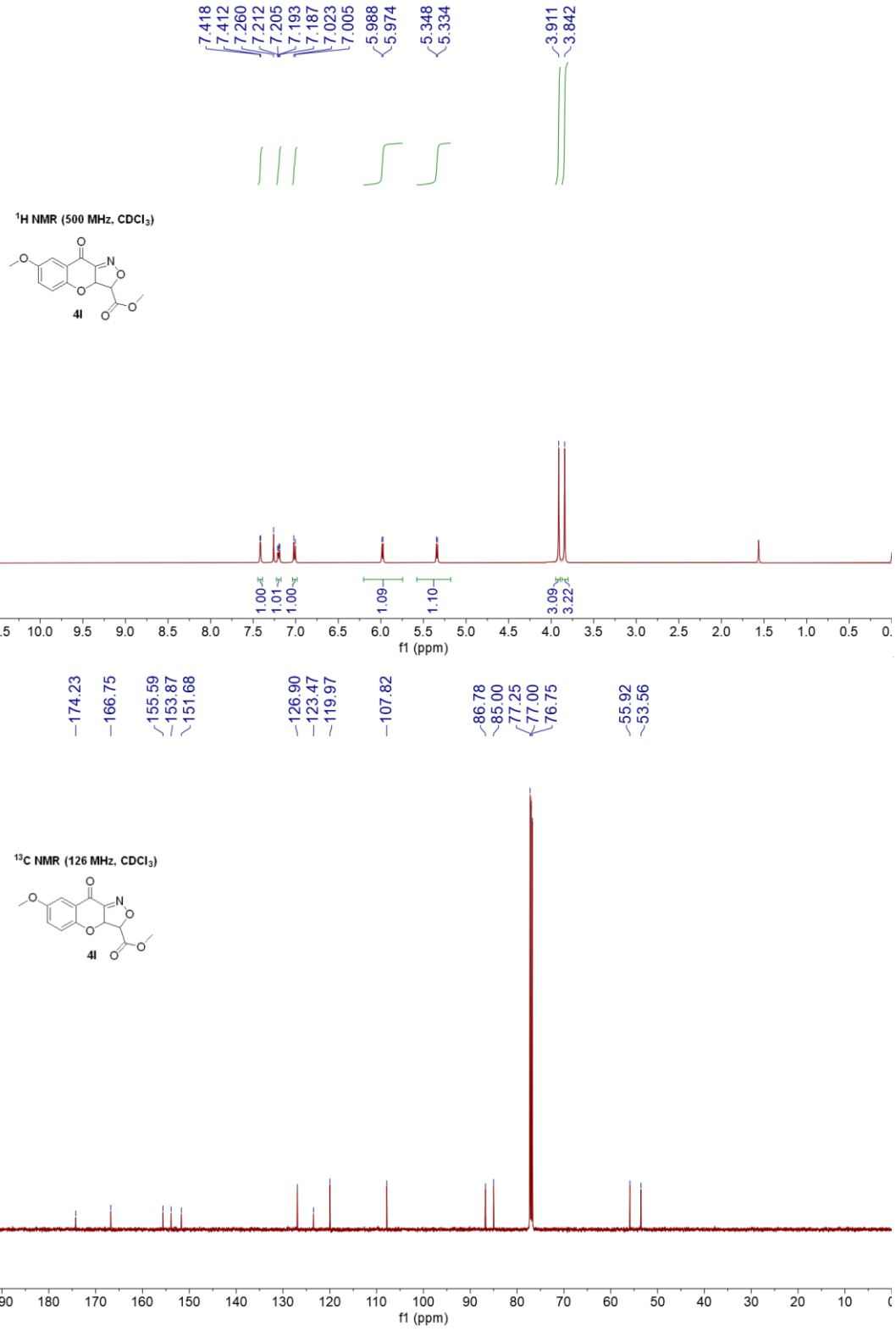
4j

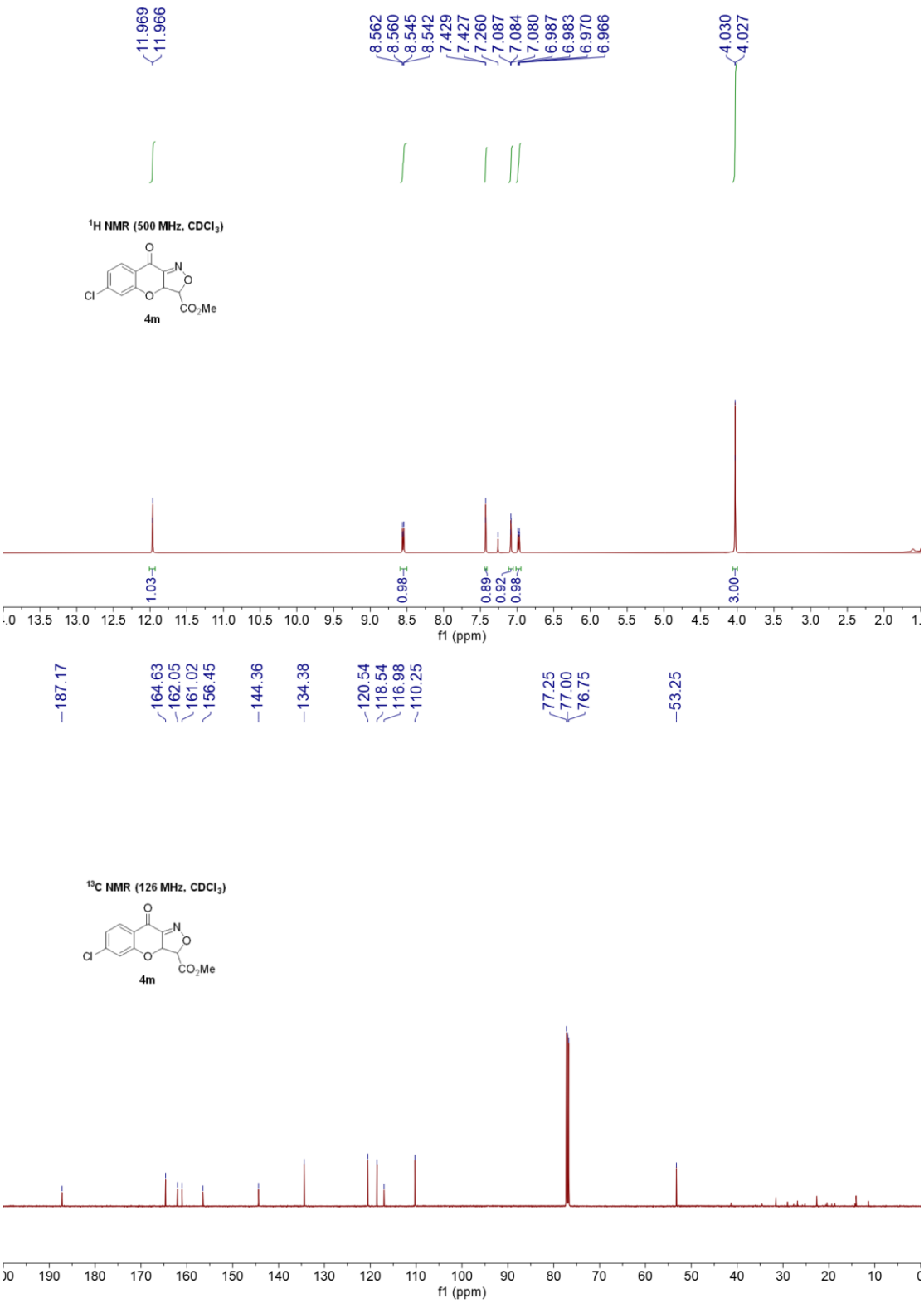
^{13}C NMR (101 MHz, $CDCl_3$)

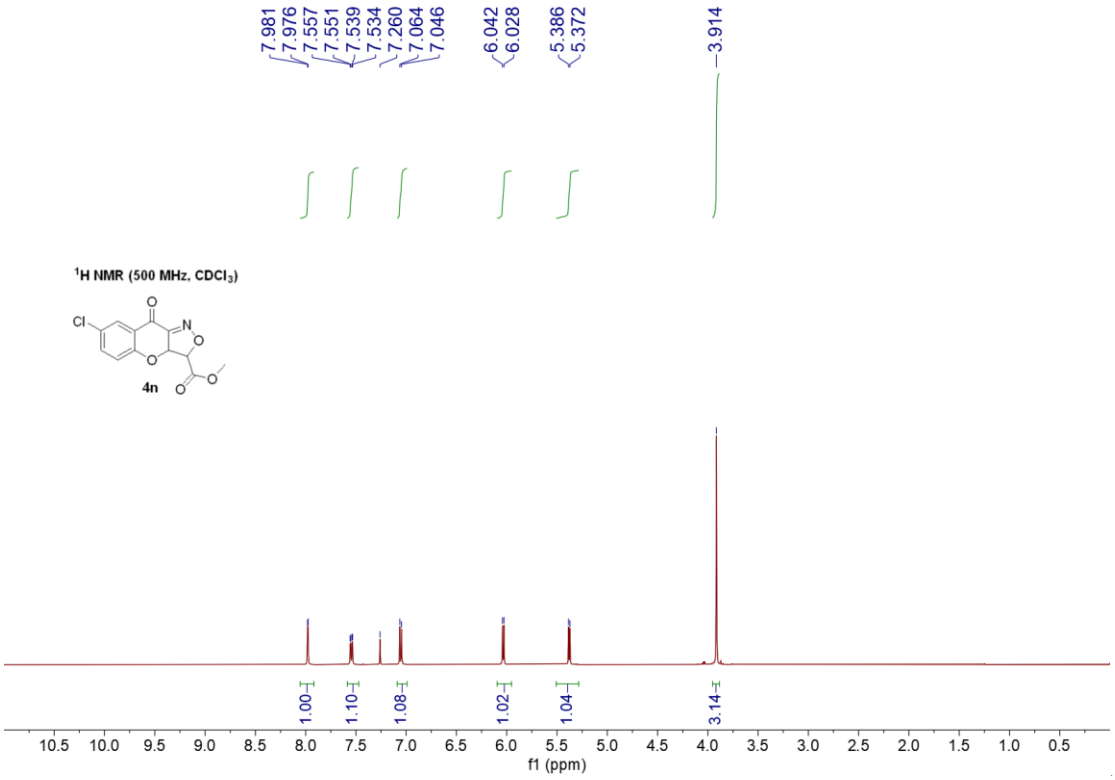


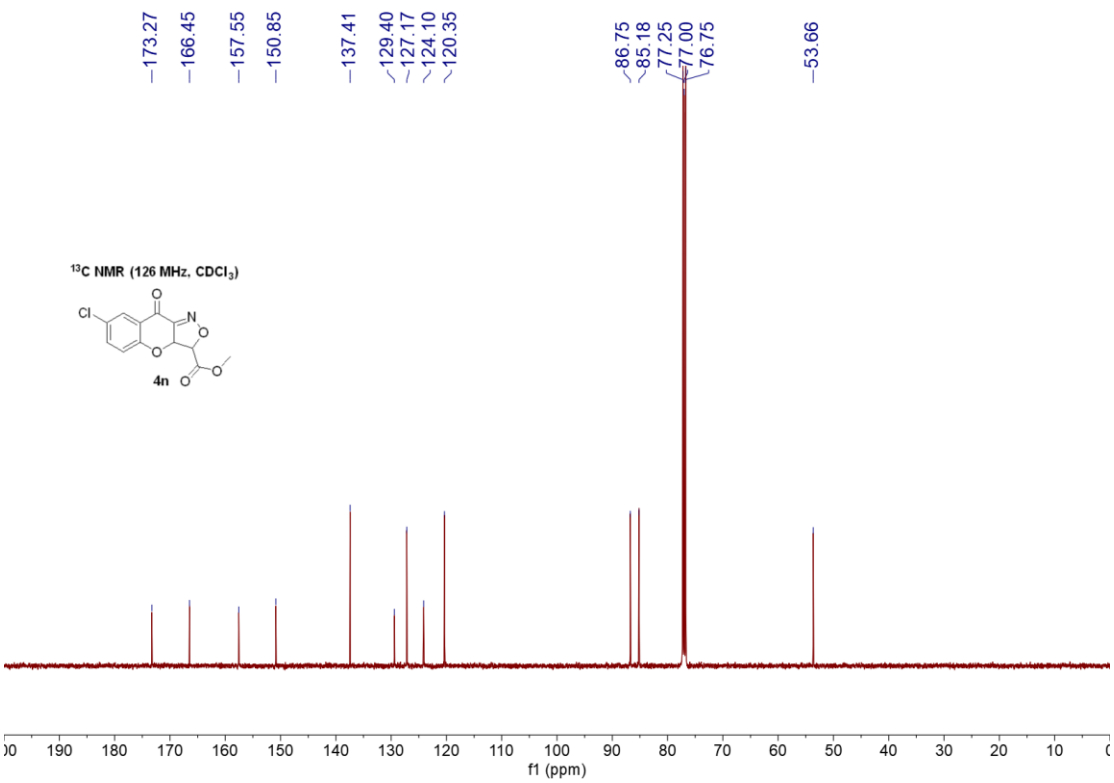
4j

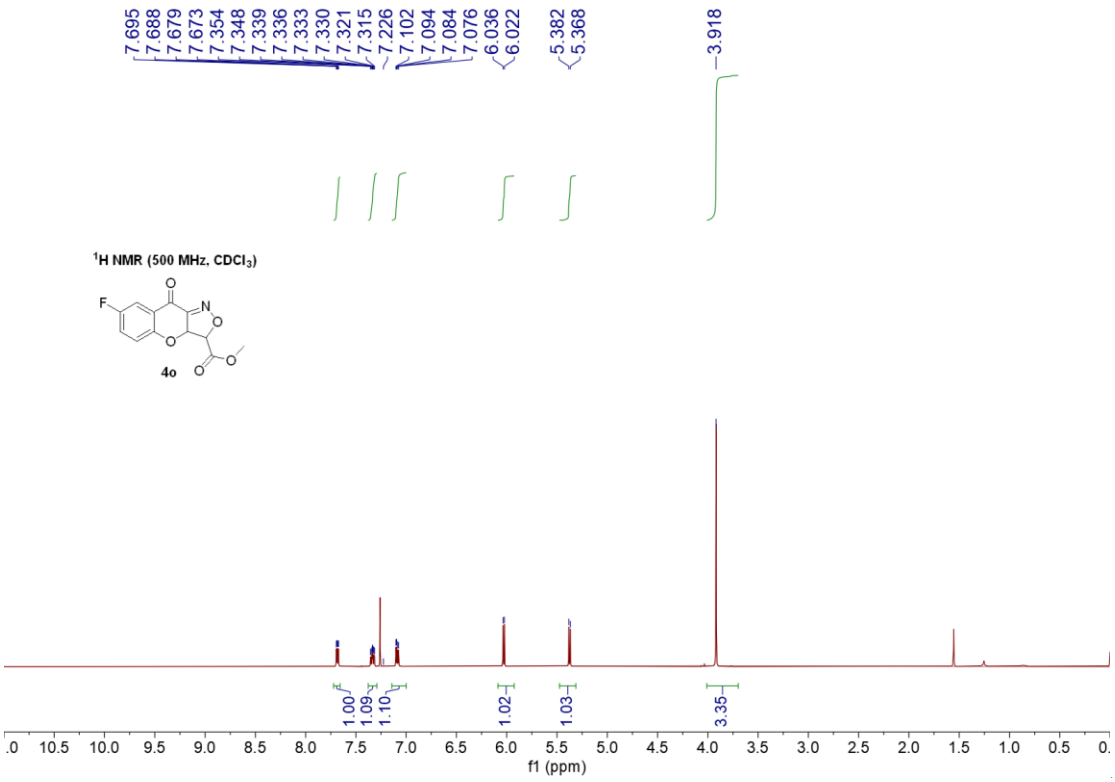

7.817
7.423
7.401
6.987
6.970
5.994
5.980
5.354
5.340
3.909
2.358
^{1}H NMR (500 MHz, CDCl$_3$)
4k
0.86
0.97
0.95
0.89
0.89
2.73
3.00
f1 (ppm)
174.44
166.75
157.28
151.64
138.73
133.39
127.41
122.98
118.41
86.67
84.97
77.32
77.00
76.68
53.52
20.37
^{13}C NMR (101 MHz, CDCl$_3$)
4k
f1 (ppm)

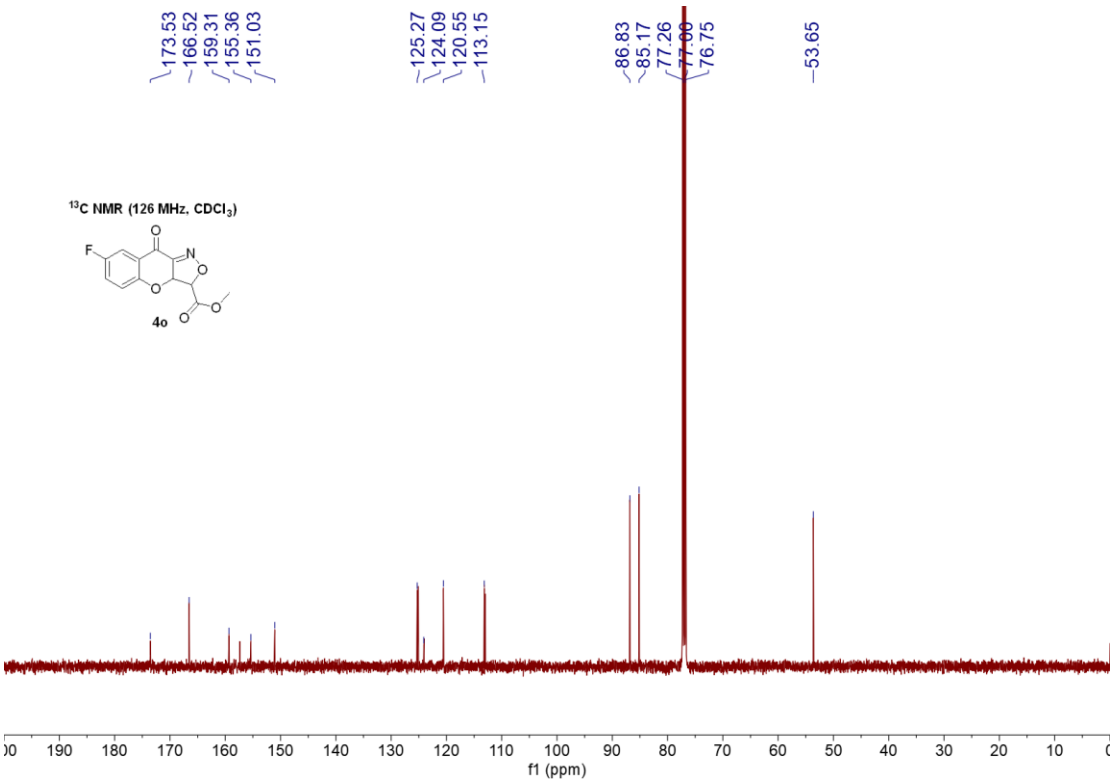

7.418
7.412
7.260
7.212
7.205
7.193
7.187
7.023
7.005
5.988
5.974
5.348
5.334
3.911
3.842
^{1}H NMR (500 MHz, CDCl$_3$)
4l
1.00
1.01
1.00
1.09
1.10
3.09
3.22
f1 (ppm)
174.23
166.75
155.59
153.87
151.68
126.90
123.47
119.97
107.82
86.78
85.00
77.25
77.00
76.75
55.92
53.56
^{13}C NMR (126 MHz, CDCl$_3$)
4l
f1 (ppm)

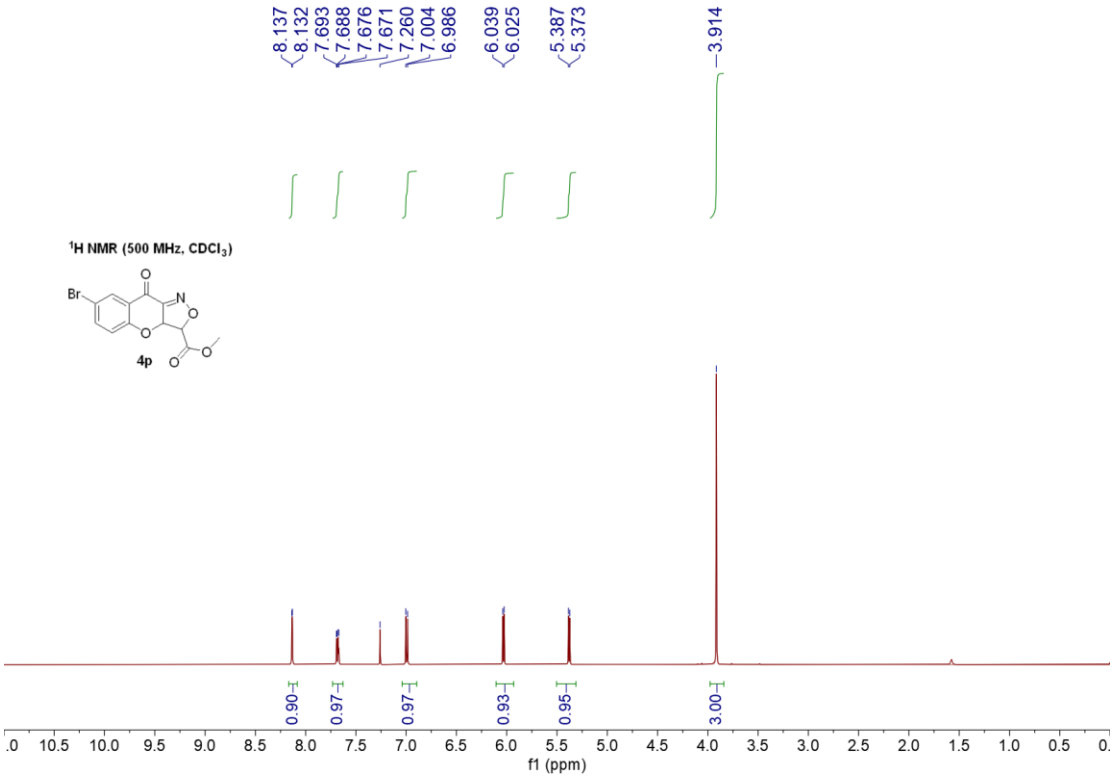

11.969
11.966
8.562
8.560
8.545
8.542
7.429
7.427
7.260
7.087
7.084
7.080
6.987
6.983
6.970
6.966
4.030
4.027
^{1}H NMR (500 MHz, CDCl$_3$)
4m
1.03
0.98
0.89
0.92
0.98
3.00
f1 (ppm)
187.17
164.63
162.05
161.02
156.45
144.36
134.38
120.54
118.54
116.98
110.25
77.25
77.00
76.75
53.25
^{13}C NMR (126 MHz, CDCl$_3$)
4m
f1 (ppm)

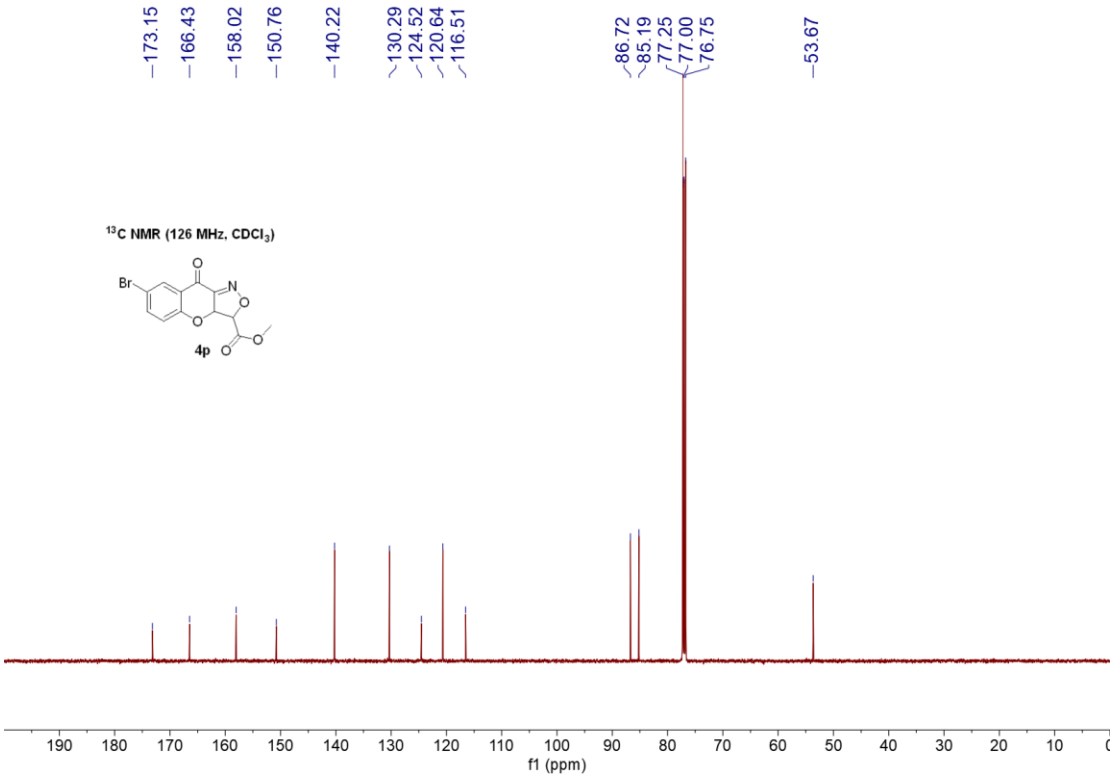

7.981
7.976
7.557
7.551
7.539
7.534
7.260
7.064
7.046
6.042
6.028
5.386
5.372
3.914
1H NMR (500 MHz, CDCl3)
4n
1.00
1.10
1.08
1.02
1.04
3.14
f1 (ppm)

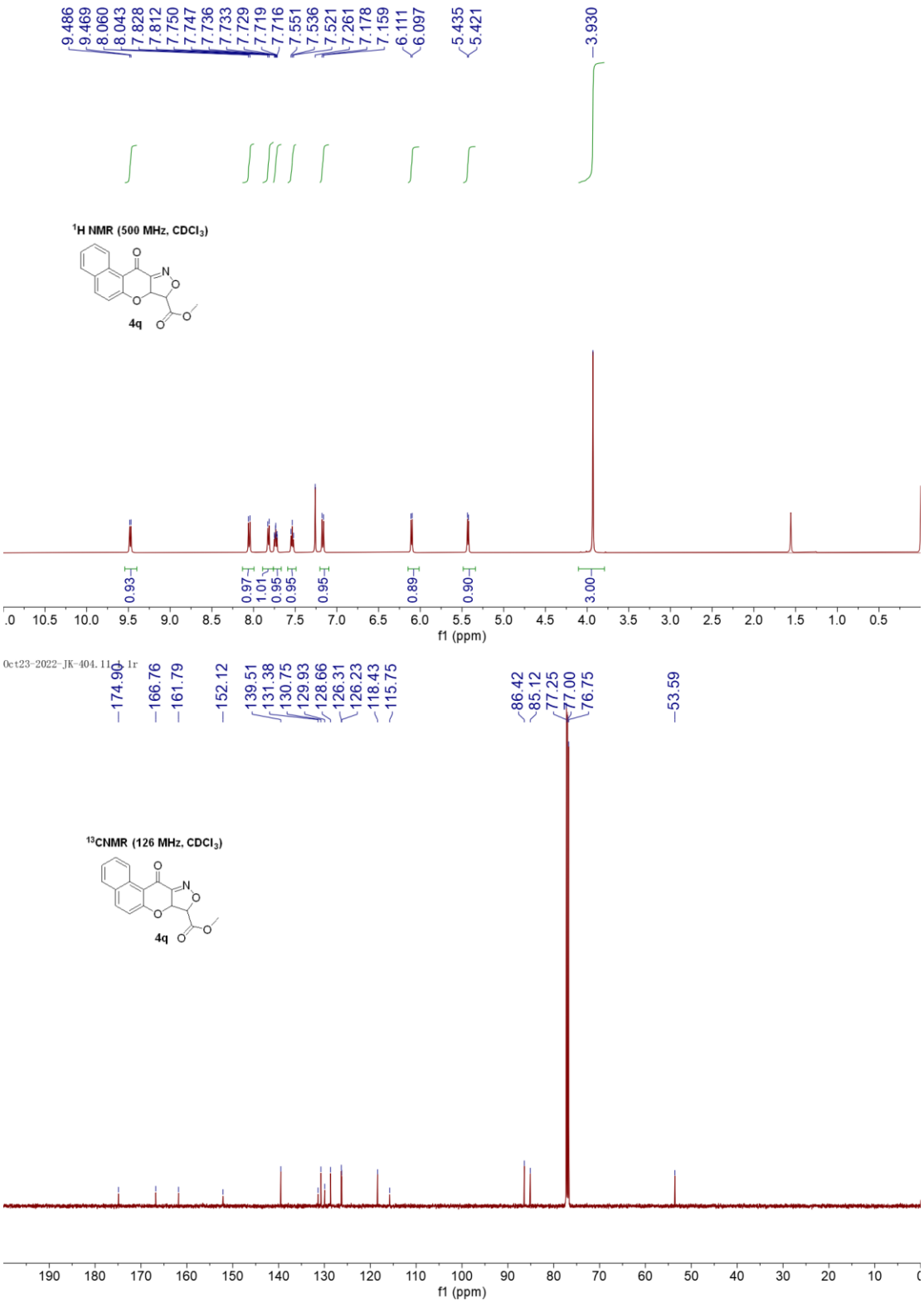

173.27
166.45
157.55
150.85
137.41
129.40
127.17
124.10
120.35
86.75
85.18
77.25
77.00
76.75
53.66
13C NMR (126 MHz, CDCl3)
4n
f1 (ppm)

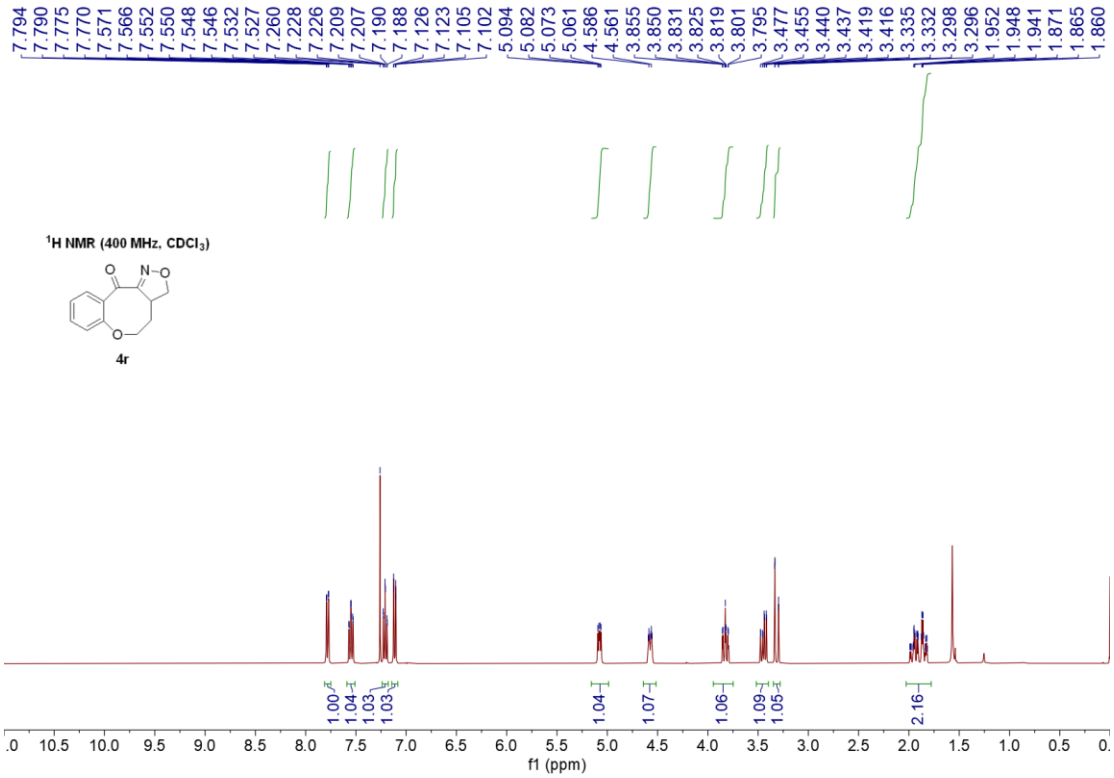

7.695
7.688
7.679
7.673
7.354
7.348
7.339
7.336
7.333
7.330
7.321
7.315
7.226
7.102
7.094
7.084
7.076
6.036
6.022
5.382
5.368
3.918
1H NMR (500 MHz, CDCl3)
4o
1.00
1.09
1.10
1.02
1.03
3.35
f1 (ppm)

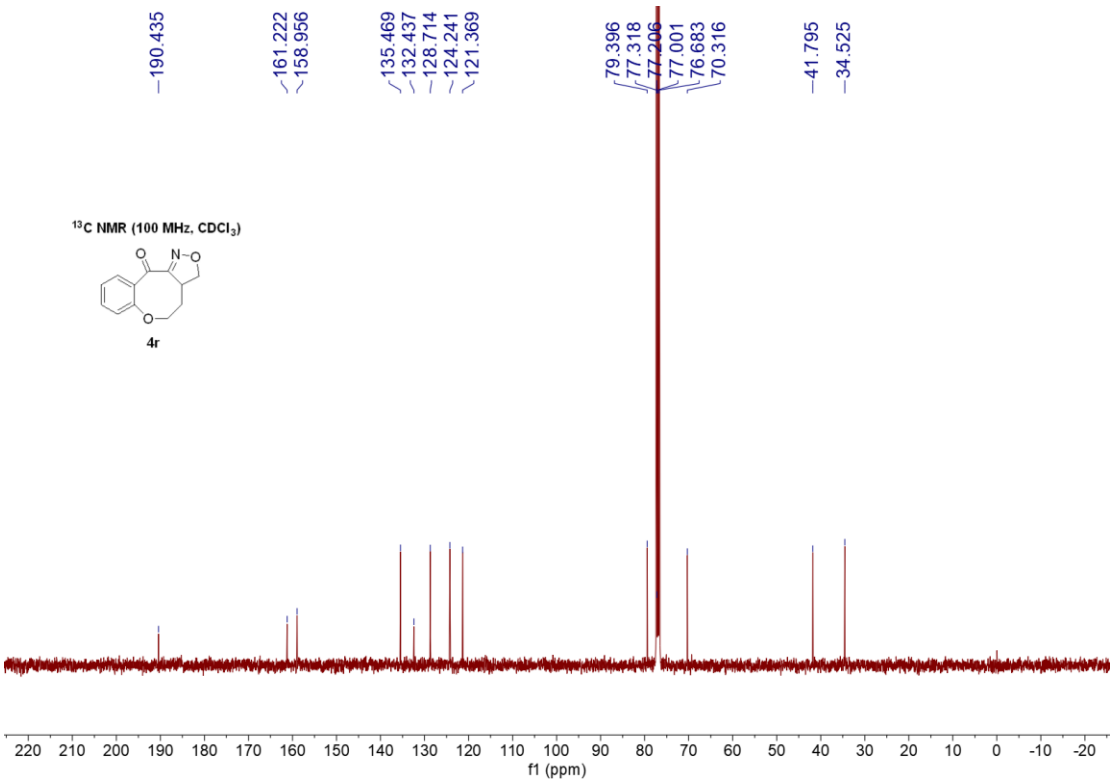

173.53
166.52
159.31
155.36
151.03
125.27
124.09
120.55
113.15
86.83
85.17
77.26
77.00
76.75
53.65
13C NMR (126 MHz, CDCl3)
4o
f1 (ppm)

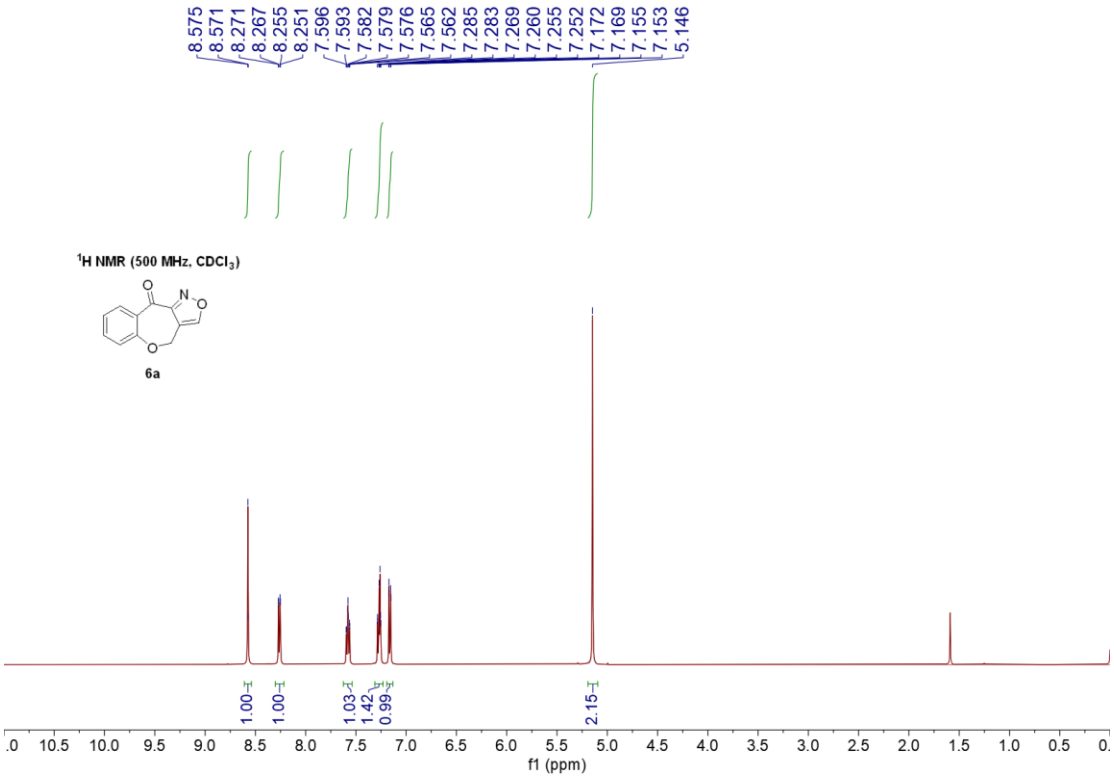

8.137
8.132
7.693
7.688
7.676
7.671
7.260
7.004
6.986
6.039
6.025
5.387
5.373
3.914
^{1}H NMR (500 MHz, CDCl$_3$)
Br
O
N
O
O
O
O
4p
0.90
0.97
0.97
0.93
0.95
3.00
f1 (ppm)

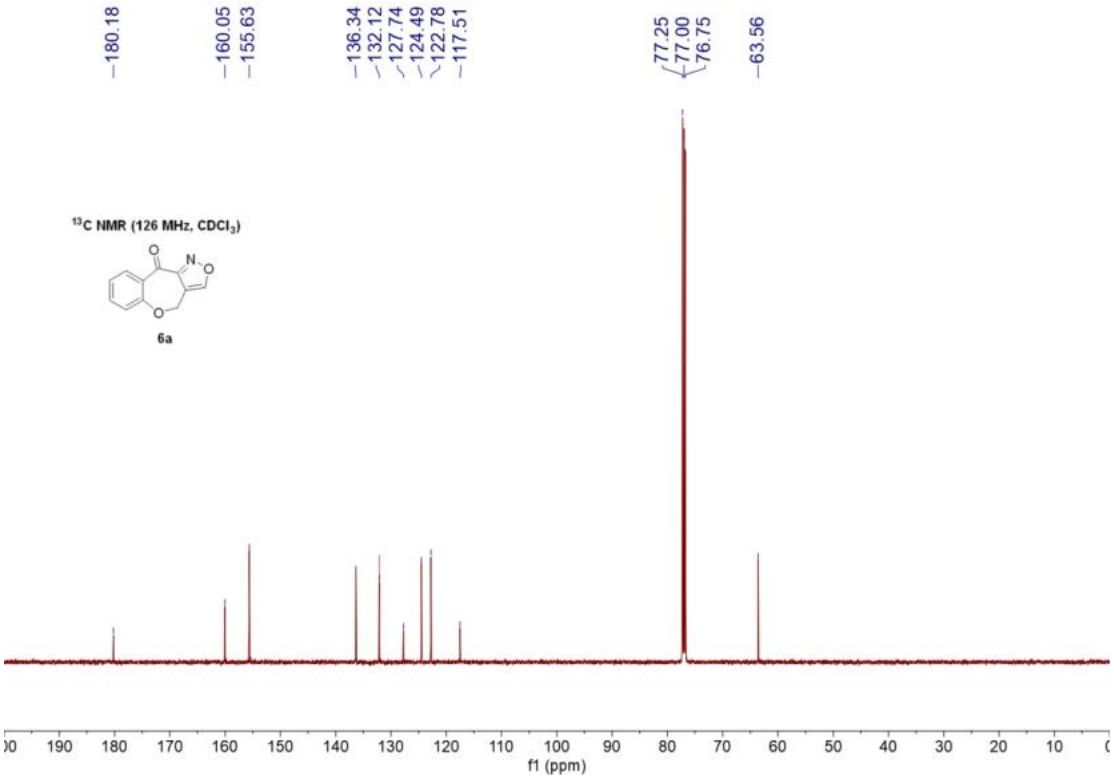

173.15
166.43
158.02
150.76
140.22
130.29
124.52
120.64
116.51
86.72
85.19
77.25
77.00
76.75
53.67
^{13}C NMR (126 MHz, CDCl$_3$)
Br
O
N
O
O
O
O
4p
f1 (ppm)

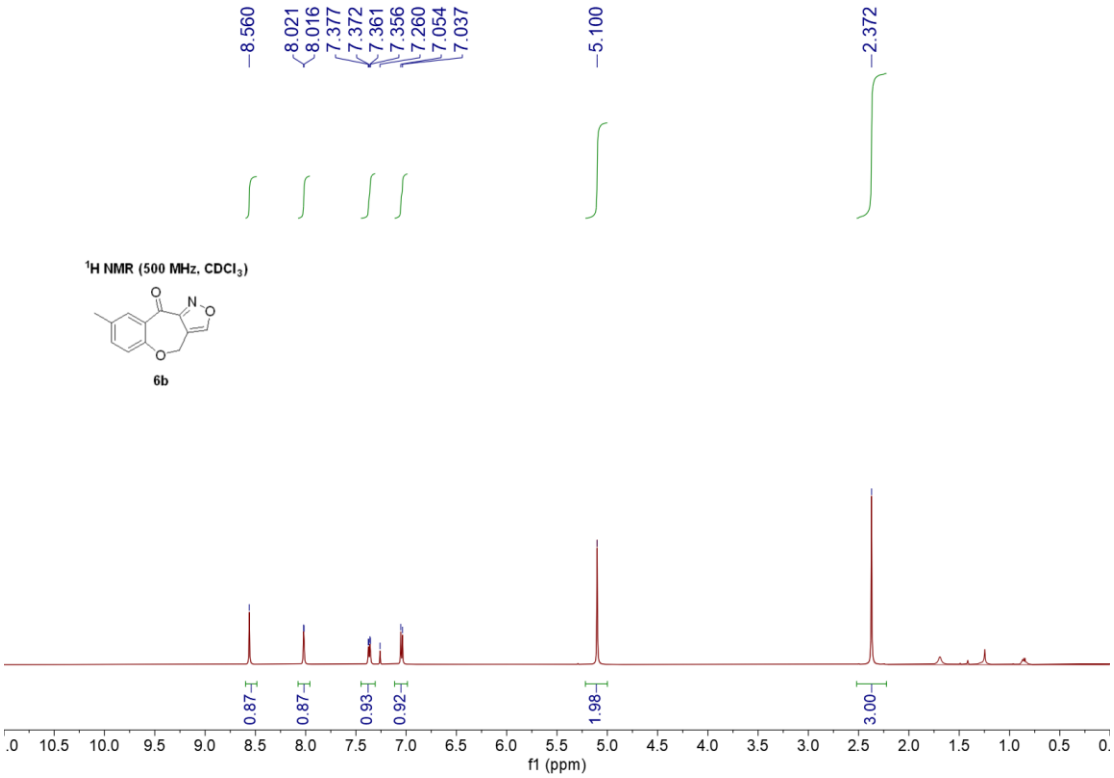

9.486
9.469
8.060
8.043
7.828
7.812
7.750
7.747
7.736
7.733
7.729
7.719
7.716
7.551
7.536
7.521
7.261
7.178
7.159
6.111
6.097
5.435
5.421
3.930
^{1}H NMR (500 MHz, CDCl$_3$)
4q
0.93
0.97
1.01
0.95
0.95
0.95
0.89
0.90
3.00
f1 (ppm)
Oct23-2022-JK-404.11.1r
174.90
166.76
161.79
152.12
139.51
131.38
130.75
129.93
128.66
126.31
126.23
118.43
115.75
86.42
85.12
77.25
77.00
76.75
53.59
^{13}CNMR (126 MHz, CDCl$_3$)
4q
f1 (ppm)

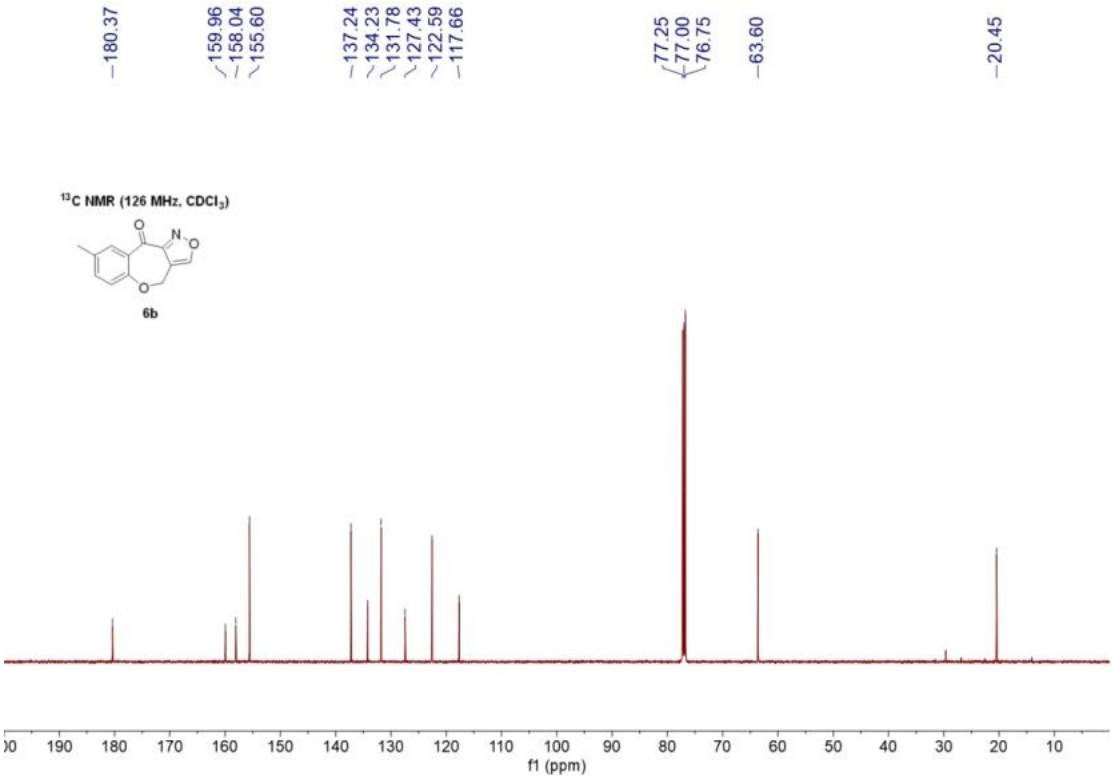

7.794
7.790
7.775
7.770
7.571
7.566
7.552
7.550
7.548
7.546
7.532
7.527
7.260
7.228
7.226
7.209
7.207
7.190
7.188
7.126
7.123
7.105
7.102
5.094
5.082
5.073
5.061
4.586
4.561
3.855
3.850
3.831
3.825
3.819
3.801
3.795
3.477
3.455
3.440
3.437
3.419
3.416
3.335
3.332
3.298
3.296
1.952
1.948
1.941
1.871
1.865
1.860
1H NMR (400 MHz, CDCl3)
4r
1.00
1.04
1.03
1.03
1.04
1.07
1.06
1.09
1.05
2.16
f1 (ppm)

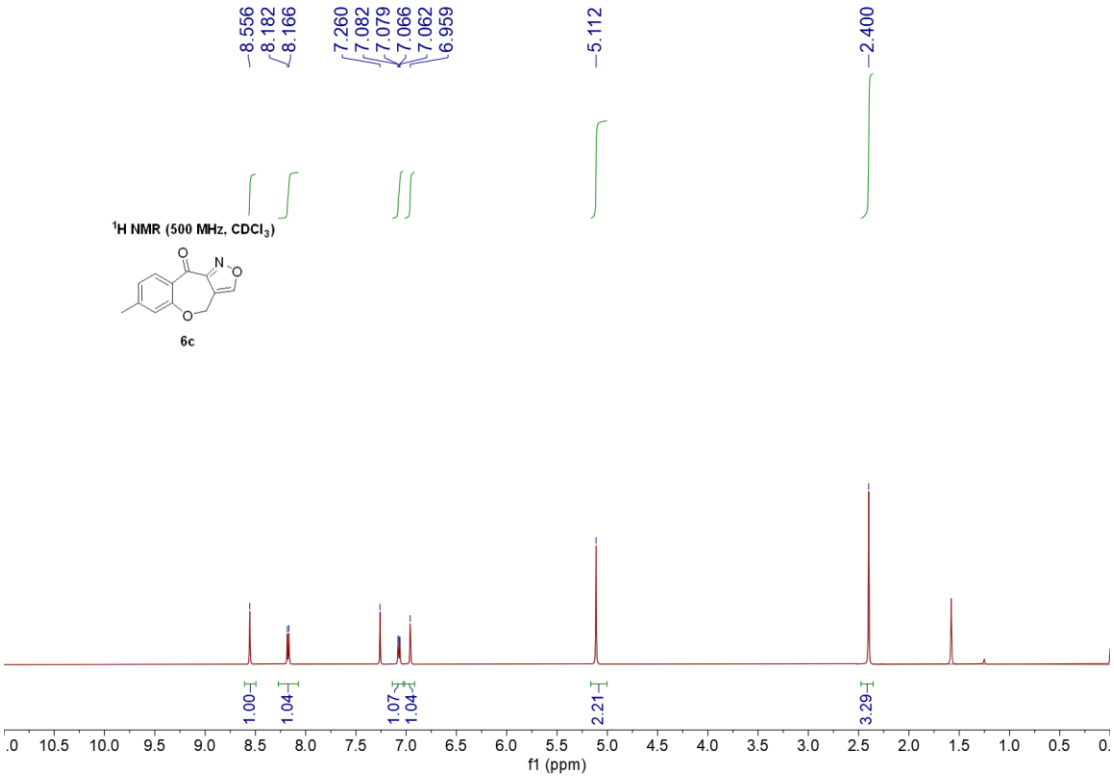

190.435
161.222
158.956
135.469
132.437
128.714
124.241
121.369
79.396
77.318
77.206
77.001
76.683
70.316
41.795
34.525
13C NMR (100 MHz, CDCl3)
4r
f1 (ppm)

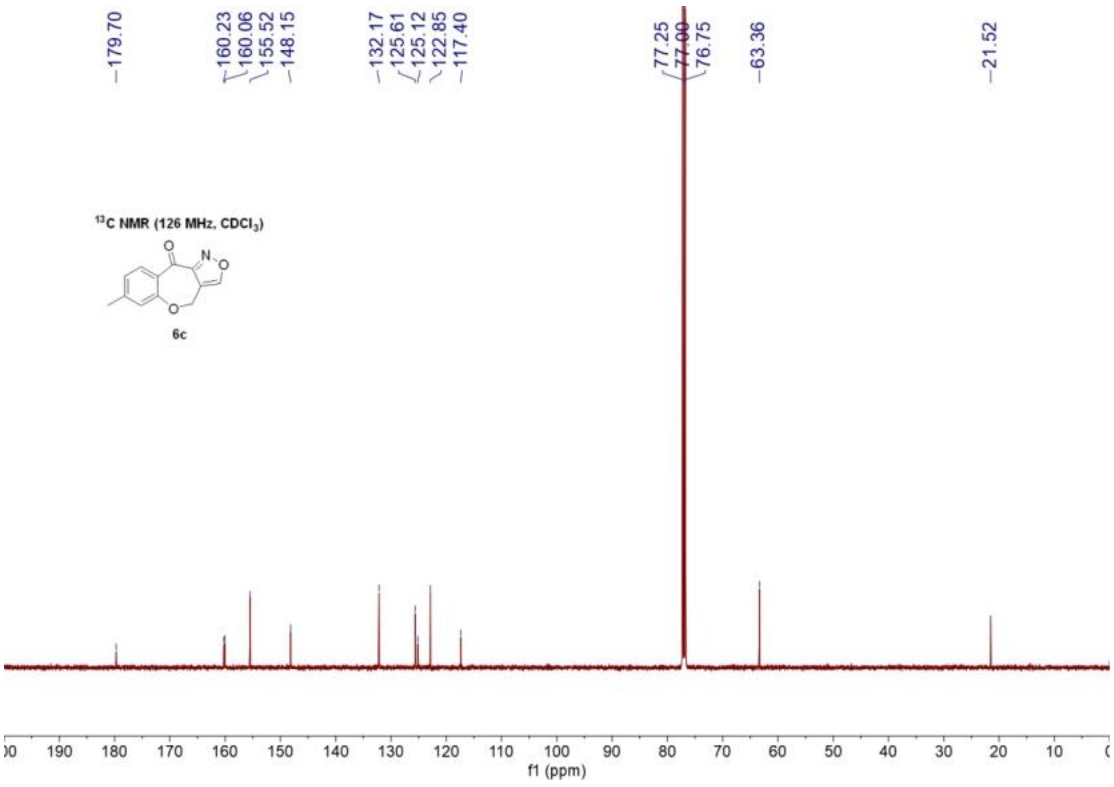

8.575
8.571
8.271
8.267
8.255
8.251
7.596
7.593
7.582
7.579
7.576
7.565
7.562
7.285
7.283
7.269
7.260
7.255
7.252
7.172
7.169
7.155
7.153
5.146
1H NMR (500 MHz, CDCl3)
6a
1.00
1.00
1.03
1.42
0.99
2.15
f1 (ppm)

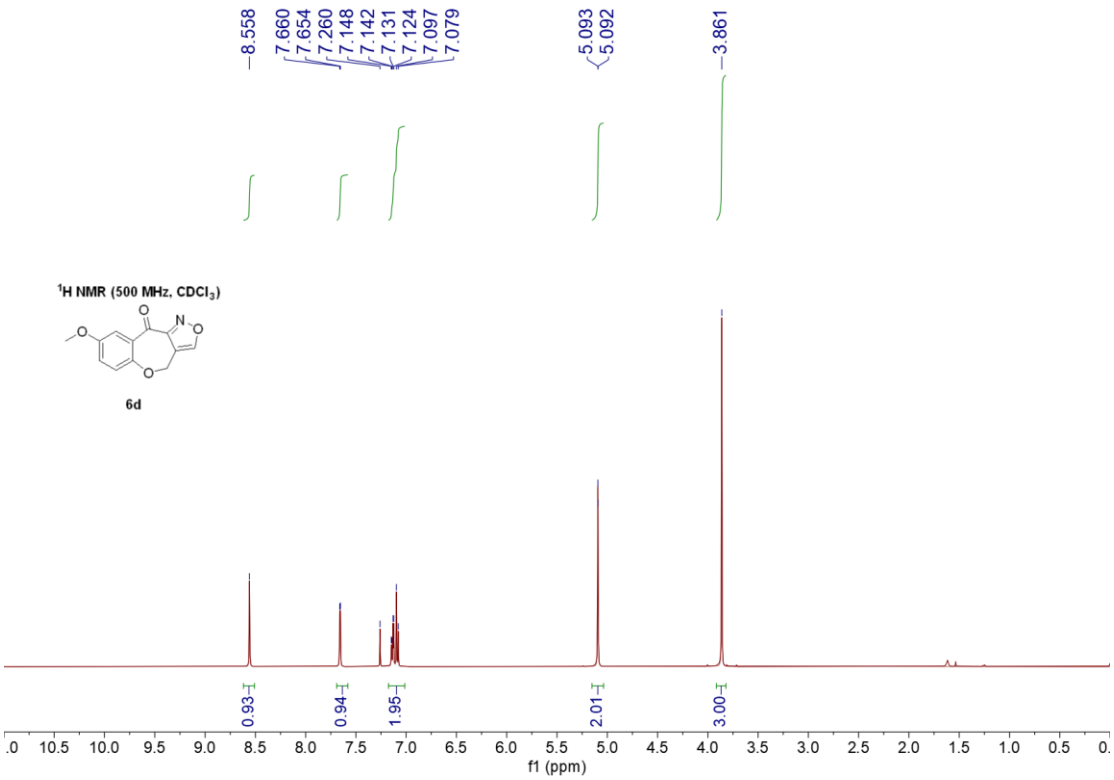

180.18
160.05
155.63
136.34
132.12
127.74
124.49
122.78
117.51
77.25
77.00
76.75
63.56
13C NMR (126 MHz, CDCl3)
6a
f1 (ppm)

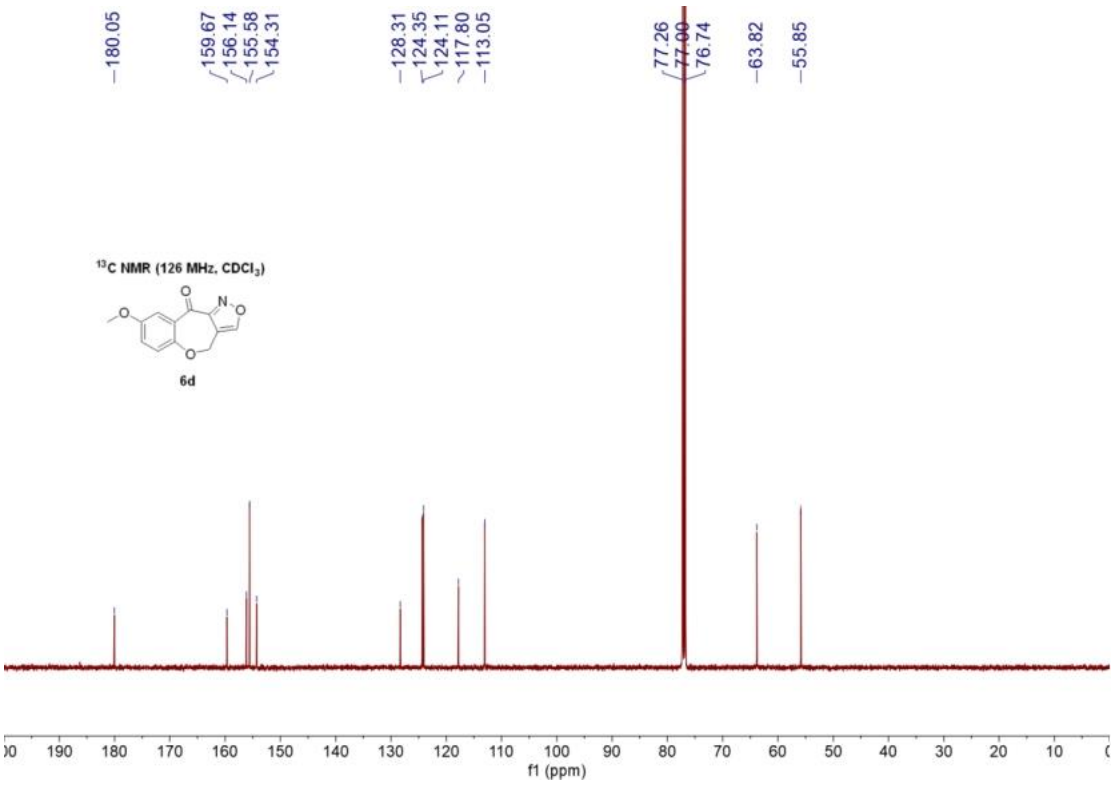

8.560
8.021
8.016
7.377
7.372
7.361
7.356
7.260
7.054
7.037
5.100
2.372
¹H NMR (500 MHz, CDCl₃)
6b
0.87
0.87
0.93
0.92
1.98
3.00
f1 (ppm)

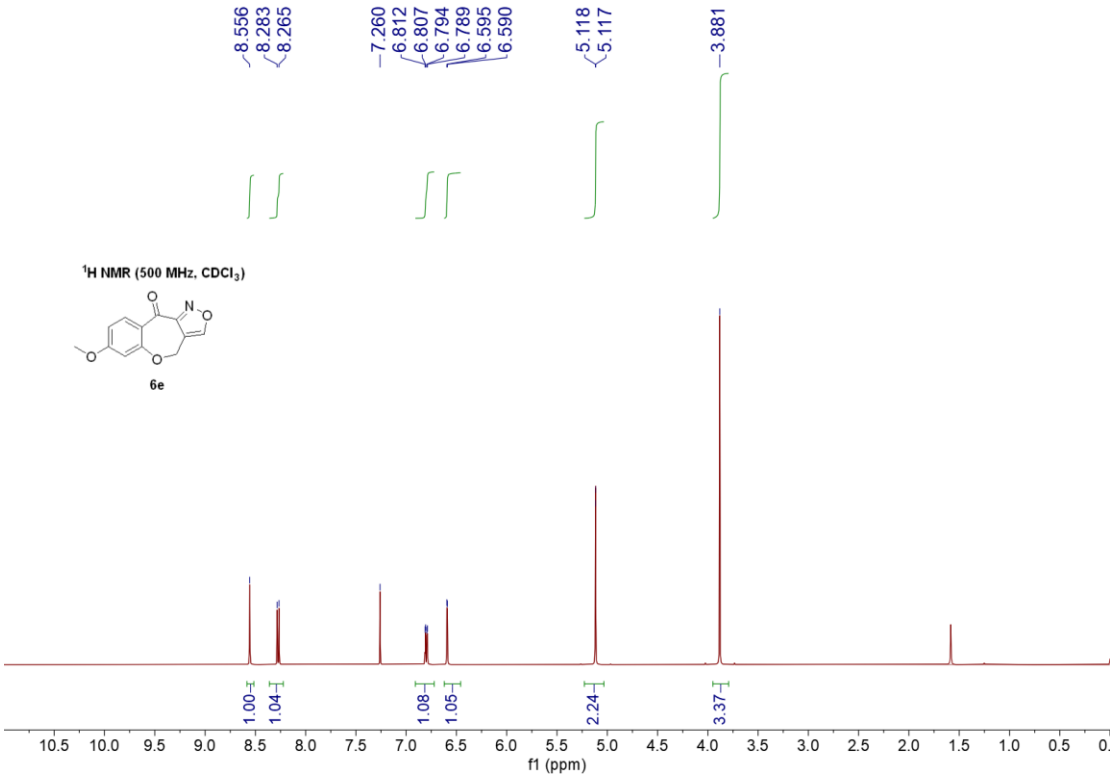

180.37
159.96
158.04
155.60
137.24
134.23
131.78
127.43
122.59
117.66
77.25
77.00
76.75
63.60
20.45
¹³C NMR (126 MHz, CDCl₃)
6b
f1 (ppm)

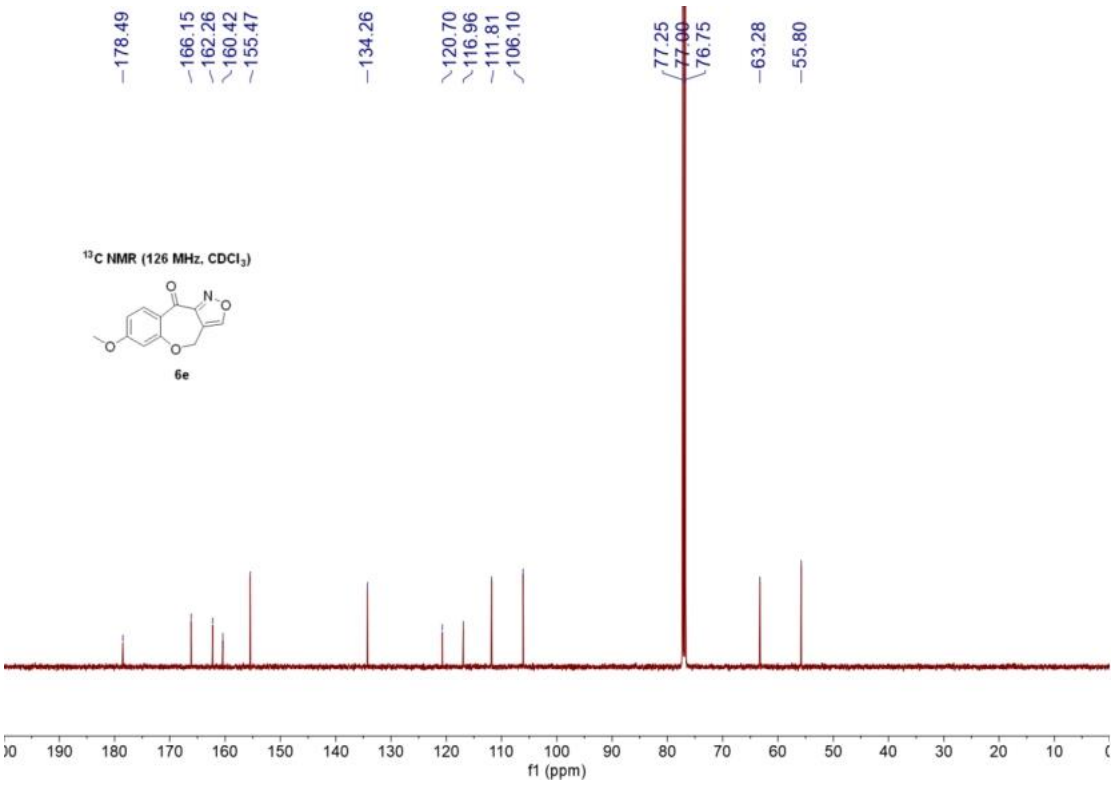

8.556
8.182
8.166
7.260
7.082
7.079
7.066
7.062
6.959
5.112
2.400
^{1}H NMR (500 MHz, CDCl$_3$)
6c
1.00
1.04
1.07
1.04
2.21
3.29
f1 (ppm)

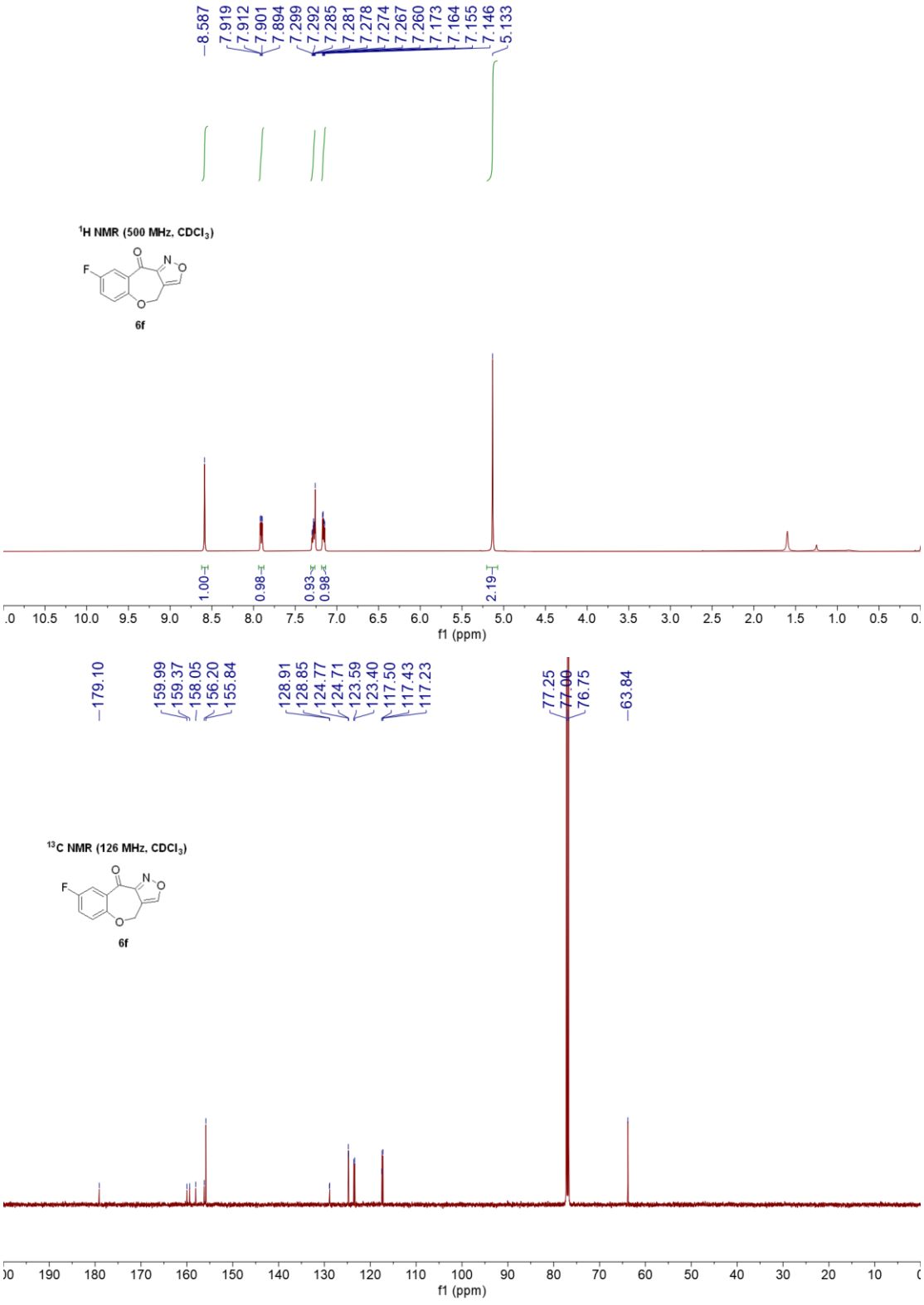

179.70
160.23
160.06
155.52
148.15
132.17
125.61
125.12
122.85
117.40
77.25
77.00
76.75
63.36
21.52
^{13}C NMR (126 MHz, CDCl$_3$)
6c
f1 (ppm)

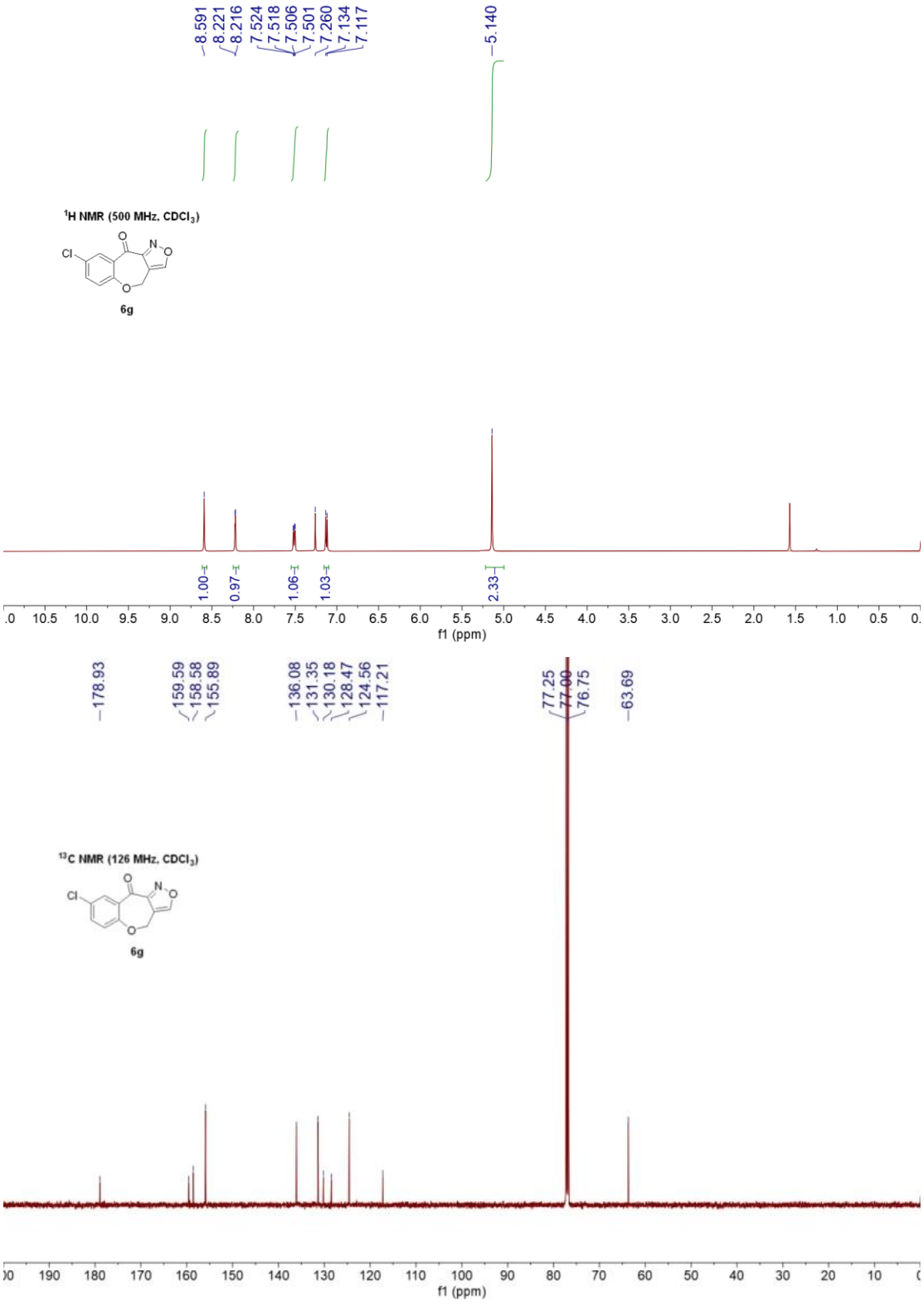

8.558
7.660
7.654
7.260
7.148
7.142
7.131
7.124
7.097
7.079
5.093
5.092
3.861
^{1}H NMR (500 MHz, CDCl$_3$)
6d
0.93
0.94
1.95
2.01
3.00
f1 (ppm)

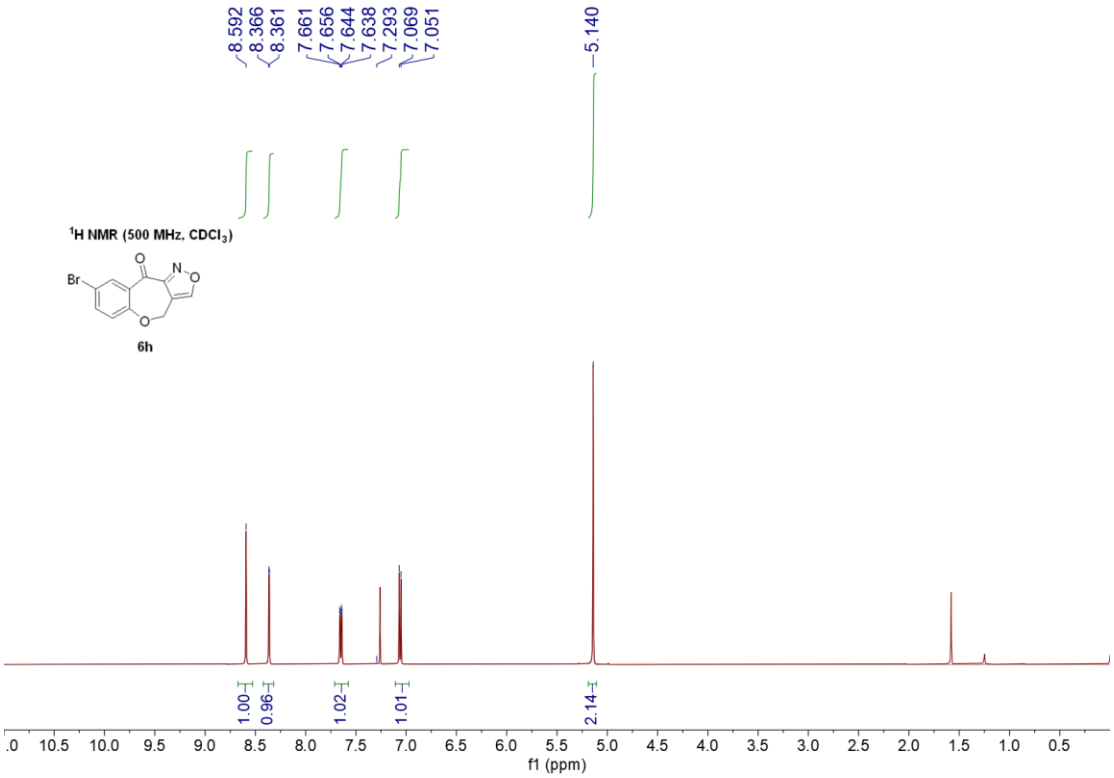

180.05
159.67
156.14
155.58
154.31
128.31
124.35
124.11
117.80
113.05
77.26
77.00
76.74
63.82
55.85
^{13}C NMR (126 MHz, CDCl$_3$)
6d
f1 (ppm)

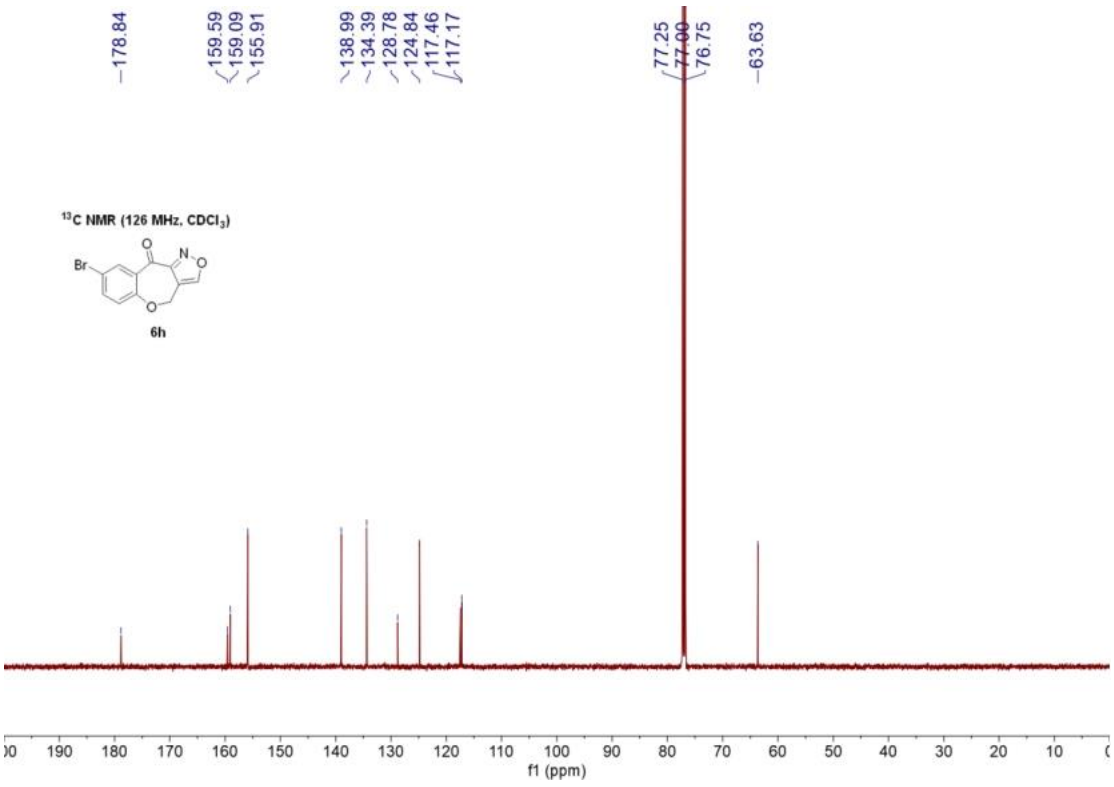

8.556
8.283
8.265
7.260
6.812
6.807
6.794
6.789
6.595
6.590
5.118
5.117
3.881
1H NMR (500 MHz, CDCl3)
6e
1.00
1.04
1.08
1.05
2.24
3.37
f1 (ppm)

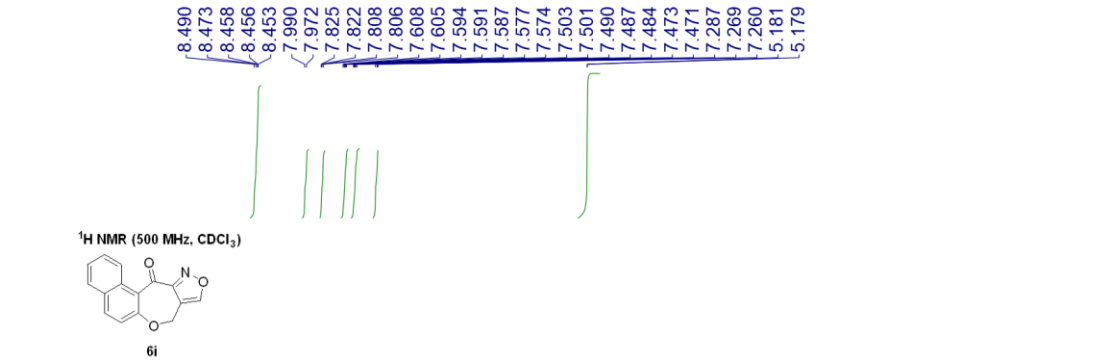

178.49
166.15
162.26
160.42
155.47
134.26
120.70
116.96
111.81
106.10
77.25
77.00
76.75
63.28
55.80
13C NMR (126 MHz, CDCl3)
6e
f1 (ppm)


8.587
7.919
7.912
7.901
7.894
7.299
7.292
7.285
7.281
7.278
7.274
7.267
7.260
7.173
7.164
7.155
7.146
5.133
1H NMR (500 MHz, CDCl3)
6f
1.00
0.98
0.93
0.98
2.19
f1 (ppm)
179.10
159.99
159.37
158.05
156.20
155.84
128.91
128.85
124.77
124.71
123.59
123.40
117.50
117.43
117.23
77.25
77.00
76.75
63.84
13C NMR (126 MHz, CDCl3)
6f
f1 (ppm)


8.591
8.221
8.216
7.524
7.518
7.506
7.501
7.260
7.134
7.117
5.140
1H NMR (500 MHz, CDCl3)
Cl
O
N
O
O
6g
1.00
0.97
1.06
1.03
2.33
f1 (ppm)
178.93
159.59
158.58
155.89
136.08
131.35
130.18
128.47
124.56
117.21
77.25
77.00
76.75
63.69
13C NMR (126 MHz, CDCl3)
6g
f1 (ppm)

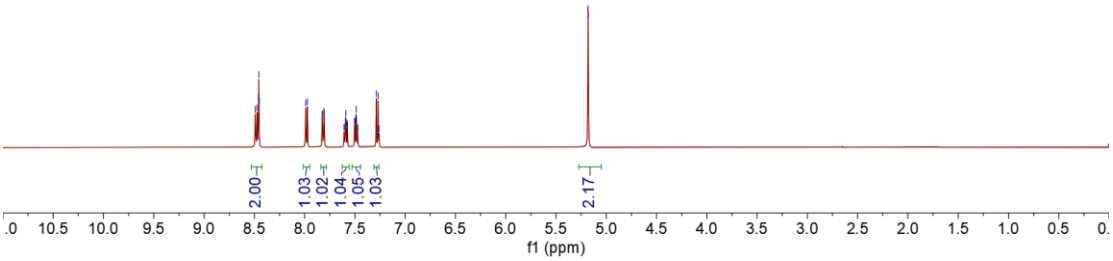

8.592
8.366
8.361
7.661
7.656
7.644
7.638
7.293
7.069
7.051
5.140
1H NMR (500 MHz, CDCl3)
Br
O
N
O
O
6h
1.00
0.96
1.02
1.01
2.14
f1 (ppm)


178.84
159.59
159.09
155.91
138.99
134.39
128.78
124.84
117.46
117.17
77.25
77.00
76.75
63.63
13C NMR (126 MHz, CDCl3)
Br
O
N
O
O
6h
f1 (ppm)

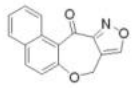


^{1}H NMR (500 MHz, $CDCl_3$)

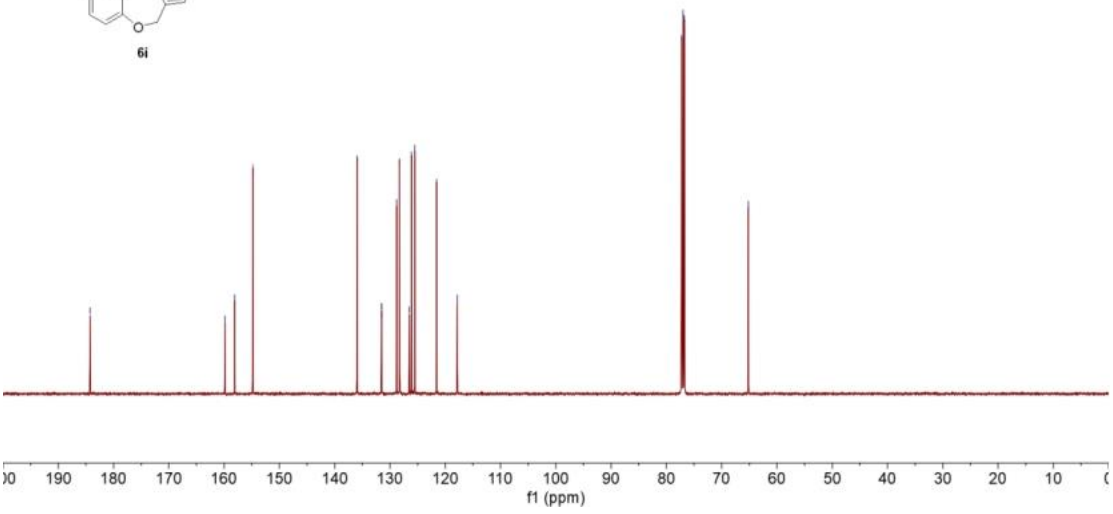
6i

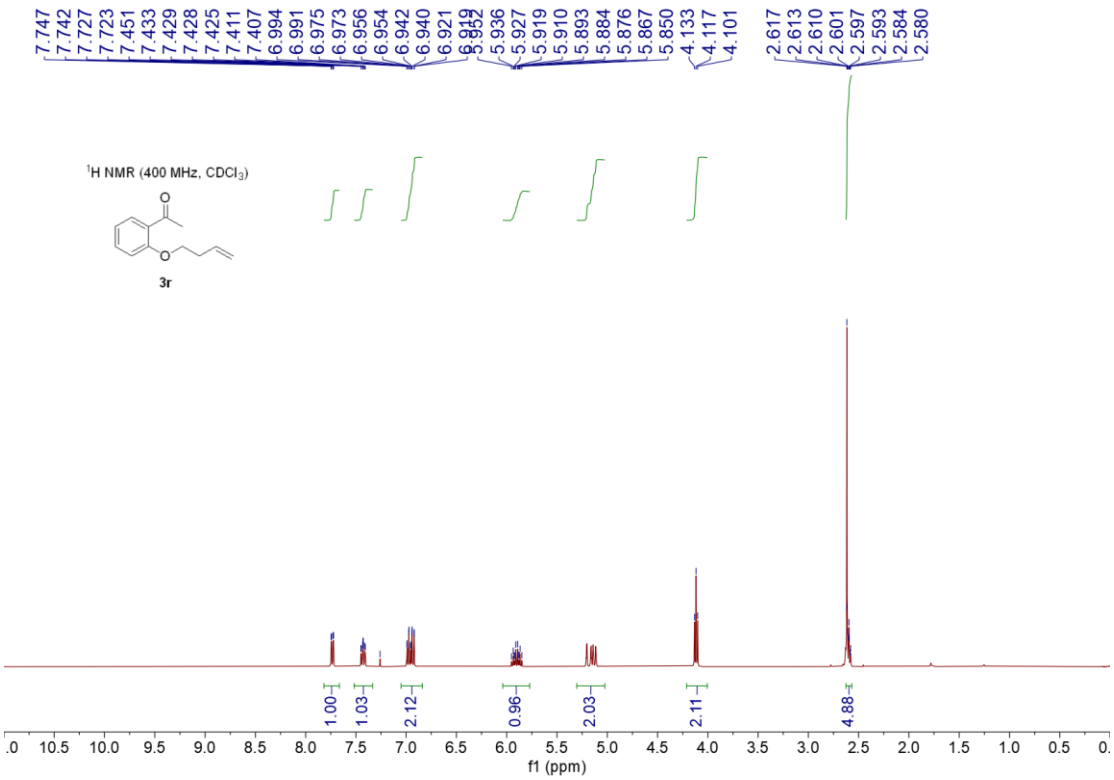


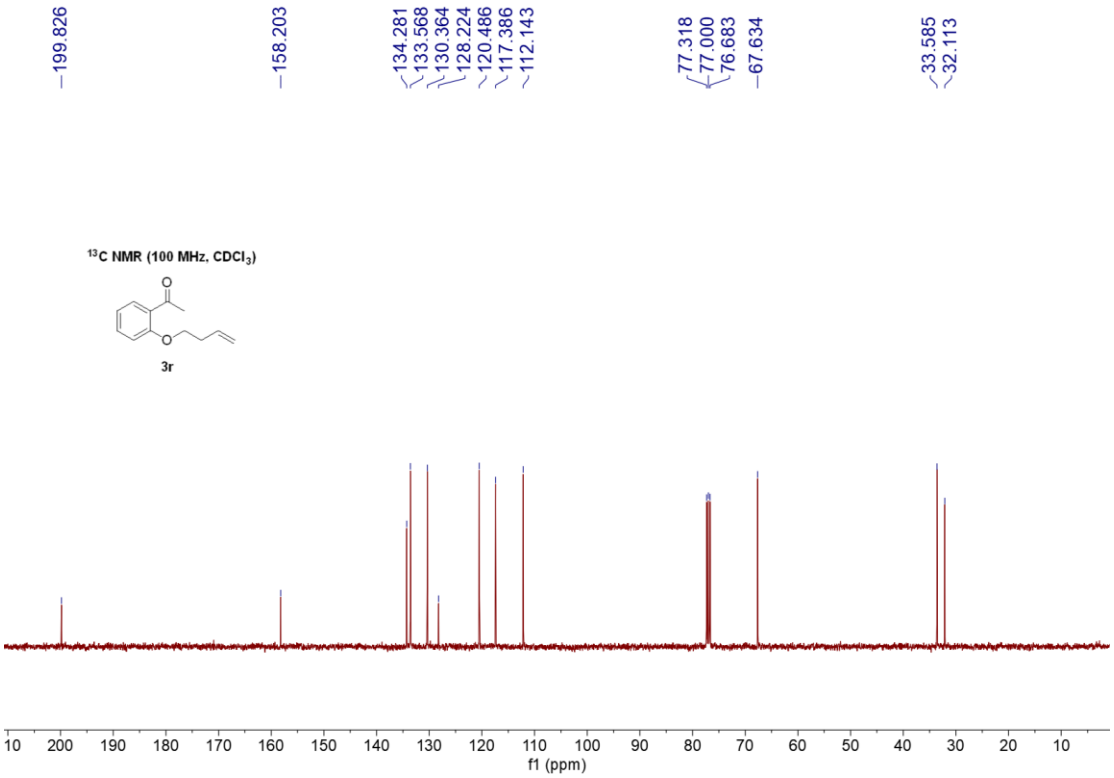
^{13}C NMR (126 MHz, $CDCl_3$)



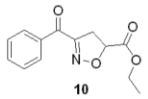
6i



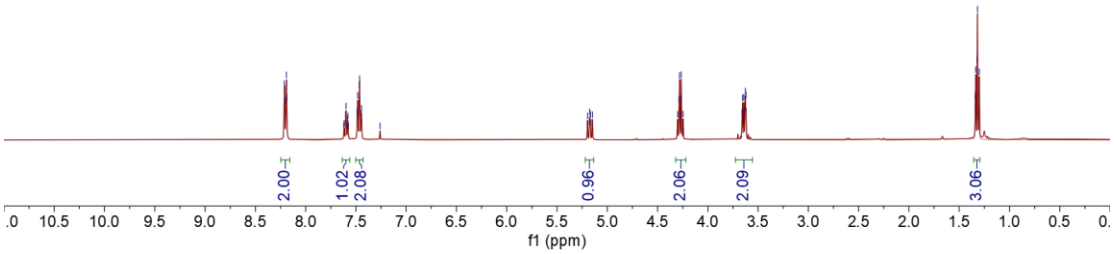

7.747
7.742
7.727
7.723
7.451
7.433
7.429
7.428
7.425
7.411
7.407
6.994
6.991
6.975
6.973
6.956
6.954
6.942
6.940
6.921
5.936
5.927
5.919
5.910
5.893
5.884
5.876
5.867
5.850
4.133
4.117
4.101
2.617
2.613
2.610
2.601
2.597
2.593
2.584
2.580
1H NMR (400 MHz, CDCl3)
3r
1.00
1.03
2.12
0.96
2.03
2.11
4.88
f1 (ppm)


199.826
158.203
134.281
133.568
130.364
128.224
120.486
117.386
112.143
77.318
77.000
76.683
67.634
33.585
32.113
13C NMR (100 MHz, CDCl3)
3r
f1 (ppm)

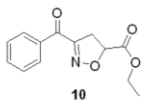
^{1}H NMR (400 MHz, $CDCl_3$)



10



^{13}C NMR (100 MHz, $CDCl_3$)



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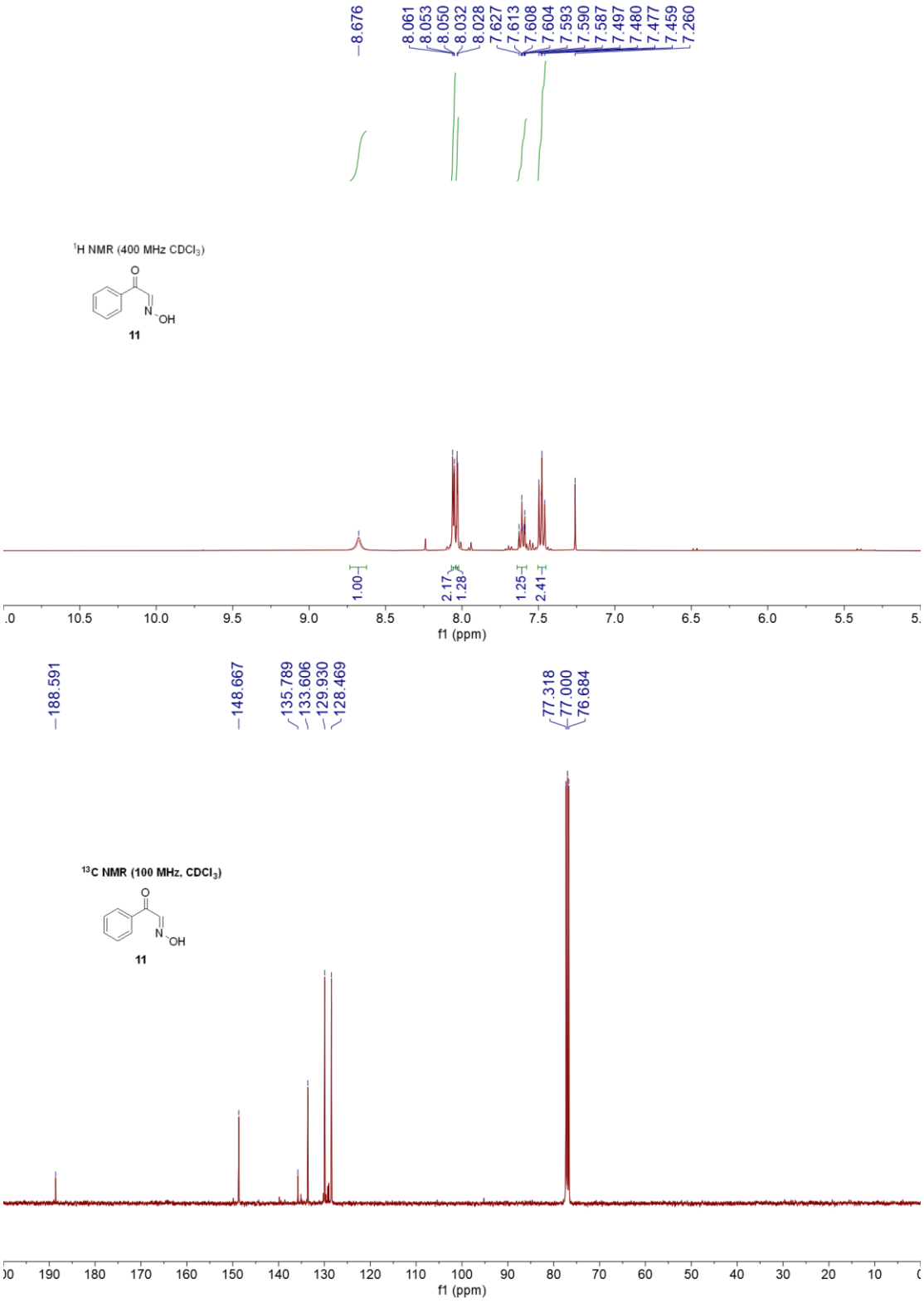
8.676
8.061
8.053
8.050
8.032
8.028
7.627
7.613
7.608
7.604
7.593
7.590
7.587
7.497
7.480
7.477
7.459
7.260
^{1}H NMR (400 MHz CDCl$_3$)
11
1.00
2.17
1.28
1.25
2.41
f1 (ppm)
188.591
148.667
135.789
133.606
129.930
128.469
77.318
77.000
76.684
^{13}C NMR (100 MHz, CDCl$_3$)
11
f1 (ppm)