Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information for:

Synthesis of Model Bacteriochlorophylls Containing Substituents of Native Rings A, C and E

Duy T. M. Chung, Phuong Vy Tran, Khiem Chau Nguyen, Pengzhi Wang, and Jonathan S. Lindsey*

Department of Chemistry
North Carolina State University
Raleigh, NC 27695-8204
e-mail: jlindsey@ncsu.edu

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1. Single-crystal X-ray data

Table S1. Single-crystal X-ray structure data for **7**

CCDC registry	2083658
Chemical formula	C_6H_6BrNO
Formula weight (g/mol)	188.03
Temperature (K)	100(2)
Wavelength (Å)	1.54178
Crystal size (mm)	0.052 × 0.066 × 0.232
Crystal habit	Colorless rod
Crystal system	monoclinic
Space group	P 1 21/c 1
Unit cell dimensions, *a* (Å)	11.2353(7)
Unit cell dimensions, *b* (Å)	7.3127(5)
Unit cell dimensions, *c* (Å)	15.8256(10)
α, deg	90
β, deg	90.408(2)
γ, deg	90
Volume ($Å^3$)	1300.20(15)
Z	8
Density (calculated) (g/cm^3)	1.921
Absorption coefficient (mm^{-1})	7.888
F(000)	736
Theta range for data collection, deg	3.93 to 72.93
Index ranges	-13<=h<=13, -9<=k<=9, -19<=l<=18
Reflections collected	19445
Independent reflections	2562 [R(int) = 0.0446]
R_1	0.0320
wR_2	0.0826
R_1 (all data)	0.0323
wR_2 (all data)	0.0828
Largest diff. peak and hole ($eÅ^{-3}$)	1.004 and -0.434
R.M.S. deviation from mean ($eÅ^{-3}$)	0.110

Table S2. Single-crystal X-ray structure data for **8**

CCDC registry	2083659
Chemical formula	$C_{13}H_{12}BrNO_3S$
Formula weight (g/mol)	342.21
Temperature (K)	100(2)
Wavelength (Å)	0.71073
Crystal size (mm)	0.098 × 0.180 × 0.223
Crystal habit	Colorless block
Crystal system	triclinic
Space group	P -1
Unit cell dimensions, *a* (Å)	8.3674(3)
Unit cell dimensions, *b* (Å)	8.5936(3)
Unit cell dimensions, *c* (Å)	10.4526(3)
α, deg	88.161(2)
β, deg	88.2410(10)
γ, deg	63.805(2)
Volume ($Å^3$)	673.95(4)
Z	2
Density (calculated) (g/cm^3)	1.686
Absorption coefficient (mm^{-1})	3.207
F(000)	344
Theta range for data collection, deg	1.95 to 30.51
Index ranges	-11<=h<=11, -12<=k<=12, -14<=l<=14
Reflections collected	39430
Independent reflections	4118 [R(int) = 0.0483]
R_1	0.0338
wR_2	0.0882
R_1 (all data)	0.0441
wR_2 (all data)	0.0931
Largest diff. peak and hole ($eÅ^{-3}$)	1.894 and -0.624
R.M.S. deviation from mean ($eÅ^{-3}$)	0.081

Table S3. Single-crystal X-ray structure data for **10**

CCDC registry	2083662
Chemical formula	$C_{22}H_{30}BrN_2O_{7.50}S$
Formula weight (g/mol)	554.45
Temperature (K)	100(2)
Wavelength (Å)	1.54178
Crystal size (mm)	0.057 × 0.102 × 0.183
Crystal habit	Colorless plate
Crystal system	monoclinic
Space group	*C*2/c
Unit cell dimensions, *a* (Å)	36.3995(13)
Unit cell dimensions, *b* (Å)	6.3576(2)
Unit cell dimensions, *c* (Å)	25.0600(9)
α, deg	90
β, deg	123.6400(10)
γ, deg	90
Volume ($Å^3$)	4828.1(3)
Z	8
Density (calculated) (g/cm^3)	1.526
Absorption coefficient (mm^{-1})	3.545
F(000)	2296
Theta range for data collection, deg	2.92 to 79.59
Index ranges	-46<=h<=42, -8<=k<=7, -30<=l<=31
Reflections collected	49434
Independent reflections	5163 [R(int) = 0.0246]
R_1	0.0232
wR_2	0.0609
R_1 (all data)	0.0234
wR_2 (all data)	0.0610
Largest diff. peak and hole ($eÅ^{-3}$)	0.385 and -0.295
R.M.S. deviation from mean ($eÅ^{-3}$)	0.050

Table S4. Single-crystal X-ray structure data for **11**

CCDC registry	2083661
Chemical formula	$C_{26}H_{34}N_2O_{10}S$
Formula weight (g/mol)	566.61
Temperature (K)	100(2)
Wavelength (Å)	0.71073
Crystal size (mm)	0.161 × 0.184 × 0.260
Crystal habit	Colorless plate
Crystal system	Monoclinic
Space group	C 1 2/c 1
Unit cell dimensions, *a* (Å)	29.6209(10)
Unit cell dimensions, *b* (Å)	12.7399(4)
Unit cell dimensions, *c* (Å)	16.3799(6)
α, deg	90
β, deg	116.8250(10)
γ, deg	90
Volume ($Å^3$)	5516.1(6)
Z	8
Density (calculated) (g/cm^3)	1.365
Absorption coefficient (mm^{-1})	0.176
F(000)	2400
Theta range for data collection, deg	2.46 to 32.04
Index ranges	-44<=h<=44, -18<=k<=18, -24<=l<=24
Reflections collected	98657
Independent reflections	9585 [R(int) = 0.0560]
R_1	0.0383
wR_2	0.0936
R_1 (all data)	0.0535
wR_2 (all data)	0.1026
Largest diff. peak and hole ($eÅ^{-3}$)	0.387 and -0.380
R.M.S. deviation from mean ($eÅ^{-3}$)	0.052

Table S5. Single-crystal X-ray structure data for **15**

CCDC registry	2083660
Chemical formula	C_7H_8INO
Formula weight (g/mol)	249.04
Temperature (K)	108
Wavelength (Å)	0.71073
Crystal size (mm)	0.11 × 0.10 × 0.09
Crystal habit	Colorless block
Crystal system	Orthorhombic
Space group	*P* b c a
Unit cell dimensions, *a* (Å)	8.8097(5)
Unit cell dimensions, *b* (Å)	12.6229(8)
Unit cell dimensions, *c* (Å)	14.4382(9)
α, deg	90
β, deg	90
γ, deg	90
Volume (Å^3)	1605.59(17)
Z	8
Density (calculated) (g/cm^3)	2.061
Absorption coefficient (mm^{-1})	3.920
F(000)	944
Theta range for data collection, deg	2.82 to 33.11
Index ranges	-13<=h<=13, -19<=k<=19, -22<=l<=22
Reflections collected	67230
Independent reflections	3062 [R(int) = 0.059]
R_1	0.0198
wR_2	0.0388
R_1 (all data)	0.0310
wR_2 (all data)	0.0415
Largest diff. peak and hole (eÅ^{-3})	0.716 and -0.850
R.M.S. deviation from mean (eÅ^{-3})	0.117

2. Absorption spectrum of unknown Knoevenagel product

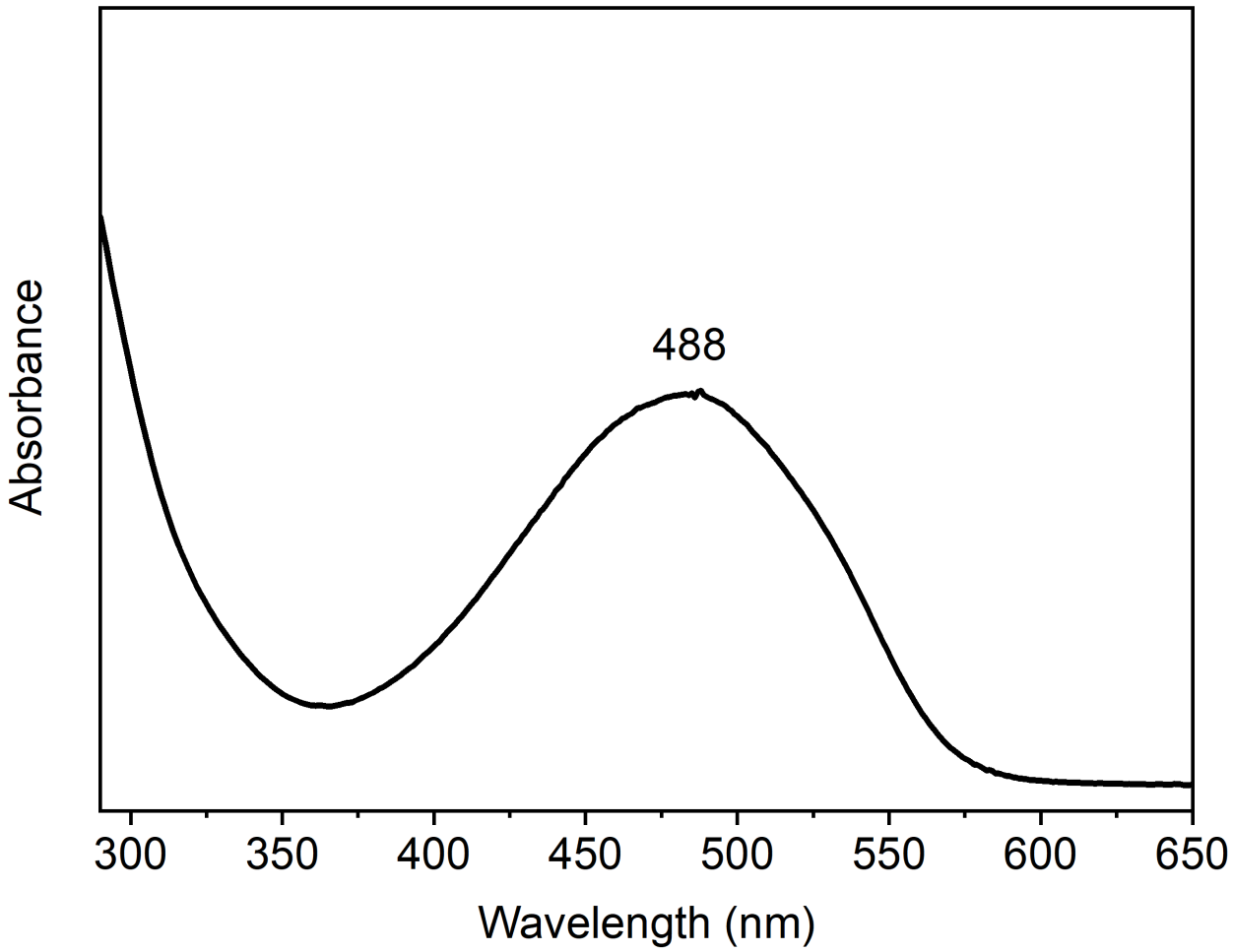


Figure S1. Absorption spectrum of the unknown side product in the Knoevenagel reaction of preparing **3bb**.

3. Stereochemistry via NOESY for bacteriochlorophyll analogues

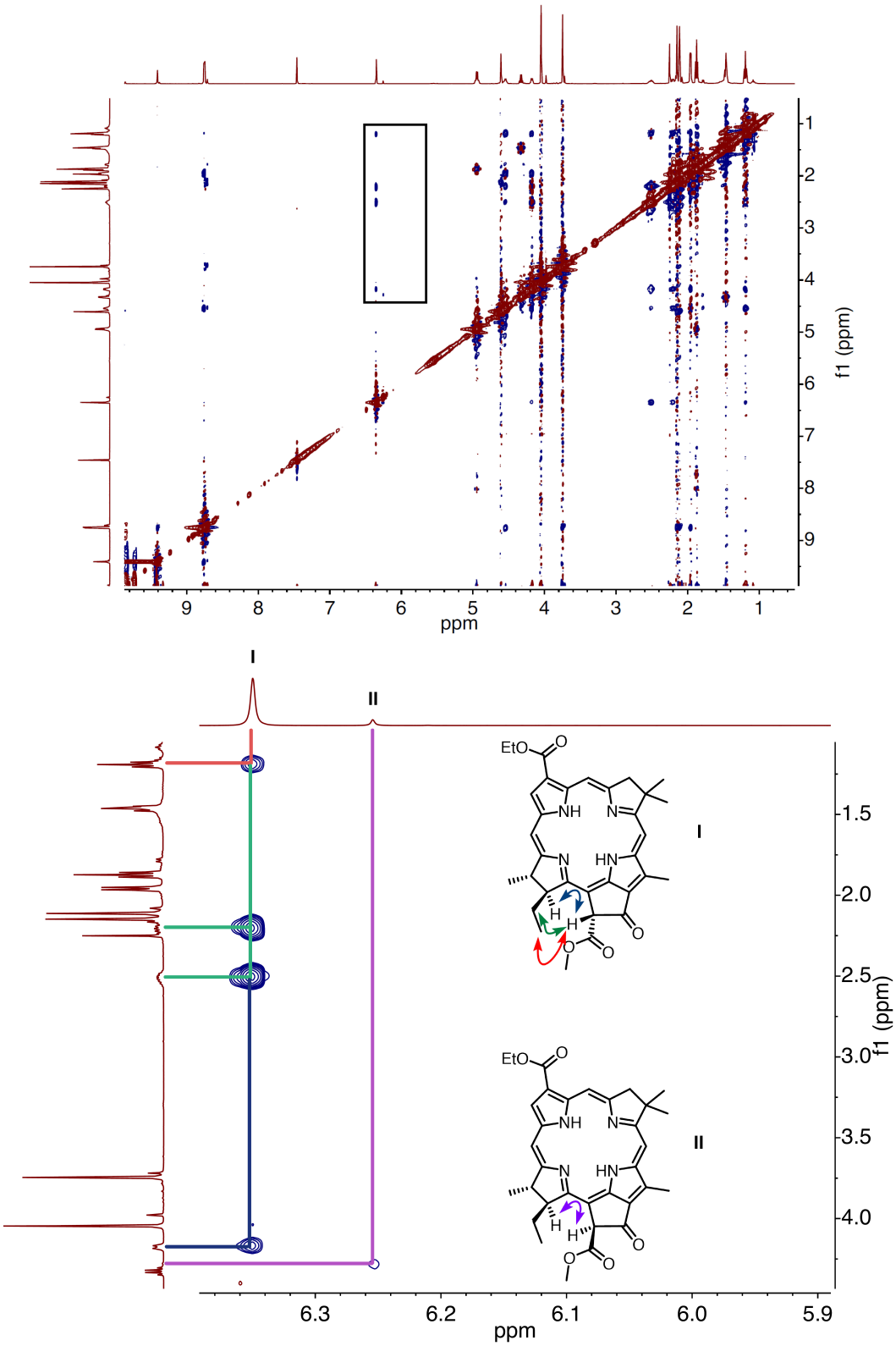


Figure S2. Full NOESY spectrum of **BC-ab** sample (top) and enlarged region showing the correlations supporting the configuration assignment of each epimer in the sample (bottom).

4. Chromatography for Knoevenagel and double-ring closure reactions

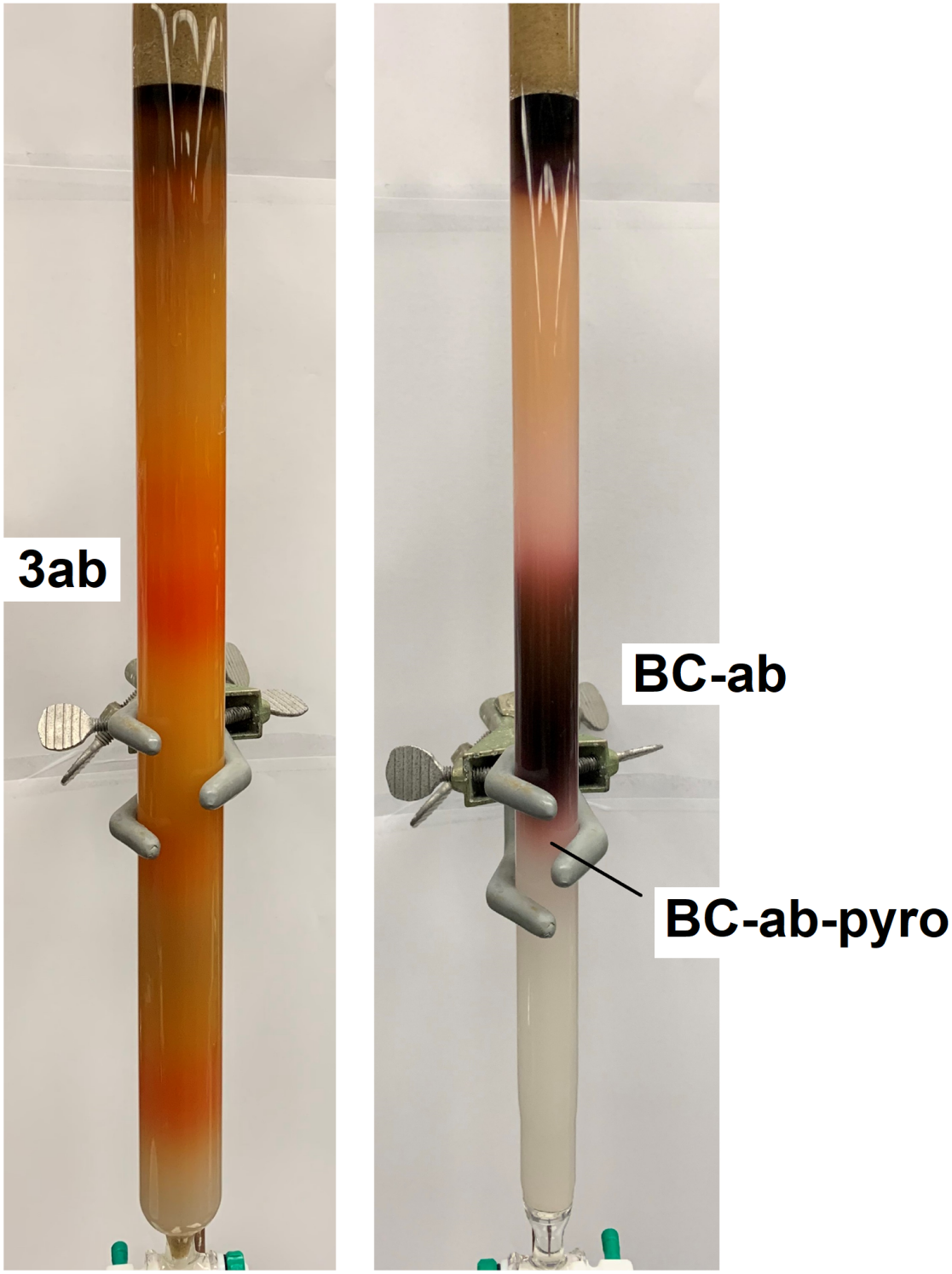


Figure S3. Column chromatography for reaction mixtures following Knoevenagel reaction (left) and one-flask double-ring closure (right) in preparation of **BC-ab**.

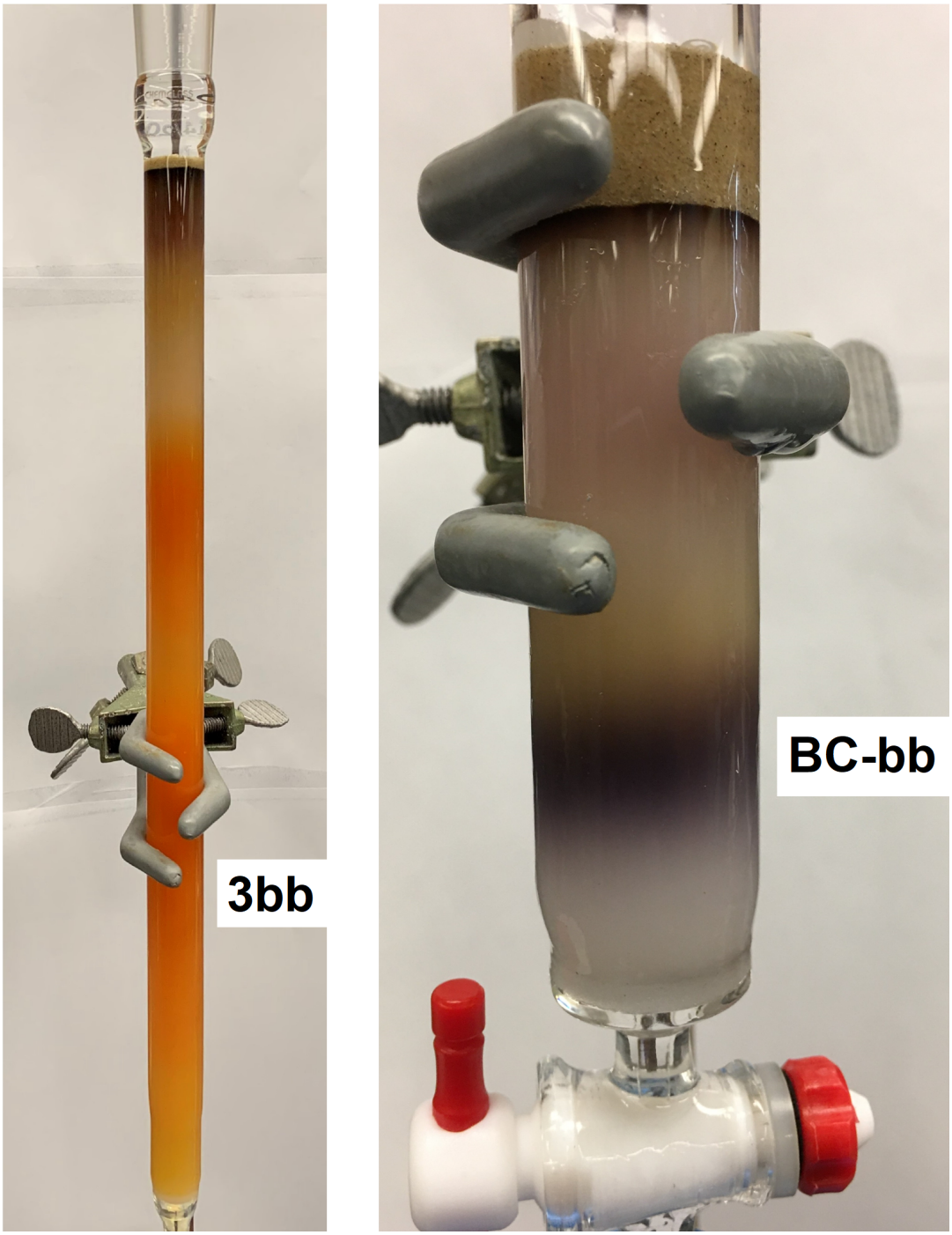
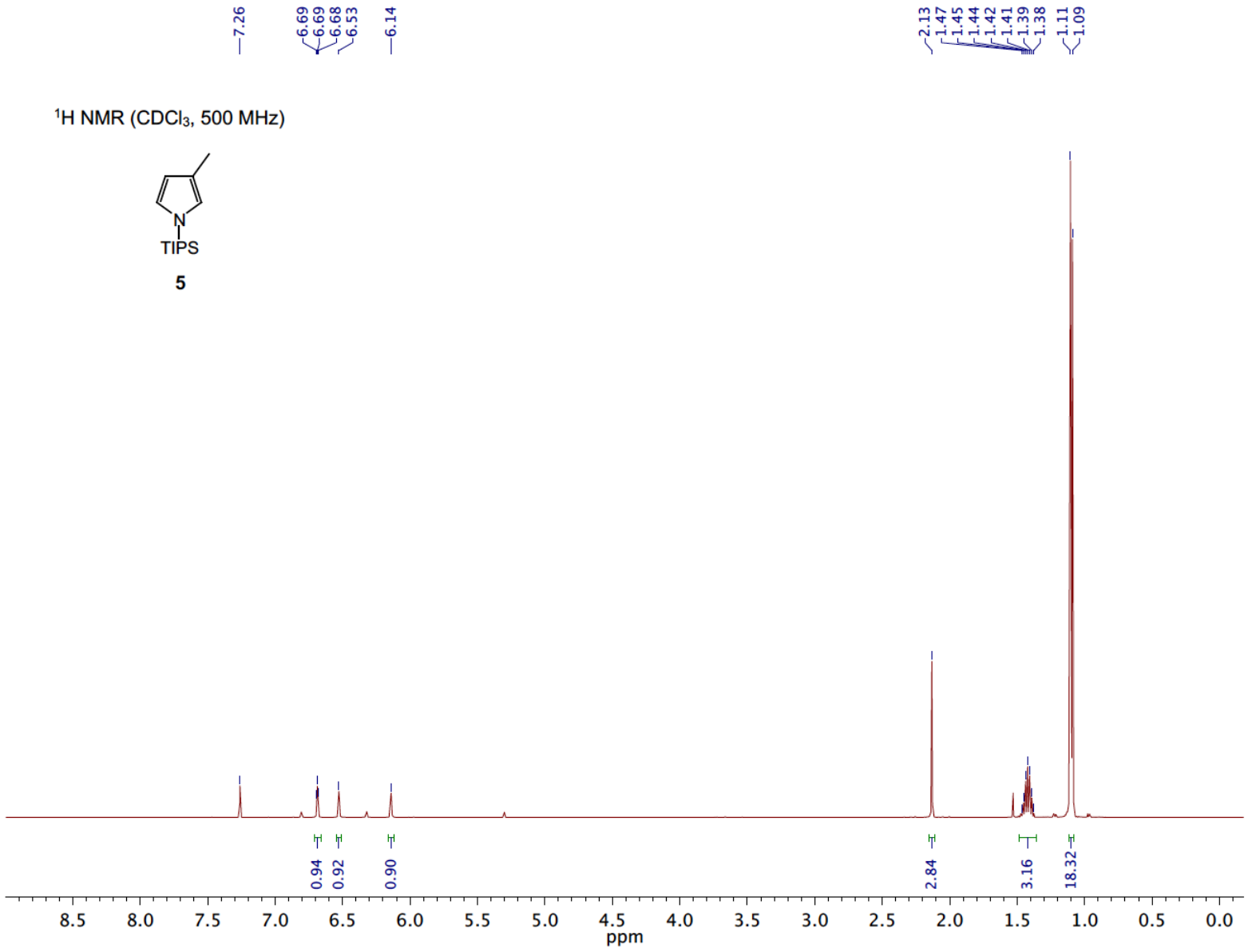
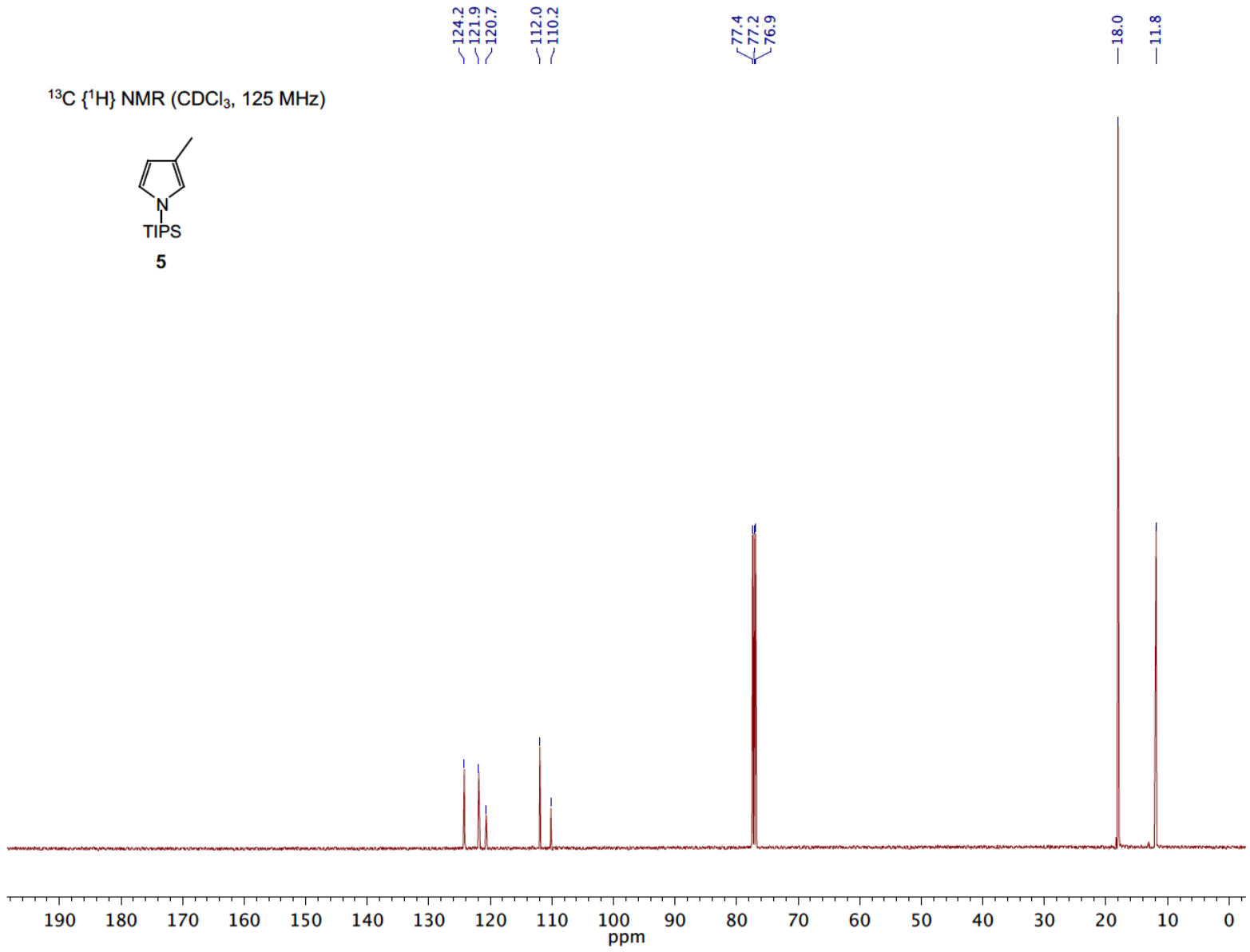
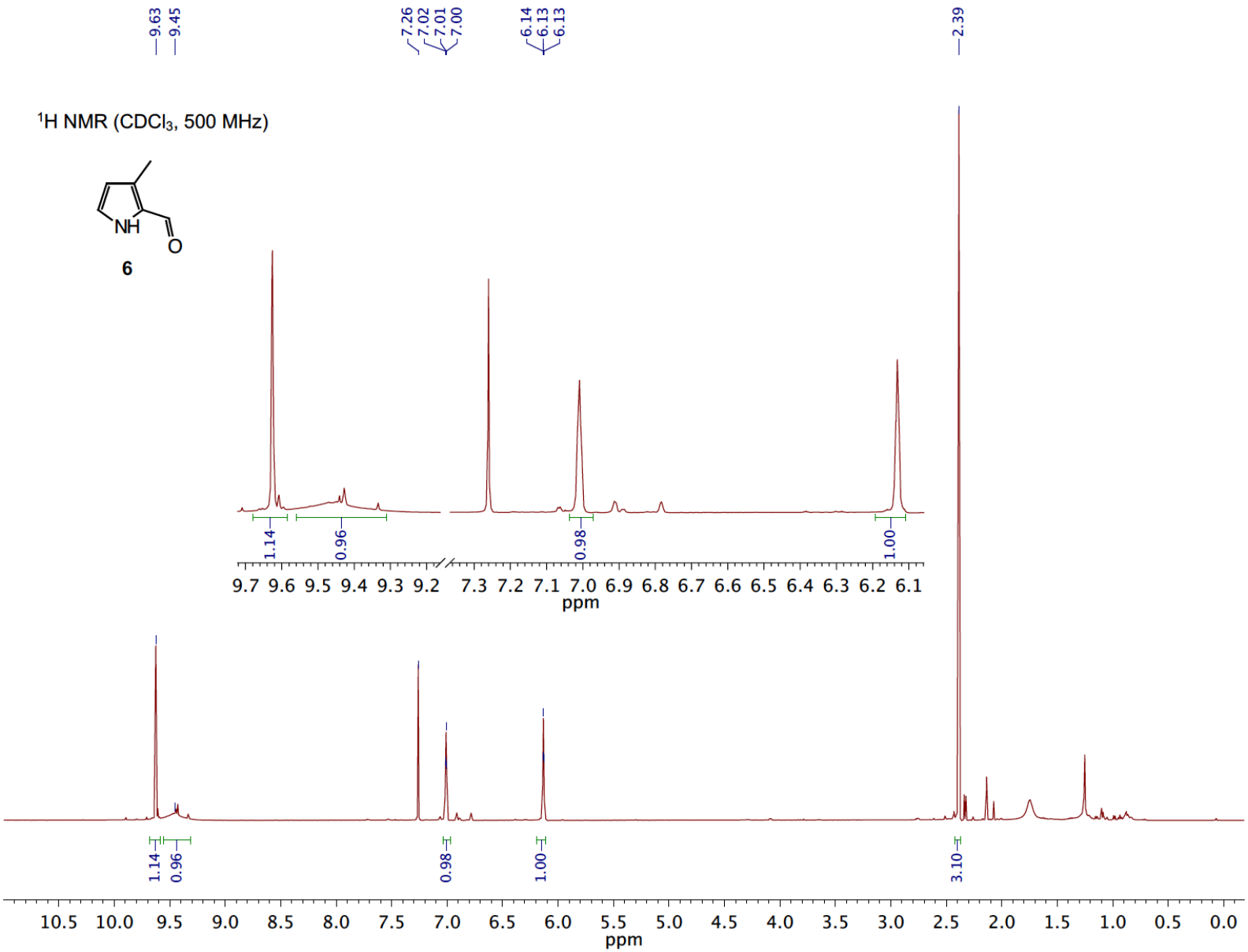


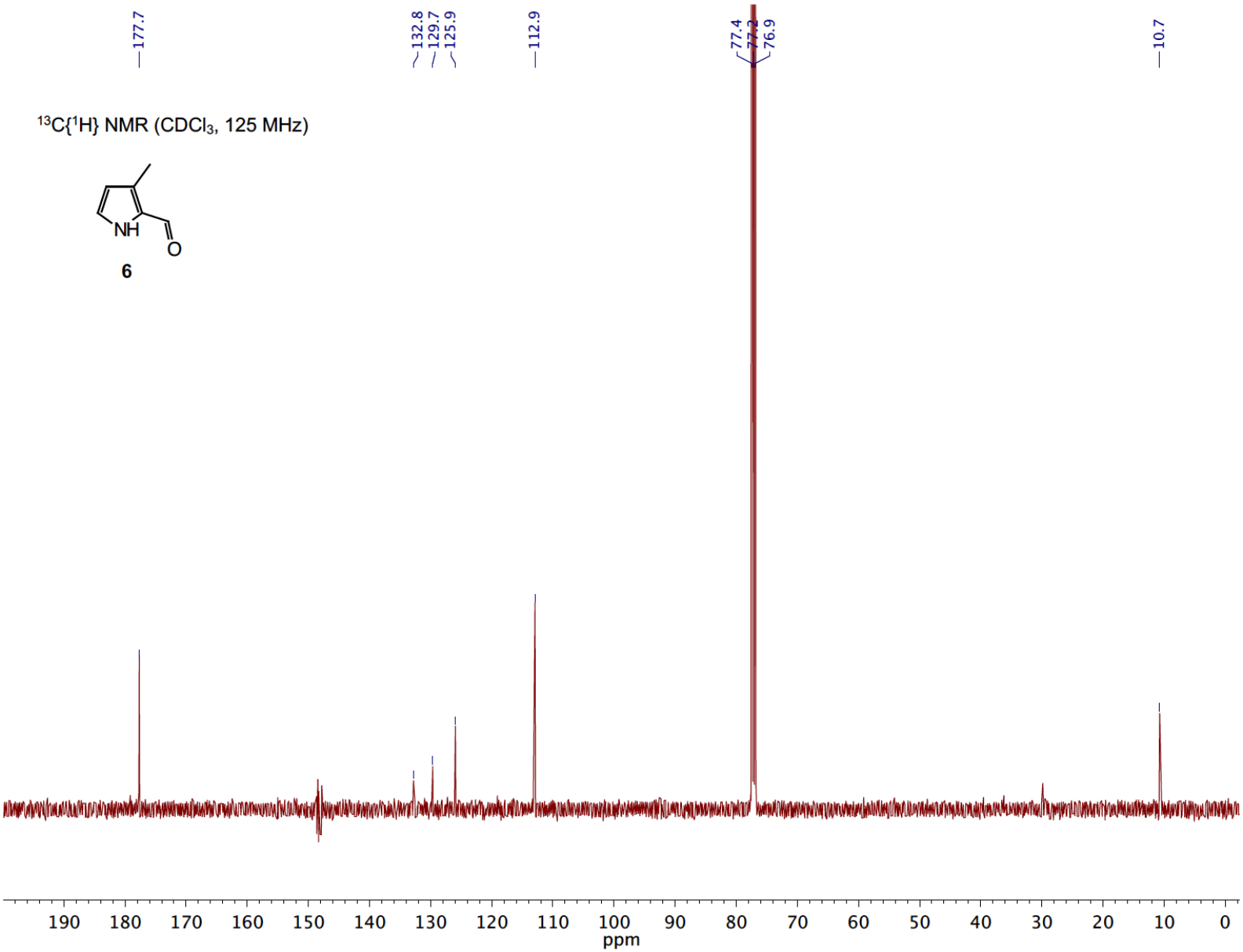
Figure S4. Column chromatography for reaction mixtures following Knoevenagel reaction (left) and one-flask double-ring closure (right) in preparation of **BC-bb**.

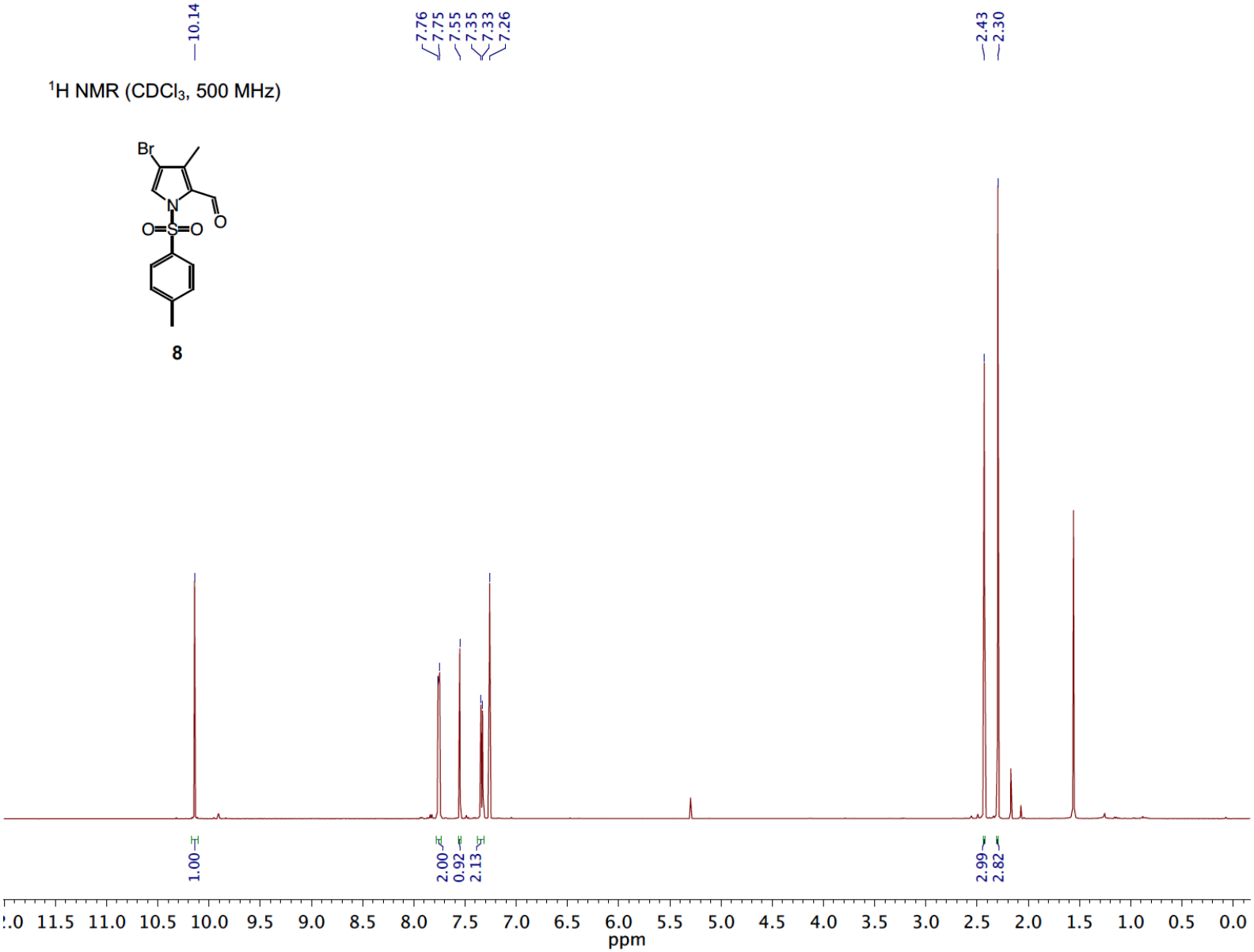
5. NMR spectra

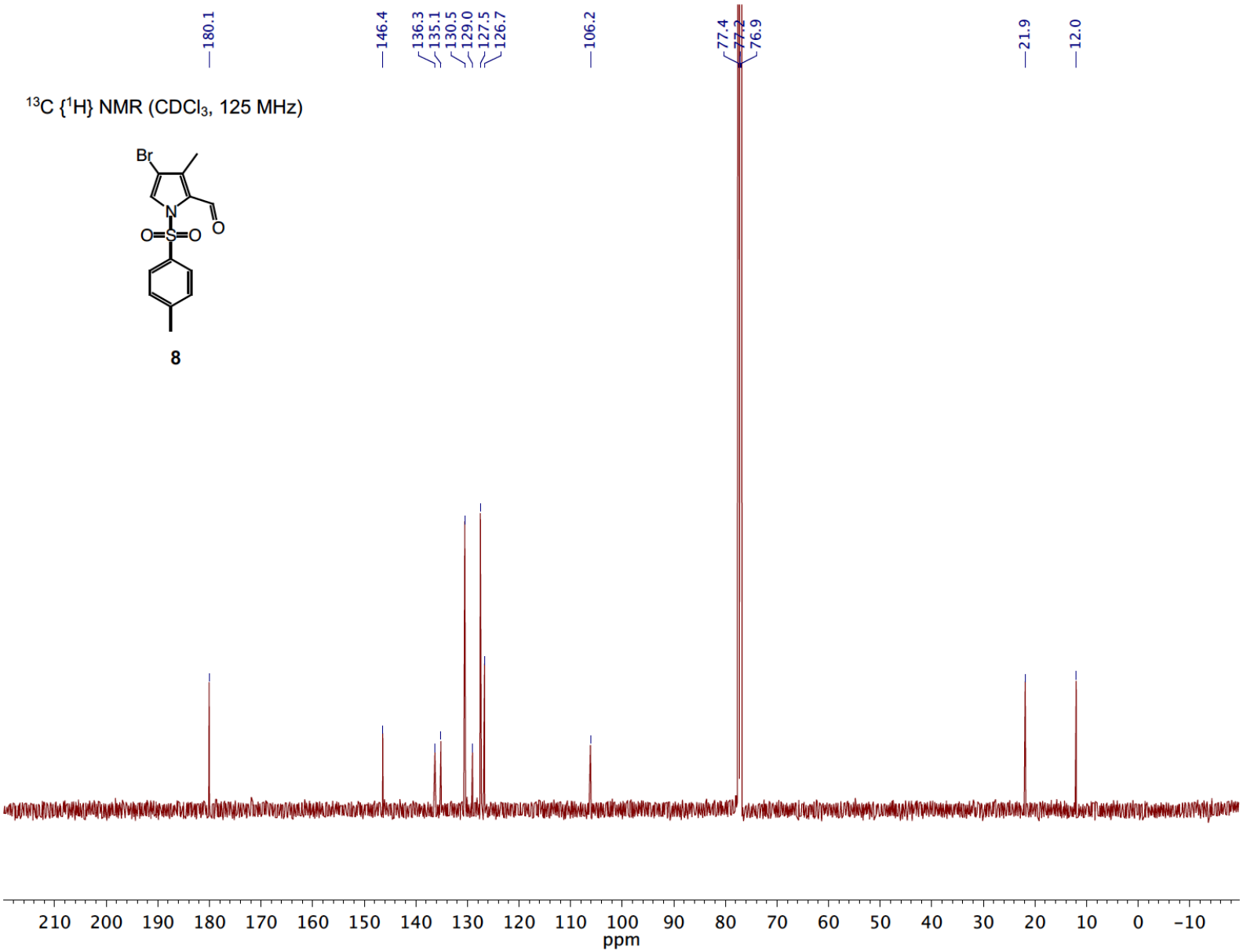

7.26
6.69
6.69
6.68
6.53
6.14
2.13
1.47
1.45
1.44
1.42
1.41
1.39
1.38
1.11
1.09
^{1}H NMR ($CDCl_3$, 500 MHz)
N
TIPS
5
0.94
0.92
0.90
2.84
3.16
18.32
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


124.2
121.9
120.7
112.0
110.2
77.4
77.2
76.9
18.0
11.8
^{13}C {^{1}H} NMR ($CDCl_3$, 125 MHz)
N
TIPS
5
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

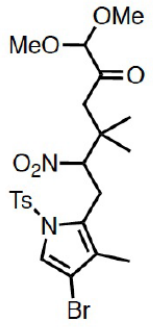

9.63
9.45
7.26
7.02
7.01
7.00
6.14
6.13
6.13
2.39
^{1}H NMR ($CDCl_3$, 500 MHz)
NH
O
6
1.14
0.96
0.98
1.00
9.7 9.6 9.5 9.4 9.3 9.2 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1
ppm
1.14
0.96
0.98
1.00
3.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm


177.7
132.8
129.7
125.9
112.9
77.4
77.2
76.9
10.7
13C{1H} NMR (CDCl3, 125 MHz)
NH
O
6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


10.14
7.76
7.75
7.55
7.35
7.33
7.26
2.43
2.30
1H NMR (CDCl3, 500 MHz)
Br
N
O
S
O
O
8
1.00
2.00
0.92
2.13
2.99
2.82
ppm


180.1
146.4
136.3
135.1
130.5
129.0
127.5
126.7
106.2
77.4
77.2
76.9
21.9
12.0
13C {1H} NMR (CDCl3, 125 MHz)
Br
N
O
S
O
O
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm

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



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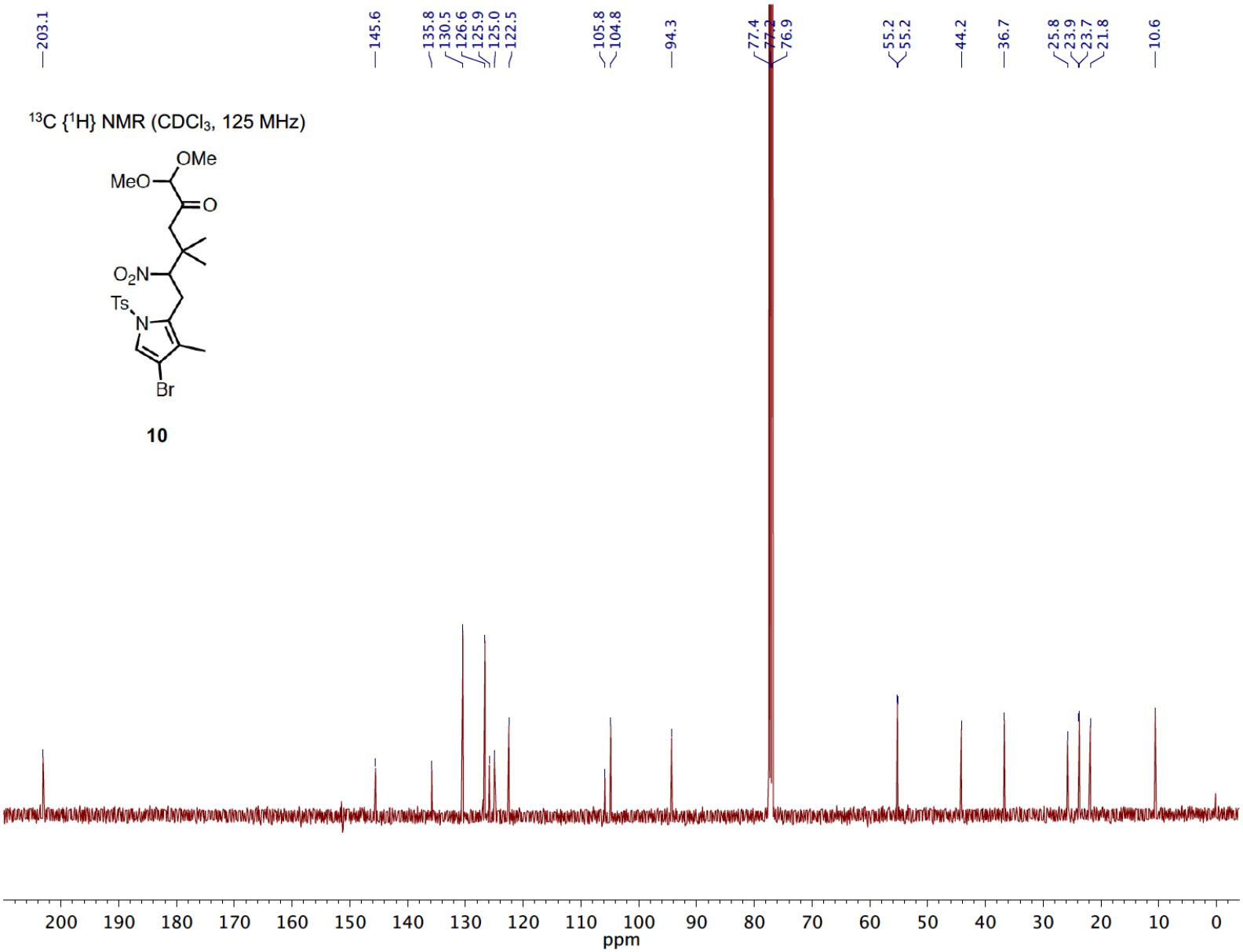
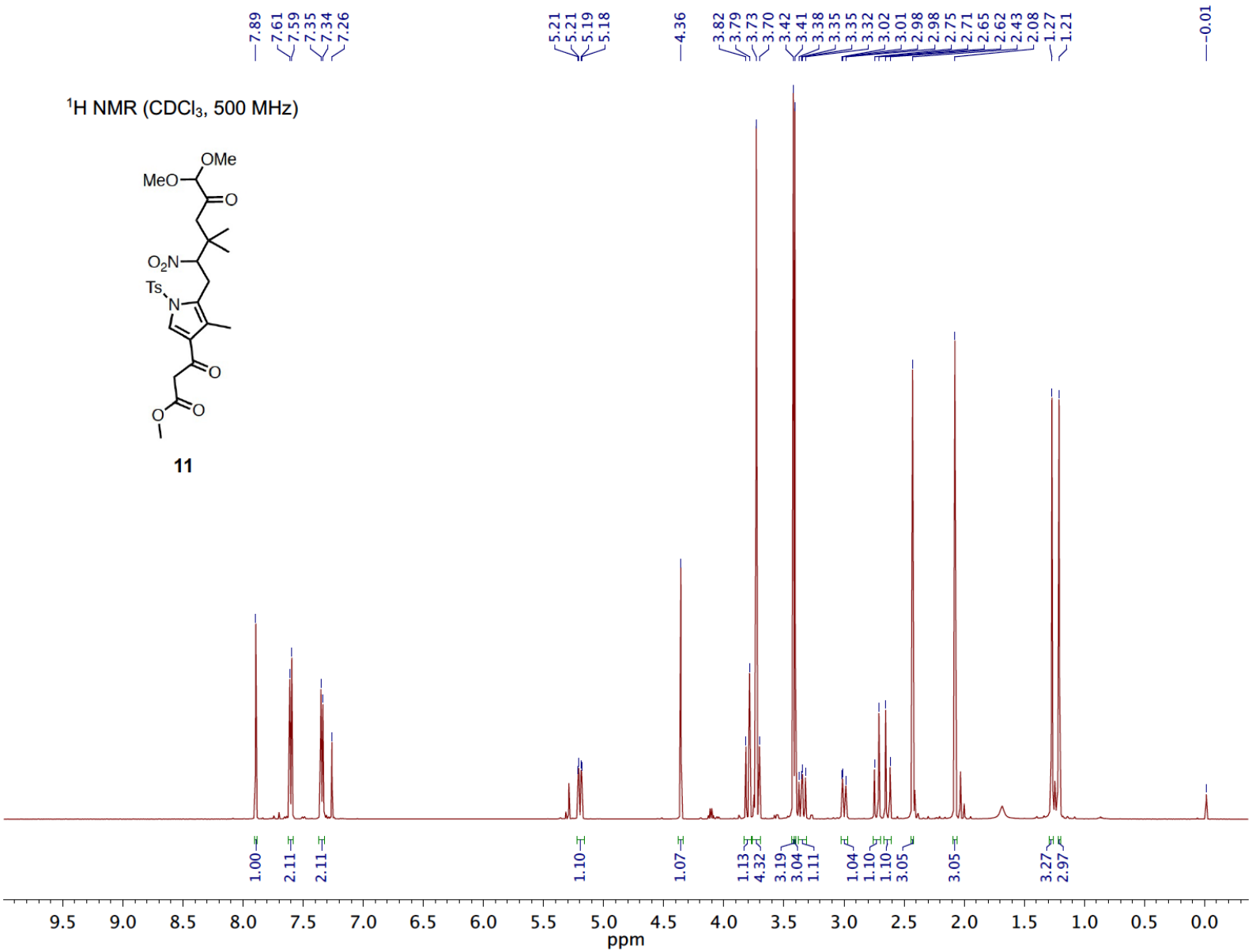

203.1
145.6
135.8
130.5
126.6
125.9
125.0
122.5
105.8
104.8
94.3
77.4
77.2
76.9
55.2
55.2
44.2
36.7
25.8
23.9
23.7
21.8
10.6
^{13}C {^{1}H} NMR ($CDCl_3$, 125 MHz)
OMe
MeO
O
O_2N
Ts
N
Br
10
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm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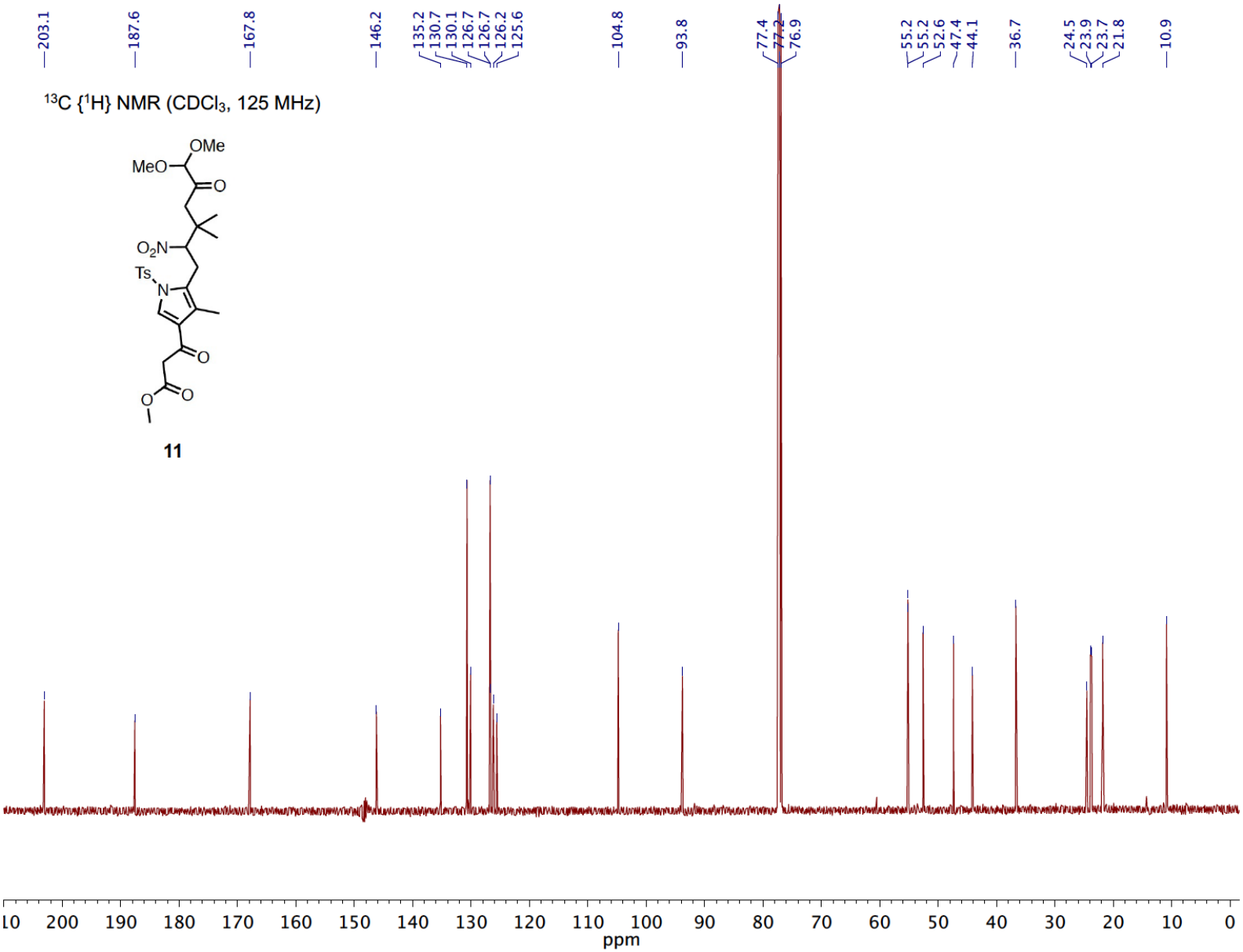
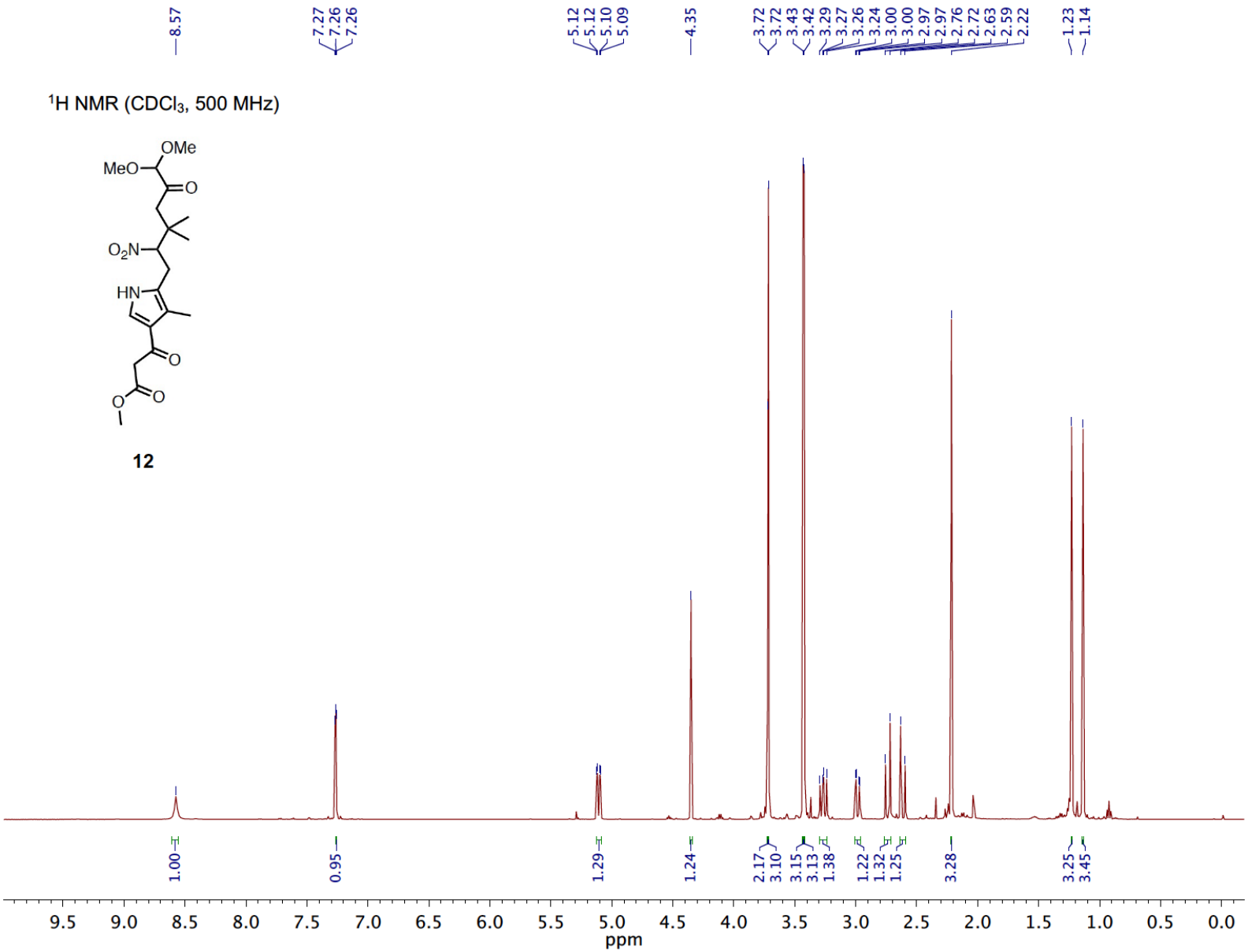
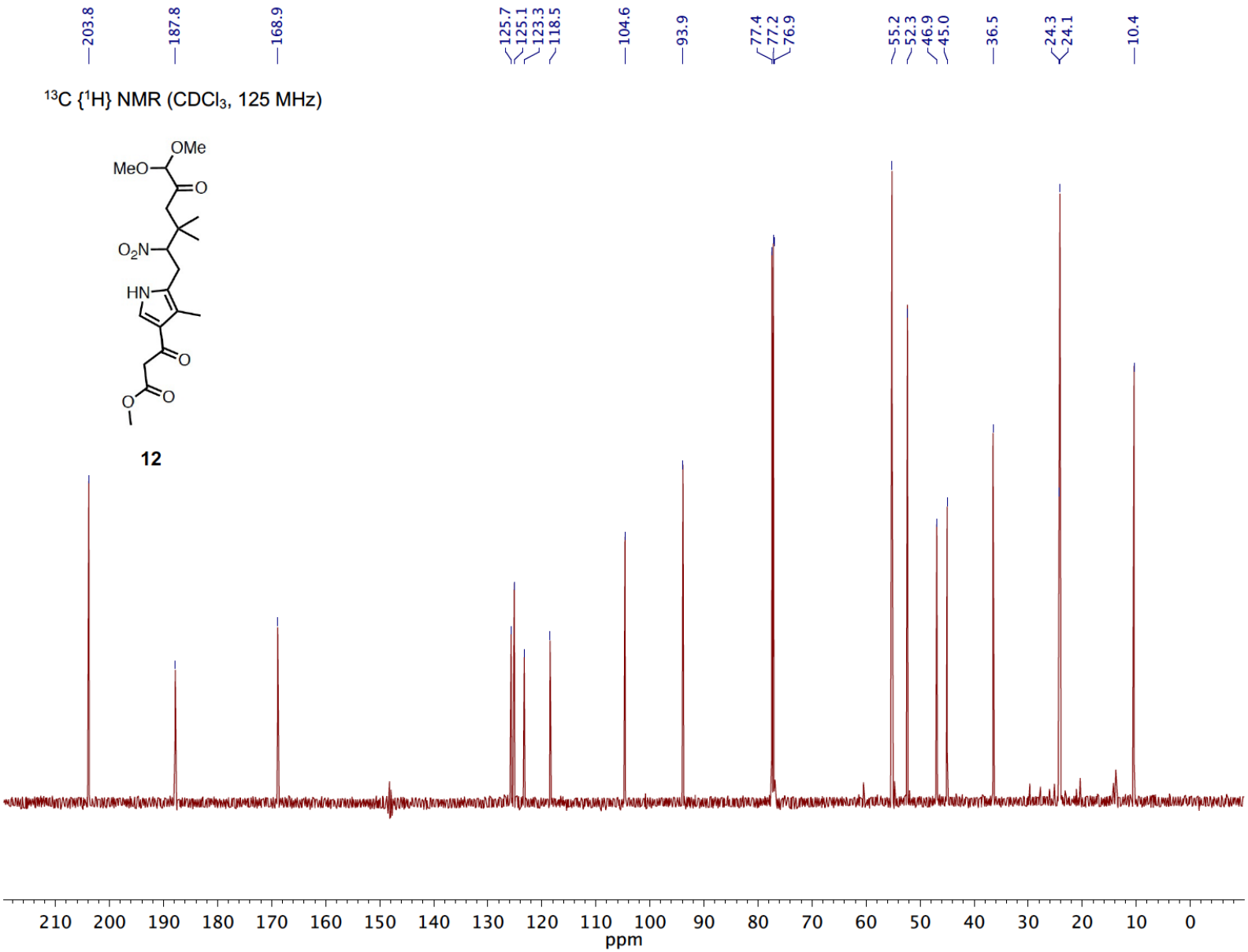
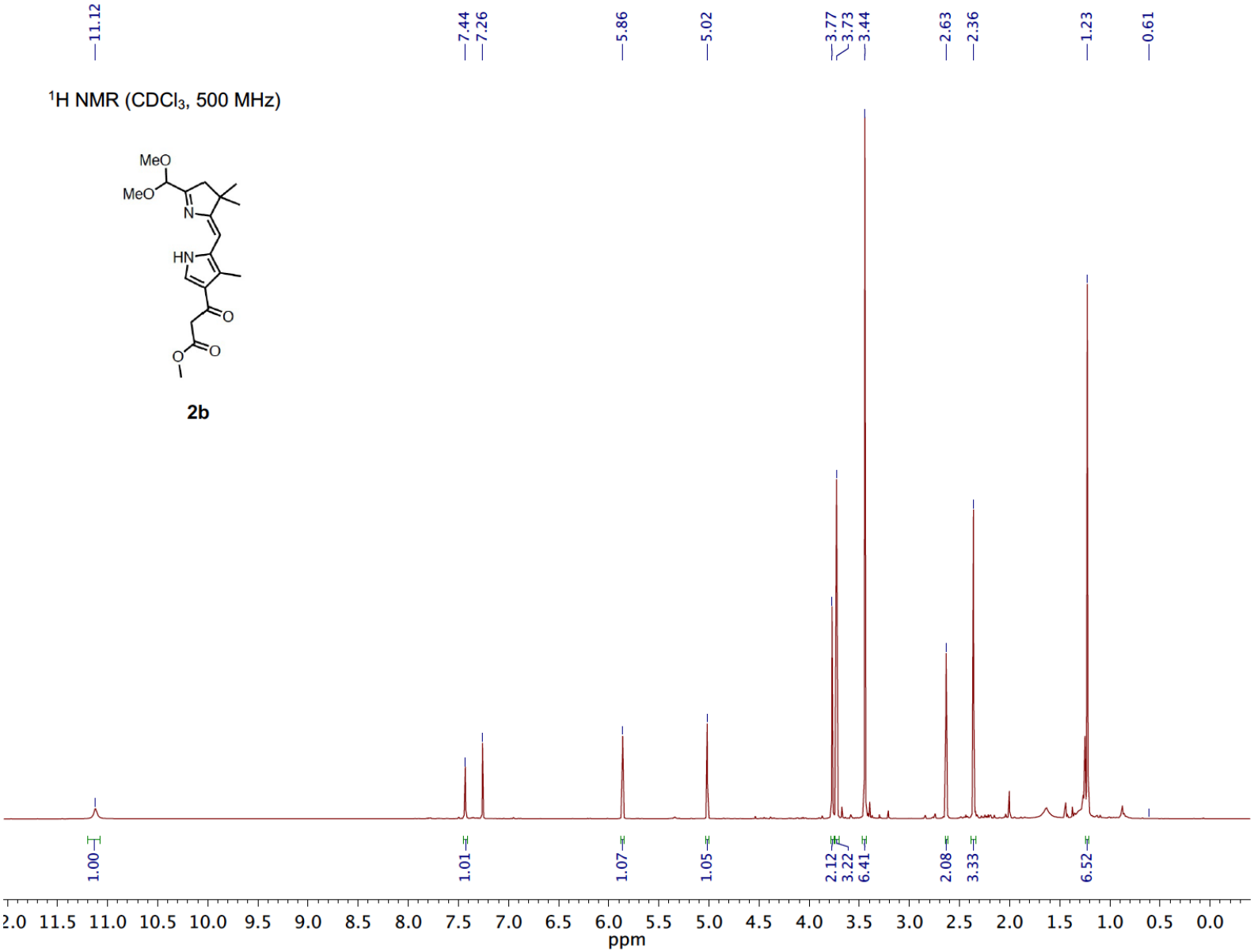
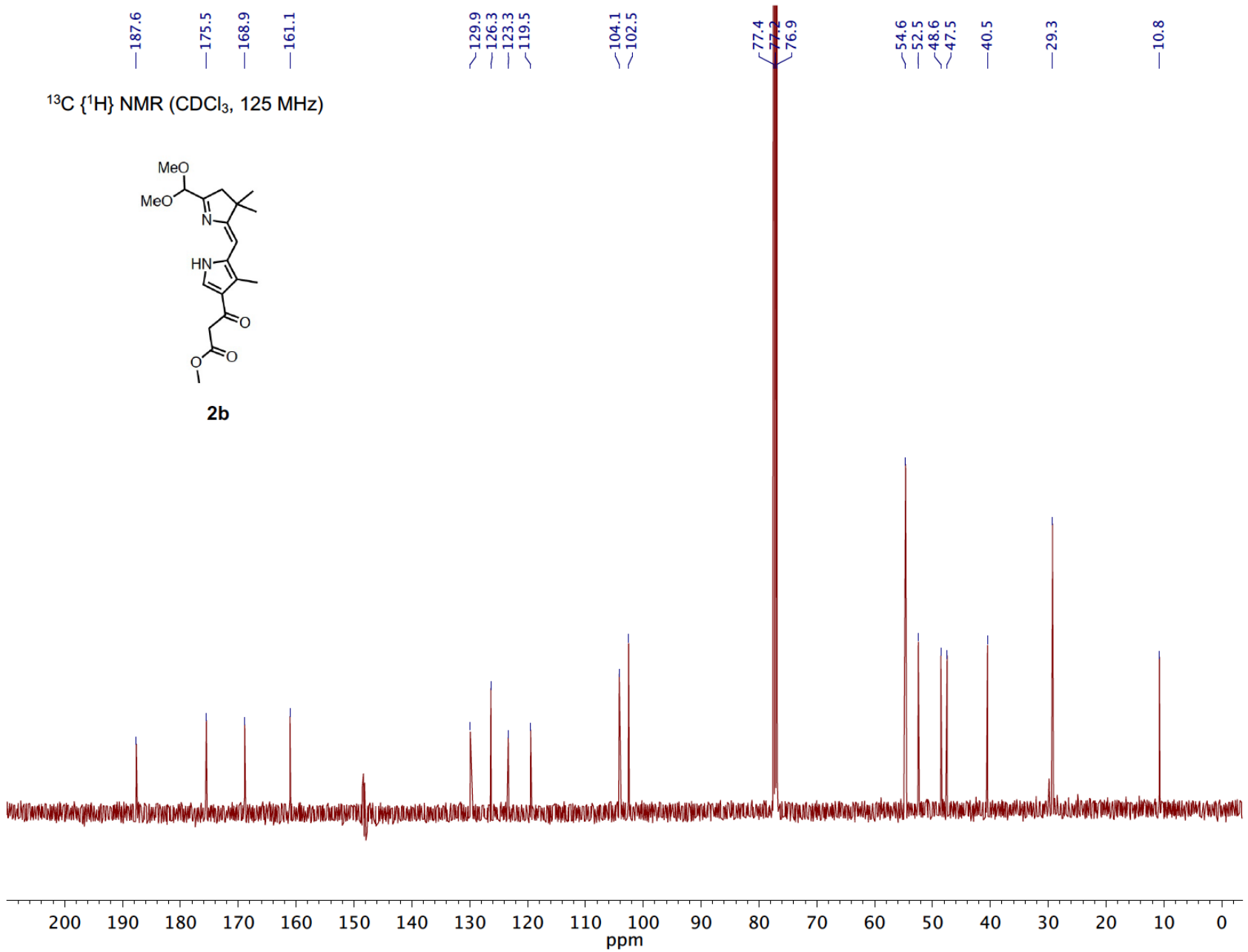
7.61
7.59
7.35
7.34
7.26
5.21
5.21
5.19
5.18
4.36
3.82
3.79
3.73
3.70
3.42
3.41
3.38
3.35
3.35
3.32
3.02
3.01
2.98
2.98
2.75
2.71
2.65
2.62
2.43
2.08
1.27
1.21
0.01
1H NMR (CDCl3, 500 MHz)
OMe
MeO
O
O2N
Ts
N
O
O
O
O
11
1.00
2.11
2.11
1.10
1.07
1.13
4.32
3.19
3.04
1.11
1.04
1.10
1.10
3.05
3.05
3.27
2.97
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

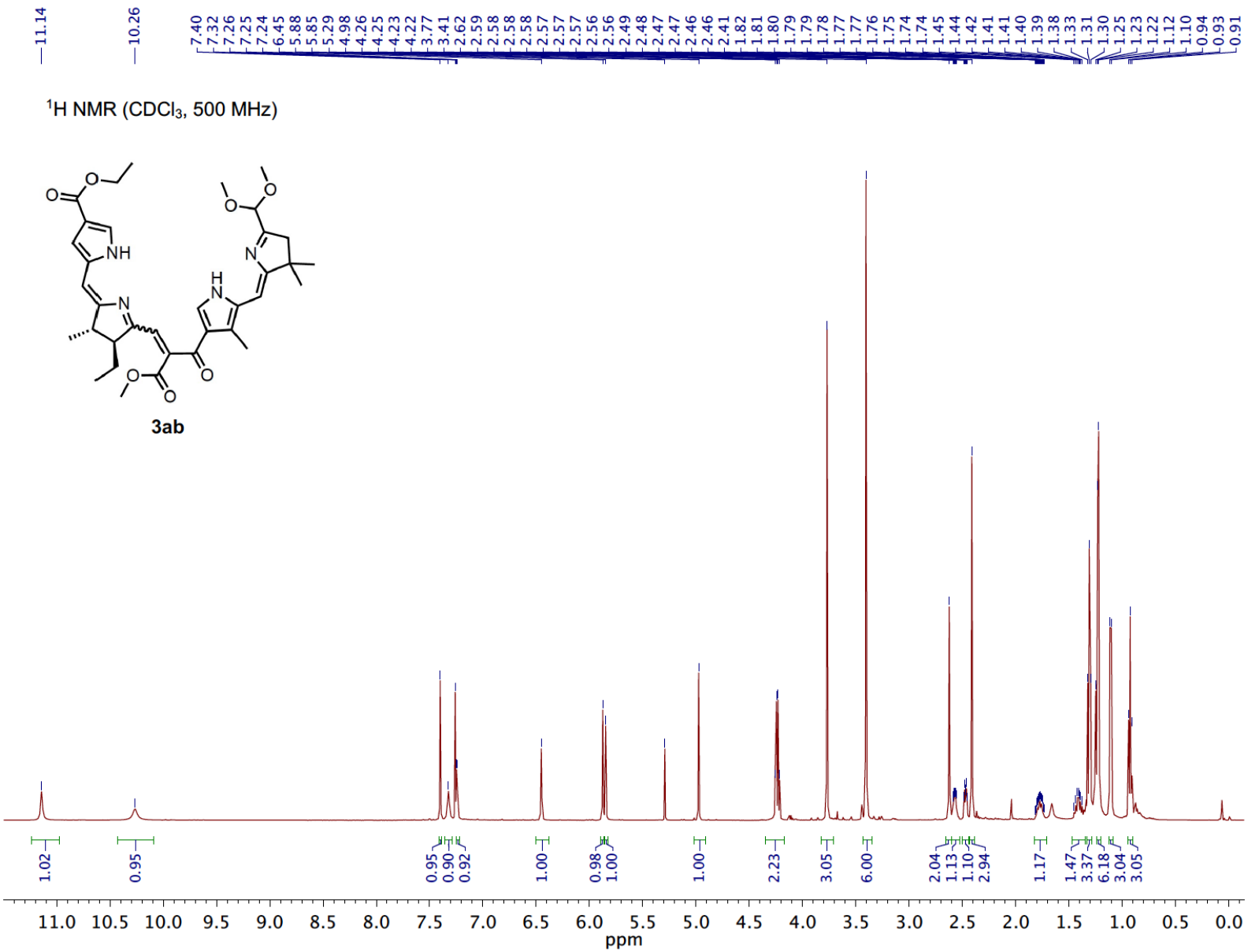

203.1
187.6
167.8
146.2
135.2
130.7
130.1
126.7
126.7
126.2
125.6
104.8
93.8
77.4
77.2
76.9
55.2
55.2
52.6
47.4
44.1
36.7
24.5
23.9
23.7
21.8
10.9
^{13}C {^{1}H} NMR ($CDCl_3$, 125 MHz)
OMe
MeO
O
O_2N
Ts
N
O
O
O
O
11
ppm

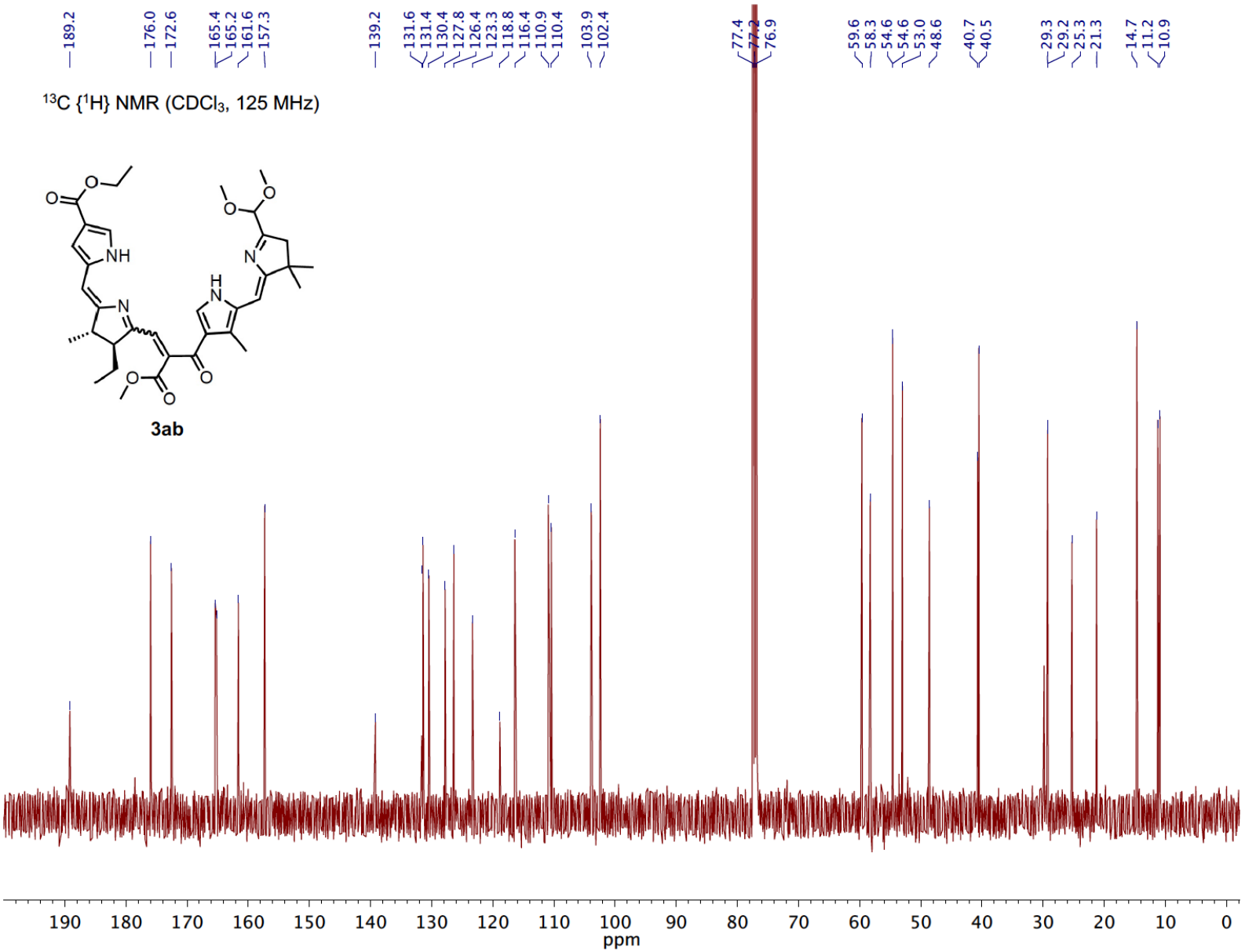

8.57
7.27
7.26
7.26
5.12
5.12
5.10
5.09
4.35
3.72
3.72
3.43
3.42
3.29
3.27
3.26
3.24
3.00
3.00
2.97
2.97
2.76
2.72
2.63
2.59
2.22
1.23
1.14
1H NMR (CDCl3, 500 MHz)
OMe
MeO
O
O2N
HN
O
O
O
O
12
1.00
0.95
1.29
1.24
2.17
3.10
3.15
3.13
1.38
1.22
1.32
1.25
3.28
3.25
3.45
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

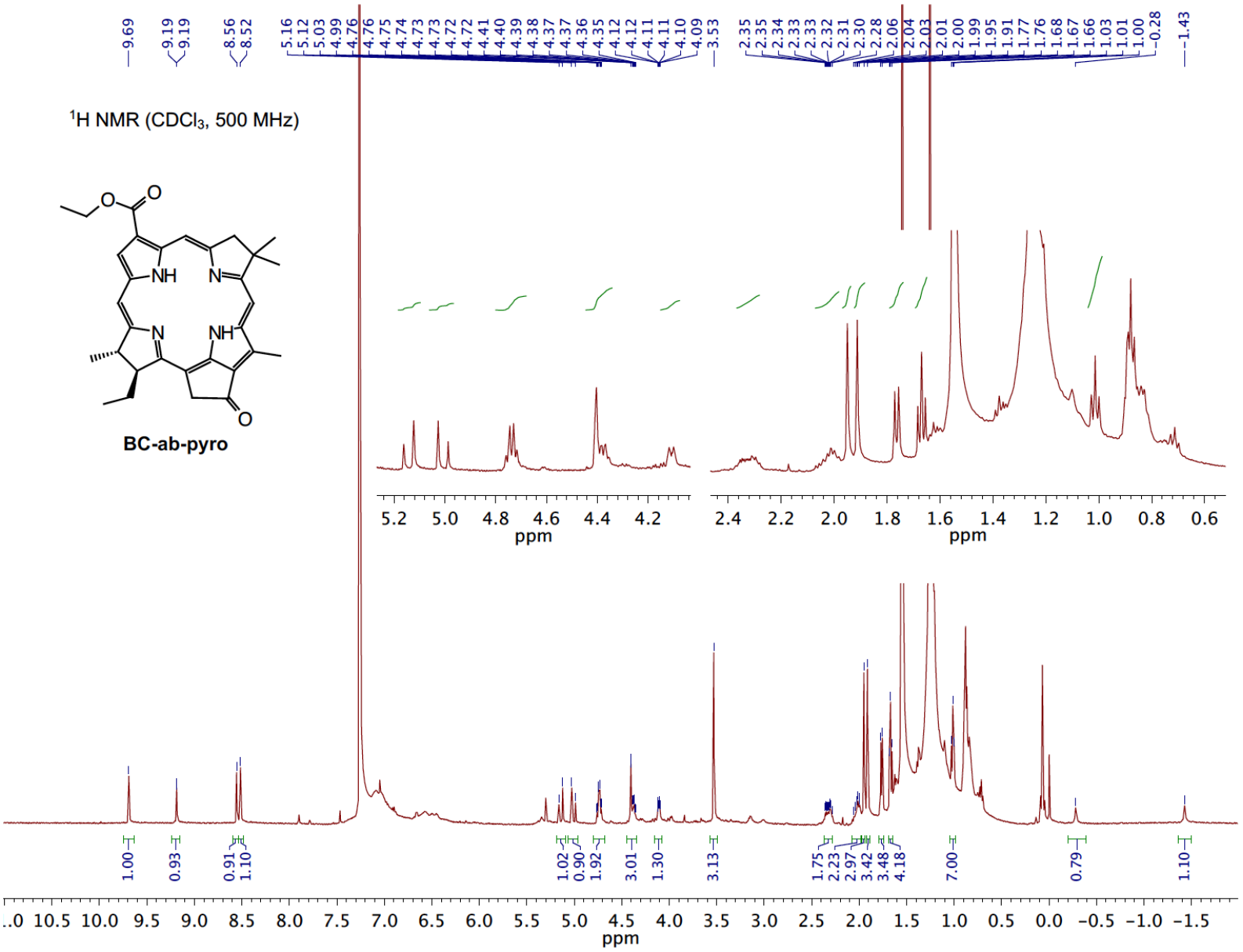

203.8
187.8
168.9
125.7
125.1
123.3
118.5
104.6
93.9
77.4
77.2
76.9
55.2
52.3
46.9
45.0
36.5
24.3
24.1
10.4
13C {1H} NMR (CDCl3, 125 MHz)
OMe
MeO
O
O2N
HN
O
O
O
12
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

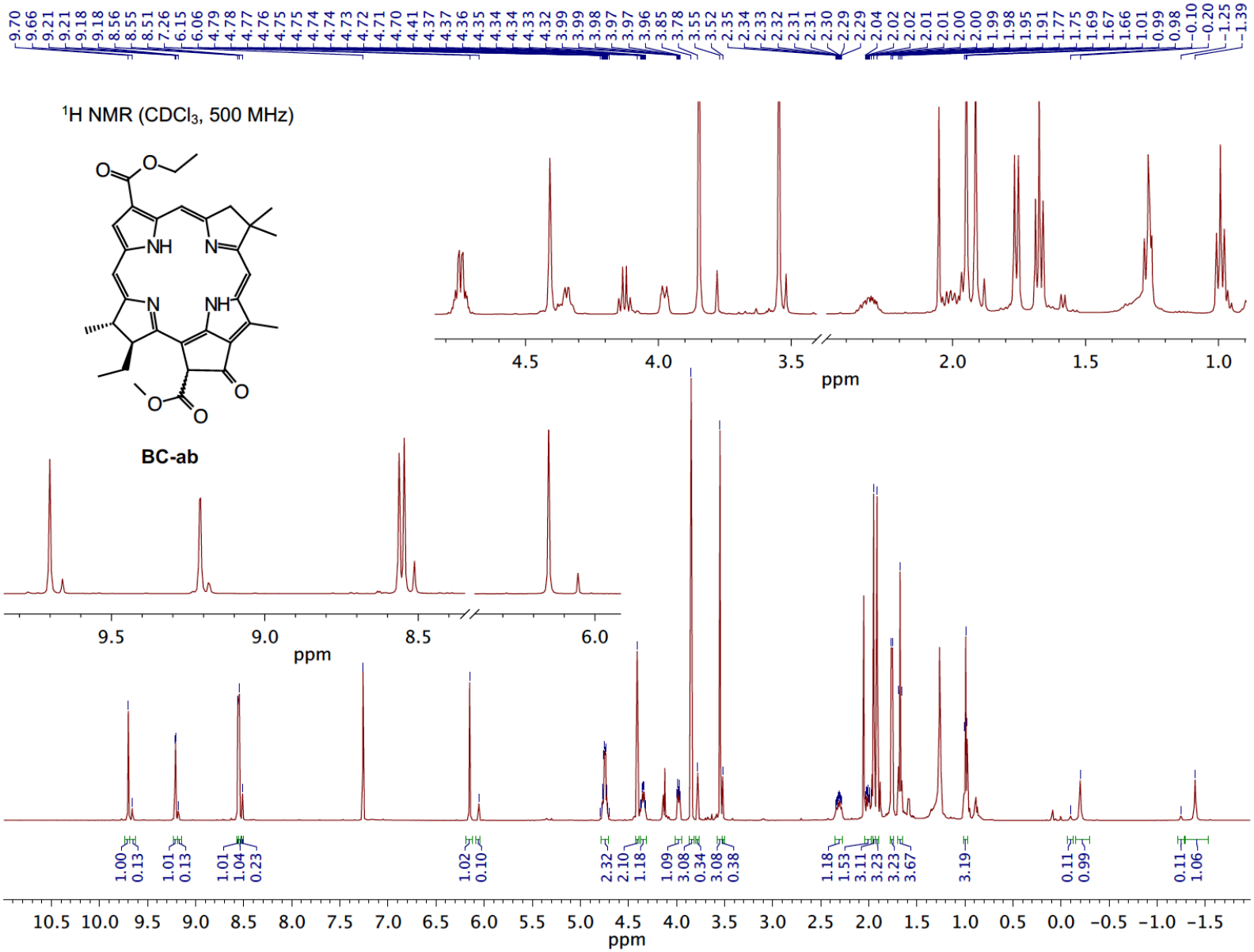

11.12
7.44
7.26
5.86
5.02
3.77
3.73
3.44
2.63
2.36
1.23
0.61
^{1}H NMR ($CDCl_3$, 500 MHz)
MeO
MeO
N
HN
O
O
O
O
2b
1.00
1.01
1.07
1.05
2.12
3.22
6.41
2.08
3.33
6.52
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

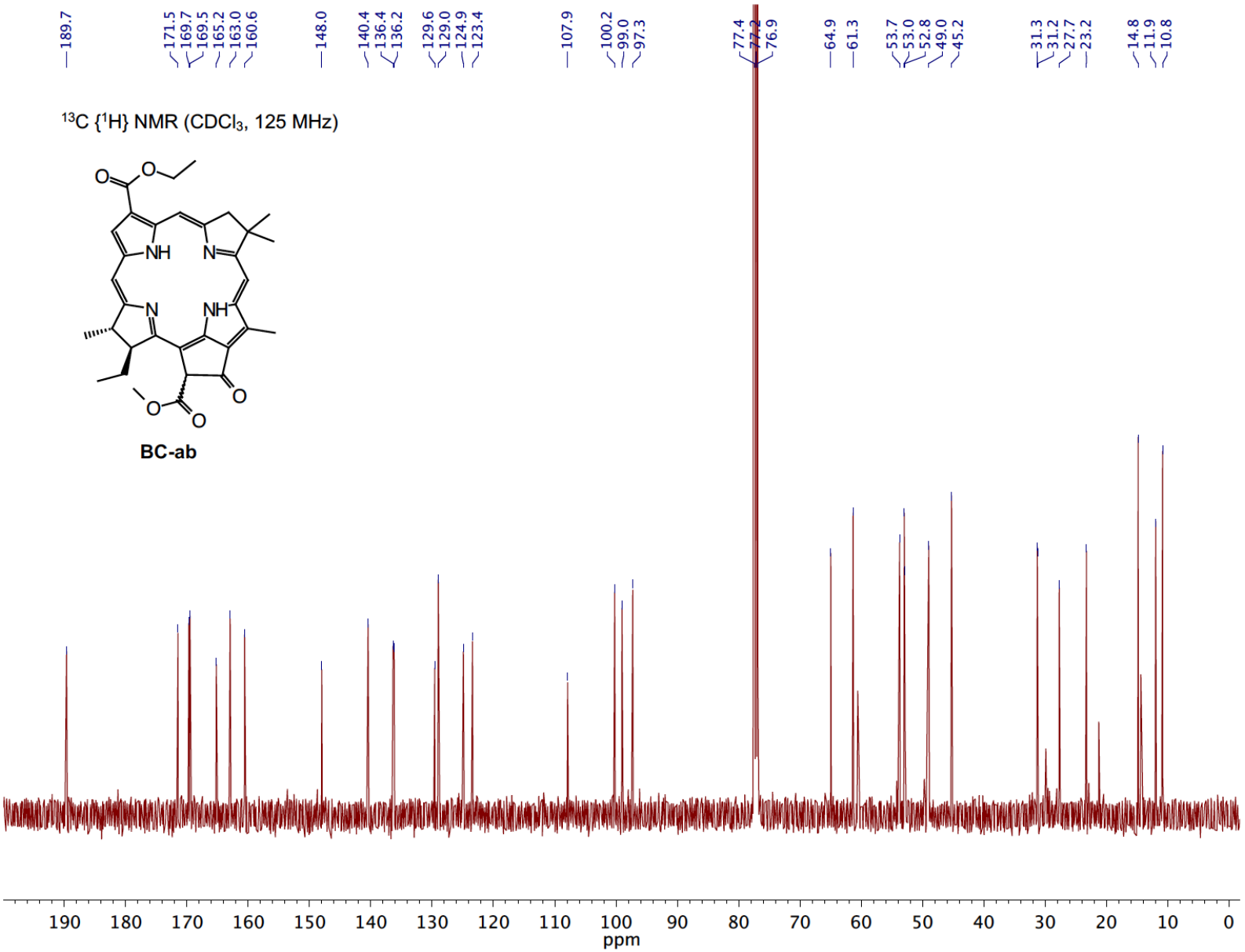

187.6
175.5
168.9
161.1
129.9
126.3
123.3
119.5
104.1
102.5
77.4
77.2
76.9
54.6
52.5
48.6
47.5
40.5
29.3
10.8
^{13}C {^{1}H} NMR ($CDCl_3$, 125 MHz)
MeO
MeO
N
HN
O
O
O
2b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

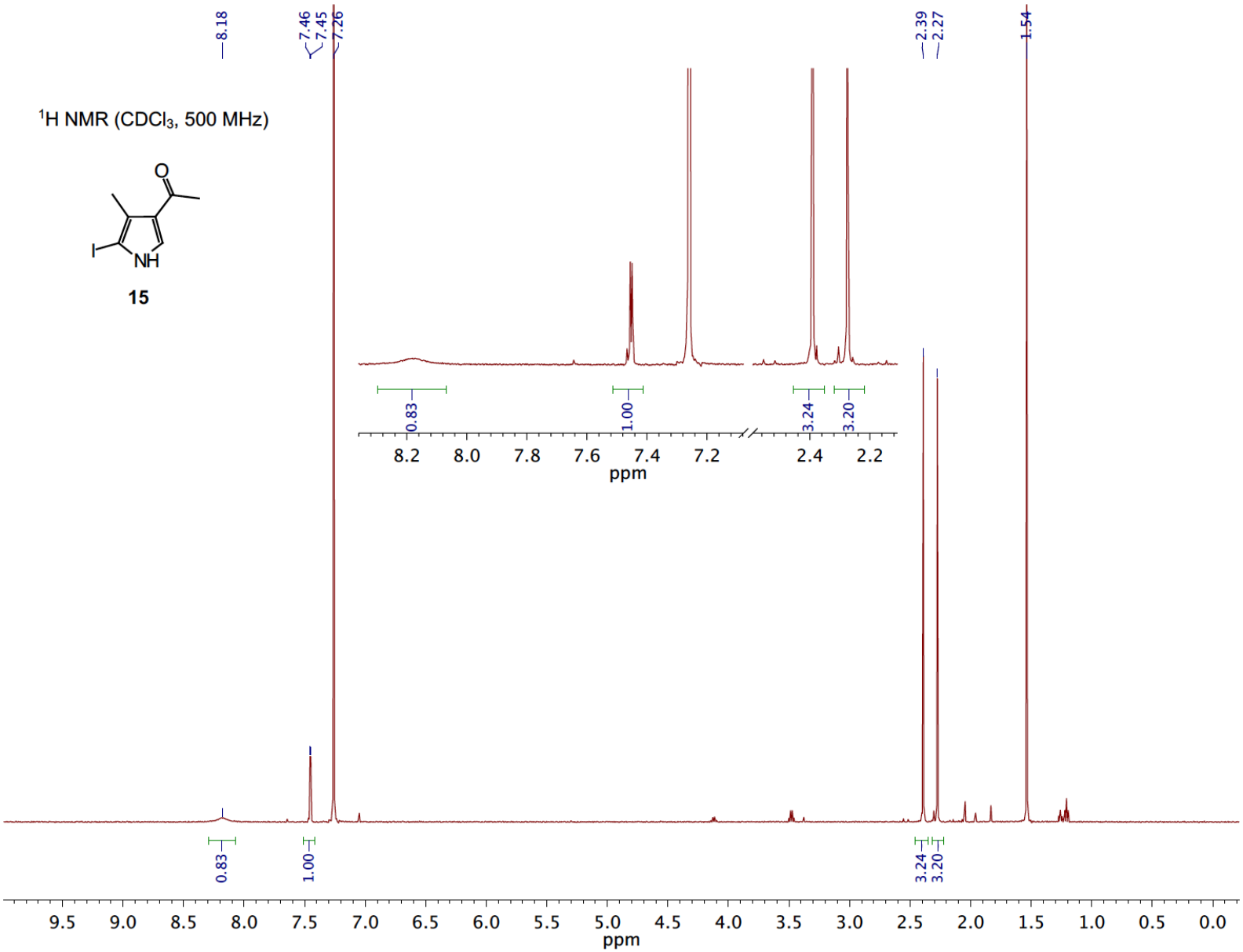

11.14
10.26
7.40 7.32 7.26 7.25 7.24 6.45 5.88 5.85 5.29 4.98 4.26 4.25 4.23 4.22 3.77 3.41 2.62 2.59 2.58 2.58 2.58 2.57 2.57 2.57 2.56 2.56 2.49 2.48 2.47 2.47 2.46 2.46 2.41 1.82 1.81 1.80 1.79 1.79 1.78 1.77 1.77 1.76 1.75 1.74 1.74 1.45 1.44 1.42 1.41 1.41 1.40 1.39 1.38 1.33 1.31 1.30 1.25 1.23 1.22 1.12 1.10 0.94 0.93 0.91
1H NMR (CDCl3, 500 MHz)
3ab
1.02 0.95 0.95 0.90 0.92 1.00 0.98 1.00 1.00 2.23 3.05 6.00 2.04 1.13 1.10 2.94 1.17 1.47 3.37 6.18 3.04 3.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

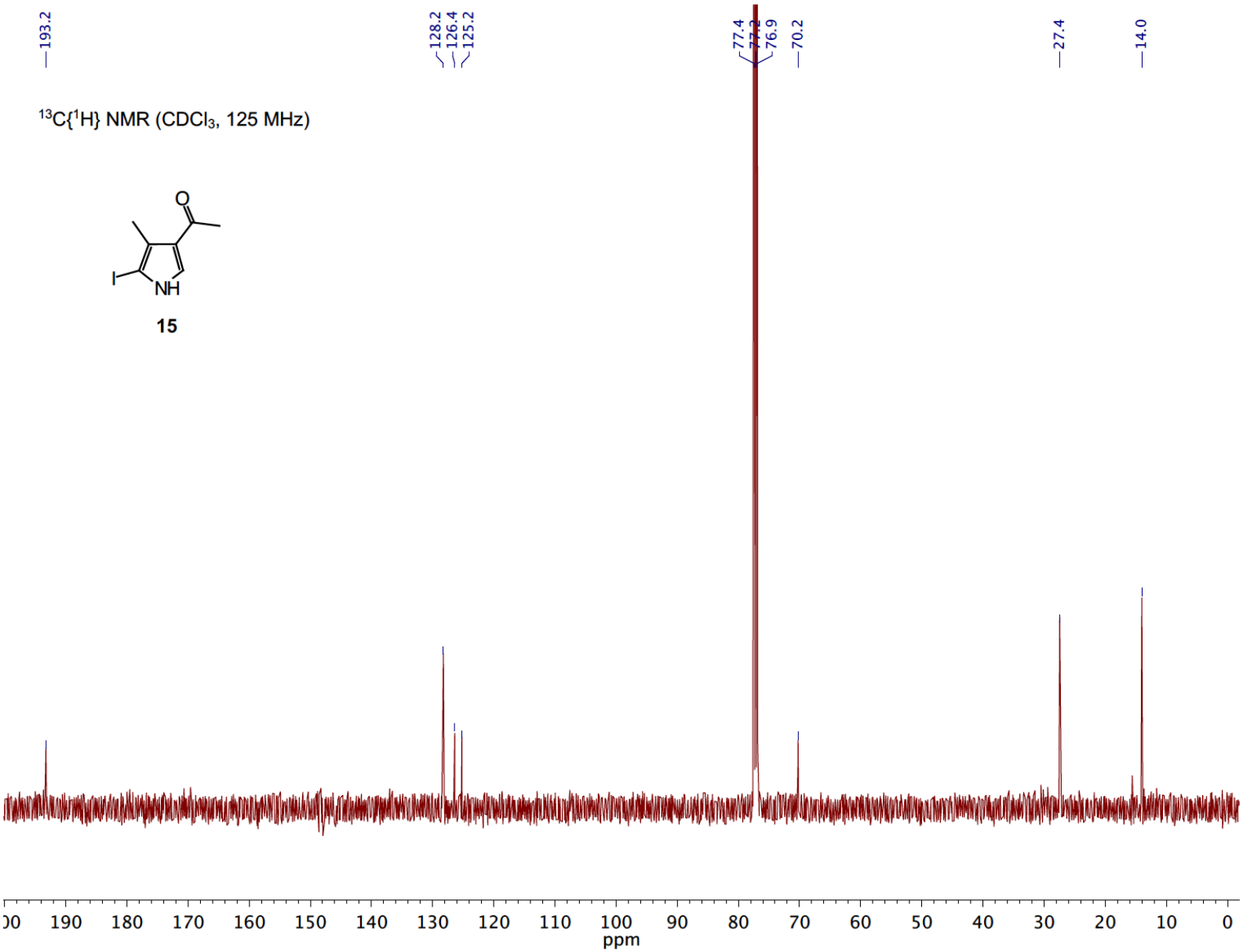

189.2
176.0
172.6
165.4
165.2
161.6
157.3
139.2
131.6
131.4
130.4
127.8
126.4
123.3
118.8
116.4
110.9
110.4
103.9
102.4
77.4
77.2
76.9
59.6
58.3
54.6
54.6
53.0
48.6
40.7
40.5
29.3
29.2
25.3
21.3
14.7
11.2
10.9
13C {1H} NMR (CDCl3, 125 MHz)
3ab
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


^{1}H NMR ($CDCl_3$, 500 MHz)
BC-ab-pyro
ppm

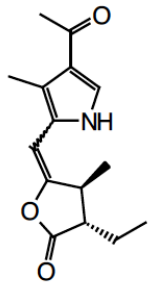

9.70 9.66 9.21 9.21 9.18 9.18 8.56 8.55 8.51 7.26 6.15 6.06 4.79 4.78 4.77 4.76 4.75 4.75 4.74 4.74 4.73 4.72 4.71 4.70 4.41 4.37 4.37 4.36 4.35 4.34 4.34 4.33 4.32 3.99 3.99 3.98 3.97 3.97 3.96 3.85 3.78 3.55 3.52 2.35 2.34 2.33 2.32 2.31 2.31 2.30 2.29 2.29 2.04 2.02 2.02 2.02 2.01 2.01 2.00 2.00 1.99 1.98 1.95 1.91 1.77 1.75 1.69 1.67 1.66 1.01 0.99 0.98 -0.10 -0.20 -1.25 -1.39
^{1}H NMR ($CDCl_3$, 500 MHz)
BC-ab
ppm
ppm
ppm
1.00 0.13 1.01 0.13 1.01 1.04 0.23 1.02 0.10 2.32 2.10 1.18 1.09 3.08 0.34 3.08 0.38 1.18 1.53 3.11 3.23 3.23 3.67 3.19 0.11 0.99 0.11 1.06


189.7
171.5
169.7
169.5
165.2
163.0
160.6
148.0
140.4
136.4
136.2
129.6
129.0
124.9
123.4
107.9
100.2
99.0
97.3
77.4
77.2
76.9
64.9
61.3
53.7
53.0
52.8
49.0
45.2
31.3
31.2
27.7
23.2
14.8
11.9
10.8
13C {1H} NMR (CDCl3, 125 MHz)
BC-ab
ppm

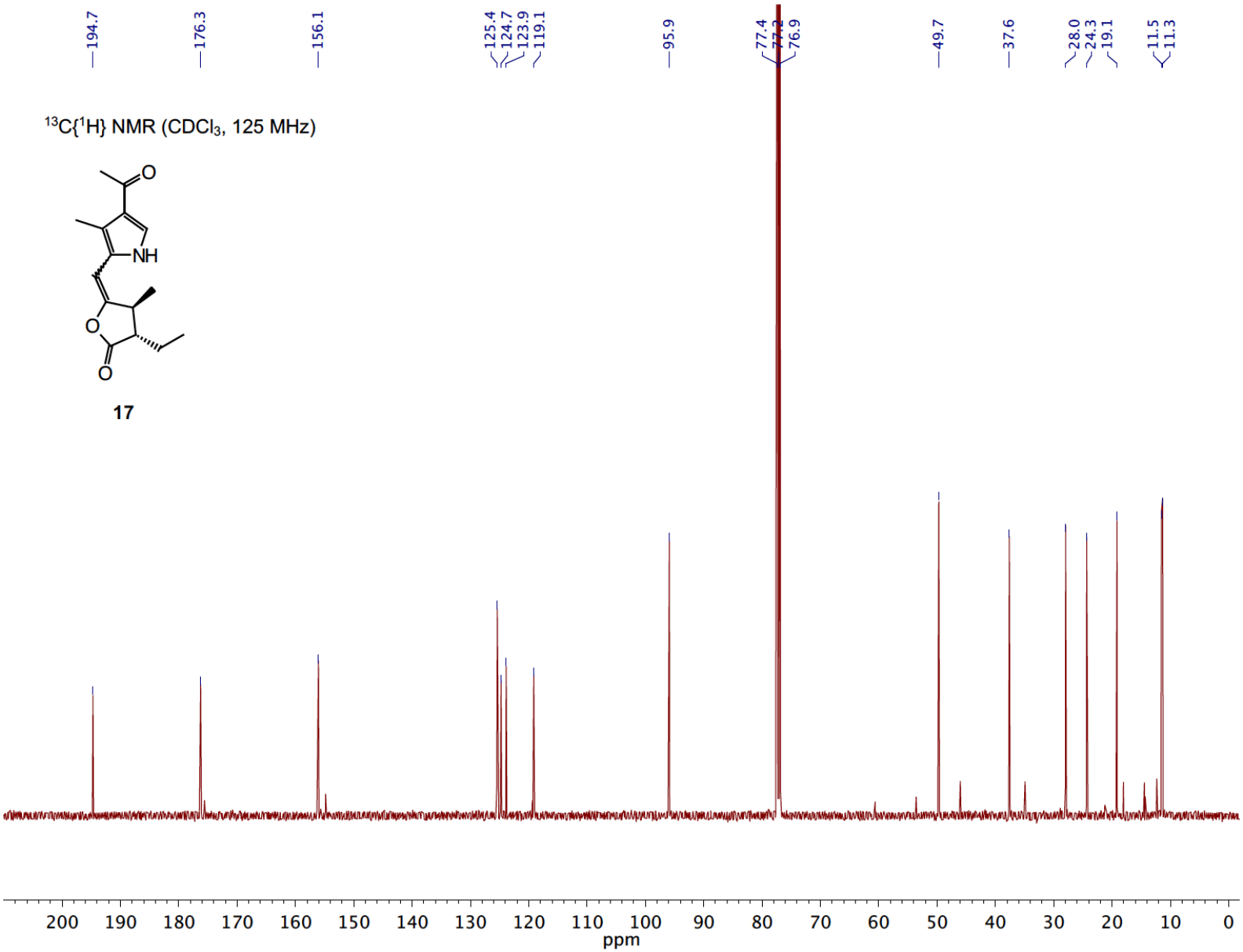

^{1}H NMR ($CDCl_3$, 500 MHz)
O
I
NH
15
8.18
7.46
7.45
7.26
2.39
2.27
1.54
0.83
1.00
3.24
3.20
ppm

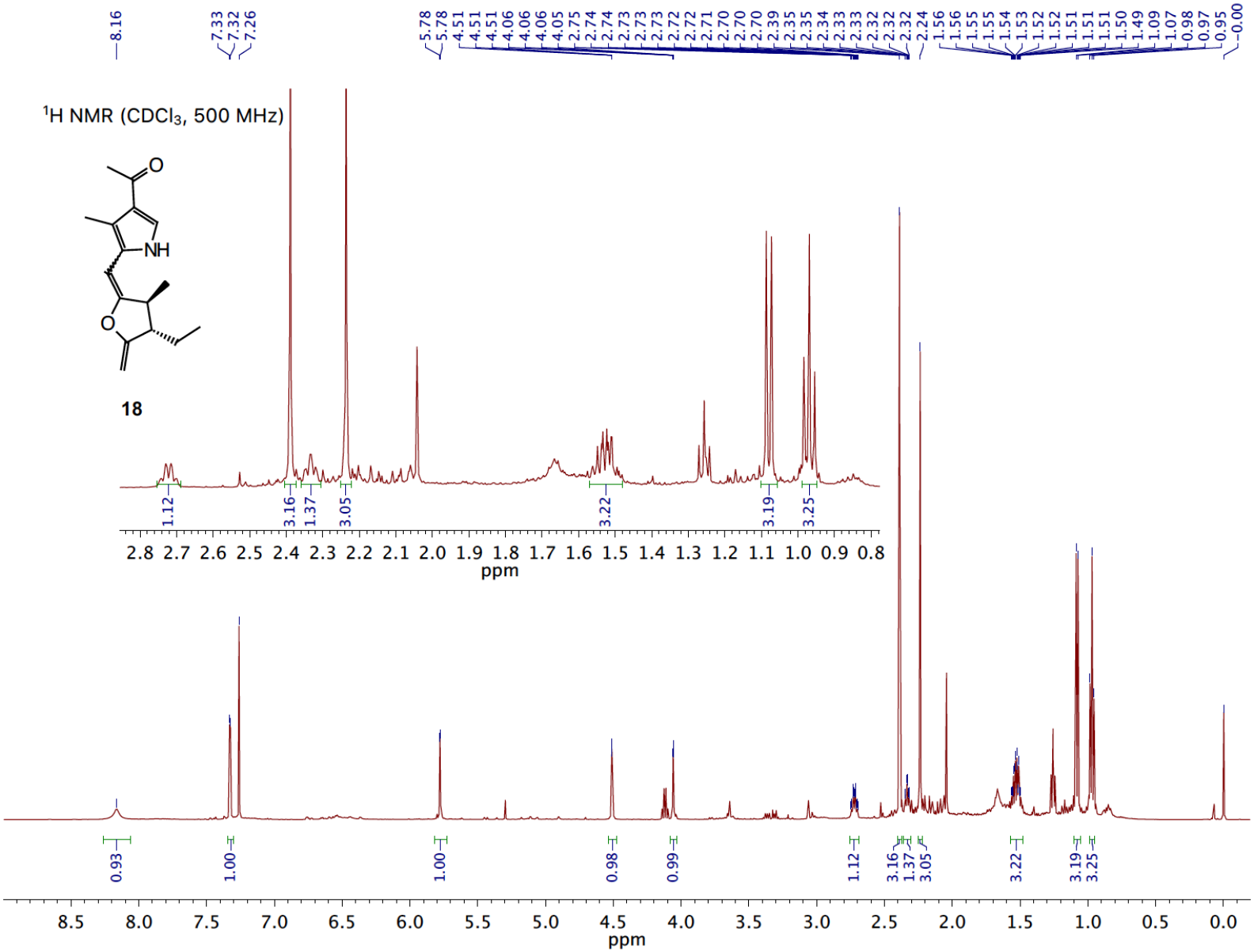

193.2
128.2
126.4
125.2
77.4
77.2
76.9
70.2
27.4
14.0
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz)
O
I
NH
15
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

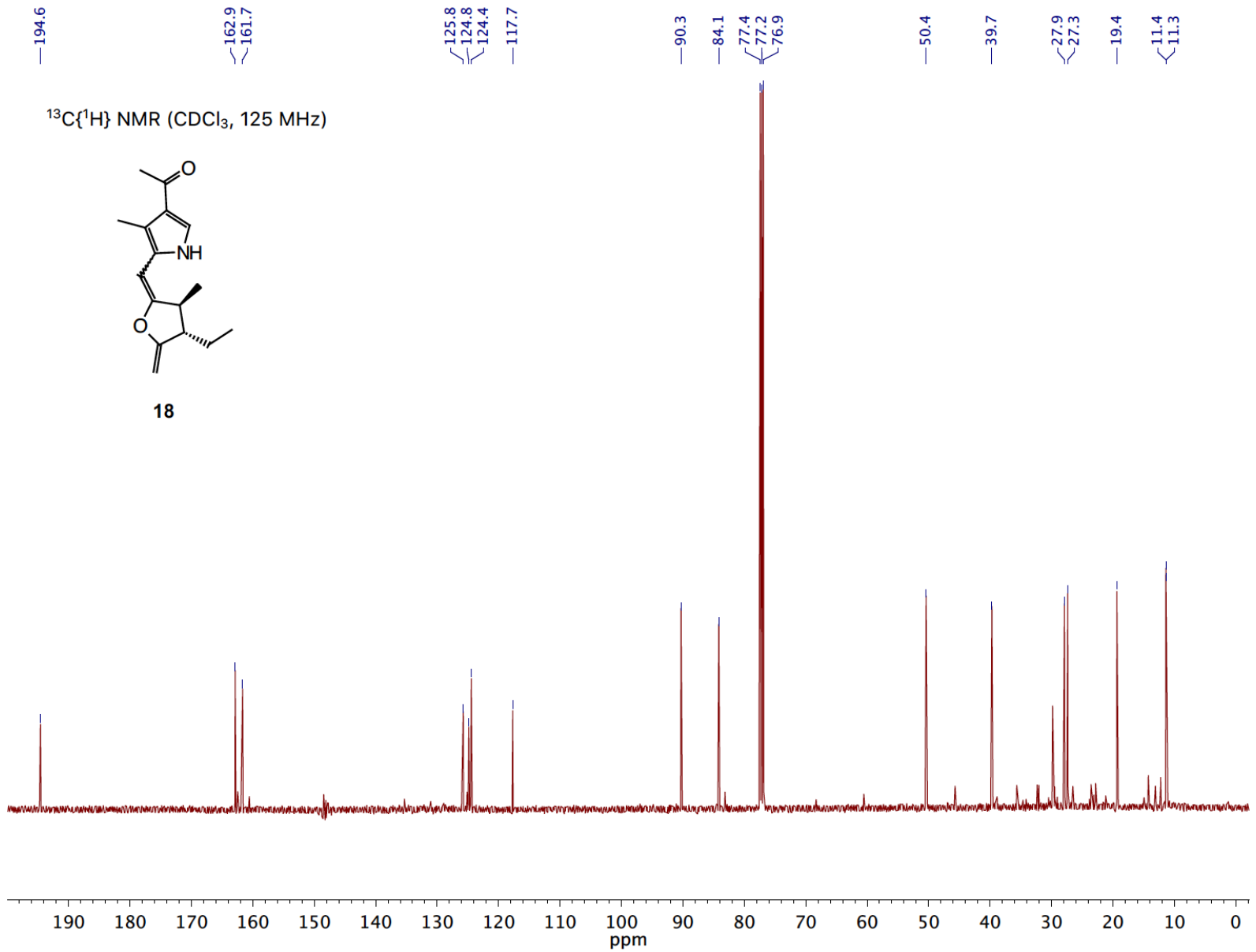
^{1}H NMR ($CDCl_3$, 500 MHz)

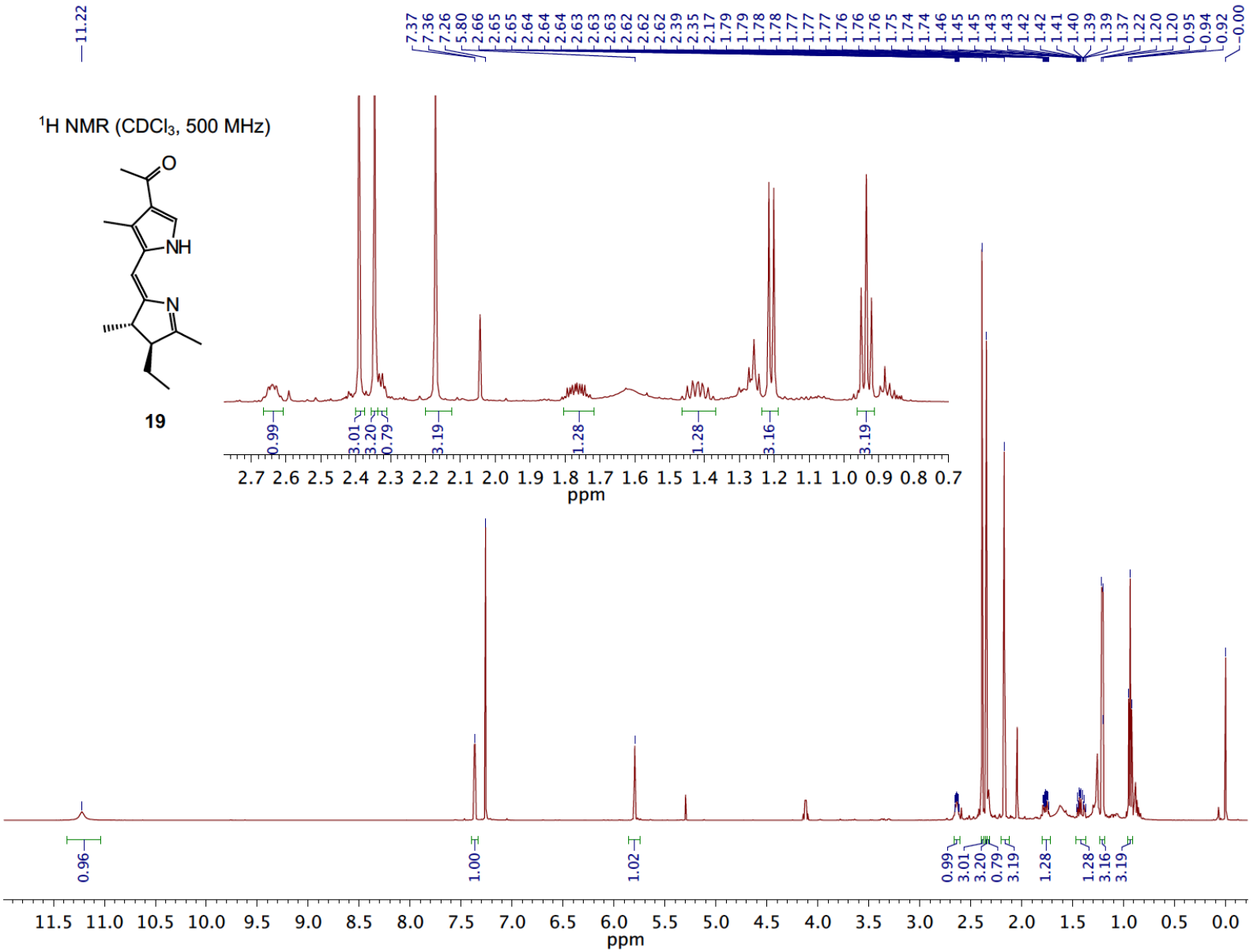


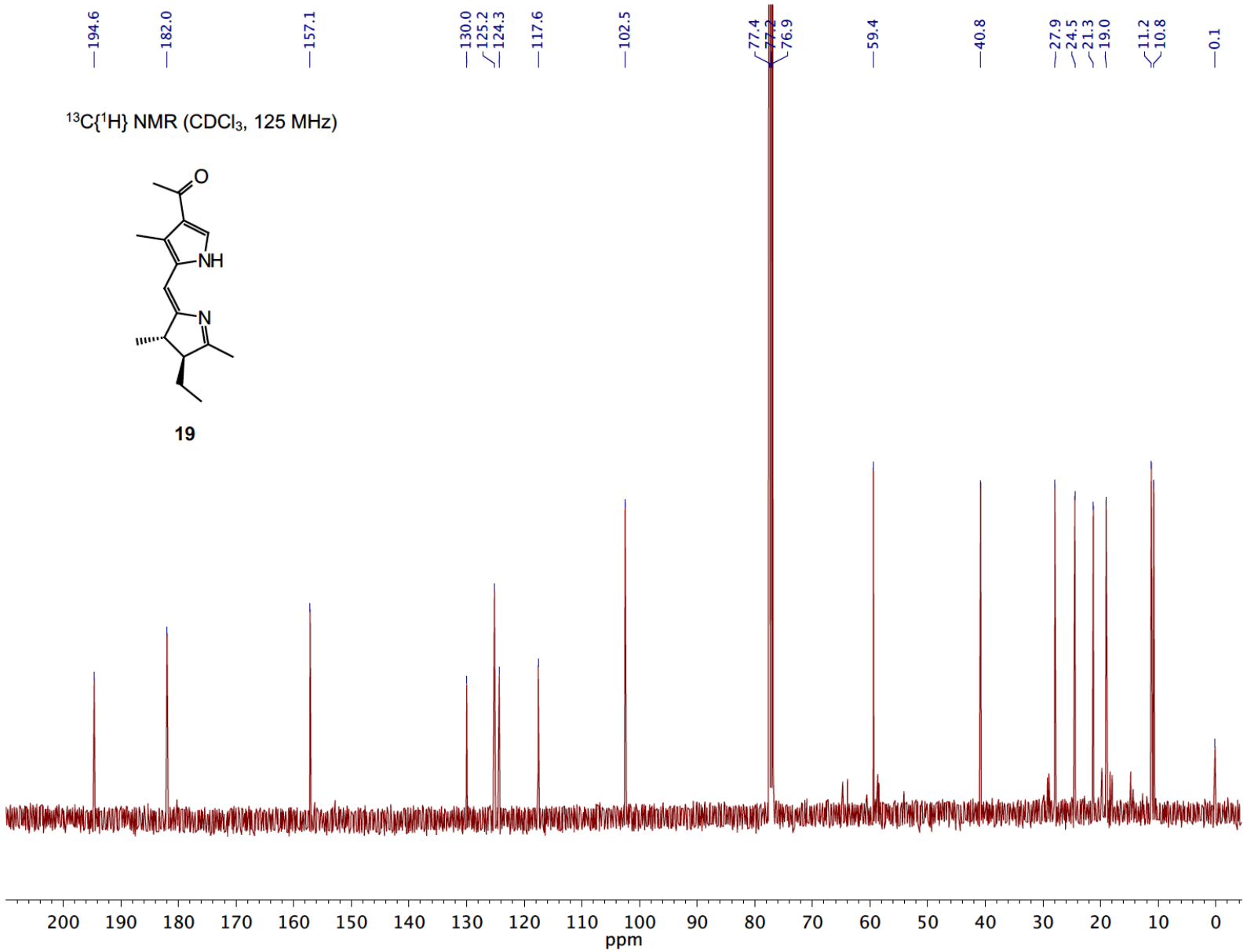
17

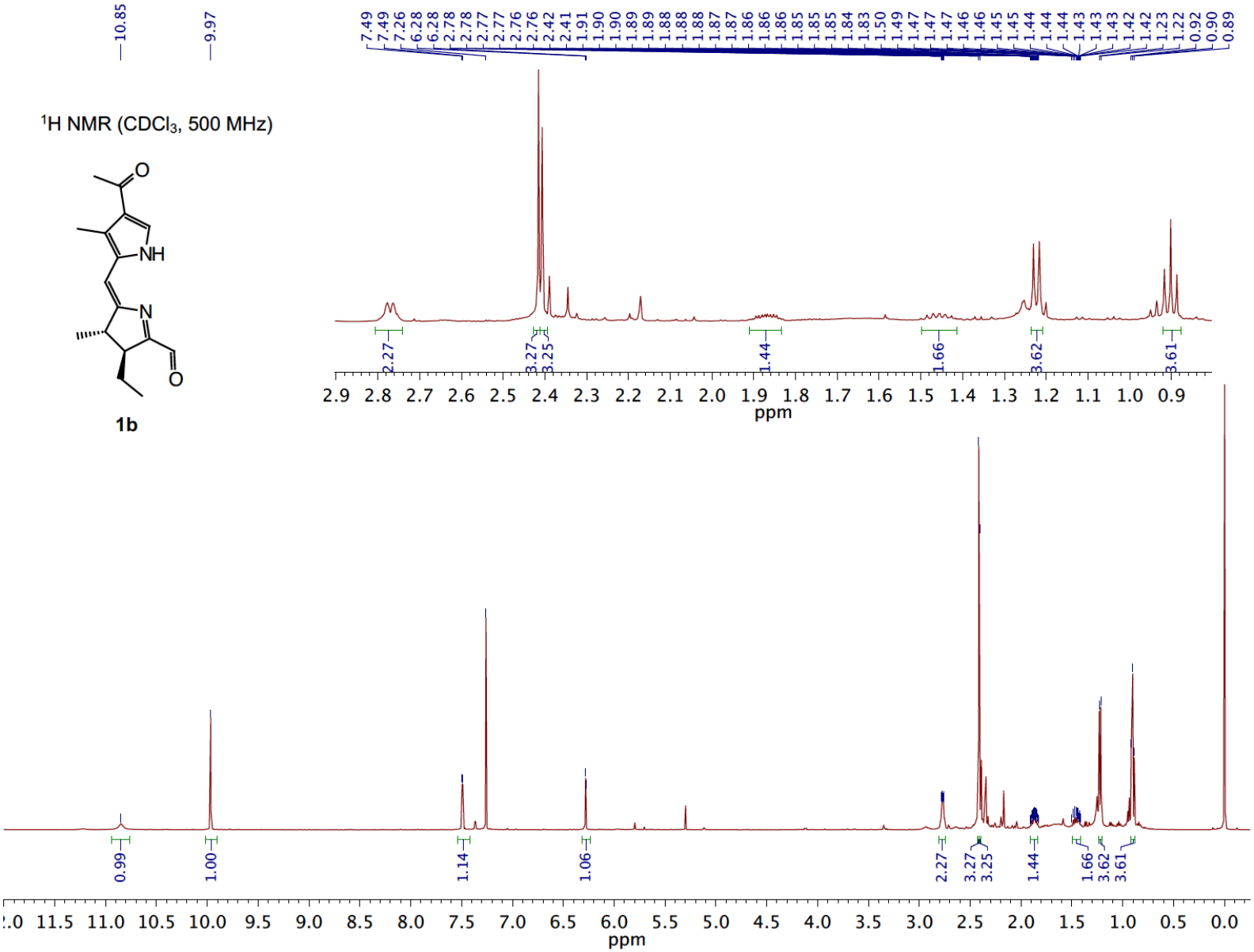

194.7
176.3
156.1
125.4
124.7
123.9
119.1
95.9
77.4
77.2
76.9
49.7
37.6
28.0
24.3
19.1
11.5
11.3
13C{1H} NMR (CDCl3, 125 MHz)
O
NH
O
O
17
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

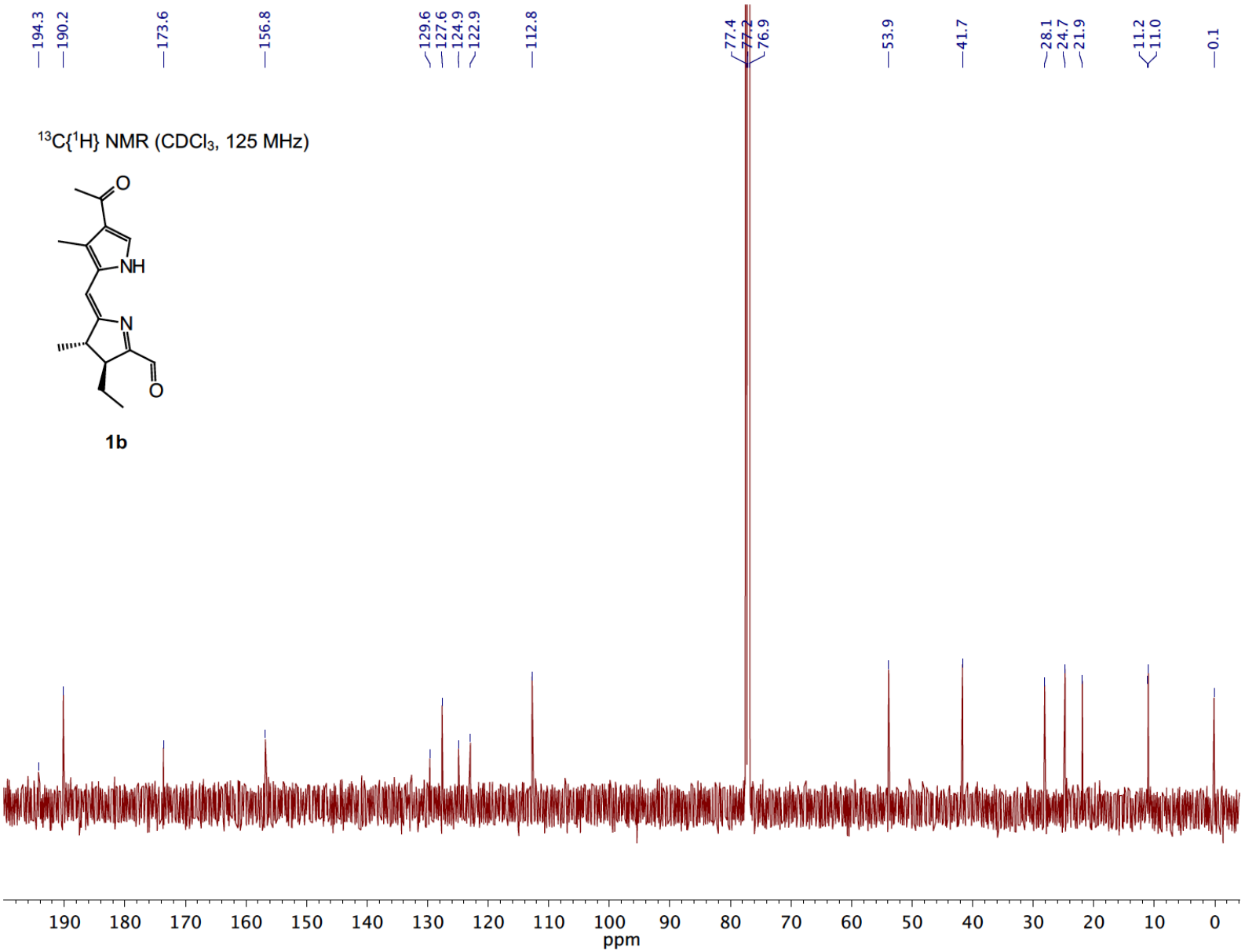

^{1}H NMR ($CDCl_3$, 500 MHz)
18
ppm

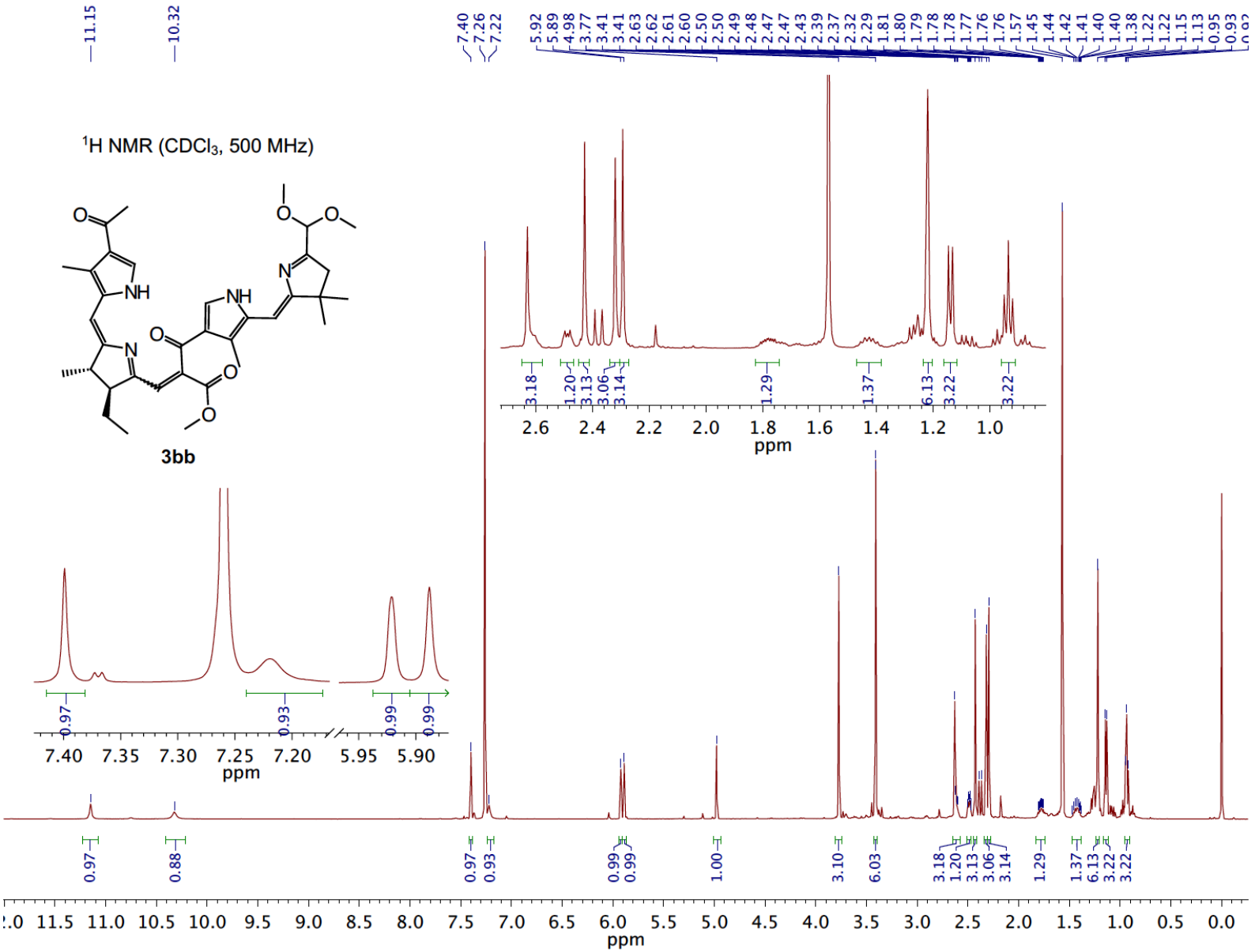

194.6
162.9
161.7
125.8
124.8
124.4
117.7
90.3
84.1
77.4
77.2
76.9
50.4
39.7
27.9
27.3
19.4
11.4
11.3
13C{1H} NMR (CDCl3, 125 MHz)
O
NH
O
18
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

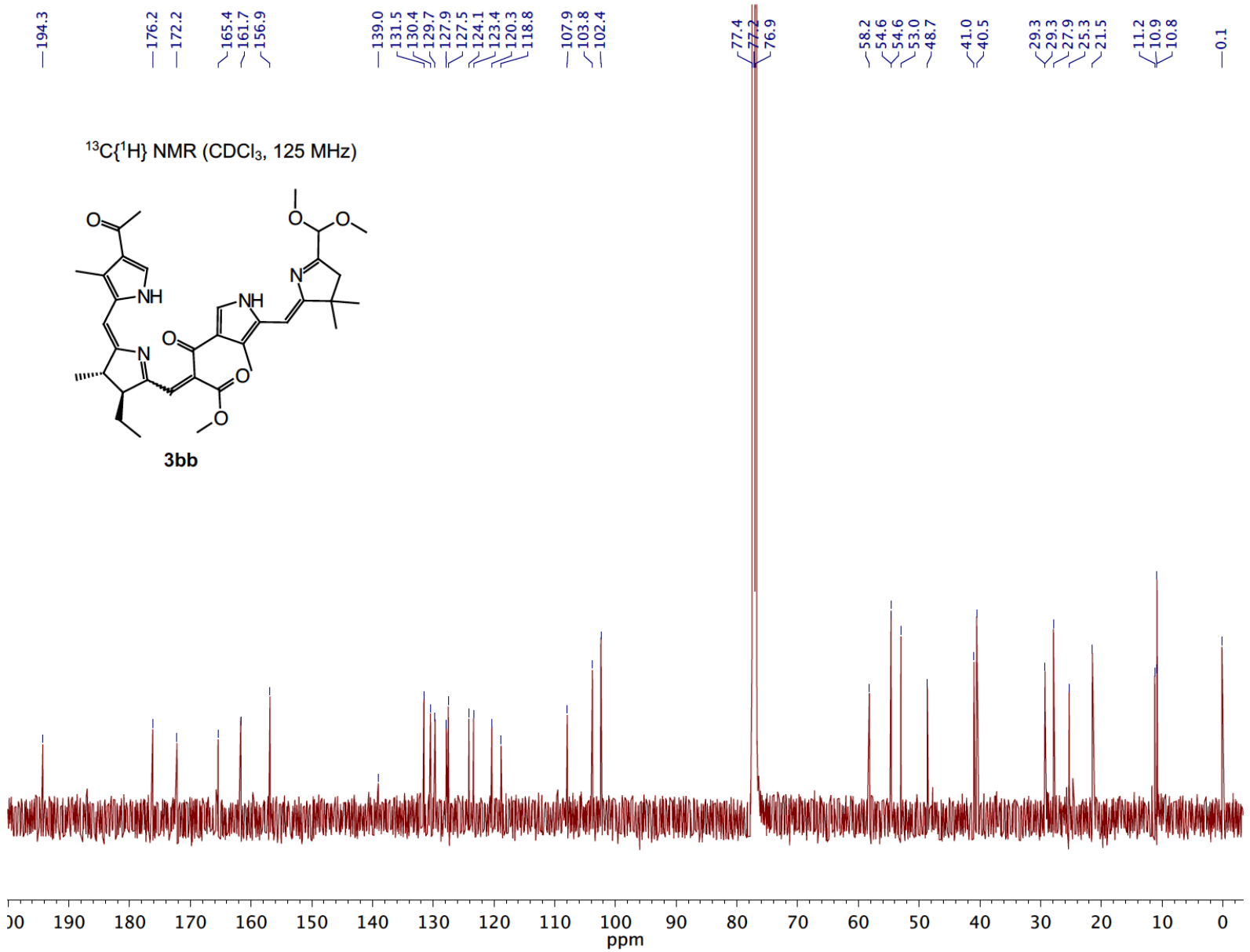

11.22
7.37 7.36 7.26 5.80 2.66 2.65 2.65 2.64 2.64 2.64 2.63 2.63 2.63 2.62 2.62 2.62 2.39 2.35 2.17 1.79 1.79 1.78 1.78 1.77 1.77 1.77 1.76 1.76 1.76 1.75 1.74 1.74 1.46 1.45 1.45 1.43 1.43 1.42 1.42 1.41 1.40 1.39 1.39 1.37 1.22 1.20 1.20 0.95 0.94 0.92 -0.00
1H NMR (CDCl3, 500 MHz)
O
NH
N
19
0.99 3.01 3.20 0.79 3.19 1.28 1.28 3.16 3.19
2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7
ppm
0.96 1.00 1.02 0.99 3.01 3.20 0.79 3.19 1.28 1.28 3.16 3.19
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

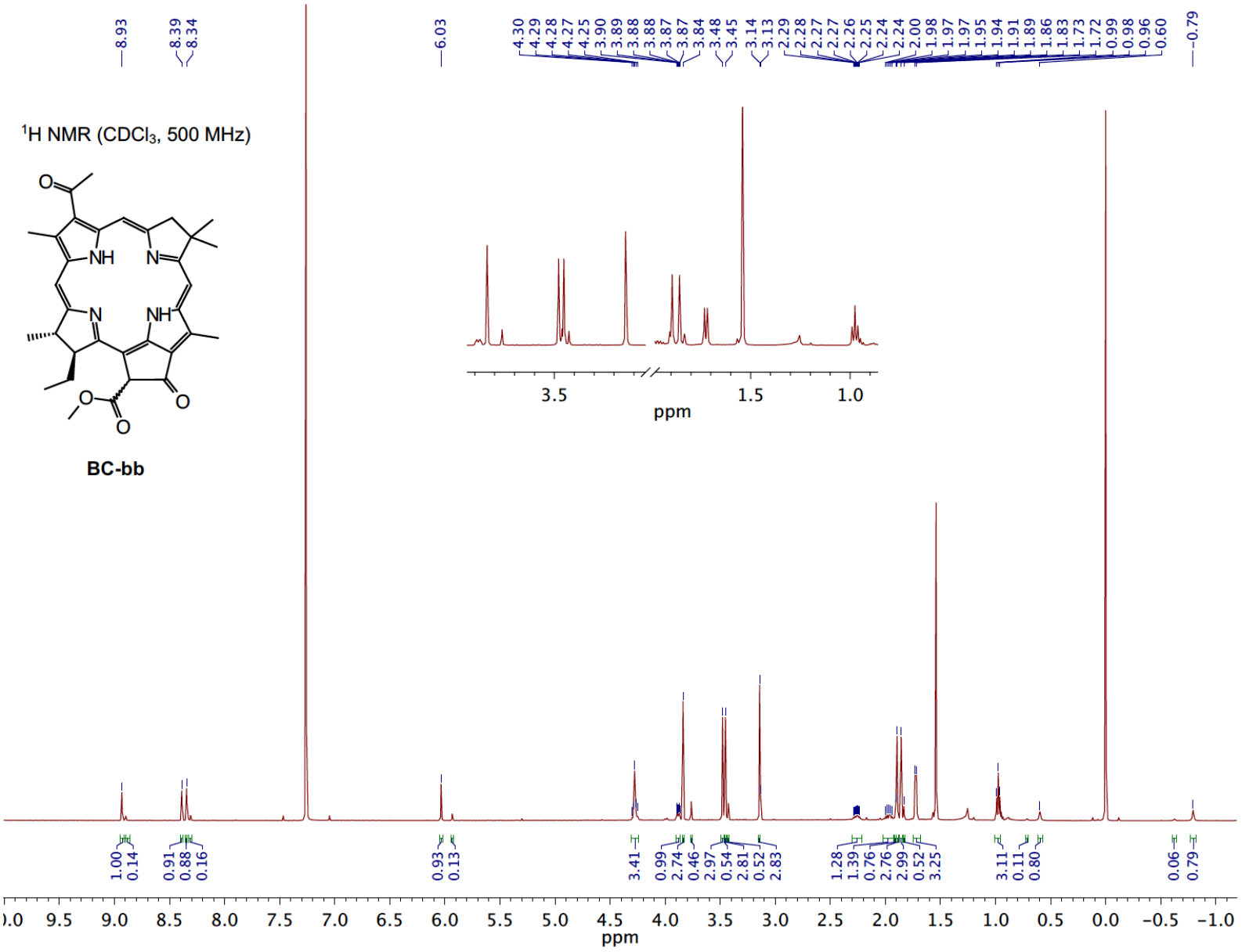

194.6
182.0
157.1
130.0
125.2
124.3
117.6
102.5
77.4
77.2
76.9
59.4
40.8
27.9
24.5
21.3
19.0
11.2
10.8
0.1
13C{1H} NMR (CDCl3, 125 MHz)
O
NH
N
19
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

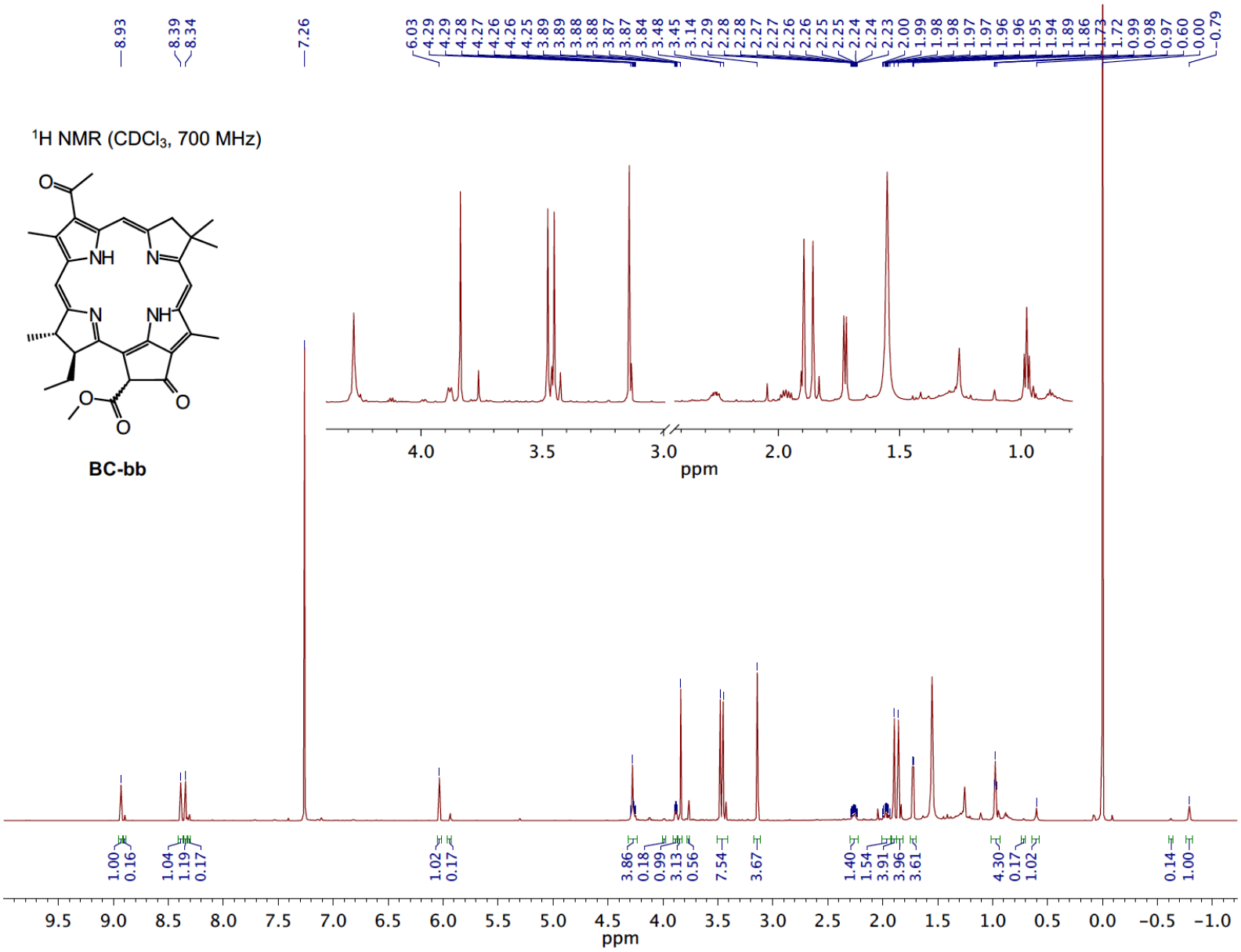

10.85
9.97
7.49 7.49 7.26 6.28 6.28 2.78 2.78 2.77 2.77 2.76 2.76 2.42 2.41 1.91 1.90 1.90 1.89 1.89 1.88 1.88 1.88 1.87 1.87 1.86 1.86 1.86 1.85 1.85 1.85 1.84 1.83 1.50 1.49 1.47 1.47 1.47 1.46 1.46 1.45 1.45 1.44 1.44 1.44 1.43 1.43 1.43 1.42 1.42 1.23 1.22 0.92 0.90 0.89
1H NMR (CDCl3, 500 MHz)
O
NH
N
O
1b
2.27
3.27
3.25
1.44
1.66
3.62
3.61
2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9
ppm
0.99
1.00
1.14
1.06
2.27
3.27
3.25
1.44
1.66
3.62
3.61
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

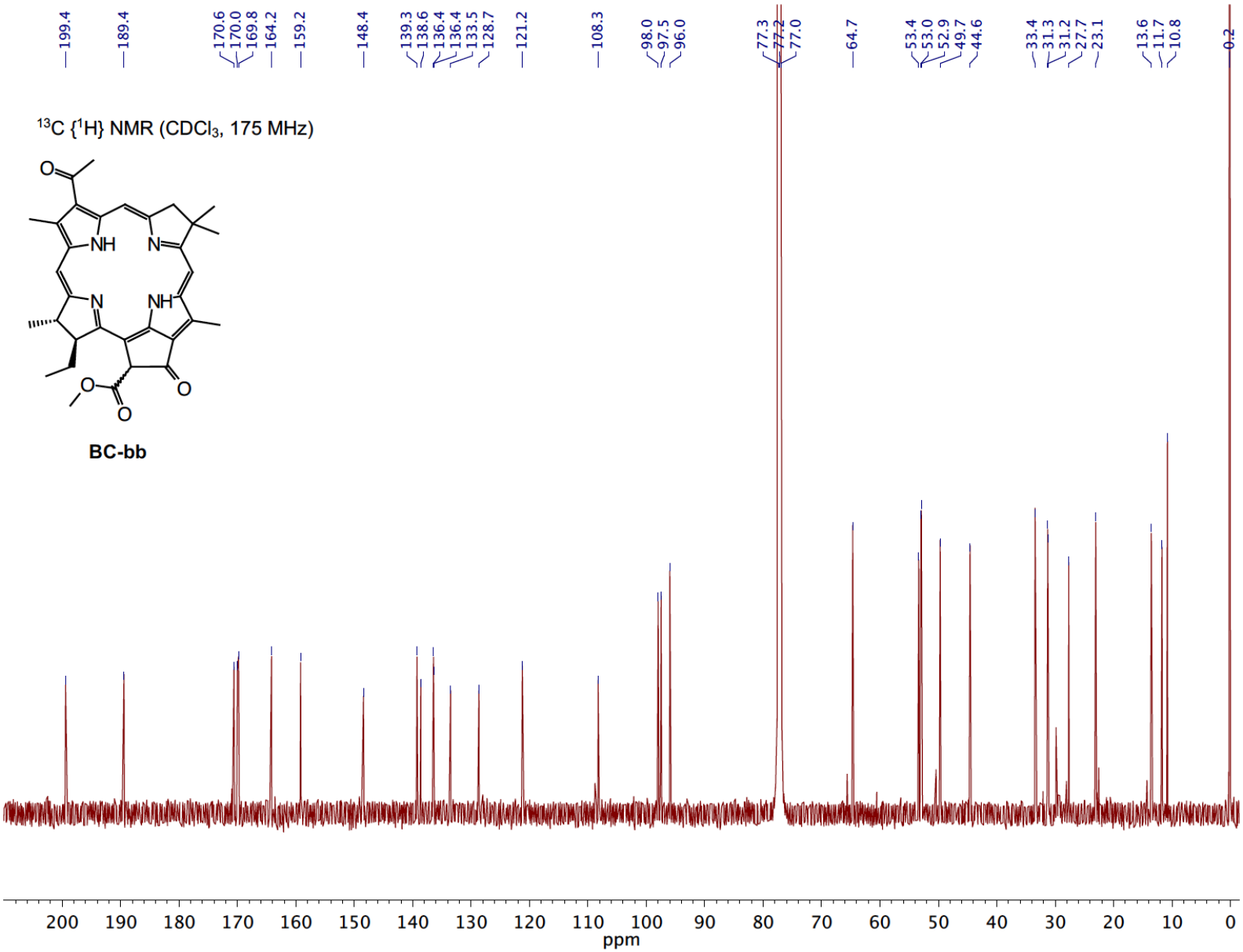

194.3
190.2
173.6
156.8
129.6
127.6
124.9
122.9
112.8
77.4
77.2
76.9
53.9
41.7
28.1
24.7
21.9
11.2
11.0
0.1
13C{1H} NMR (CDCl3, 125 MHz)
O
NH
N
O
1b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


11.15
10.32
7.40
7.26
7.22
5.92
5.89
4.98
3.77
3.41
3.41
2.63
2.62
2.61
2.60
2.50
2.50
2.49
2.48
2.47
2.47
2.43
2.39
2.37
2.32
2.29
1.81
1.80
1.79
1.78
1.78
1.77
1.76
1.76
1.57
1.45
1.44
1.42
1.41
1.40
1.40
1.38
1.22
1.22
1.15
1.13
0.95
0.93
1H NMR (CDCl3, 500 MHz)
3bb
ppm
ppm


194.3
176.2
172.2
165.4
161.7
156.9
139.0
131.5
130.4
129.7
127.9
127.5
124.1
123.4
120.3
118.8
107.9
103.8
102.4
77.4
77.2
76.9
58.2
54.6
54.6
53.0
48.7
41.0
40.5
29.3
29.3
27.9
25.3
21.5
11.2
10.9
10.8
0.1
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz)
3bb
ppm


^{1}H NMR ($CDCl_3$, 500 MHz)
BC-bb
ppm


^{1}H NMR ($CDCl_3$, 700 MHz)
BC-bb
ppm


199.4
189.4
170.6
170.0
169.8
164.2
159.2
148.4
139.3
138.6
136.4
136.4
133.5
128.7
121.2
108.3
98.0
97.5
96.0
77.3
77.2
77.0
64.7
53.4
53.0
52.9
49.7
44.6
33.4
31.3
31.2
27.7
23.1
13.6
11.7
10.8
0.2
^{13}C {^{1}H} NMR ($CDCl_3$, 175 MHz)
BC-bb
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm