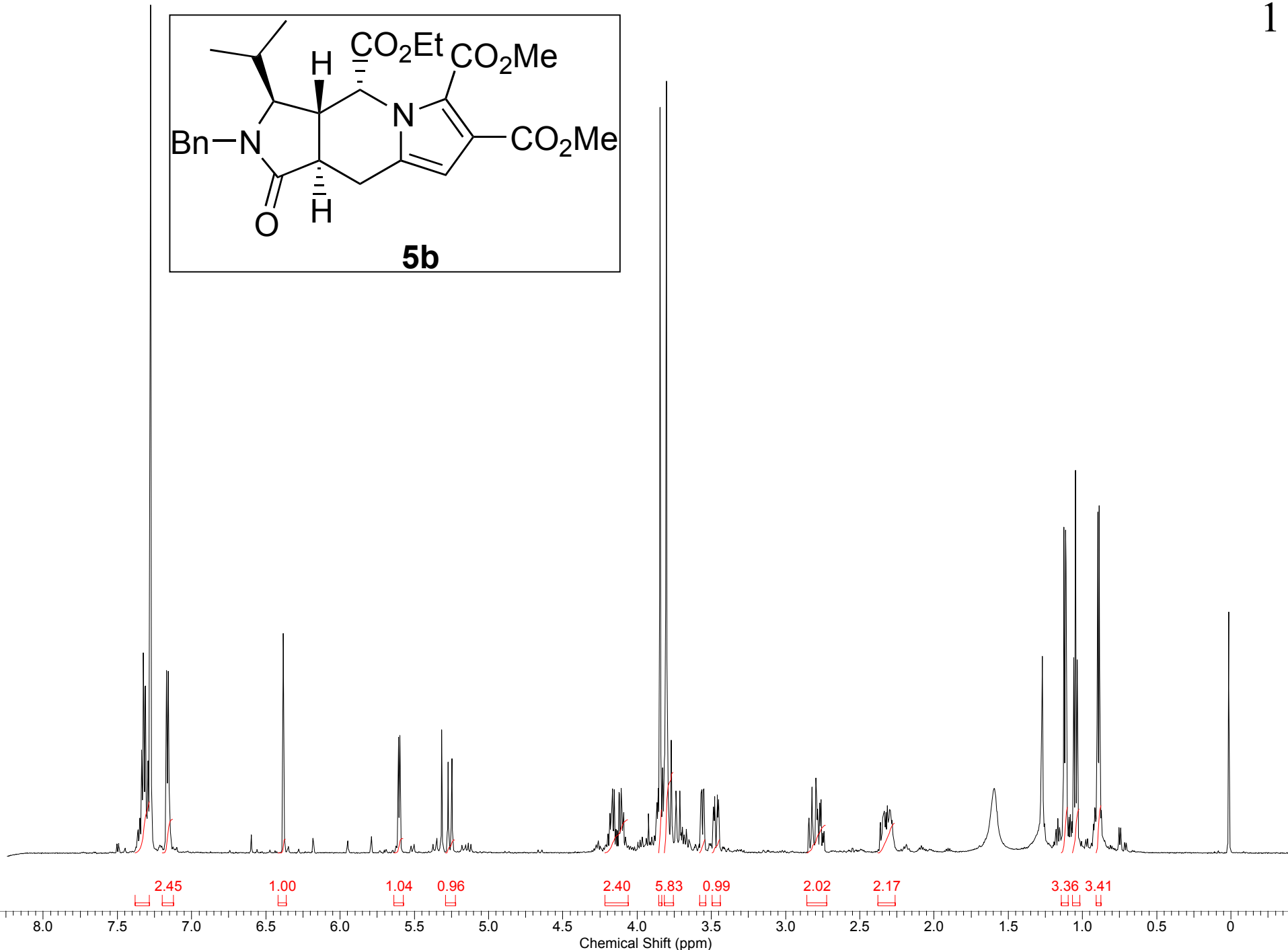
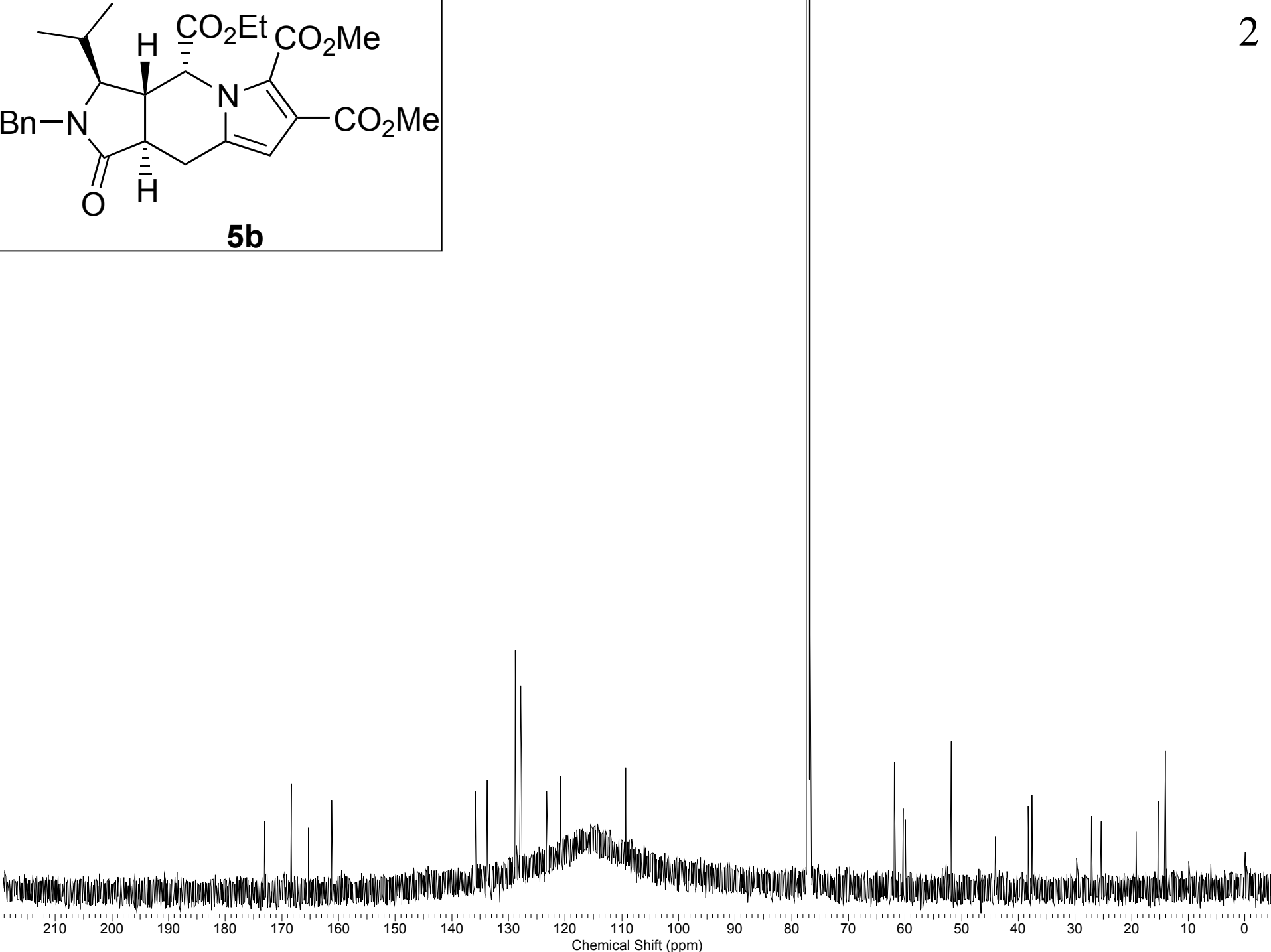
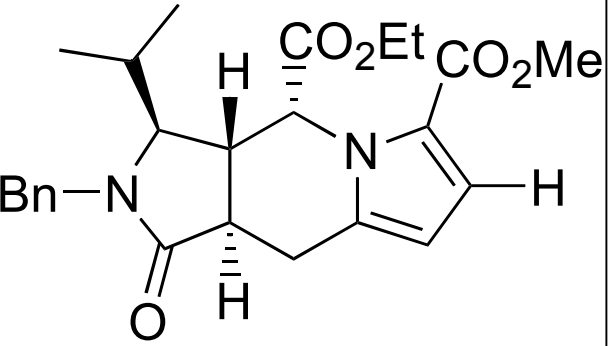
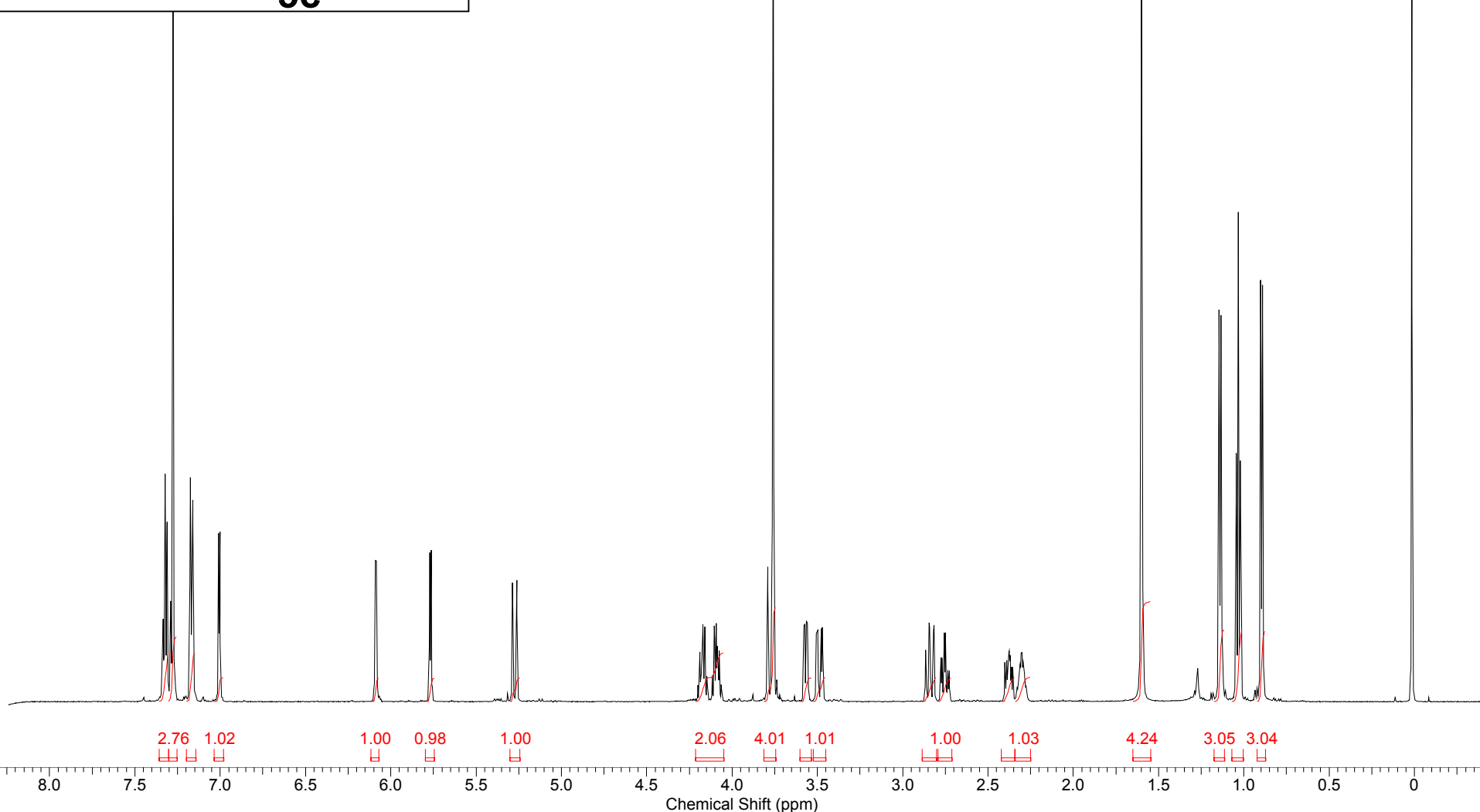

CO2Et
CO2Me
H
N
Bn—N
CO2Me
O
H
5b
2.45
1.00
1.04
0.96
2.40
5.83
0.99
2.02
2.17
3.36
3.41
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

H
CO2Et
CO2Me
N
Bn—N
CO2Me
O
H
5b


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

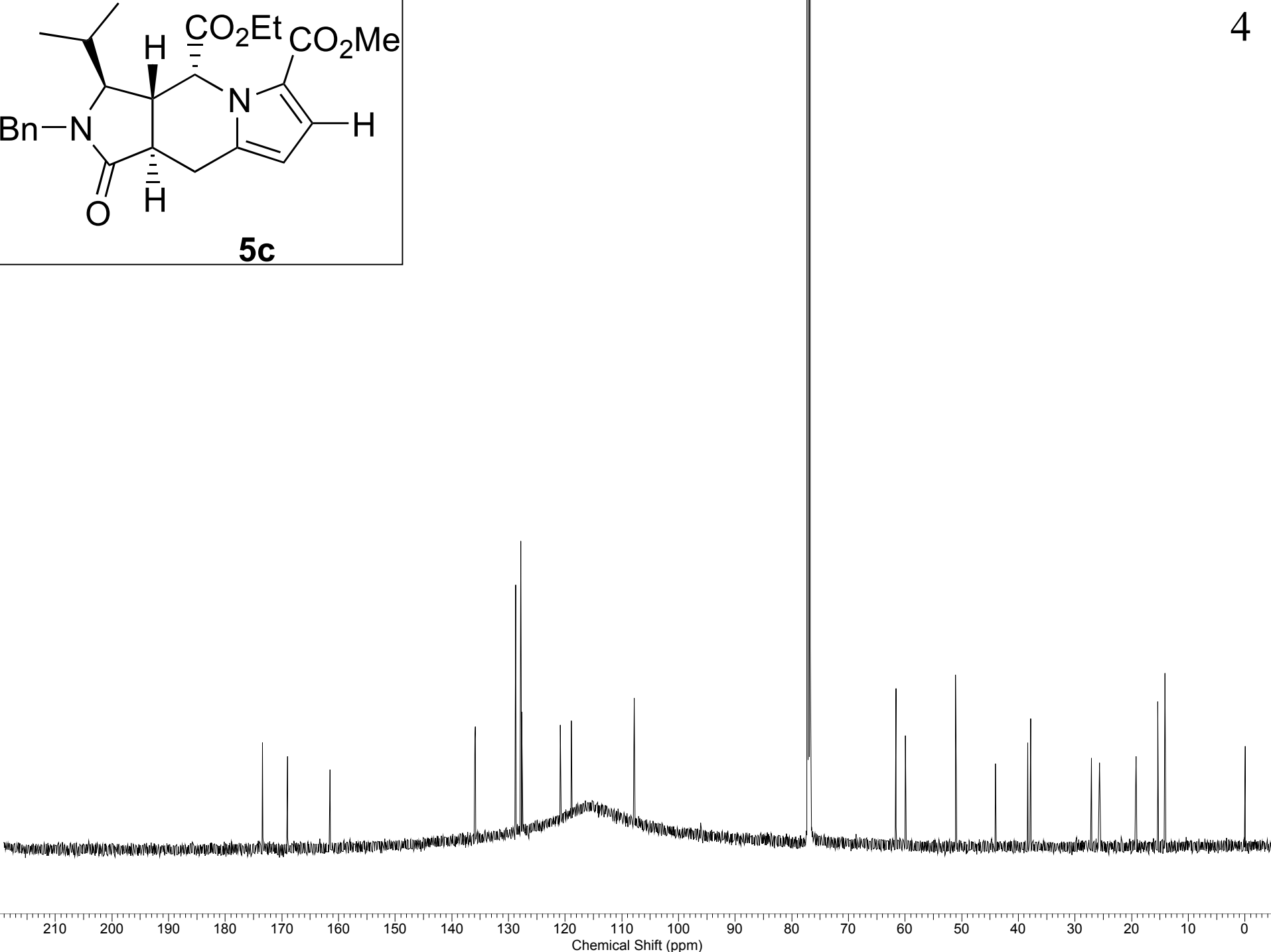

CO2Et
CO2Me
H
N
Bn—N
H
O
H

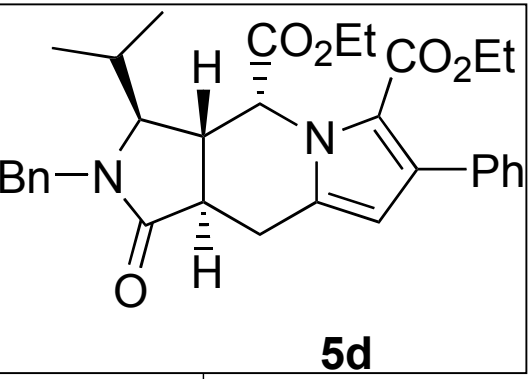
5c


2.76
1.02
1.00
0.98
1.00
2.06
4.01
1.01
1.00
1.03
4.24
3.05
3.04
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
Chemical Shift (ppm)

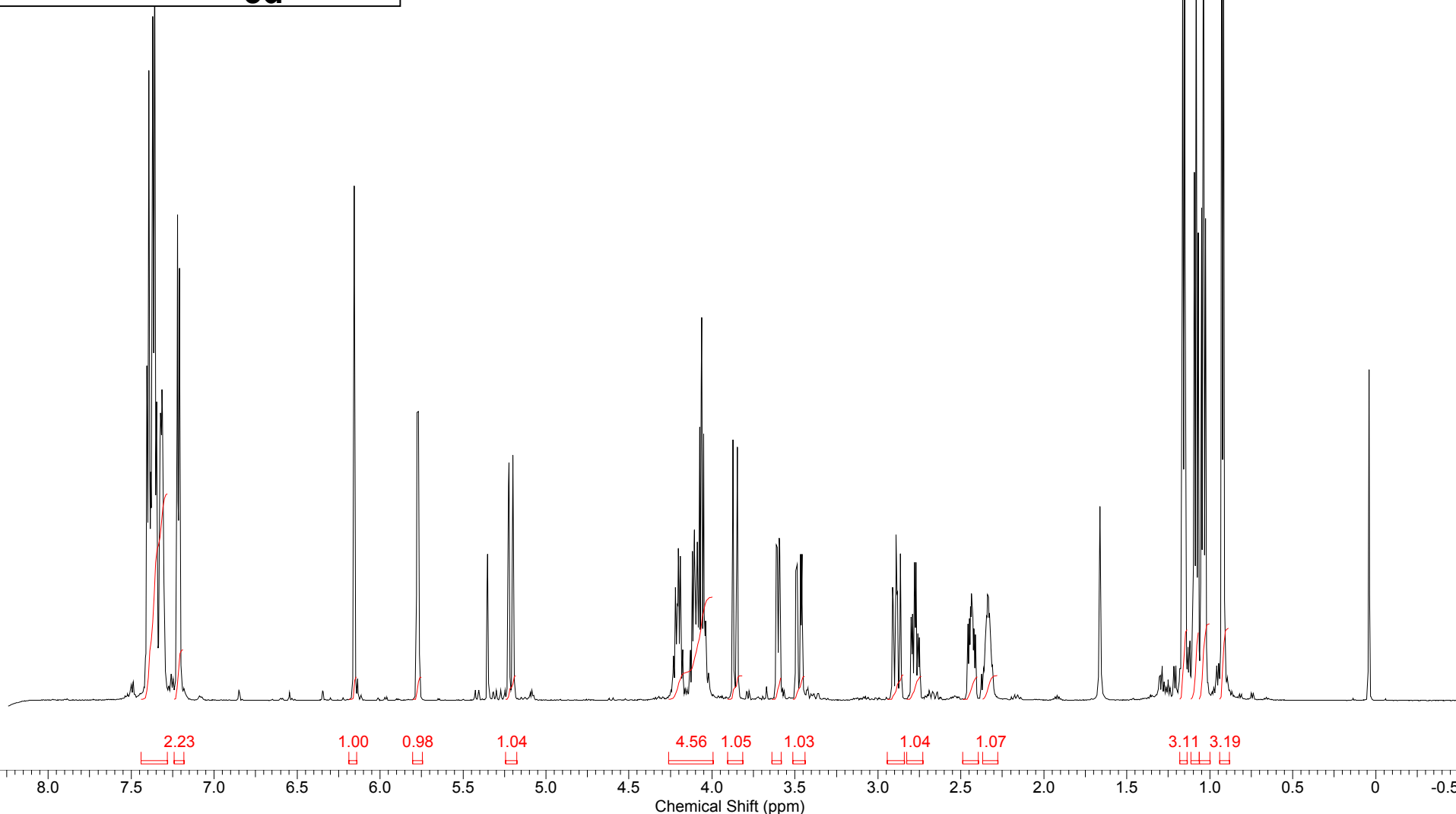
CO2Et
CO2Me
H
N
Bn—N
H
O
H

5c


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

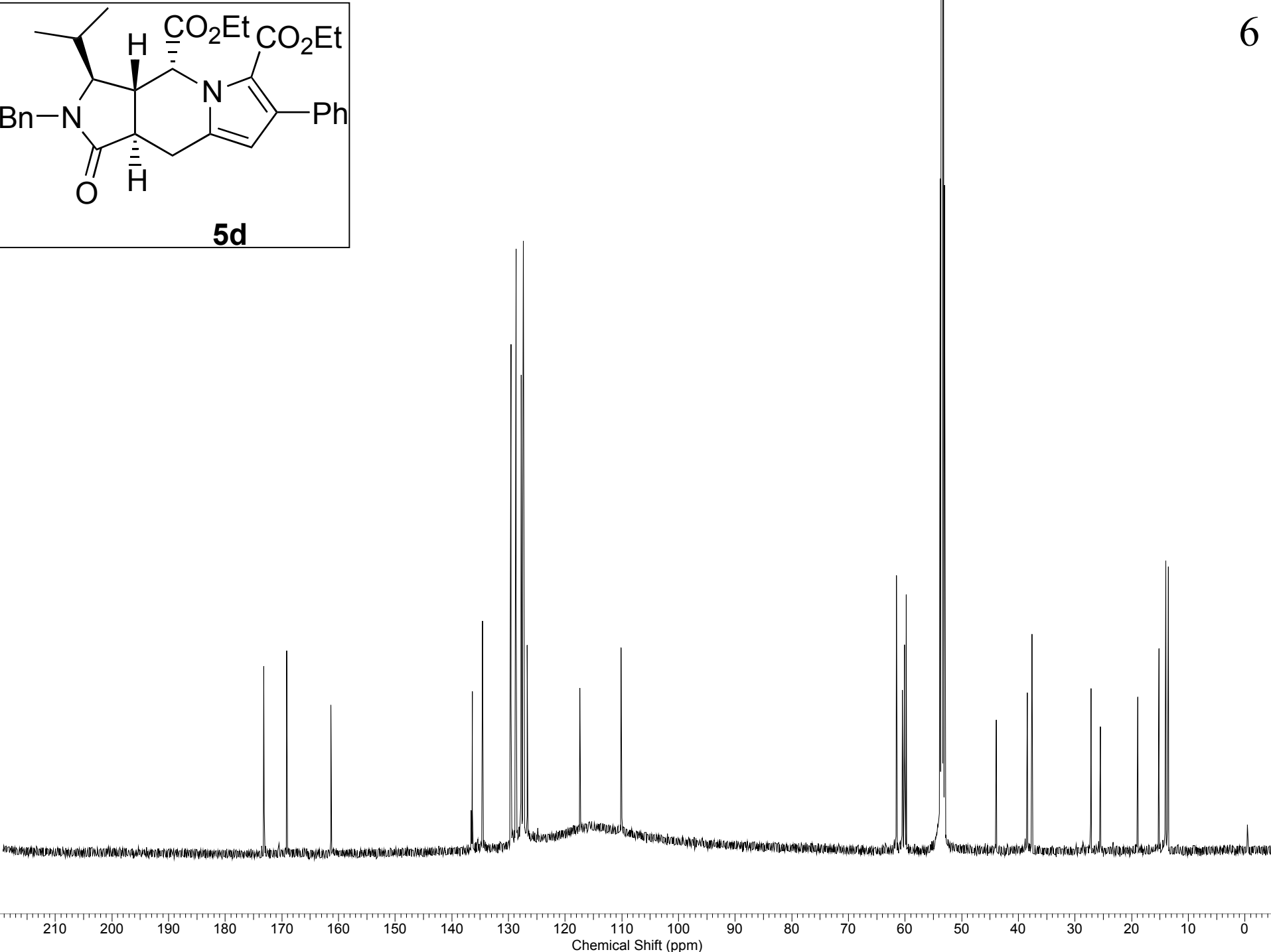

H
CO2Et
CO2Et
N
Bn—N
Ph
O
H

5d


2.23
1.00
0.98
1.04
4.56
1.05
1.03
1.04
1.07
3.11
3.19
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
-0.5
Chemical Shift (ppm)

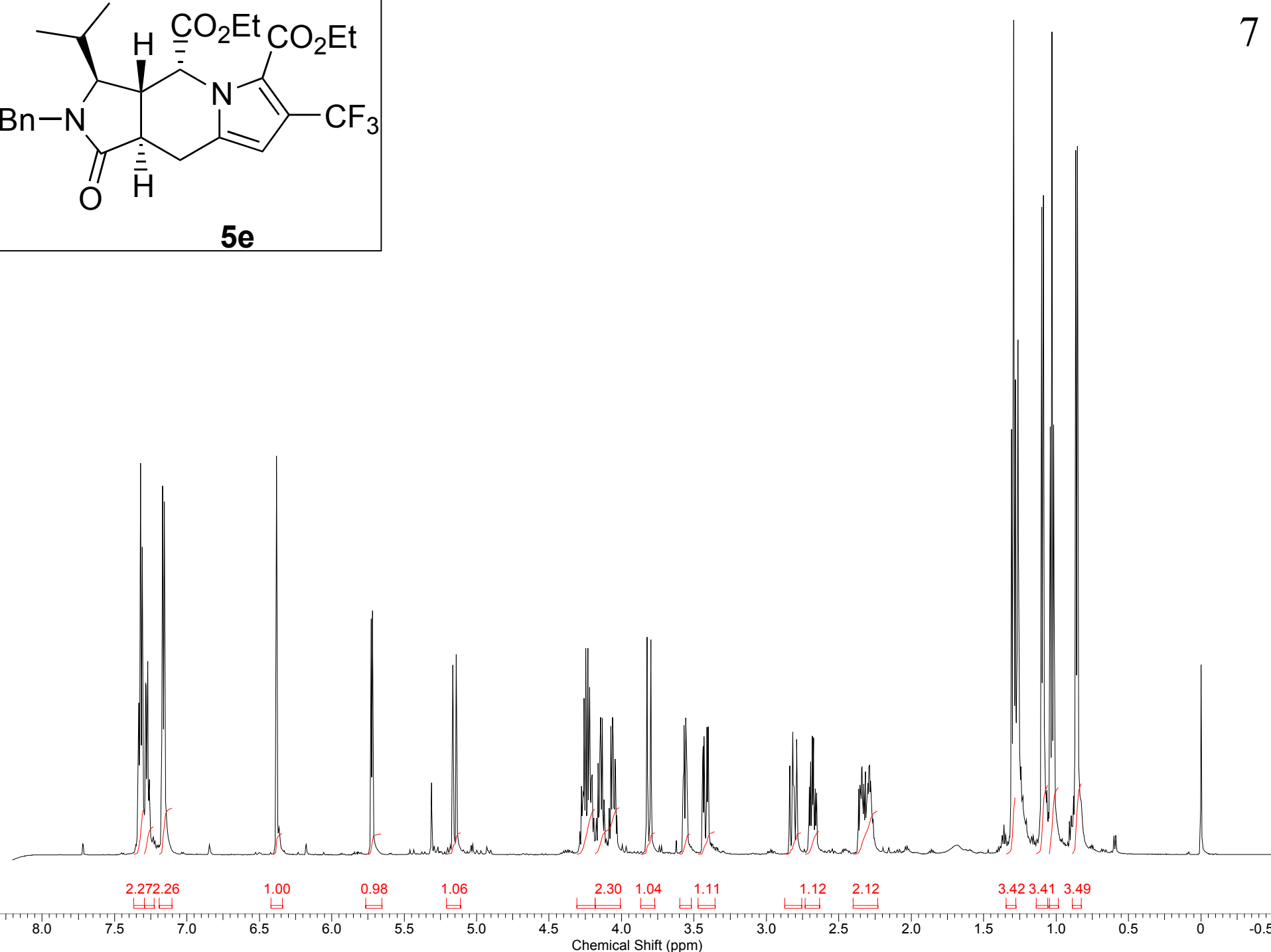
CO2Et
CO2Et
H
N
Bn—N
Ph
O
H

5d


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

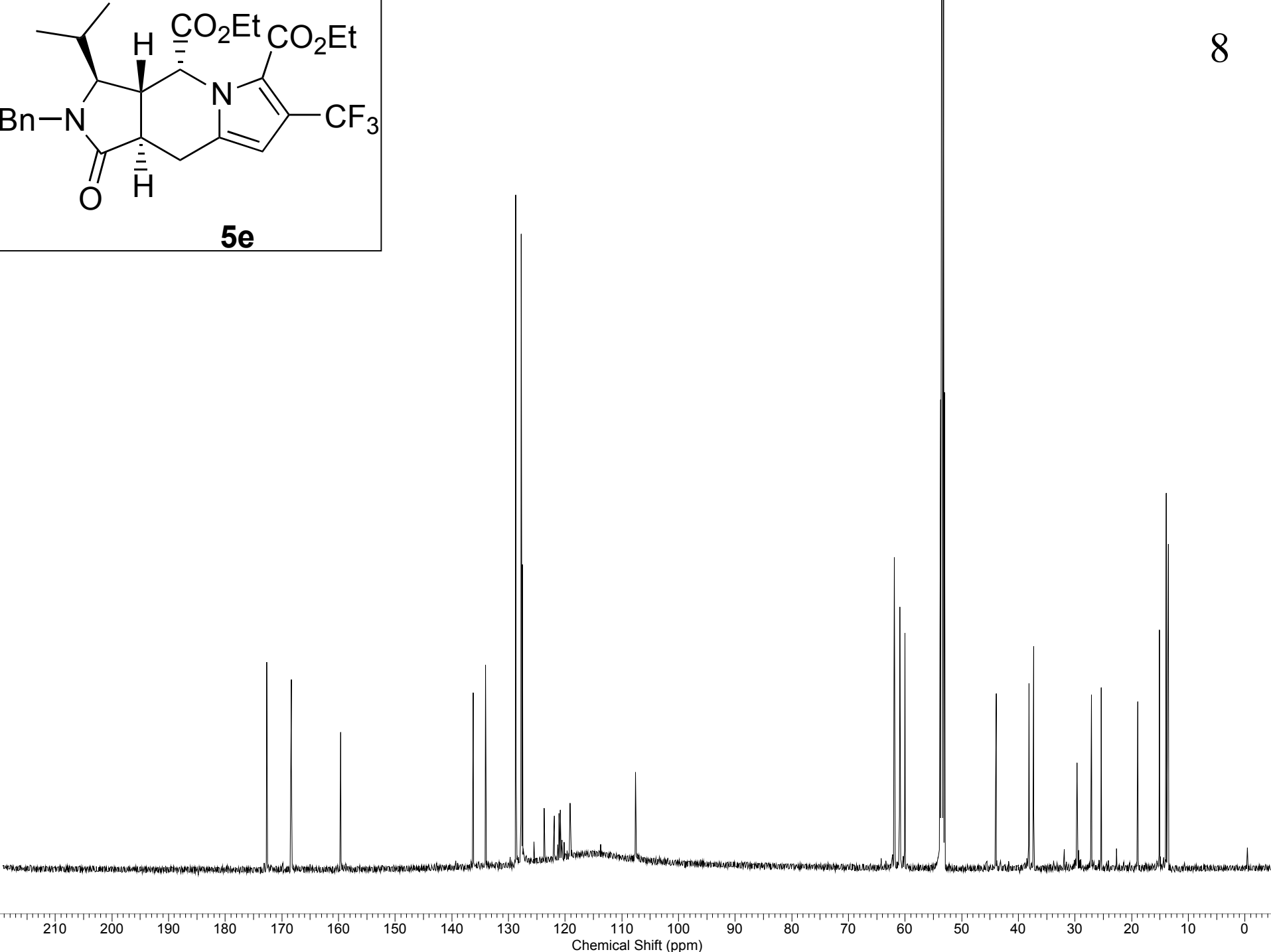
CO2Et
CO2Et
H
N
Bn–N
CF3
O
H

5e

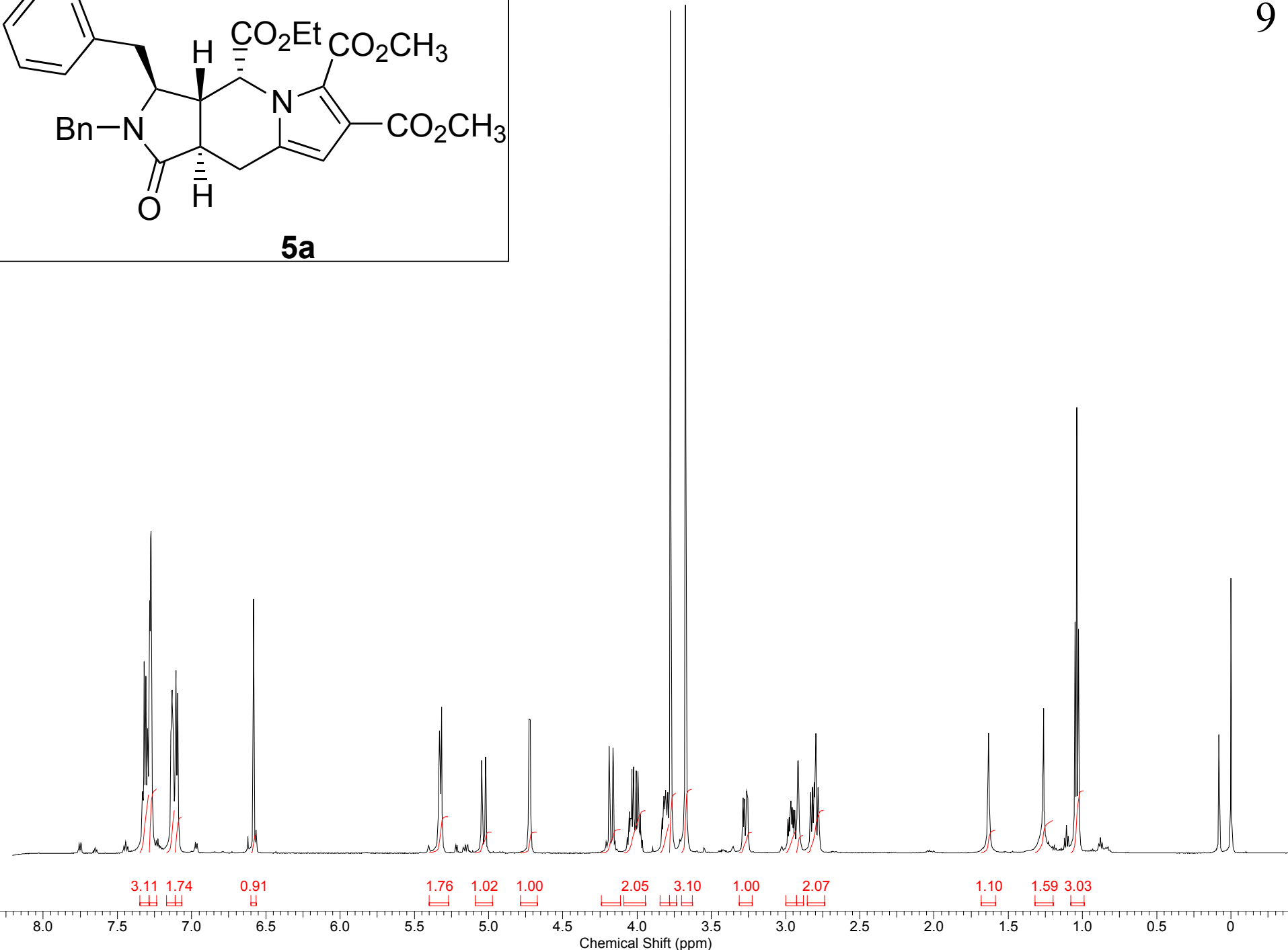

2.27 2.26
1.00
0.98
1.06
2.30
1.04
1.11
1.12
2.12
3.42 3.41
3.49
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
-0.5
Chemical Shift (ppm)

CO2Et
CO2Et
H
N
Bn−N
CF3
O
H

5e

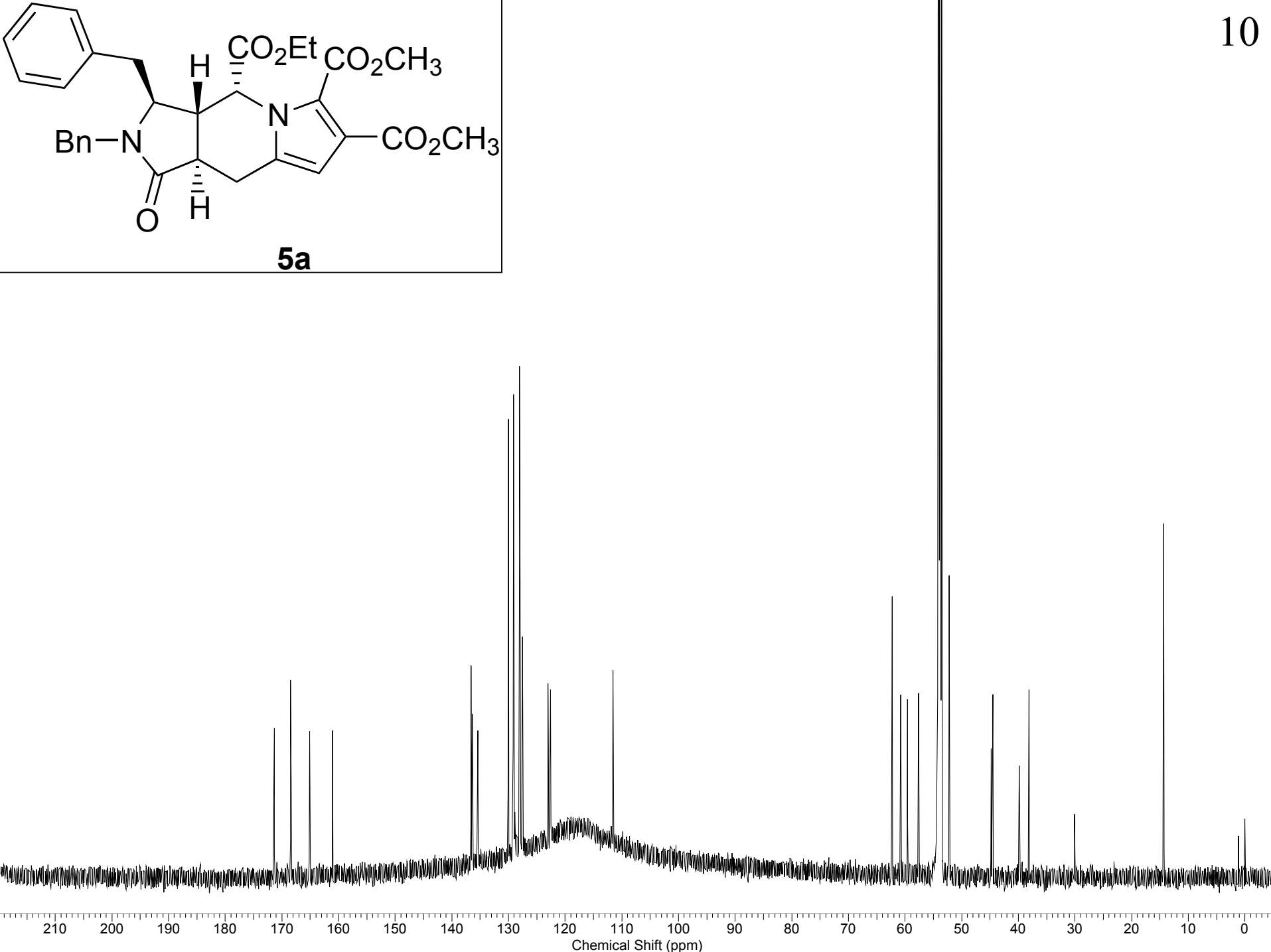

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

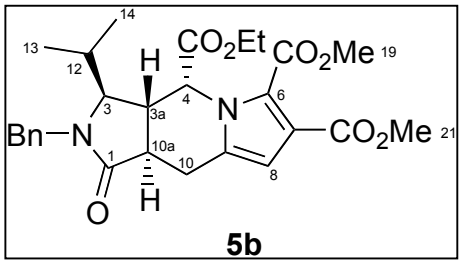
CO2Et
CO2CH3
H
N
Bn—N
CO2CH3
O
H
5a


3.11
1.74
0.91
1.76
1.02
1.00
2.05
3.10
1.00
2.07
1.10
1.59
3.03
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
Chemical Shift (ppm)

H
CO2Et
CO2CH3
N
Bn—N
CO2CH3
O
H

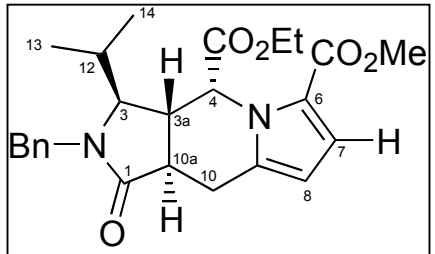
5a


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)



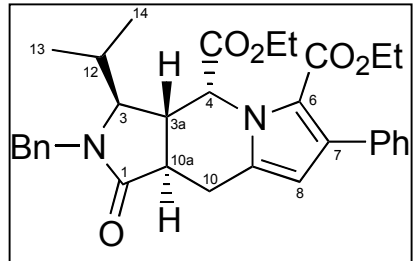
5b

Obs nOe / (intensity)
10eq-8 (m)
10eq-10ax, 10a (s)
4-13 (s)
4-3a (s)
3-10a (m)
3-12 (s)



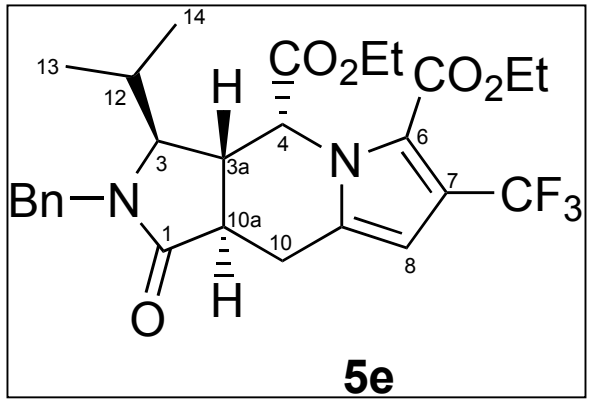
5c

Obs nOe / (intensity)
8-7 (s)
8-10eq (s)
8-10ax (m)
4-18 (ww)
4-3a (s)
4-14 (s)
3-10a (w)
3-13 (m)
3-3a (w)
10eq-10a (m)
3a-10ax (s)
3a-14 (s)
12-4 (w)
12-3 (s)
12-13,14 (s)
13-3a (m)
13-4 (s)
7-18 (w)



5d

Obs nOe / (intensity)
8-phenyl (s)
8-10eq (s)
8-10ax (m)
4-3a (s)
4-13 (s)
4-12 (w)
4-3 (w)
3-10a (s)
3-12 (s)
3-13 (s)
10eq-10a (m)
3a-13 (m)
3a-14 (s)
3a-10ax (s)
12-13,14 (s)



5e

Obs nOe / (intensity)
4-3a (s)
4-13 (s)
10eq-8 (m)
10eq-10a (s)
10ax-8 (m)
10ax-3a (s)
3a-4 (s)
12-3 (s)
14-3a,12 (s)

C-F Couplings: C21-F J = 267.9,
C7-F J = 37.3, C6-F J = 3.29, C8-F J = 4.39

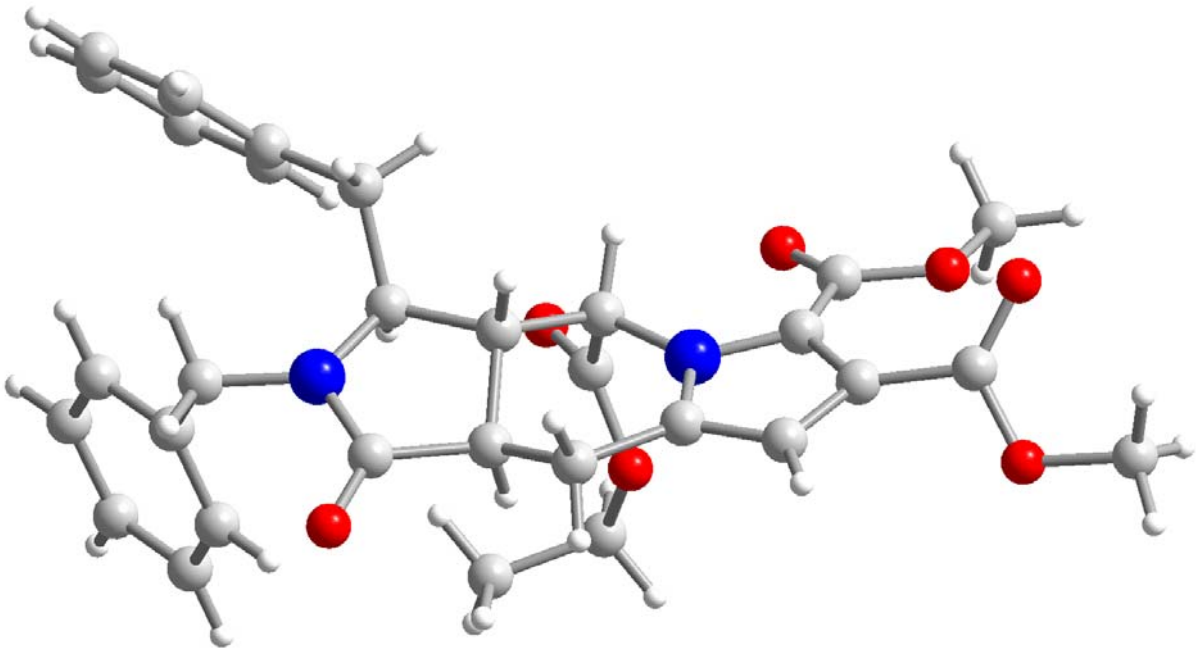


Figure 1: Ball and Stick Diagram of 5a

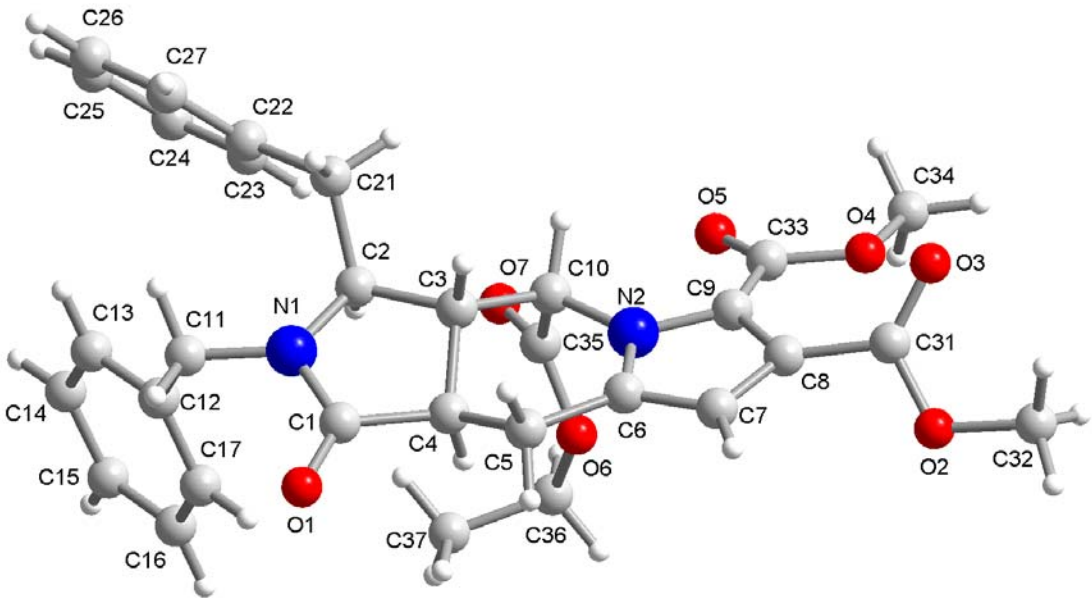


Figure 2: Labeled Ball and Stick Diagram of 5a

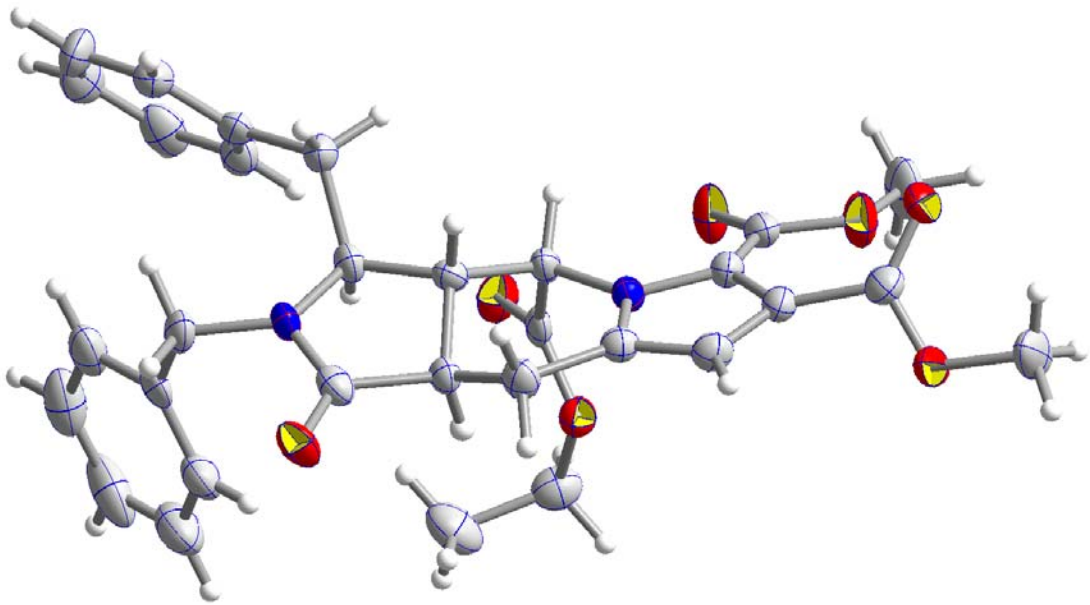


Figure 3: ORTEP Diagram of 5a

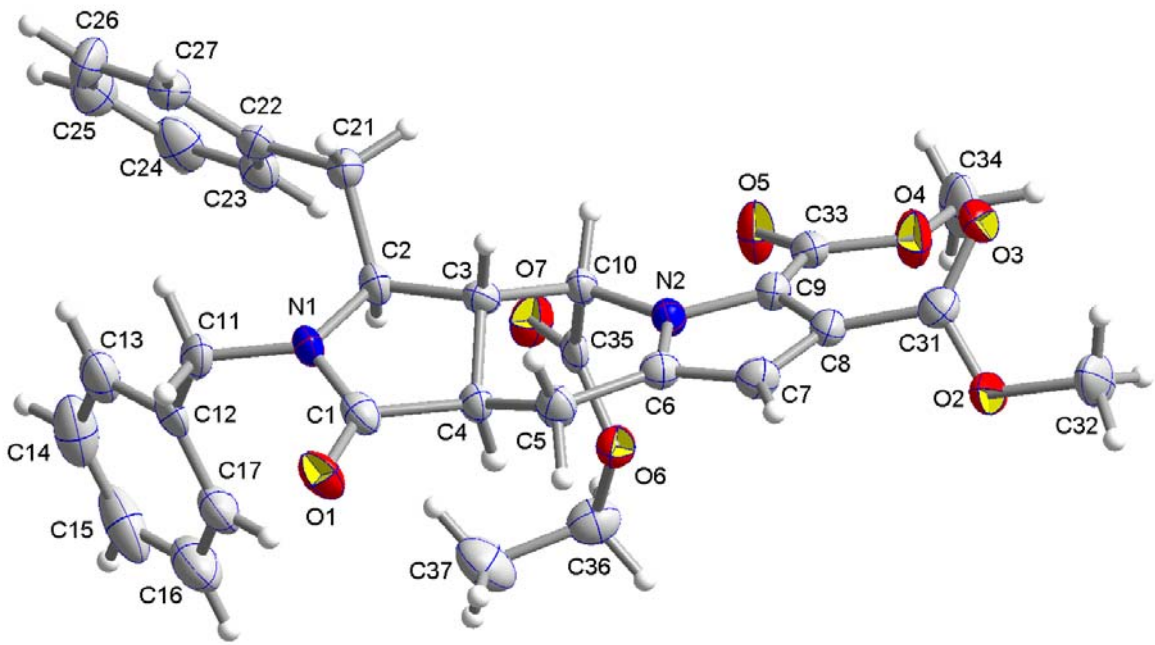


Figure 4: Labeled ORTEP Diagram of 5a

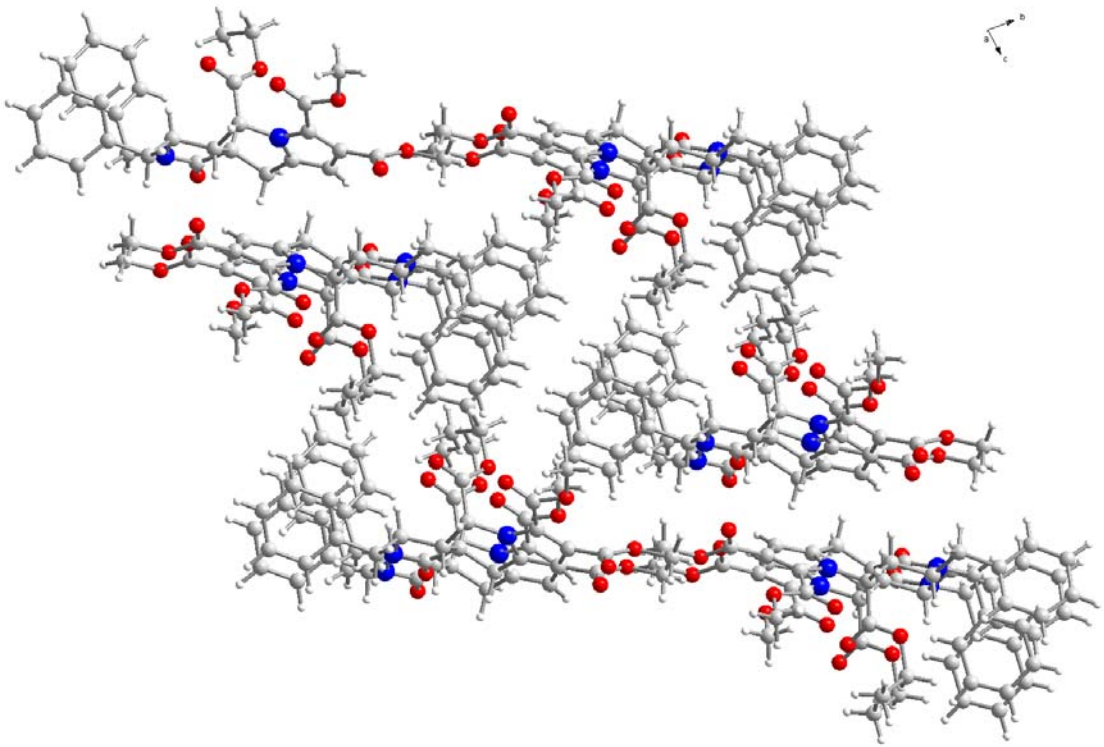


Figure 5: Packing Diagram of 5a