Supporting information

For

Reaction of Pyrrolobenzothiazines with Schiff Bases and Carbodiimides: Approach to Angular 6/5/5/5-Tetracyclic Spiroheterocycles

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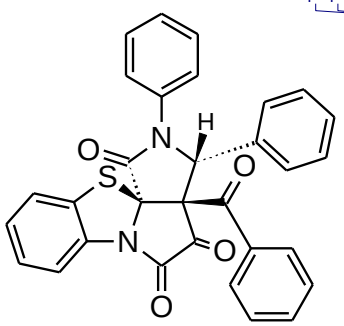
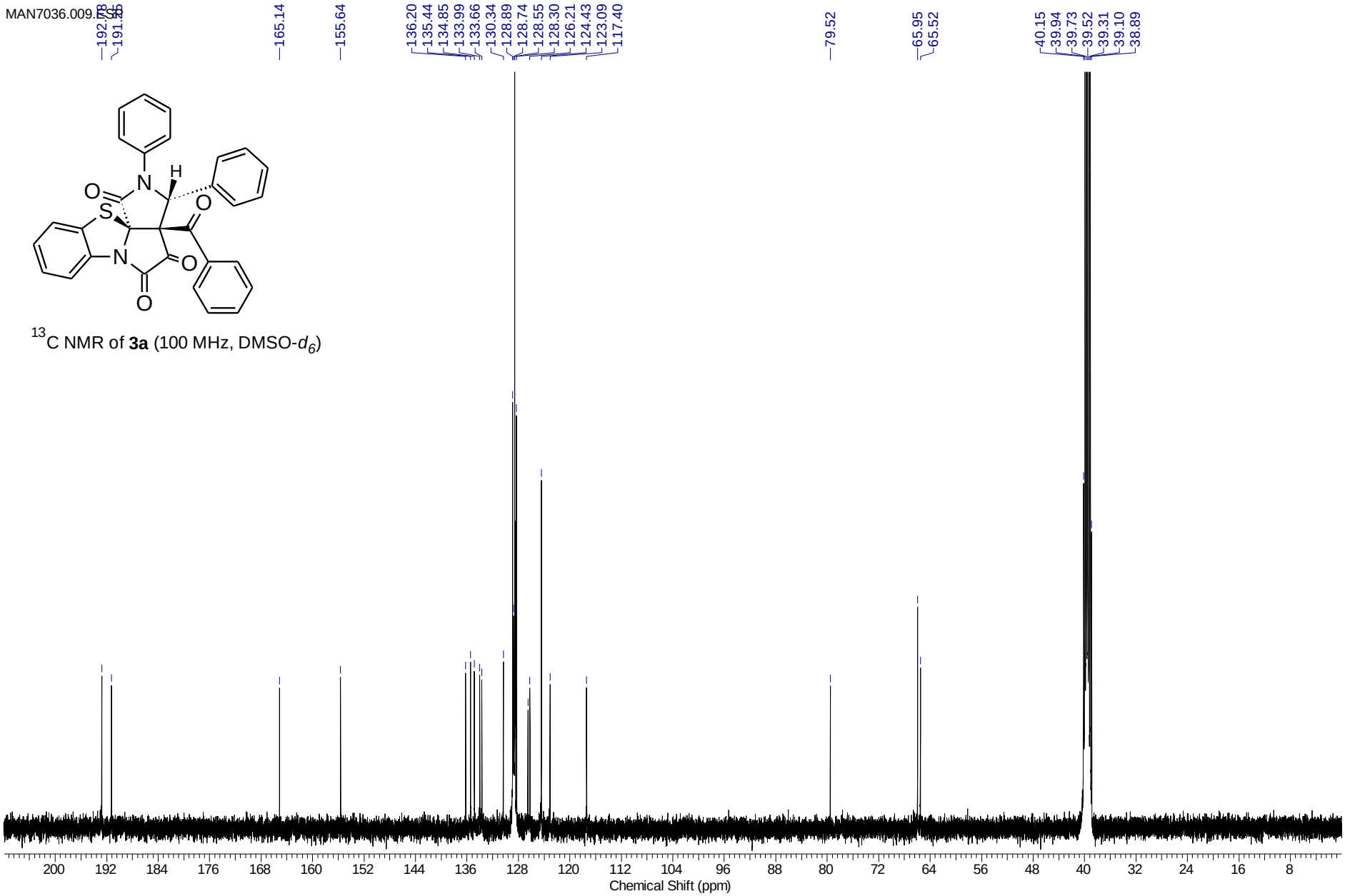
MAN7036.008.ESP

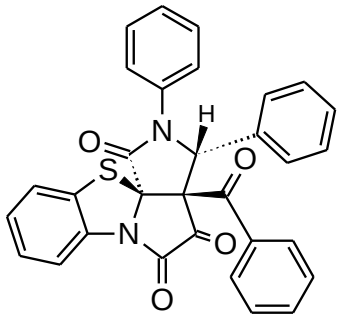


^{1}H NMR of **3a** (400 MHz, DMSO-d_6)



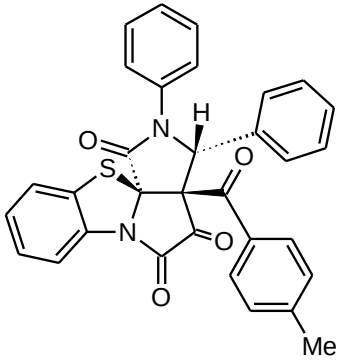
^{13}C NMR of **3a** (100 MHz, DMSO-d_6)

MAN7036.010.ESP

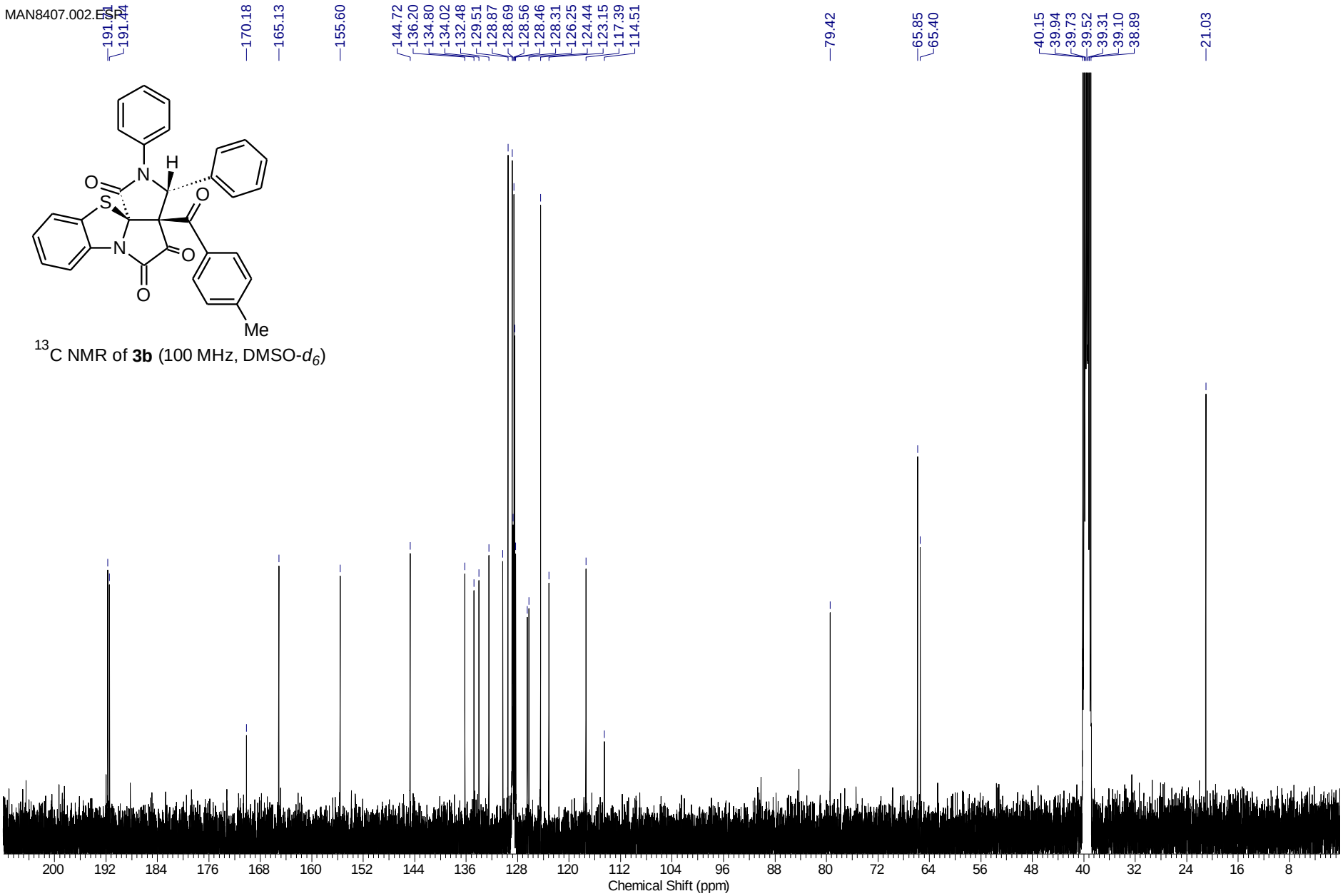


DEPT135 of **3a** (100 MHz, DMSO-d_6)

MAN8407.001.ESP



^{1}H NMR of **3b** (400 MHz, DMSO-d_6)



^{13}C NMR of **3b** (100 MHz, DMSO-d_6)

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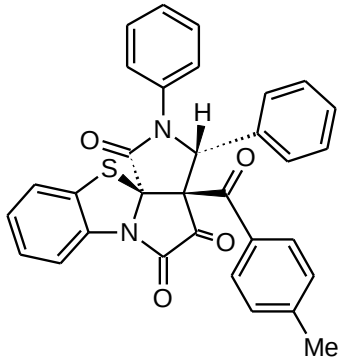
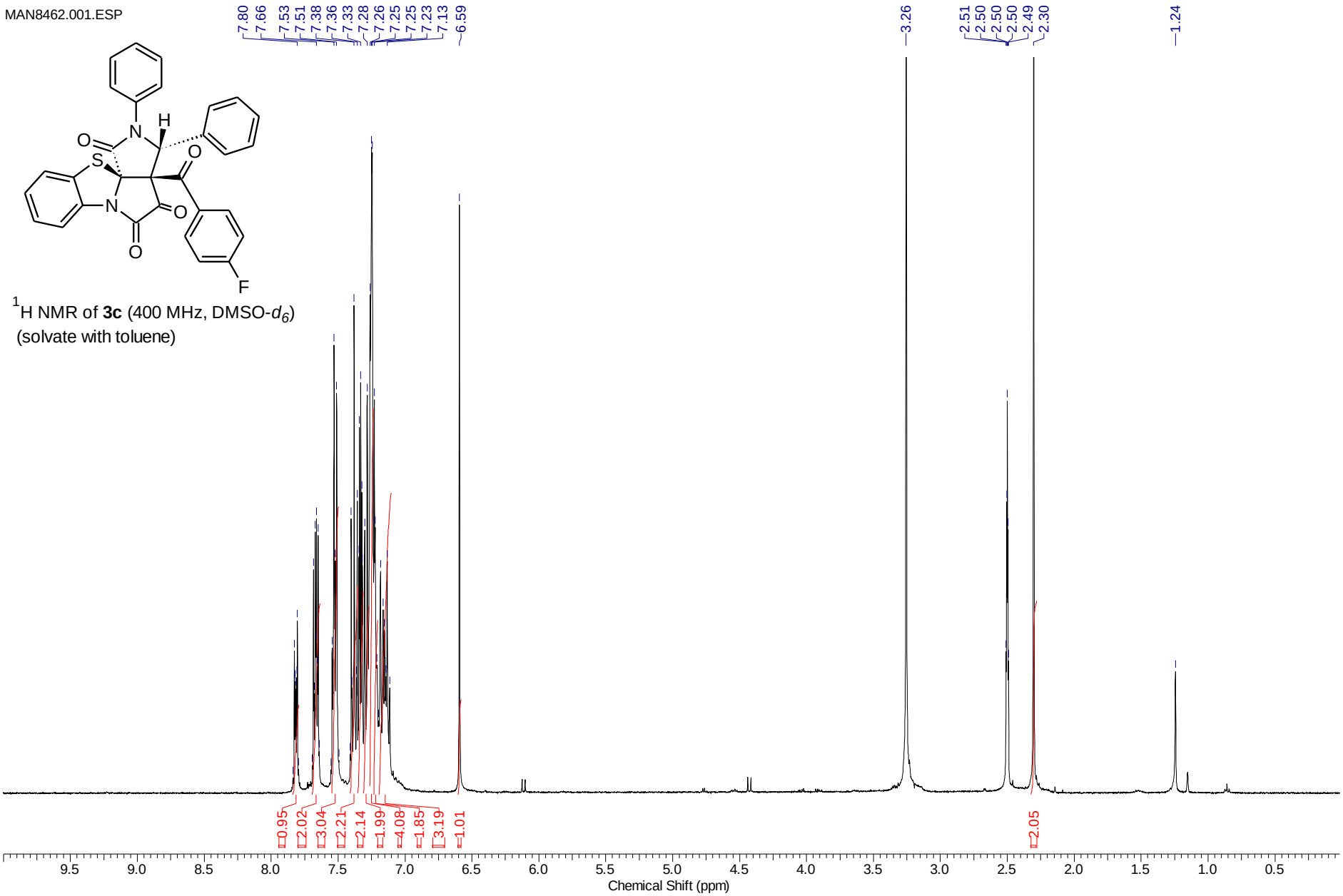
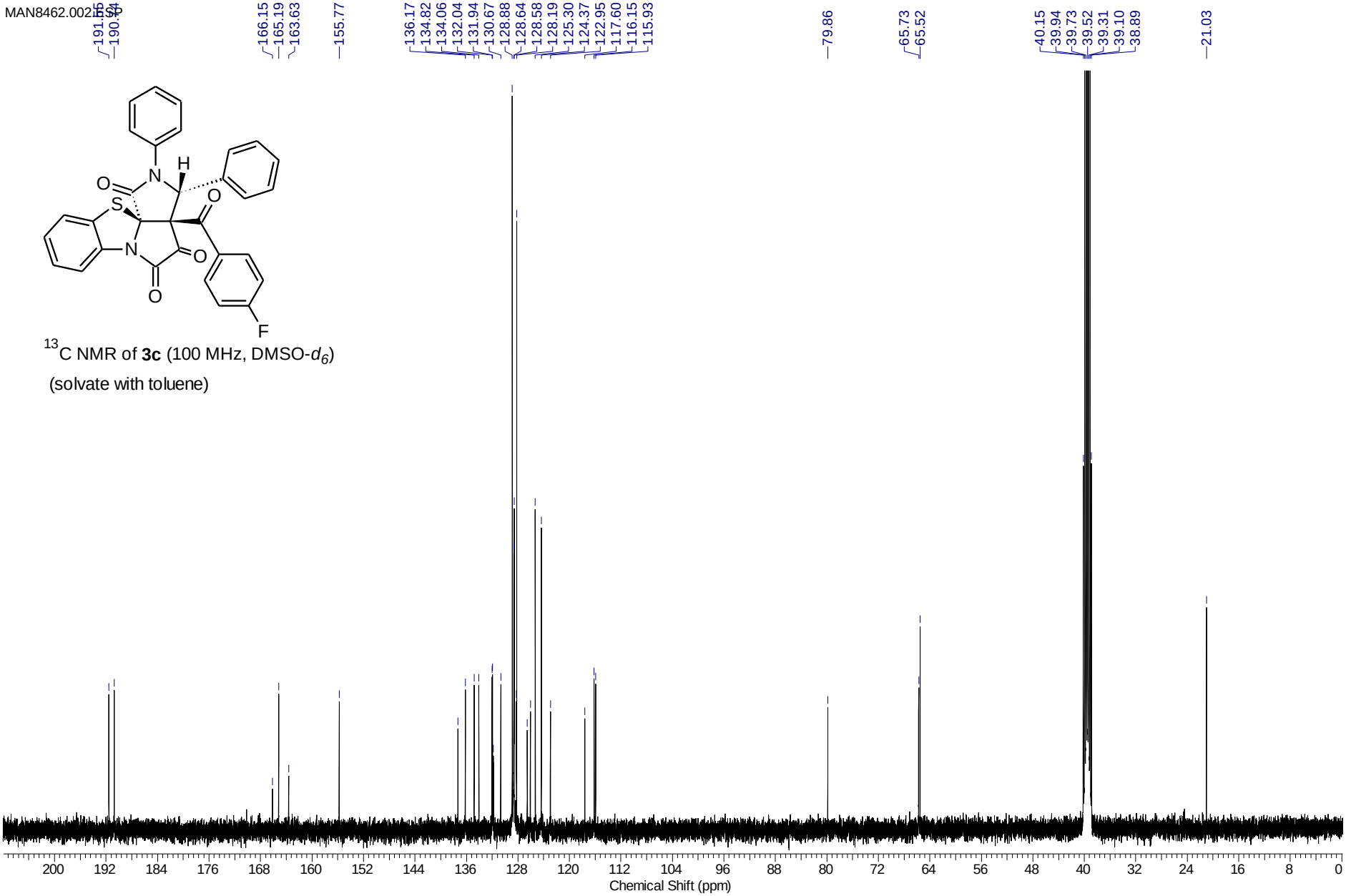


DEPT135 of **3b** (100 MHz, DMSO-d_6)



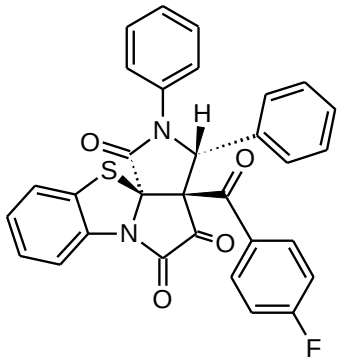
^{1}H NMR of **3c** (400 MHz, DMSO-d_6)
(solvate with toluene)



^{13}C NMR of **3c** (100 MHz, DMSO-d_6)

(solvate with toluene)

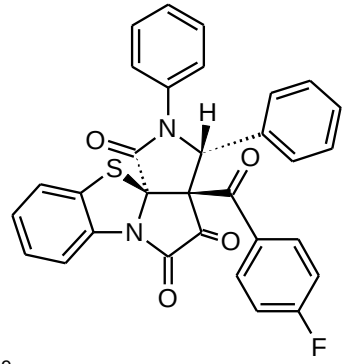
MAN8462.003.ESP



DEPT135 of **3c** (100 MHz, DMSO-d_6)

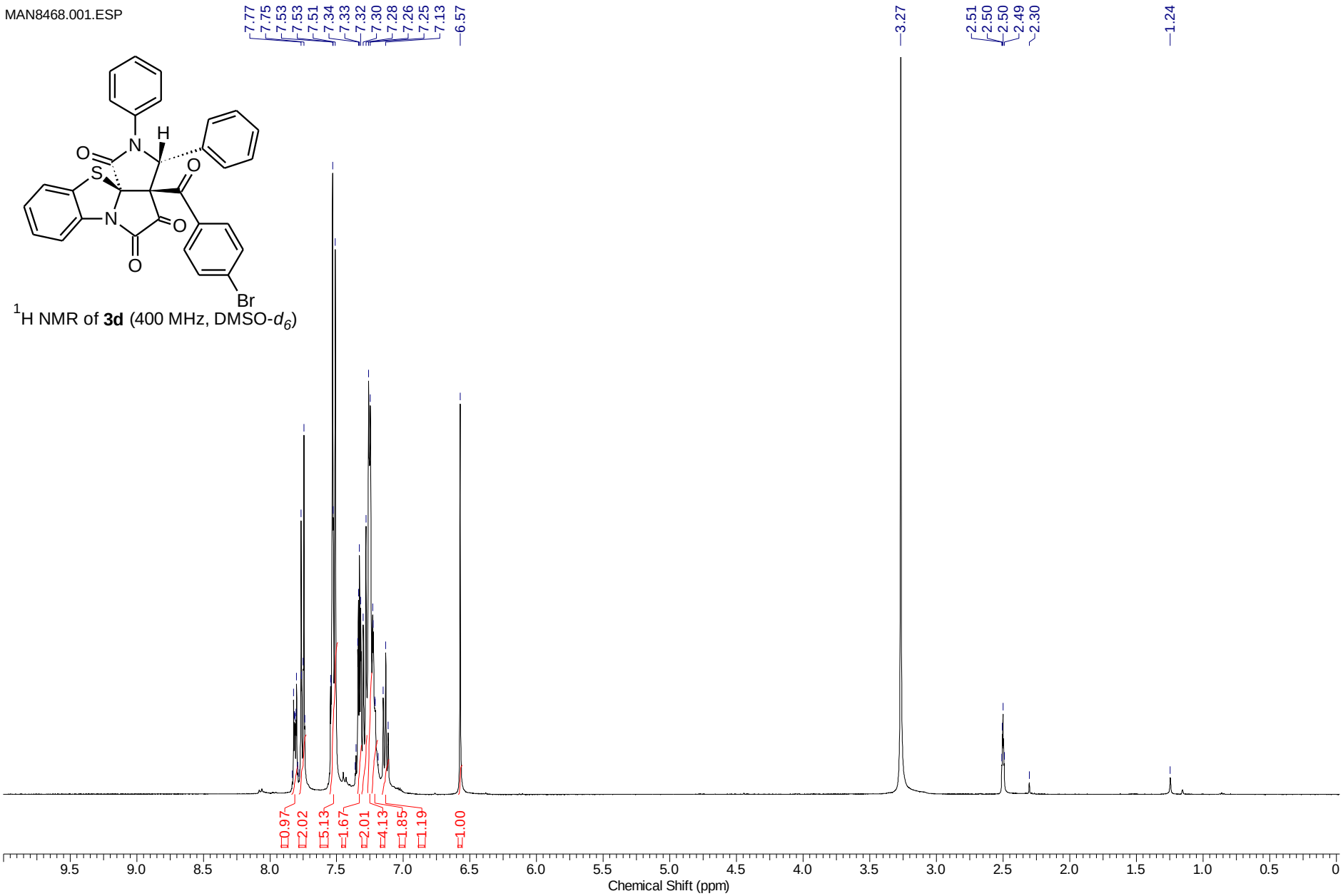
(solvate with toluene)

MAN8462.004.ESP

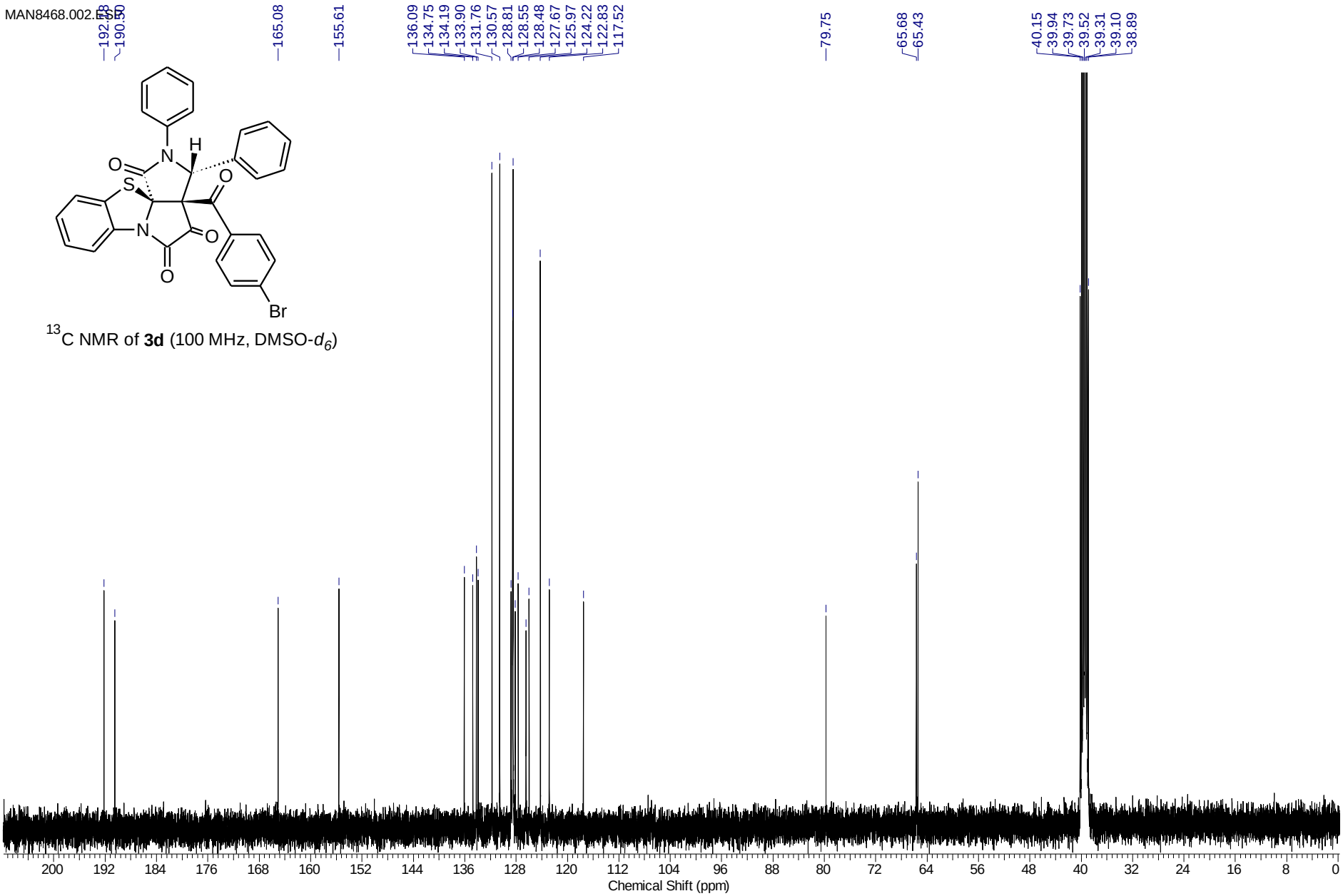


^{19}F NMR of **3c** (376 MHz, DMSO-d_6)

(solvate with toluene)

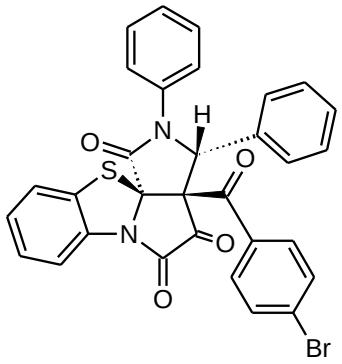


^{1}H NMR of **3d** (400 MHz, DMSO-d_6)



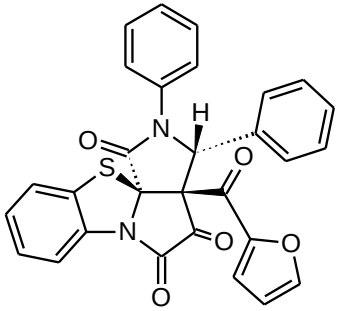
^{13}C NMR of **3d** (100 MHz, DMSO-d_6)

MAN8468.003.ESP

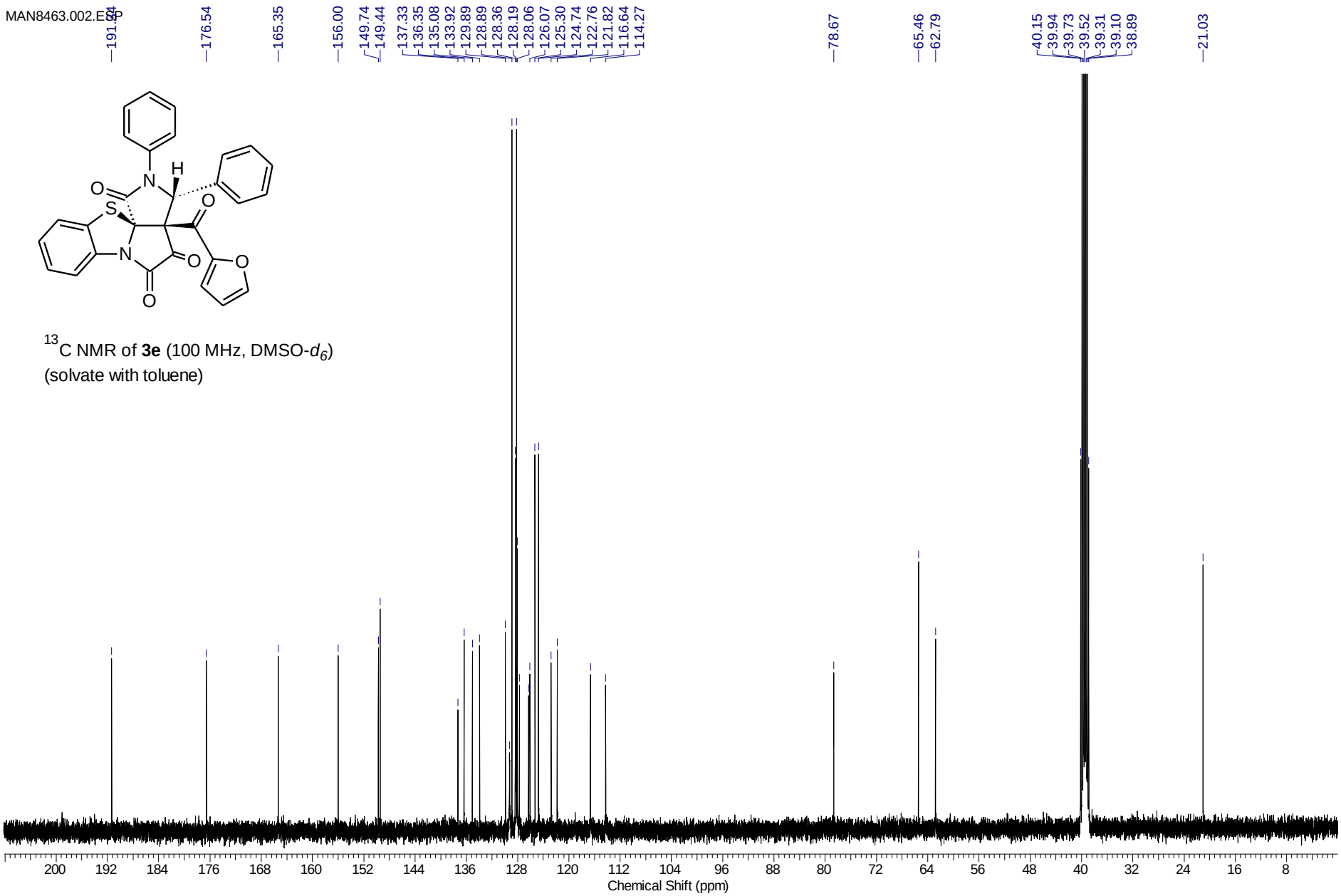


DEPT135 of **3d** (100 MHz, DMSO-d_6)

MAN8463.001.ESP



^{1}H NMR of **3e** (400 MHz, DMSO-d_6)
(solvate with toluene)



^{13}C NMR of **3e** (100 MHz, DMSO-d_6)
(solvate with toluene)

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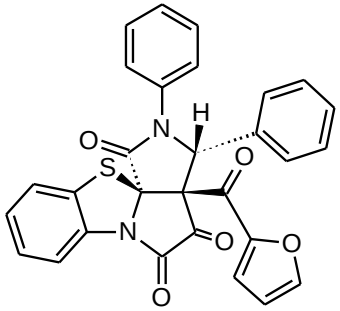

DEPT135 of **3e** (100 MHz, DMSO-d_6)
(solvate with toluene)

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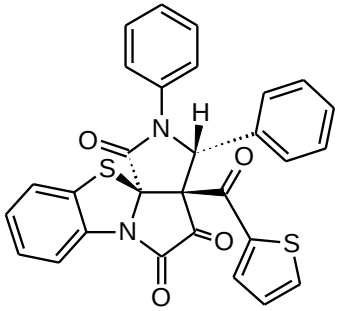
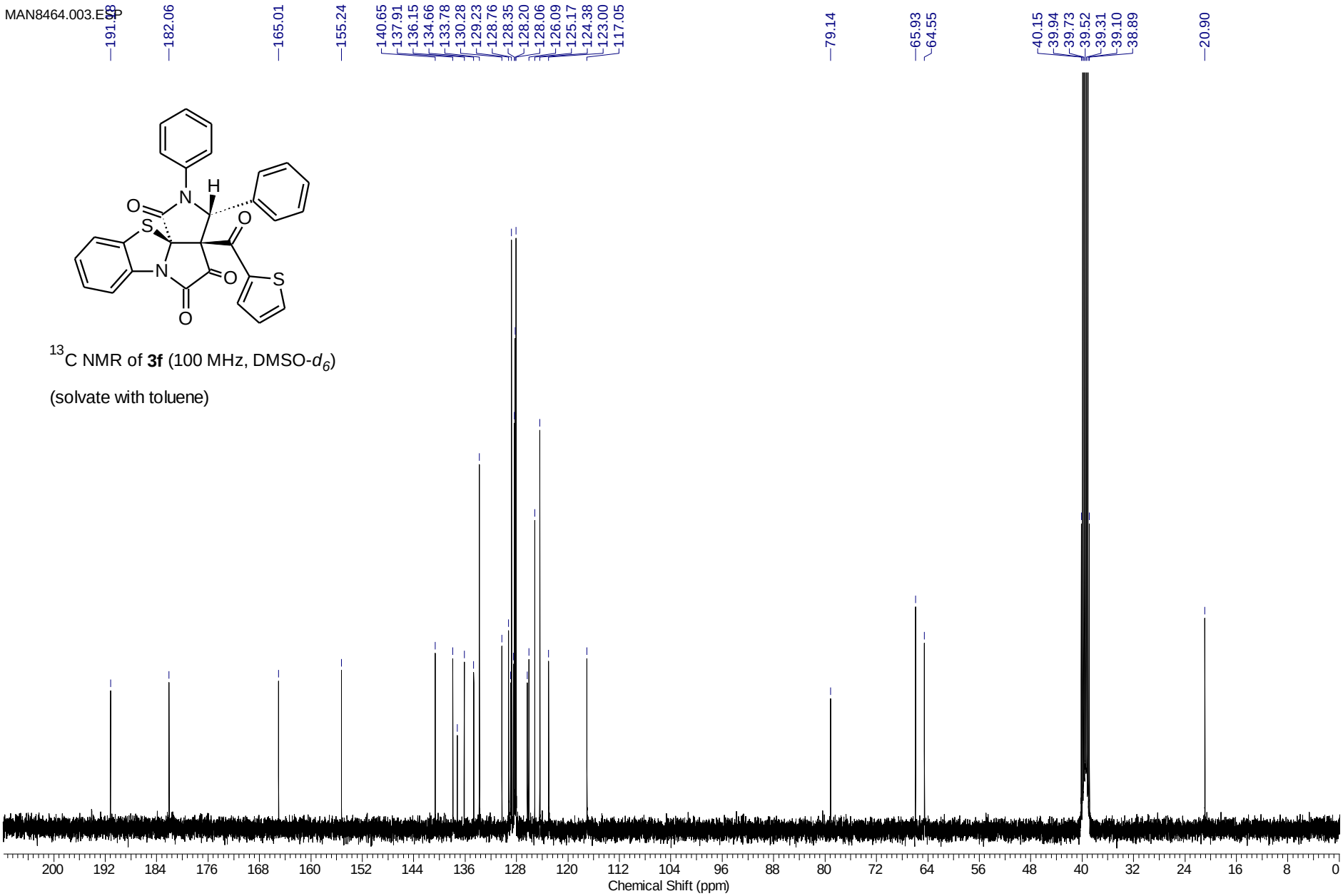


^{1}H NMR of **3f** (400 MHz, DMSO-d_6)

(solvate with toluene)



^{13}C NMR of **3f** (100 MHz, DMSO-d_6)

(solvate with toluene)

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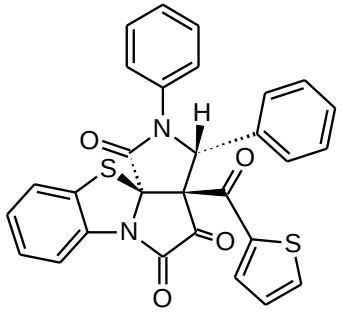
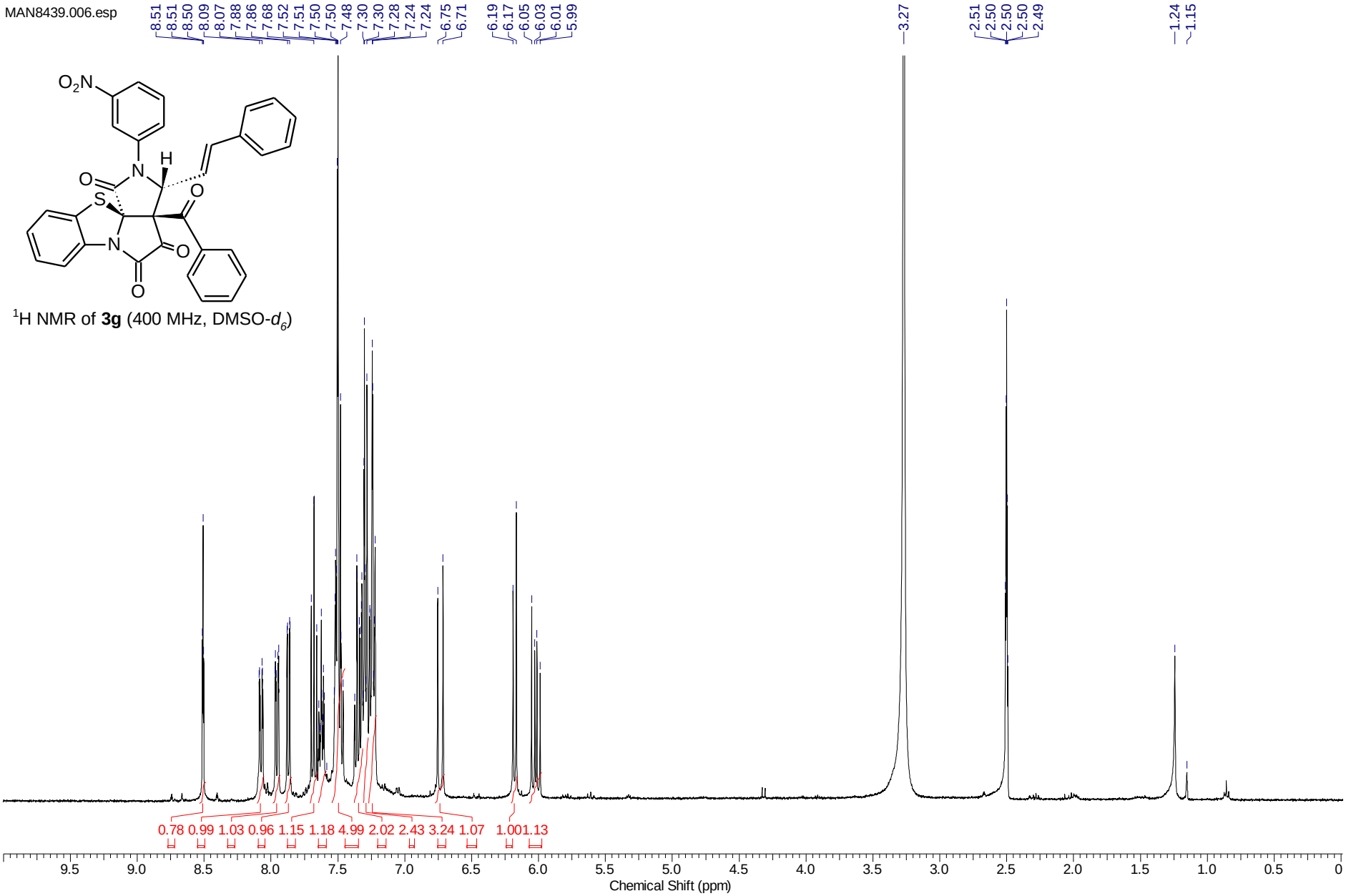
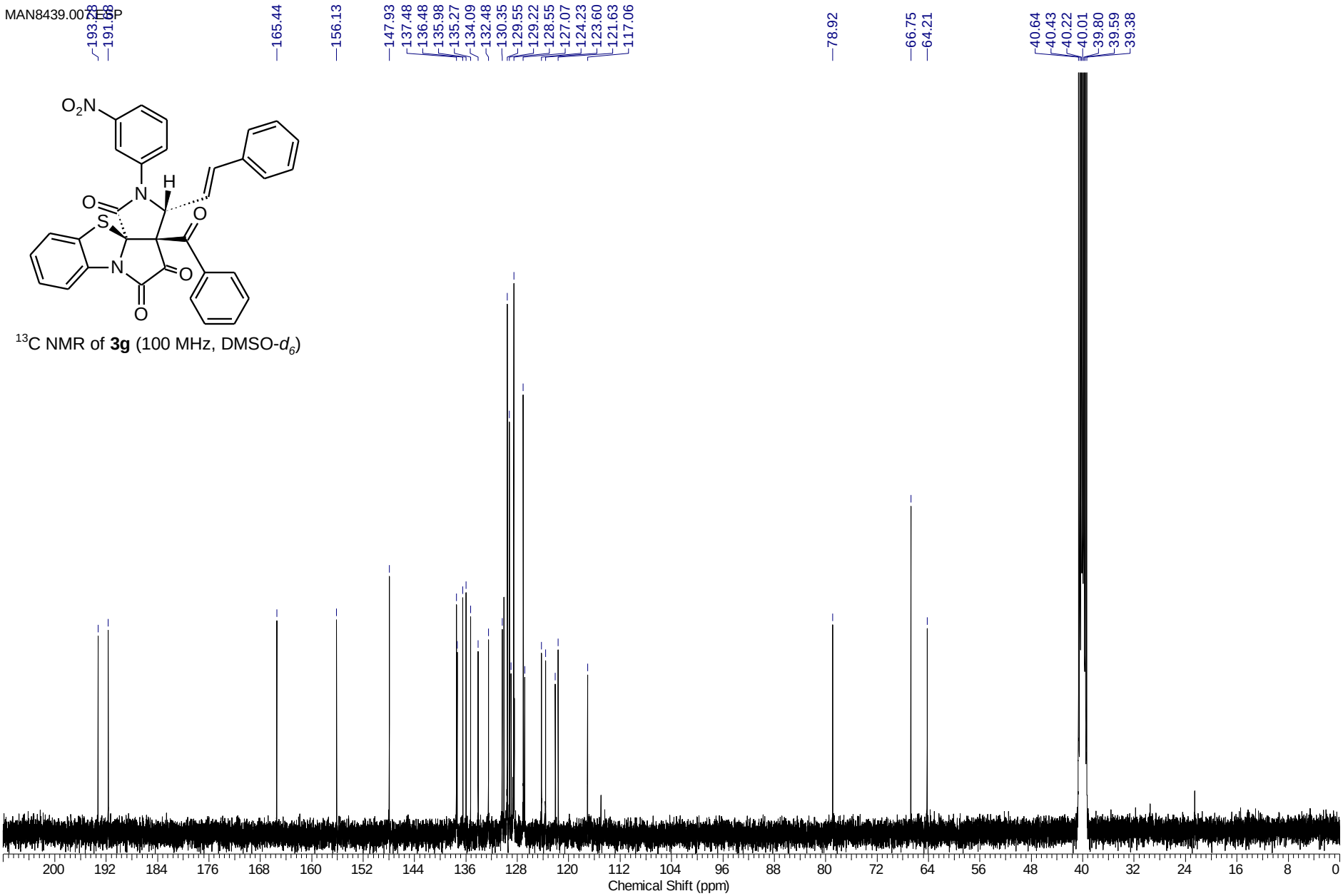


DEPT135 of **3f** (100 MHz, DMSO-d_6)

(solvate with toluene)



^{1}H NMR of **3g** (400 MHz, DMSO-d_6)



^{13}C NMR of **3g** (100 MHz, DMSO-d_6)

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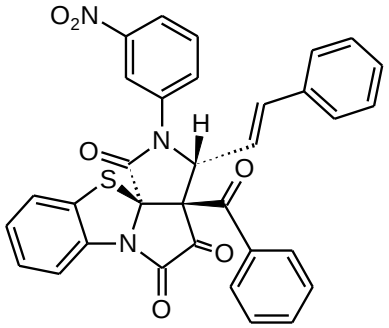

DEPT135 of **3g** (100 MHz, DMSO-d_6)

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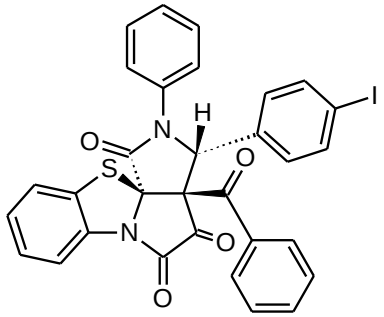
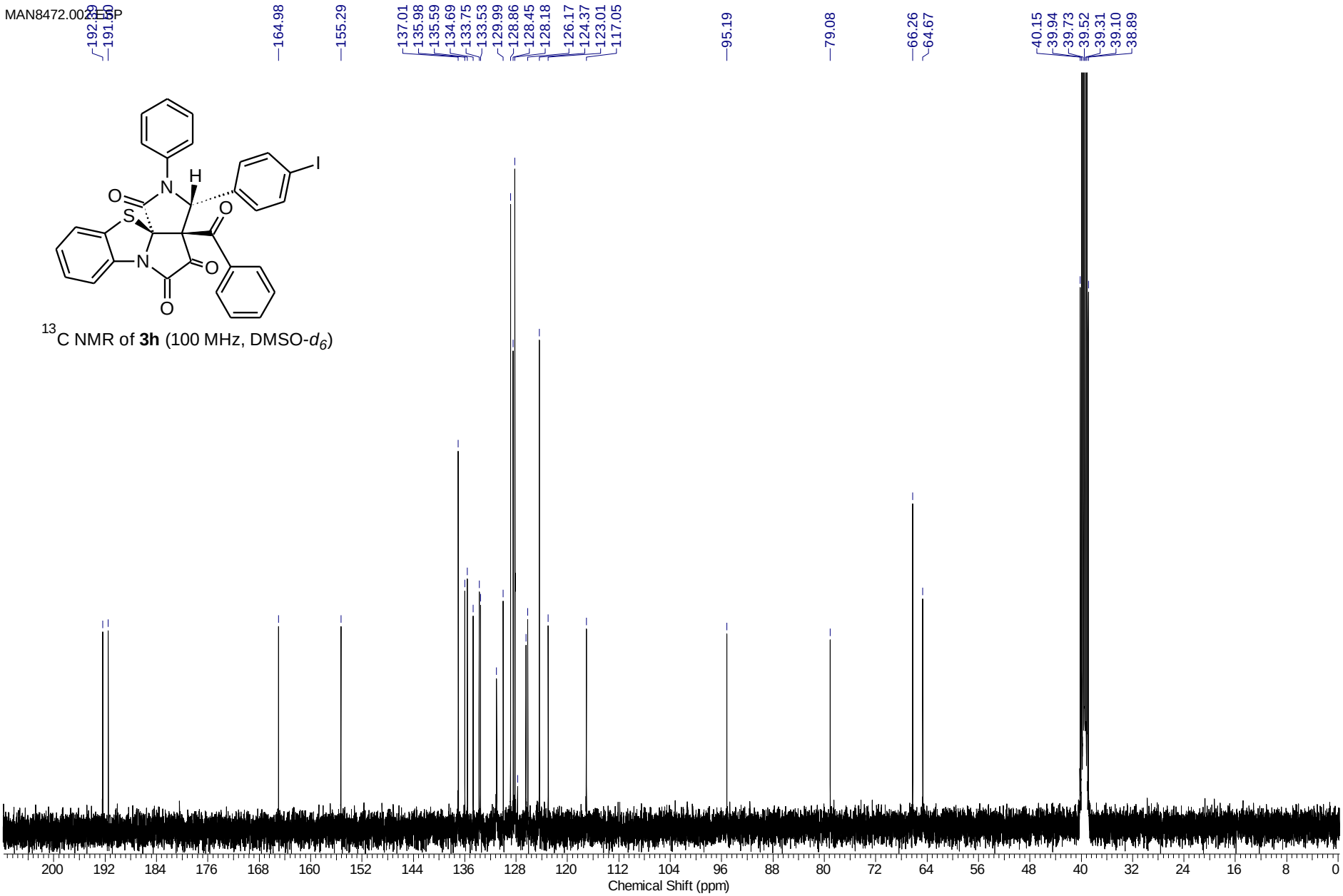


^{1}H NMR of **3h** (400 MHz, DMSO-d_6)



^{13}C NMR of **3h** (100 MHz, DMSO-d_6)

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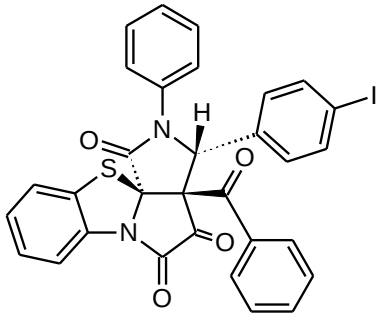
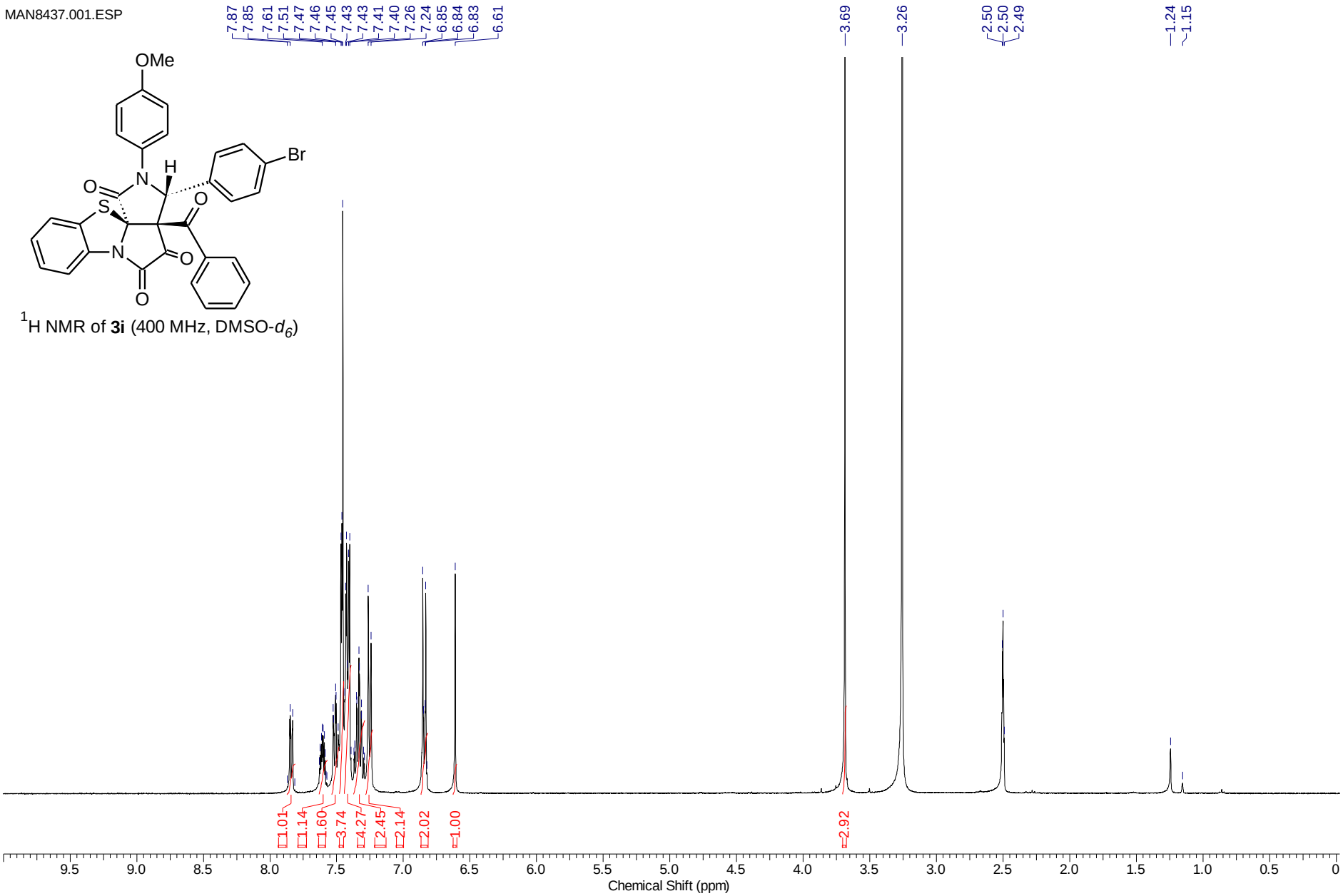
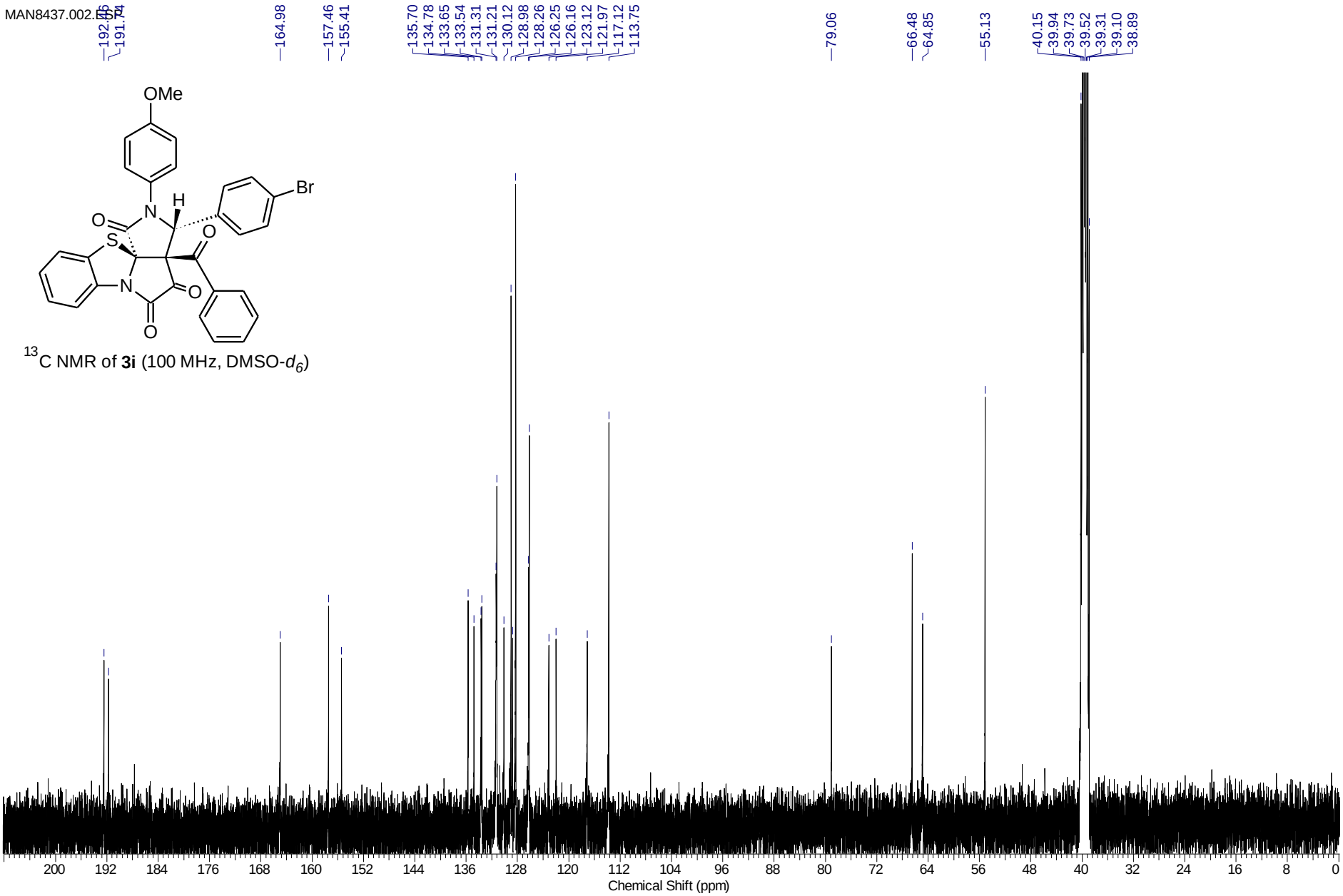


DEPT135 of **3h** (100 MHz, DMSO-d_6)

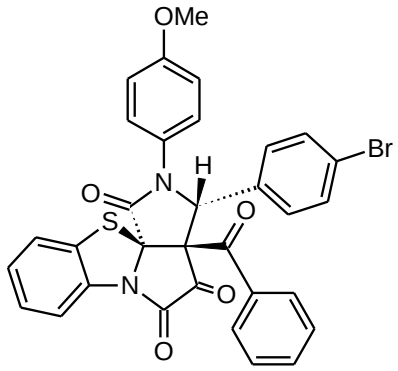


^{1}H NMR of **3i** (400 MHz, DMSO-d_6)

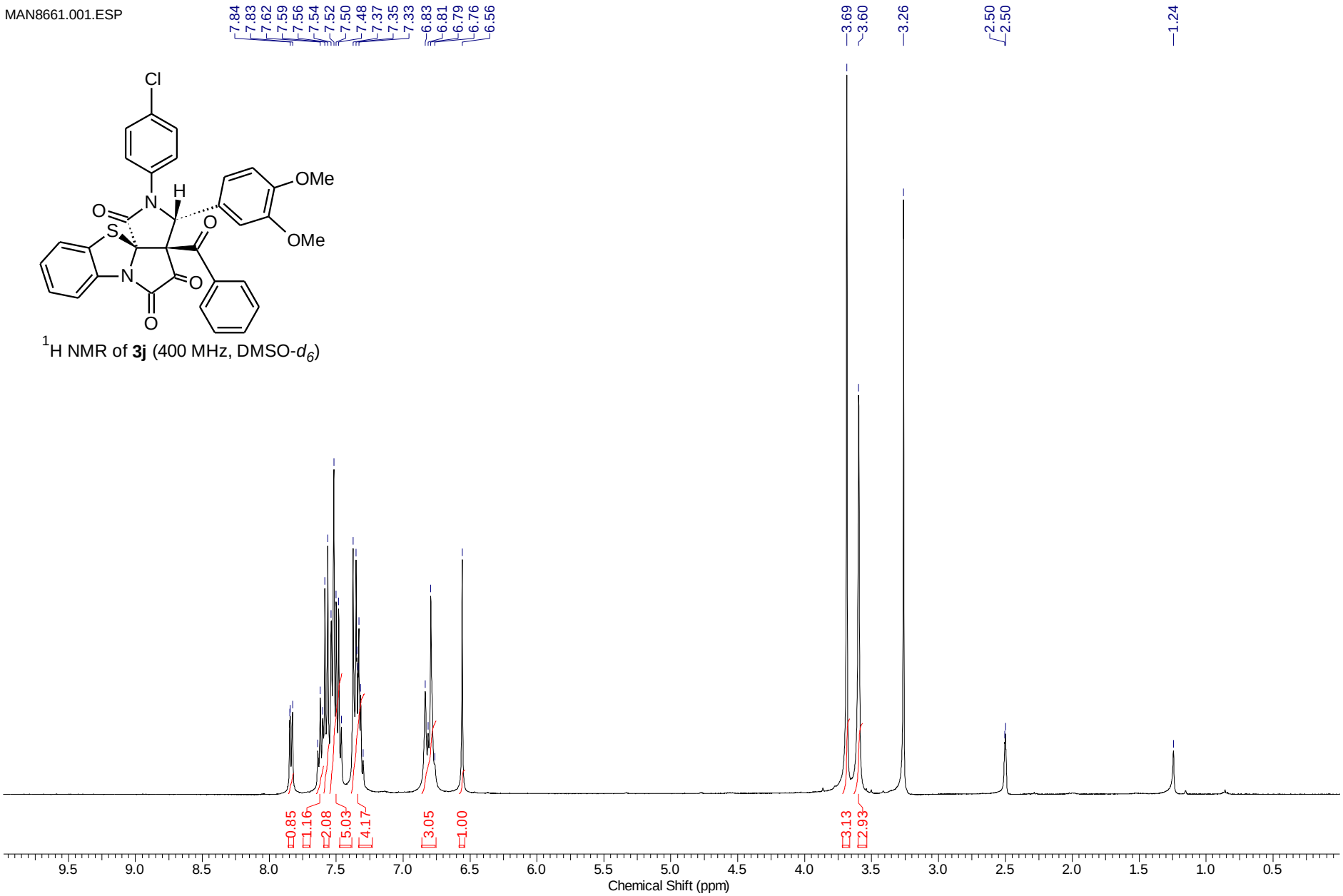


^{13}C NMR of **3i** (100 MHz, DMSO-d_6)

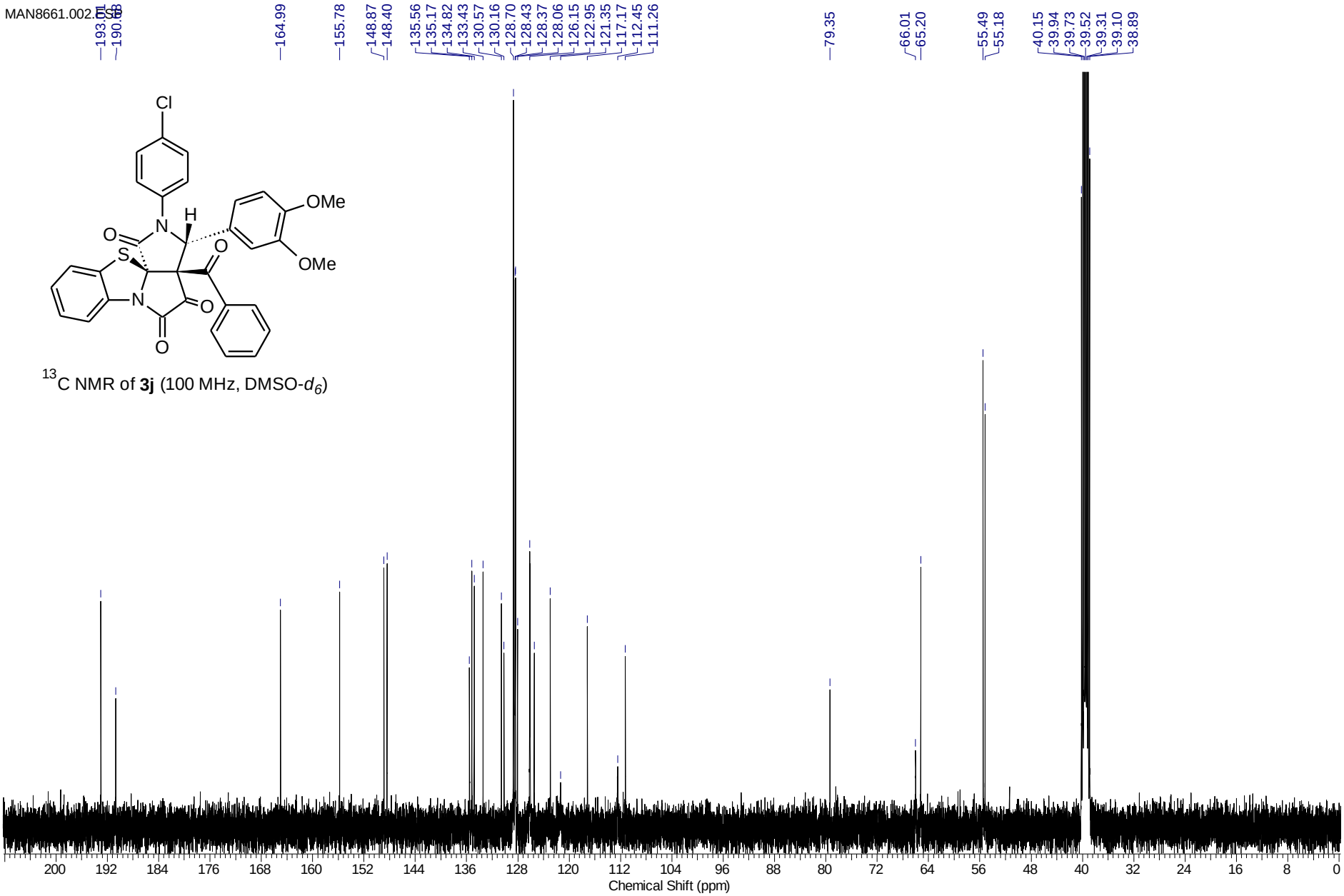
MAN8437.003.ESP



DEPT135 of **3i** (100 MHz, DMSO-d_6)



^{1}H NMR of **3j** (400 MHz, DMSO-d_6)



^{13}C NMR of **3j** (100 MHz, DMSO-d_6)

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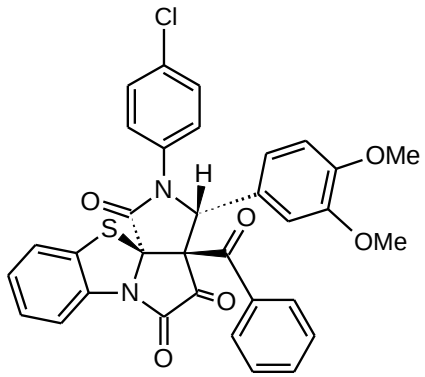
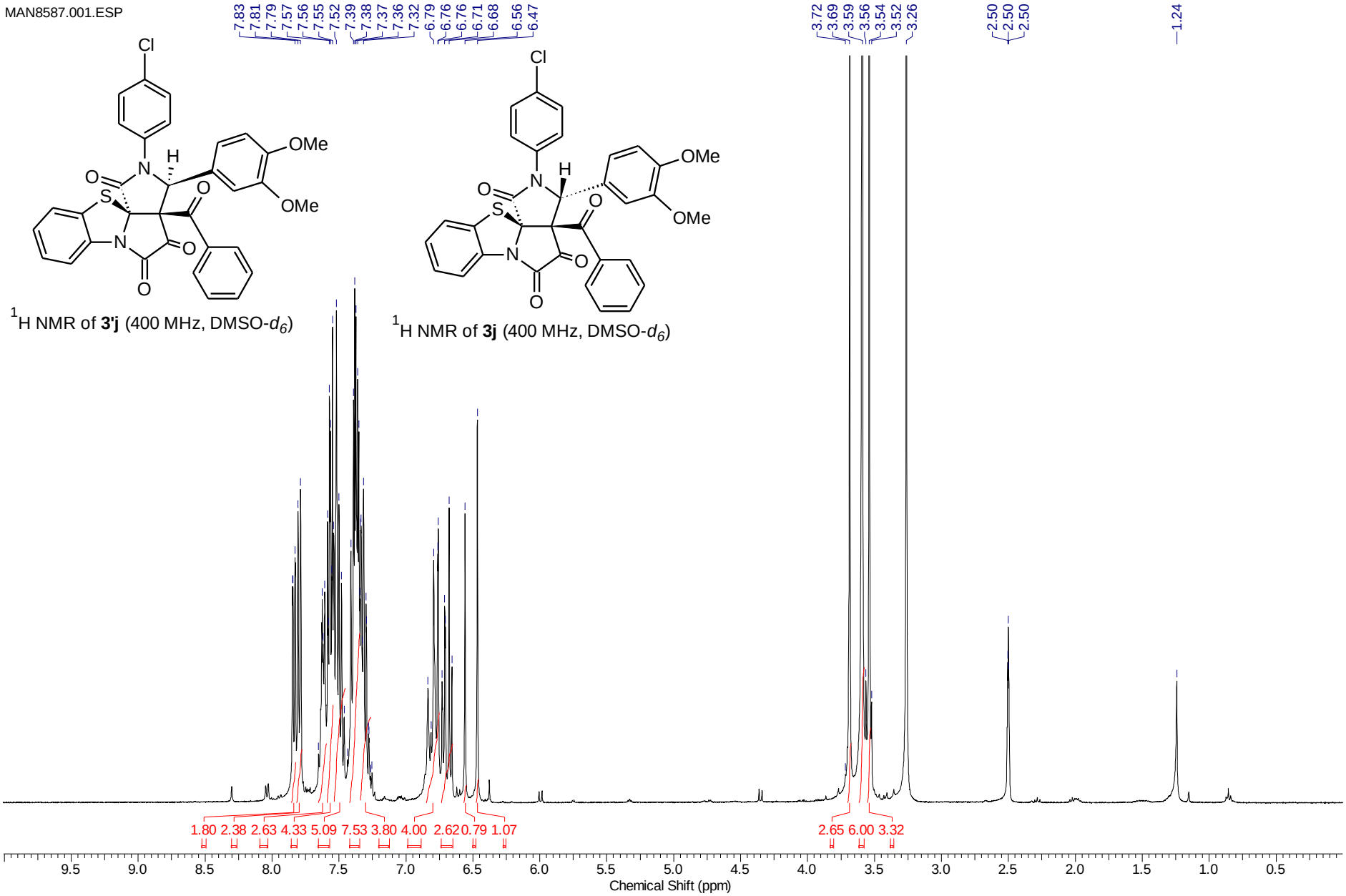


DEPT135 of **3j** (100 MHz, DMSO-d_6)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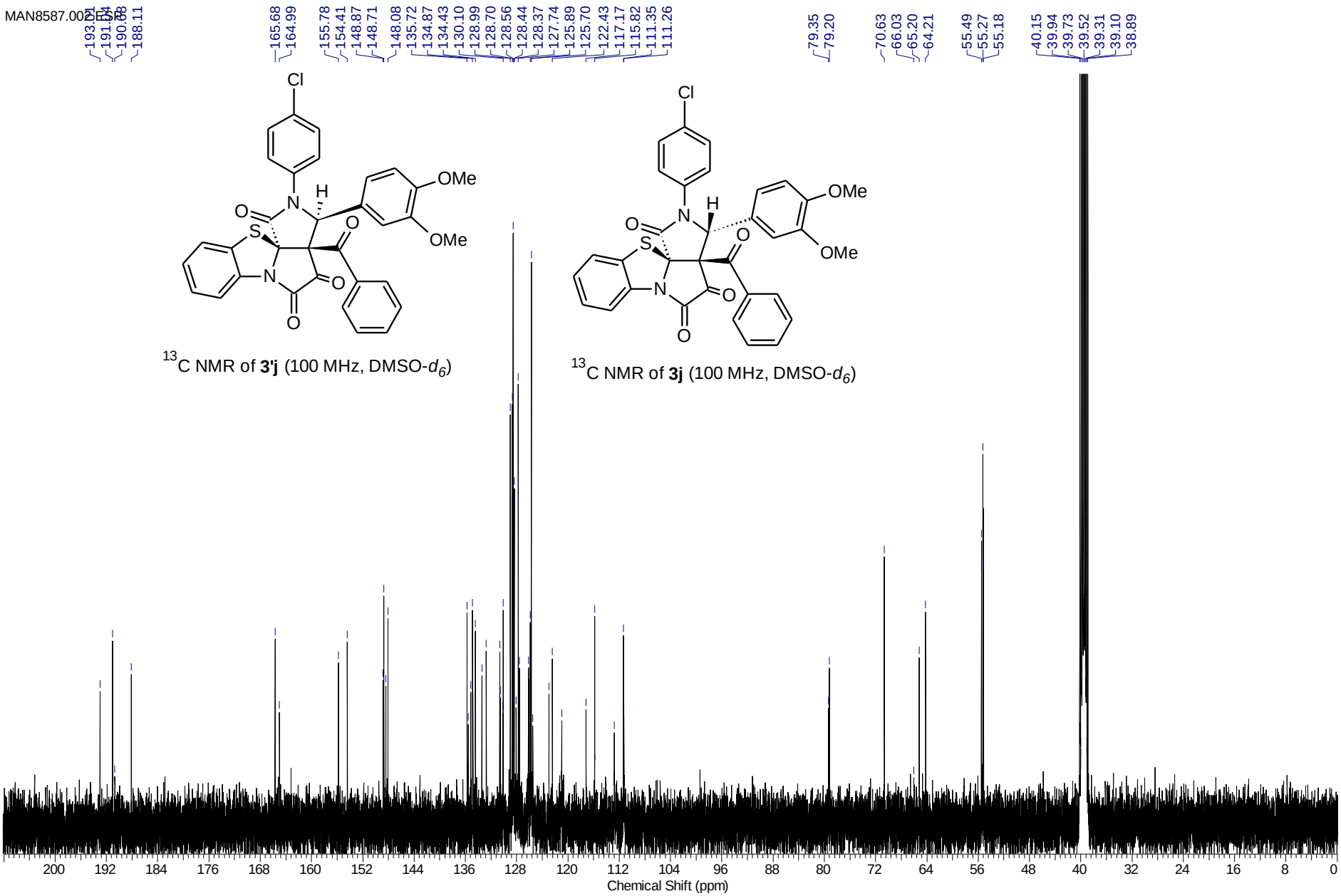
7.83 7.81 7.79 7.57 7.56 7.55 7.52 7.39 7.38 7.37 7.36 7.32 6.79 6.76 6.76 6.71 6.68 6.56 6.47
3.72 3.69 3.59 3.56 3.54 3.52 3.26
2.50 2.50 2.50
1.24
Cl
OMe
OMe
H
N
O
S
O
O
O
O
1H NMR of 3'j (400 MHz, DMSO-d6)
1H NMR of 3j (400 MHz, DMSO-d6)
1.80 2.38 2.63 4.33 5.09 7.53 3.80 4.00 2.62 0.79 1.07
2.65 6.00 3.32
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
Chemical Shift (ppm)



^{13}C NMR of **3'j** (100 MHz, DMSO-d_6)

^{13}C NMR of **3j** (100 MHz, DMSO-d_6)

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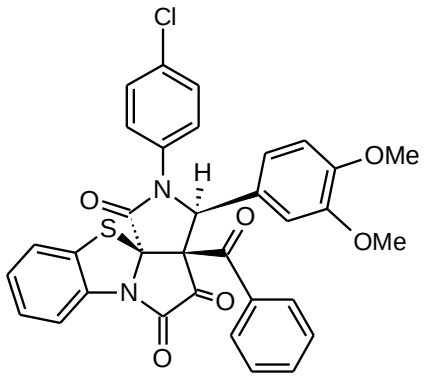
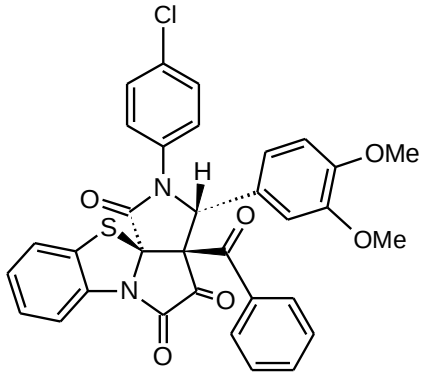


DEPT135 of **3'j** (100 MHz, DMSO-d_6)

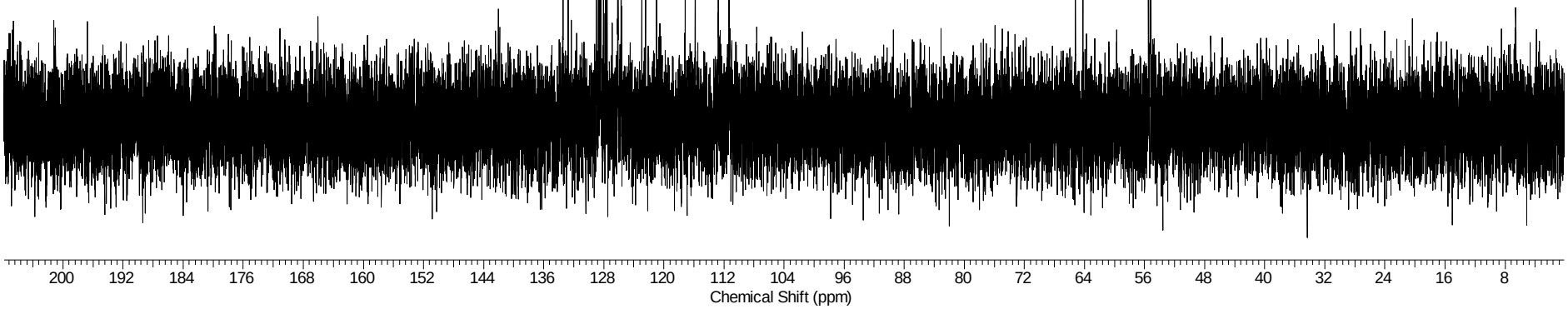


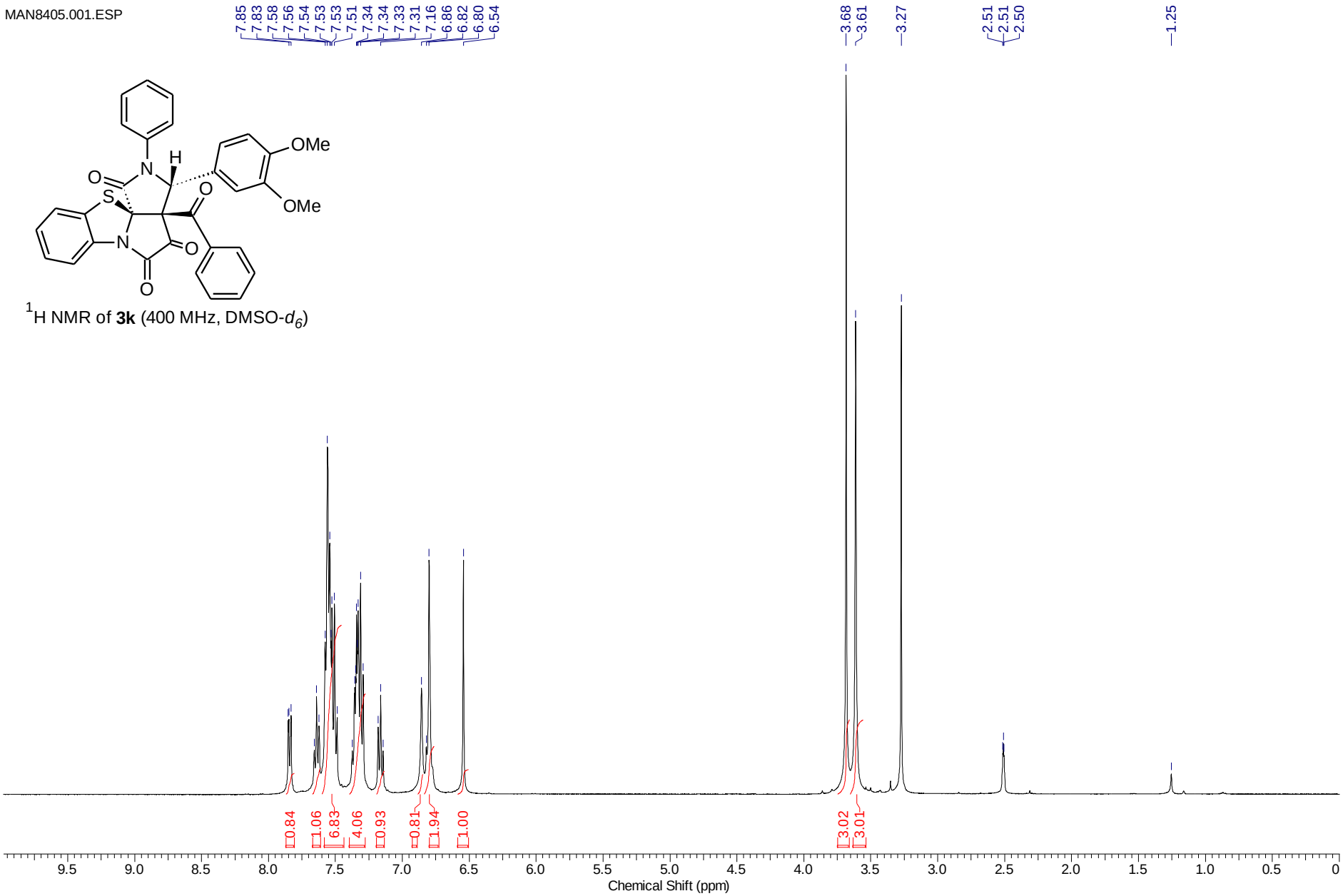
DEPT135 of **3j** (100 MHz, DMSO-d_6)

133.43
132.73
128.99
128.69
128.56
128.37
128.06
127.73
127.56
126.09
125.70
122.42
117.17
115.82
112.76
111.35
111.25

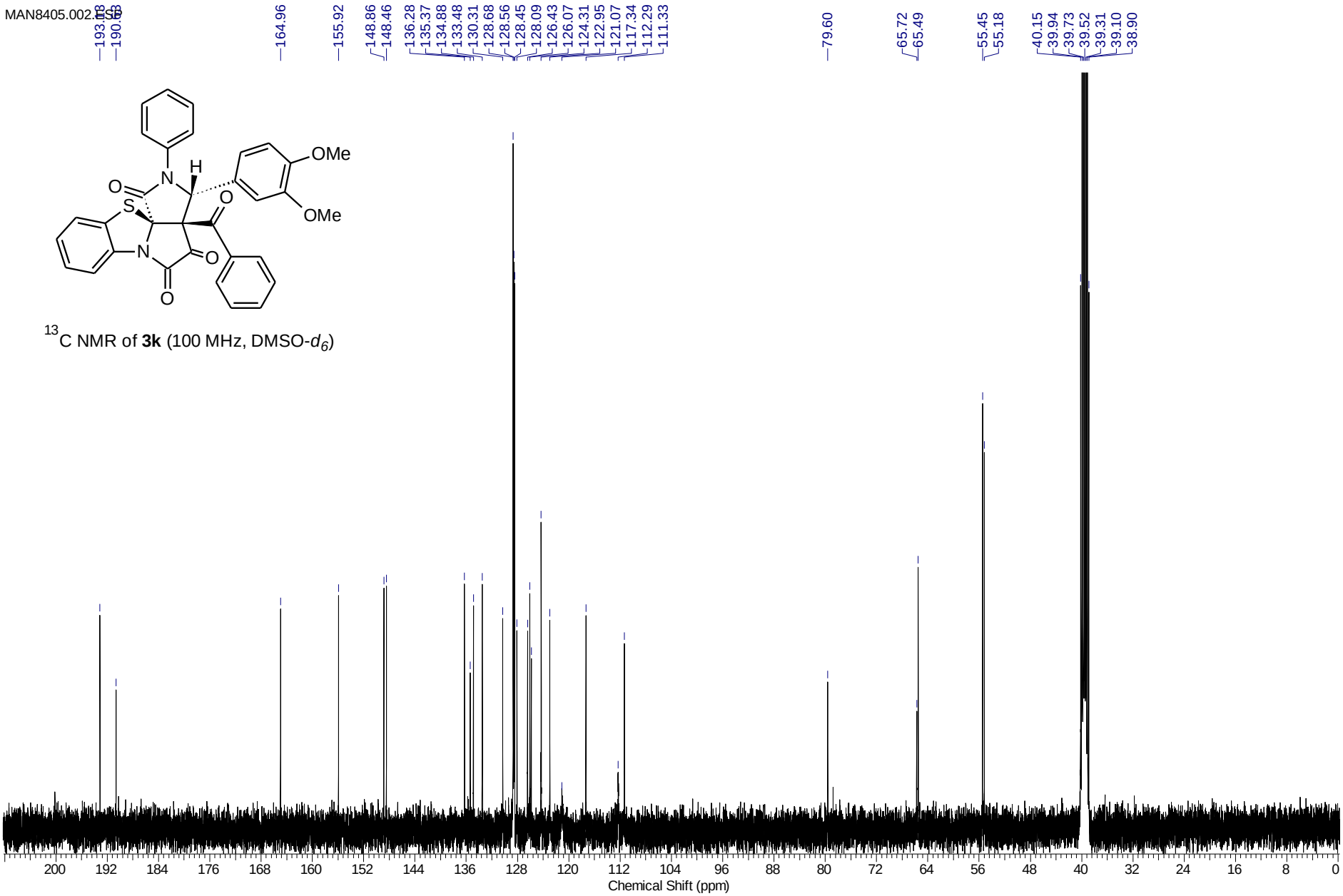
65.20
64.20

55.49
55.27
55.18





^{1}H NMR of **3k** (400 MHz, DMSO-d_6)



^{13}C NMR of **3k** (100 MHz, DMSO-d_6)

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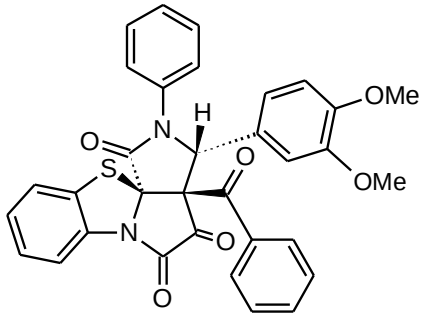

DEPT135 of **3k** (100 MHz, DMSO-d_6)

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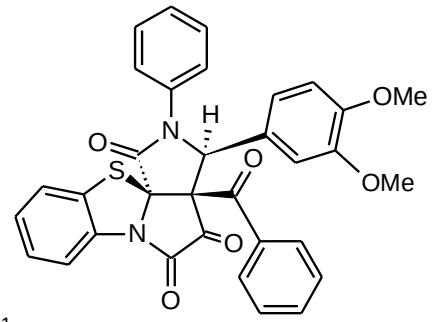
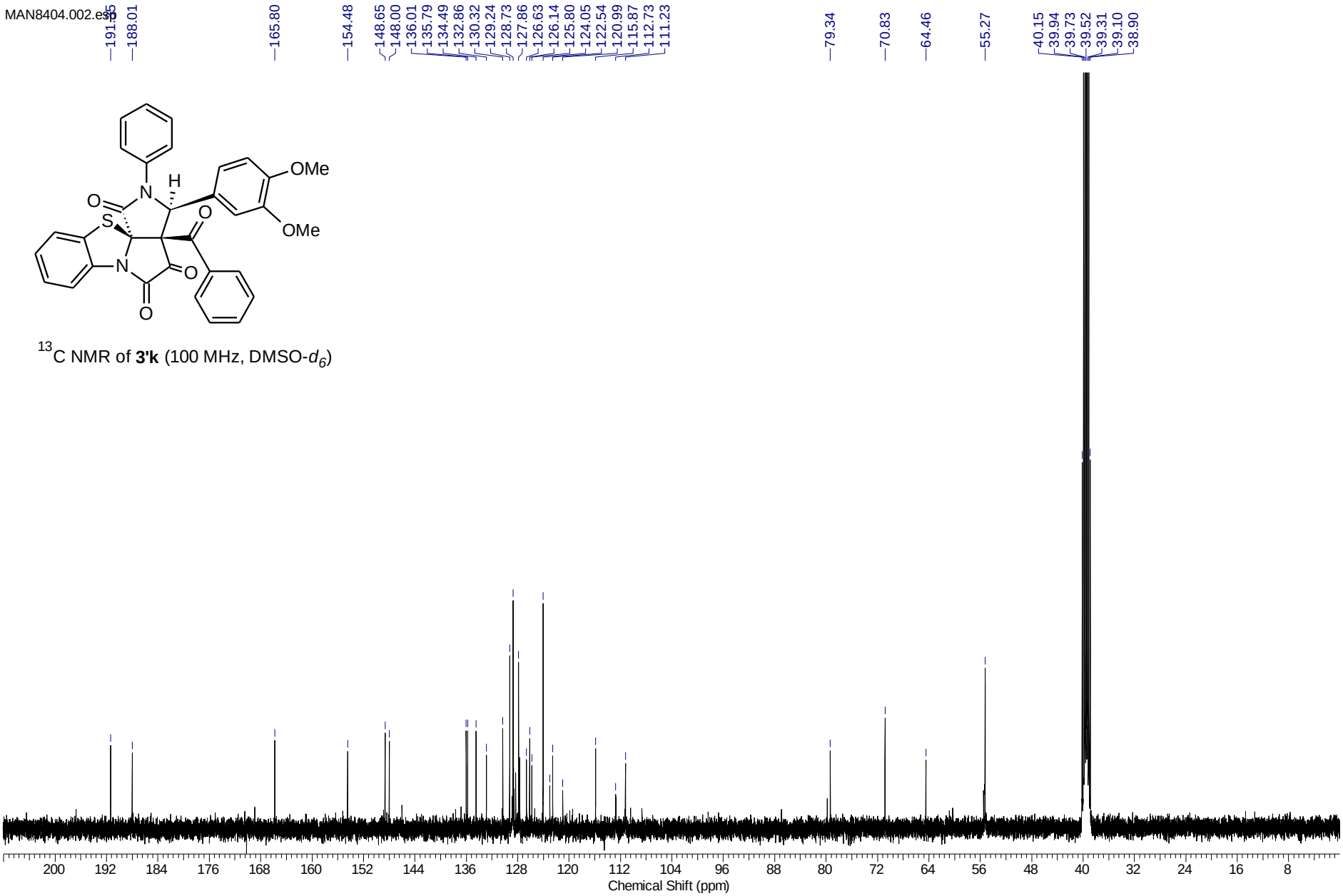


^{1}H NMR of **3'k** (400 MHz, DMSO-d_6)



^{13}C NMR of **3'k** (100 MHz, DMSO-d_6)

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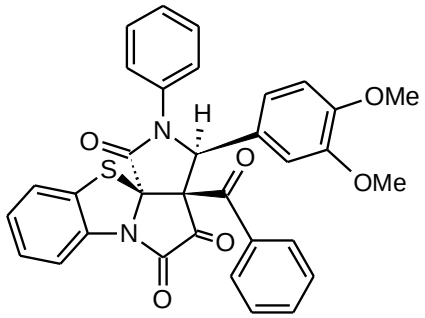
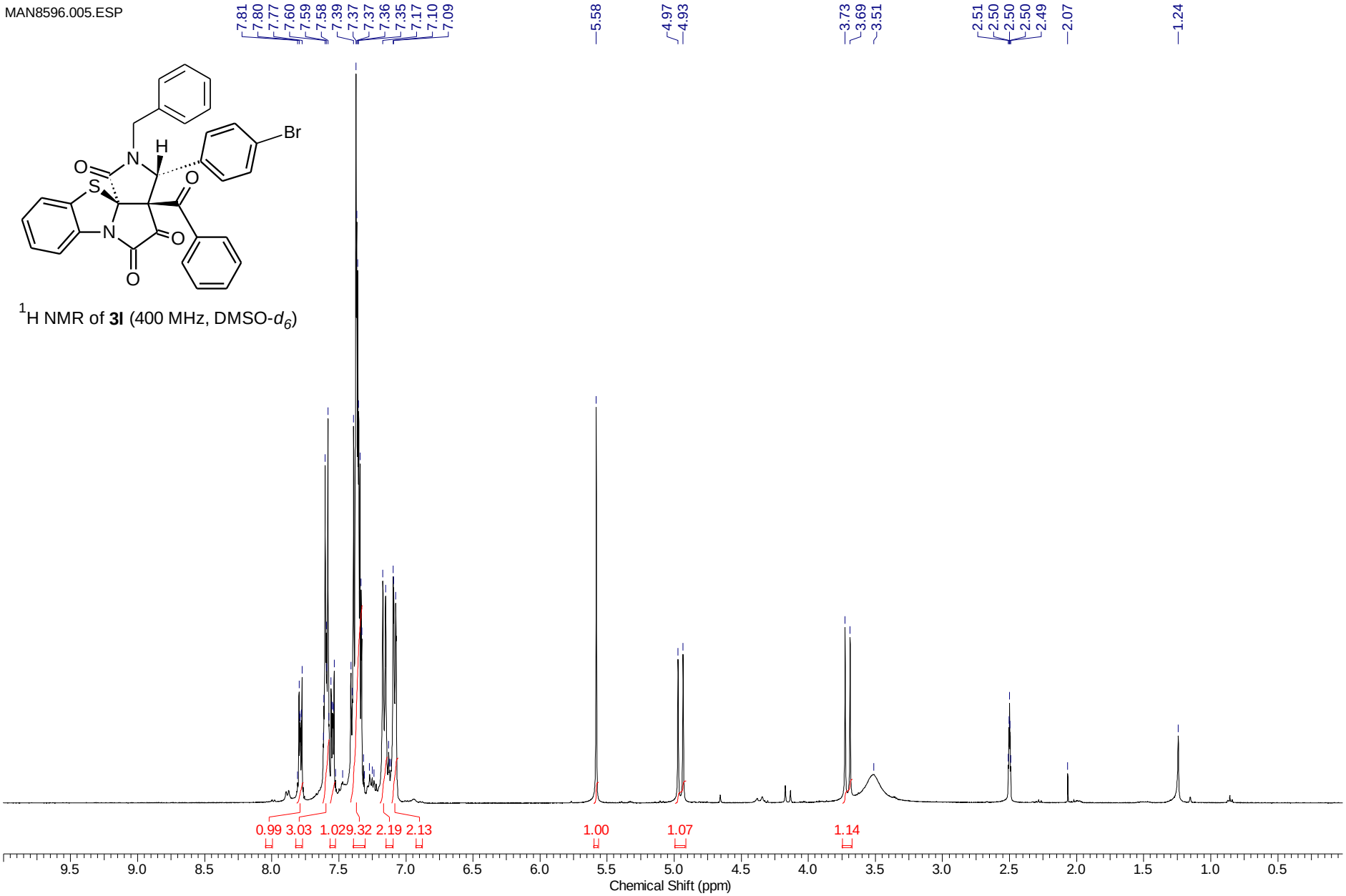
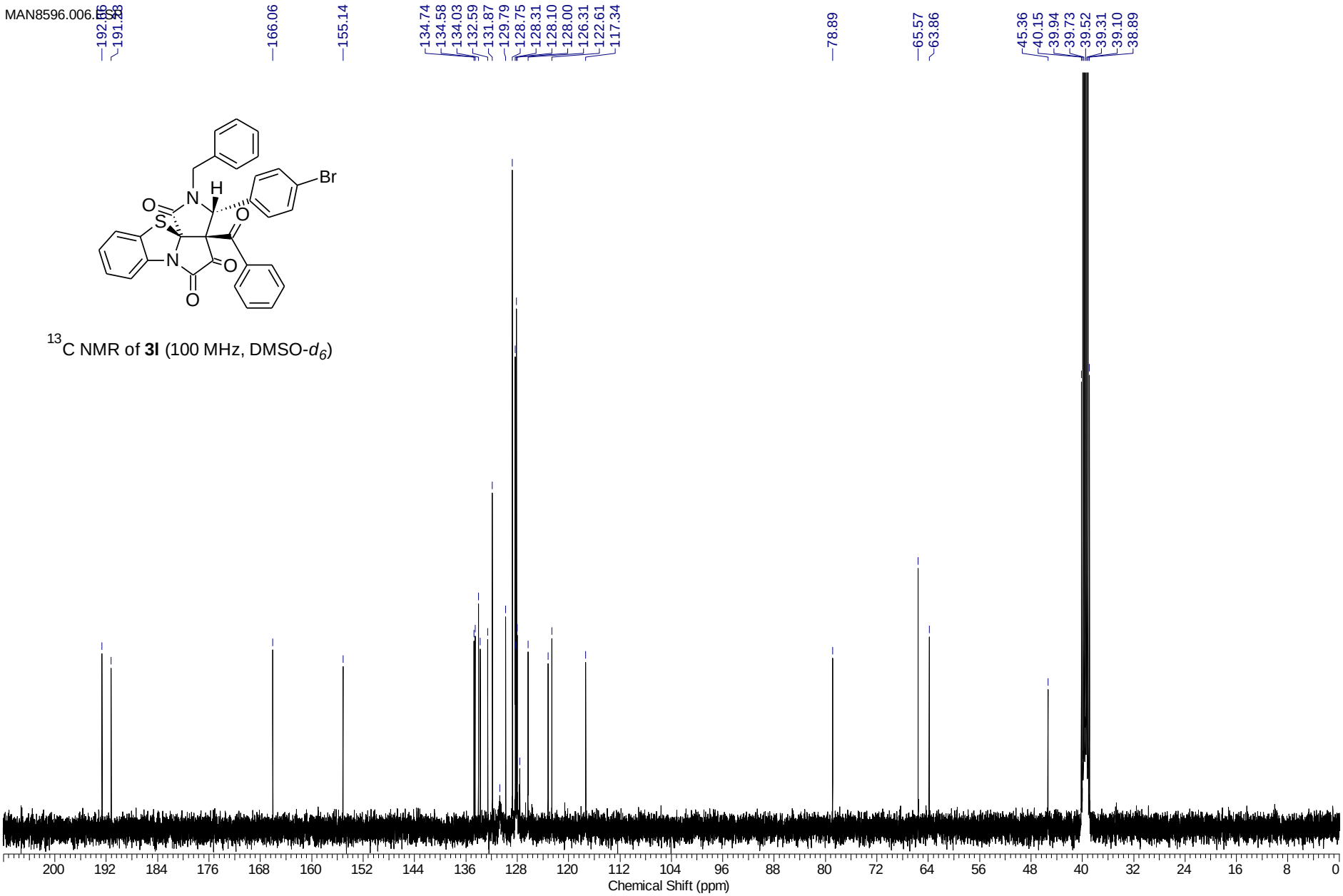


DEPT135 of **3k** (100 MHz, DMSO-d_6)



^{1}H NMR of **3l** (400 MHz, DMSO-d_6)



^{13}C NMR of **3l** (100 MHz, DMSO-d_6)

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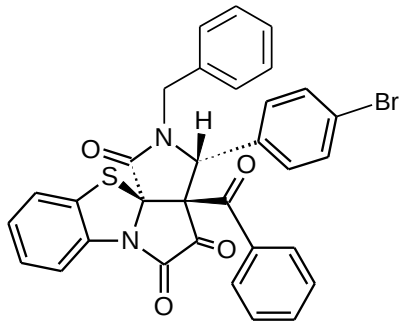
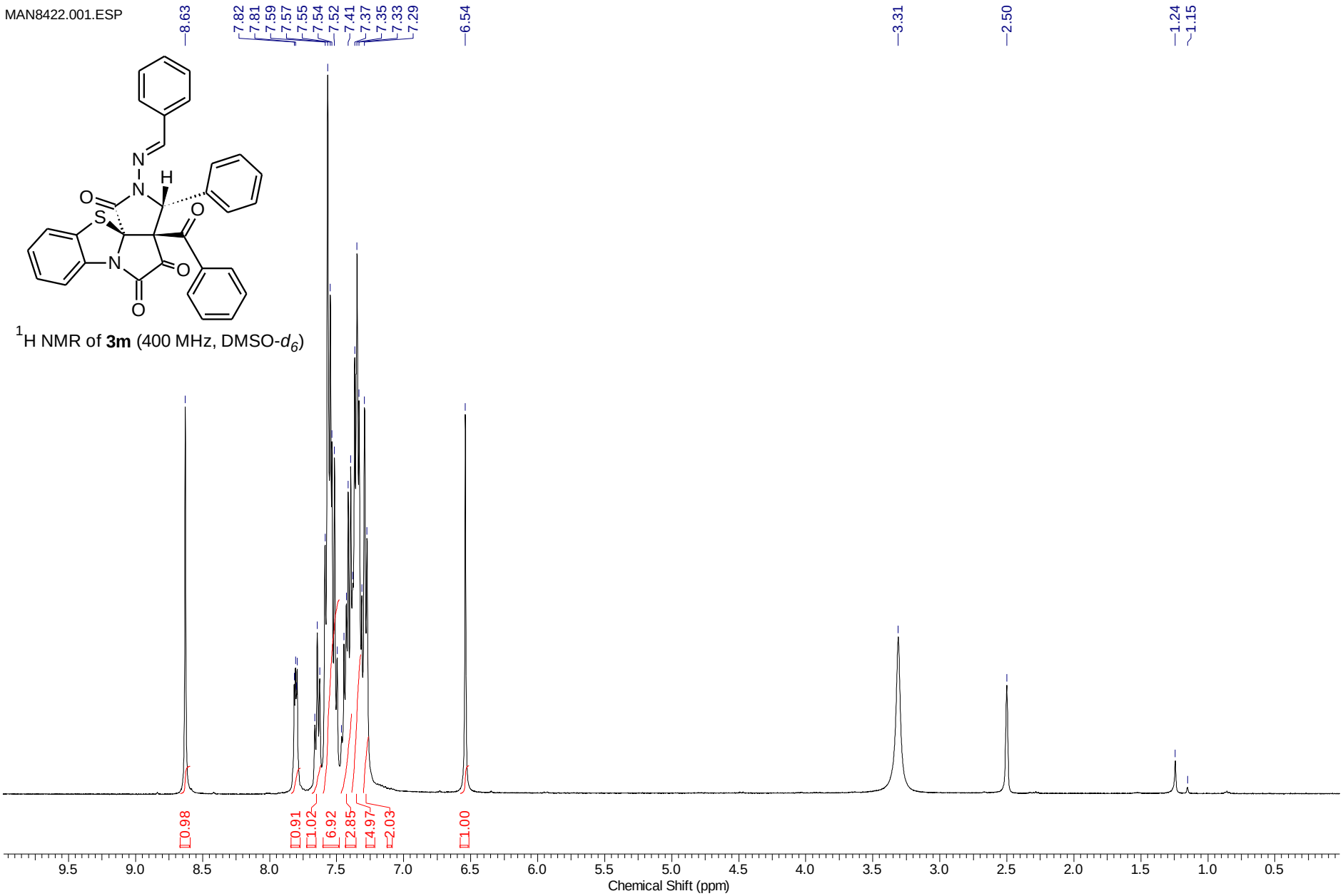
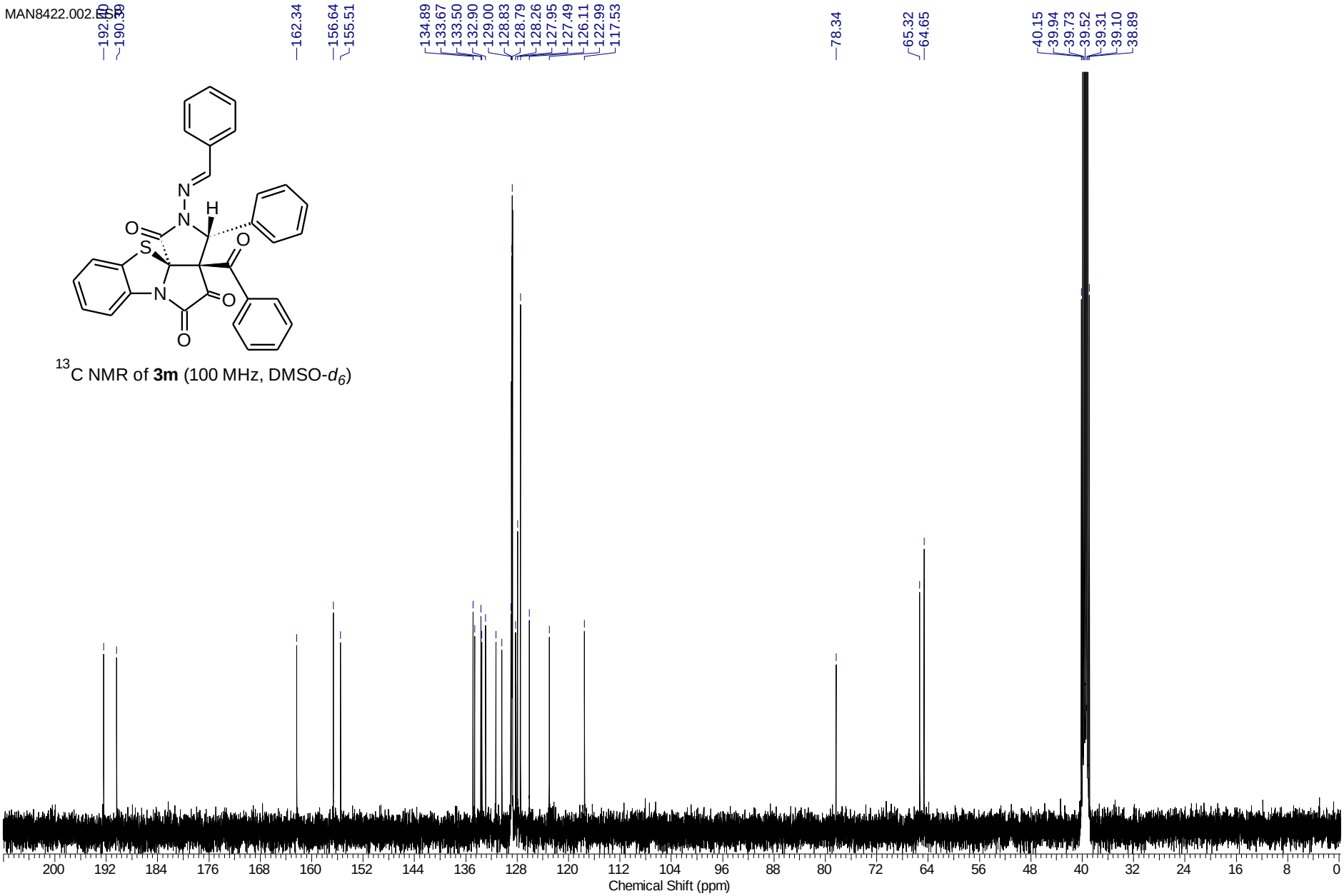


DEPT135 of **3l** (100 MHz, DMSO-d_6)

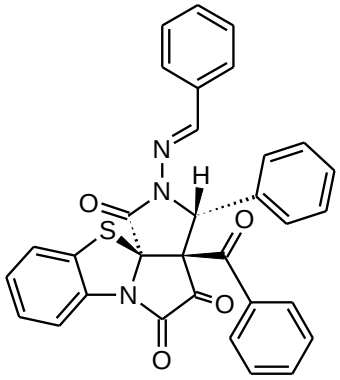


^{1}H NMR of **3m** (400 MHz, DMSO-d_6)



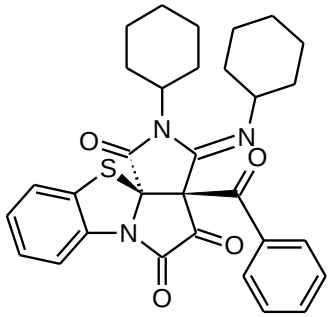
^{13}C NMR of **3m** (100 MHz, DMSO-d_6)

MAN8422.003.ESP



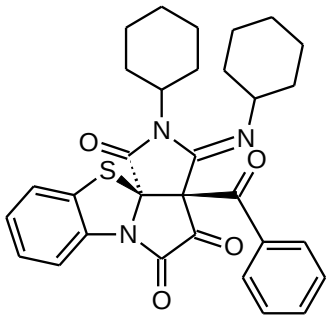
DEPT135 of **3m** (100 MHz, DMSO-d_6)

MAN7116.004.ESP



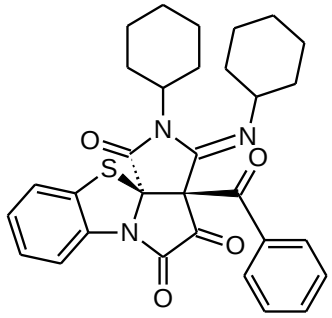
^{1}H NMR of **8a** (400 MHz, $CDCl_3$)

MAN7116.002.ESP



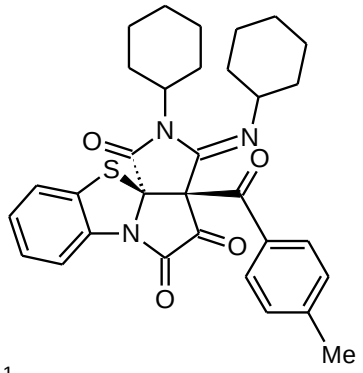
^{13}C NMR of **8a** (100 MHz, $CDCl_3$)

MAN7116.003.ESP

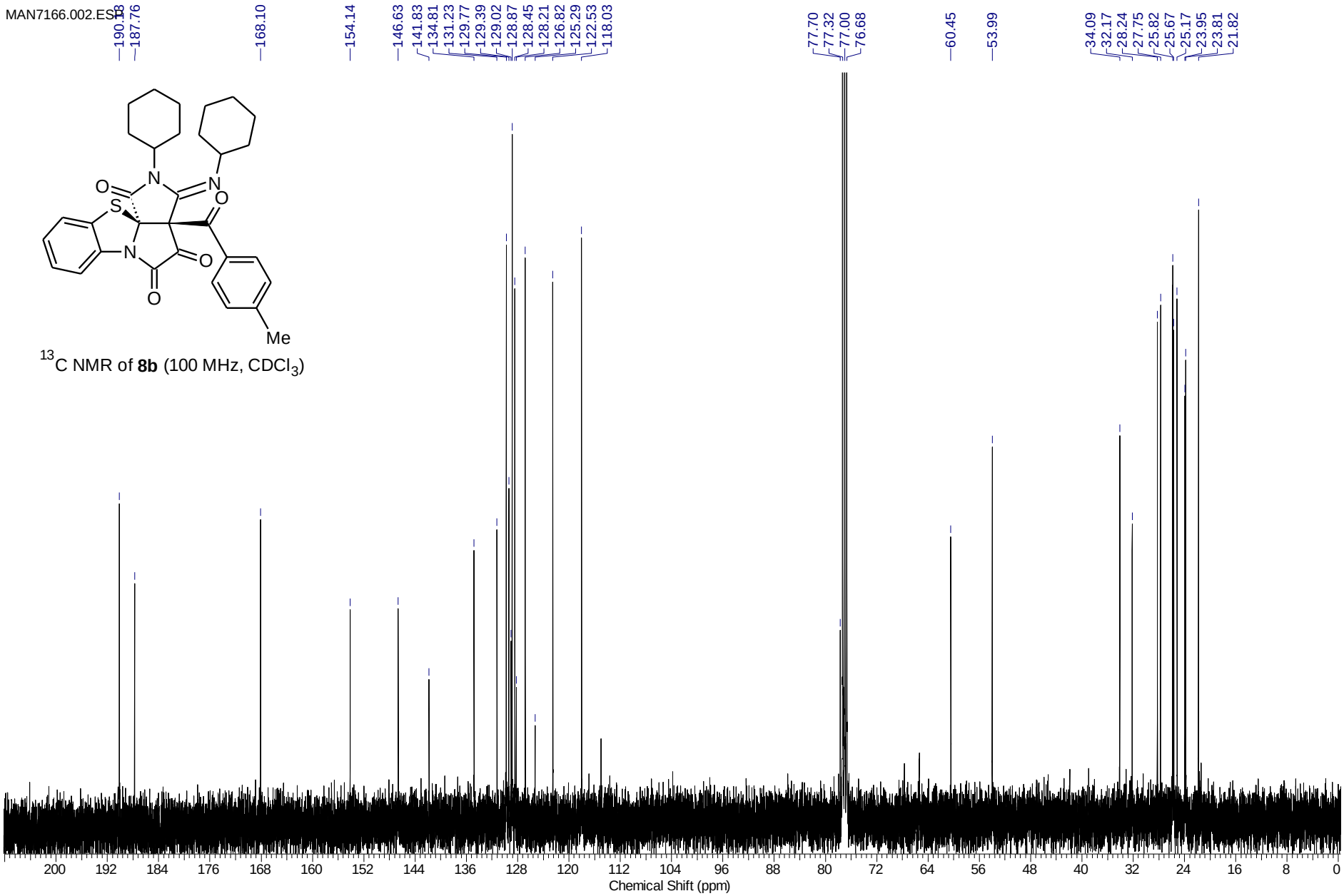


^{13}C NMR of **8a** (100 MHz, $CDCl_3$)

MAN7166.004.ESP

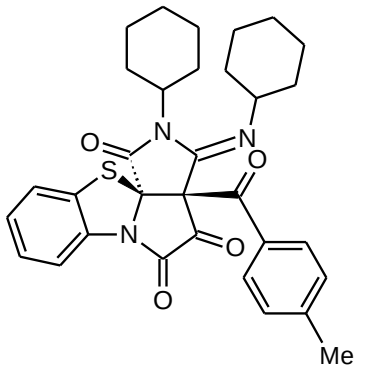


^{1}H NMR of **8b** (400 MHz, $CDCl_3$)



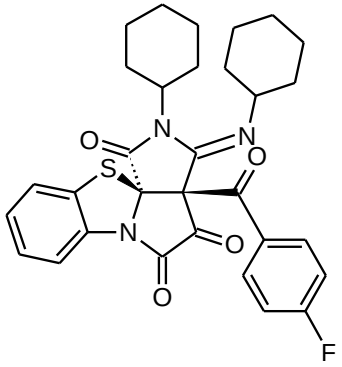
^{13}C NMR of **8b** (100 MHz, $CDCl_3$)

MAN7166.003.ESP



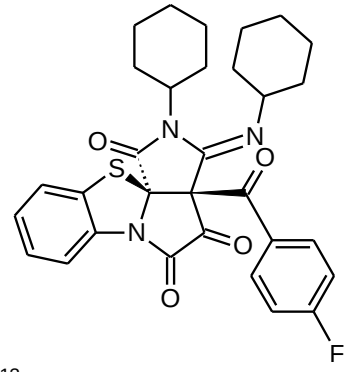
DEPT135 of **8b** (100 MHz, $CDCl_3$)

MAN8476.001.ESP



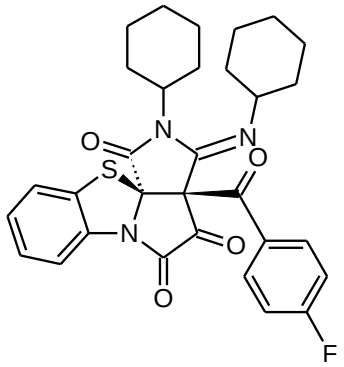
^{1}H NMR of **8c** (400 MHz, $CDCl_3$)

MAN8476.002.ESP



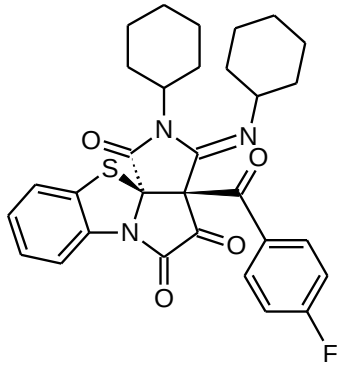
^{13}C NMR of **8c** (100 MHz, $CDCl_3$)

MAN8476.003.ESP



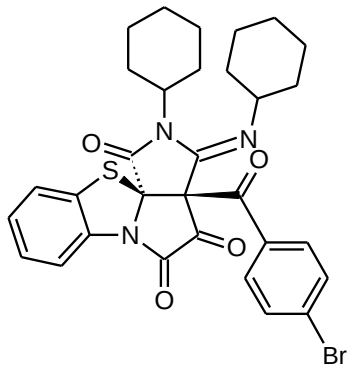
DEPT135 of **8c** (100 MHz, $CDCl_3$)

MAN8476.004.ESP

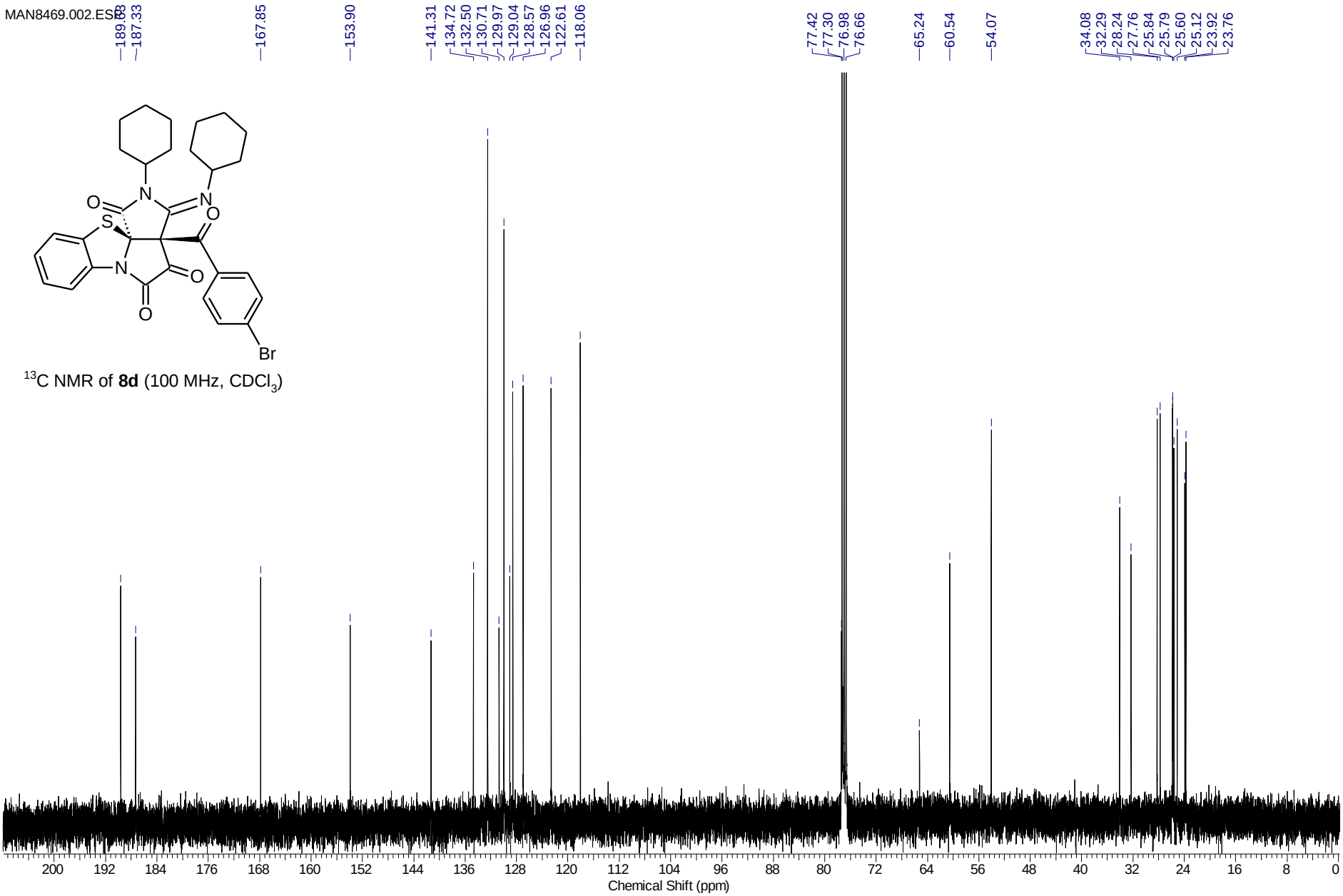


^{19}F NMR of **8c** (376 MHz, $CDCl_3$)

MAN8469.001.ESP

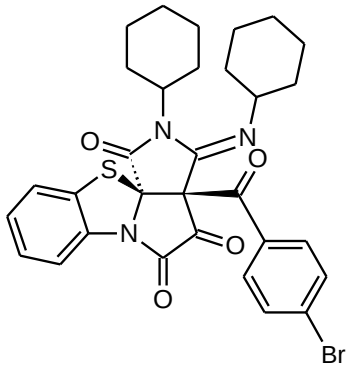


^{1}H NMR of **8d** (400 MHz, $CDCl_3$)



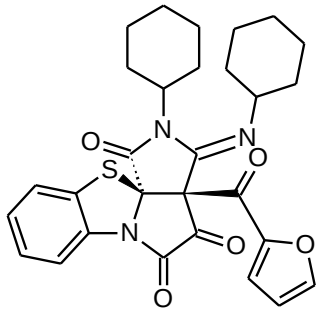
^{13}C NMR of **8d** (100 MHz, $CDCl_3$)

MAN8469.003.ESP

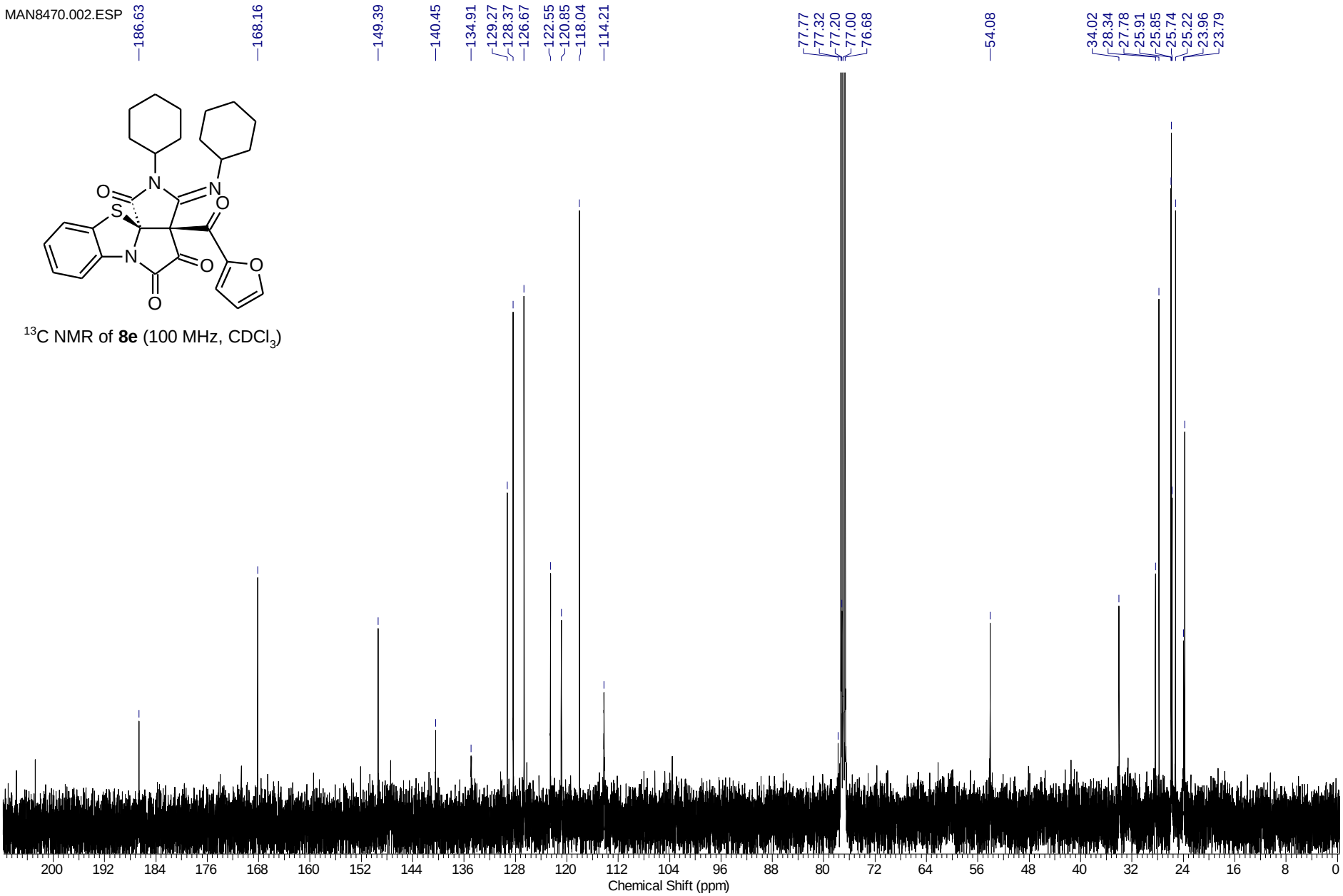


DEPT135 of **8d** (100 MHz, $CDCl_3$)

MAN8470.001.ESP

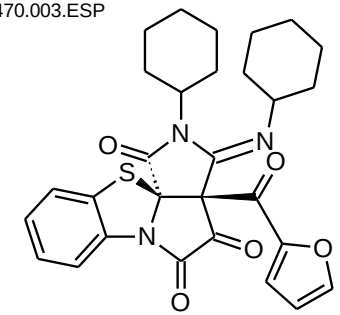


^{1}H NMR of **8e** (400 MHz, $CDCl_3$)



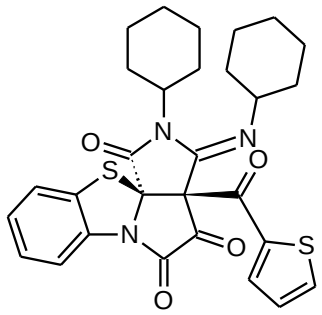
^{13}C NMR of **8e** (100 MHz, $CDCl_3$)

MAN8470.003.ESP



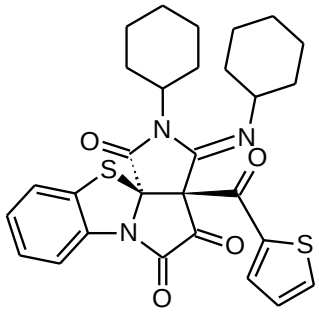
DEPT135 of **8e** (100 MHz, $CDCl_3$)

MAN8471.001.ESP



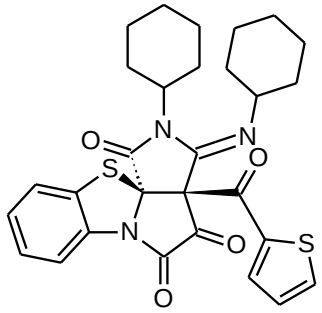
^{1}H NMR of **8f** (400 MHz, $CDCl_3$)

MAN8471.002.ESP



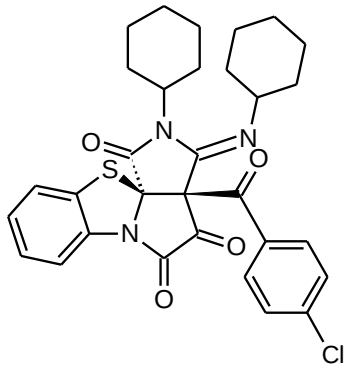
^{13}C NMR of **8f** (100 MHz, $CDCl_3$)

MAN8471.003.ESP

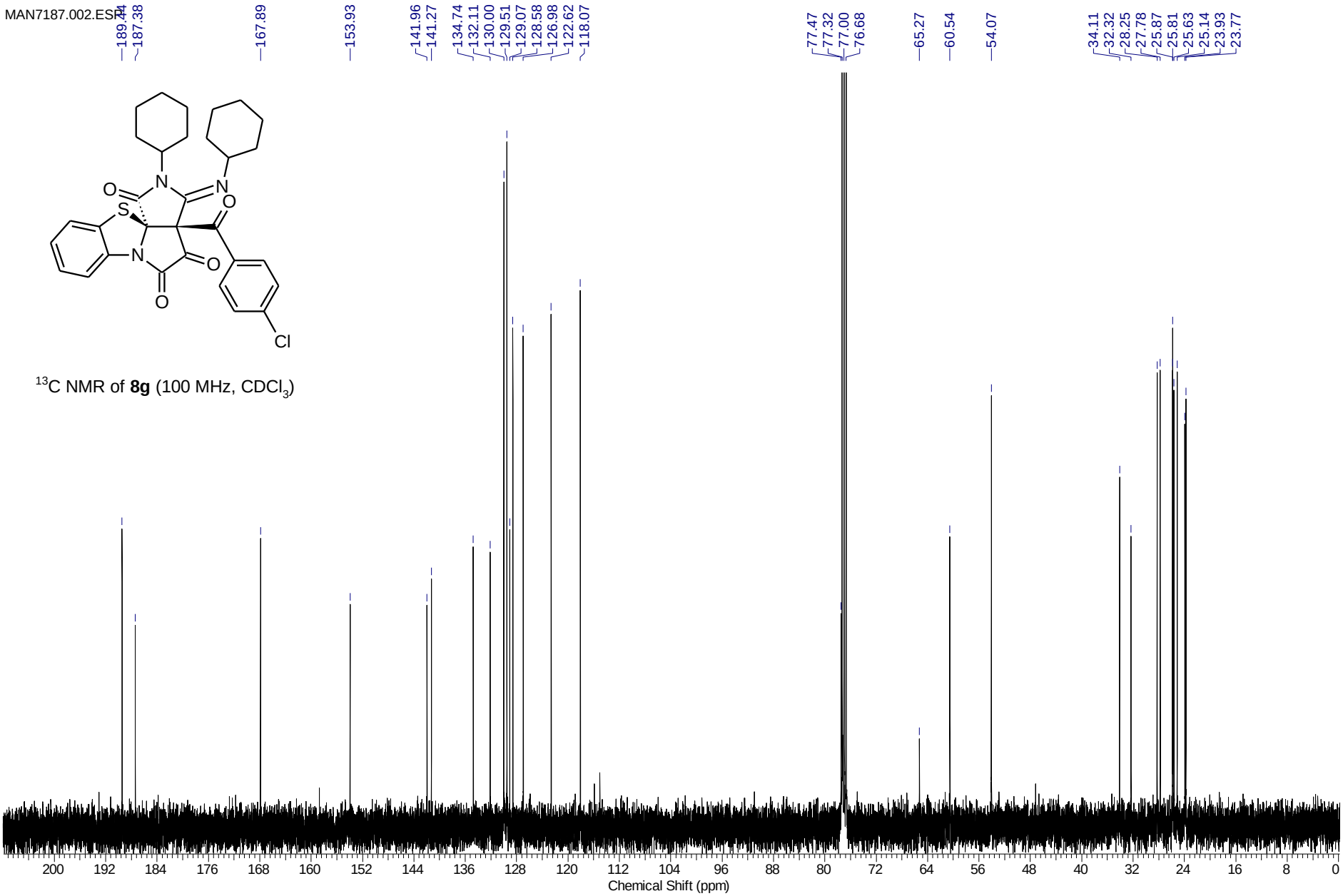


DEPT135 of **8f** (100 MHz, $CDCl_3$)

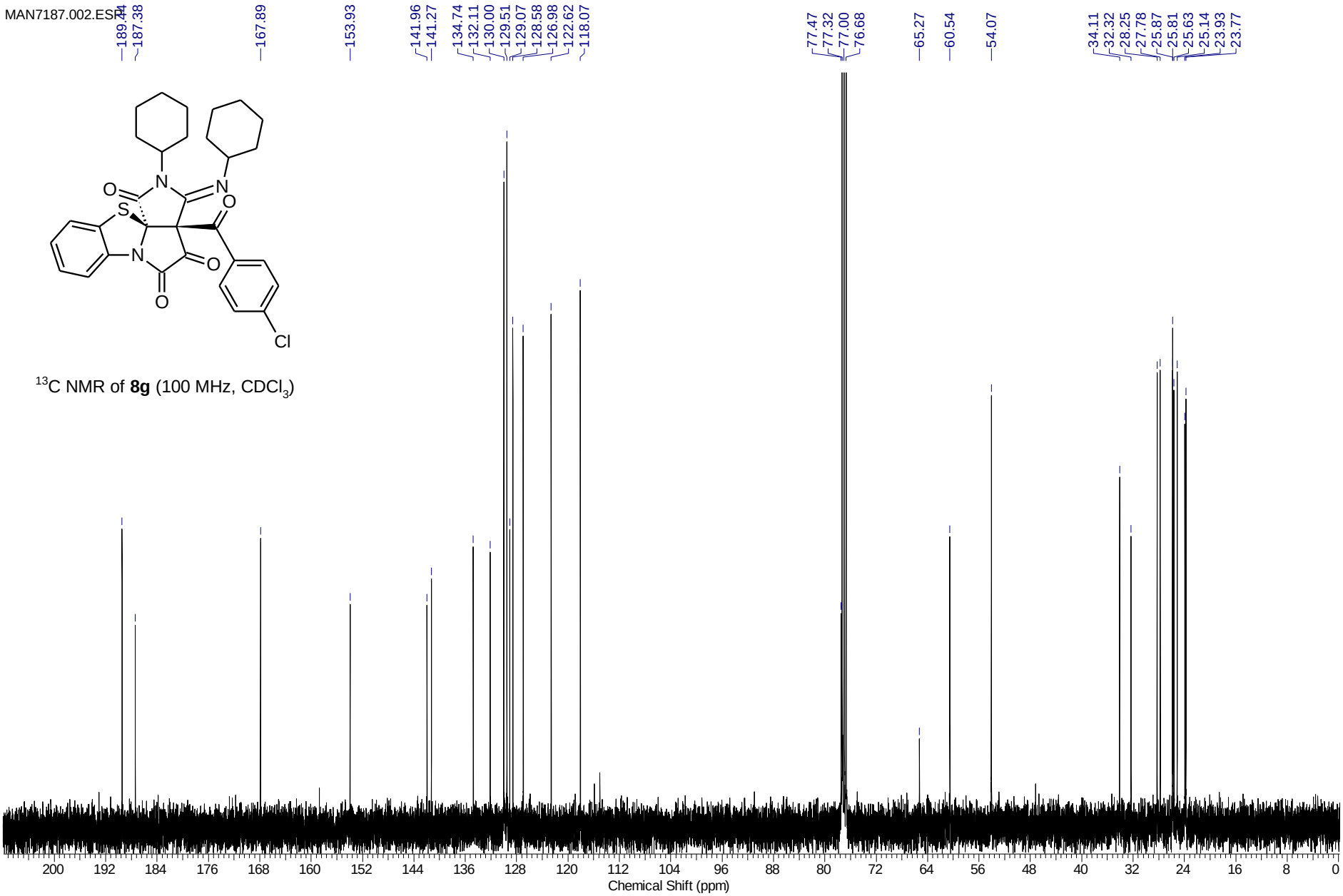
MAN7187.001.ESP



^{1}H NMR of **8g** (400 MHz, $CDCl_3$)

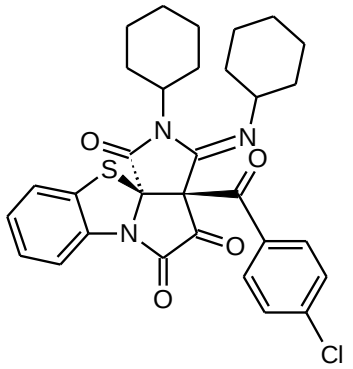


^{13}C NMR of **8g** (100 MHz, $CDCl_3$)

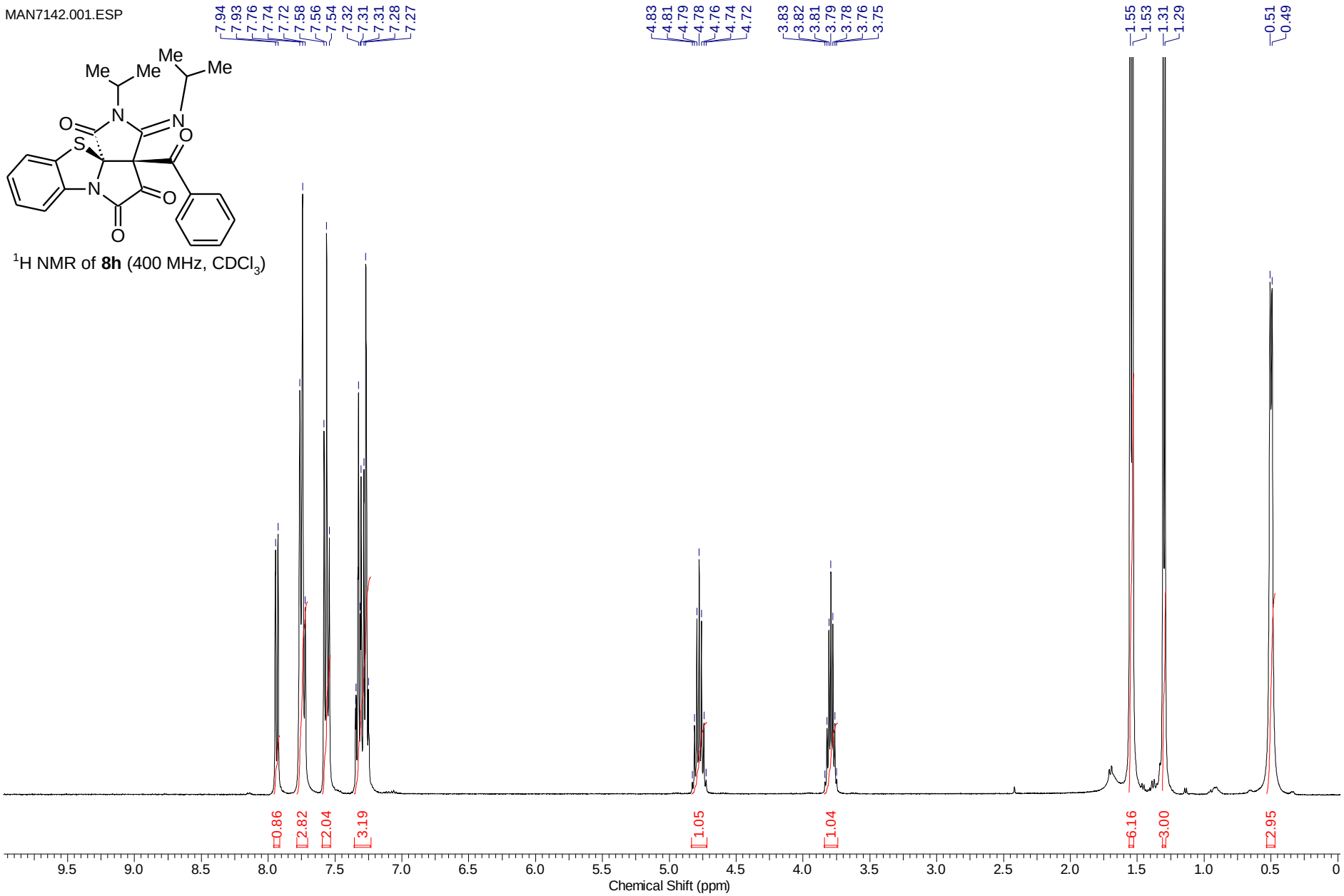


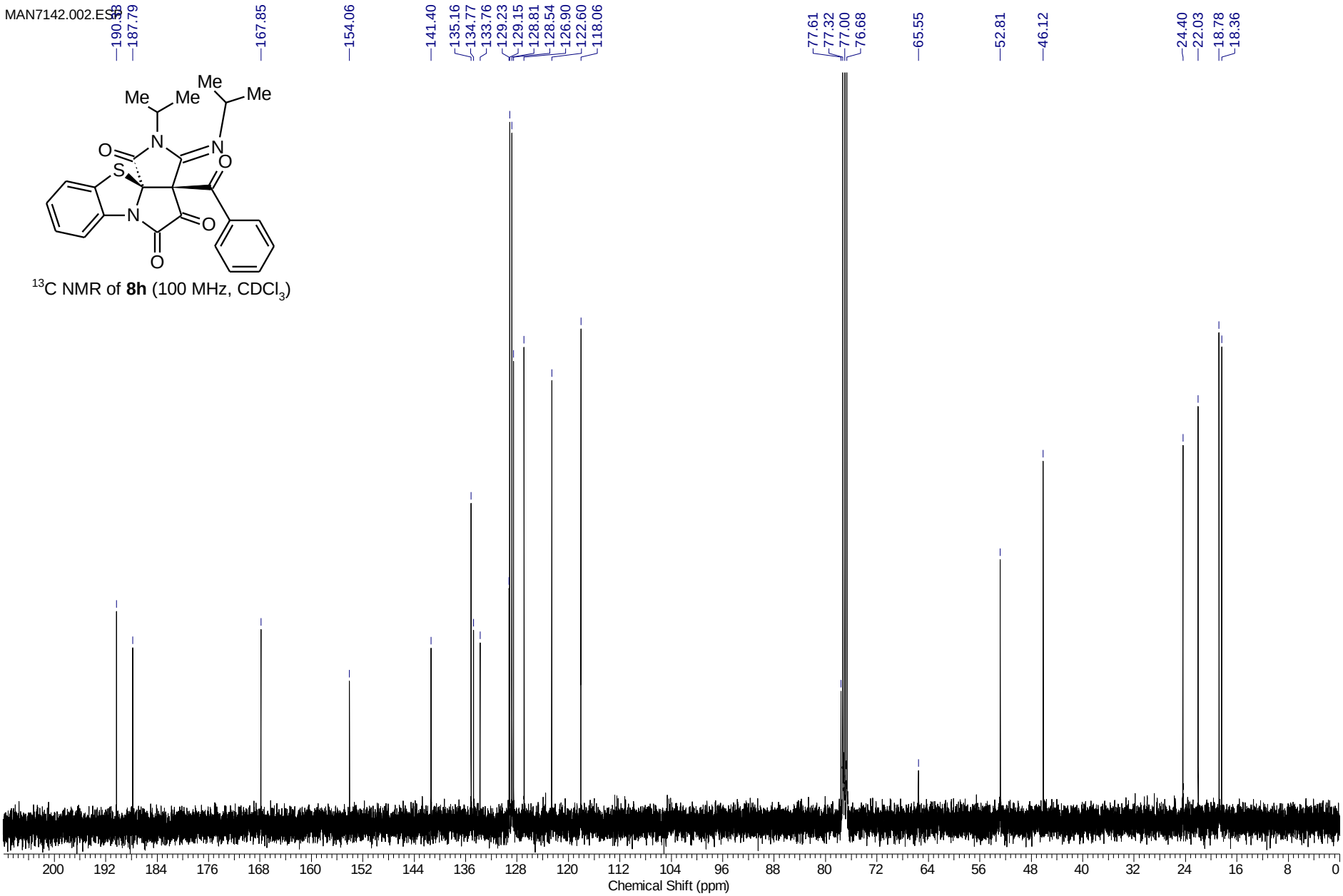
^{13}C NMR of **8g** (100 MHz, $CDCl_3$)

MAN7187.003.ESP



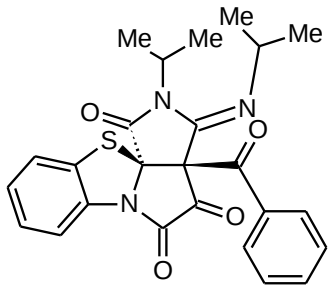
DEPT135 of **8g** (100 MHz, $CDCl_3$)


MAN7142.001.ESP
7.94
7.93
7.76
7.74
7.72
7.58
7.56
7.54
7.32
7.31
7.31
7.28
7.27
4.83
4.81
4.79
4.78
4.76
4.74
4.72
3.83
3.82
3.81
3.79
3.78
3.76
3.75
1.55
1.53
1.31
1.29
0.51
0.49
Me
Me
Me
Me
O
S
N
N
O
N
O
O
O
1H NMR of 8h (400 MHz, CDCl3)
0.86
2.82
2.04
3.19
1.05
1.04
6.16
3.00
2.95
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
Chemical Shift (ppm)

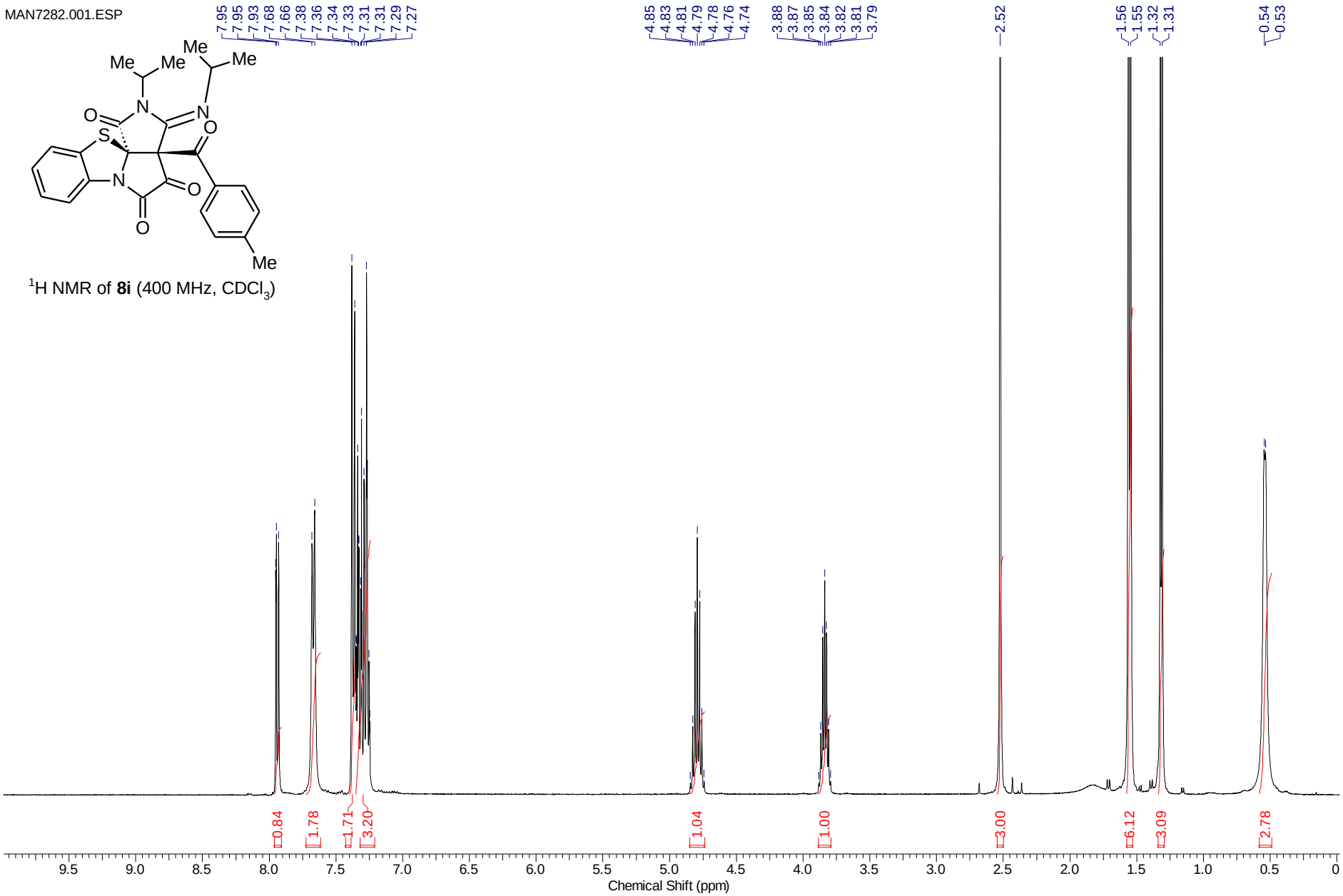


^{13}C NMR of **8h** (100 MHz, $CDCl_3$)

MAN7142.003.ESP



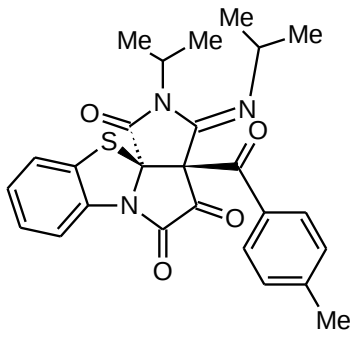
DEPT135 of **8h** (100 MHz, $CDCl_3$)



^{1}H NMR of **8i** (400 MHz, $CDCl_3$)

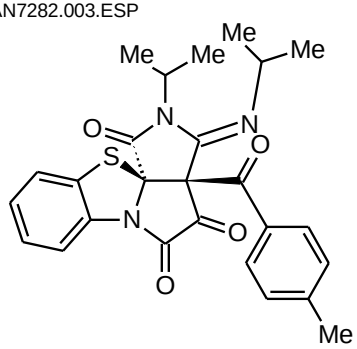
MAN7282.002.ESP

189.79
187.84
167.91
154.11
146.76
141.60
134.78
131.17
129.85
129.30
128.96
128.48
126.85
122.55
118.04
115.01
77.69
77.32
77.00
76.68
65.52
52.72
46.09
24.41
22.12
21.81
18.78
18.35



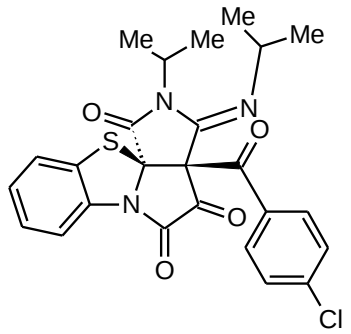
^{13}C NMR of **8i** (100 MHz, $CDCl_3$)

MAN7282.003.ESP

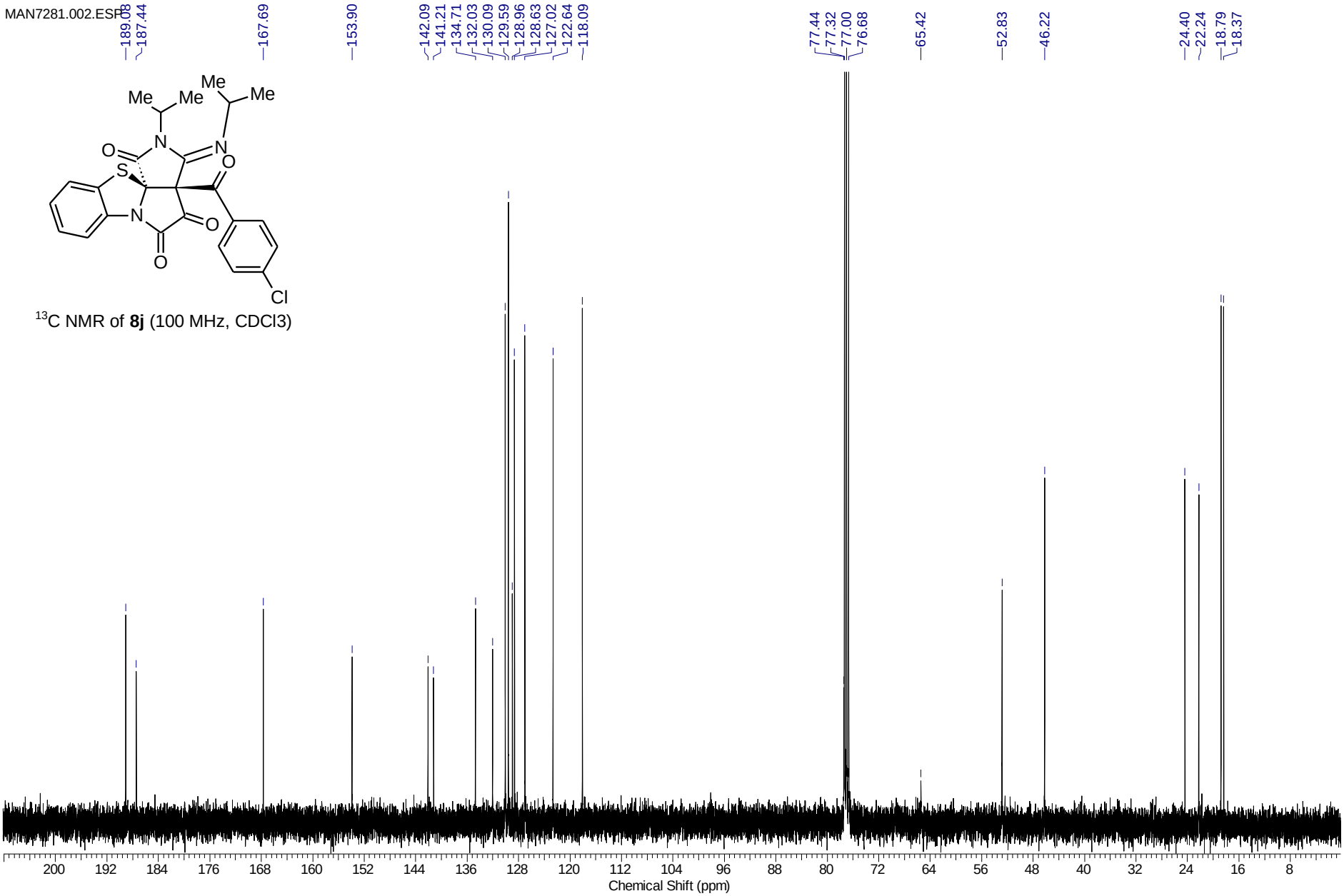


DEPT135 of **8i** (100 MHz, $CDCl_3$)

MAN7281.001.ESP

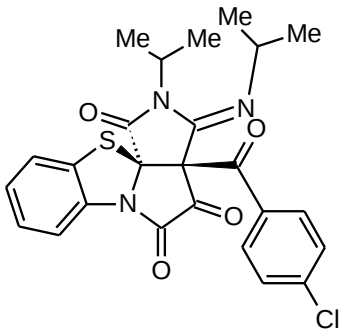


^{1}H NMR of **8j** (400 MHz, CDCl3)



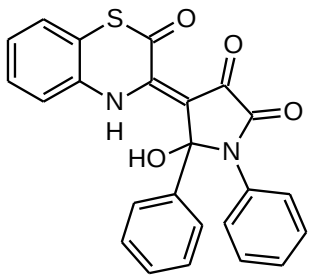
^{13}C NMR of **8j** (100 MHz, CDCl3)

MAN7281.003.ESP



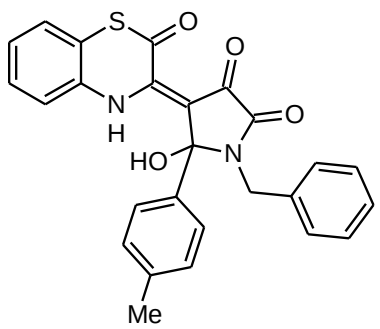
DEPT135 of **8j** (100 MHz, CDCl3)

MAN8285.001.esp

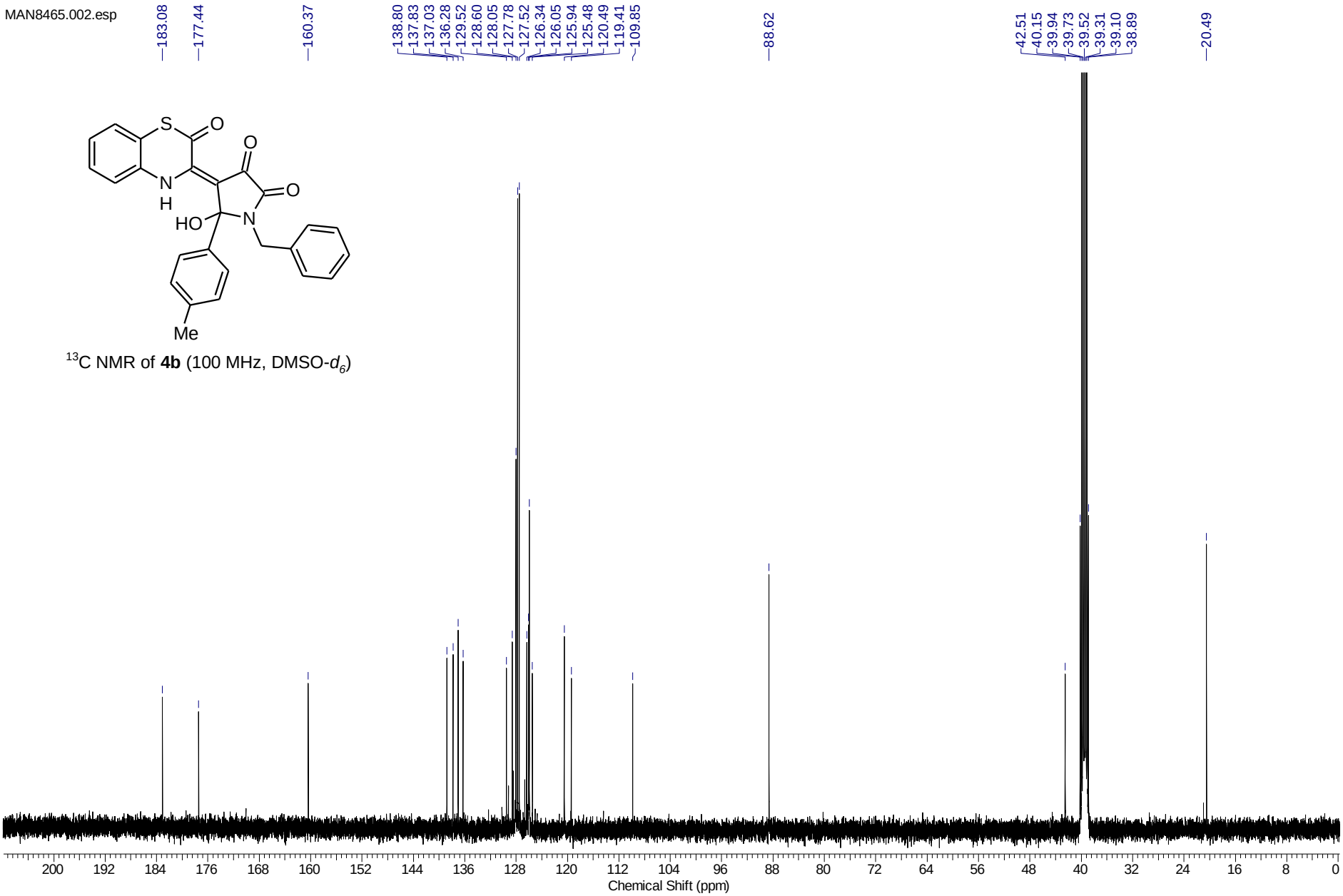


^{1}H NMR of **4a** (400 MHz, DMSO-d_6)

MAN8465.001.esp

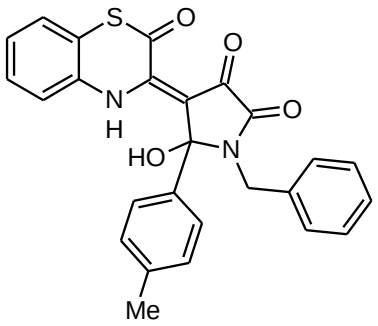


^{1}H NMR of **4b** (400 MHz, DMSO-d_6)

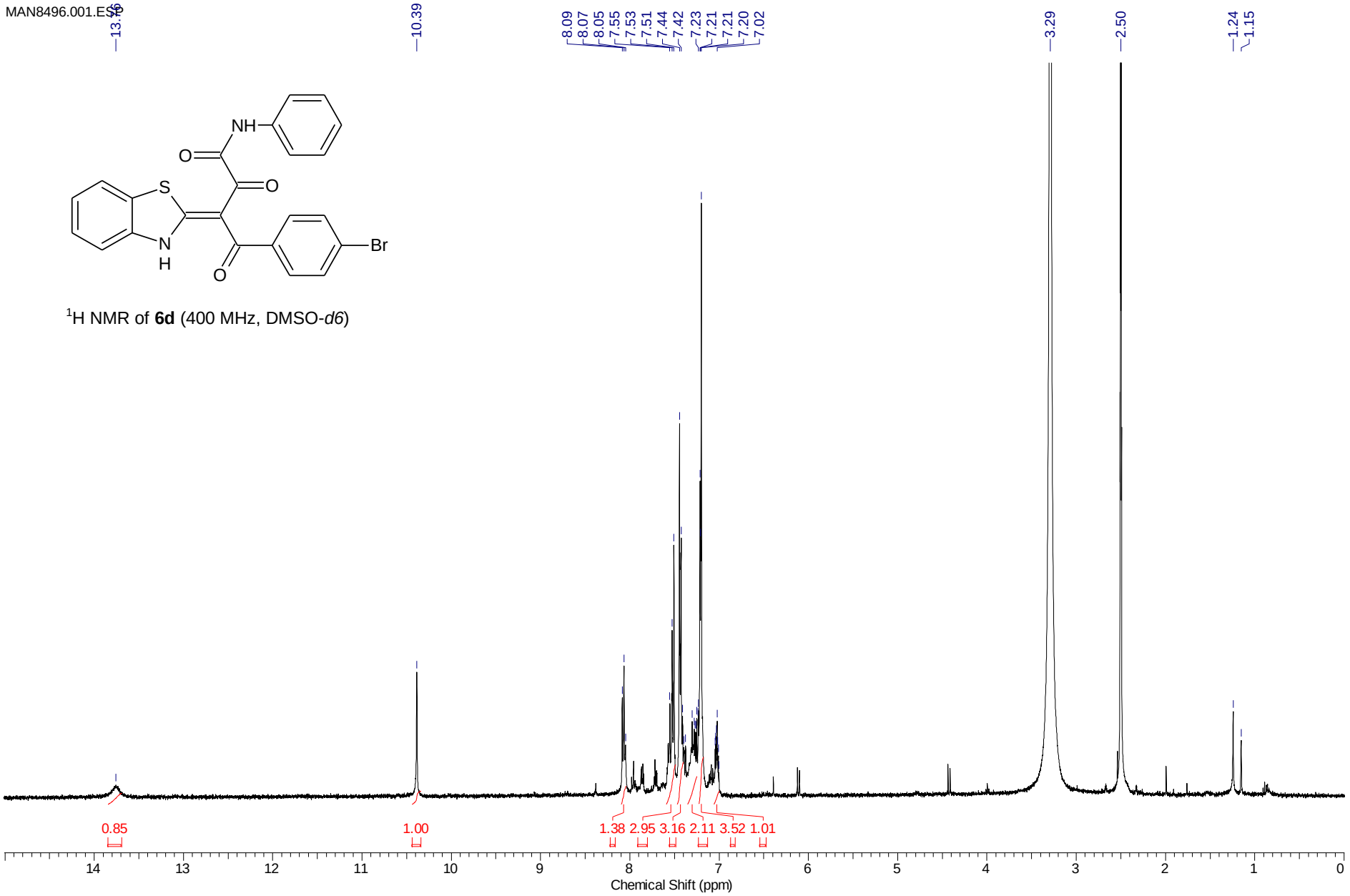


^{13}C NMR of **4b** (100 MHz, DMSO-d_6)

MAN8465.003.esp



DEPT135 of **4b** (100 MHz, DMSO-d_6)


MAN8496.001.ESP
13.15
10.39
8.09
8.07
8.05
7.55
7.53
7.51
7.44
7.42
7.23
7.21
7.21
7.20
7.02
3.29
2.50
1.24
1.15
NH
O
O
S
N
H
O
Br
1H NMR of 6d (400 MHz, DMSO-d6)
0.85
1.00
1.38
2.95
3.16
2.11
3.52
1.01
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

Calculated total electronic energies (E, in Hartree), enthalpies (H, in Hartree), Gibbs free energies (G, in Hartree), and entropies (S, cal/mol•K) for optimized equilibrium model structures.

Model structure	E	H	G	S
2a	-556.505478837	-556.288000	-556.337930	105.087
1a	-1444.70735189	-1444.455577	-1444.525748	147.689
OC	-2001.22427330	-2000.752484	-2000.853026	211.608
I2	-2001.20499337	-2000.732654	-2000.826957	198.477
3a	-2001.27537318	-2000.801112	-2000.892382	192.095
3'a	-2001.28342773	-2000.808838	-2000.899955	191.773
TS	-2001.21741473	-2000.745789	-2000.837371	192.749
TS’	-2001.21575382	-2000.744961	-2000.834876	189.242

ORTEP images of X-ray crystal structures of compounds 3a, 4b, 6d, 8a

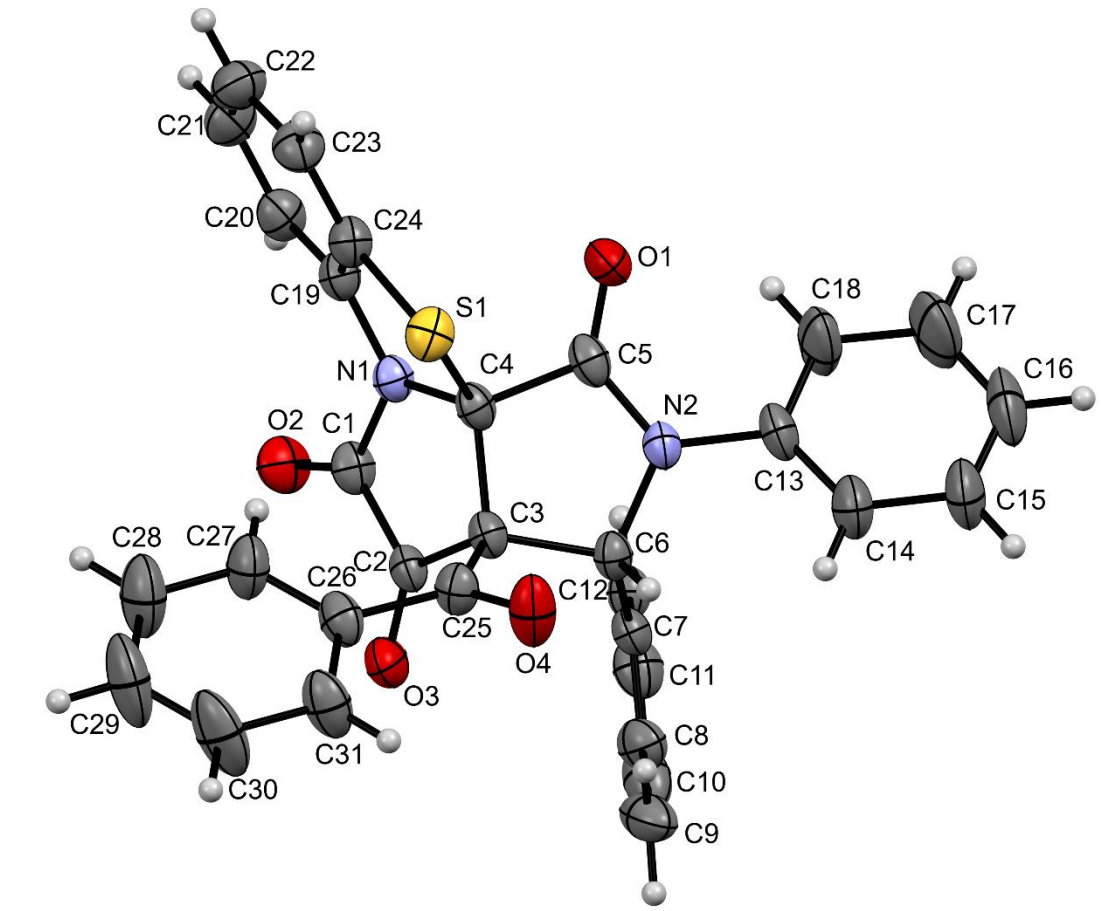


Figure S1. *Molecular structure of compound* ***3a*** *showing 30% probability amplitude displacement ellipsoids (CCDC 2341688). Toluene solvate molecule is not shown.*

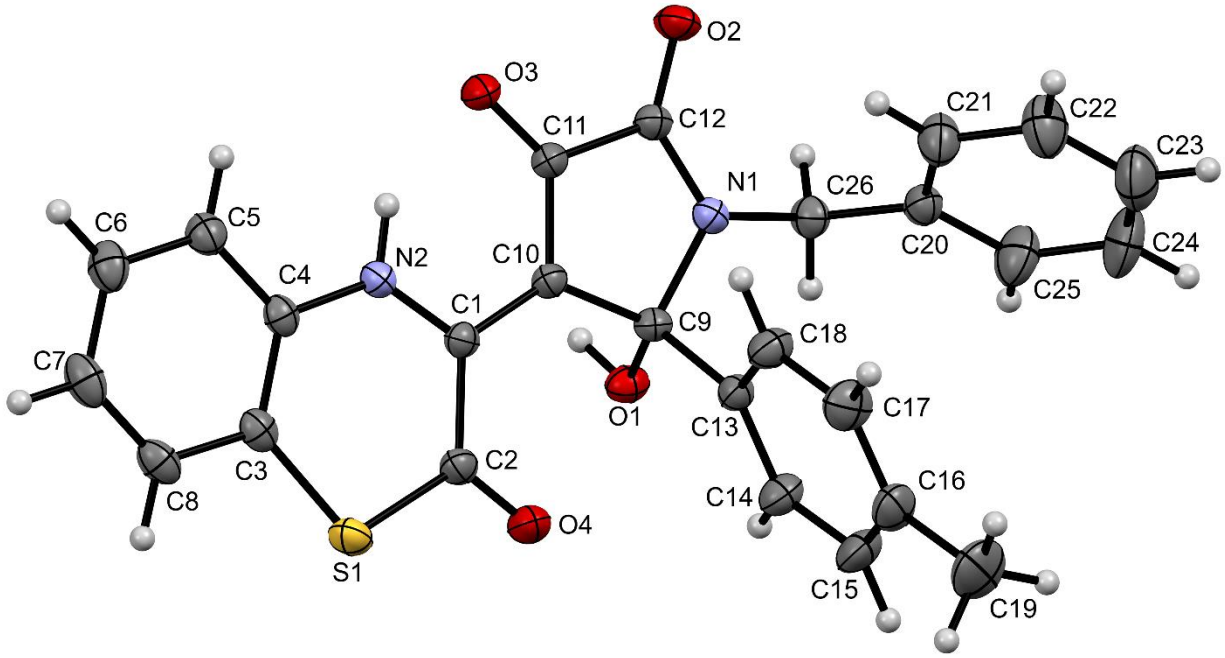


Figure S2. *Molecular structure of compound* ***4b*** *showing 30% probability amplitude displacement ellipsoids (CCDC 2341690).*

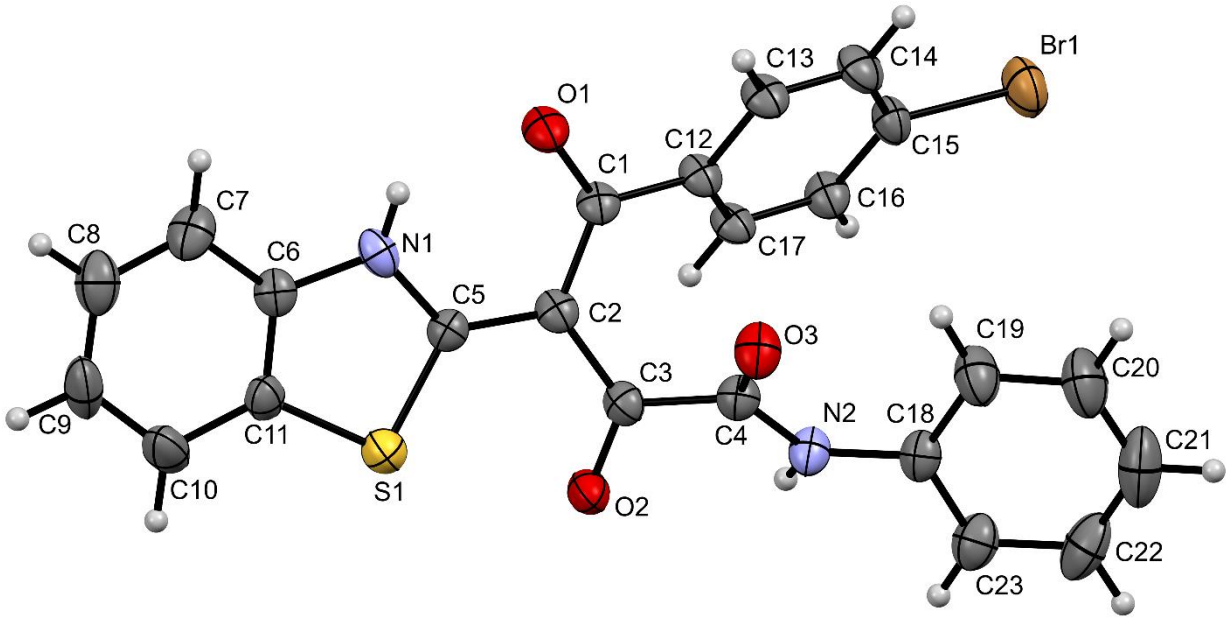


Figure S3. *Molecular structure of compound* ***6d*** *showing 30% probability amplitude displacement ellipsoids (CCDC 2341691).*

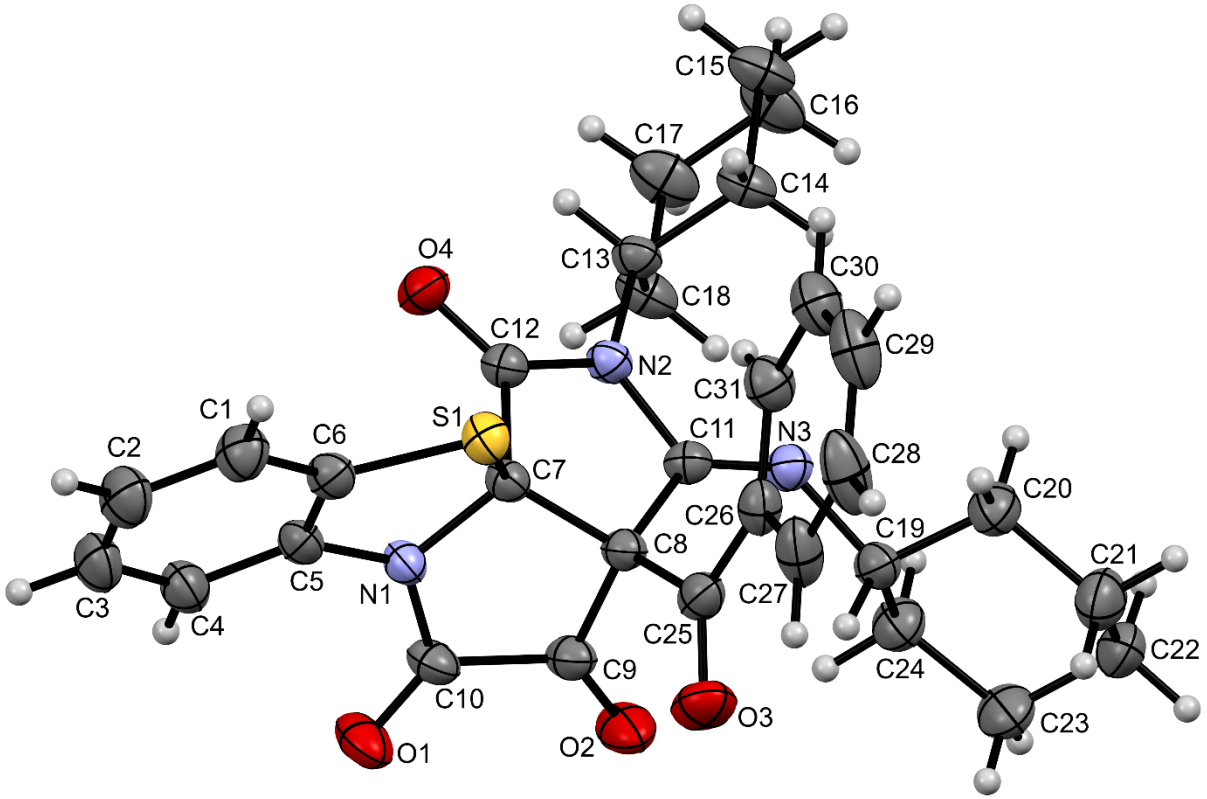


Figure S4. *Molecular structure of compound* ***8a*** *showing 30% probability amplitude displacement ellipsoids (CCDC 2341689).*