# Electronic Supplimentary Information

# Cu(I)-catalysed cross-coupling reaction of *in situ* generated azomethine ylides towards easy construction of fused *N*-heterocycles

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## 1. Materials and methods

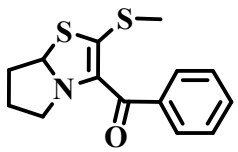
All reagents were purchased from commercial suppliers and used without further purification, unless otherwise specified. Commercially supplied ethyl acetate and petroleum ether were distilled before use. Petroleum ether used in our experiments was in the boiling range of 60-80 ºC. Column chromatography was performed on silica gel (100-200 mesh, 0.075-0.150 mm). Analytical thin layer chromatography was performed on 0.25 mm extra hard silica gel plates with UV-254 fluorescent indicator. $^{1}$H-NMR and $^{13}$C-NMR spectra (300 MHz & 400 MHz) were recorded at ambient temperature using 300 MHz & 400 MHz spectrometers (300 MHz & 400 MHz for $^{1}$H and 75 & 100 MHz for $^{13}$C). Chemical shift is reported in ppm from internal reference tetramethylsilane and coupling constant in Hz. Proton multiplicities are represented as s (singlet), brs (broad singlet), d (doublet), dd (double doublet), t (triplet), q (quartet), and m (multiplet). Infrared spectra were recorded on FT-IR spectrometer (IR Spectrophotometer) in thin film (KBr) or neat. HR-MS data were acquired by electron spray ionization technique on a Q-tof-micro quadriple mass spectrophotometer (Qtof ESI-MS). X-RAY crystallographic data was taken in a CCD difractometer.

## 2. General procedure for the synthesis of 5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazoles (6a-p).

In a dry seal tube, 1.1 mmol of L-Prolinee (**1**) and 1 mmol of phenylglyoxal (**2**) were dissolved in anhydrous toluene (5 mL), and the reaction mixture was stirred at 140 ºC. After 5-10 minutes, when reaction mixture turned red, 1 mmol of dialkyl trithiocarbonate (**3**), 1.0 mmol of $K_2CO_3$ and 5 mol% of CuI were added. The seal tube was immediately sealed and the reaction mixture was stirred at 110 ºC. The progress of reaction was monitored by thin layer chromatography (TLC). The post-reaction mixture was extracted with ethyl acetate (2x10 mL). The combined organic layer was washed with water (3x10 mL) and brine (1x10 mL). It was dried over activated $Na_2SO_4$, filtered and evaporated in a rotary evaporator under reduced pressure at room temperature. Purification of the crude product mixture by column chromatography on silica gel (100-200 mesh) with ethyl acetate-petroleum ether (1:9 v/v) as an eluent afforded the corresponding 5,6,7,7a-tetrahydropyrrolo[2,1-*b*]thiazole (**6a-p)**. All the synthesised compounds were characterized by relevent spectroscopic analysis and finally structure was confirmed through the single crystal XRD analysis of compound **6a**.

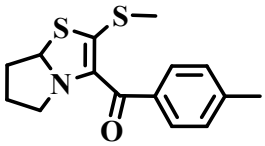
## 3. Characterization data of the synthesized 5,6,7,7a-tetrahydropyrrolo[2,1-*b*]thiazoles (6a-p)

### 3.1. (2-(Methylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(phenyl)methanone (6a)



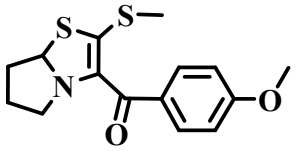

Compound **6a** was prepared using L-proline, phenylglyoxal and dimethyl trithiocarbonate as starting materials to obtain the product as yellow solid; yield: 93% (258 mg, 0.93 mmol); m.p. 63-65 ºC; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.16- 8.12 (m, 2H), 7.50-7.37 (m, 3H), 6.06 (t, *J* = 4.2 Hz, 1H), 2.88 (d, *J* = 6.6 Hz, 2H), 2.53 (s, 3H), 2.42 (d, *J* = 8.7 Hz, 1H), 2.31 (d, *J* = 8.7 Hz, 1H), 2.10 (brs, 1H), 1.88 (brs, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 184.0, 138.7, 137.3, 131.5, 129.3, 128.0, 78.2, 54.8, 31.4, 30.9, 25.1, 20.4; FT-IR (KBr, $cm^{-1}$): 3130, 2935, 1650, 1599, 1442, 1320; HR-MS (*m*/*z*) for: $C_{14}H_{16}NOS_2$ (M+H): Calculated, 278.0673, found 278.0677.

### 3.2. (2-(Methylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(p-tolyl)methanone (6b)



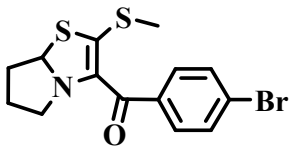
Compound **6b** was prepared using L-proline, 4-methylphenylglyoxal and dimethyl trithiocarbonate as starting materials to obtain the product as brown gummy liquid; yield: 89% (259 mg, 0.89 mmol); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.05 (d, $J$ = 8.1 Hz, 2H), 7.19 (d, $J$ = 8.1 Hz, 2H), 6.05 (t, $J$ = 4.2 Hz, 1H), 2.93- 2.86 (m, 2H), 2.51 (s, 3H), 2.46- 2.42 (m, 1H), 2.39 (s, 3H), 2.32 (d, $J$ = 6.3 Hz, 1H), 2.15-2.03 (m, 1H), 1.88 (d, $J$ = 7.2 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 183.8, 142.2, 137.2, 135.9, 129.5, 128.7, 77.9, 54.8, 31.5, 29.7, 25.1, 21.7, 20.3; FT-IR (neat, cm$^{-1}$): 3101, 2910, 1625, 1573, 1409, 1295; HR-MS (*m*/*z*) for: $C_{15}H_{17}NNaOS_2$ (M+Na): Calculated, 314.0649, found 314.0652.

### 3.3. (4-Methoxyphenyl)(2-(methylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)methanone (6c)



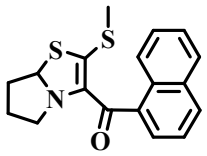
Compound **6c** was prepared using L-proline, 4-methoxyphenylglyoxal and dimethyl trithiocarbonate as starting materials to obtain the product as yellow gummy liquid; yield: 90% (277 mg, 0.90 mmol); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.21 (dd, $J_1$ = 6.9 Hz, $J_2$ = 2.1 Hz, 2H), 6.90 (dd, $J_1$ = 6.9 Hz, $J_2$ = 2.1 Hz, 2H), 6.04 (t, $J$ = 4.2 Hz, 1H), 3.87 (s, 3H), 2.95-2.88 (m, 2H), 2.51 (s, 3H), 2.41 (d, $J$ = 7.2 Hz, 1H), 2.32 (br s, 1H), 2.11 (br s, 1H), 1.89 (br s, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 182.8, 162.4, 137.5, 131.8, 131.3, 113.2, 77.8, 55.3, 54.6, 31.6, 29.7, 25.1, 20.4; FT-IR (neat, cm$^{-1}$): 3091, 2902, 1615, 1565, 1403, 1280; HR-MS (*m*/*z*) for: $C_{15}H_{17}NNaO_2S_2$ (M+Na): Calculated, 330.0598, found 330.0595.

### 3.4. (4-Bromophenyl)(2-(methylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)methanone (6d)



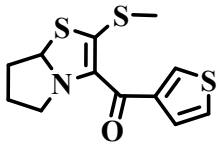
Compound **6d** was prepared using L-proline, 4-bromophenylglyoxal and dimethyl trithiocarbonate as starting materials to obtain the product yellow gummy liquid; yield: 85% (303 mg, 0.85 mmol); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.04 (d, $J$ = 8.7 Hz, 2H), 7.53 (d, $J$ = 8.7 Hz, 2H), 6.06 (t, $J$ = 3.9 Hz, 1H), 2.91-2.82 (m, 2H), 2.54 (s, 3H), 2.44-2.39 (m, 1H), 2.34-2.30 (m, 1H), 2.19-2.05 (m, 1H), 1.90 (t, $J$ = 6.9 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 182.4, 137.4, 136.9, 131.3, 131.0, 126.4, 78.5, 54.9, 31.3, 29.7, 25.1, 20.4; FT-IR (neat, cm$^{-1}$): 3120, 2931, 16345, 1597, 1435, 1318; HR-MS (*m*/*z*) for: $C_{14}H_{15}BrNOS_2$ (M+H): Calculated, 355.9778, found 355.9782 (One of the major peaks).

### 3.5. (2-(Methylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(naphthalen-1-yl)methanone (6e)



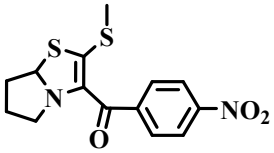
Compound **6e** was prepared using L-proline, naphthalene-1-glyoxal and dimethyl trithiocarbonate as starting materials to obtain the product as brown liquid; yield: 86% (282 mg, 0.86 mmol); $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.17-8.15 (m, H), 7.93-7.86 (m, 2H), 7.74 (d, $J$ = 6.8 Hz, 1H), 7.54-7.46 (m, 3H), 6.01-5.99 (m, 1H), 2.89-2.83 (m, 1H), 2.71-2.66 (m, 1H), 2.52 (s, 3H), 2.35-2.20 (m, 2H), 2.08-2.01 (m, 1H), 1.79-1.70 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 187.1, 138.6, 137.6, 133.5, 130.5, 130.4, 128.2, 126.8, 126.5, 126.1, 125.7, 124.7, 78.4, 55.1, 31.2, 29.8, 25.1, 20.4; FT-IR (neat, cm$^{-1}$): 3141, 2942, 1657, 1605, 1445, 1327; HR-MS (*m*/*z*) for: $C_{18}H_{18}NOS_2$ (M+H): Calculated, 328.0830, found 328.0833.

### 3.6. (2-(Methylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(thiophen-3-yl)methanone (6f)



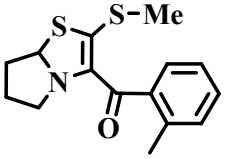
Compound **6f** was prepared using L-proline, thiophene-3-glyoxal and dimethyl trithiocarbonate as starting materials to obtain the product as a brown solid; yield: 90% (255 mg, 0.90 mmol); m.p. 64-66 °C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.55 (dd, $J_1$ = 3.0 Hz, $J_2$ = 1.2 Hz, 1H), 7.78 (dd, $J_1$ = 5.1 Hz, $J_2$ = 1.2 Hz, 1H), 7.24 (dd, $J_1$ = 5.1 Hz, $J_2$ = 3.0 Hz, 1H), 6.06 (dd, $J_1$ = 5.4 Hz, $J_2$ = 2.7 Hz, 1H), 3.21-3.13 (m, 1H), 2.98-2.90 (m, 1H), 2.53 (s, 3H), 2.47-2.39 (m, 1H), 2.37-2.29 (m, 1H), 2.25-2.16 (m, 1H), 2.03-1.92 (m, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 177.1, 141.8, 137.1, 132.7, 128.9, 124.8, 78.9, 54.8, 31.1, 29.7, 25.2, 20.4; FT-IR (KBr, cm$^{-1}$): 3112, 2922, 1638, 1586, 1424, 1305; HR-MS (*m*/*z*) for: $C_{12}H_{13}NNaOS_3$ (M+Na): Calculated, 306.0057, found 306.0060.

### 3.7. (2-(Methylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(4-nitrophenyl)methanone (6g)



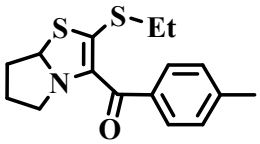
Compound **6g** was prepared using L-proline, 4-nitrophenylglyoxal and dimethyl trithiocarbonate as starting materials to obtain the product as brown solid; yield: 78% (251 mg, 0.78 mmol); m.p. 68-80 °C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.30-8.24 (m, 4H), 6.10 (t, $J$ = 4 Hz, 1H), 2.84 (t, $J$ = 6.8 Hz, 2H), 2.58 (s, 3H), 2.47-2.42 (m, 1H), 2.36-2.28 (m, 1H), 2.23-2.11 (m, 1H), 1.93-1.89 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 181.2, 149.1, 144.0, 136.7, 130.2, 123.2, 79.2, 55.2, 31.1, 29.7, 25.1, 20.5; FT-IR (KBr, cm$^{-1}$): 3150, 2968, 1679, 1618, 1469, 1354; HR-MS (*m*/*z*) for: $C_{14}H_{15}N_2O_3S_2$ (M+H): Calculated, 323.0524, found 323.0527.

### 3.8. (2-(Methylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(o-tolyl)methanone (6h)



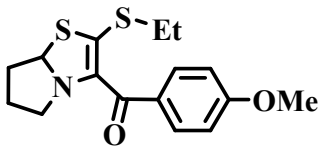
Compound **6h** was prepared using L-proline, 2-methylphenylglyoxal and dimethyl trithiocarbonate as starting materials to obtain the product brown gummy liquid; yield: 75% (218 mg, 0.75 mmol); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.43-7.40 (m, 1H), 7.32-7.27 (m, 1H), 7.21-7.17 (m, 2H), 5.96 (t, *J* = 4.2 Hz, 1H), 2.88-2.80 (m, 2H), 2.51 (s, 3H), 2.40 (s, 3H), 2.36-2.19 (m, 2H), 2.09-2.02 (m, 1H), 1.84-1.77 (m, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 188.0, 140.3, 138.3, 135.9, 130.4, 129.5, 127.8, 125.2, 78.2, 54.6, 31.3, 29.7, 25.2, 20.2, 19.8; FT-IR (neat, $cm^{-1}$): 3098, 2907, 1627, 1571, 1413, 1295; HR-MS (*m*/*z*) for: $C_{15}H_{18}NOS_2$ (M+H): Calculated, 292.0830, found 292.0834.

### 3.9. (2-(Ethylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(p-tolyl)methanone (6i)



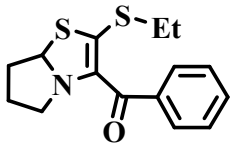

Compound **6i** was prepared using L-proline, 4-methylphenylglyoxal and diethyl trithiocarbonate as starting materials to obtain the product yellow gummy liquid; yield: 87% (265 mg, 0.87 mmol); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.07-8.04 (m, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 6.01 (t, *J* = 4.2 Hz, 1H), 3.03-2.84 (m, 4H), 2.40 (s, 3H), 2.33-2.29 (m, 1H), 2.09-2.06 (m, 1H), 1.88 (d, *J* = 11.1 Hz, 1H), 1.75 (brs, 1H), 1.36 (t, *J* = 7.5 Hz, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 184.0, 142.3, 138.0, 136.0, 129.6, 128.7, 77.6, 54.6, 31.6, 31.4, 29.7, 25.1, 21.7, 14.8; FT-IR (neat, $cm^{-1}$): 3096, 2909, 1625, 1573, 1411, 1292; HR-MS (*m*/*z*) for: $C_{16}H_{20}NOS_2$ (M+H): Calculated, 306.0986, found 306.0990.

### 3.10. (2-(Ethylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(4-methoxyphenyl)methanone (6j)




Compound **6j** was prepared using L-proline, 4-methoxylphenylglyoxal and diethyl trithiocarbonate as starting materials to obtain the product as a brown gummy liquid; yield: 88% (283 mg, 0.88 mmol); $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.21-8.19 (m, 2H), 6.91-6.89 (m, 2H), 6.01-5.99 (m, 1H), 3.87 (d, *J* = 1.2 Hz, 3H), 3.01-2.96 (m, 2H), 2.90-2.86 (m, 2H), 2.44-2.39 (m, 1H), 2.33-2.29 (m, 1H), 2.11-2.07 (m, 1H), 1.91-1.86 (m, 1H), 1.38-1.34 (m, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 183.0, 162.5, 138.0, 131.8, 131.3, 113.2, 77.4, 55.3, 54.5, 31.6, 31.4, 29.7, 25.0, 14.8; FT-IR (neat, $cm^{-1}$): 3080, 2890, 1606, 1555, 1392, 1371; HR-MS (*m*/*z*) for: $C_{16}H_{20}NO_2S_2$ (M+H): Calculated, 322.0935, found 322.0939.

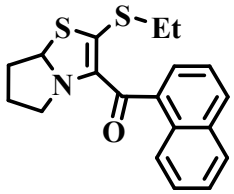
### 3.11. (2-(Ethylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(phenyl)methanone (6k)




Compound **6k** was prepared using L-proline, phenylglyoxal and diethyl trithiocarbonate as starting materials to obtain the product as a yellow gummy liquid; yield: 90% (262 mg, 0.90 mmol); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.14-8.11 (m, 2H), 7.51-7.37 (m, 3H), 6.03 (t, *J* = 4.2 Hz, 1H), 3.03 (t, *J* = 7.2 Hz, 1H), 2.94-2.84 (m, 3H), 2.46-2.41 (m, 1H), 2.38-2.27 (m, 1H), 2.09-2.02 (m, 1H), 1.88 (d, *J* = 8.4 Hz,

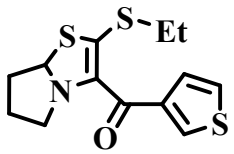
1H), 1.37 (t, *J* = 7.2 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 184.3, 138.6, 137.7, 131.7, 129.4, 128.0, 77.8, 54.7, 31.5, 31.1, 29.7, 25.1, 14.8; FT-IR (neat, $cm^{-1}$): 3106, 2916, 1629, 1579, 1418, 1299; HR-MS (*m*/*z*) for: $C_{15}H_{18}NOS_2$ (M+H): Calculated, 292.0830, found 292.0831.

### 3.12. (2-(Ethylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(naphthalen-1-yl)methanone (6l)



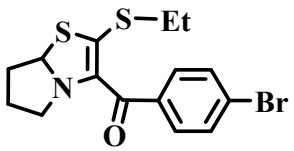

Compound **6l** was prepared using L-proline, naphthalene-1-glyoxal and diethyl trithiocarbonate as starting materials to obtain the product as a brown gummy liquid; yield: 82% (280 mg, 0.82 mmol); $^1$H NMR (300 MHz, $CDCl_3$): δ 8.19-8.16 (m, 1H), 7.92-7.86 (m, 2H), 7.74 (d, *J* = 6.9 Hz, 1H), 7.61-7.45 (m, 3H), 5.95 (s, 1H), 3.02-2.88 (m, 3H), 2.71 (brs, 1H), 2.35-2.25 (m, 2H), 2.06 (brs, 1H), 1.74 (brs, 1H), 1.37-1.32 (m, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 187.3, 139.3, 137.9, 133.5, 130.4, 128.4, 128.1, 126.7, 126.5, 126.0, 125.7, 124.6, 77.9, 54.8, 31.5, 31.4, 29.7, 25.1, 14.8; FT-IR (neat, $cm^{-1}$): 3145, 2945, 1652, 1609, 1451, 1322; HR-MS (*m*/*z*) for: $C_{19}H_{20}NOS_2$ (M+H): Calculated, 342.0986, found 342.0989.

### 3.13. (2-(Ethylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)(thiophen-3-yl)methanone (6m)



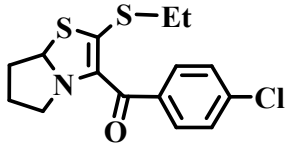

Compound **6m** was prepared using L-proline, thiophene-3-glyoxal and diethyl trithiocarbonate as starting materials to obtain the product as brown gummy liquid; yield: 86% (256 mg, 0.86 mmol); $^1$H NMR (400 MHz, $CDCl_3$): δ 8.55 (d, *J* = 3.2 Hz, 1H), 7.78 (d, *J* = 5.2 Hz, 1H), 7.25-7.23 (m, 1H), 6.04-6.02 (m, 1H), 3.18-3.13 (m, 1H), 3.08-3.00 (m, 1H), 2.95-2.89 (m, 2H), 2.48-2.41 (m, 1H), 2.37-2.30 (m, 1H), 2.22-2.16 (m, 1H), 1.99-1.90 (m, 1H), 1.37 (t, *J* = 7.2 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 173.1, 141.9, 137.3, 132.8, 129.0, 124.7, 78.6, 54.7, 31.4, 31.2, 29.7, 25.2, 14.7; FT-IR (neat, $cm^{-1}$): 3110, 2919, 1635, 1590, 1430, 1302; HR-MS (*m*/*z*) for: $C_{13}H_{15}NNaOS_3$ (M+Na): Calculated, 320.0213, found 320.0209.

### 3.14. (4-Bromophenyl)(2-(ethylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)methanone (6n)



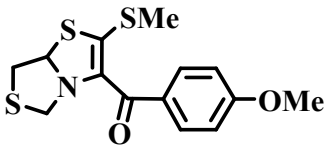

Compound **6n** was prepared using L-proline, 4-bromophenylglyoxal and diethyl trithiocarbonate as starting materials to obtain the product as yellow gummy liquid; yield: 80% (256 mg, 0.80 mmol); $^1$H NMR (300 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.4 Hz, 2H), 7.54 (d, *J* = 8.4 Hz, 2H), 6.02 (s, 1H), 3.04-2.82 (m, 4H), 2.42 (d, *J* = 7.5 Hz, 1H), 2.33 (brs, 1H), 2.19-2.06 (m, 1H), 1.89 (brs, 1H), 1.38 (t, *J* = 7.5 Hz, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 182.6, 137.5, 131.9, 131.3, 131.1, 129.9, 78.2, 54.8, 31.5, 31.3, 29.7, 25.1, 14.7; FT-IR (neat, $cm^{-1}$): 3122, 2936, 1641, 1593, 1430, 1314; HR-MS (*m*/*z*) for: $C_{15}H_{17}BrNOS_2$ (M+H): Calculated, 369.9935, found 369.9937 (One of the major peaks).

### 3.15. (4-Chlorophenyl)(2-(ethylthio)-5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazol-3-yl)methanone (6o)




Compound **6o** was prepared using L-proline, 4-chlorophenylglyoxal and diethyl trithiocarbonate as starting materials to obtain the product as yellow gummy liquid; yield: 81% (264 mg, 0.81 mmol); $^1$H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, $J$ = 8.0 Hz, 2H), 7.37 (d, $J$ = 8.0 Hz, 2H), 6.03 (t, $J$ = 4.0 Hz, 1H), 3.03 (t, $J$ = 7.6 Hz, 1H), 2.95-2.81 (m, 3H), 2.46-2.42 (m, 1H), 2.35-2.30 (m, 1H), 2.12-2.03 (m, 1H), 1.89 (d, $J$ = 8.4 Hz, 1H), 1.38 (t, $J$ = 7.2 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 182.5, 137.8, 137.2, 137.0, 130.9, 128.3, 78.1, 54.8, 31.5, 31.3, 29.7, 25.1, 14.7; FT-IR (neat, cm$^{-1}$): 3126, 2934, 1645, 1596, 1435, 1320; HR-MS (*m*/*z*) for: $C_{15}H_{17}ClNOS_2$ (M+H): Calculated, 326.0440, found 326.0443 (One of the majo peaks).

### 3.16. (4-methoxyphenyl)(2-(methylthio)-7,7a-dihydro-5*H*-thiazolo[4,3-*b*]thiazol-3-yl)methanone (6p)



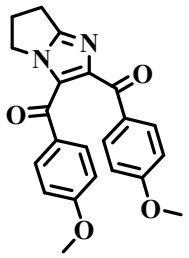

Compound **6p** was prepared using L-timonacic, 4-methoxyphenylglyoxal and dimethyl trithiocarbonate as starting materials to obtain the product as yellow gummy liquid (It has been performed at 80 °C); yield: 70% (228 mg, 0.70 mmol); $^1$H NMR (300 MHz, $CDCl_3$): δ 8.03 (d, $J$ = 8.7 Hz, 2H), 6.94 (d, $J$ = 9.0 Hz, 2H), 5.54 (t, $J$ = 5.4 Hz, 1H), 4.26 (d, $J$ = 9.9 Hz, 1H), 4.09 (d, $J$ = 9.9 Hz, 1H), 3.89 (s, 3H), 3.46 (dd, $J_1$ = 11.7 Hz, $J_2$ = 6.0 Hz, 1H ), 3.27 (dd, $J_1$ = 11.7 Hz, $J_2$ = 5.4 Hz, 1H), 2.37 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 184.8, 163.4, 131.8, 130.7, 125.4, 113.7, 74.0, 57.3, 55.5, 39.1, 19.0; FT-IR (neat, cm$^{-1}$): 3120, 2930, 1636, 1585, 1422, 1301; HR-MS (*m*/*z*) for: $C_{14}H_{16}NO_2S_3$ (M+H): Calculated, 326.0343, found 326.0347.

## 4. General procedure for the synthesis of symmetrical 6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazoles (7a-k)

In a dry seal tube, 1.1 mmol of L-prolinee (**1**) and 1 mmol of phenylglyoxal **(2)** were dissolved in anhydrous toluene (5 mL), and the reaction mixture was stirred at 140 ºC. After 5-10 minutes, when reaction mixture turned red, 1 mmol of p-toluenesulfonamide **(4)**, 1 mmol of phenylglyoxal **(2),** 1.0 mmol of $K_2CO_3$ and 5 mol% of CuI were added. The seal tube was immediately sealed and the reaction mixture was stirred at 110 ºC. The progress of reaction was monitored by thin layer chromatography (TLC). The post-reaction mixture was extracted with ethyl acetate (2x10 mL). The combined organic layer was washed with water (3x10 mL) and brine (1x10 mL). It was dried over activated $Na_2SO_4$, filtered and evaporated in a rotary evaporator under reduced pressure at room temperature. Purification of the crude product mixture by column chromatography on silica gel (100-200 mesh) with ethyl acetate-petroleum ether (1:1 v/v) as an eluent afforded the corresponding **(7a-k)** 6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazole. All the synthesised compounds were characterized by relevent spectroscopic analysis.

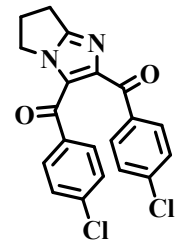
**5. Characterization data of the synthesized symmetrical 6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazoles (7a-k)**

**5.1. (6,7-Dihydro-5*H*-pyrrolo[1,2-*a*]imidazole-2,3-diyl)bis((4-methoxyphenyl)methanone) (7a)[1]**



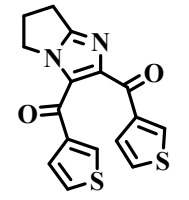
Compound **7a** was prepared using L-proline, 4-methoxyphenylglyoxal and p-toluenesulfonamide as starting materials to obtain the product as a brown solid; yield: 88% (331 mg, 0.88 mmol); m.p. 176-178 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.95 (d, $J$ = 9.0 Hz, 2H), 7.68 (d, $J$ = 8.7 Hz, 2H), 6.84 (d, $J$ = 9.0 Hz, 2H), 6.75 (d, $J$ = 9.0 Hz, 2H), 4.24 (t, $J$ = 6.9 Hz, 2H), 3.83 (s, 3H), 3.78 (s, 3H), 2.99 (t, $J$ = 7.5 Hz, 2H) 2.74-2.66 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 187.4, 185.4, 163.3, 163.1, 156.1, 147.9, 132.3, 131.2, 130.7, 130.5, 129.6, 113.5, 113.3, 55.3, 55.2, 45.4, 25.9, 23.1; FT-IR (KBr, cm$^{-1}$): 2922, 1601, 1552, 1521, 1461, 1432, 1290, 1173; HR-MS (*m*/*z*) for: $C_{22}H_{20}N_2NaO_4$ (M+Na): Calculated, 399.1321, found 399.1322.

**5.2. (6,7-Dihydro-5*H*-pyrrolo[1,2-*a*]imidazole-2,3-diyl)bis((4-chlorophenyl)methanone) (7b)[1]**



Compound **7b** was prepared using L-proline, 4-chlorophenylglyoxal and p-toluenesulfonamide as starting materials to obtain the product as a pale yellow solid; yield: 87% (335 mg, 0.87 mmol); m.p. 178-180 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.93 (d, $J$ = 8.4 Hz, 2H), 7.65 (d, $J$ = 8.4 Hz, 2H), 7.38 (d, $J$ = 8.1 Hz, 2H), 7.31-7.28 (m, 2H), 4.30 (t, $J$ = 7.2 Hz, 2H), 3.03 (d, $J$ = 7.2 Hz, 2H), 2.75 (t, $J$ = 7.2 Hz, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ; 187.2, 185.6, 156.9, 147.8, 139.5, 139.4, 136.3, 135.6, 131.6, 130.2, 129.8, 128.8, 128.5, 45.8, 26.1, 23.3; FT-IR (KBr, cm$^{-1}$): 2930, 2851, 1657, 1632, 1586, 1376, 1217; HR-MS (*m*/*z*) for: $C_{20}H_{15}Cl_2N_2O_2$ (M+H): Calculated, 385.0511, found 385.0515 (One of the major peaks).

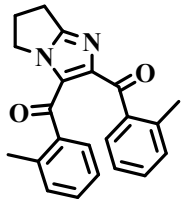
**5.3. (6,7-Dihydro-5*H*-pyrrolo[1,2-*a*]imidazole-2,3-diyl)bis(thiophen-3-ylmethanone) (7c)**



Compound **7c** was prepared using L-proline, thiophene-3-glyoxal and p-toluenesulfonamide as starting materials to obtain the product as a brown solid; yield: 89% (292 mg, 0.89 mmol); m.p. 124-126 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.47-8.46 (m, 1H), 7.84 (dd, $J_1$ = 2.7 Hz, $J_2$ = 0.9 Hz, 1H), 7.58 (dd, $J_1$ = 5.1

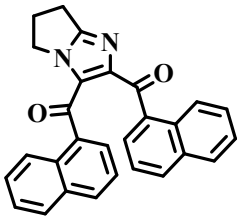
Hz, $J_2$ = 0.9 Hz, 1H), 7.39 (dd, $J_1$ = 5.1 Hz, $J_2$ = 0.9 Hz, 1H), 7.25-7.22 (m, 2H), 4.24 (t, $J$ = 7.2 Hz, 2H), 3.02 (t, $J$ = 7.2 Hz, 2H), 2.76-2.66 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 181.8, 180.4, 156.3, 147.8, 142.1, 141.8, 135.2, 133.6, 130.6, 128.2, 127.3, 126.5, 125.7, 45.5, 26.1, 23.3; FT-IR (KBr, cm$^{-1}$): 2952, 1632, 1590, 1561, 1501, 1470, 1331, 1209; HR-MS (*m*/*z*) for: $C_{16}H_{12}N_2NaO_2S_2$ (M+Na): Calculated, 351.0238, found 351.0240.

### 5.4. (6,7-Dihydro-5*H*-pyrrolo[1,2-*a*]imidazole-2,3-diyl)bis(o-tolylmethanone) (7d)



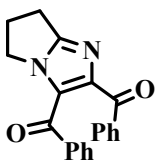
Compound **7d** was prepared using L-proline, 2-methylphenylglyoxal and p-toluenesulfonamide as starting materials to obtain the product as a brown solid; yield: 75% (258 mg, 0.75 mmol); m.p. 114-116 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.38-7.21 (m, 4H), 7.14-7.02 (m, 4H), 4.35 (t, $J$ = 7.5 Hz, 2H), 3.02 (t, $J$ = 7.8 Hz, 2H), 2.76-2.71 (m, 2H), 2.28 (s, 3H), 2.20 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 191.3, 188.1, 157.4, 149.9, 138.8, 138.2, 138.1, 137.7, 131.4, 131.4, 131.2, 131.2, 130.6, 130.1, 129.2, 125.2, 125.1, 46.2, 26.2, 23.3, 20.9, 20.2; FT-IR (KBr, cm$^{-1}$): 2935, 1615, 1584, 1541, 1480, 1449, 1312, 1201; HR-MS (*m*/*z*) for: $C_{22}H_{21}N_2O_2$ (M+H): Calculated, 345.1603, found 345.1606.

### 5.5. (6,7-Dihydro-5*H*-pyrrolo[1,2-*a*]imidazole-2,3-diyl)bis(naphthalen-1-ylmethanone) (7e)



Compound **7e** was prepared using L-proline, naphthalene-1-glyoxal and p-toluenesulfonamide as starting materials to obtain the product as a dark brown solid; yield: 85% (354 mg, 0.85 mmol); m.p. 100-102 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.16 (d, $J$ = 7.8 Hz, 1H), 8.03-8.00 (m, 1H), 7.57-7.25 (m, 10H), 6.99 (t, $J$ = 7.5 Hz, 2H), 4.44 (t, $J$ = 7.2 Hz, 2H), 3.09 (d, $J$ = 7.2 Hz, 2H), 2.83-2.73 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 190.5, 187.1, 157.9, 150.3, 136.1, 135.7, 133.2, 133.1, 132.1, 131.3, 130.0, 129.7, 129.4, 128.8, 128.1, 127.9, 127.1, 126.3, 126.1, 125.9, 125.2, 124.0, 123.7, 46.4, 26.2, 23.4; FT-IR (KBr, cm$^{-1}$): 2955, 1648, 1592, 1579, 1518, 1487, 1348, 1211; HR-MS (*m*/*z*) for: $C_{28}H_{21}N_2O_2$ (M+H): Calculated, 417.1603, found 417.1601.

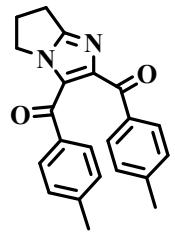
### 5.6. (6,7-Dihydro-5*H*-pyrrolo[1,2-*a*]imidazole-2,3-diyl)bis(phenylmethanone) (7f)[1]



Compound **7f** was prepared using L-proline, phenylglyoxal and p-toluenesulfonamide as starting materials to obtain the product as a yellow solid; yield: 90% (285 mg, 0.90 mmol); m.p. 160-162 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.87-7.84 (m, 2H), 7.67-7.64 (m, 2H), 7.52-7.42 (m, 2H), 7.38-7.25 (m, 4H),

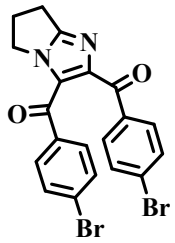
4.36-4.31 (m, 2H), 3.05 (t, $J$ = 7.5 Hz, 2H), 2.81-2.70 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 189.1, 186.9, 156.9, 148.5, 138.2, 137.6, 132.9, 132.7, 130.0, 129.7, 128.9, 128.4, 128.2, 45.8, 26.1, 23.4; FT-IR (KBr, cm$^{-1}$): 2962, 1641, 1599, 1572, 1510, 1481, 1340, 1220; HR-MS (*m*/*z*) for: $C_{20}H_{17}N_2O_2$ (M+H): Calculated, 317.1290, found 317.1287.

**5.7. (6,7-Dihydro-5*H*-pyrrolo[1,2-*a*]imidazole-2,3-diyl)bis(p-tolylmethanone) (7g)**



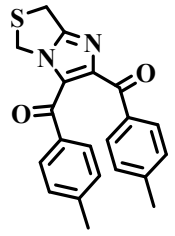
Compound **7g** was prepared using L-proline, 4-methylphenylglyoxal and p-toluenesulfonamide as starting materials to obtain the product as a brown solid; yield: 89% (306 mg, 0.89 mmol); m.p. 98-100 °C; $^1$H NMR (300 MHz, $DCl_3$): 7.81 (d, $J$ = 8.1 Hz, 2H), 7.59 (d, $J$ = 8.1 Hz, 2H), 7.17 (d, $J$ = 7.8 Hz, 2H), 7.07 (d, $J$ = 7.8 Hz, 2H), 4.30 (t, $J$ = 7.2 Hz, 2H), 3.02 (t, $J$ = 7.5 Hz, 2H), 2.75-2.70 (m, 2H), 2.39 (s, 3H), 2.33 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 188.8, 186.6, 156.5, 148.5, 143.7, 143.5, 135.5, 135.1, 130.2, 129.8, 129.1, 129.0, 128.8, 45.7, 26.1, 23.3, 21.7, 21.7; FT-IR (KBr, cm$^{-1}$): 2945, 1620, 1578, 1553, 1493, 1463, 1320, 1202; HR-MS (*m*/*z*) for: $C_{22}H_{21}N_2O_2$ (M+H): Calculated, 345.1603, found 345.1607.

**5.8. (6,7-Dihydro-5*H*-pyrrolo[1,2-*a*]imidazole-2,3-diyl)bis((4-bromophenyl)methanone) (7h)**



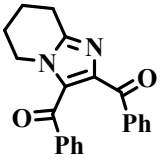
Compound **7h** was prepared using L-proline, 4-bromophenylglyoxal and p-toluenesulfonamide as starting materials to obtain the product as a brown solid; yield: 86% (408 mg, 0.86 mmol); m.p. 164-170 °C; $^1$H NMR (300 MHz, $CDCl_3$): δ 7.87-7.84 (m, 2H), 7.58-7.54 (m, 4H), 7.47-7.44 (m, 2H), 4.29 (t, $J$ = 7.5 Hz, 2H), 3.03 (t, $J$ = 7.5 Hz, 2H), 2.79-2.72 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 187.5, 185.8, 157.0, 148.0, 136.7, 136.0, 131.7, 131.7, 131.6, 131.5, 130.3, 129.8, 128.2, 45.8, 26.1, 23.3 FT-IR (KBr, cm$^{-1}$): 2980, 1663, 1615, 1590, 1531, 1501, 1363, 1241; HR-MS (*m*/*z*) for: $C_{20}H_{15}Br_2N_2O_2$ (M+H): Calculated, 472.9500, found 472.9497 (One of the peak).

**5.9. (5H,7H-imidazo[1,2-c]thiazole-2,3-diyl)bis(p-tolylmethanone) (7i)**



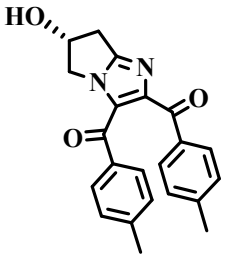
Compound **7i** was prepared using L-timonacic acid, 4-methylphenylglyoxal and p-toluenesulfonamide as starting materials to obtain the product as a brown sticky liquid (It has been performed at 80 °C); yield: 75% (272 mg, 0.75 mmol); $^1$H NMR (300 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.1 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.08 (d, *J* = 7.8 Hz, 2H), 5.31 (t, *J* = 1.8 Hz, 2H), 4.20 (t, *J* = 1.8 Hz, 2H), 2.40 (s, 3H), 2.34 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 188.4, 186.1, 153.7, 149.2, 144.1, 143.9, 135.1, 134.6, 130.2, 129.1, 129.1, 128.9, 128.1, 46.7, 26.9, 21.7, 21.6; FT-IR (neat, cm$^{-1}$): 2985, 1675, 1625, 1570, 1551, 1509, 1383, 1249; HR-MS (*m*/*z*) for: $C_{21}H_{19}N_2O_2S$ (M+H): Calculated, 363.1167, found 363.1171.

**5.10. (5,6,7,8-tetrahydroimidazo[1,2-a]pyridine-2,3-diyl)bis(phenylmethanone) (7j)**




Compound **7j** was prepared using L-pipecolic acid, phenylglyoxal and p-toluenesulfonamide as starting materials to obtain the product as a yellow sticky liquid; yield: 72% (238 mg, 0.72 mmol); $^1$H NMR (300 MHz, $CDCl_3$): δ 7.84-7.81 (m, 2H), 7.66-7.63 (m, 2H), 7.50-7.42 (m, 2H), 7.35-7.27 (m, 4H), 4.22 (t, *J* = 6.9 Hz, 2H), 3.07 (t, *J* = 5.7 Hz, 2H), 2.09-2.03 (m, 4H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 189.2, 187.7, 148.0, 143.8, 138.6, 137.8, 133.0, 132.6, 131.7, 129.9, 129.0, 128.4, 128.1, 45.2, 25.1, 22.7, 20.1; FT-IR (neat, cm$^{-1}$): 3020, 1695, 1652, 1598, 1581, 1539, 1399, 1269; HR-MS (*m*/*z*) for: $C_{21}H_{19}N_2O_2$ (M+H): Calculated, 331.1447, found 331.1451.

**5.11. (R)-(6-hydroxy-6,7-dihydro-5H-pyrrolo[1,2-a]imidazole-2,3-diyl)bis(phenylmethanone) (7k)**




Compound **7k** was prepared using L-4-hydroxyproline, 4-methylphenylglyoxal and *p*-toluenesulfonamide as starting materials to obtain the product as a brown sticky liquid; yield: 74% (267 mg, 0.74 mmol); $^1$H NMR (300 MHz, $CDCl_3$): δ 7.82 (d, *J* = 8.1 Hz, 2H), 7.63 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 7.8 Hz, 2H), 7.06 (d, *J* = 7.8 Hz, 2H), 5.78-5.68 (m, 1H), 4.76-4.71 (m, 1H), 4.50-4.43 (m, 1H), 3.78-3.70 (m, 1H), 3.49-3.43 (m, 1H), 2.84 (brs, 1H), 2.38 (s, 3H), 2.32 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 188.8, 186.5, 155.0, 149.0, 144.6, 143.9, 135.8, 135.3, 132.3, 130.9, 130.1, 128.8, 128.7, 65.6, 48.6, 30.6, 21.7, 21.4; FT-IR (neat, cm$^{-1}$): 3330, 3025, 1685, 1660, 1585, 1590, 1545, 1389, 1280; HR-MS (*m*/*z*) for: $C_{22}H_{21}N_2O_3$ (M+H): Calculated, 361.1552, found 361.1556.

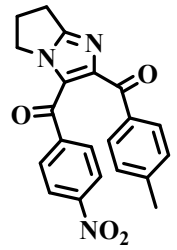
**6. General procedure for the synthesis of unsymmetrical 6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazoles (8a-n)**

In a dry seal tube, 1.1 mmol of L-prolinee (**1**) and 1 mmol of phenylglyoxal (**2**) were dissolved in anhydrous toluene (5 mL), and the reaction mixture was stirred at 140 ºC. After 5-10 minutes, when reaction mixture turned red, 1 mmol of immine (prepared by phenylglyoxal and p-toluenesulfonamide) (**5**), 1.0 mmol of $K_2CO_3$ and 5 mol% of CuI were added. The seal tube was immediately sealed and the

reaction mixture was stirred at 110 °C. The progress of the reaction was monitored by thin layer chromatography (TLC). The post-reaction mixture was extracted with ethyl acetate (2x10 mL). The combined organic layer was washed with water (3x10 mL) and brine (1x10 mL). It was dried over activated $Na_2SO_4$, filtered and evaporated in a rotary evaporator under reduced pressure at room temperature. Purification of the crude product mixture by column chromatography on silica gel (100-200 mesh) with ethyl acetate-petroleum ether (1:1 v/v) as an eluent afforded the corresponding 6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazole (**8a-n)**. All the synthesised compounds were characterized by relevent spectroscopic analyses and finally structure was confirmed through the single crystal XRD analysis of compound **8c**.

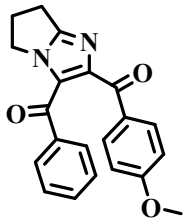
**7. Characterization data of the synthesized unsymmetrical 6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazoles (8a-n)**

**7.1. (2-(4-Methylbenzoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-3-yl)(4-nitrophenyl)methanone (8a)**



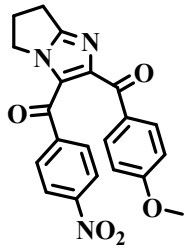
Compound **8a** was prepared using L-proline, 4-nitrophenylglyoxal and immine (prepared by 4-methylphenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as brown solid; yield: 86% (323 mg, 0.86 mmol); m.p.-138-140 °C; $^1$H NMR (300 MHz, $CDCl_3$): δ 8.13 (d, *J* = 8.7 Hz, 2H), 7.86-7.81 (m, 4H), 7.22 (d, *J* = 8.1 Hz, 2H), 4.38 (t, *J* = 7.2 Hz, 2H), 3.07 (t, *J* = 7.5 Hz, 2H), 2.80-2.76 (m, 2H), 2.42 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 188.5, 185.0, 157.7, 150.2, 149.8, 144.3, 143.3, 134.4, 130.4, 129.5, 129.1, 128.8, 123.5, 46.2, 26.1, 23.4, 21.7; FT-IR (KBr, cm$^{-1}$): 2982, 1662, 1615, 1590, 1532, 1499, 1361, 1241; HR-MS (*m*/*z*) for: $C_{21}H_{18}N_3O_4$ (M+H): Calculated, 376.1297, found 376.1301.

**7.2. (3-Benzoyl-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-2-yl)(4-methoxyphenyl)methanone (8b)**



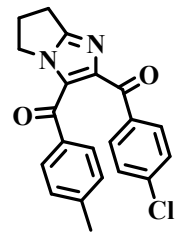
Compound **8b** was prepared using L-proline, phenylglyoxal and immine (prepared by 4-methoxyphenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as dark brown gummy liquid; yield: 92% (319 mg, 0.92 mmol); $^1$H NMR (300 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 7.2 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 2H), 6.83 (d, *J* = 8.7 Hz, 2H), 4.32-4.27 (m, 2H), 3.83 (s, 3H), 3.01 (t, *J* = 7.5 Hz, 2H), 2.71 (t, *J* = 7.5 Hz, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 187.6, 186.8, 163.2, 156.7, 149.0, 138.1, 132.7, 132.3, 130.4, 129.2, 128.7, 128.2, 113.3, 55.3, 45.7, 26.0, 23.2; FT-IR (neat, cm$^{-1}$): 2942, 1620, 1579, 1555, 1500, 1465, 1325, 1212; HR-MS (*m*/*z*) for: $C_{21}H_{18}N_2NaO_3$ (M+Na): Calculated, 369.1215, found 369.1212.

**7.3. (2-(4-Methoxybenzoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-3-yl)(4-nitrophenyl)methanone (8c)**



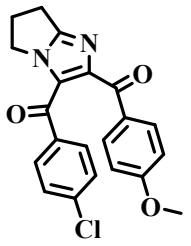
Compound **8c** was prepared using L-proline, 4-nitrophenylglyoxal and immine (prepared by 4-methoxyphenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as dark brown solid; yield: 89% (348 mg, 0.89 mmol); m.p. 122-124 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.11 (d, *J* = 8.7 Hz, 2H), 7.94 (d, *J* = 9.0 Hz, 2H), 7.80 (d, *J* = 8.7 Hz, 2H), 6.89 (d, *J* = 9.0 Hz, 2H), 4.37 (t, *J* = 7.2 Hz, 2H), 3.87 (s, 3H), 3.05 (t, *J* = 7.5 Hz, 2H), 2.79-2.74 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 187.3, 184.9, 163.8, 157.7, 150.4, 149.7, 143.3, 132.7, 129.8, 129.4, 128.6, 123.5, 113.7, 55.5, 46.2, 26.1, 23.4; FT-IR (KBr, $cm^{-1}$): 2955, 1646, 1595, 1576, 1517, 1484, 1347, 1215; HR-MS (*m*/*z*) for: $C_{21}H_{18}N_3O_5$ (M+H): Calculated, 392.1246, found 392.1248.

**7.4. (2-(4-Chlorobenzoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-3-yl)(p-tolyl)methanone (8d)**



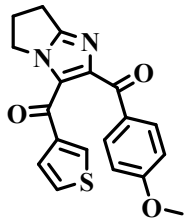
Compound **8d** was prepared using L-proline, 4-methylphenylglyoxal and immine (prepared by 4-chlorophenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as off white solid; yield: 88% (321 mg, 0.88 mmol); m.p. 168-170 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.90 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.1 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 8.1 Hz, 2H), 4.28 (t, *J* = 7.2 Hz, 2H), 3.04 (t, *J* = 7.2 Hz, 2H), 2.76-2.71 (m, 2H), 2.35 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 187.4, 186.5, 156.5, 147.2, 144.1, 139.1, 135.9, 135.3, 131.5, 130.2, 129.2, 129.1, 128.4, 45.7, 26.1, 23.3, 21.7; FT-IR (KBr, $cm^{-1}$): 2960, 1645, 1596, 1576, 1514, 1485, 1335, 1222; HR-MS (*m*/*z*) for: $C_{21}H_{17}ClN_2NaO_2$ (M+Na): Calculated, 387.0876, found 387.0871 (one of the major peaks).

**7.5. (3-(4-Chlorobenzoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-2-yl)(4-methoxyphenyl)methanone (8e)**



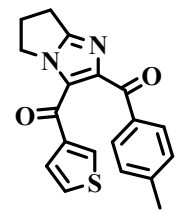
Compound **8e** was prepared using L-proline, 4-chlorophenylglyoxal and immine (prepared by 4-methoxyphenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as yellow solid; yield: 90% (343 mg, 0.90 mmol); m.p. 174-176 °C; $^1$H NMR (300 MHz, $CDCl_3$): δ 7.94 (d, $J$ = 8.7 Hz, 2H), 7.62 (d, $J$ = 8.4 Hz, 2H), 7.25 (d, $J$ = 8.4 Hz, 2H), 6.88 (d, $J$ = 8.7 Hz, 2H), 4.31 (t, $J$ = 7.5 Hz, 2H), 3.87 (s, 3H), 3.03 (t, $J$ = 7.5 Hz, 2H), 2.76-2.71 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 187.5, 185.6, 163.5, 156.9, 149.3, 139.1, 136.6, 132.5, 130.3, 130.2, 128.6, 116.9, 113.5, 55.5, 45.8, 26.1, 23.3; FT-IR (KBr, cm$^{-1}$): 2952, 1630, 1581, 1561, 1501, 1471, 1330, 1211; HR-MS (*m*/*z*) for: $C_{21}H_{18}ClN_2O_3$ (M+H): Calculated, 381.1006, found 381.1009 (one of the major peaks).

### 7.6. (2-(4-Methoxybenzoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-3-yl)(thiophen-3-yl)methanone (8f)



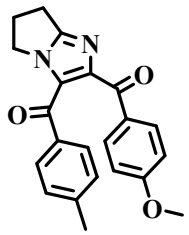
Compound **8f** was prepared using L-proline, thiophene-3-glyoxal and immine (prepared by 4-methoxyphenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as a brown solid; yield: 89% (314 mg, 0.89 mmol); m.p. 130-132 °C; $^1$H NMR (300 MHz, $CDCl_3$): δ 7.96-7.90 (m, 2H), 7.77-7.76 (m, 1H), 7.31-7.29 (m, 1H), 7.16 (dd, $J_1$ = 5.1 Hz, $J_2$ = 3.0 Hz, 1H), 6.85 (d, $J$ = 8.7 Hz, 2H), 4.29 (t, $J$ = 7.2 Hz, 2H), 3.84 (s, 3H), 3.01 (t, $J$ = 7.5 Hz, 2H), 2.76-2.66 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 188.0, 180.0, 163.4, 156.7, 148.6, 142.2, 133.2, 132.3, 130.6, 130.1, 127.2, 126.5, 113.5, 55.5, 45.7, 26.1, 23.3; FT-IR (KBr, cm$^{-1}$): 2950, 1630, 1589, 1562, 1500, 1471, 1330, 1210; HR-MS (*m*/*z*) for: $C_{19}H_{17}N_2O_3S$ (M+H): Calculated, 353.0960, found 353.0958.

### 7.7. (2-(4-Methylbenzoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-3-yl)(thiophen-3-yl)methanone (8g)



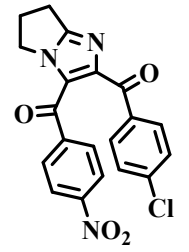
Compound **8g** was prepared using L-proline, thiophene-3-glyoxal and immine (prepared by 4-methylphenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as brown solid; yield: 91% (306 mg, 0.91 mmol) m.p. 138-140 °C; $^1$H NMR (300 MHz, $CDCl_3$): δ 7.82-7.75 (m, 3H), 7.28 (dd, $J_1$ = 5.1 Hz, $J_2$ = 1.2 Hz, 1H), 7.18-7.14 (m, 3H), 4.28 (t, $J$ = 7.2 Hz, 2H), 3.00 (t, $J$ = 7.5 Hz, 2H), 2.73-2.68 (m, 2H), 2.37 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 189.0, 180.0, 156.7, 148.4, 143.6, 142.2, 135.1, 133.2, 130.3, 130.0, 128.9, 127.2, 126.4, 45.7, 26.1, 23.3, 21.7; FT-IR (KBr, cm$^{-1}$): 2957, 1635, 1594, 1567, 1505, 1475, 1334, 1213; HR-MS (*m*/*z*) for: $C_{19}H_{17}N_2O_2S$ (M+H): Calculated, 337.1011, found 337.1015.

**7.8. (2-(4-Methoxybenzoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-3-yl)(p-tolyl)methanone (8h)**



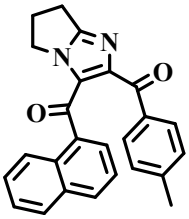
Compound **8h** was prepared using L-proline, 4-methylphenylglyoxal and immine (prepared by 4-methoxyphenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as a brown solid; yield: 91% (328 mg, 0.91 mmol); m.p. 75-77 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.93 (d, $J$ = 9.0 Hz, 2H), 7.60 (d, $J$ = 8.1 Hz, 2H), 7.08 (d, $J$ = 8.1 Hz, 2H), 6.87-6.84 (m, 2H), 4.32-4.27 (m, 2H), 3.86 (s, 3H), 3.03 (t, $J$ = 7.5 Hz, 2H), 2.75-2.70 (m, 2H), 2.33 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 187.7, 186.6, 163.3, 156.5, 148.7, 143.7, 135.5, 132.5, 130.6, 129.6, 129.1, 128.8, 113.4, 55.4, 45.7, 26.1, 23.3, 21.6; FT-IR (KBr, cm$^{-1}$): 2925, 1601, 1545, 1530, 1470, 1440, 1301, 1182; HR-MS (*m*/*z*) for: $C_{22}H_{21}N_2O_3$ (M+H): Calculated, 361.1552, found 361.1556.

**7.9. (2-(4-Chlorobenzoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-3-yl)(4-nitrophenyl)methanone (8i)**



Compound **8i** was prepared using L-proline, 4-nitrophenylglyoxal and immine (prepared by 4-chlorophenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as a brown solid; yield: 85% (336 mg, 0.85 mmol); m.p. 206-208 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.17 (d, $J$ = 8.7 Hz, 2H), 7.98 (d, $J$ = 8.4 Hz, 2H), 7.86 (d, $J$ = 8.4 Hz, 2H), 7.41 (d, $J$ = 8.7 Hz, 2H), 4.36 (t, $J$ = 7.2 Hz, 2H), 3.07 (t, $J$ = 7.5 Hz, 2H), 2.80-2.76 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 187.1, 185.0, 157.5, 149.9, 149.0, 143.0, 139.8, 135.1, 131.8, 129.5, 129.4, 128.7, 123.6, 46.1, 26.1, 23.4; FT-IR (KBr, cm$^{-1}$): 2999, 1682, 1635, 1611, 1552, 1523, 1385, 1261; HR-MS (*m*/*z*) for: $C_{20}H_{14}ClN_3NaO_4$ (M+Na): Calculated, 418.0571, found 418.0569 (one of the major peaks).

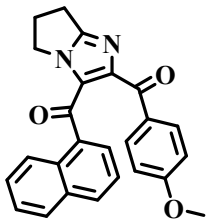
**7.10. (3-(1-Naphthoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-2-yl)(p-tolyl)methanone (8j)**



Compound **8j** was prepared using L-proline, naphthalene-1-glyoxal and immine (prepared by 4-methylphenylglyoxal and *p*-toluenesulfonamide) as starting materials to obtain the product as brown solid; yield: 80% (304 mg, 0.80 mmol); m.p. 64-66 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.18-8.15 (m, 1H),

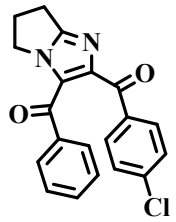
7.78 (d, *J* = 8.1 Hz, 1H), 7.70-7.67 (m, 1H), 7.52-7.40 (m, 3H), 7.28-7.21 (m, 3H), 6.71 (d, *J* = 7.8 Hz, 2H), 4.46 (t, *J* = 7.2 Hz, 2H), 3.05 (t, *J* = 7.5 Hz, 2H), 2.82-2.72 (m, 2H), 2.03 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 190.0, 186.9, 158.2, 150.1, 143.0, 136.3, 135.4, 133.5, 132.6, 130.4, 129.7, 128.7, 128.7, 128.4, 128.0, 127.1, 126.4, 125.4, 124.0, 46.5, 26.2, 23.3, 21.3; FT-IR (KBr, $cm^{-1}$): 2954, 1632, 1590, 1565, 1502, 1472, 1331, 1208; HR-MS (*m*/*z*) for: $C_{25}H_{21}N_2O_2$ (M+H): Calculated, 381.1603, found 381.1605.

**7.11. (3-(1-Naphthoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-2-yl)(4-methoxyphenyl)methanone (8k)**



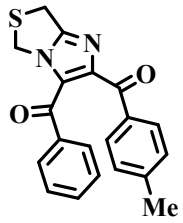
Compound **8k** was prepared using L-proline, naphthalene-1-glyoxal and immine (prepared by 4-methoxyphenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as dark brown solid; yield: 84% (333 mg, 0.84 mmol); m.p. 98-100 $^{o}$C ; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.21-8.17 (m, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.71-7.68 (m, 1H), 7.52-7.33 (m, 5H), 7.26-7.21 (m, 1H), 6.42-6.39 (m, 2H), 4.45 (t, *J* = 7.2 Hz, 2H), 3.60 (s, 3H), 3.03 (t, *J* = 7.8 Hz, 2H), 2.80-2.70 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 188.8, 186.9, 162.7, 158.1, 150.5, 136.3, 133.5, 132.5, 131.0, 130.8, 130.1, 129.8, 128.6, 128.0, 127.1, 126.3, 125.4, 124.0, 113.0, 55.1, 46.5, 26.2, 23.4; FT-IR (KBr, $cm^{-1}$): 2955, 1623, 1581, 1558, 1492, 1463, 1321, 1200; HR-MS (*m*/*z*) for: $C_{25}H_{21}N_2O_3$ (M+H): Calculated, 397.1552, found 397.1550.

**7.12. (2-(4-Methylbenzoyl)-6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazol-3-yl)(thiophen-3-yl)methanone (8l)**



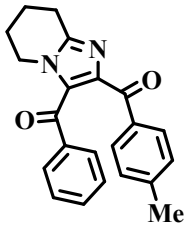
Compound **8l** was prepared using L-proline, phenylglyoxal and immine (prepared by 4-chlorophenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as a yellow solid; yield: 87% (305 mg, 0.87 mmol); m.p. 113-115 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 8.87 (d, *J* = 8.4 Hz, 2H), 7.69-7.66 (m, 2H), 7.50-7.44 (m, 1H), 7.36-7.28 (m, 4H), 4.30 (t, *J* = 7.2 Hz, 2H), 3.03 (t, *J* = 7.5 Hz, 2H), 2.79-2.71 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 187.5, 186.9, 156.8, 148.0, 139.1, 138.0, 135.9, 133.0, 131.5, 130.0, 128.9, 128.5, 128.4, 45.8, 26.1, 23.3; FT-IR (KBr, $cm^{-1}$): 2967, 1646, 1606, 1578, 1516, 1486, 1347, 1228; HR-MS (*m*/*z*) for: $C_{20}H_{16}ClN_2O_2$ (M+H): Calculated, 351.0900, found 351.0904 (one of the major peaks).

### 7.13. (3-benzoyl-5H,7H-imidazo[1,2-c]thiazol-2-yl)(p-tolyl)methanone (8m)




Compound **8m** was prepared using L-timonacic acid, phenylglyoxal and immine (prepared by 4-methylphenylglyoxal and *p*-toluenesulfonamide) as starting materials to obtain the product as a yellow sticky liquid (It has been performed at 80 °C); yield: 73% (254 mg, 0.73 mmol); $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, *J* = 6.8 Hz, 2H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.52 (t, *J* = 6.8 Hz, 1H), 7.39-7.36 (m, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 5.21 (d, *J* = 2.0 Hz, 2H), 4.22 (d, *J* = 2.0 Hz, 2H), 2.40 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 188.8, 186.4, 154.1, 149.3, 144.0, 137.8, 137.1, 133.2, 130.0, 128.9, 128.5, 128.4, 128.3, 46.9, 27.1, 21.1; FT-IR (neat, $cm^{-1}$): 2977, 1636, 1626, 1568, 1525, 1475, 1360, 1240; HR-MS (*m*/*z*) for: $C_{20}H_{17}N_2O_2S$ (M+H): Calculated, 349.1011, found 349.1015.

### 7.14. (3-benzoyl-5,6,7,8-tetrahydroimidazo[1,2-a]pyridin-2-yl)(p-tolyl)methanone (8n)



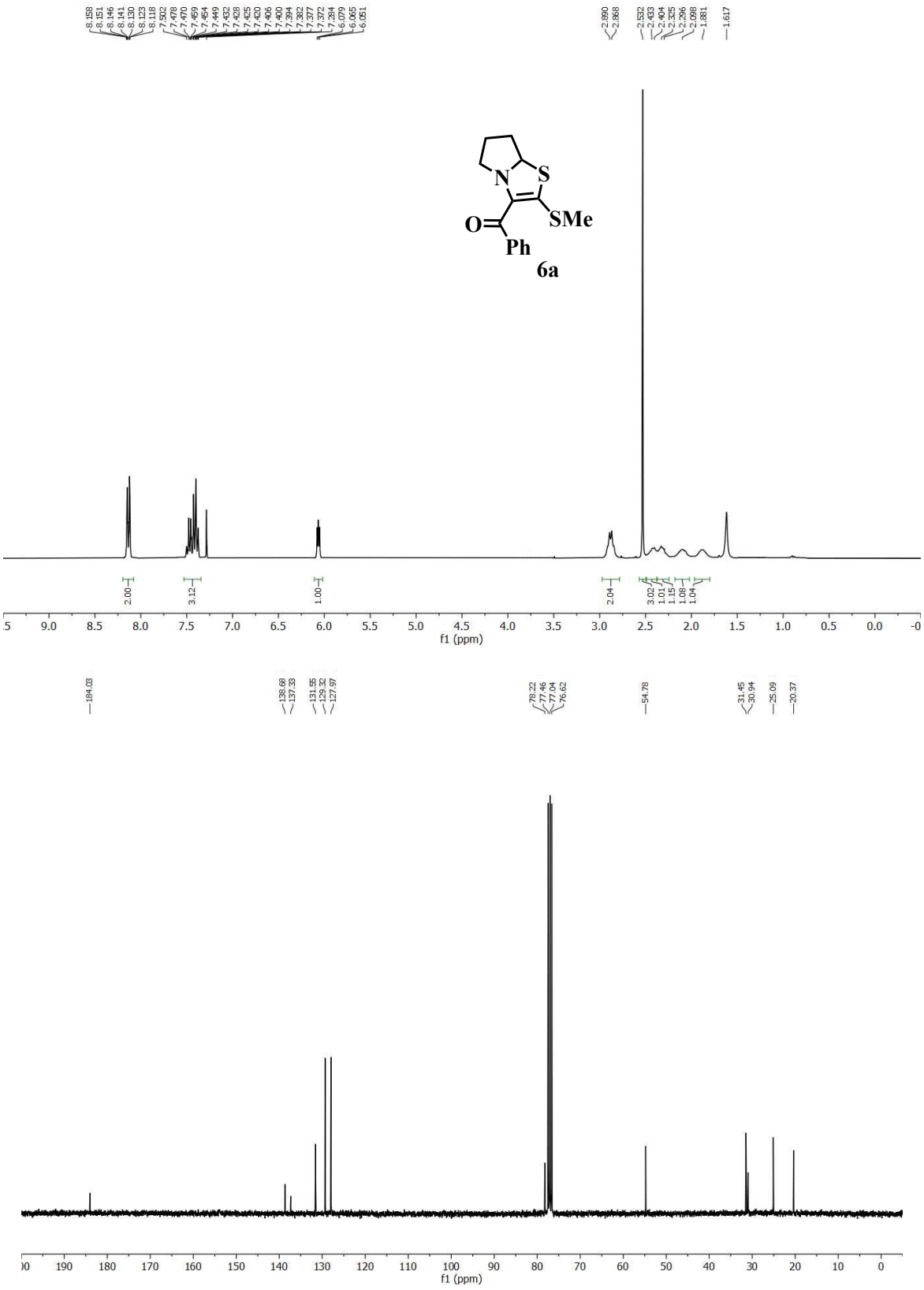

Compound **8n** was prepared using L-pipecolic acid, phenylglyoxal and immine (prepared by 4-methylphenylglyoxal and p-toluenesulfonamide) as starting materials to obtain the product as a brown sticky liquid; yield: 70% (241 mg, 0.70 mmol); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.1 Hz, 2H), 7.59 (d, *J* = 8.1 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 2H), 7.08 (d, *J* = 7.8 Hz, 2H), 4.21-4.17 (m, 2H), 3.07-3.03 (m, 2H), 2.38 (s, 3H), 2.07-2.03 (m, 4H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 188.8, 187.4, 147.6, 143.9, 143.3, 136.0, 135.3, 132.9, 131.9, 130.1, 129.2, 129.1, 128.7, 45.0, 25.0, 22.7, 21.6, 20.2; FT-IR (neat, $cm^{-1}$): 2967, 1645, 1615, 1576, 1514, 1483, 1354, 1249; HR-MS (*m*/*z*) for: $C_{22}H_{21}N_2O_2$ (M+H): Calculated, 345.1603, found 345.1607.

## 8. Reference

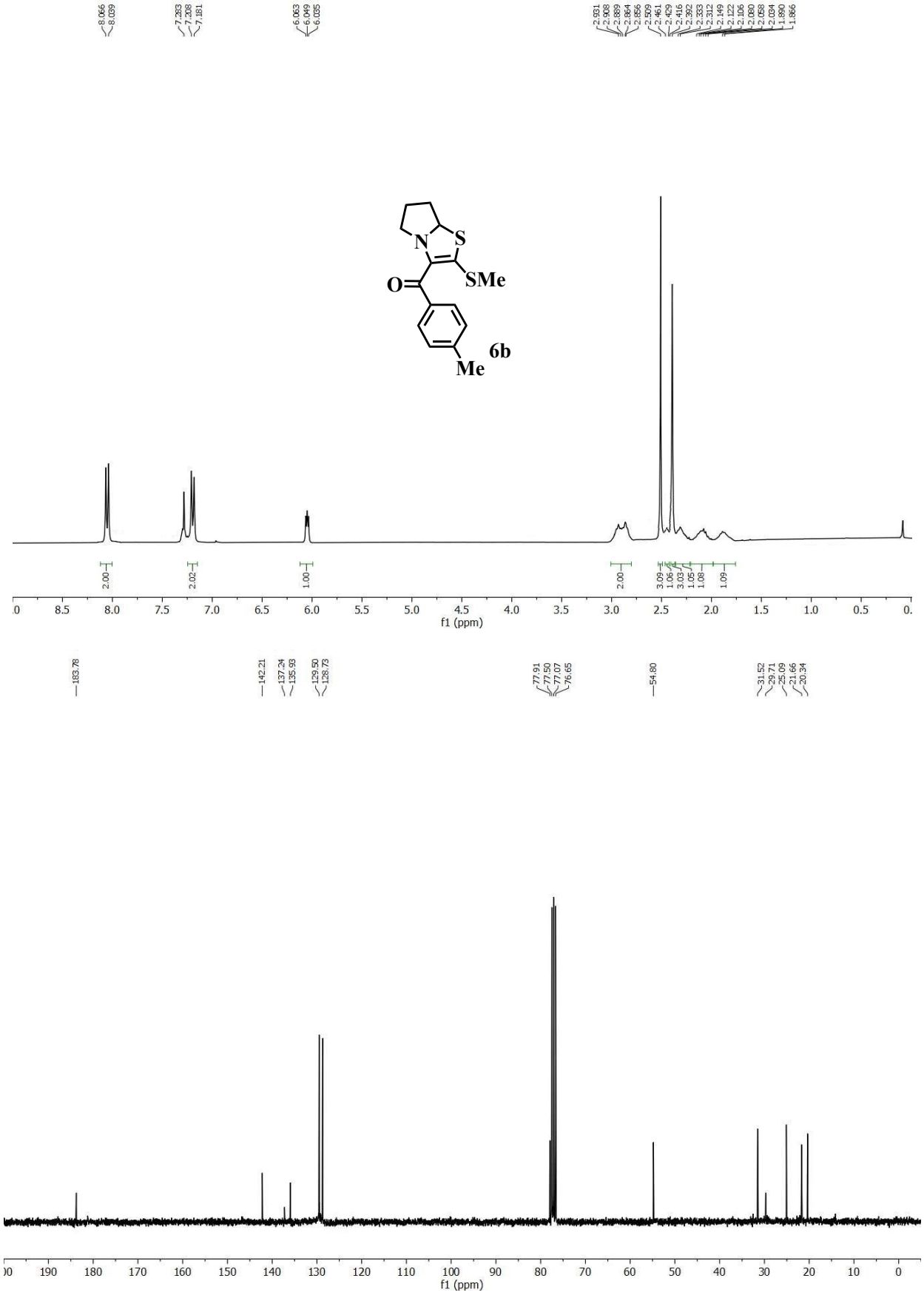
1. C. N. Reddy, M. Sathish, S. Adhikary, J. B. Nanubolu, A. Alarifi, R. A. Maurya and A. Kamal, *Org. Biomol. Chem.,* 2017, **15**, 2730.

## 9. $^{1}H$ and $^{13}C$ NMR spectra of synthesised 5,6,7,7*a*-tetrahydropyrrolo[2,1-*b*]thiazole (6a-p) and 6,7-dihydro-5*H*-pyrrolo[1,2-*a*]imidazole (7a-k, 8a-n)

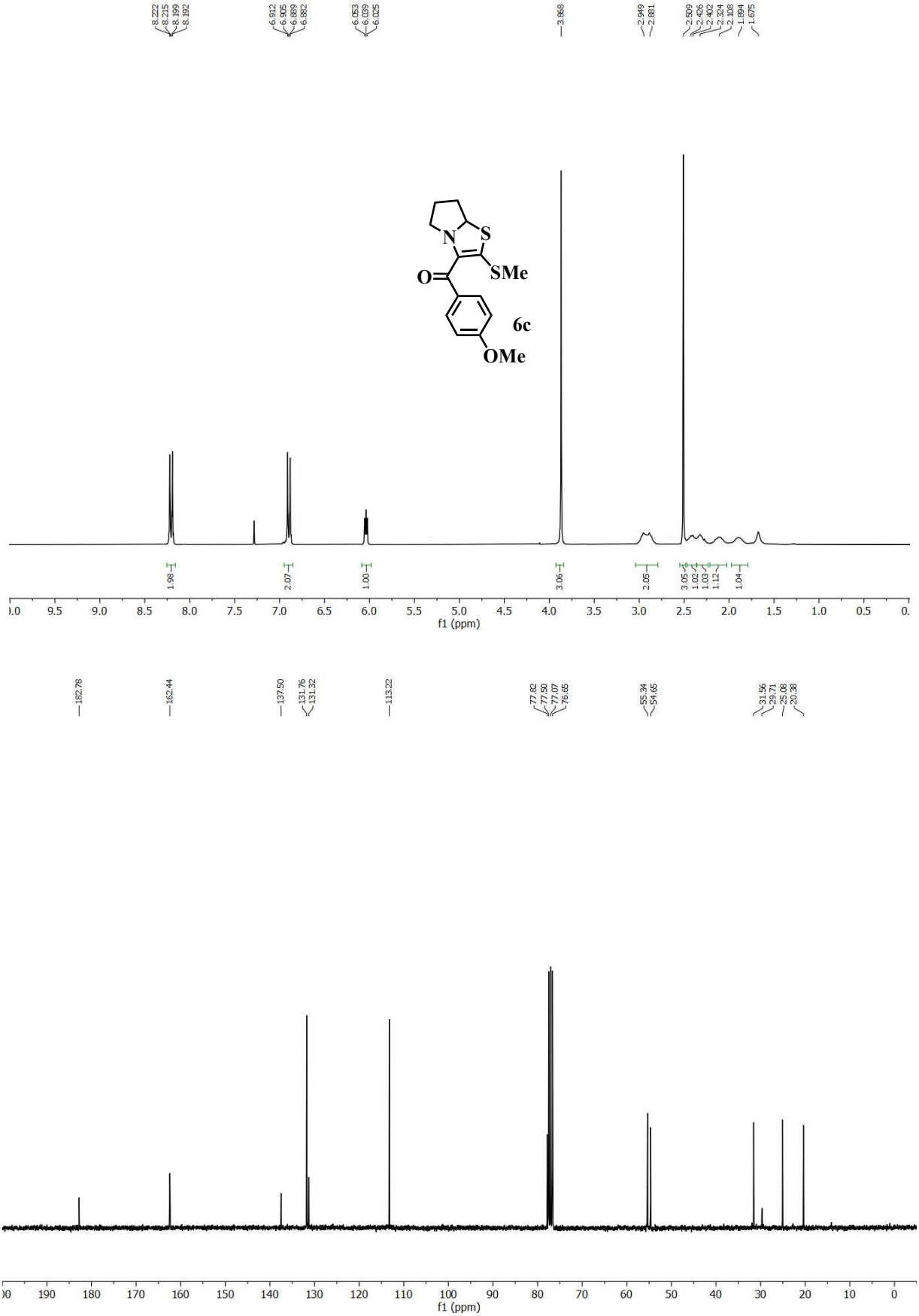
**SI Figure 1:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6a**



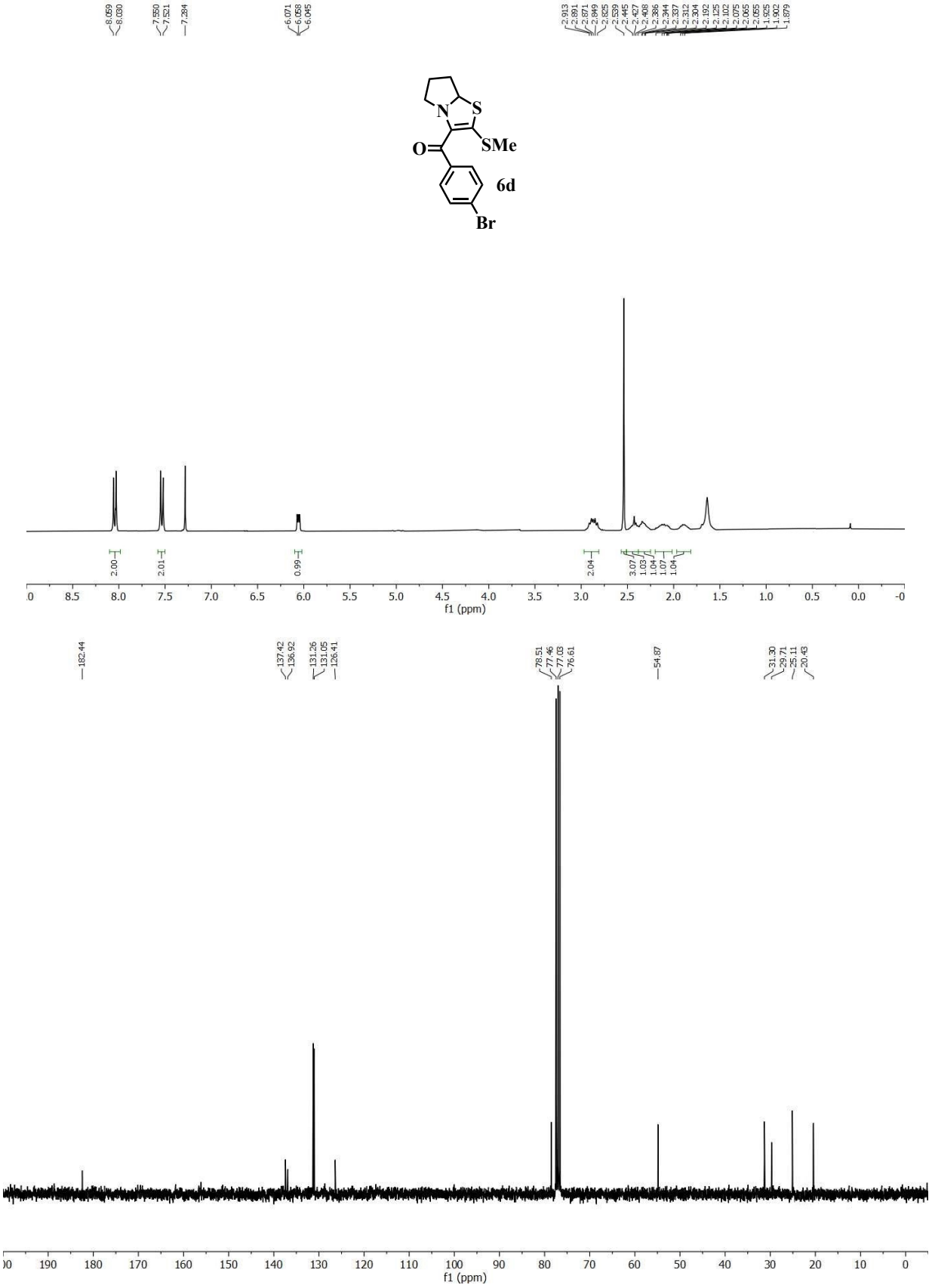
**SI Figure 2:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6b**



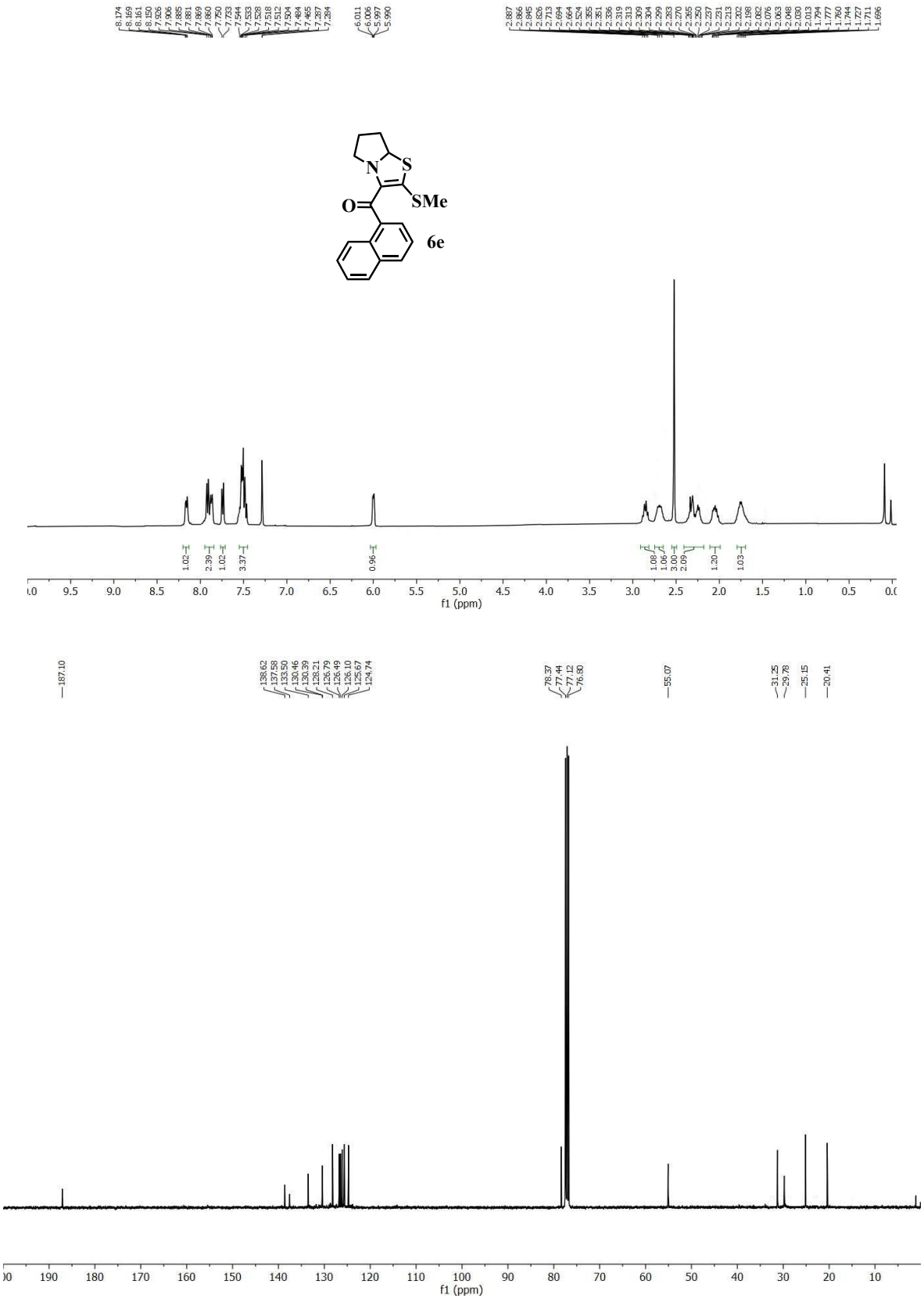
**SI Figure 3:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6c**



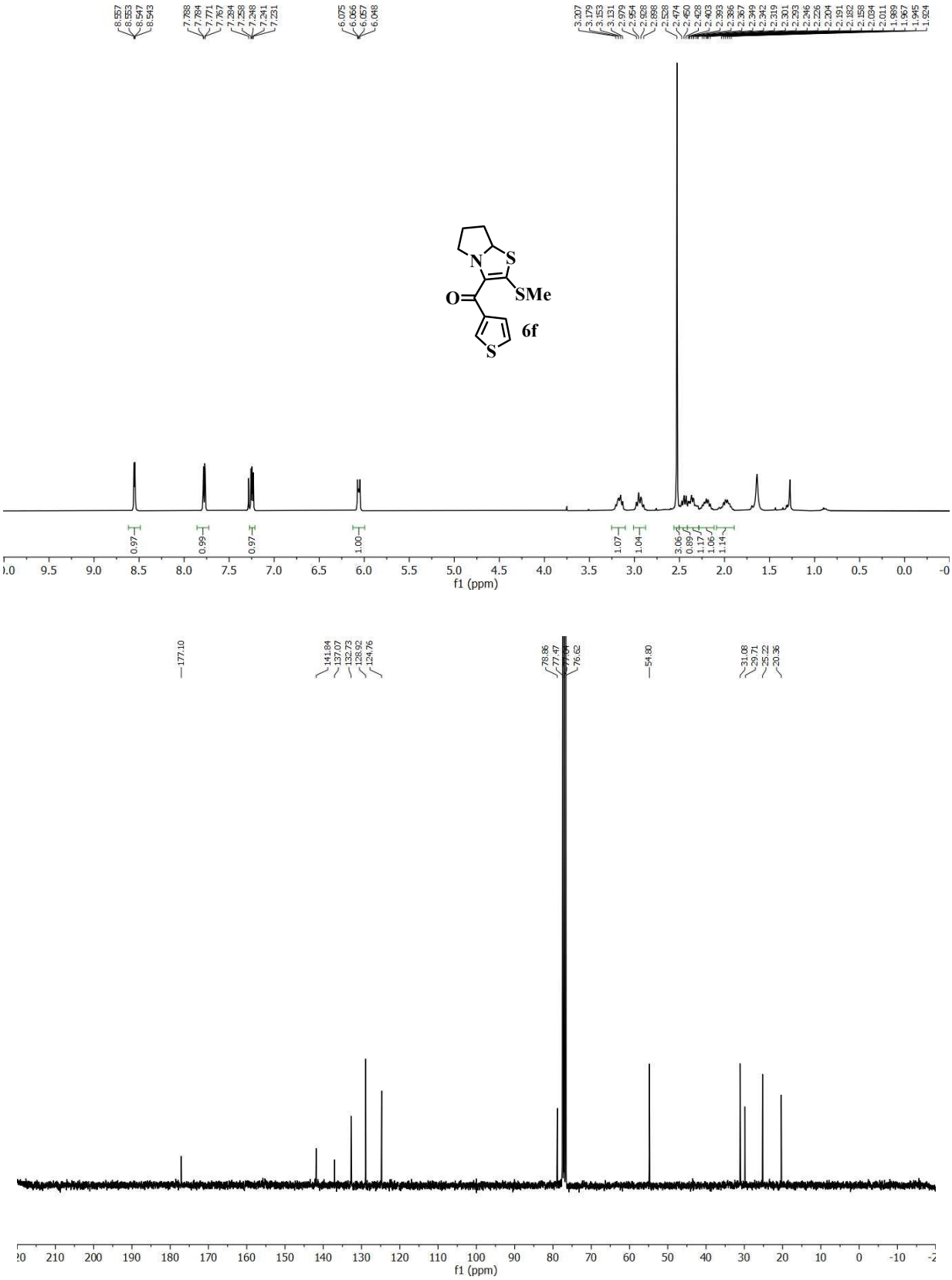
**SI Figure 4:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6d**



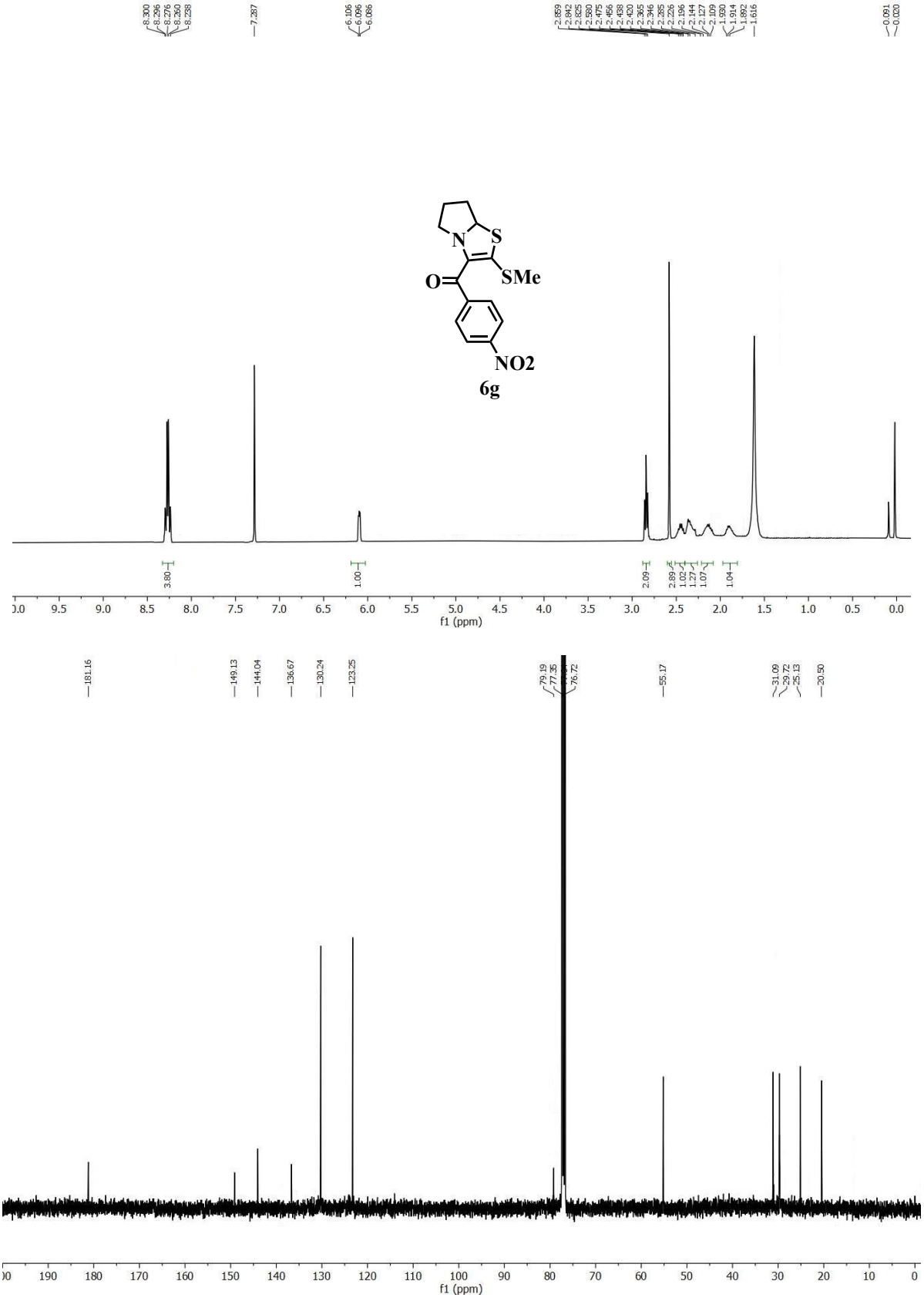
**SI Figure 5:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6e**



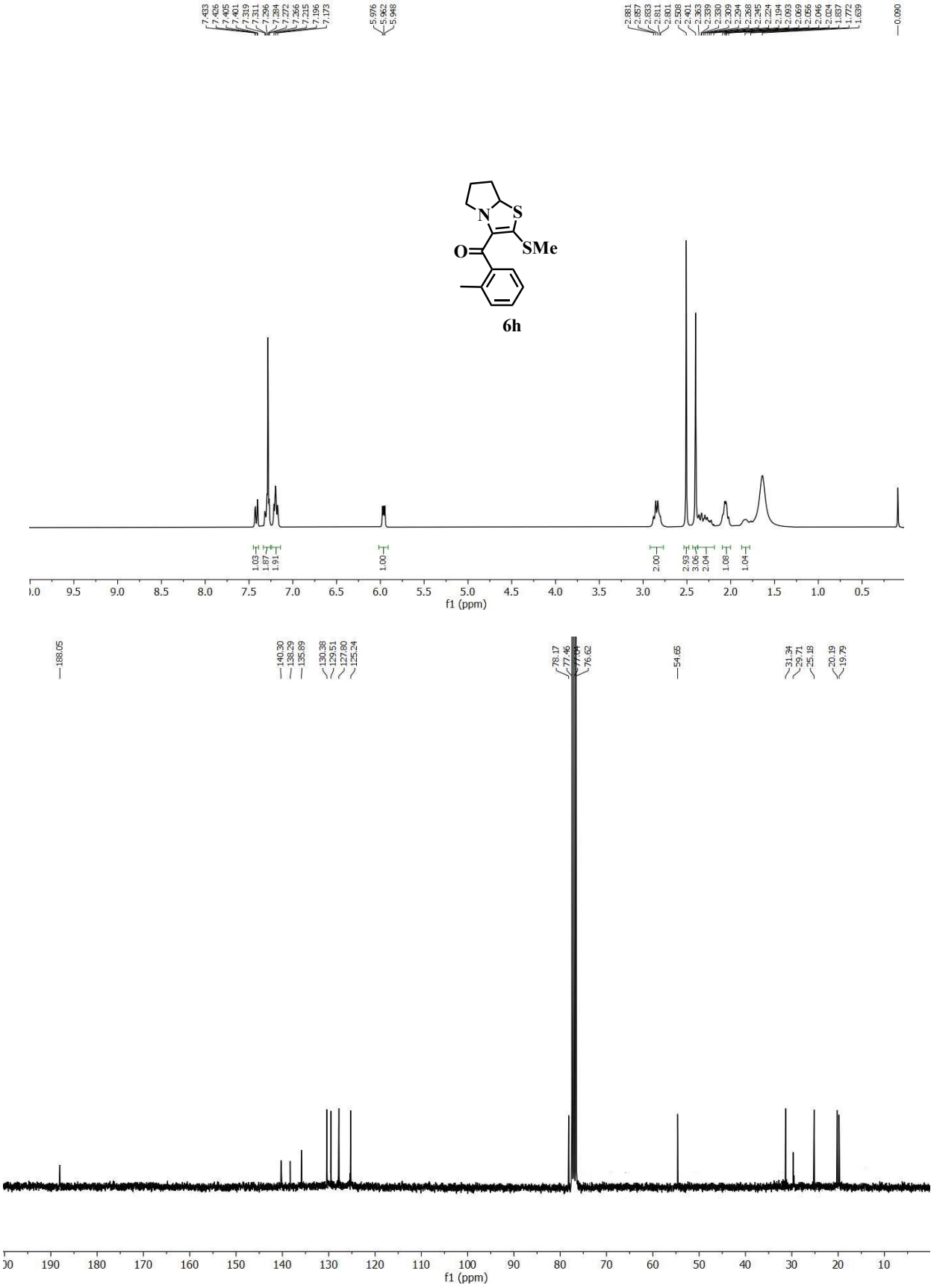
**SI Figure 6:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6f**



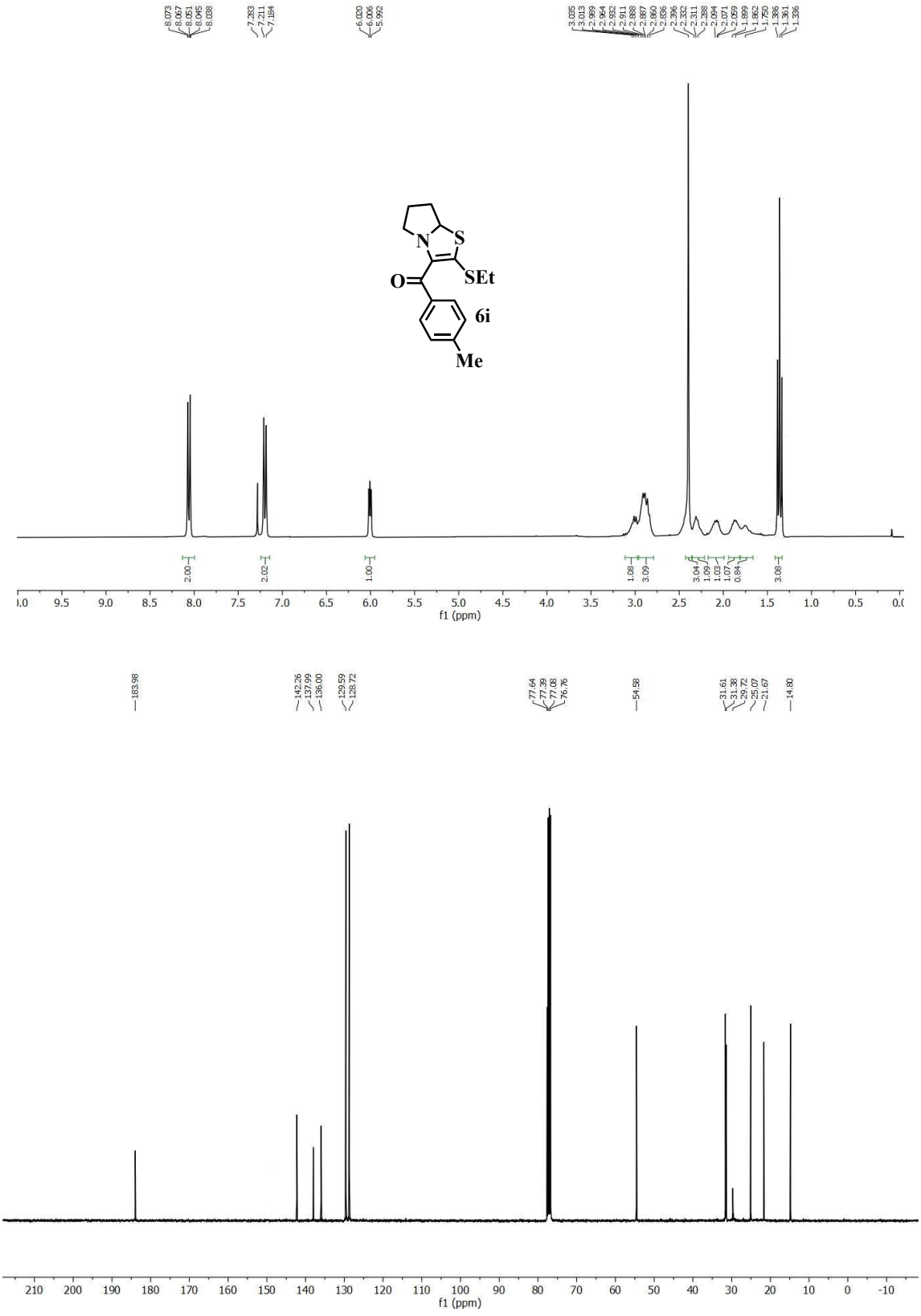
**SI Figure 7:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6g**



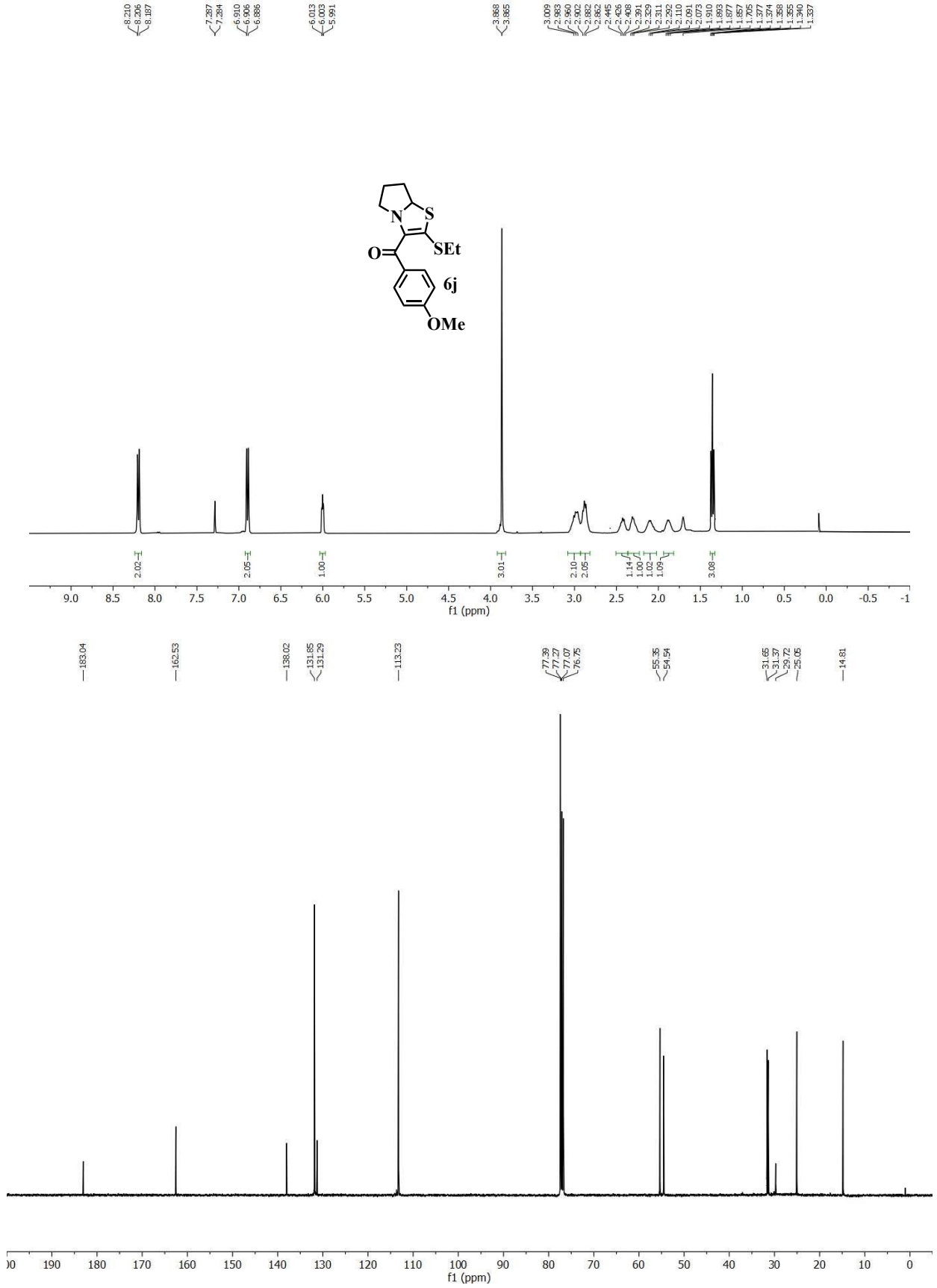
**SI Figure 8:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6h**



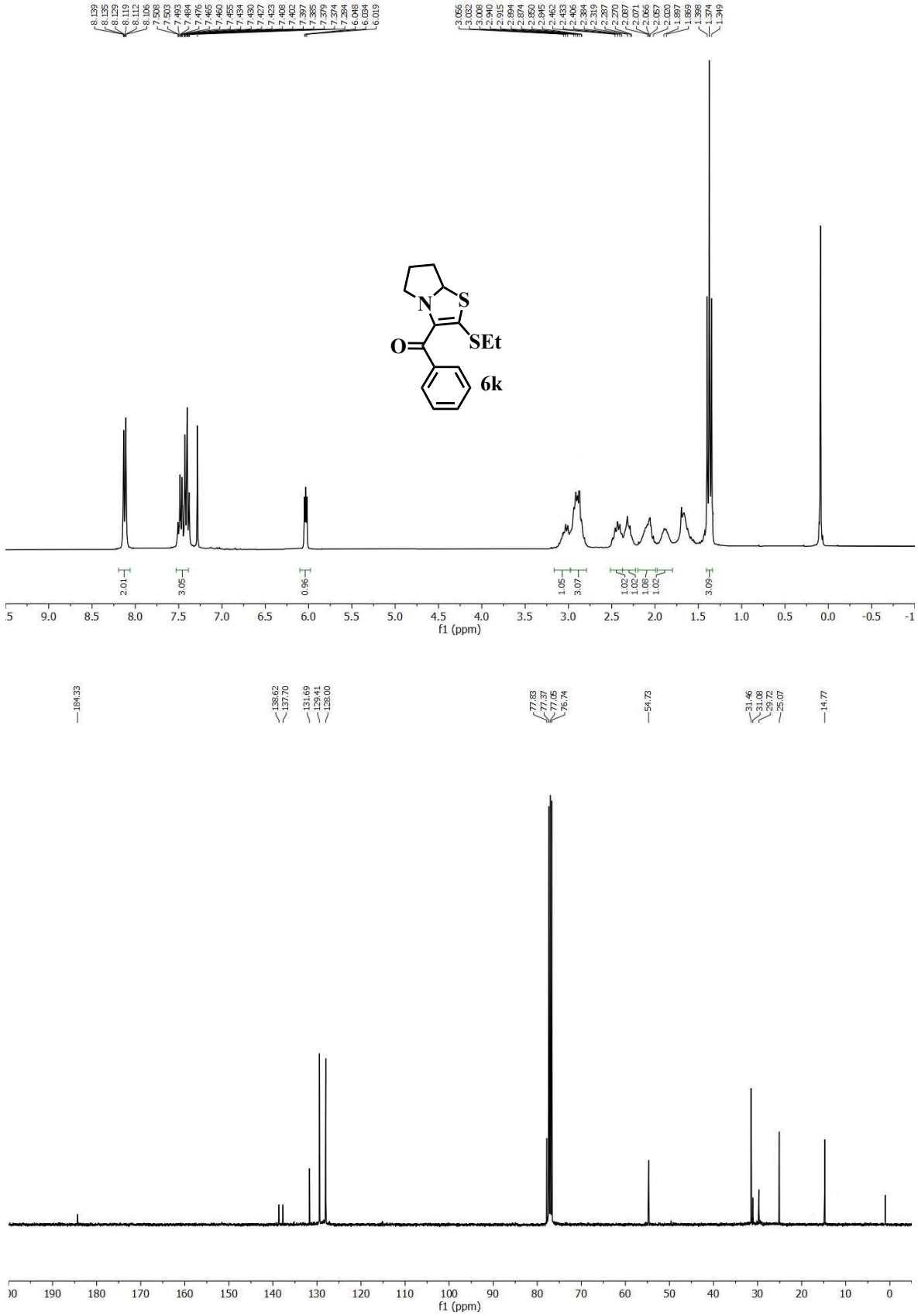
**SI Figure 9:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6i**



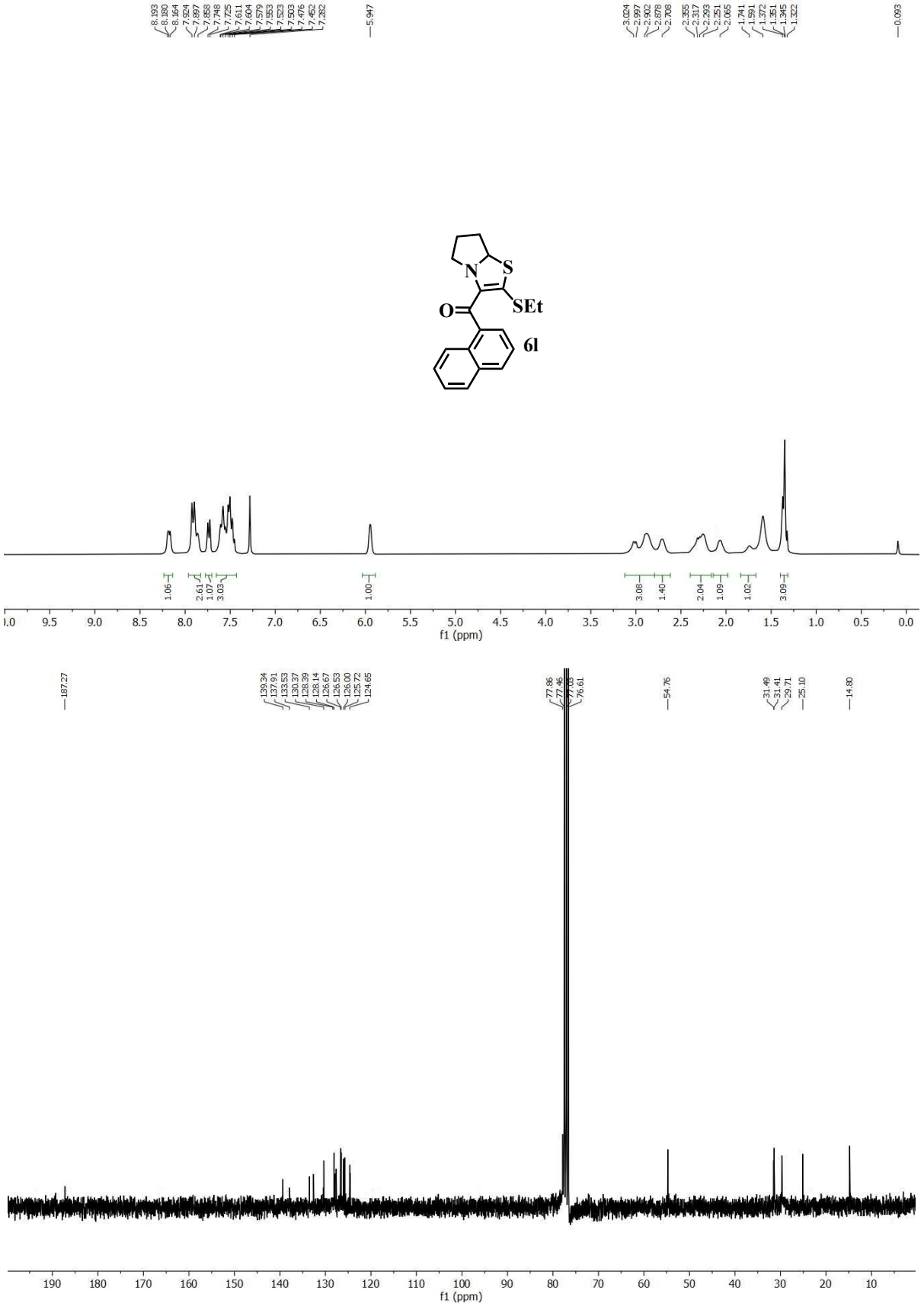
**SI Figure 10:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6j**



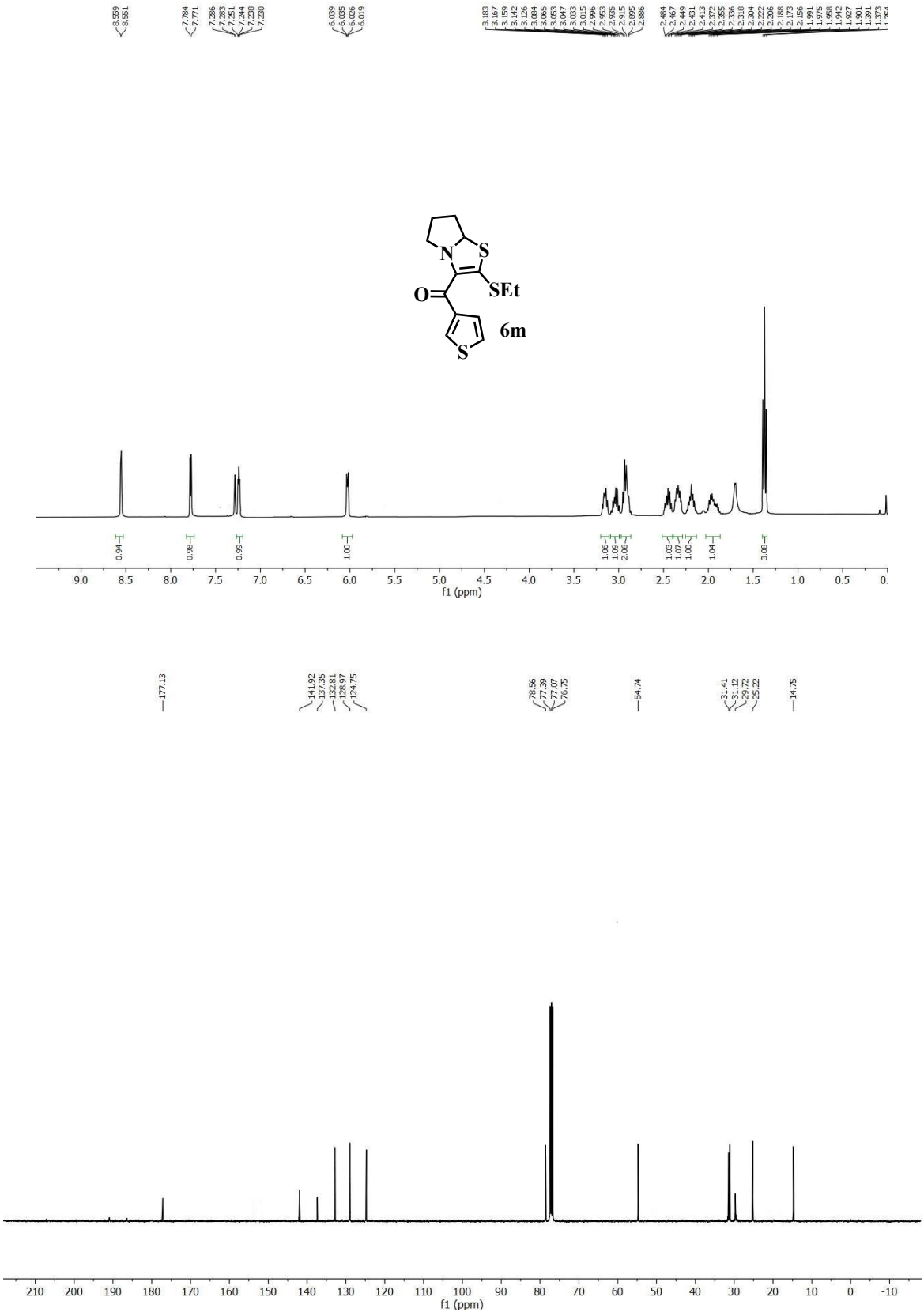
**SI Figure 11:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6k**



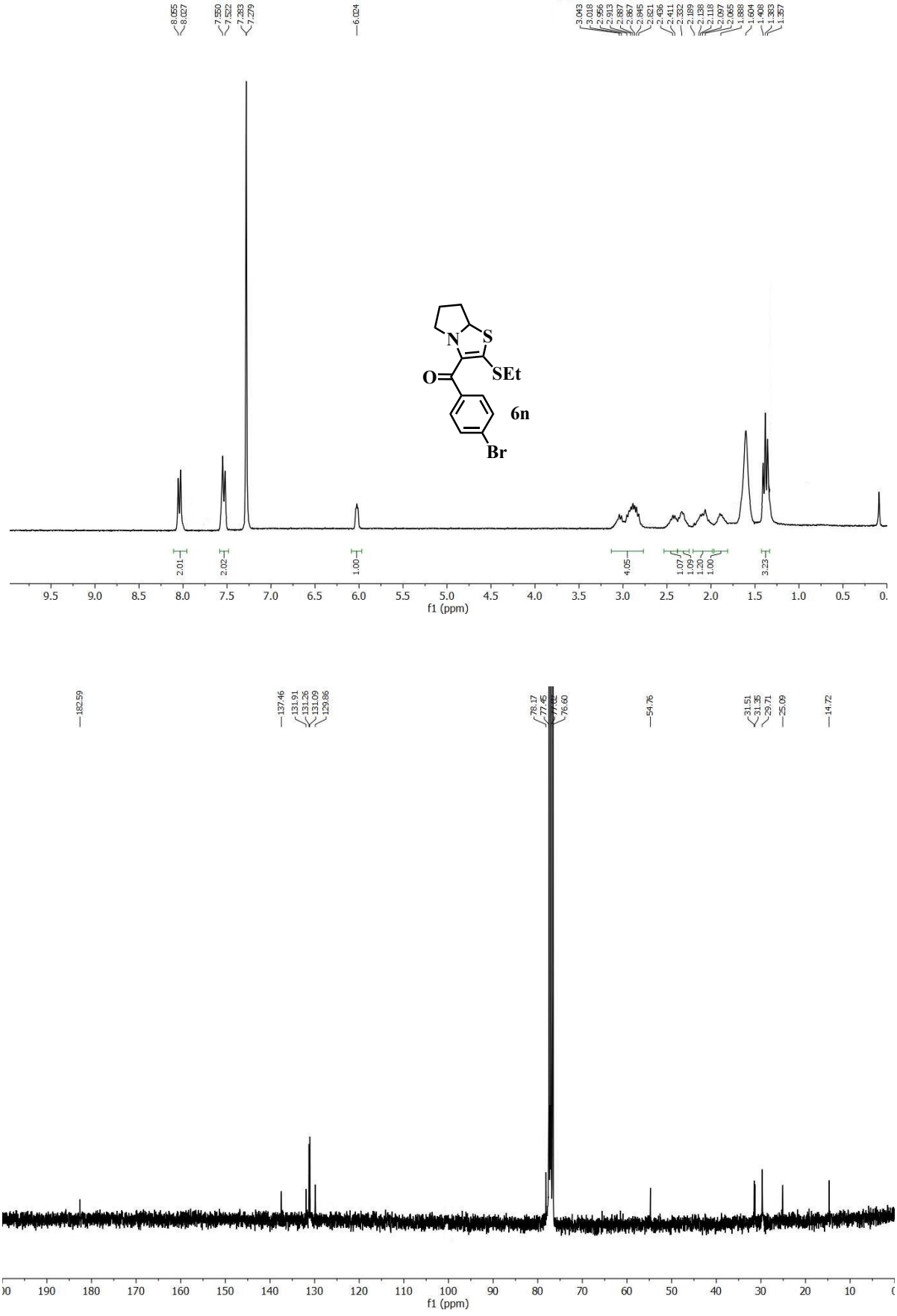
**SI Figure 12:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6l**



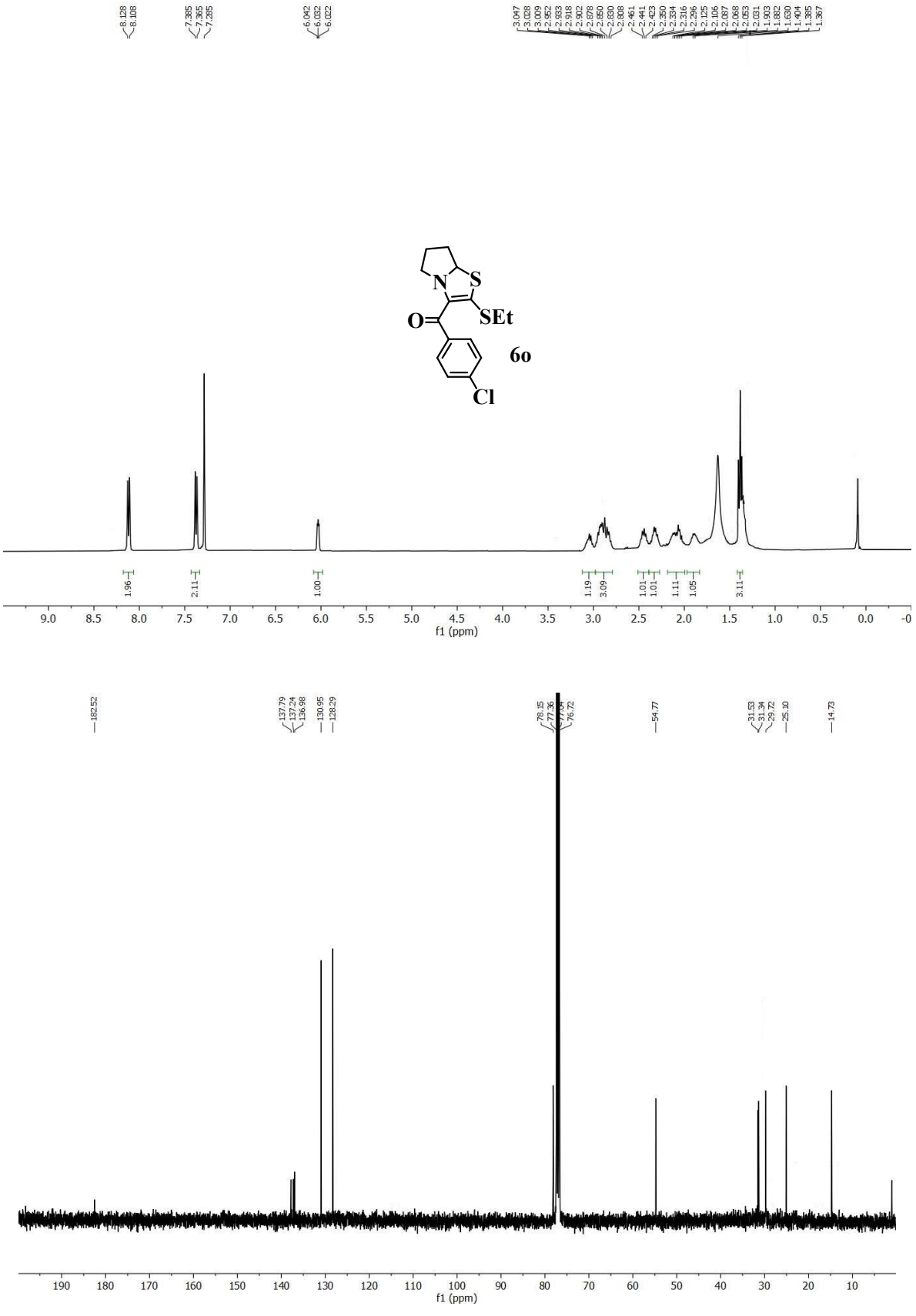
**SI Figure 13:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6m**



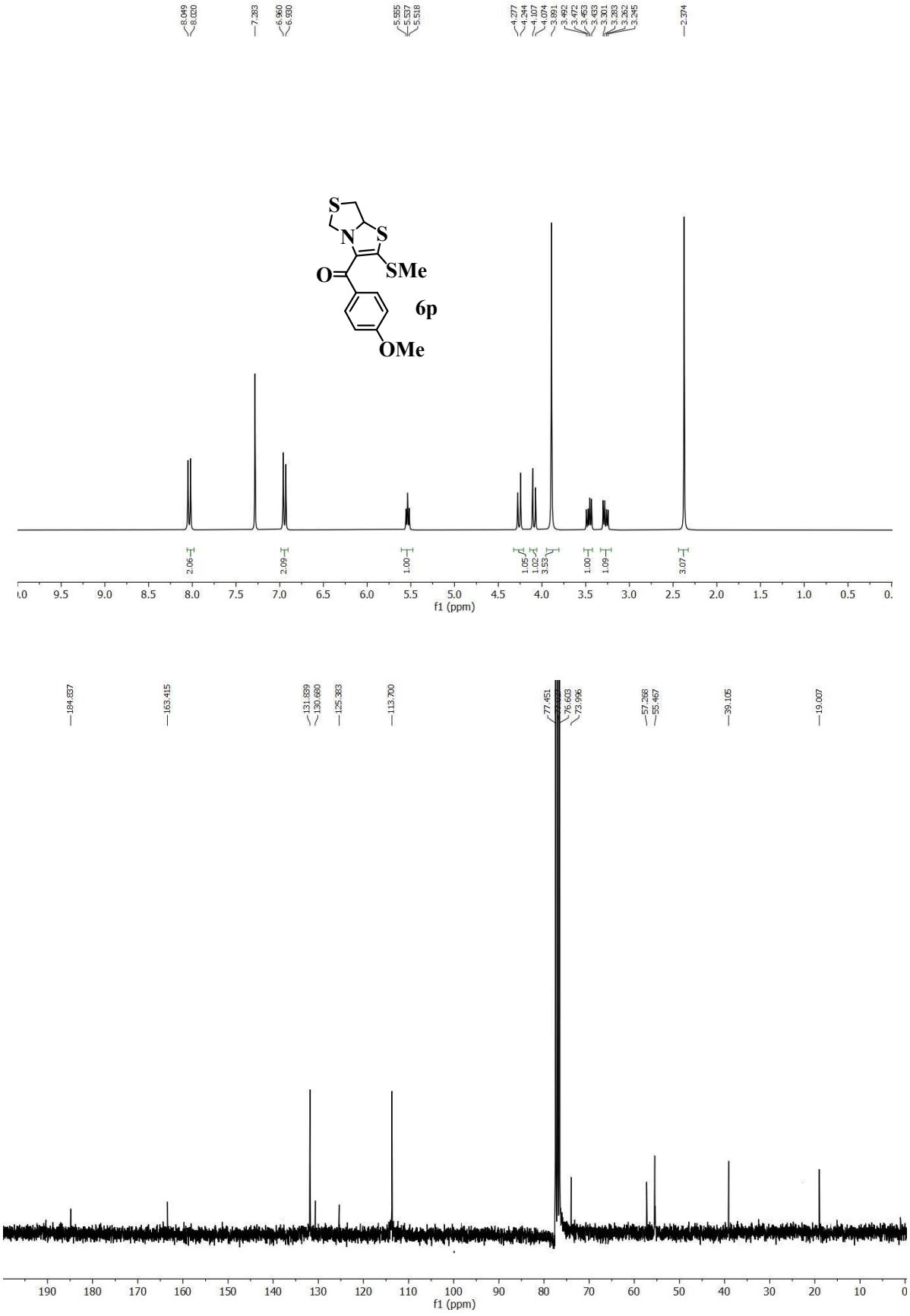
**SI Figure 14:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6n**



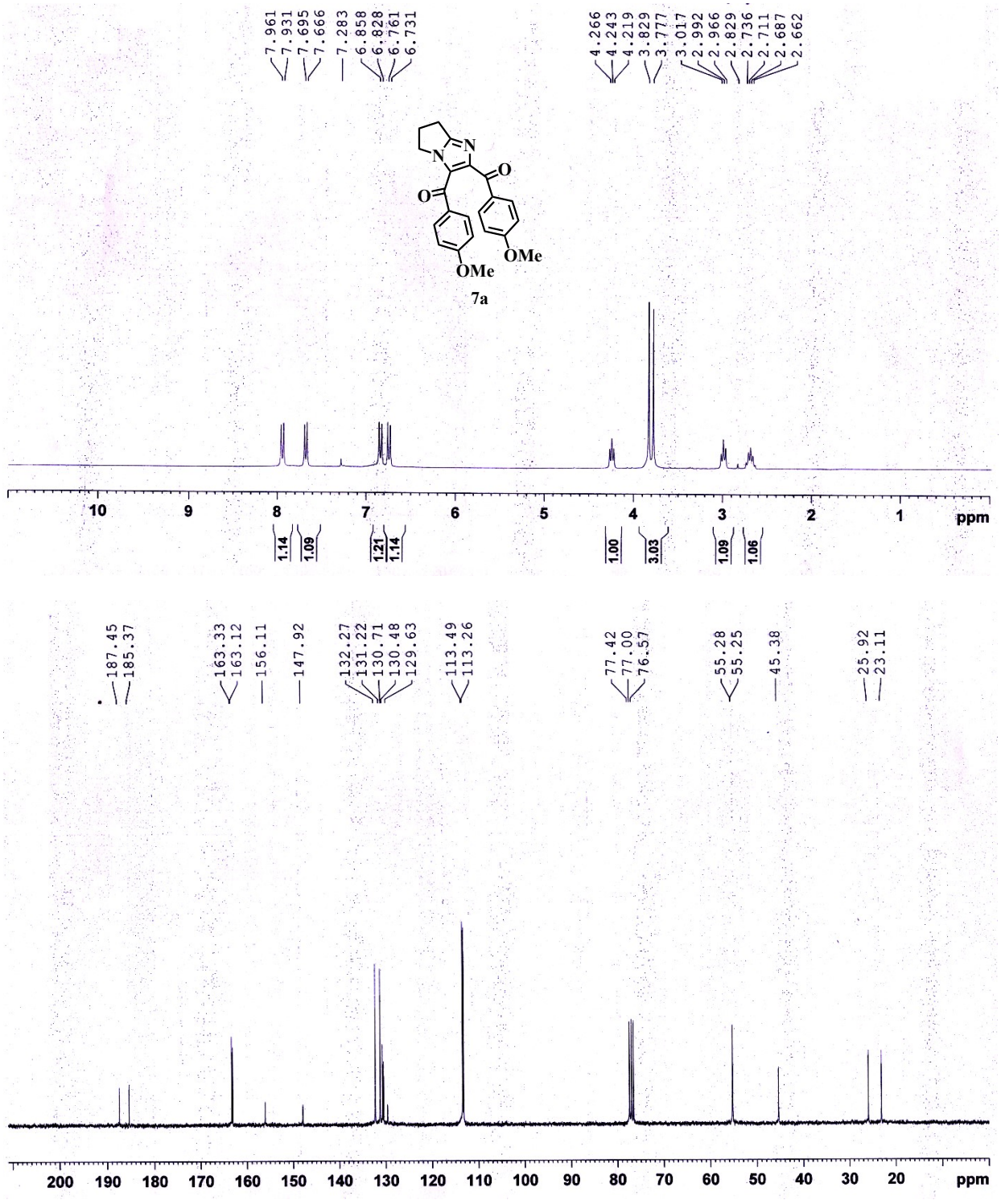
**SI Figure 15: $^{1}H$ and $^{13}C$-NMR spectra of compound 6o**



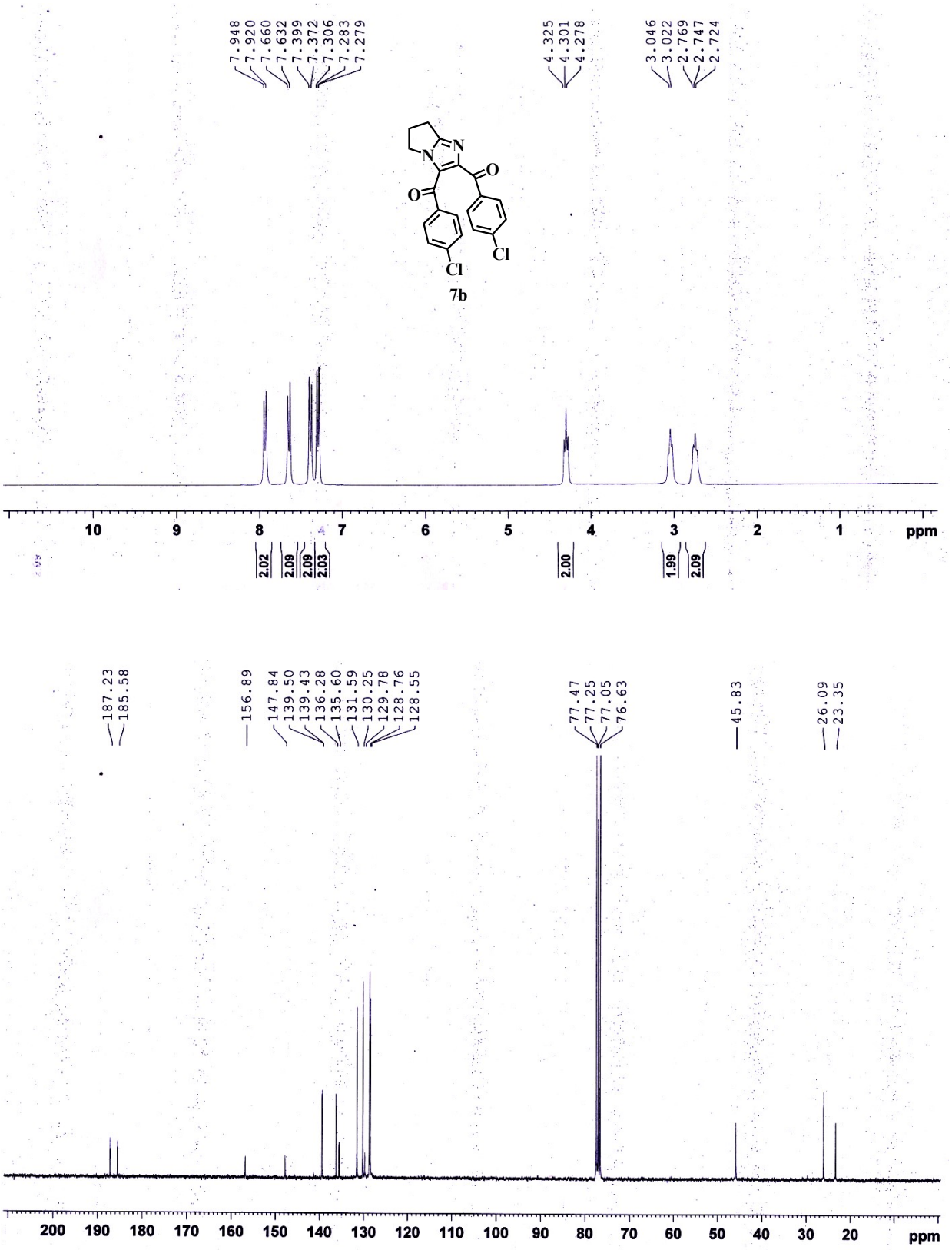
**SI Figure 16:** $^{1}H$ and $^{13}C$-NMR spectra of compound **6p**



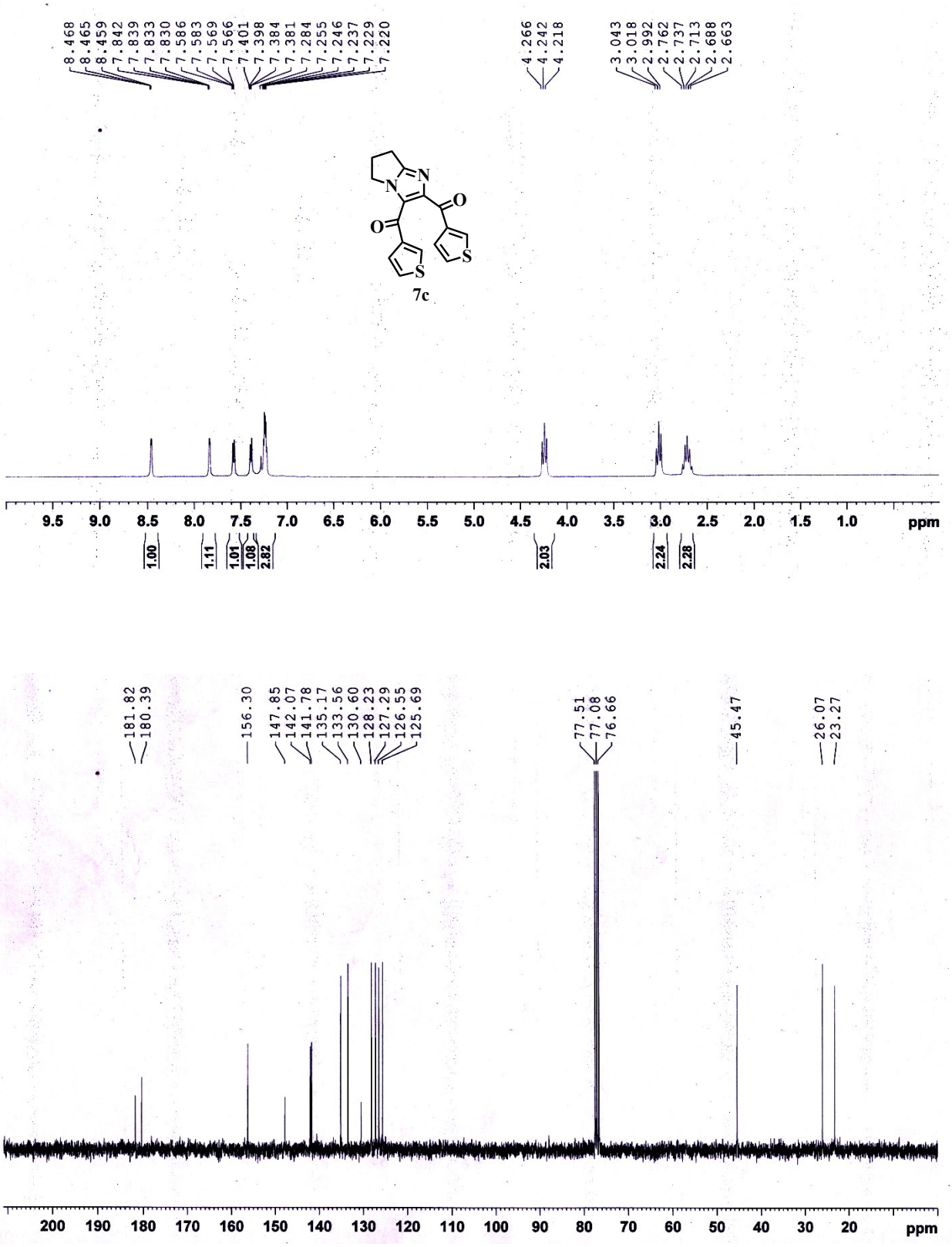
**SI Figure 17:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7a**



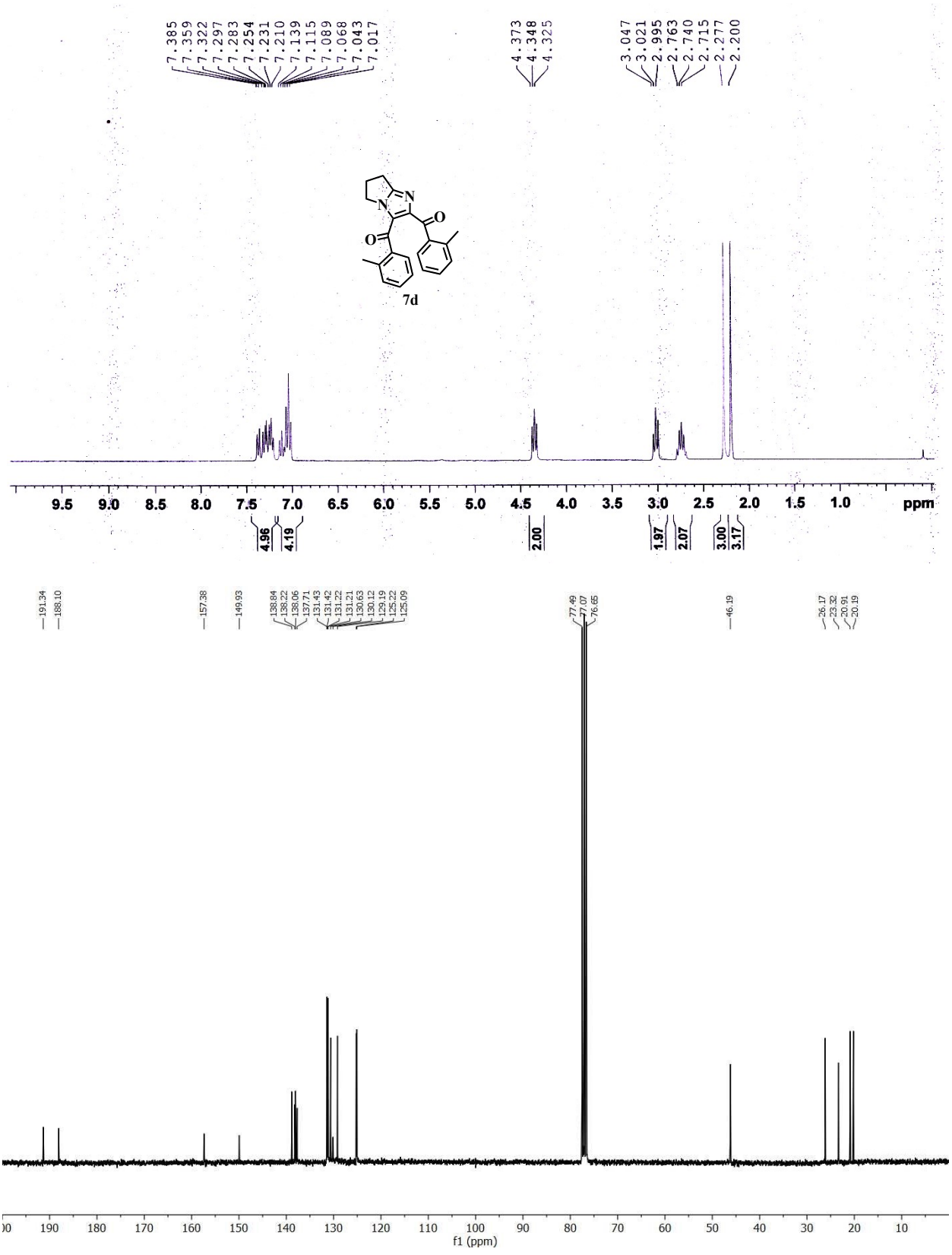
**SI Figure 18:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7b**



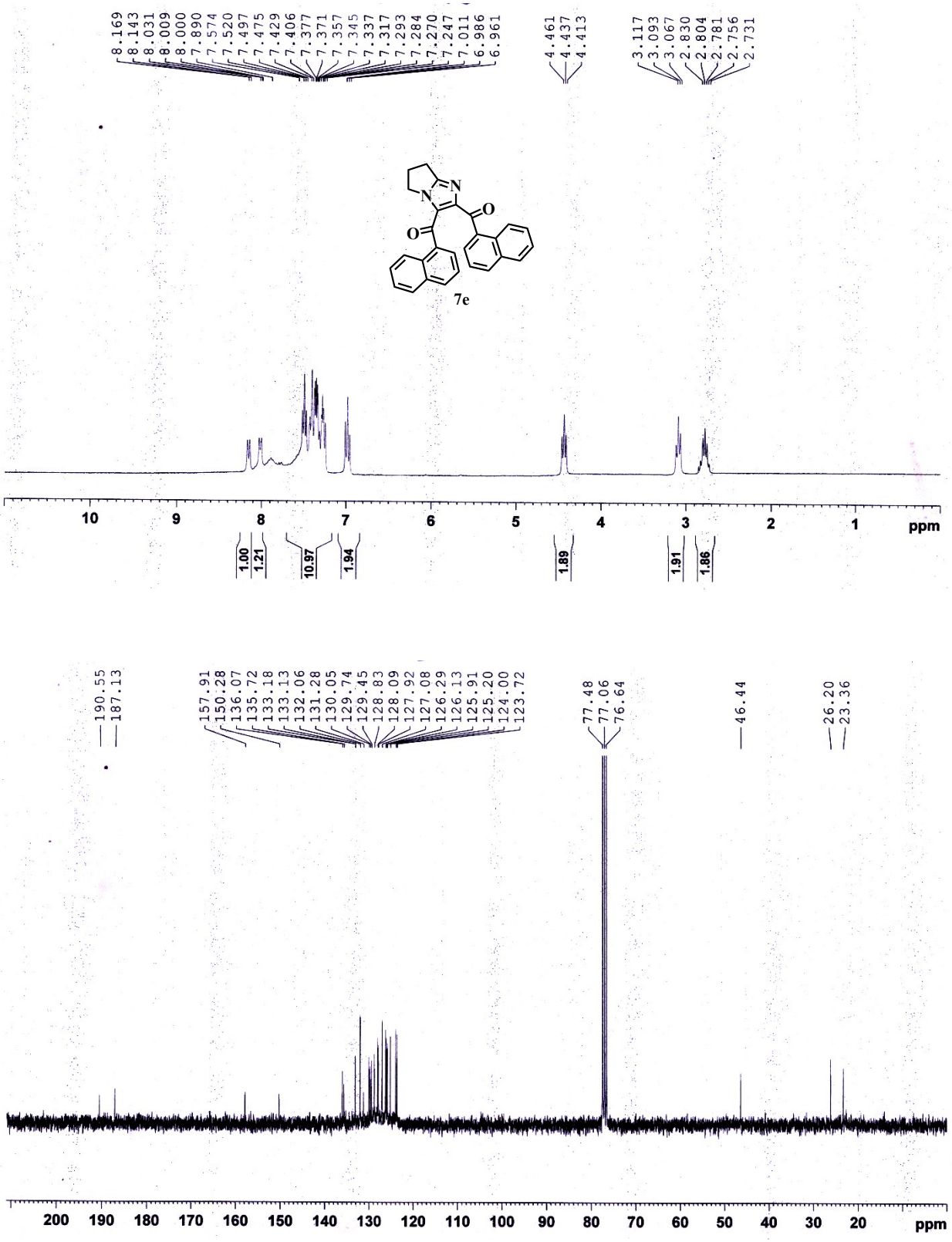
**SI Figure 19:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7c**



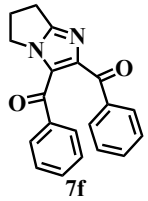
**SI Figure 20:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7d**



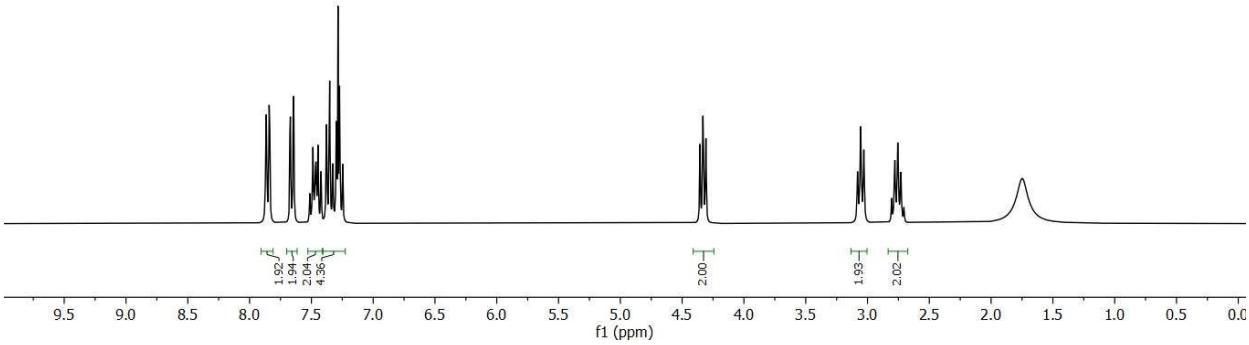
**SI Figure 21:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7e**

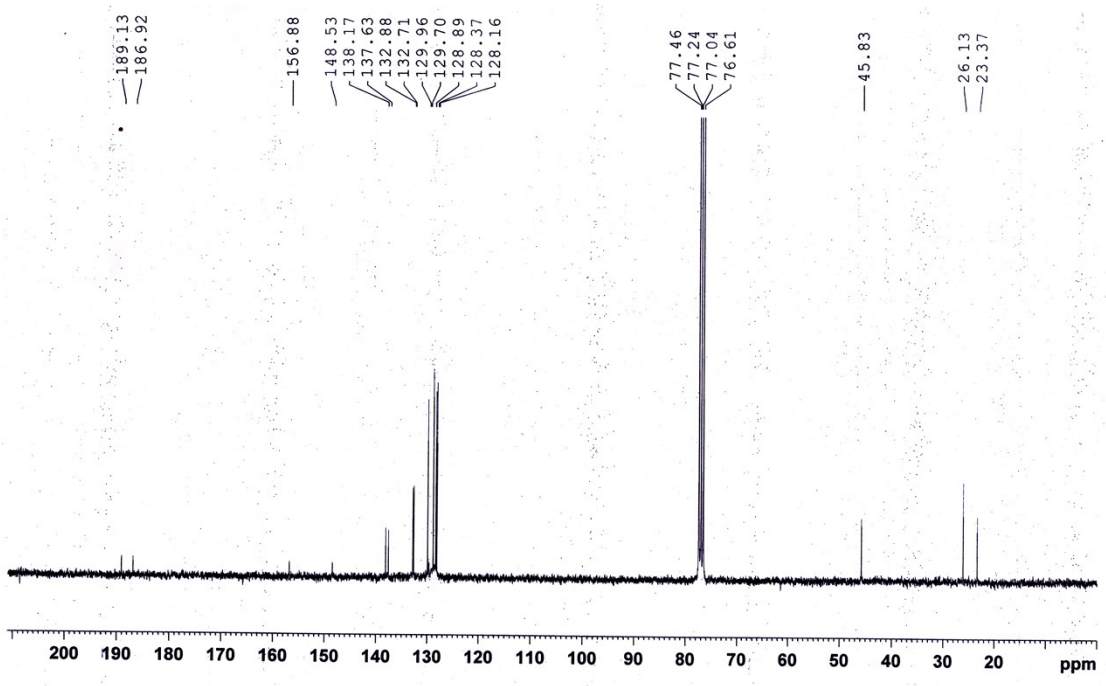


**SI Figure 22:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7f**

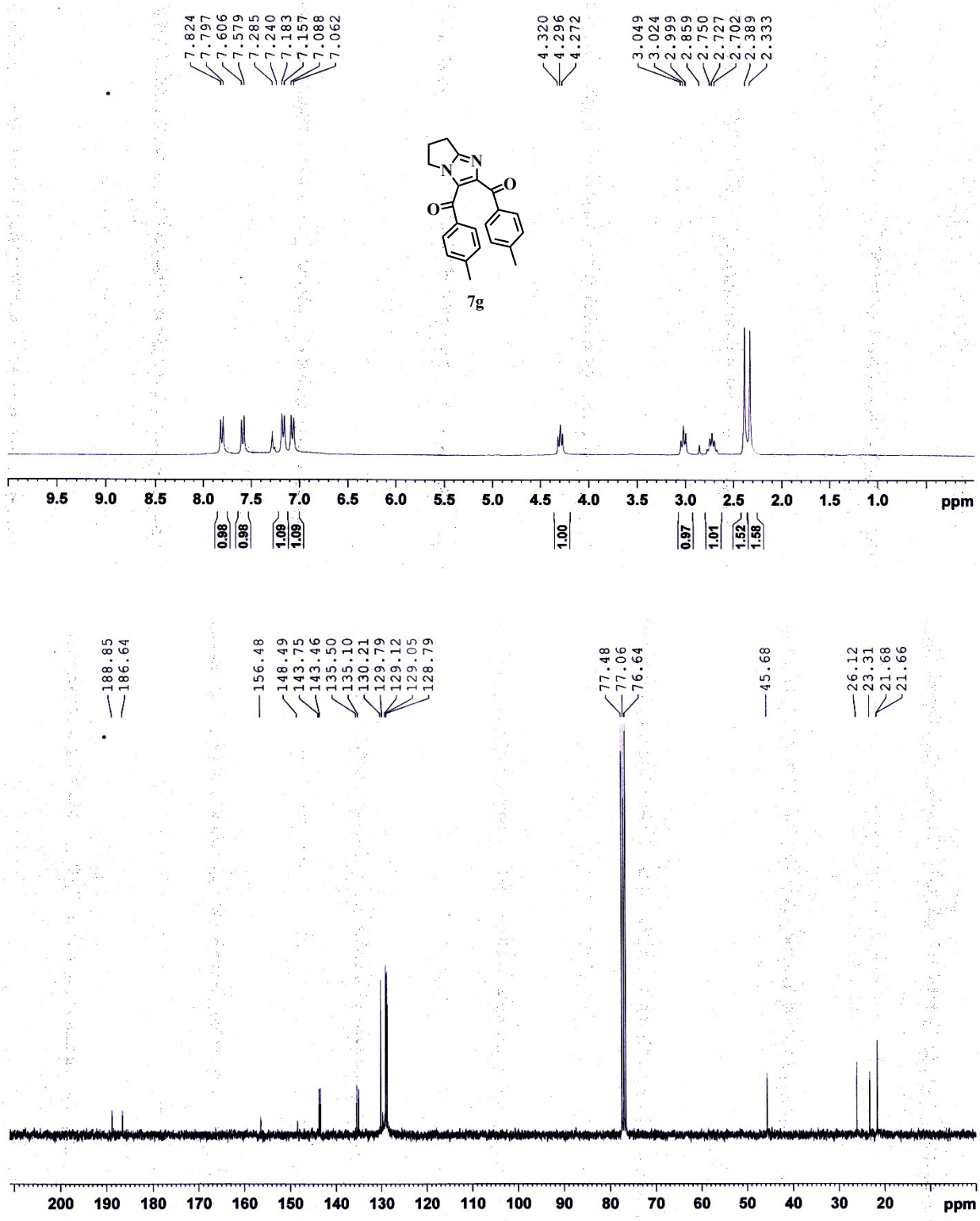




7f

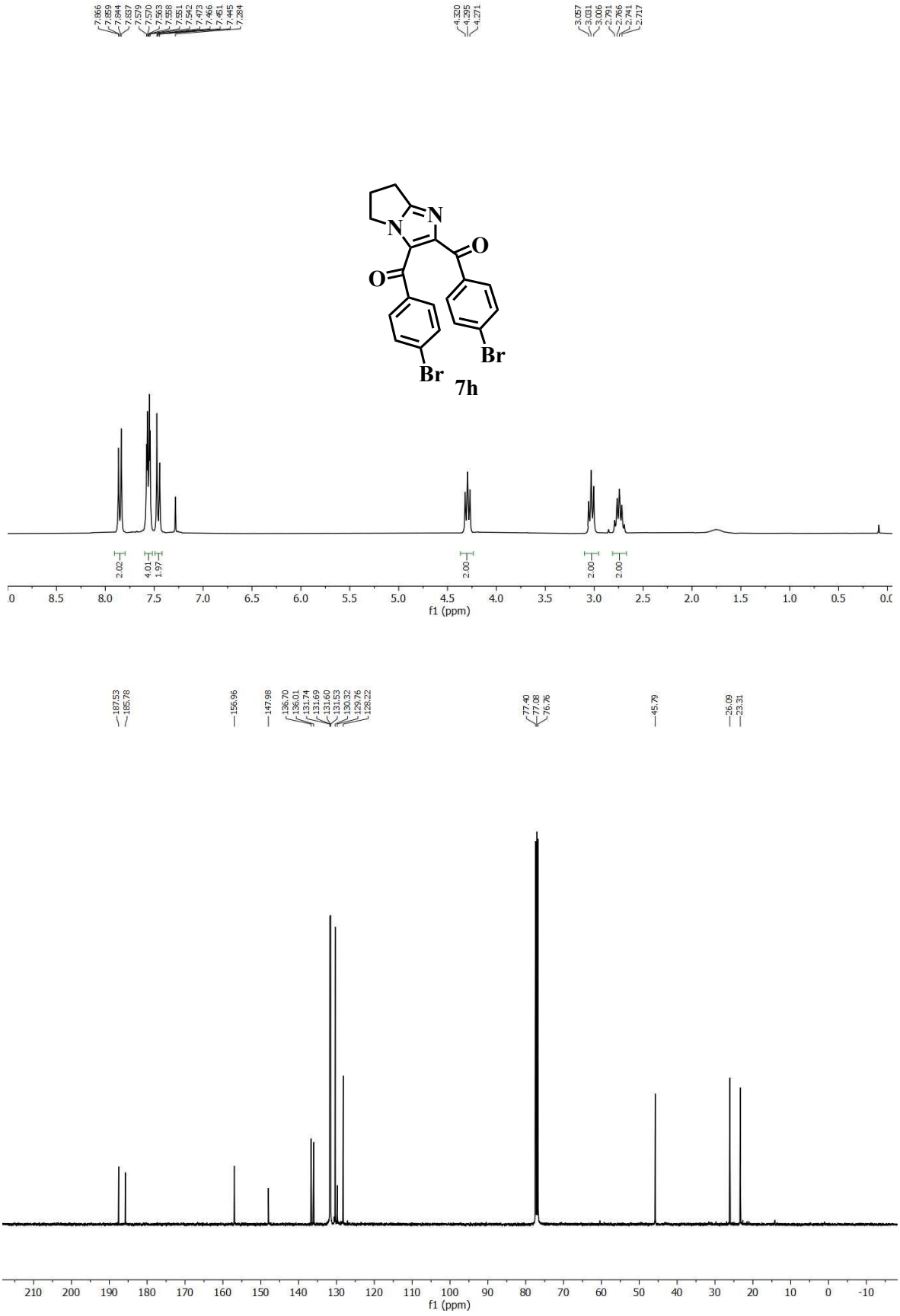


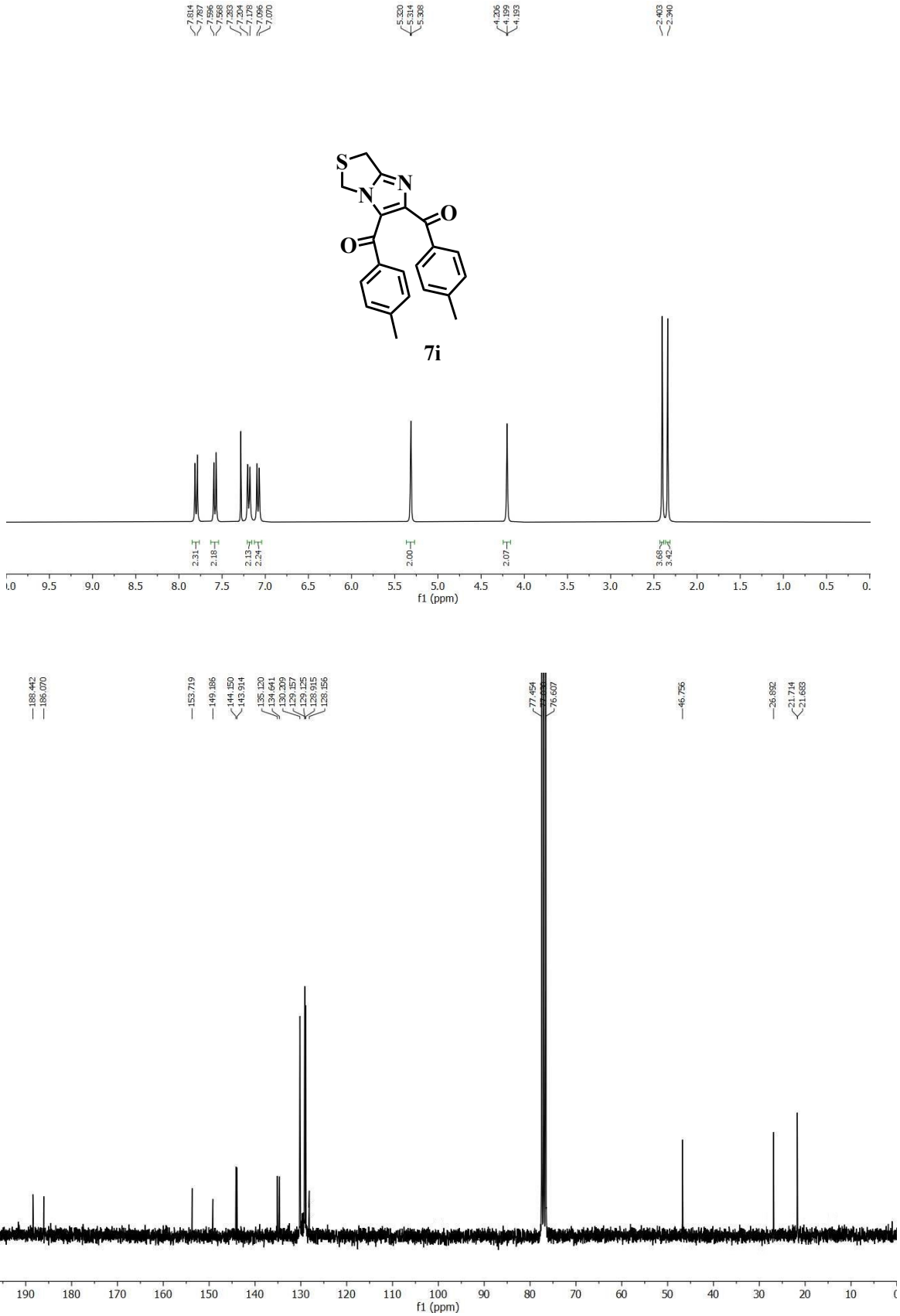
**SI Figure 23:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7g**



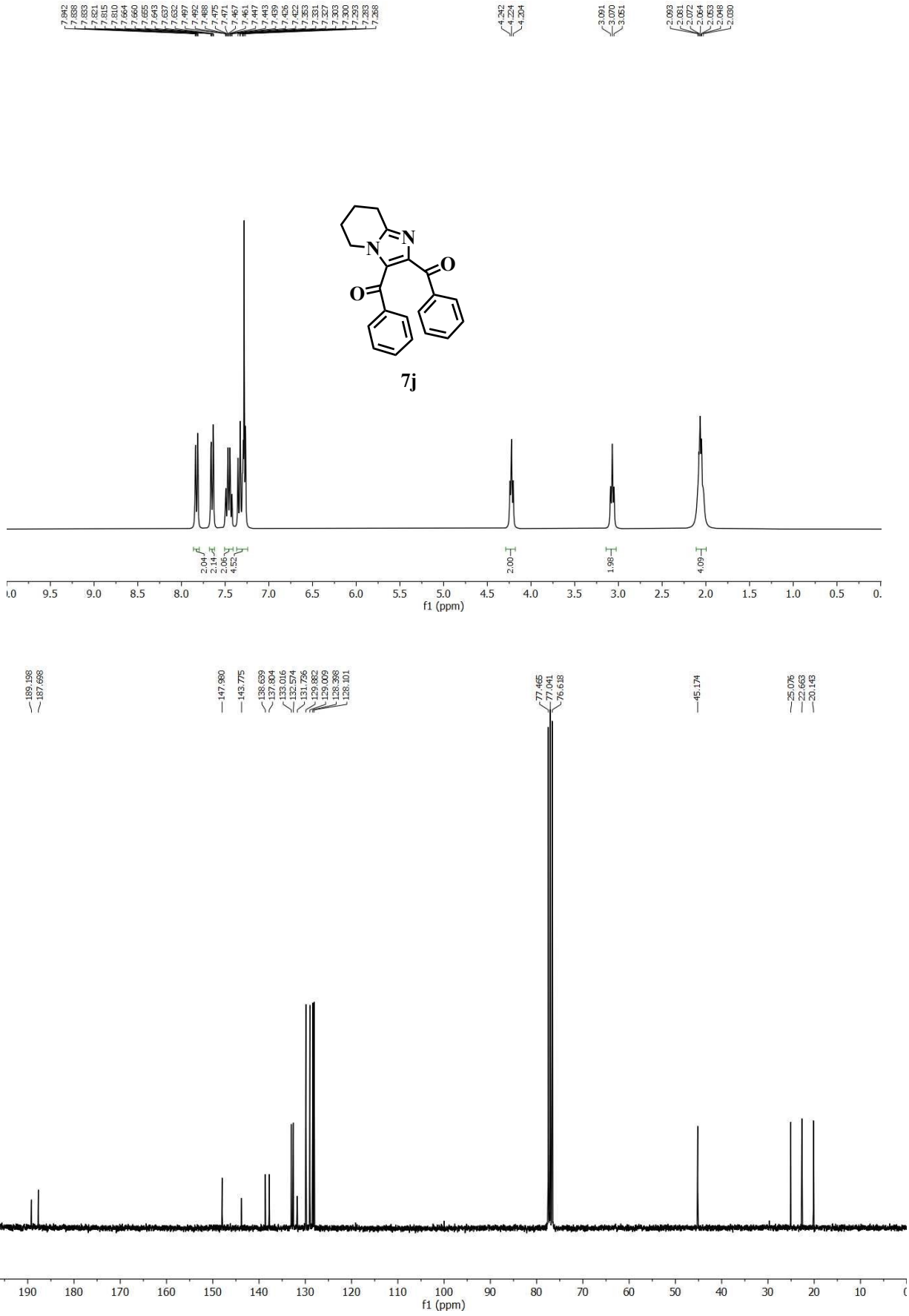
**SI Figure 24:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7h**



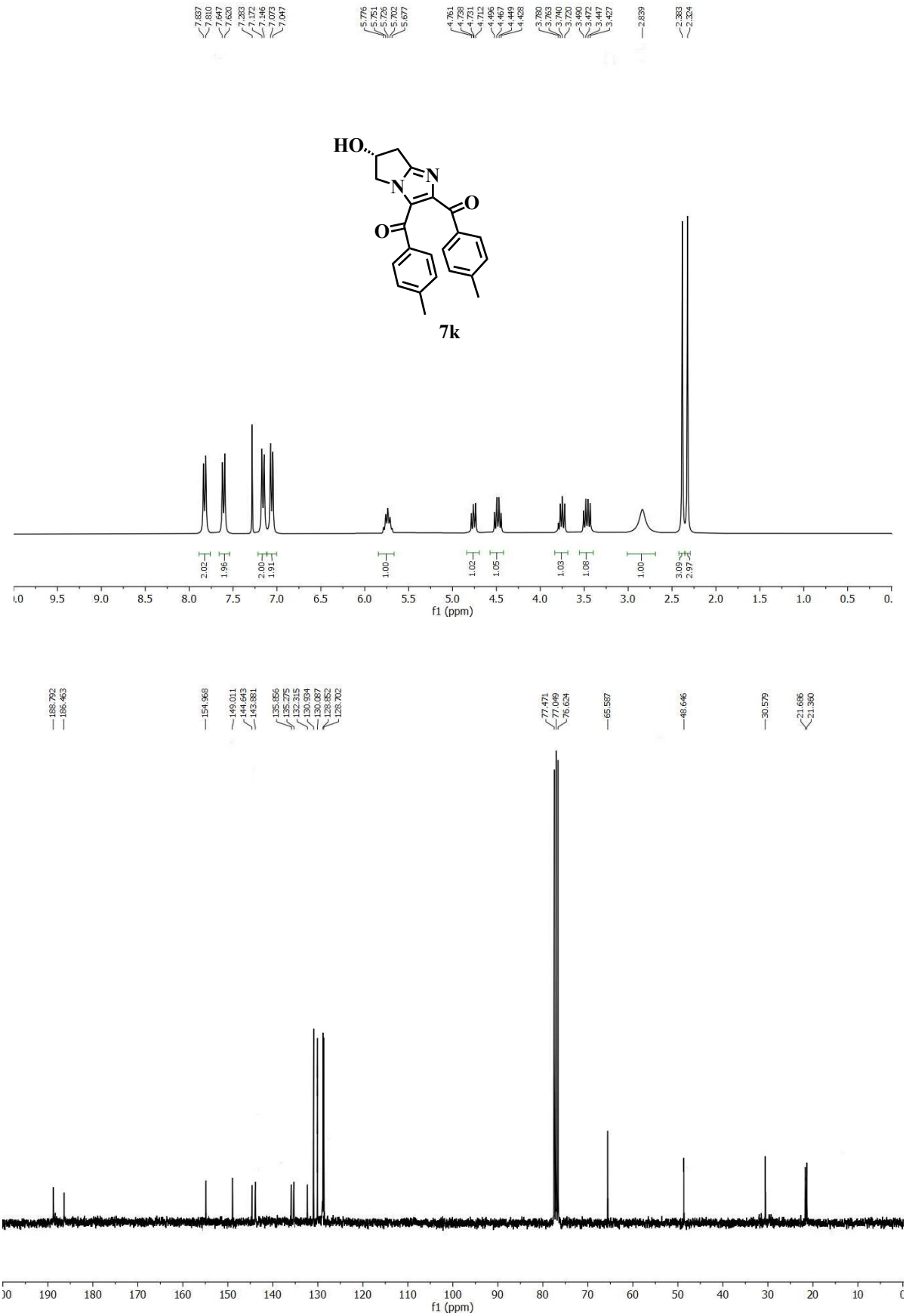
**SI Figure 25:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7i**



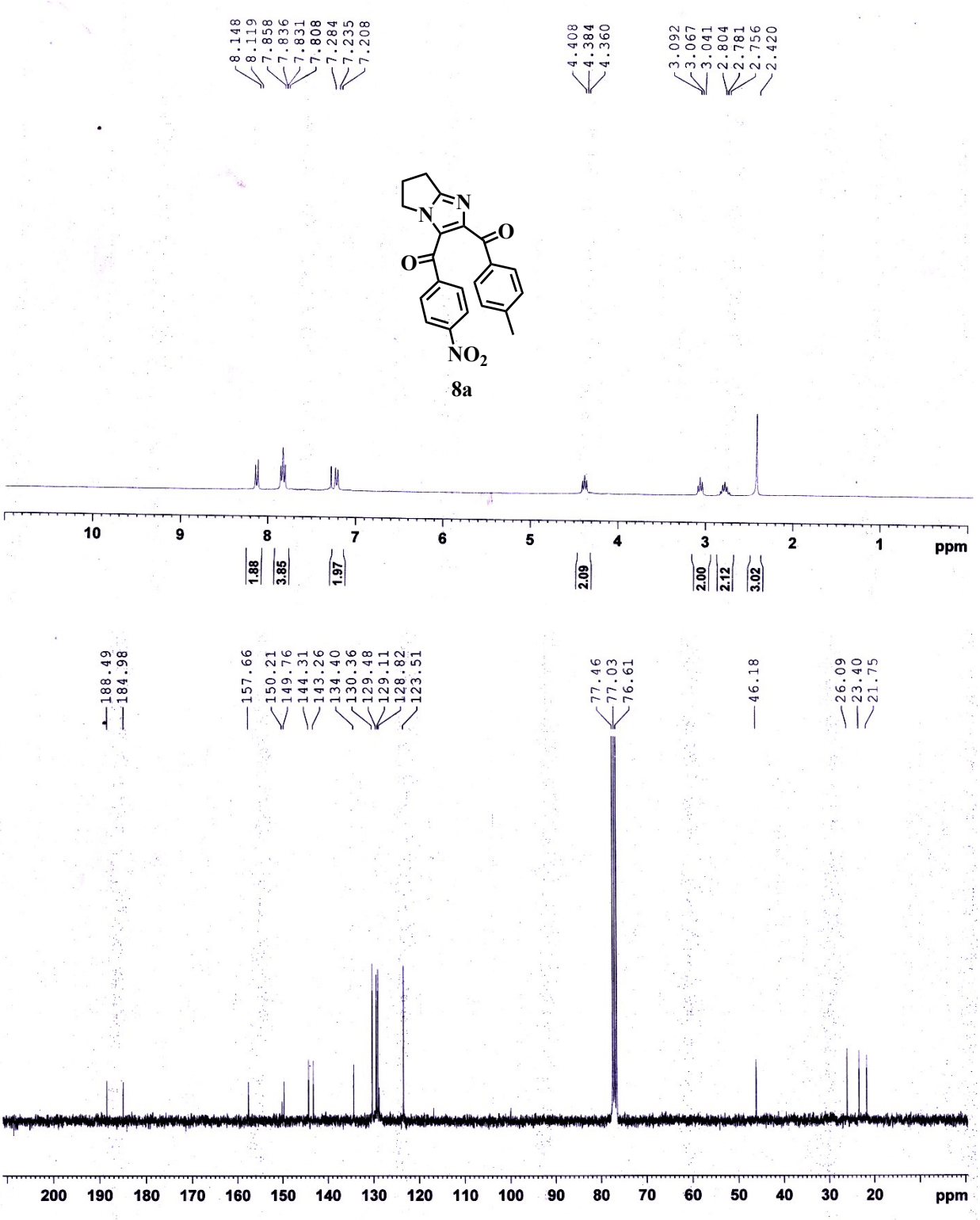
**SI Figure 26:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7j**



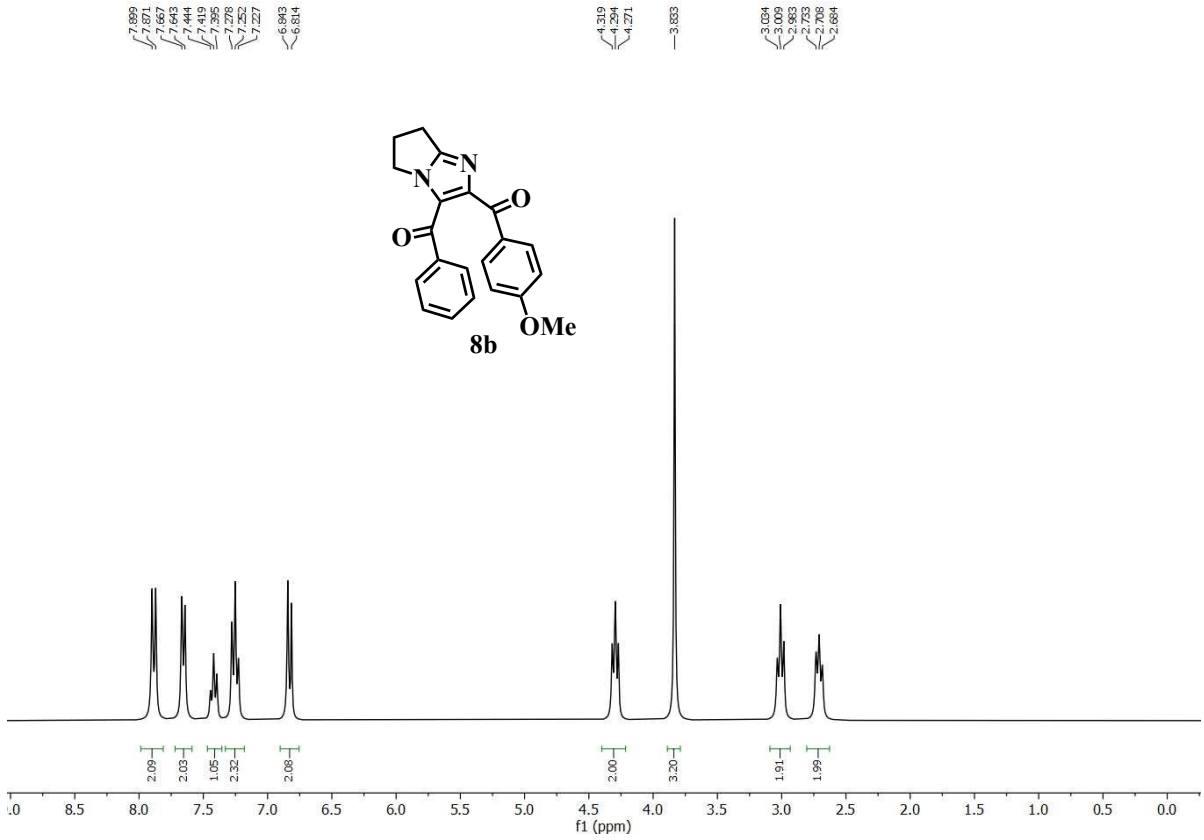
**SI Figure 27:** $^{1}H$ and $^{13}C$-NMR spectra of compound **7k**

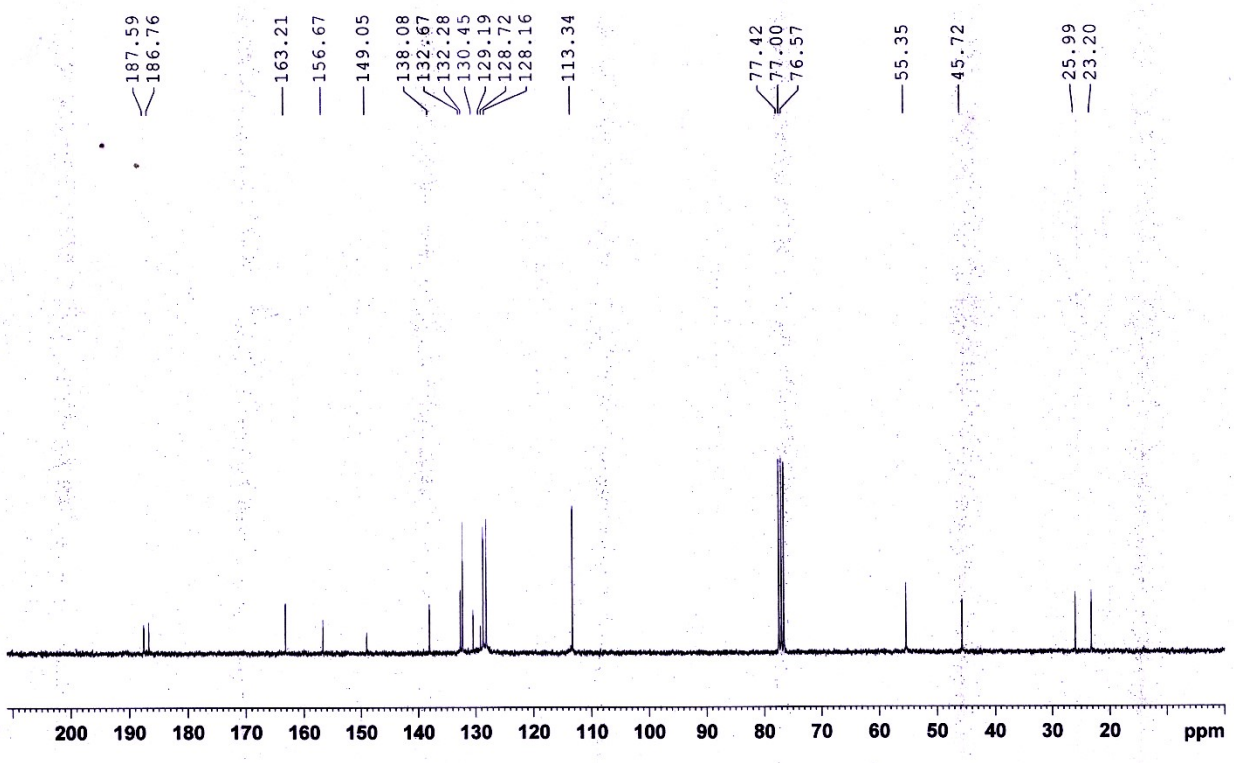


**SI Figure 28:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8a**

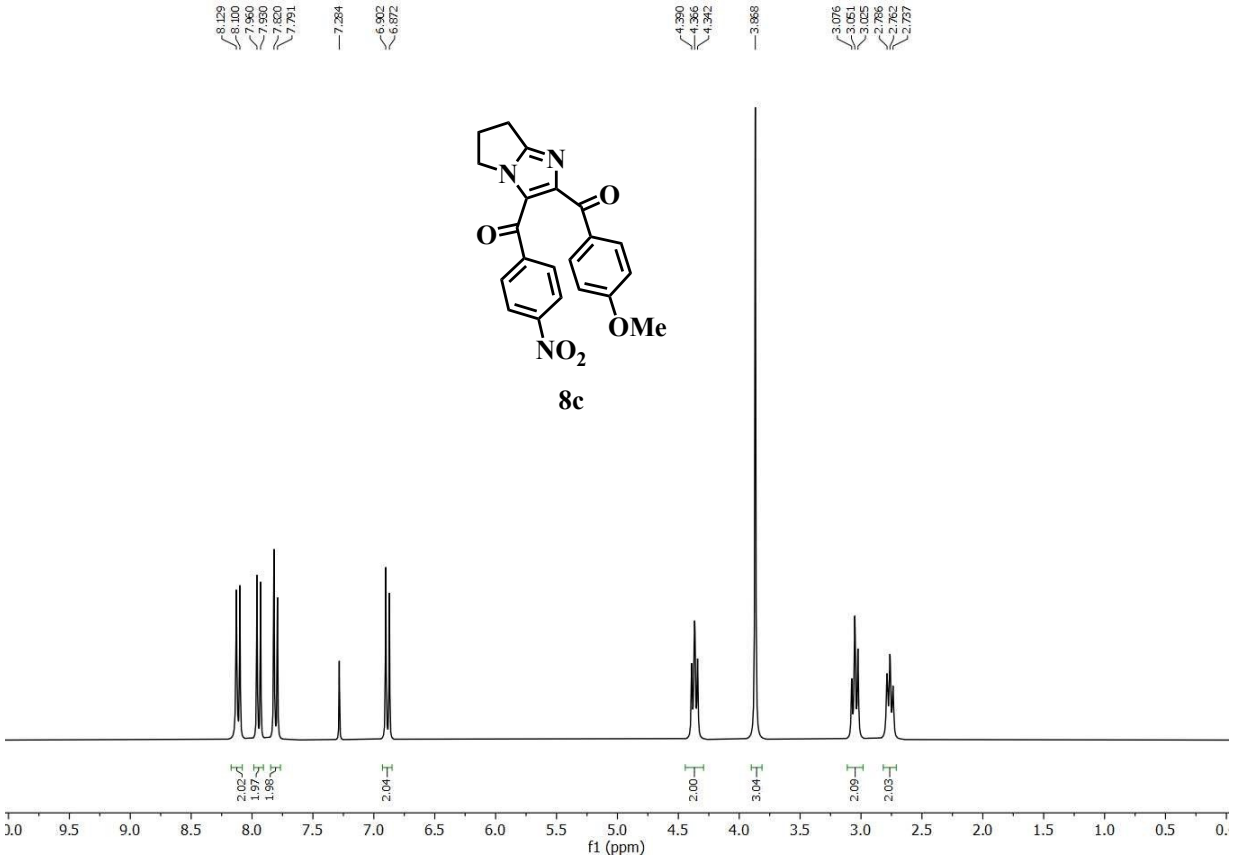


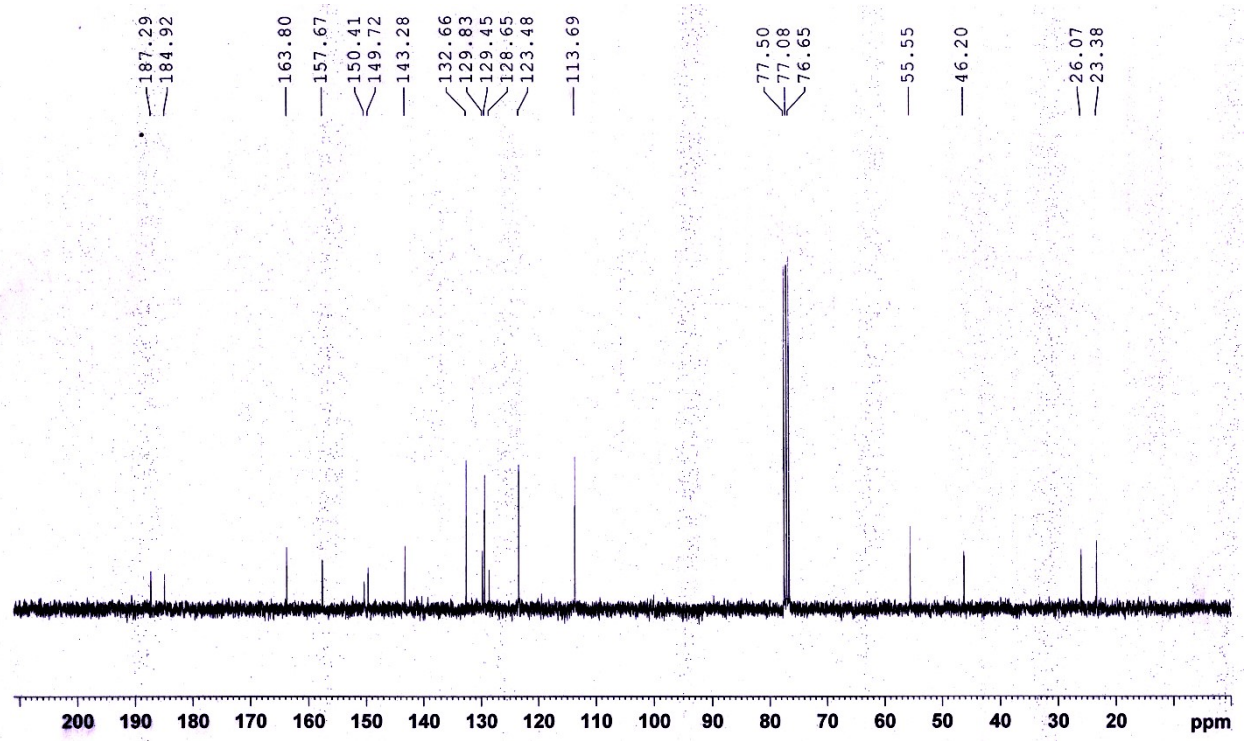
**SI Figure 29:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8b**



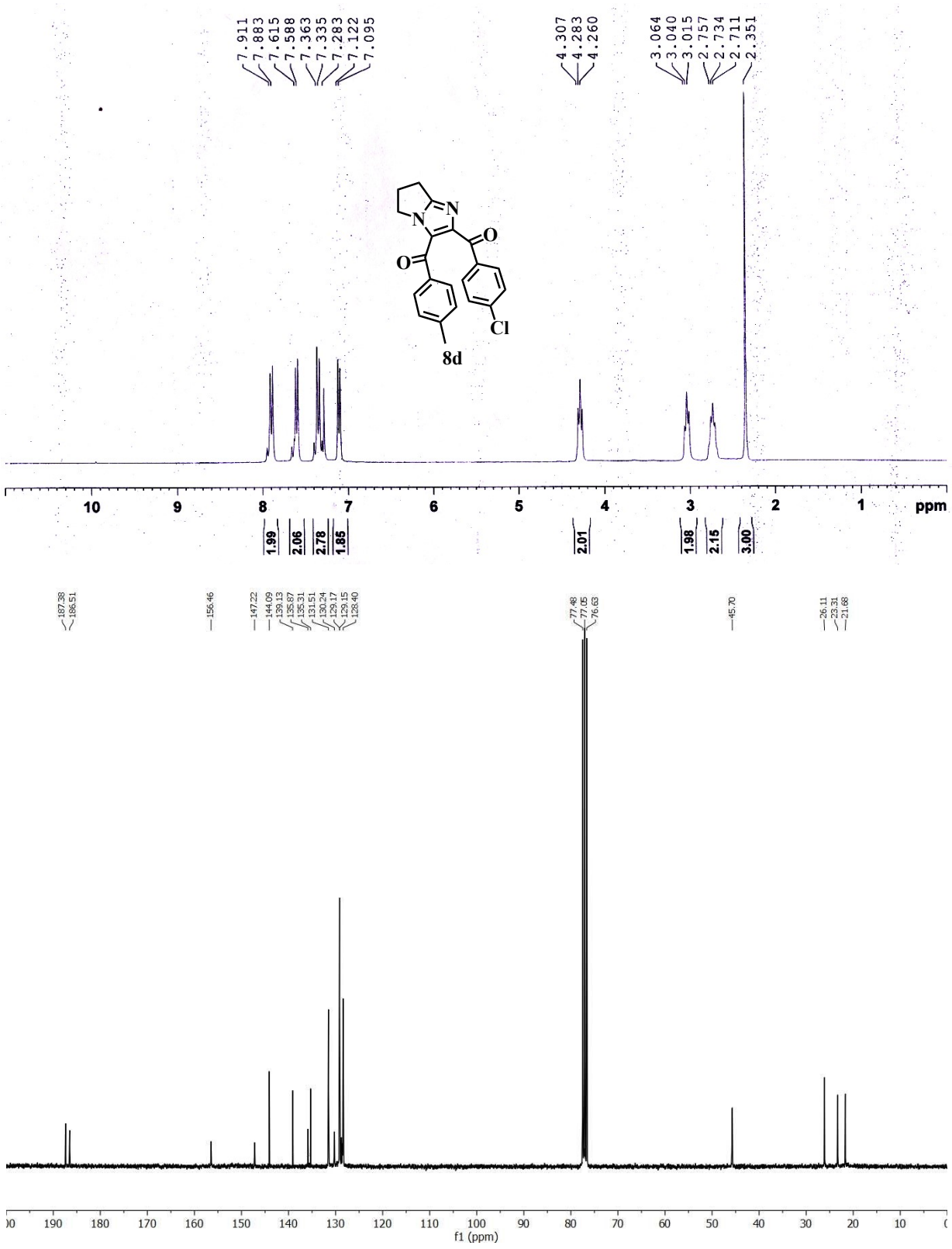



**SI Figure 30:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8c**

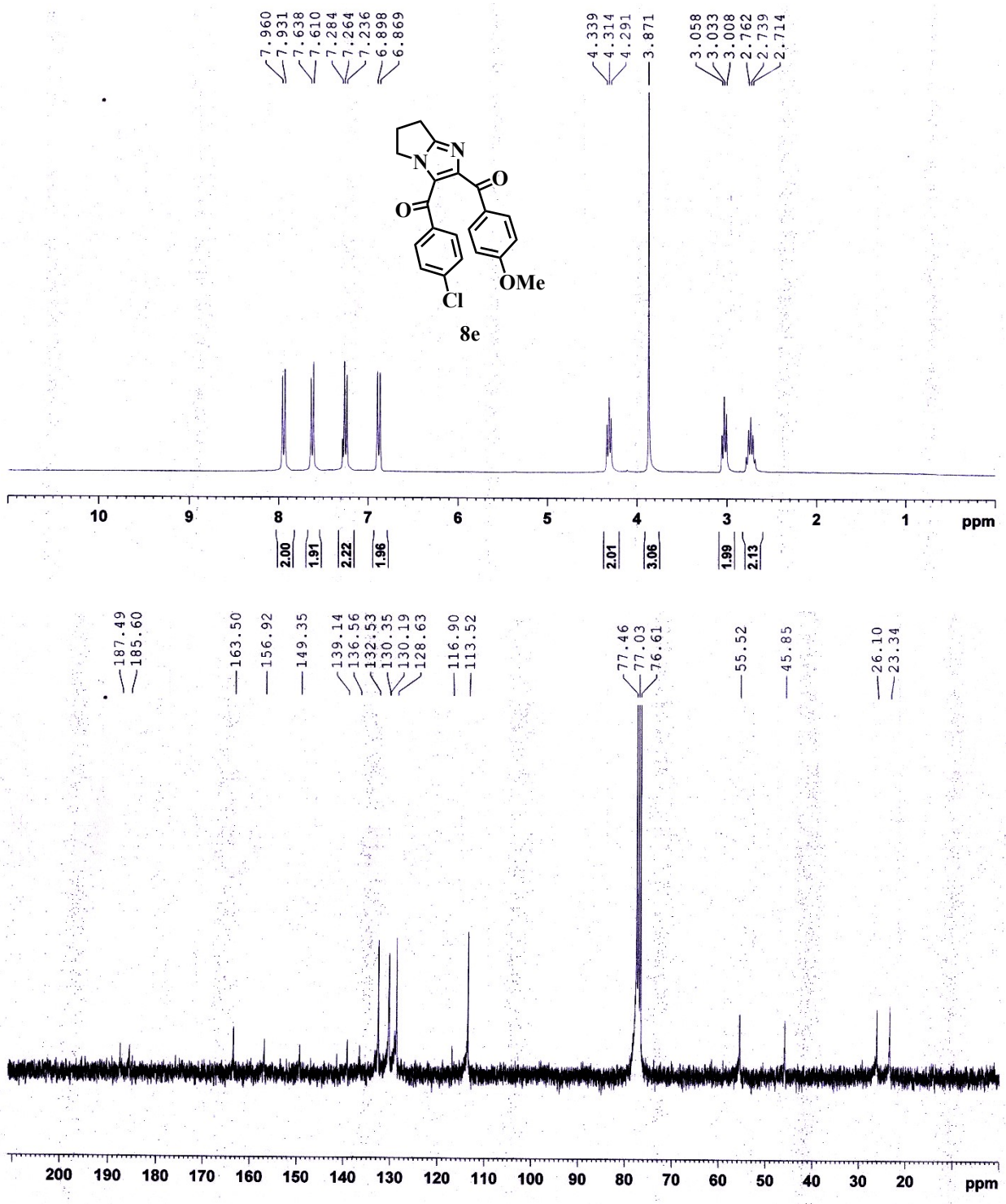


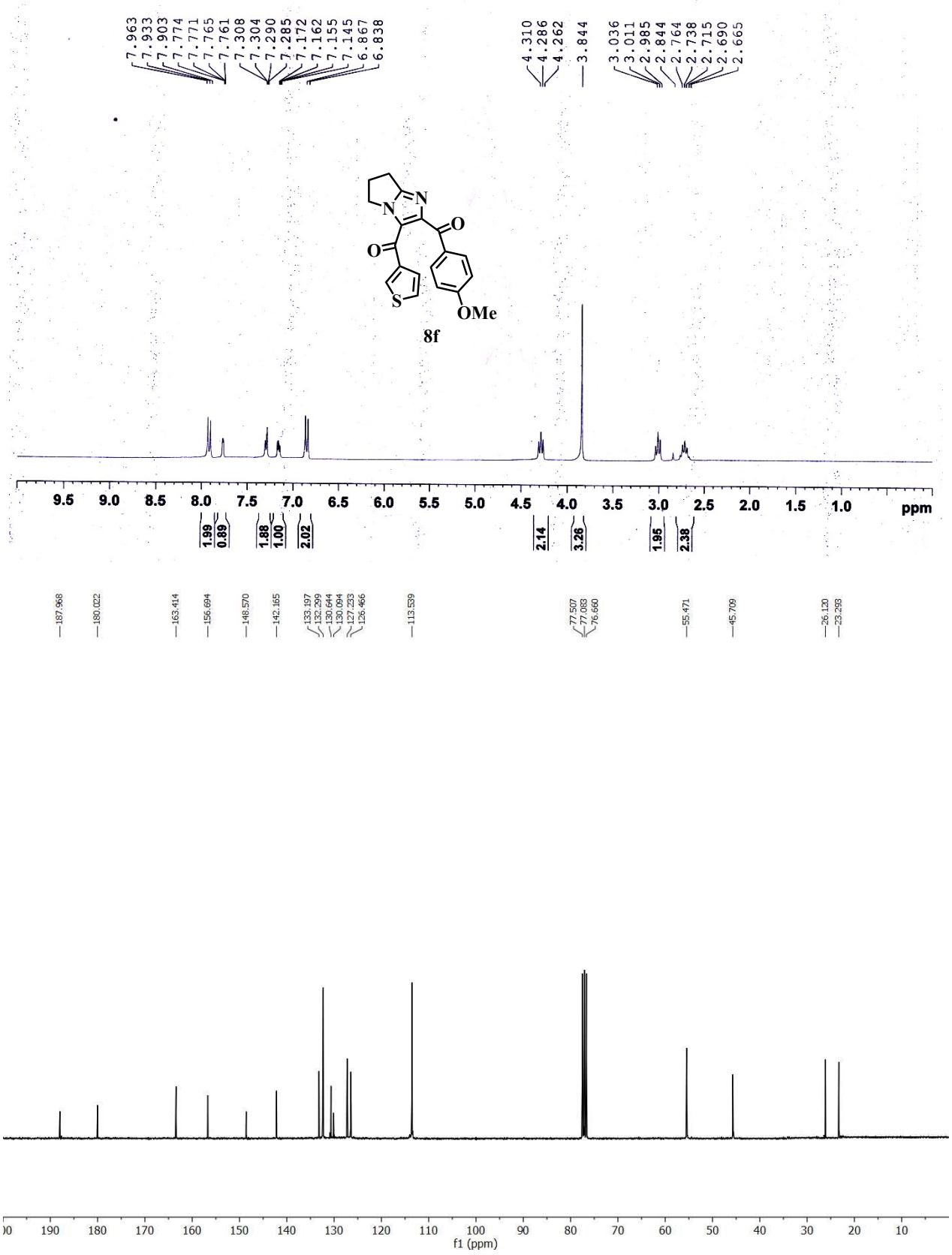
**SI Figure 31:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8d**



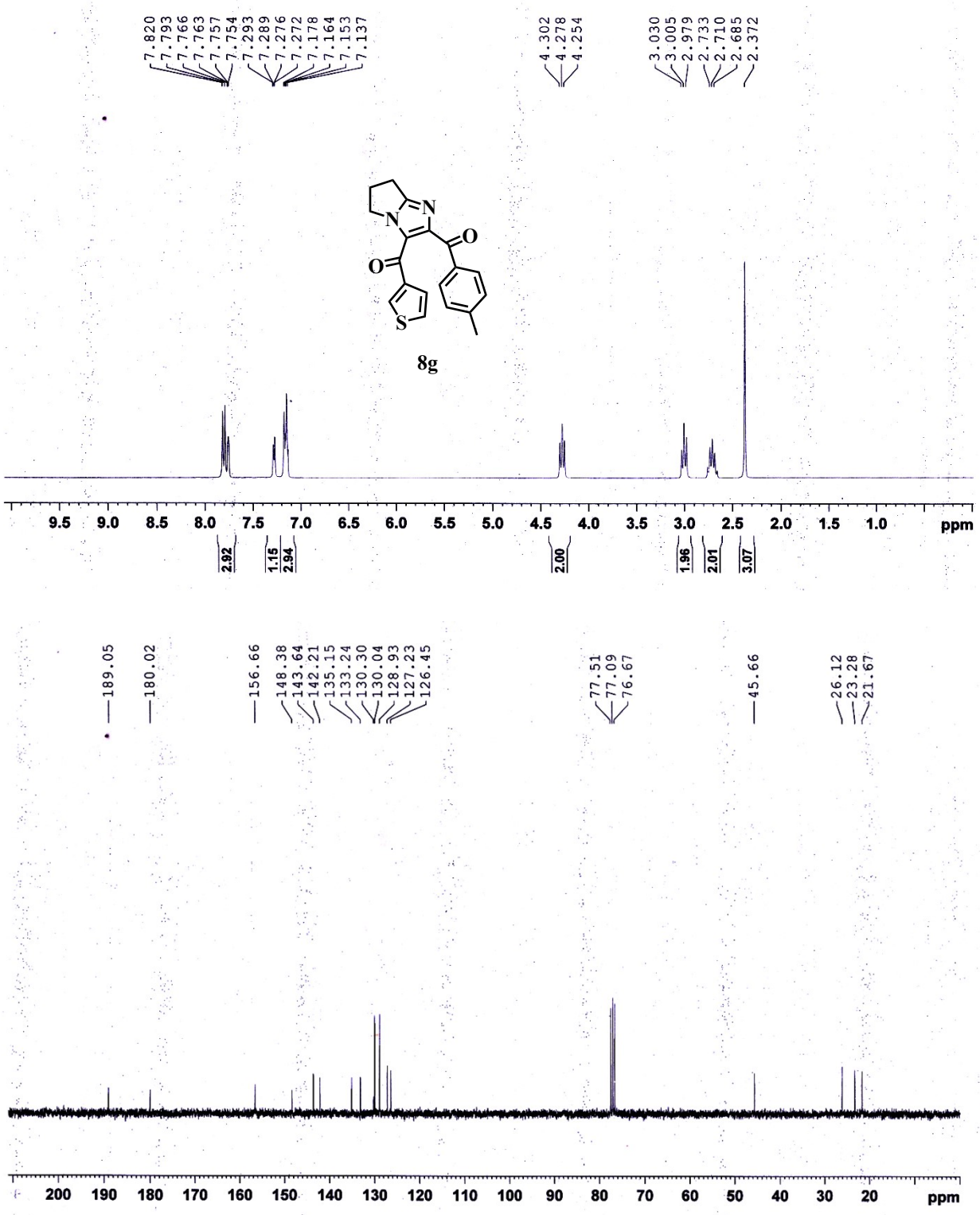
**SI Figure 32:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8e**



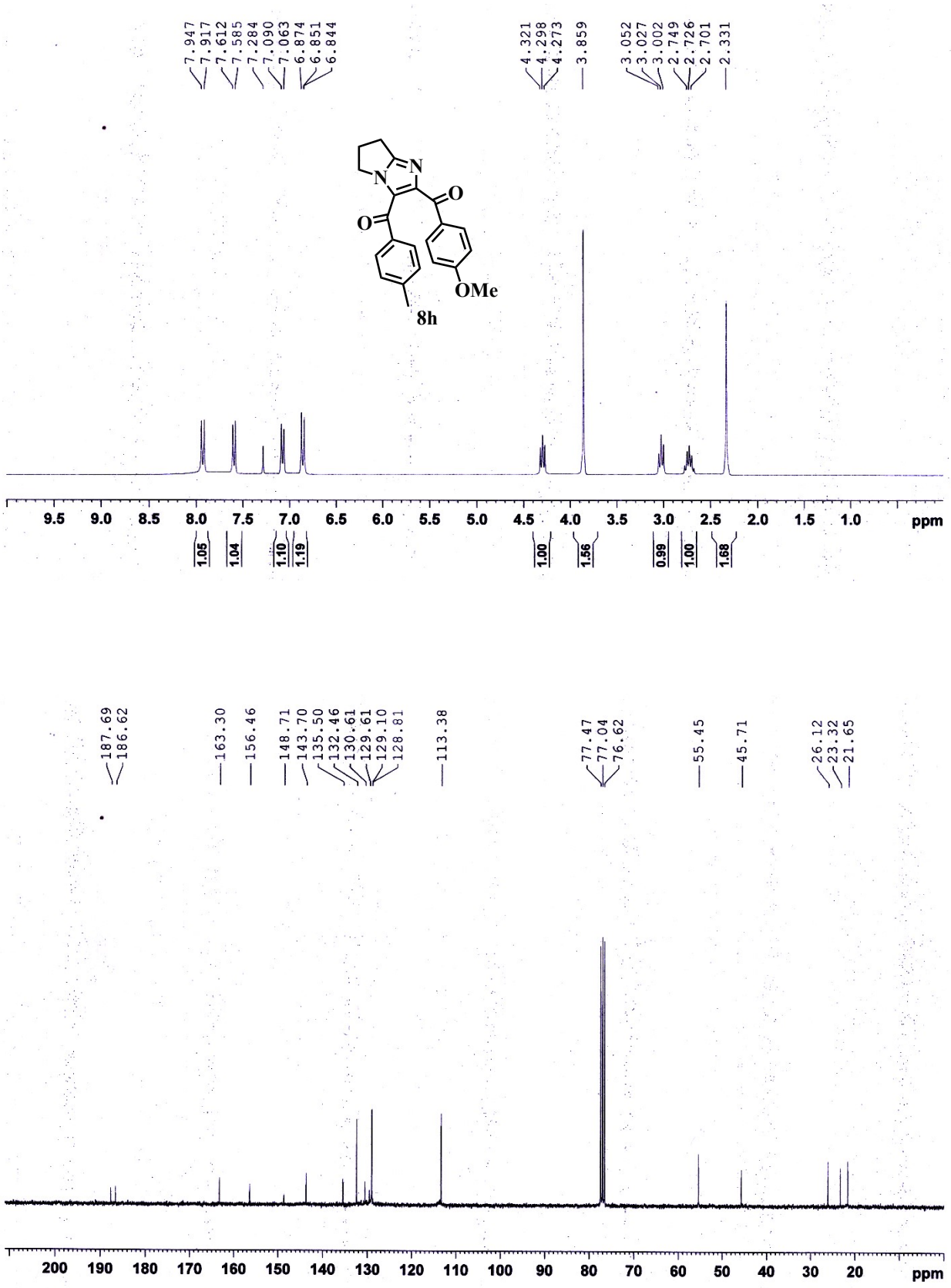
**SI Figure 33:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8f**



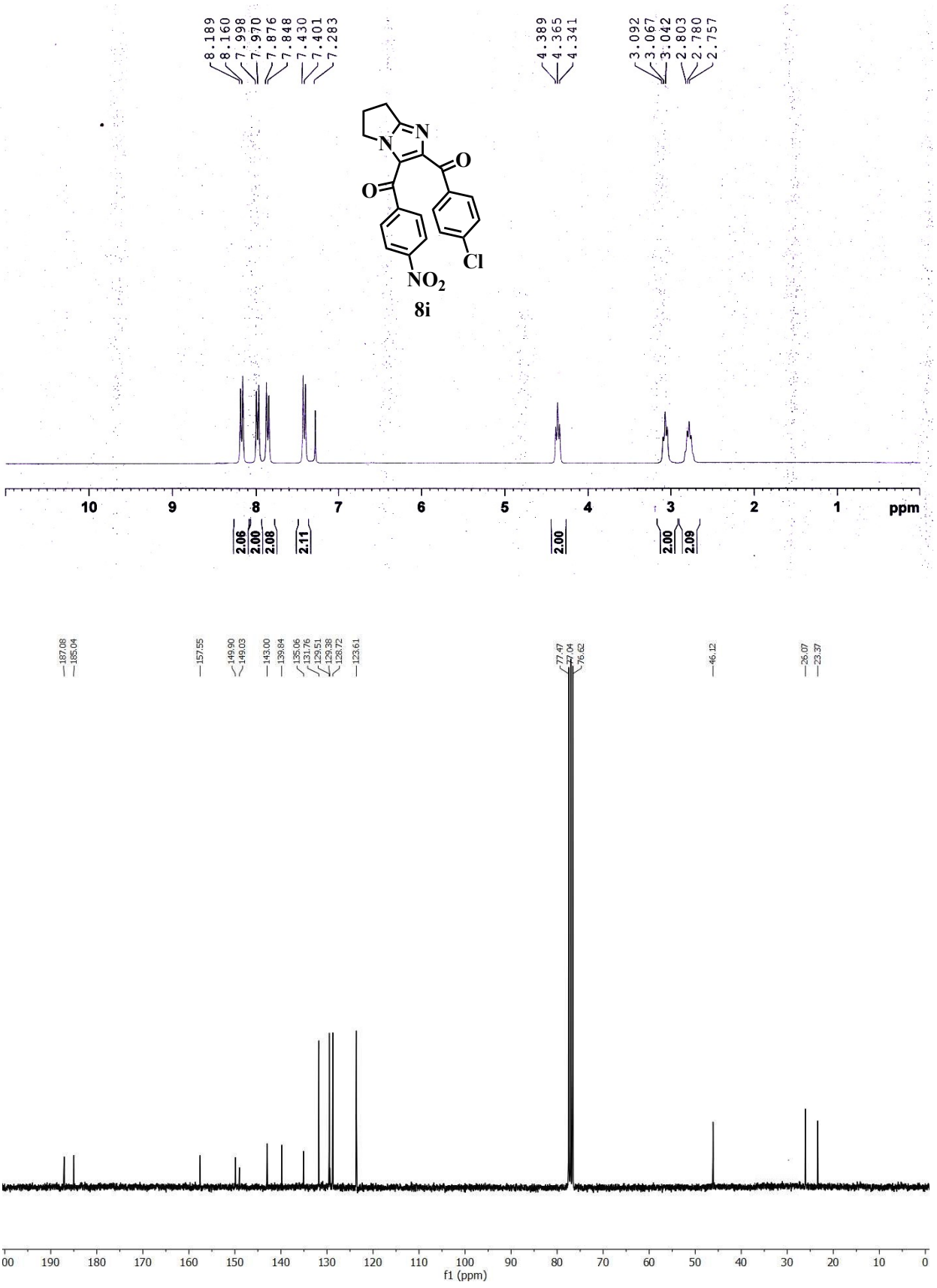
**SI Figure 34:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8g**



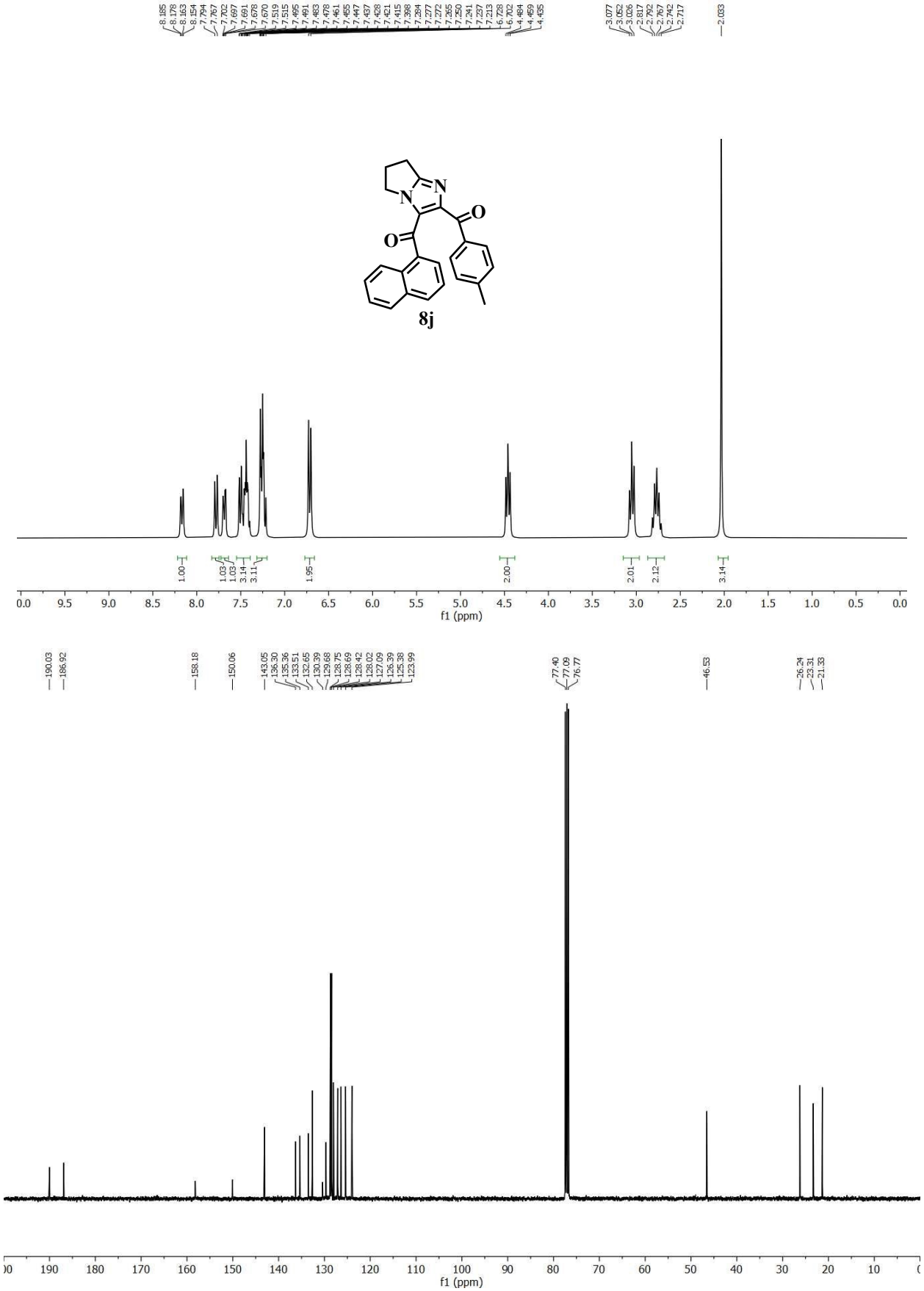
**SI Figure 35:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8h**



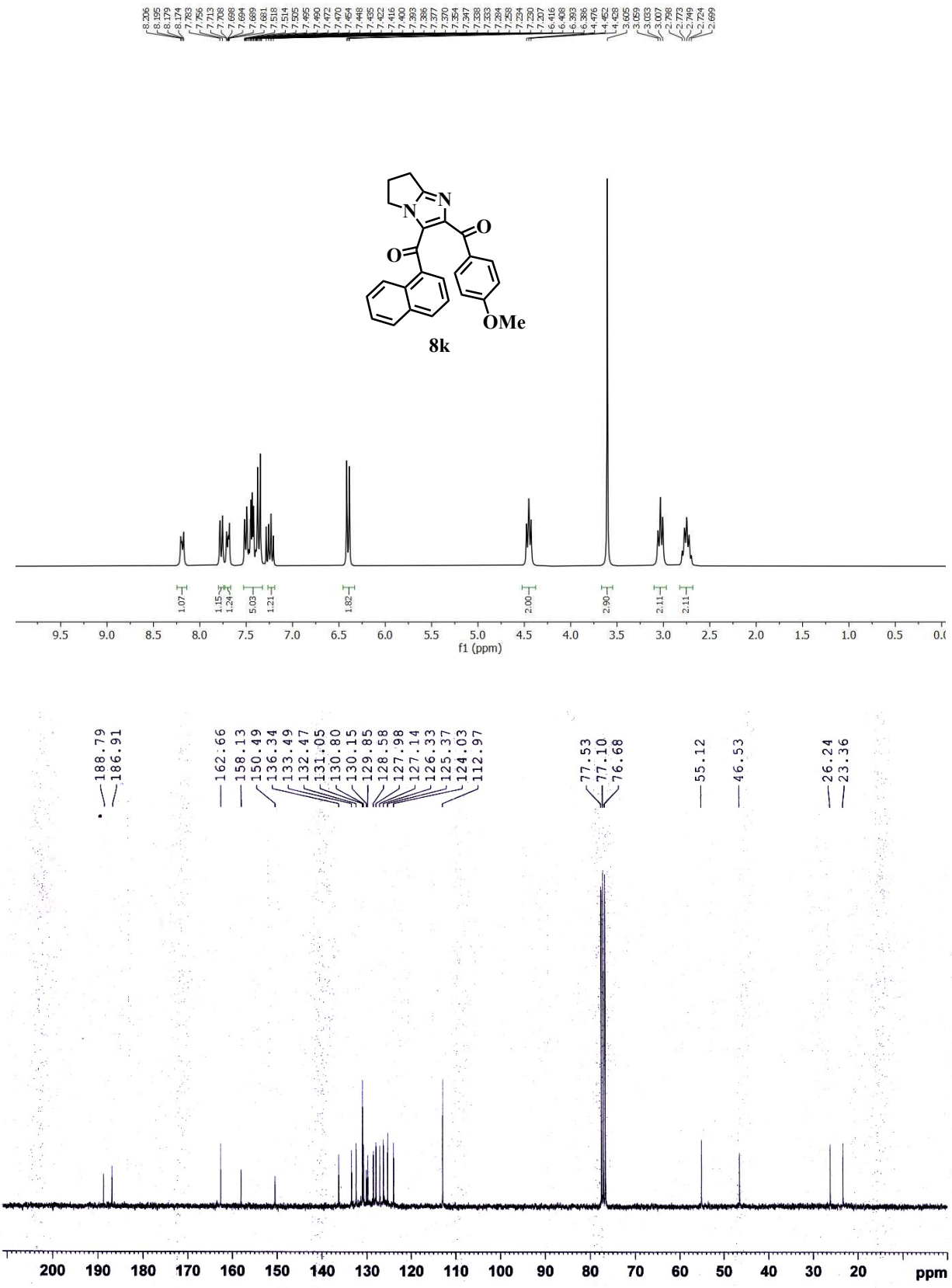
**SI Figure 36:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8i**



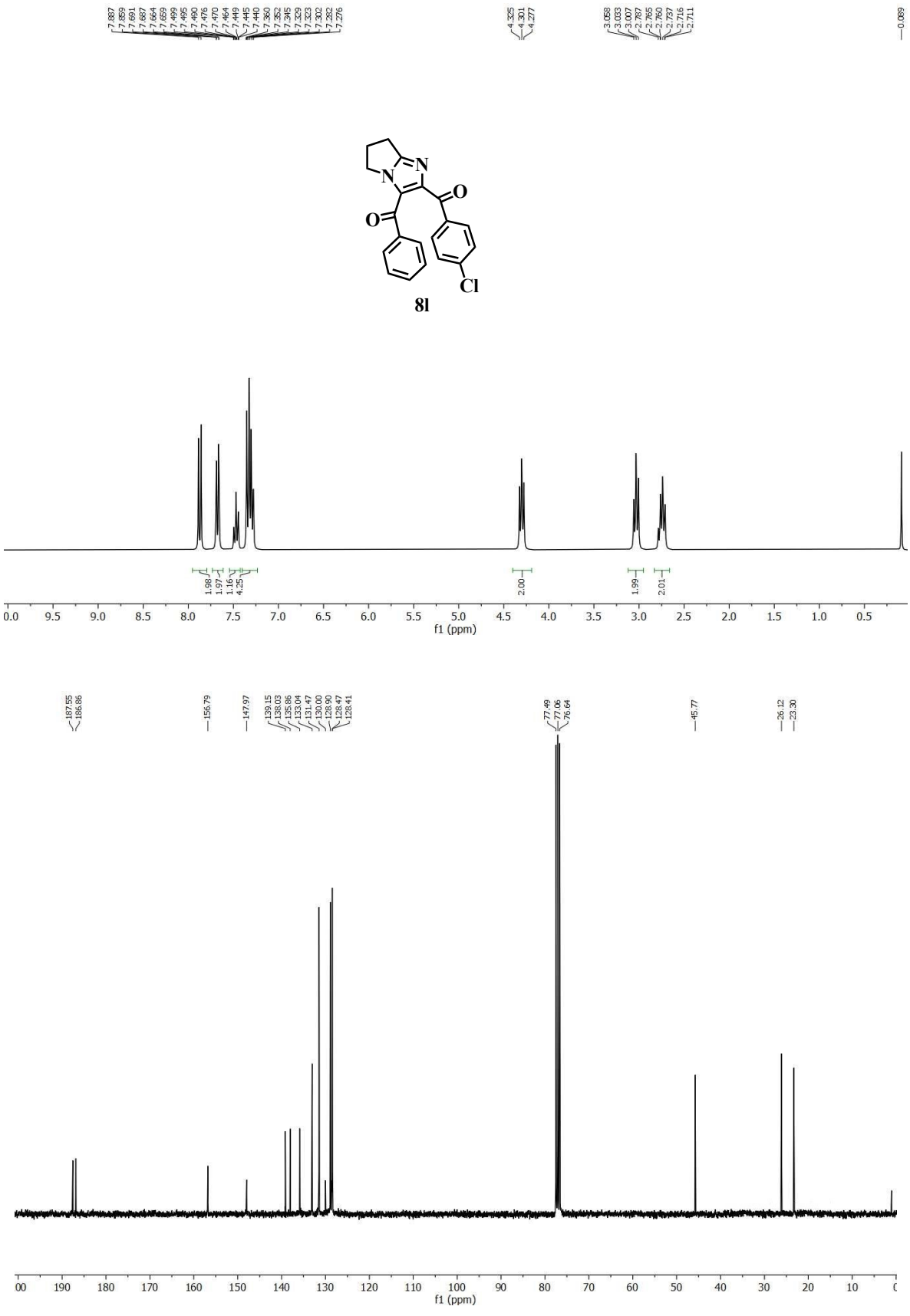
**SI Figure 37:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8j**



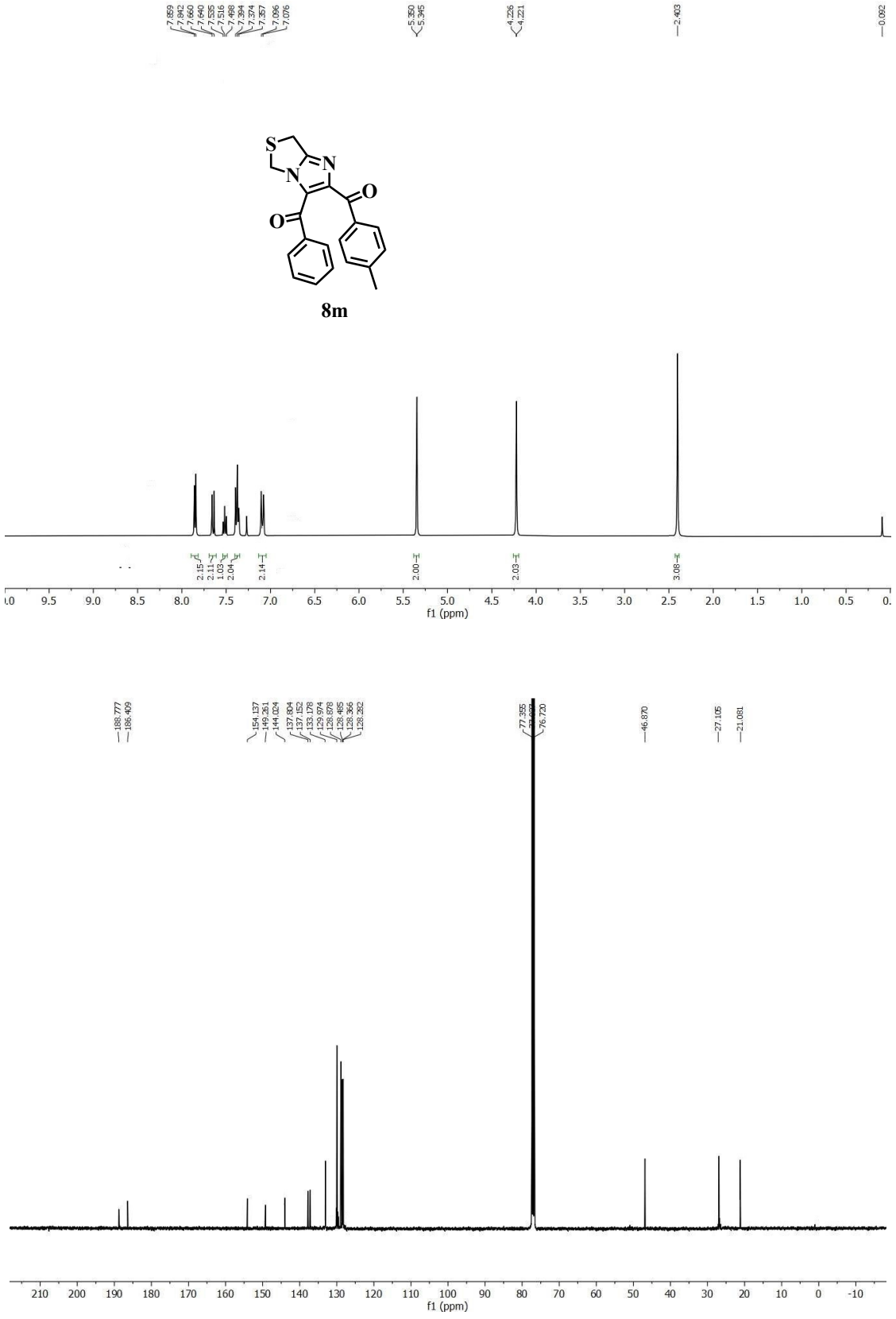
**SI Figure 38:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8k**



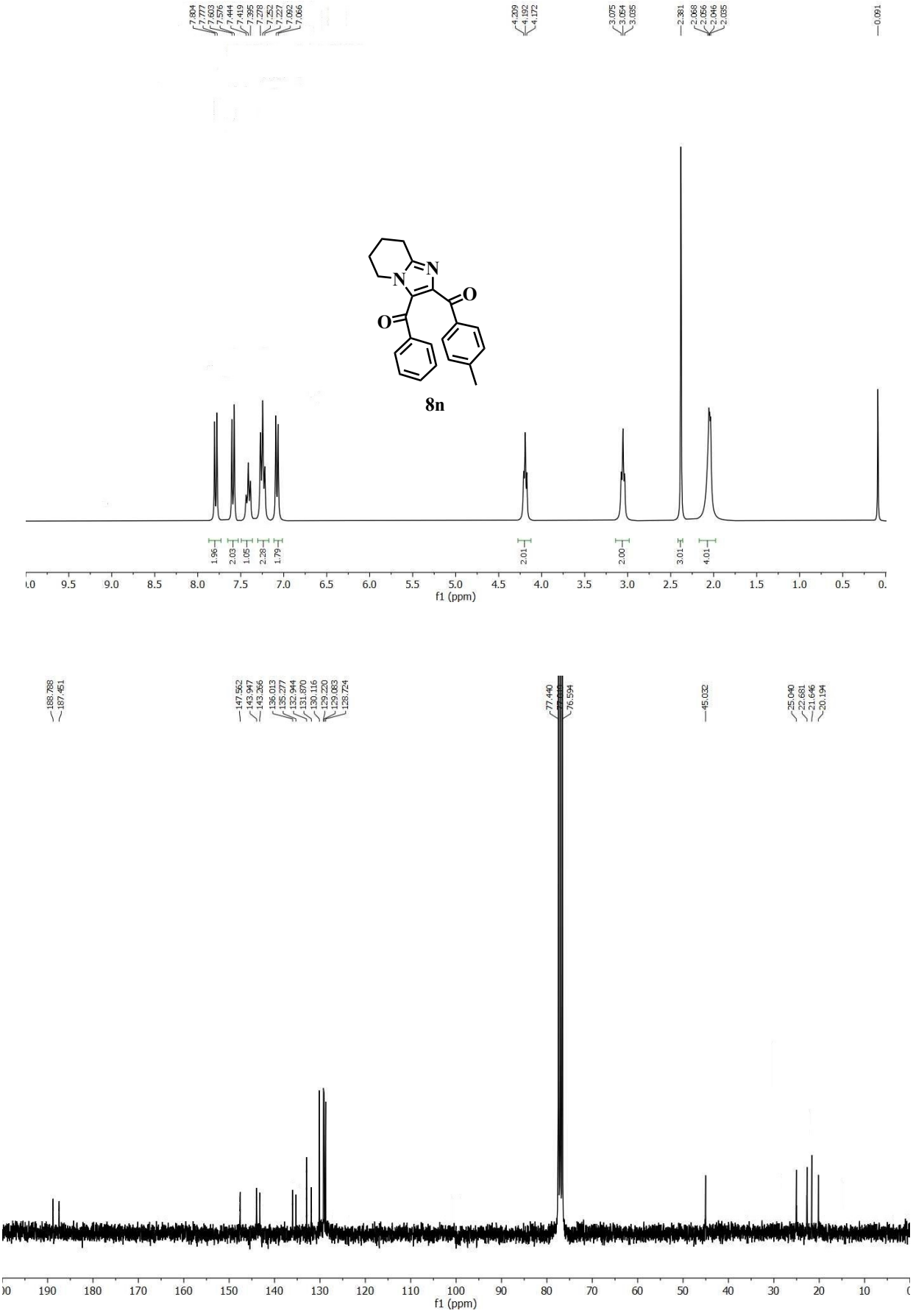
**SI Figure 39:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8l**



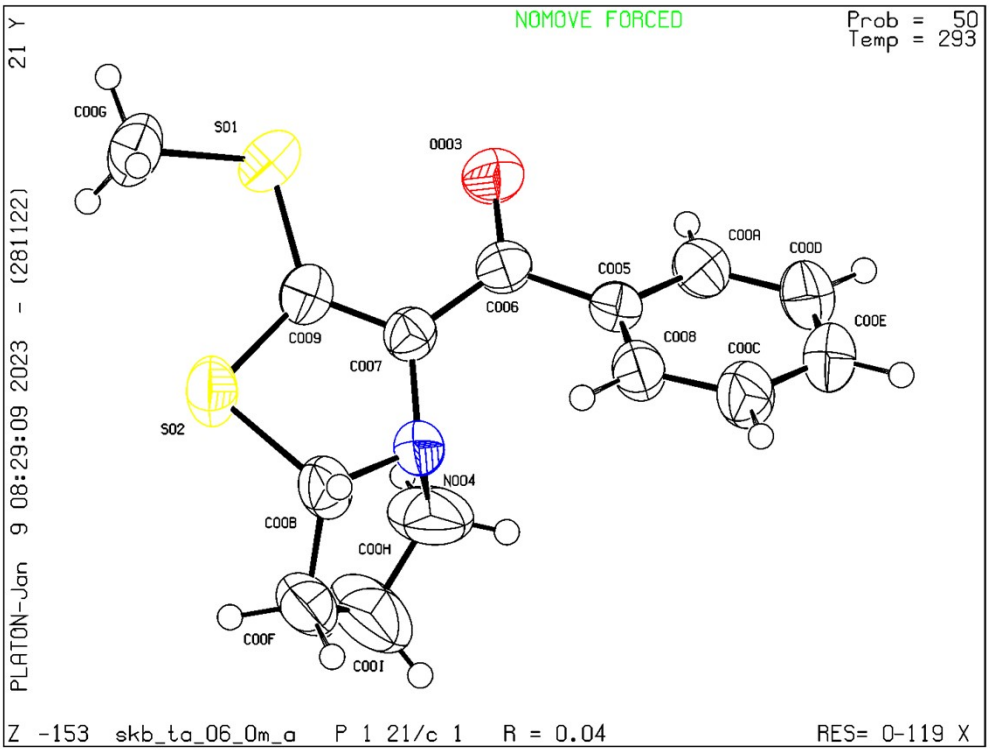
**SI Figure 40:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8m**



**SI Figure 41:** $^{1}H$ and $^{13}C$-NMR spectra of compound **8n**

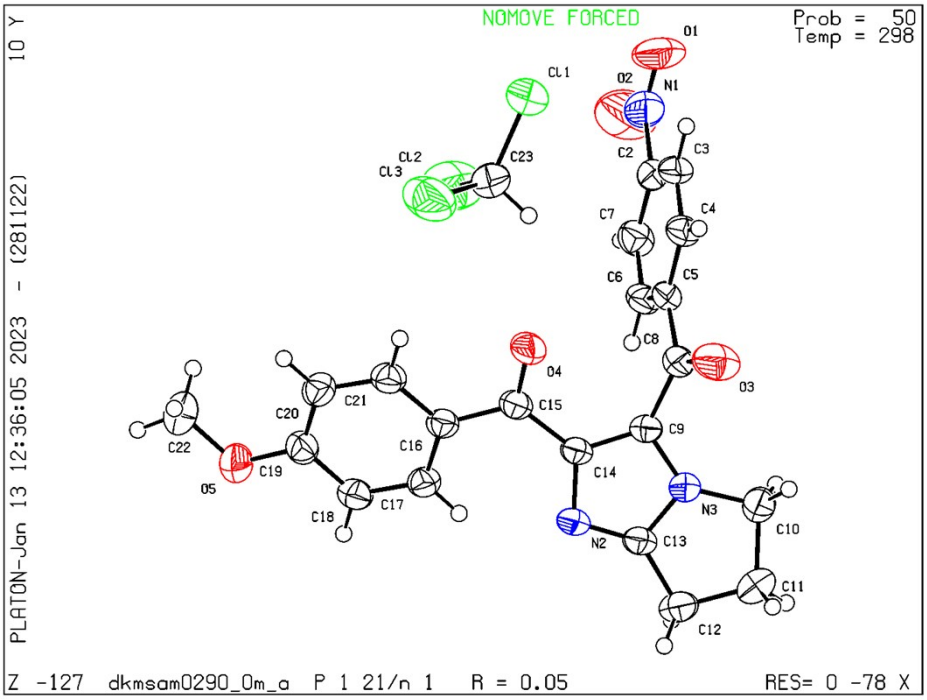


**10. Crystal summary data of compound 6a** (CCDC 2239889)




- Chemical formula and formula weight (M): $C_{14}$ $H_{15}$ N O $S_2$ and 277.39
- Crystal system: Monoclinic Unit-cell dimensions (angstrom, degrees) and volume, with edges: a 15.095(9) b 7.738(5) c 11.649(7) 90.00, 91.42(2) 90.00, 1360.1(14)
- Temperature: 296 K
- Space group symbol: P 1 21/c 1
- No. of formula units in unit cell (Z): 4
- Number of reflections measured and/or number of independent reflections, Rint: 2920
- Final R values (and whether quoted for all or obrserved data): 0.0410

**11. Crystal summary data of compound 8c** (CCDC 2239890)




- Chemical formula and formula weight (M): $C_{22}H_{18}Cl_3N_3O_5$ and 510.74
- Crystal system: Monoclinic Unit-cell dimensions (angstrom, degrees) and volume, with edges: a 13.558(3) b 7.3045(19) c 23.523(6), 90.00, 103.417(4), 90.00, 2266.0(10)
- Temperature: 298 K
- Space group symbol: P 1 21/n 1
- No. of formula units in unit cell (Z): 4
- Number of reflections measured and/or number of independent reflections, Rint: 4357
- Final R values (and whether quoted for all or obrserved data): 0.0492