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Supporting Information

Developing a Straightforward Route Toward Synthesis of Arylaminomaleimides by Palladium-Catalyzed Arylation of One-Pot Synthesized Aminomaleimides

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1. Experimental

1.1. Materials and characterization techniques

Anhydrous solvents were prepared by standard drying methods from commercially available solvents. Other solvents were used as received. Palladium(II) acetate [$Pd(OAc)_2$], palladium(II) chloride [$PdCl_2$], palladium(II) bis(acetylacetonate) [$Pd(acac)_2$], tris(dibenzylideneacetone)dipalladium(0) [$Pd(dba)_2$], and bis(acetonitrile)dichloropalladium(II) [$Pd(ACN)_2Cl_2$], dimethyl acetylenedicarboxylate, aryl iodides and all other used compounds were commercial and acquired from Sigma Aldrich Co. or other companies. The synthesized compounds identified through obtained ^1H NMR and ^{13}C NMR spectra by a Bruker UltraShield 400 MHz (100 MHz for ^{13}C) or a Varian-INOVA 500 MHz (125 MHz for ^{13}C) in $CDCl_3$ with the tetramethylsilane (TMS) as the internal standard. Chemical shifts (δ) are recorded and presented in parts per million (ppm). Electron ionization mass spectrometry analyses (EI-MS) were performed using an Agilent 5975C Mass Spectrum. The CHN elemental analyses were recorded using a Thermo Finnigan Flash EA 1112 Elemental Analyzer.

1.2. General synthesizing procedure of 3-aminomaleimides

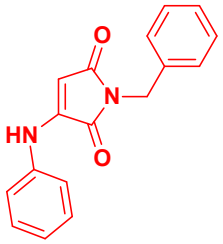
3-Aminomaleimides **1a-h** synthesized according to the previously reported method [1]. Briefly, 10 mmol of R^1NH_2 amine was added slowly to a cooled solution comprising 10 mmol of dimethyl acetylenedicarboxylate in 20 mL methanol at 0 ºC. The reaction continued for 30 min at room temperature. After that, 50 mmol of R^2NH_2 amine was slowly added to the reaction pot and stirring of the reaction continued overnight. Finally, the obtained precipitate was filtered and washed with hexane, followed by recrystallization in hot ethanol. That results in obtaining the desired 3-aminomaleimides (**1a-h**) as the formed solid. The compounds **1a** [1], **1d** [2, 3], and **1h** [1] have been reported previously.

1.3. General procedure for palladium-catalyzed synthesis of 3-aryl-4-aminomaleimides

In a 5 mL vial containing 1 mL of a solvent, an amount of 0.1 mmol of synthesized 3-aminomaleimide (**1a-h)**, 0.2 mmol of desired aryl iodides (**2a-g**; or a given amount), 0.2 mmol of sodium bicarbonate (or a mentioned amount of other bases), and 10 mol% of palladium catalyst (respect to **1a-h** amount) were added with a stirrer bar. Then the vial was caped and put in a pre-heated oil at a desired temperature for 24 hours. Then, the vial was cooled to room temperature, and the desired product (**3aa**-**he**) after removal of the solvent, was purified using column chromatography on silica gel (solvent: ethylacetate-hexane).

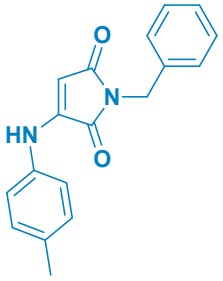
2. Experimental characterization data

2.1. Experimental characterization data of synthesized 3-aminomaleimides



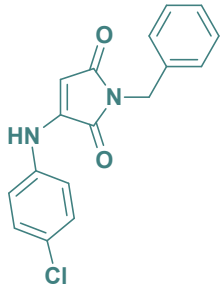
1a

1-Benzyl-3-(phenylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 60% yield. mp: 160-162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.43 (m, 7H), 7.26 (s, 1H), 7.14-7.19 (m, 3H), 5.55 (s, 1H), 4.73 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.24, 167.94, 142.29, 138.32, 136.47, 129.78, 128.67, 128.32, 127.76, 124.58, 118.79, 89.11, 41.44. Elemental Analysis Calculated for $C_{17}H_{14}N_2O_2$: C, 73.37; H, 5.07; N, 10.07. Found: C, 73.23; H, 4.91; N, 9.94.



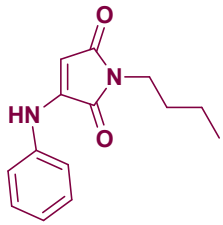
1b

1-Benzyl-3-(p-tolylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 76% yield. mp: 191-193 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.40 (m, 6H), 7.20 (d, J= 8 Hz, 2H), 7.05 (d, J= 8.4 Hz, 2H), 5.49 (s, 1H), 4.72 (s, 2H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.35, 167.97, 142.82, 136.54, 135.79, 134.48, 130.72, 128.66, 128.30, 127.88, 127.73, 118.90, 88.36, 41.39, 20.88. Elemental Analysis Calculated for $C_{18}H_{16}N_2O_2$: C, 73.95; H, 5.52; N, 9.58. Found: C, 73.76; H, 5.37; N, 9.37.



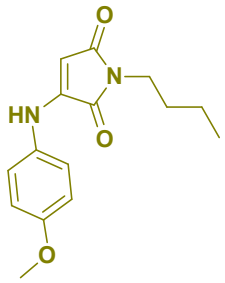
1c

1-Benzyl-3-((4-chlorophenyl)amino)-1H-pyrrole-2,5-dione. Yellow Solid; 54% yield. mp: 174-176 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.39 (m, 7H), 7.26 (s, 1H), 7.08 (d, J=8.8 Hz, 2H), 5.51 (s, 1H), 4.72 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.97, 167.76, 142.24, 136.92, 136.34, 129.87, 129.81, 128.69, 128.32, 127.82, 119.99, 89.60, 41.49. Elemental Analysis Calculated for $C_{17}H_{13}ClN_2O_2$: C, 65.29; H, 4.19; N, 8.96. Found: C, 65.51; H, 4.37; N, 9.21.



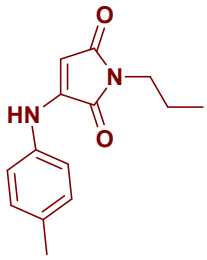
1d

1-Butyl-3-(phenylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 68% yield. mp: 131-133 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.43 (m, 2H), 7.37 (s, 1H), 7.14-7.18 (m, 3H), 5.51 (s, 1H), 3.55 (t, J=7.4 Hz, 2H), 1.61(quint, J=7.6 Hz, 2H), (sext, J=7.2 Hz, 2H), 0.95 (t, J=7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.83, 168.33, 142.34, 138.51, 129.73, 124.42, 118.73, 88.96, 37.71, 30.74, 20.03, 13.64. Elemental Analysis Calculated for $C_{14}H_{16}N_2O_2$: C, 68.83; H, 6.60; N, 11.47. Found: C, 68.54; H, 6.48; N, 11.25.



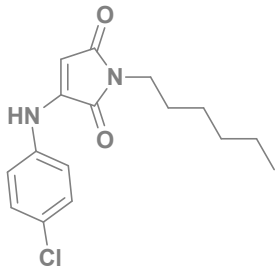
1e

1-Butyl-3-((4-methoxyphenyl) amino)-1H-pyrrole-2,5-dione. Yellow Solid; 48% yield. mp: 143-145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (s, 1H), 7.12 (d, J=9.2 Hz, 2H), 6.93 (d, J=9.2 Hz, 2H), 5.37 (s, 1H), 3.82 (s, 3H), 3.53 (t, J= 7.2 Hz, 2H), 1.60 (quint, J=7.6 Hz, 2H), 1.35 (sext, J=7.6 Hz, 2H), 0.94 (t, J=7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.95, 168.28, 156.66, 143.15, 131.56, 120.57, 114.92, 87.23, 55.56, 37.63, 30.76, 20.03, 13.64. Elemental Analysis Calculated for $C_{15}H_{18}N_2O_2$: C, 65.68; H, 6.61; N, 10.21. Found: C, 65.43; H, 6.51; N, 9.97.



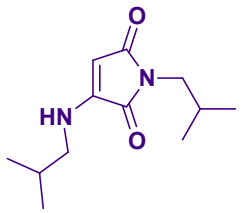
1f

1-Propyl-3-(p-tolylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 43% yield. mp:148-150 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (s, 1H), 7.21 (d, J=8.4 Hz, 2H), 7.06 (d, J=8.4 Hz, 2H), 5.45 (s, 1H), 3.51 (t, J=7.2 Hz, 2H), 2.36 (s, 3H), 1.67 (sext, J=7.6 Hz, 2H), 0.93 (t, J=7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.94, 168.36, 142.56, 135.91, 134.34, 130.25, 118.78, 88.23, 39.49, 22.02, 20.86, 11.27. Elemental Analysis Calculated for $C_{14}H_{16}N_2O_2$: C, 68.83; H, 6.60; N, 11.47. Found: C, 69.03; H, 6.74; 11. 62.



1g

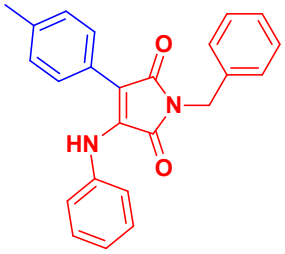
3-((4-Chlorophenyl) amino)-1-hexyl-1H-pyrrole-2,5-dione. Yellow Solid; 53% yield. mp:135-137 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (s, 1H),7.37 (d, J=8.8 Hz, 2H), 7.12(d, J=8.8 Hz, 2H), 5.43 (s, 1H), 3.55 (t, J=7.4 Hz, 2H), 1.57-1.65 (m, 2H), 1.28-1.33(m, 6H), 0.89 (t, J=6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.53, 168.17, 142.10, 137.14, 129.81, 129.63, 119.94, 89.45, 38.04, 31.35, 28.63, 26.47, 22.53, 14.01. Elemental Analysis Calculated for $C_{16}H_{19}ClN_2O_2$: C, 62.64; H, 6.24; N, 9.13. Found: C, 62.35; H, 6.08; N, 8.92.



1h

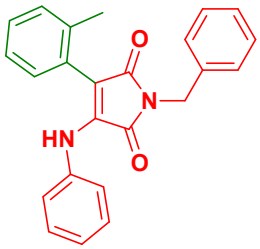
1-Isobutyl-3-(isobutylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 39% yield. mp:125-127 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.50 (s, 1H), 4.78 (s, 1H), 3.27 (d, J=7.6 Hz, 2H), 2.99 (t, J=6.4 Hz, 2H), 1.89-2.06 (m, 2H), 0.98 (d, J=6.8 Hz, 6H), 0.89 (d, J=6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.88, 167.83, 140.34, 83.69, 51.95, 44.88, 28.09, 27.93, 20.17, 20.04. Elemental Analysis Calculated for $C_{12}H_{20}N_2O_2$: C, 64.26; H, 8.99; N, 12.49. Found: C, 63.89; H, 8.73; N, 12.28.

2.2. Experimental characterization data of synthesized 3-aryl-4-aminomaleimides



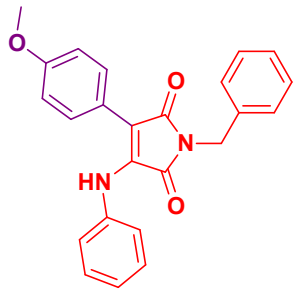
3aa

1-Benzyl-3-(phenylamino)-4-(p-tolyl)-1H-pyrrole-2,5-dione. Yellow Solid; 95% yield. mp: 166-168 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J=8.8 Hz, 2H), 7.29-7.38 (m, 3H), 7.27 (s, 1H), 7.06 (t, J=7.6 Hz, 2H), 6.99 (t, J=7.2 Hz, 1H), 6.95 (s, 4H), 6.64 (d, J=8 Hz, 2H), 4.80 (s, 2H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.99, 168.43, 137.34, 136.62, 136.35, 135.41, 129.62, 128.69, 128.68, 128.29, 127.99, 127.81, 126.33, 124.32, 121.34, 103.06, 41.81, 21.34. EI-MS m/z: 368.20 (Calcd. for $C_{24}H_{20}N_2O_2$: 368.15). Elemental Analysis Calculated for $C_{24}H_{20}N_2O_2$: C, 78.24; H, 5.47; N, 7.60. Found: C, 78.08; H, 5.32; N, 7.43.



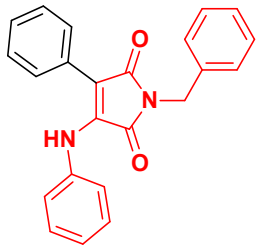
3ab

1-Benzyl-3-(phenylamino)-4-(o-tolyl)-1H-pyrrole-2,5-dione. Yellow Solid; 92% yield: mp: 131-133 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J=6.8 Hz, 2H), 7.30-7.39 (m, 4H),7.13-7.17(m, 1H),7.03-7.09 (m, 2H),6.99 (d, J=8Hz, 1H), 6.93-6.95 (m, 3H), 6.60-6.62 (m, 2H), 4.81(s, 2H), 1.97(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.71, 168.21, 137.99, 137.53, 136.64, 136.33, 130.34, 129.70, 128.71, 128.59, 128.22, 128.13, 127.80, 125.20, 124.43, 120.95, 102.31, 41.90, 20.11. EI-MS m/z: 368.20 (Calcd. for $C_{24}H_{20}N_2O_2$: 368.15). Elemental Analysis Calculated for $C_{24}H_{20}N_2O_2$: C, 78.24; H, 5.47; N, 7.60. Found: C, 78.41; H 5.62; N, 7.86.



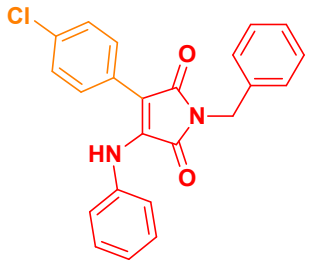
3ac

1-Benzyl-3-(4-methoxyphenyl)-4-(phenylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 83% yield. mp: 151-153 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J=6.4 Hz, 2H), 7.29-7.38 (m, 3H), 7.21, (s, 1H), 7.06 (t, J=7.6 Hz, 3H), 6.99 (d, J=8.8 Hz, 3H), 6.67 (d, J=8.8 Hz, 2H), 6.64 (d, J=8 Hz, 2H), 4.80 (s, 2H), 3.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.09, 168.49, 158.92, 136.62, 136.34, 134.86, 131.04, 128.66, 128.33, 127.78, 124.24, 121.78, 121.25, 112.82, 103.08, 55.26, 41.79. EI-MS m/z: 384.30 (Calcd. for $C_{24}H_{20}N_2O_3$: 384.15). Elemental Analysis Calculated for $C_{24}H_{20}N_2O_3$: C, 74.98; H, 5.24; N, 7.29. Found: C, 74.78; H, 5.11; N, 7.06.



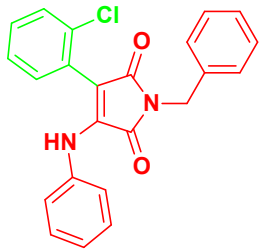
3ad

1-Benzyl-3-phenyl-4-(phenylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 94% yield. mp: 152-154 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J=8 Hz, 2H), 7.29-7.38 (m, 4H), 7.10-7.18 (m, 3H), 6.97-7.06 (m, 5H), 6.64 (d, J=7.6 Hz, 2H), 4.81 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.63, 168.23, 136.56, 136.20, 136.06, 129.72, 129.27, 128.69, 128.29, 127.82, 127.33, 127.26, 124.53, 121.52, 102.68, 41.84. EI-MS m/z: 354.20 (Calcd. for $C_{23}H_{18}N_2O_2$: 354.40). Elemental Analysis Calculated for $C_{23}H_{18}N_2O_2$: C, 77.95; H, 5.12; N, 7.90. Found: C, 77.73; H, 4.89; N, 7.81.



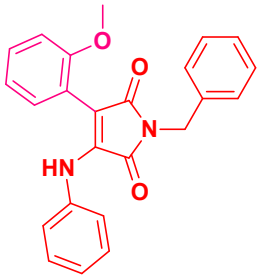
3ae

1-Benzyl-3-(4-chlorophenyl)-4-(phenylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 80% yield. mp: 137-139 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J=6.8 Hz, 2H), 7.29-7.38 (m, 4H), 7.02-7.12 (m, 5H), 6.96 (d, J=8.4 Hz, 2H), 6.65 (d, J=6.8 Hz, 2H), 4.79 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.62, 167.94, 136.41, 136.29, 135.99, 133.23, 130.89, 128.73, 128.69, 128.51, 127.90, 127.70, 127.44, 125.03, 121.73, 101.23, 41.90. EI-MS m/z: 388.30 (Calcd. for $C_{23}H_{17}ClN_2O_2$: 388.85). Elemental Analysis Calculated for $C_{23}H_{17}ClN_2O_2$: C, 71.04; H, 4.41; N, 7.20. Found: C, 70.82; H, 4.31; N, 7.11.



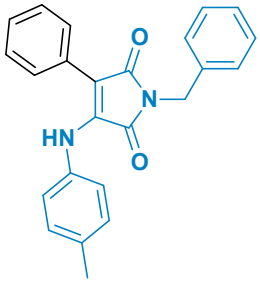
3af

1-Benzyl-3-(2-chlorophenyl)-4-(phenylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 91% yield. mp: 137-139 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J=8 Hz, 2H), 7.29-7.40 (m, 4H), 7.15 (s, 4H), 6.94-7.00 (m, 3H), 6.66-6.69 (m, 2H), 4.81 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.02, 167.70, 138.60, 136.50, 136.32, 135.16, 131.71, 129.45, 129.28, 129.02, 128.71, 128.59, 128.14, 127.81, 126.15, 124.87, 124.54, 99.50, 41.94. EI-MS m/z: 388.30 (Calcd. for $C_{23}H_{17}ClN_2O_2$: 388.85). Elemental Analysis Calculated for $C_{23}H_{17}ClN_2O_2$: C, 71.04; H, 4.41; N, 7.20. Found: C, 71.28; H, 4.63; N, 7.34.



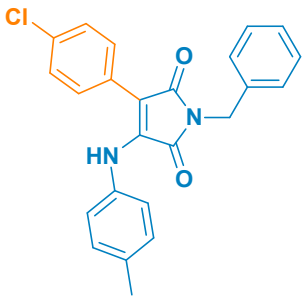
3ag

1-Benzyl-3-(2-methoxyphenyl)-4-(phenylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 49% yield. mp: 104-106 °C; (Hexan/EtOAC); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.50 (m, 3H), 7.29-7.40 (m, 4H), 7.20-7.25 (m, 1H), 6.91-7.01 (m, 4H), 6.61(d, J=7.6 Hz, 2H), 6.44 (d, J=8 Hz, 1H), 4.79 (s, 2H), 3.08 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.87, 168.53, 156.90, 137.33, 136.68, 136.67, 130.53, 129.44, 128.73, 128.64, 127.99, 127.73, 123.76, 120.01, 119.96, 119.21, 109.70, 98.50, 54.26, 41.86. EI-MS m/z: 384.30 (Calcd. for $C_{24}H_{20}N_2O_3$: 384.43). Elemental Analysis Calculated for $C_{24}H_{20}N_2O_3$: C, 74.98; H, 5.24; N, 7.29. Found: C, 74.69; H, 4.89; N, 6.97.



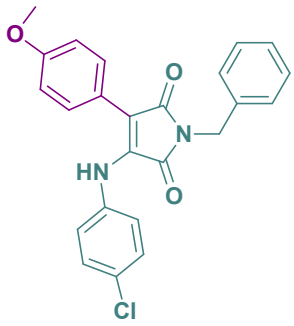
3bd

1-Benzyl-3-phenyl-4-(p-tolylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 90% yield: mp: 146-148 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J=7.2 Hz, 2H), 7.29-7.38 (m, 4H), 7.10-7.18 (m, 3H), 7.03 (d, J=7.6 Hz, 2H), 6.84 (d, J=8 Hz, 2H), 6.54 (d, J=8 Hz, 2H), 4.80 (s, 2H), 2.24 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.92, 168.27, 136.62, 136.32, 134.42, 133.74, 129.79, 129.37, 128.81, 128.68, 127.79, 127.21, 121.49, 101.95, 41.81, 20.85. EI-MS m/z: 368.30 (Calcd. for $C_{24}H_{20}N_2O_2$:368.43). Elemental Analysis Calculated for $C_{24}H_{20}N_2O_2$: C, 78.24; H, 5.47; N, 7.60. Found: C, 77.91; H, 5.12; N, 7.35.



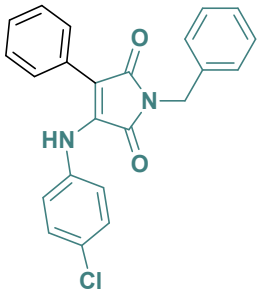
3be

1-Benzyl-3-(4-chlorophenyl)-4-(p-tolylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 78% yield. mp: 126-128 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J=6.4 Hz, 2H), 7.29-7.38 (m, 4H), 7.09 (d, J=8.8 Hz, 2H), 6.96 (d, J=8.8 Hz, 2H), 6.89 (d, J=8 Hz, 2H), 6.55 (d, J=8.4 Hz, 2H), 4.79 (s, 2H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.69, 167.96, 136.53, 136.47, 134.96, 133.49, 133.05, 130.94, 129.02, 128.71, 128.67, 127.86, 127.80, 127.38, 121.70, 100.57, 41.86, 20.88. EI-MS m/z: 402.30 (Calcd. for $C_{24}H_{19}ClN_2O_2$: 402.87). Elemental Analysis Calculated for $C_{24}H_{19}ClN_2O_2$: C, 71.55; H, 4.75; N, 6.95. Found: C, 71.38; H, 4.56; N, 6.73.



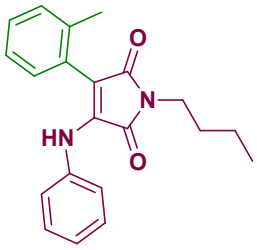
3cc

1-Benzyl-3-((4-chlorophenyl)amino)-4-(4-methoxyphenyl)-1H-pyrrole-2,5-dione. Yellow Solid; 45% yield. mp: 201-203 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J=6.4 Hz, 2H), 7.29-7.38 (m, 3H), 7.15 (s, 1H), 7.03 (t, J=8.8 Hz, 4H), 6.71 (d, J=9.2 Hz, 2H), 6.57 (d, J=8.8 Hz, 2H), 4.78 (s, 2H), 3.79 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.83, 168.35, 159.19, 136.50, 135.07, 134.42, 131.10, 129.42, 128.68, 128.64, 128.38, 127.83, 122.19, 121.46, 113.04, 103.96, 55.29, 41.85. EI-MS m/z: 418.30 (Calcd. for $C_{24}H_{19}ClN_2O_3$: 418.87). Elemental Analysis Calculated for $C_{24}H_{19}ClN_2O_3$: C, 68.82; H, 4.57; N, 6.69. Found: C, 68.65; H, 4.38; N, 6.43.



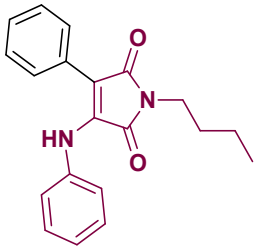
3cd

1-Benzyl-3-((4-chlorophenyl)amino)-4-phenyl-1H-pyrrole-2,5-dione. Yellow Solid; 89% yield. mp: 157-159 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J=6.4 Hz, 2H), 7.29-7.38 (m, 4H), 7.15-7.23 (m, 3H), 7.05 (d, J=6.4 Hz, 2H), 6.99 (d, J=8.8 Hz, 2H), 6.57 (d, J=8.8 Hz, 2H), 4.80 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.61, 168.13, 136.44, 135.73, 134.92, 129.76, 129.04, 128.72, 128.65, 128.34, 127.88, 127.76, 127.48, 122.50, 103.43, 41.89. EI-MS m/z: 388.30 (Calcd. for $C_{23}H_{17}ClN_2O_2$: 388.85). Elemental Analysis Calculated for $C_{23}H_{17}ClN_2O_2$: C, 71.04; H, 4.41; N, 7.20. Found: C, 70.83; H, 4.16; N, 6.97.



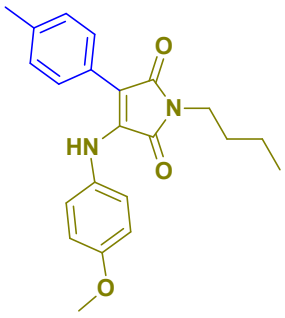
3db

1-Butyl-3-(phenylamino)-4-(o-tolyl)-1H-pyrrole-2,5-dione. Yellow Solid; 52% yield. mp: 110-112 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31(s, 1H), 7.03-7.16 (m, 3H), 6.90-6.99 (m, 4H), 6.59-6.63 (m, 2H), 3.64 (t, J=7.2 Hz, 2H), 1.96 (s, 3H), 1.69 (quint, J= 7.2 Hz, 2H), 1.40 (sext, J=7.6 Hz, 2H), 0.98 (t, J=7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.14, 168.56, 137.98, 137.24, 136.43, 130.33, 129.79, 129.67, 128.14, 125.18, 124.30, 120.81, 102.13, 38.12, 30.80, 20.08, 13.69. EI-MS m/z: 334.30 (Calcd. for $C_{21}H_{22}N_2O_2$: 334.41). Elemental Analysis Calculated for $C_{21}H_{22}N_2O_2$: C, 75.42; H, 6.63; N, 8.38. Found: C, 75.11; H, 6.49; N, 8.09.



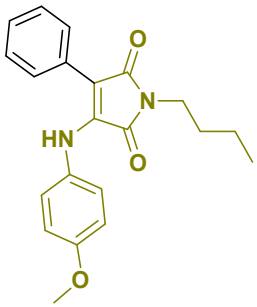
3dc

1-Butyl-3-phenyl-4-(phenylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 78% yield. mp: 178-180 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (s, 1H), 7.09-7.18 (m, 3H), 6.96-7.07 (m, 5H), 6.66 (d, J=7.6 Hz, 2H), 3.64 (t, J=7.2 Hz, 2H), 1.68 (quint, J= 7.6 Hz, 2H), 1.36 (sext, J=7.2 Hz, 2H), 0.98 (t, J=7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.30, 168.67, 136.38, 135.97, 129.74, 129.44, 128.25, 127.25, 124.43, 121.48, 102.48, 38.06, 30.82, 20.09, 13.68. EI-MS m/z: 320.30 (Calcd. for $C_{20}H_{20}N_2O_2$: 320.38). Elemental Analysis Calculated for $C_{20}H_{20}N_2O_2$: C, 74.98; H, 6.29; N, 8.74. Found: C, 75.16; H, 6.43; N, 8.96.



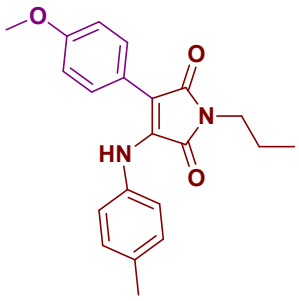
3ea

1-Butyl-3-((4-methoxyphenyl)amino)-4-(p-tolyl)-1H-pyrrole-2,5-dione. Yellow Solid; 79% yield. mp: 114-116 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (s, 1H), 6.93 (m, 4H), 6.62 (d, J=9.2 Hz, 2H), 6.59 (d, J=9.2 Hz, 2H), 3.75 (s, 3H), 3.62 (t, J=7.4 Hz, 2H), 2.28 (s, 3H), 1.66 (quint, J=7.6 Hz, 2H), 1.39 (sext, J=7.2 Hz, 2H), 0.97 (t, J=7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.52, 168.76, 156.64, 136.85, 136.11, 129.70, 129.57, 127.92, 126.49, 123.06, 113.49, 101.34, 55.50, 37.95, 30.84, 21.28, 20.09, 13.68. EI-MS m/z: 364.30 (Calcd. for $C_{22}H_{24}N_2O_3$:364.44). Elemental Analysis Calculated for $C_{22}H_{24}N_2O_3$: C, 72.50; H, 6.64; N, 7.69. Found: C, 72.18; H, 6.37; N, 7.42.



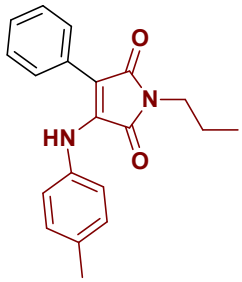
3ed

1-Butyl-3-((4-methoxyphenyl)amino)-4-phenyl-1H-pyrrole-2,5-dione. Yellow Solid; 73% yield. mp: 118-120 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (s, 1H), 7.08-7.16 (m, 3H), 7.01(dd, J=9.6 ,1.6 Hz, 2H), 6.62 (d, J=9.2 Hz, 2H), 6.56 (d, J=9.2Hz, 2H), 3.70 (s, 3H), 3.62 (t, J=7.2 Hz, 2H), 1.67 (quint, J= 7.6 Hz, 2H), 1.39 (sext, J= 7.6 Hz, 2H), 0.97 (t, J=7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.39, 168.62, 156.79, 136.75, 129.69, 129.56, 129.43, 127.18, 126.96, 123.23, 113.47, 100.98, 55.49, 37.98, 30.84, 20.10, 13.68. EI-MS m/z: 350.30 (Calcd. for $C_{21}H_{22}N_2O_3$: 350.41). Elemental Analysis Calculated for $C_{21}H_{22}N_2O_3$: C, 71.98; H, 6.33; N, 7.99. Found: C, 71.68; H, 6.13; N, 7.78.



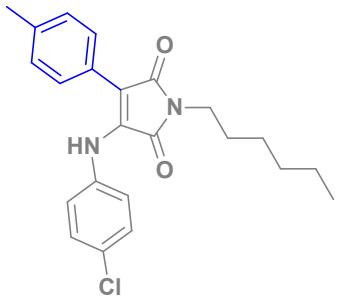
3fc

3-(4-Methoxyphenyl)-1-propyl-4-(p-tolylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 71% yield. mp: 133-135 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (s, 1H), 7.00 (d, J=8.8 Hz, 2H), 6.87 (d, J=8.4 Hz, 2H), 6.69 (d, J=8.8 Hz, 2H),6.56 (d, J=8.4, 2H) 3.78 (s, 3H), 3.58 (t, J=7.2 Hz, 2H), 2.25 (s, 3H), 1.70 (sext, J=7.2 Hz, 2H), 0.97 (t, J=7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.65, 168.92, 158.74, 134.97, 133.97, 131.08, 128.85, 122.03, 121.17, 112.79, 102.10, 55.27, 39.82, 22.09, 20.83, 11.36. EI-MS m/z: 350.30 (Calcd. for $C_{21}H_{22}N_2O_3$: 350.41). Elemental Analysis Calculated for $C_{21}H_{22}N_2O_3$: C, 71.98; H, 6.33; N, 7.99. Found: C, 71.62; H, 6.05; N, 7.68.



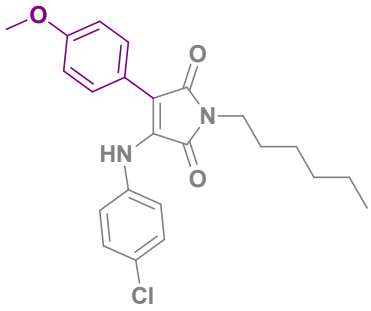
3fd

3-Phenyl-1-propyl-4-(p-tolylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 85% yield. mp: 138-140 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.10-7.18 (m, 3H), 7.05 (m, 2H), 6.84 (d, J=8 Hz, 2H), 6.56 (d, J=8.4 Hz, 2H), 3.60 (t, J=7.4 Hz, 2H), 2.24 (s, 3H), 1.68 (sext, J=7.6 Hz, 2H), 0.98 (t, J=7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.38, 168.70, 136.18, 134.25, 133.90, 129.80, 129.52, 128.77, 127.20, 127.10, 121.44, 101.76, 39.87, 22.08, 20.83, 11.38. EI-MS m/z: 320.30 (Calcd. for $C_{20}H_{20}N_2O_2$: 320.38). Elemental Analysis Calculated for $C_{20}H_{20}N_2O_2$: C, 74.98; H, 6.29; N, 8.74. Found: C, 74.63; H, 6.09; N, 8.58.



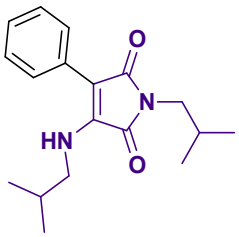
3ga

3-((4-Chlorophenyl)amino)-1-hexyl-4-(p-tolyl)-1H-pyrrole-2,5-dione. Yellow Solid; 82% yield. mp: 123-125 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (s, 1H), 6.95-7.03 (m, 6H), 6.59 (d, J=8.8 Hz, 2H), 3.61 (t, J=7.4 Hz, 2H), 2.32 (s, 3H), 1.63-1.70 (m, 2H), 1.27-1.37 (m, 6H), 0.90 (t, J=6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.18, 168.72, 137.65, 135.25, 134.99, 129.66, 129.27, 128.26, 128.19, 126.27, 122.27, 103.68, 38.37, 31.40, 28.71, 26.55, 22.55, 21.33, 14.05. EI-MS m/z: 396.30 (Calcd. for $C_{23}H_{25}ClN_2O_2$: 396.91). Elemental Analysis Calculated for $C_{23}H_{25}ClN_2O_2$: C, 69.60; H, 6.35; N, 7.06. Found: C, 69.82; H, 6.47; N, 7.29.



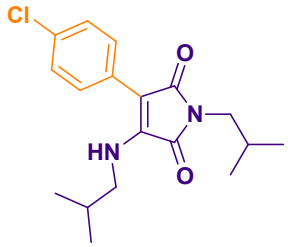
3gc

3-((4-Chlorophenyl)amino)-1-hexyl-4-(4-methoxyphenyl)-1H-pyrrole-2,5-dione. Yellow Solid; 65% yield. mp: 130-132 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (s, 1H), 7.00-7.05 (m, 4H), 6.73 (d, J=8.8 Hz, 2H), 6.59 (d, J=8.8 Hz, 2H), 3.79 (s, 3H), 3.61 (t, J=7.4 Hz, 2H), 1.64-1.71 (m, 2H), 1.27-1.38 (m, 6H), 0.89 (t, J=6.4 Hz, 3H).). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.29, 168.75, 159.12, 135.22, 134.30, 131.10, 129.26, 128.35, 122.14, 121.62, 113.03, 103.73, 55.29, 38.36, 31.38, 28.70, 26.52, 22.53, 14.03. EI-MS m/z: 412.30 (Calcd. for $C_{23}H_{25}ClN_2O_3$: 412.91). Elemental Analysis Calculated for $C_{23}H_{25}ClN_2O_3$: C, 66.90; H, 6.10; N, 6.78. Found: C, 66.71; H, 5.89; N, 6.62.



3hd

1-Isobutyl-3-(isobutylamino)-4-phenyl-1H-pyrrole-2,5-dione. Yellow Solid; 83% yield. mp: 107-109 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.39 (m, 5H), 5.56 (s, 1H), 3.35 (d, J=7.2 Hz, 2H), 2.93 (t, J= 6.8 Hz, 2H), 2.06 (hept, J=6.8 Hz, 1H), 1.92 (hept, J=6.4 Hz, 1H), 0.92 (d, J=6.8Hz, 6H), 0.75 (d, J=6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.60, 168.22, 142, 130.53, 130.34, 127.87, 127.25, 98.77, 51.50, 45.33, 28.78, 27.97, 20.14, 19.71. EI-MS m/z: 300.30 (Calcd. for $C_{18}H_{24}N_2O_2$:300.40). Elemental Analysis Calculated for $C_{18}H_{24}N_2O_2$: C, 71.97; H, 8.05; N, 9.33. Found: C, 71.68; H, 7.84; N, 9.02.



3he

3-(4-Chlorophenyl)-1-isobutyl-4-(isobutylamino)-1H-pyrrole-2,5-dione. Yellow Solid; 81% yield. mp: 99-101 °C; (Hexan/EtOAC 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J= 8.4 Hz, 2H), 7.26 (d, J=8.4 Hz, 2H), 5.62 (s, 1H), 3.34 (d, J=7.6 Hz, 2H), 2.92 (t, J=6.6 Hz, 2H), 2.04 (hept, J=6.8 Hz, 1H), 1.62(hept, J=6.8 Hz, 1H), 0.91 (d, J=6.8 Hz, 6H), 0.79 (d, J=6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.37, 167.92, 142.15, 133.15, 131.74, 128.85, 128.11, 97.46, 51.65, 45.40, 28.79, 27.95, 20.11, 19.75. EI-MS m/z: 334.30 (Calcd. for $C_{18}H_{23}ClN_2O_2$:334.84). Elemental Analysis Calculated for $C_{18}H_{23}ClN_2O_2$: C, 64.57; H, 6.92; N, 8.37. Found: C, 64.23; H, 6.71; N, 8.14.

References

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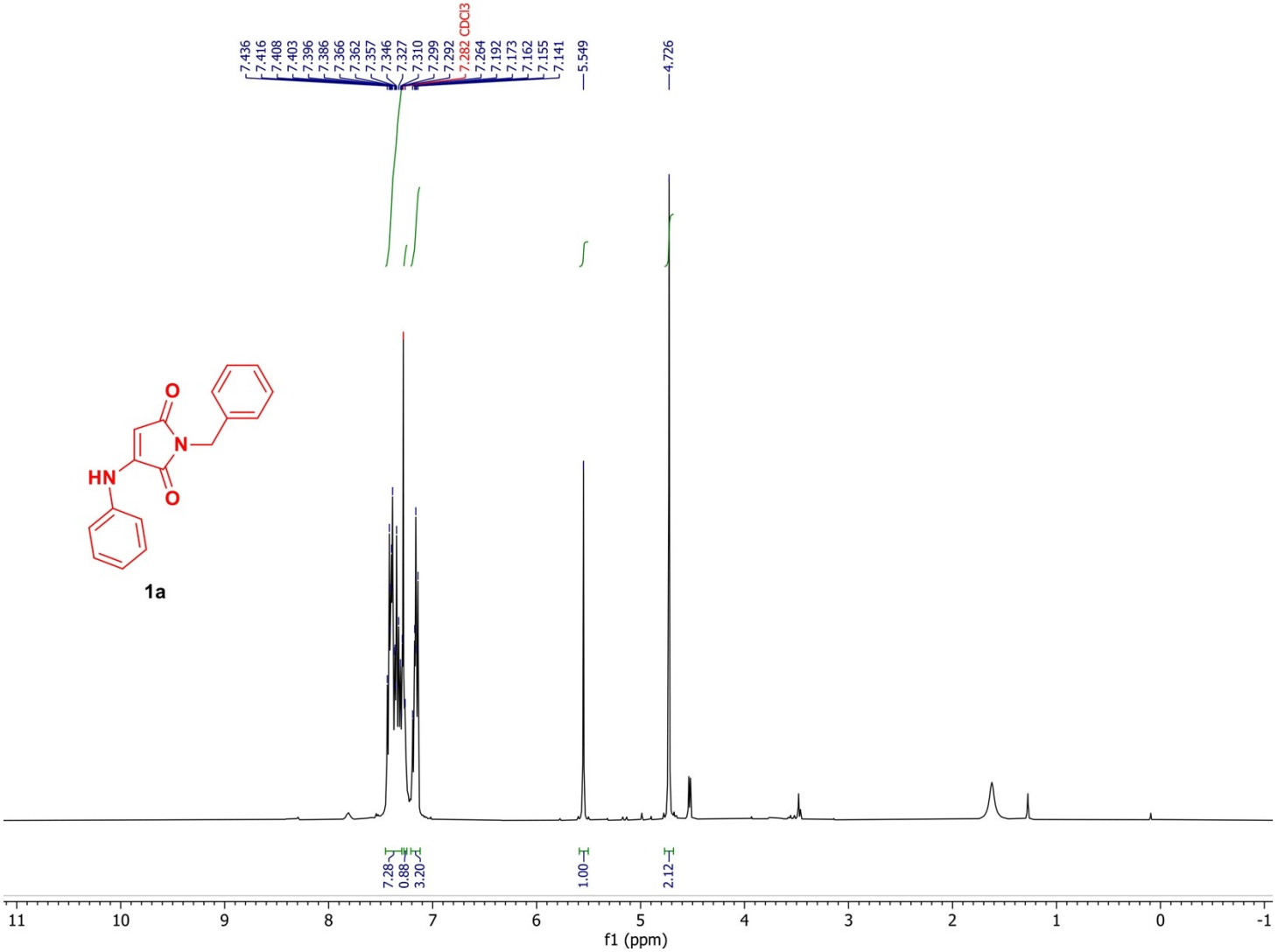
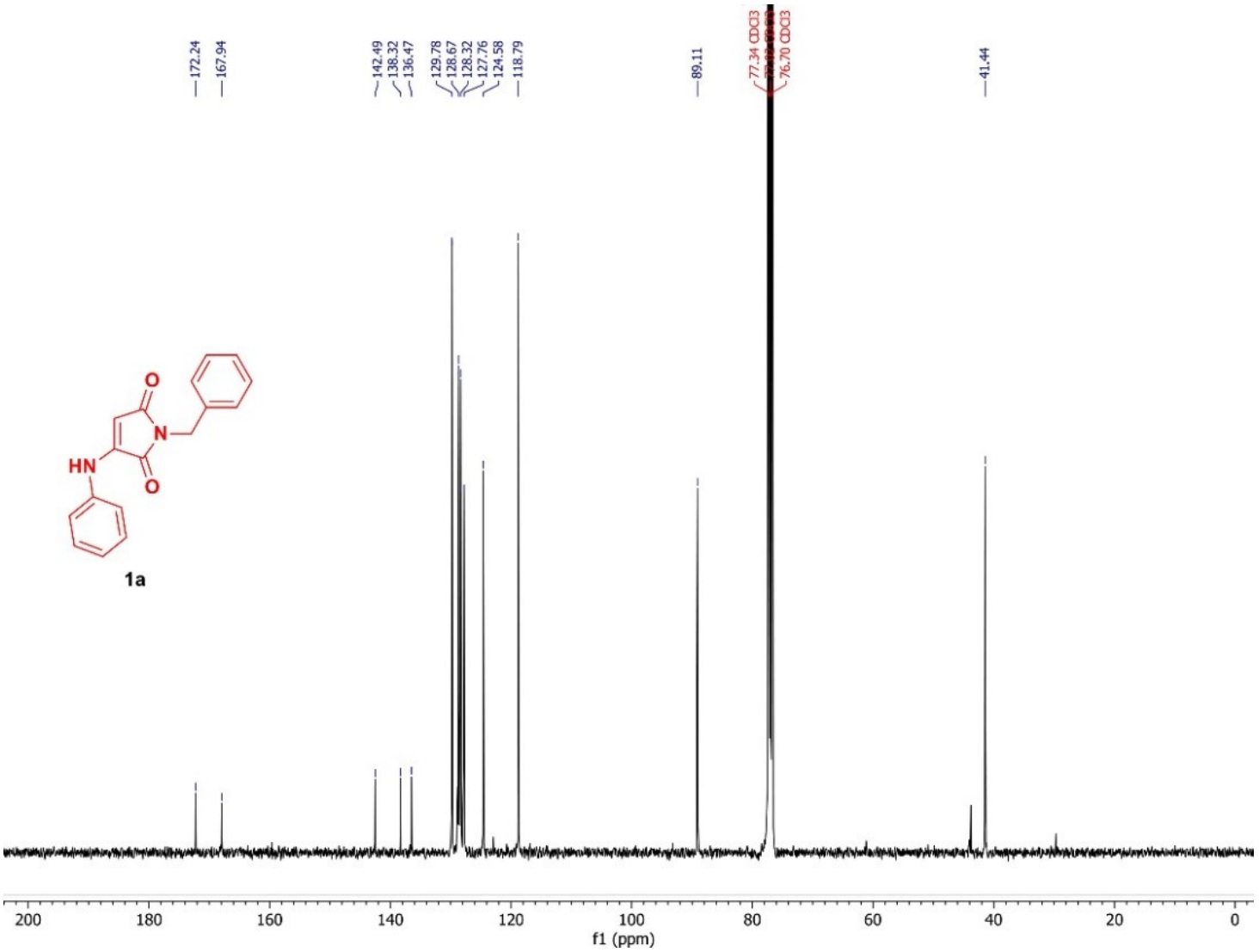
2. Q. Zhu, Z. Ye, W. Yang, X. Cai and B. Z. Tang, *J. Org. Chem.*, 2017, **82**, 1096-1104.
3. H. Imoto, K. Nohmi, K. Kizaki, S. Watase, K. Matsukawa, S. Yamamoto, M. Mitsuishic and K. Naka, *RSC Adv.*, 2015, **5**, 94344-94350.

3. ^{1}H and ^{13}C NMR spectra

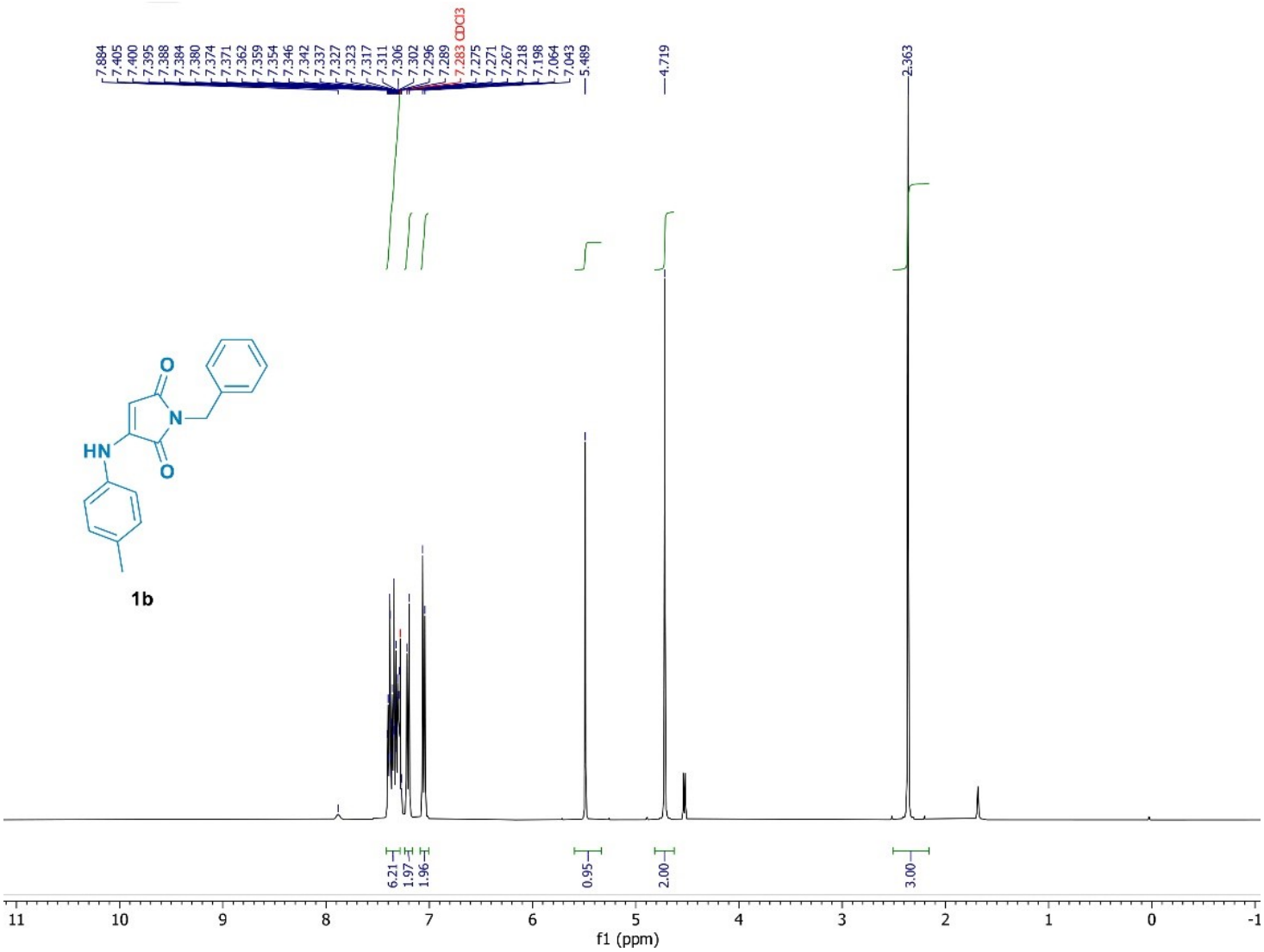
3.1. ^{1}H and ^{13}C NMR spectra of synthesized 3-aminomaleimides 1a-h



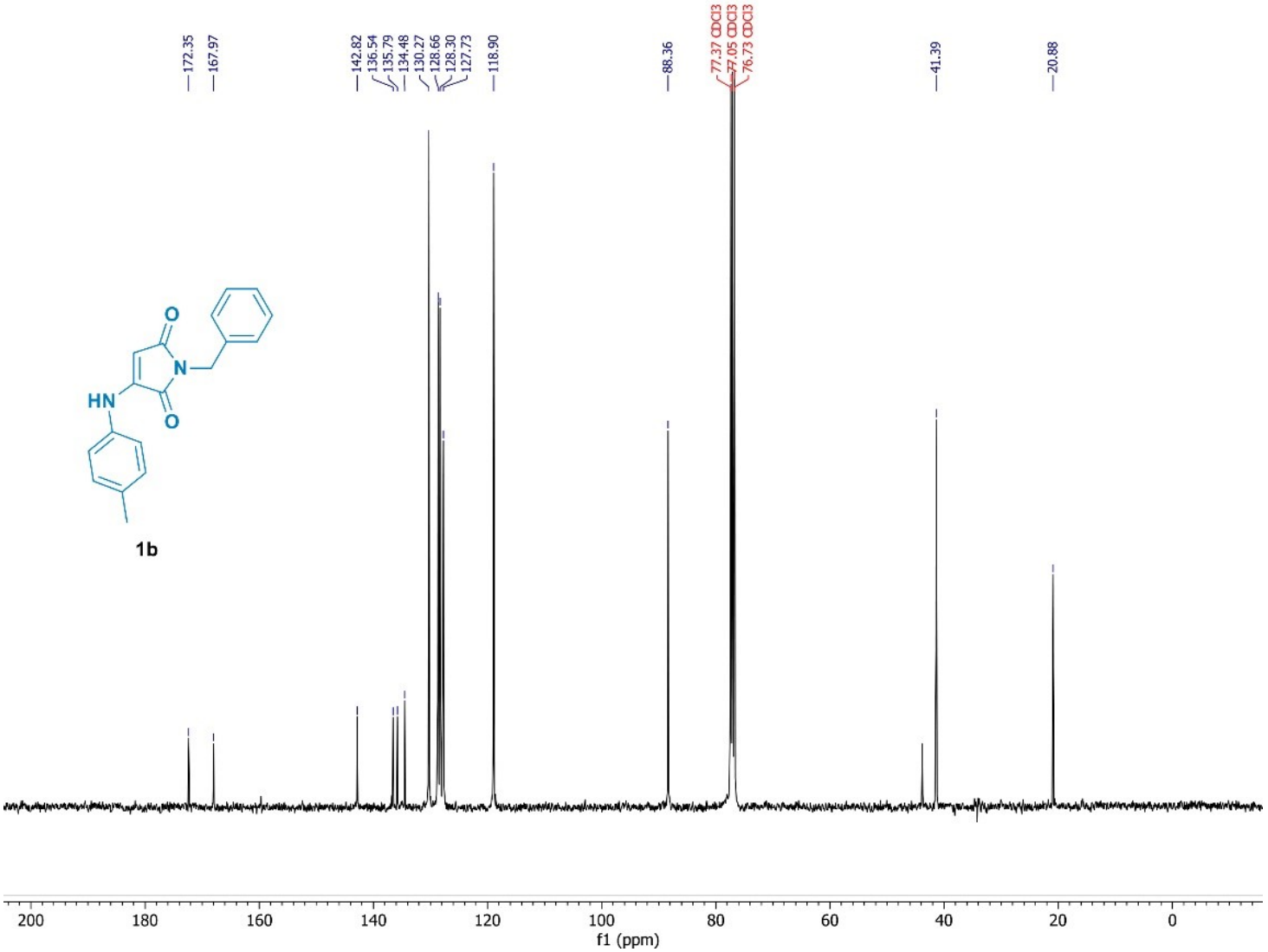
^{1}H NMR of compound **1a** ($CDCl_3$, 400 MHz)



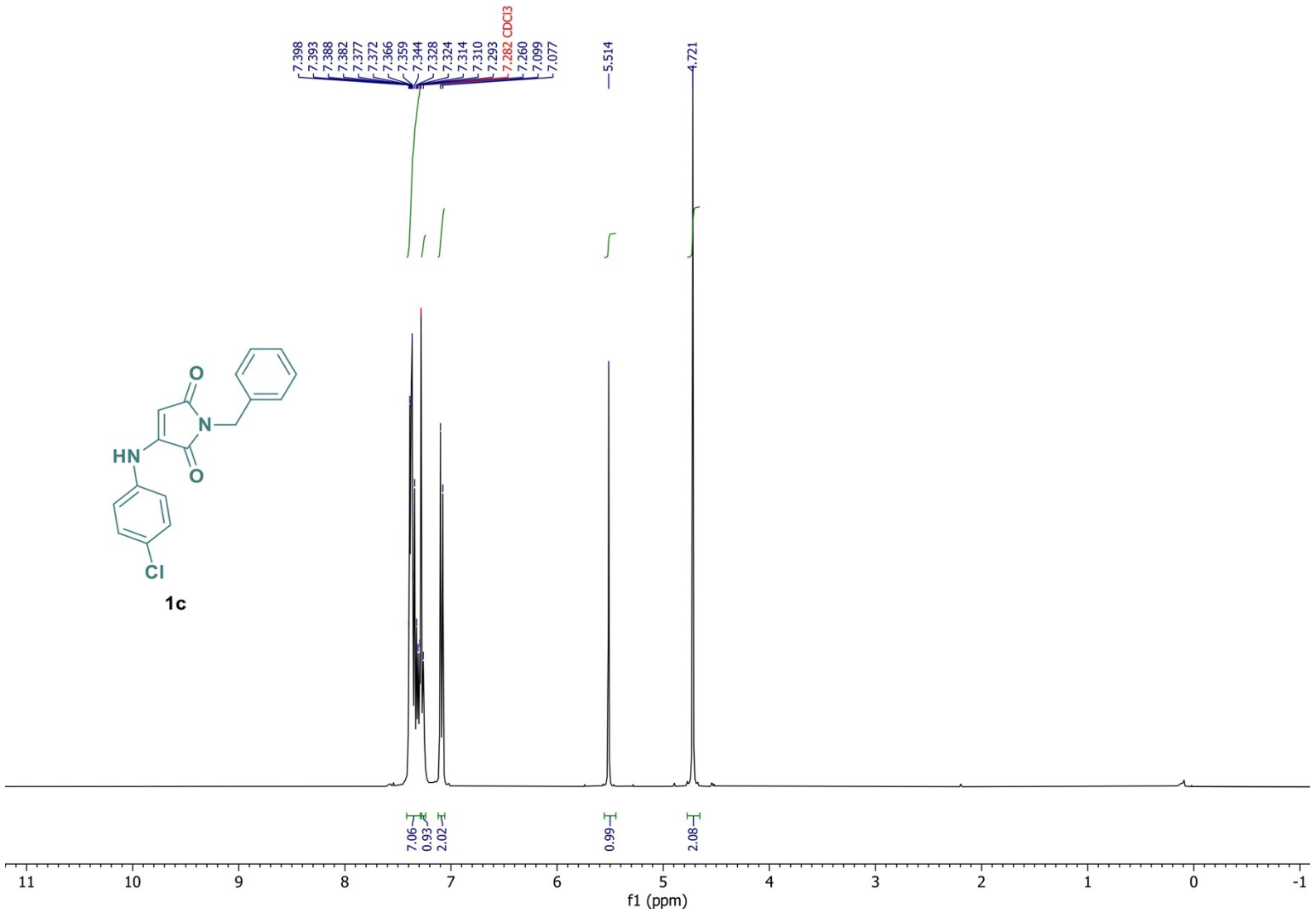
^{13}C NMR of compound **1a** ($CDCl_3$, 100 MHz)



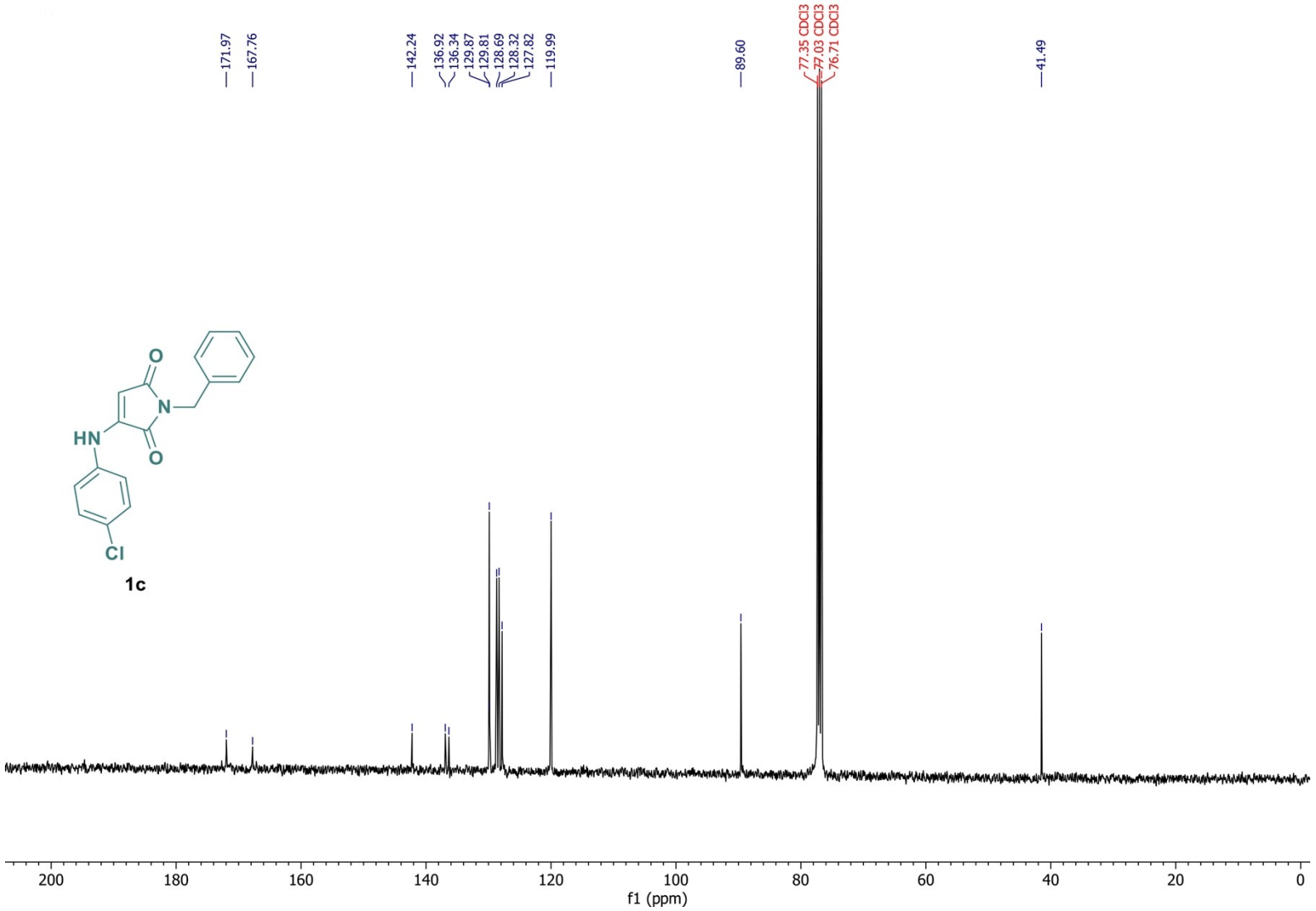
^{1}H NMR of compound **1b** ($CDCl_3$, 400 MHz)



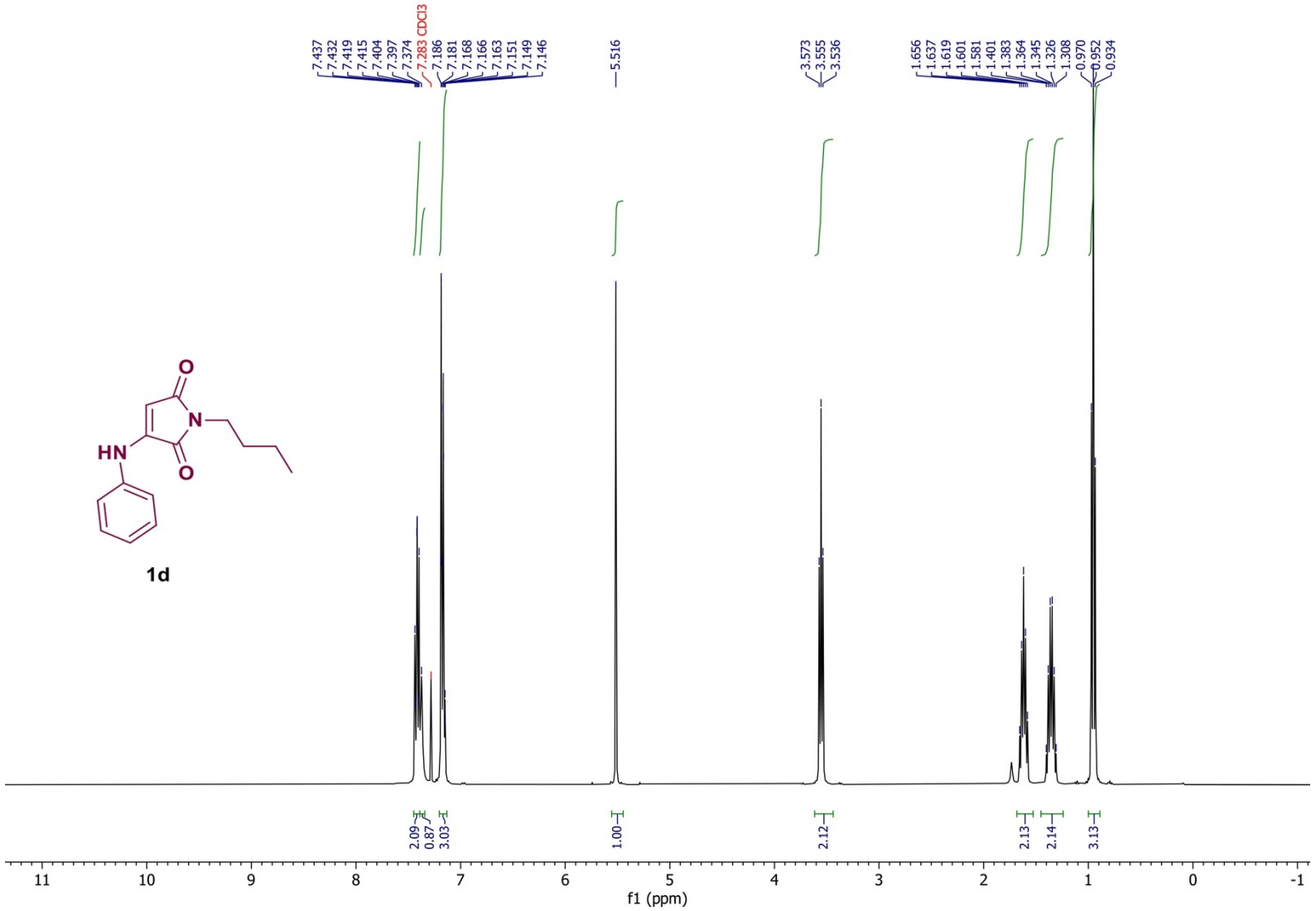
^{13}C NMR of compound **1b** ($CDCl_3$, 100 MHz)



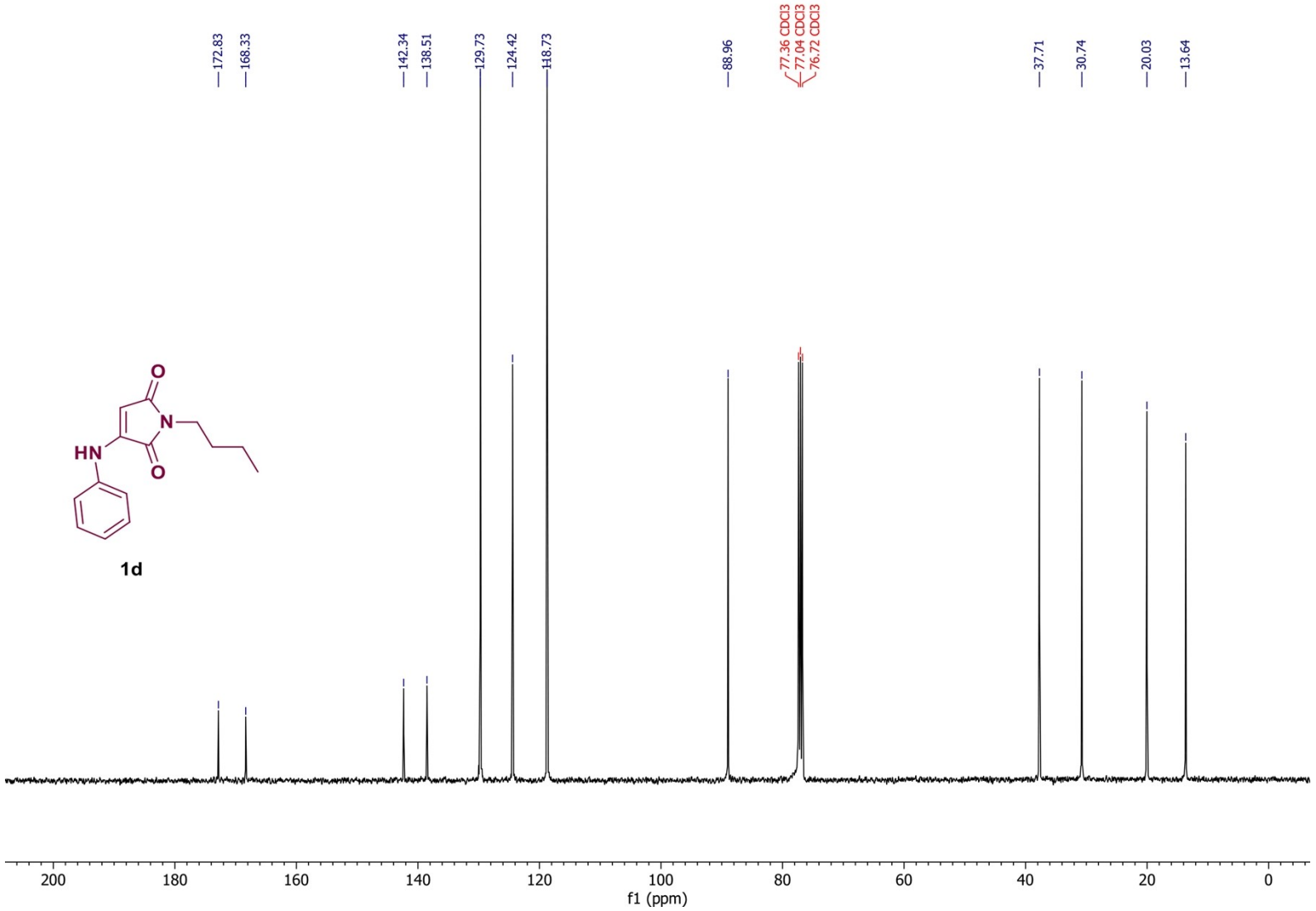
^{1}H NMR of compound **1c** ($CDCl_3$, 400 MHz)



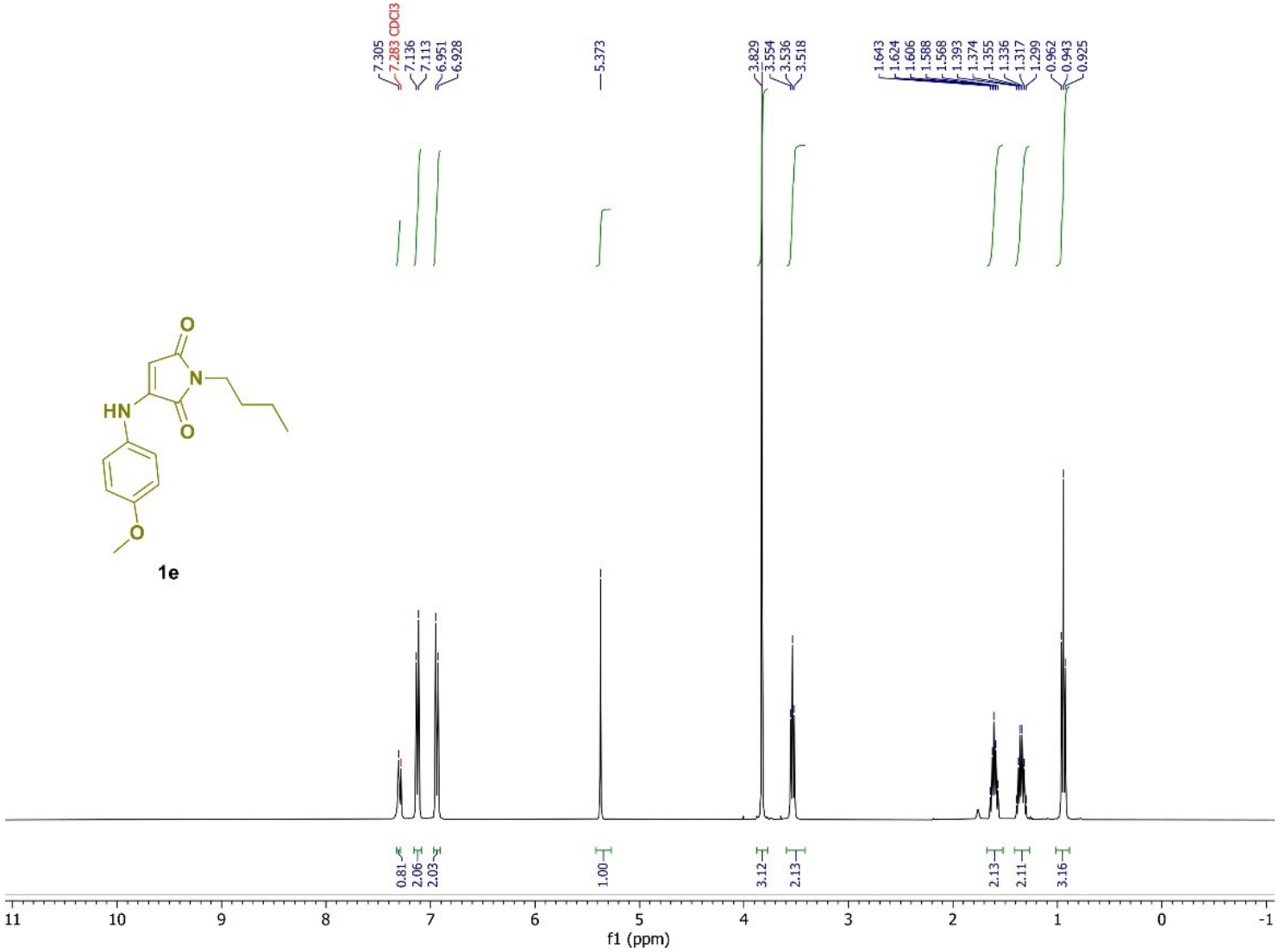
^{13}C NMR of compound **1c** ($CDCl_3$, 100 MHz)



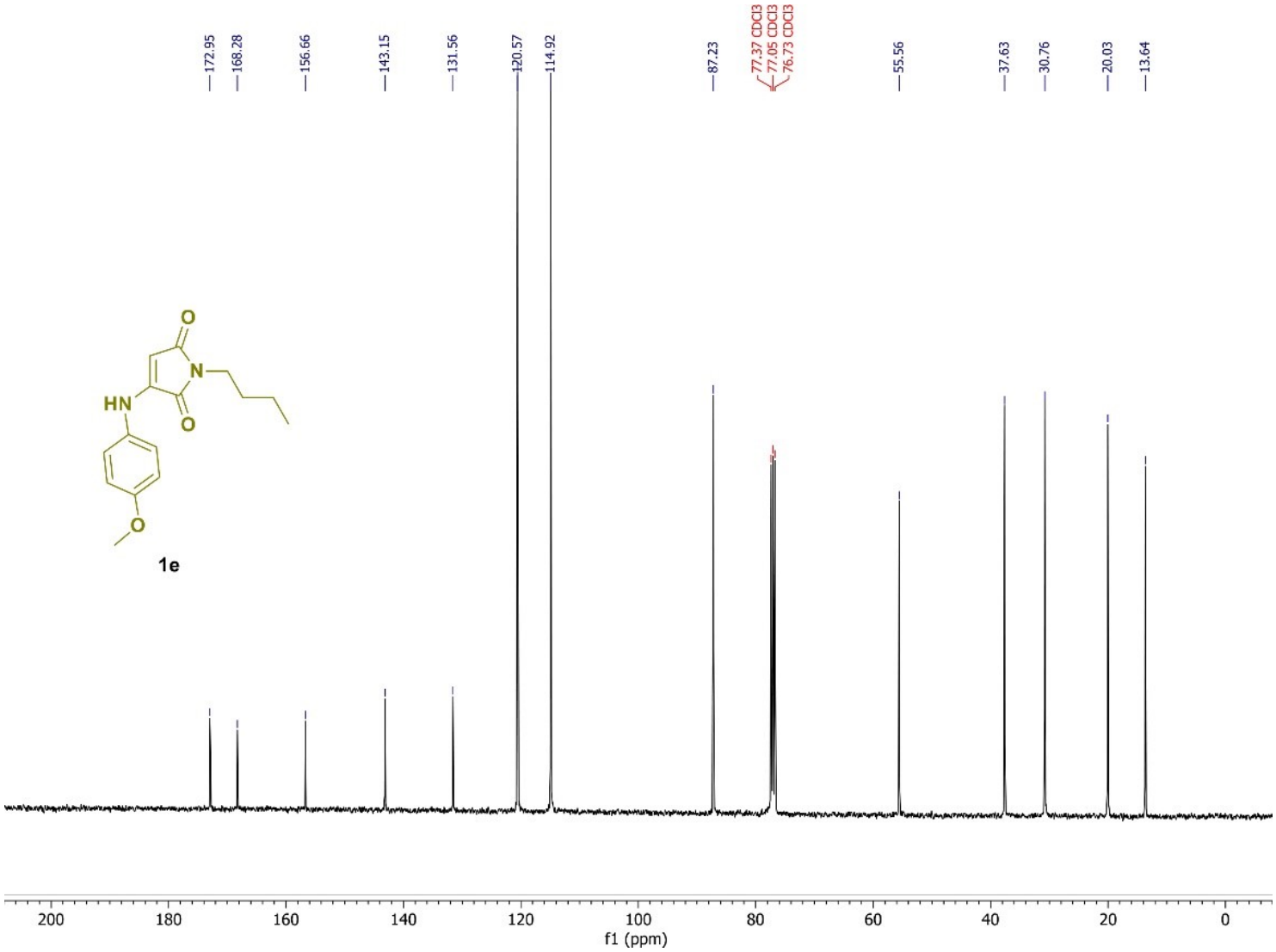
^{1}H NMR of compound **1d** ($CDCl_3$, 400 MHz)



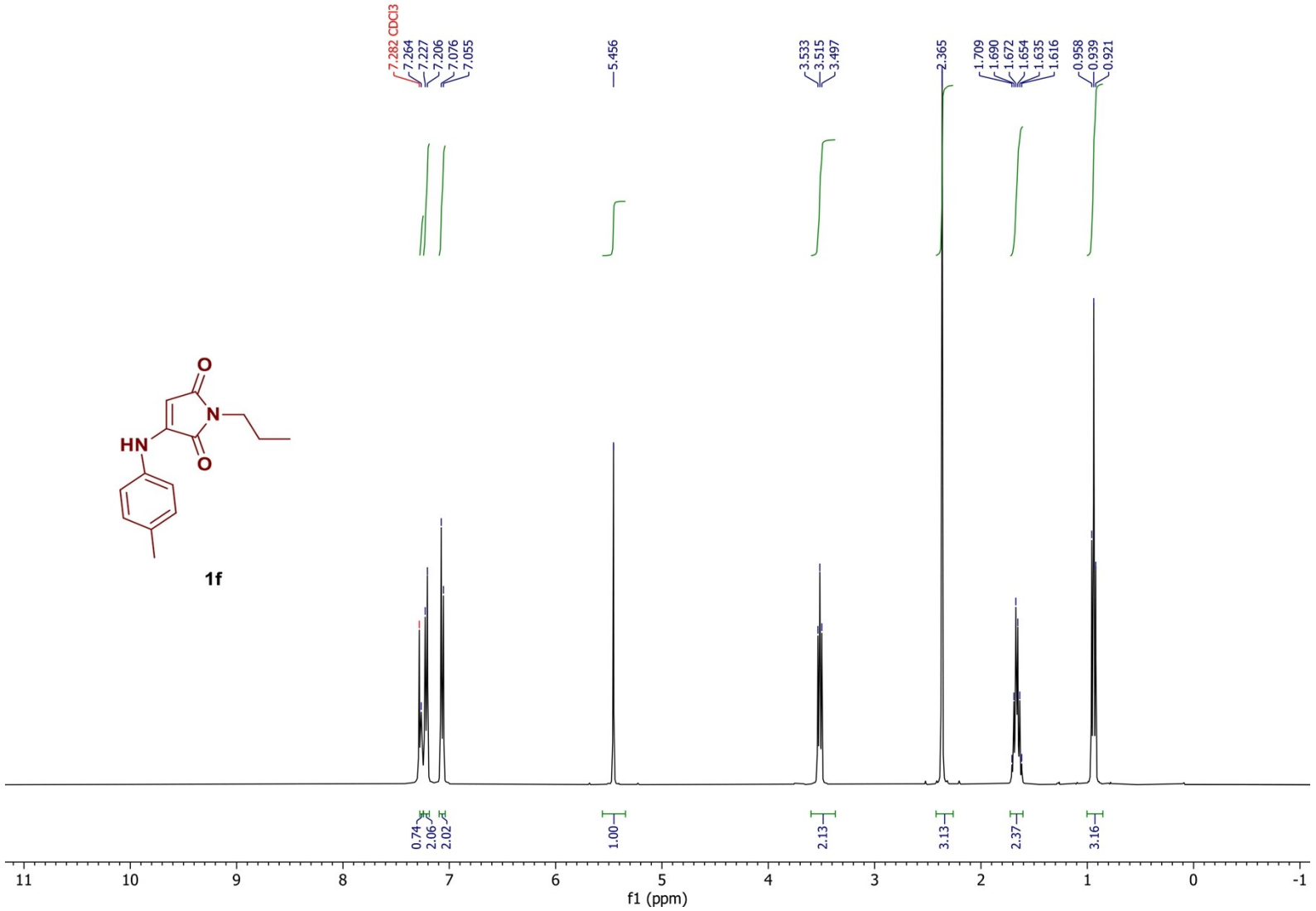
^{13}C NMR of compound **1d** ($CDCl_3$, 100 MHz)



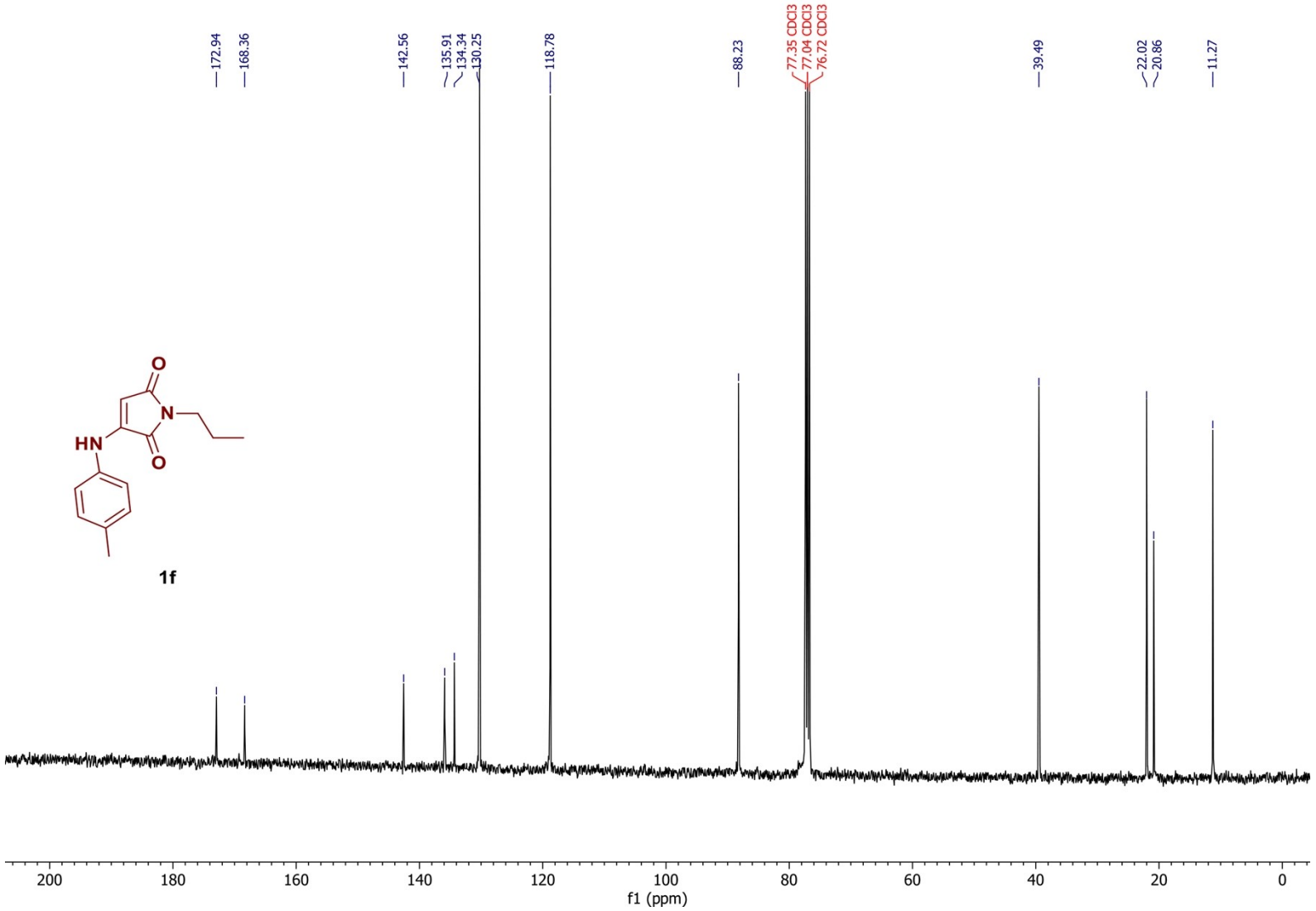
^{1}H NMR of compound **1e** ($CDCl_3$, 400 MHz)



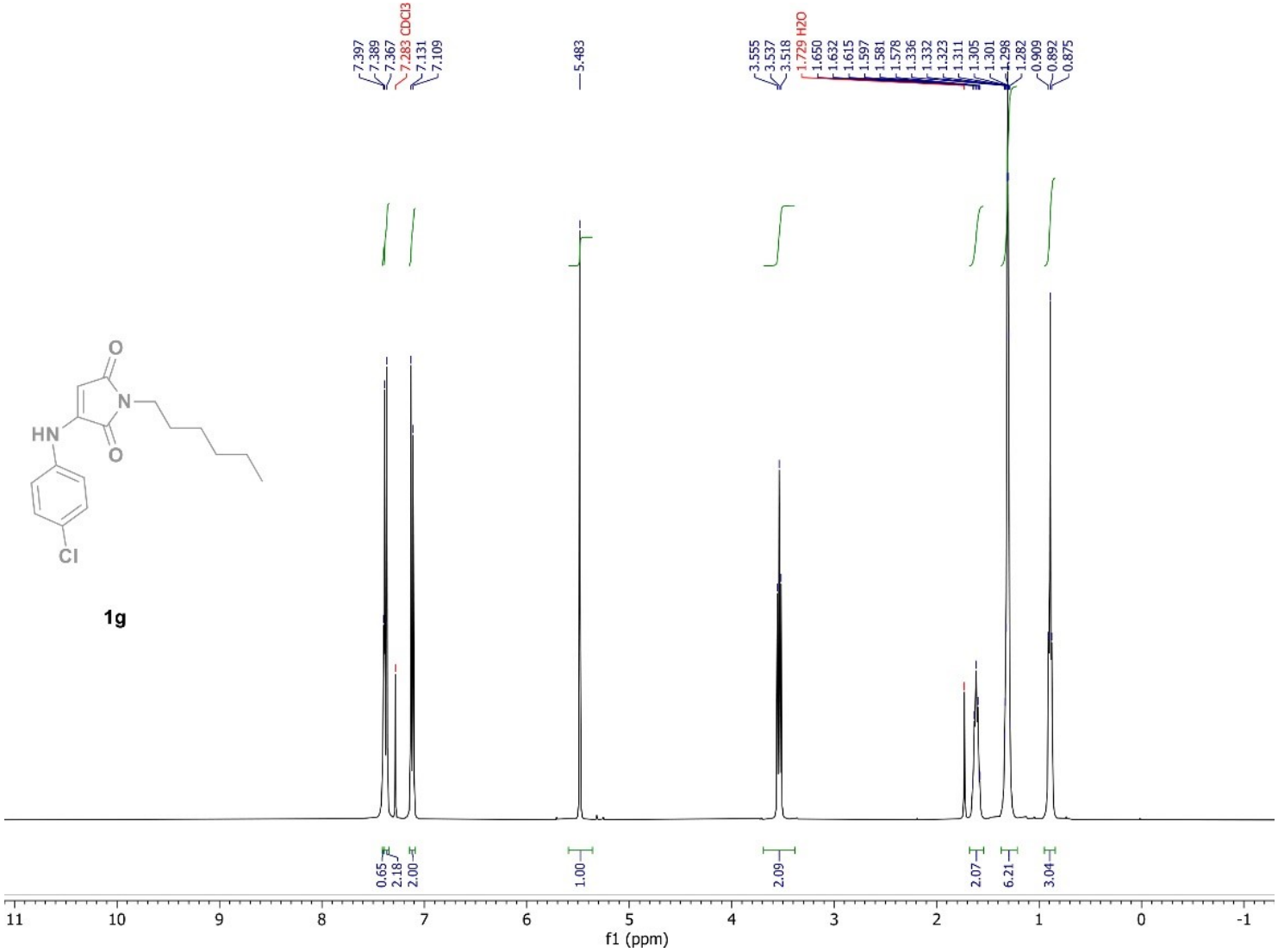
^{13}C NMR of compound **1e** ($CDCl_3$, 100 MHz)



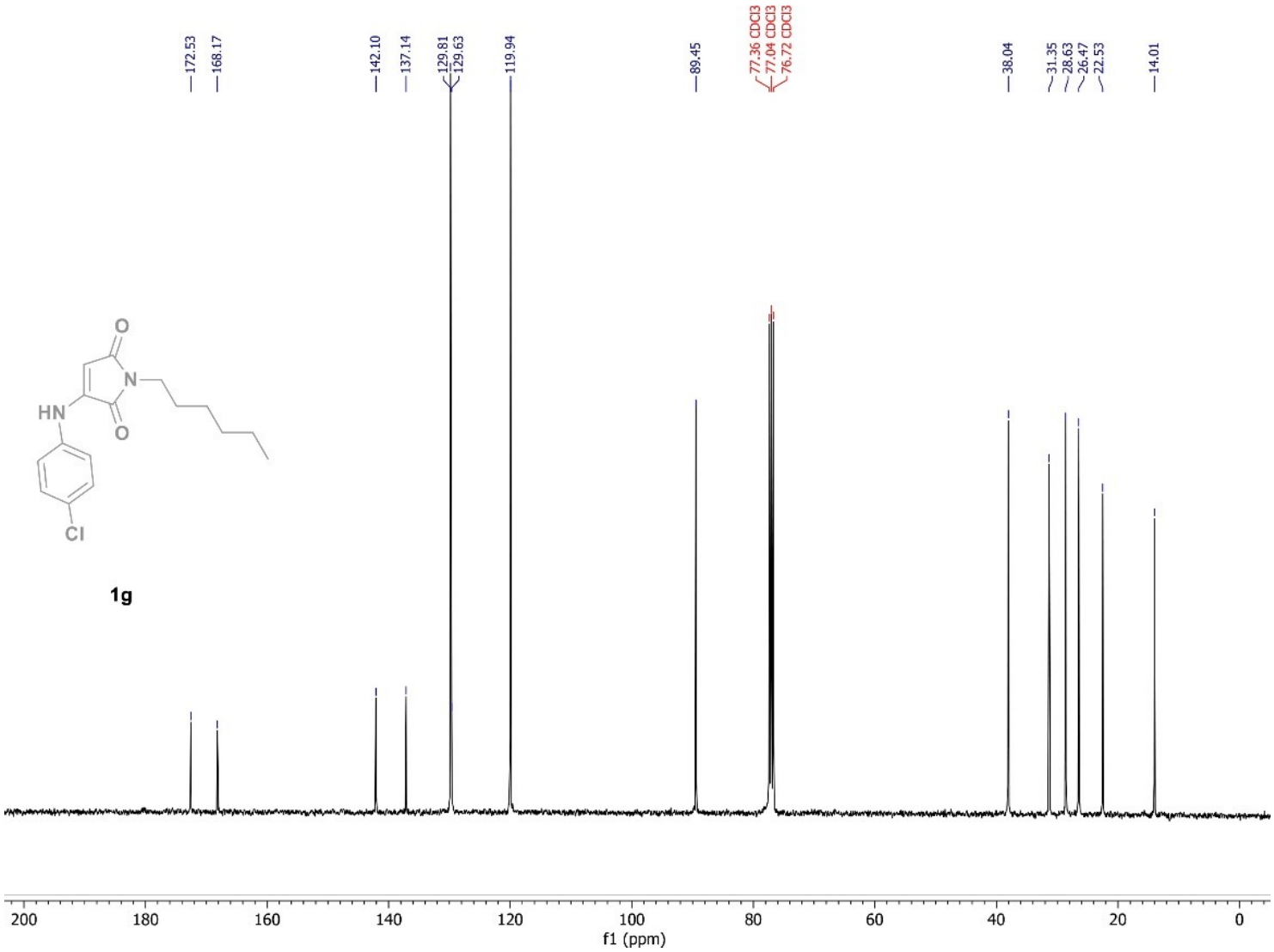
^{1}H NMR of compound **1f** ($CDCl_3$, 400 MHz)



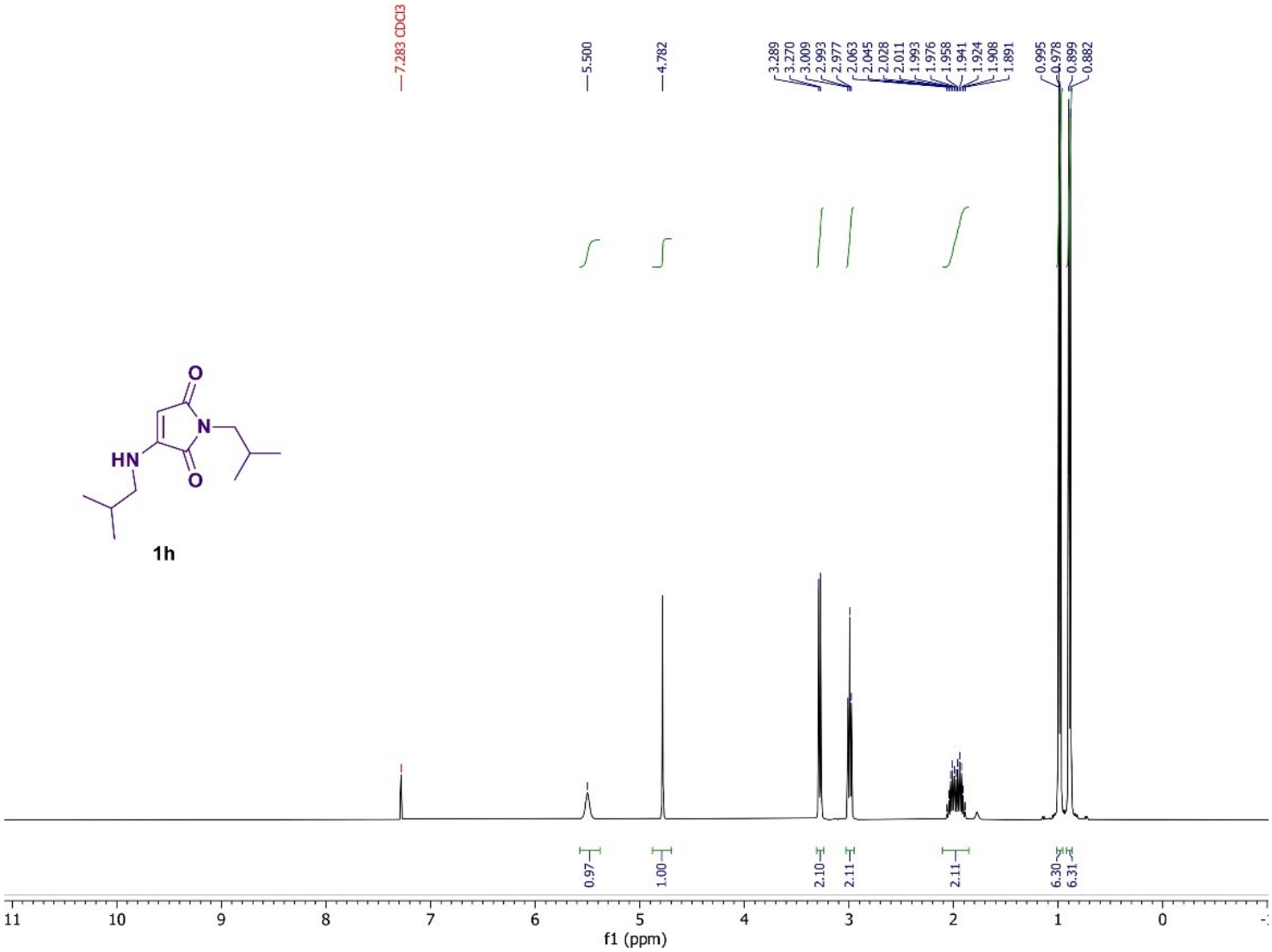
^{13}C NMR of compound **1f** ($CDCl_3$, 100 MHz)



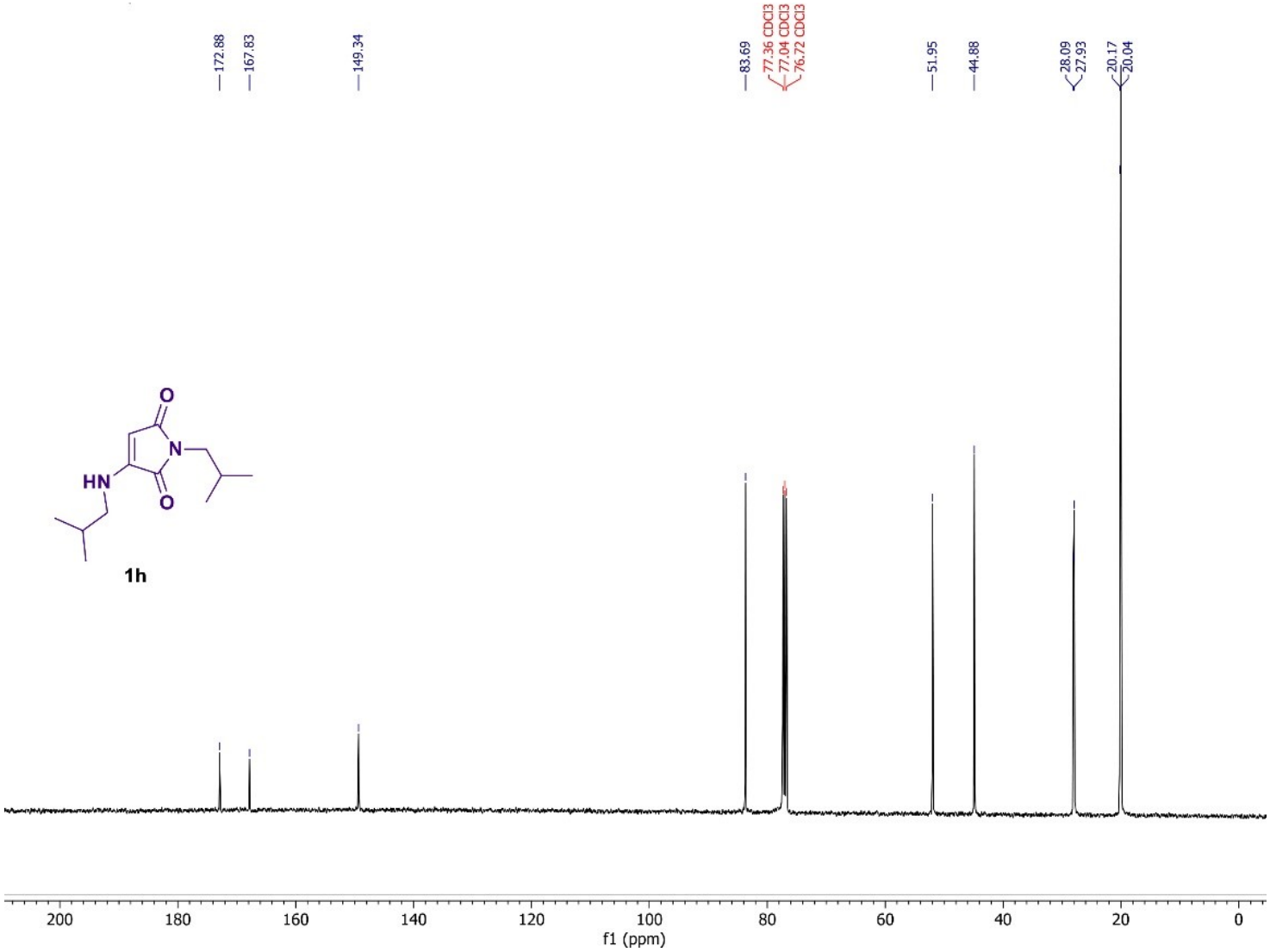
^{1}H NMR of compound **1g** ($CDCl_3$, 400 MHz)



^{13}C NMR of compound **1g** ($CDCl_3$, 100 MHz)

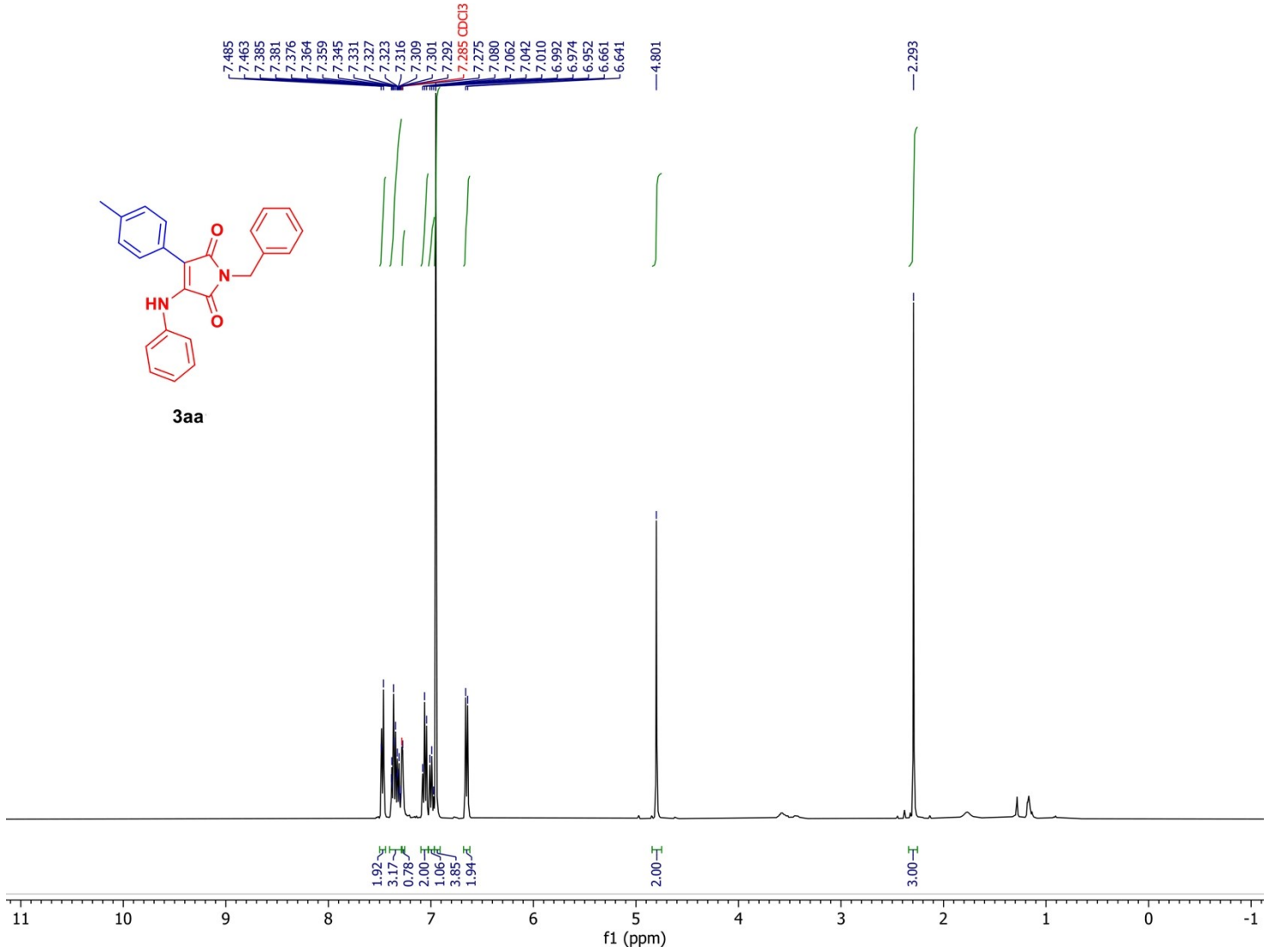


^{1}H NMR of compound **1h** ($CDCl_3$, 400 MHz)

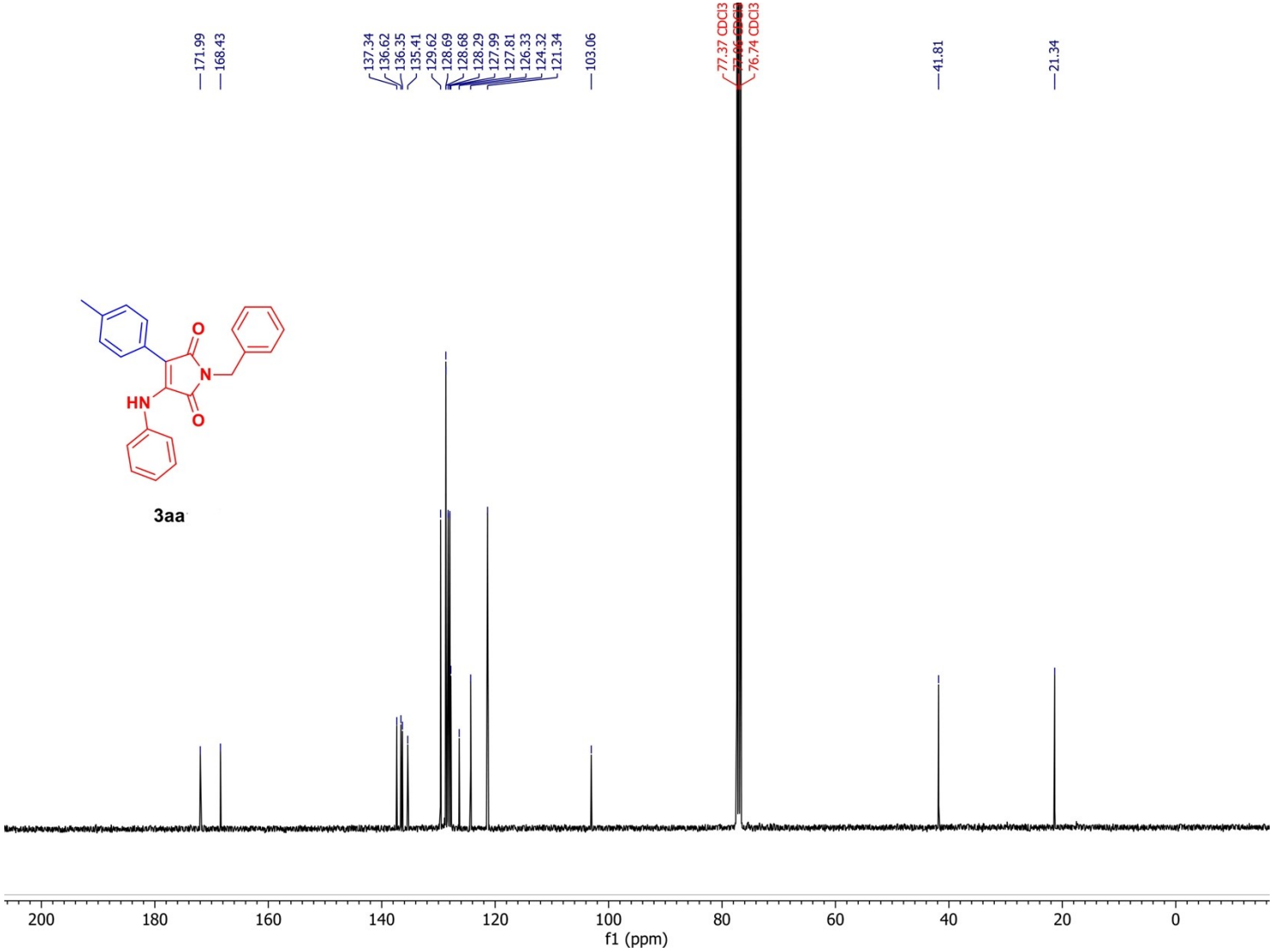


^{13}C NMR of compound **1h** ($CDCl_3$, 100 MHz)

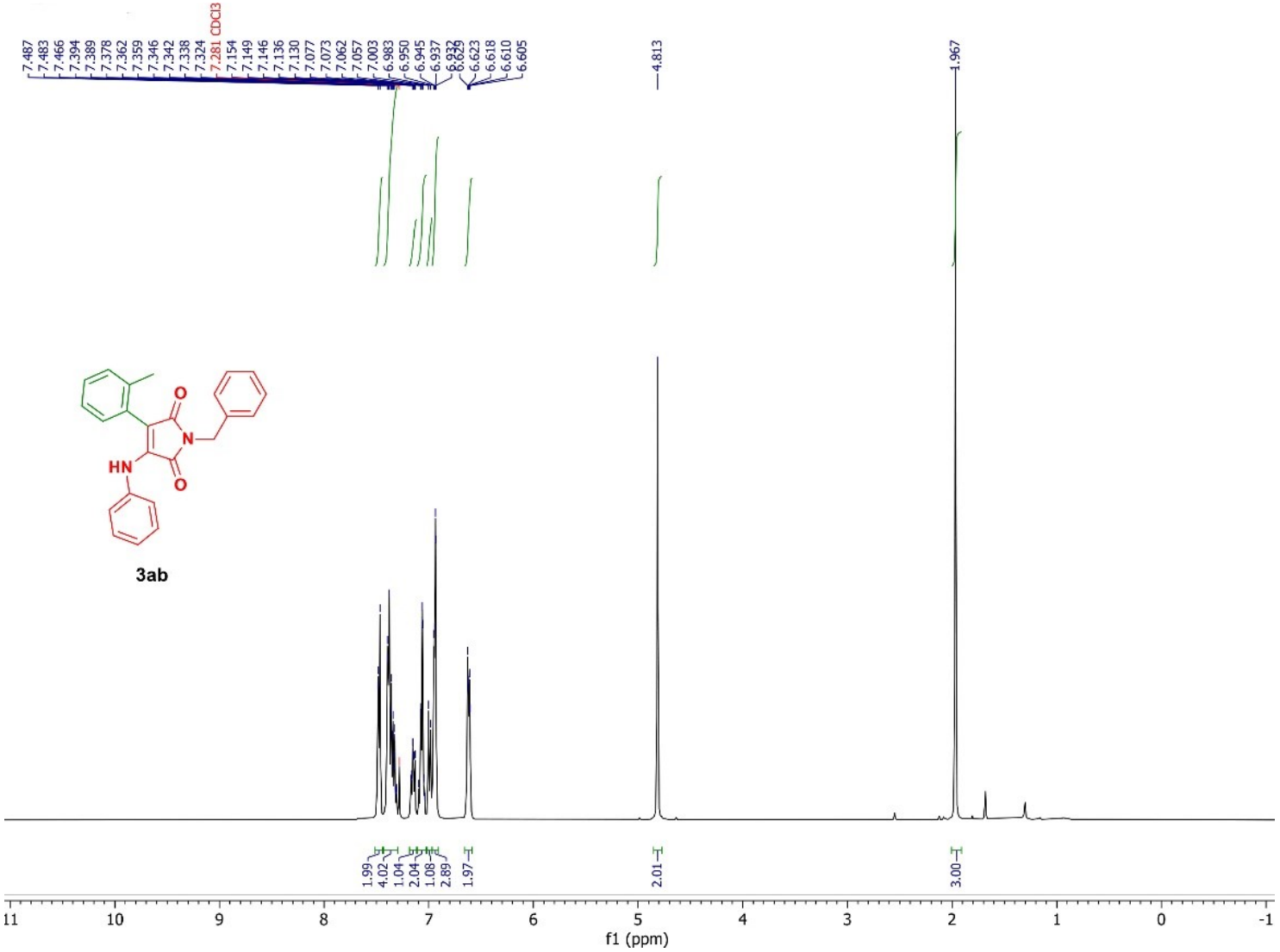
3.2. ^{1}H and ^{13}C NMR spectra of synthesized 3-aryl-4-aminomaleimides 3aa-he



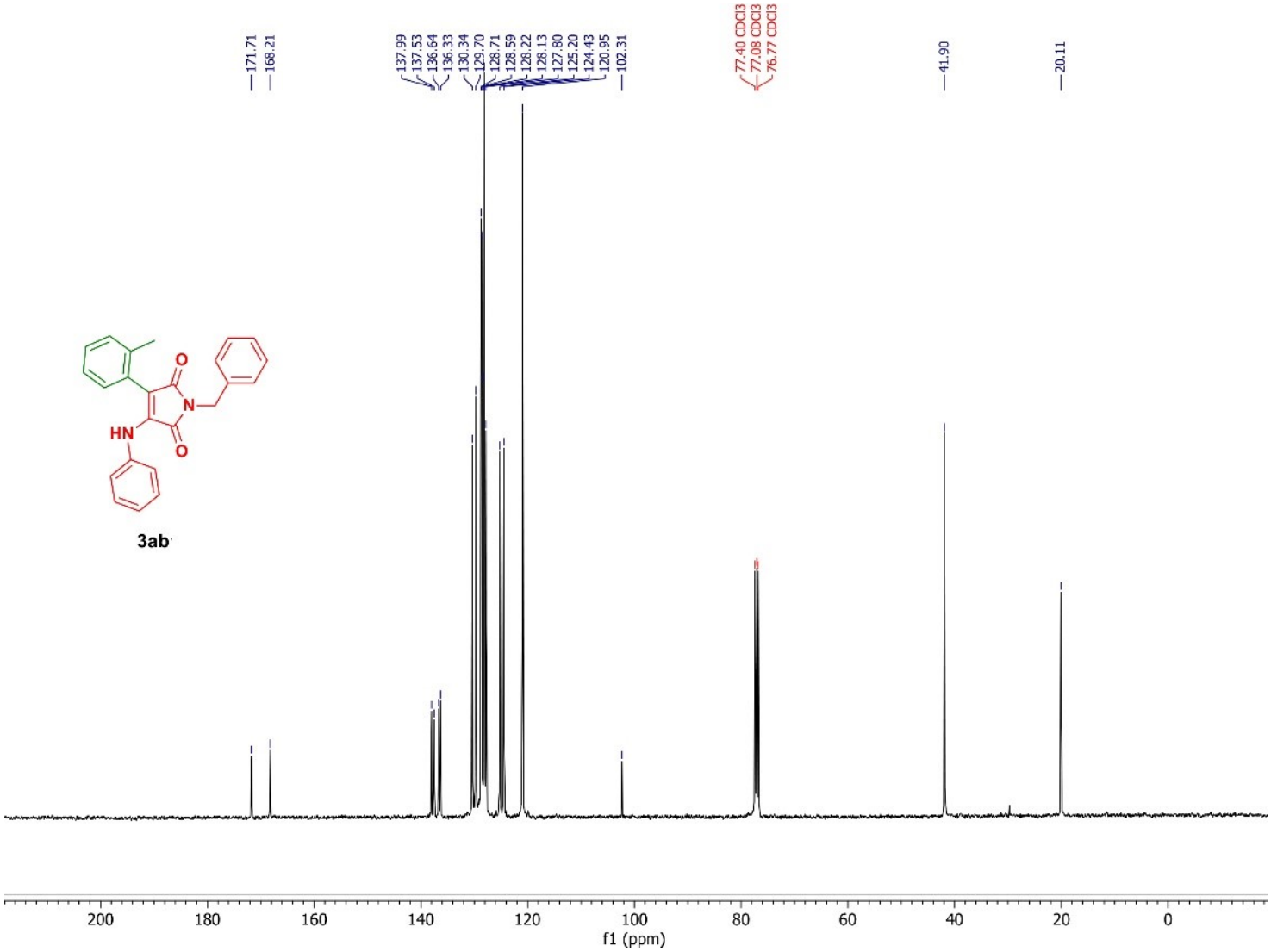
^{1}H NMR of compound **3aa** ($CDCl_3$, 400 MHz)



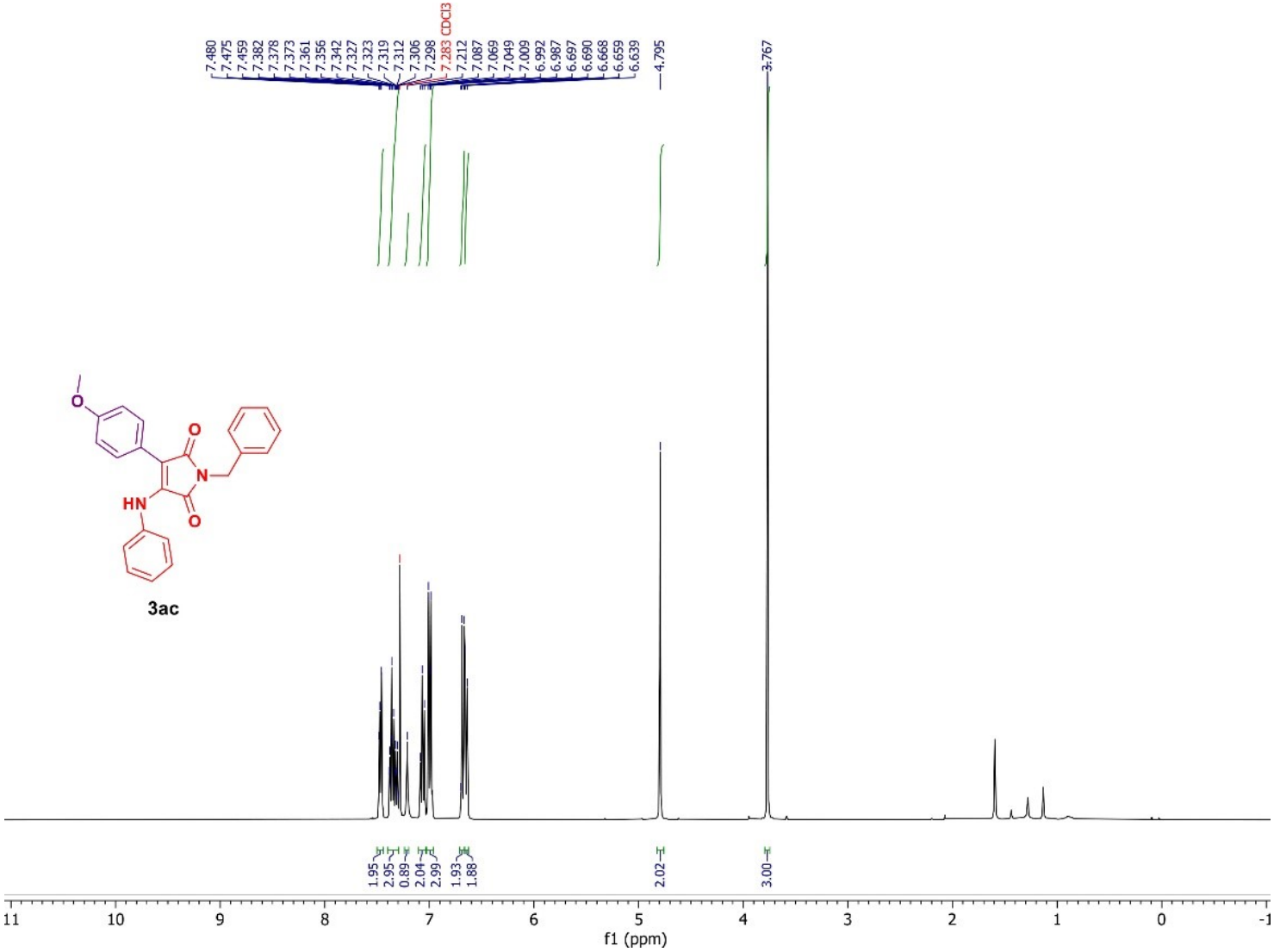
^{13}C NMR of compound **3aa** ($CDCl_3$, 100 MHz)



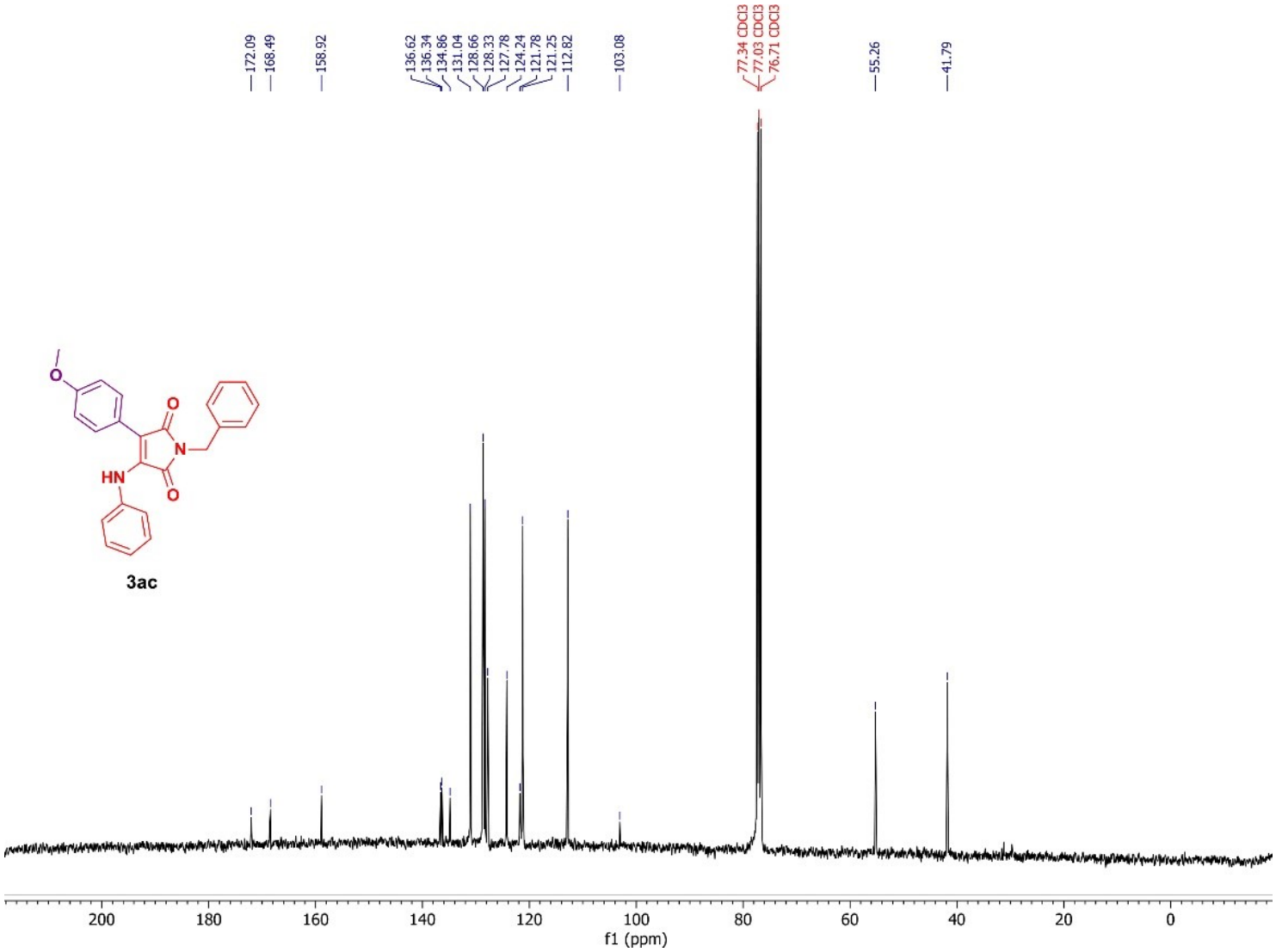
^{1}H NMR of compound **3ab** ($CDCl_3$, 400 MHz)



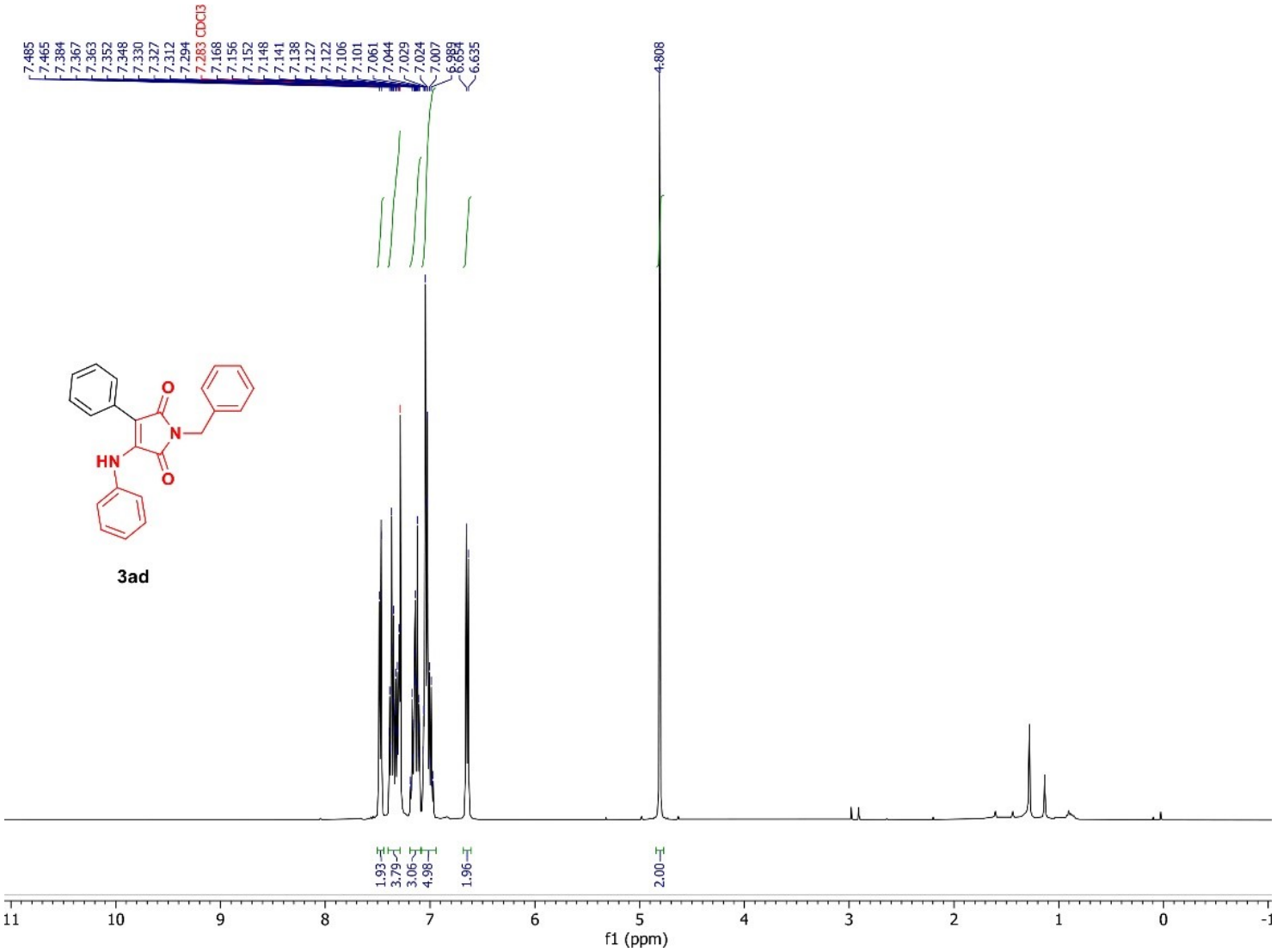
^{13}C NMR of compound **3ab** ($CDCl_3$, 100 MHz)



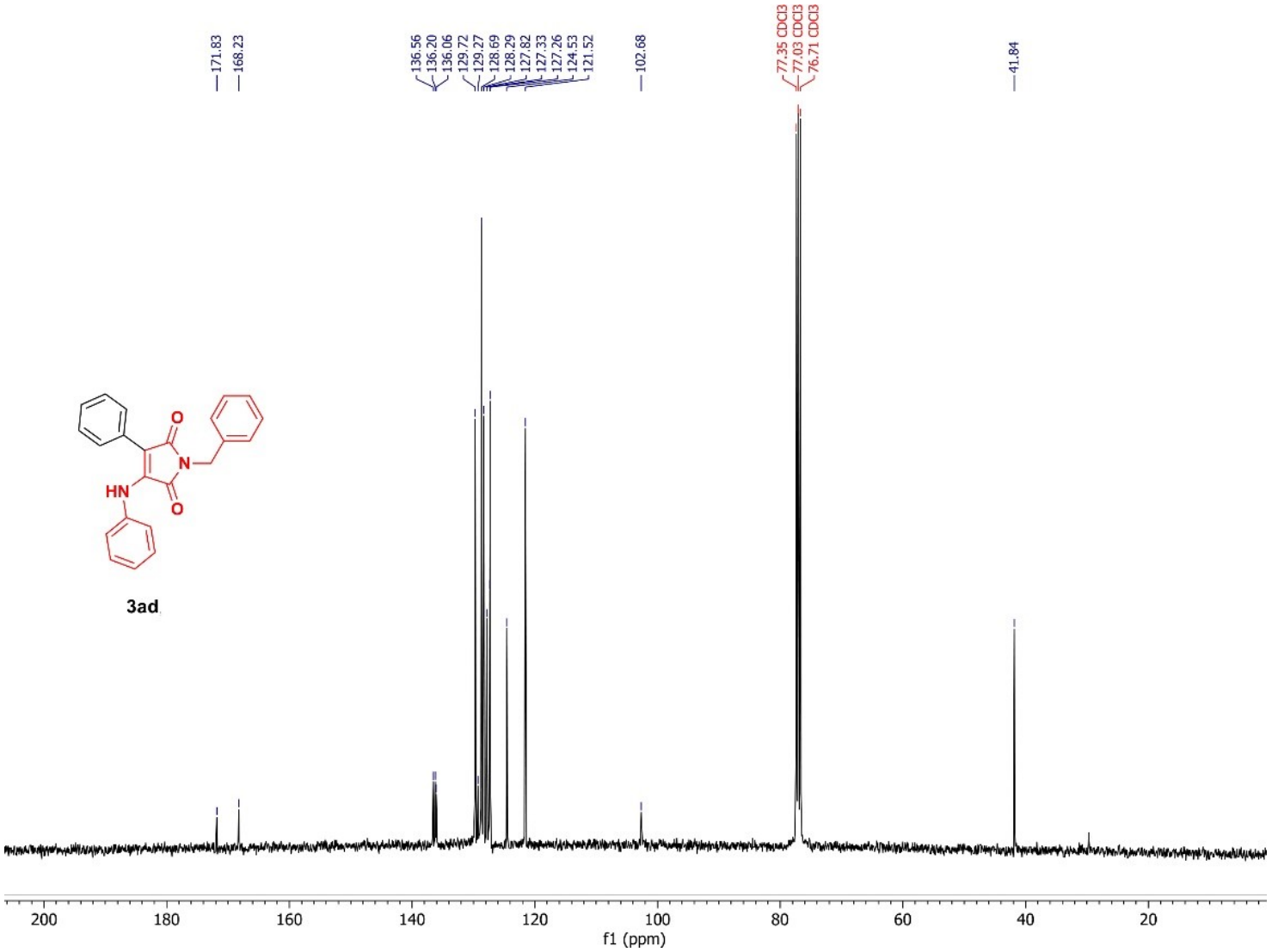
^{1}H NMR of compound **3ac** ($CDCl_3$, 400 MHz)



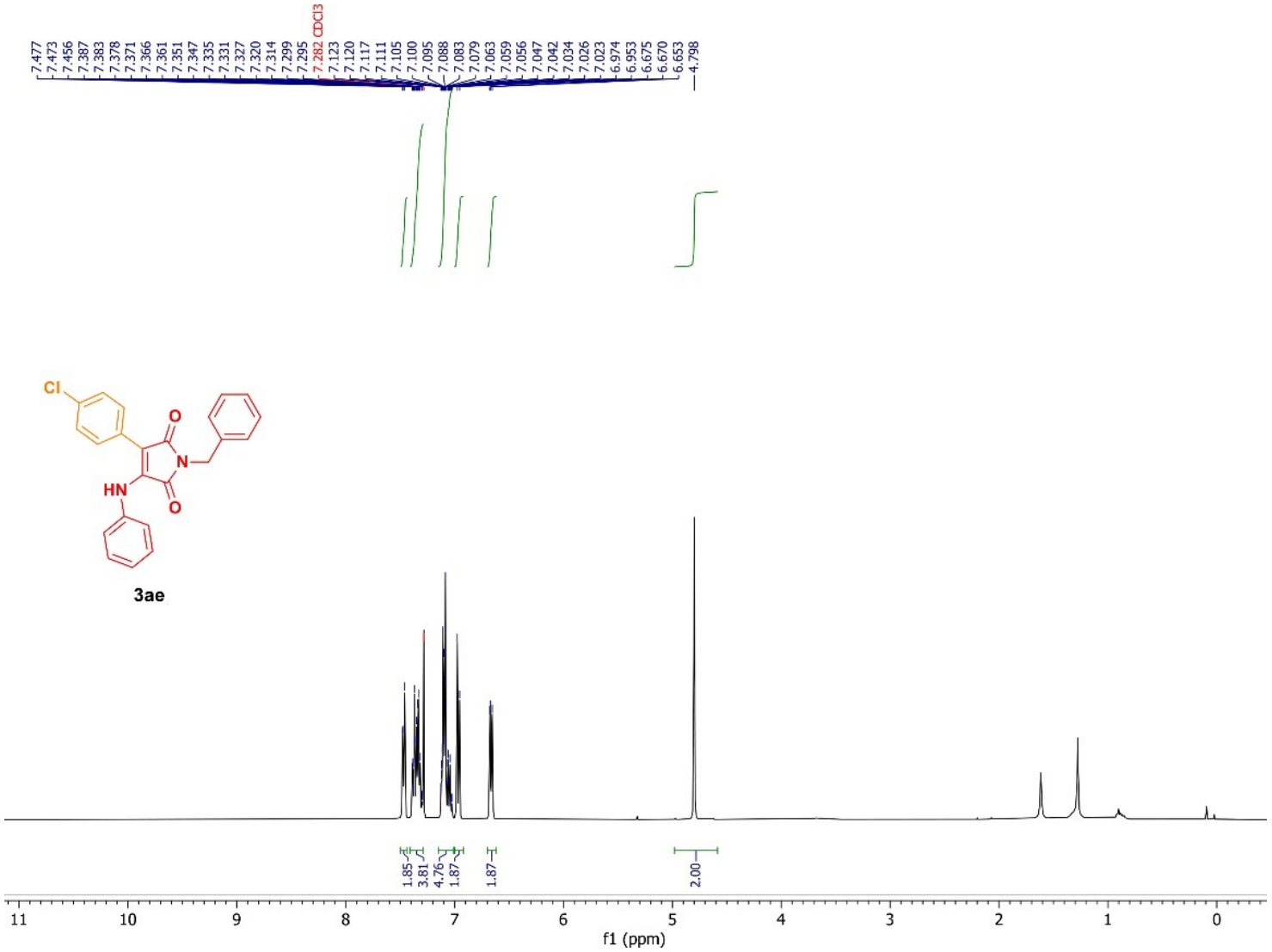
^{13}C NMR of compound **3ac** ($CDCl_3$, 100 MHz)



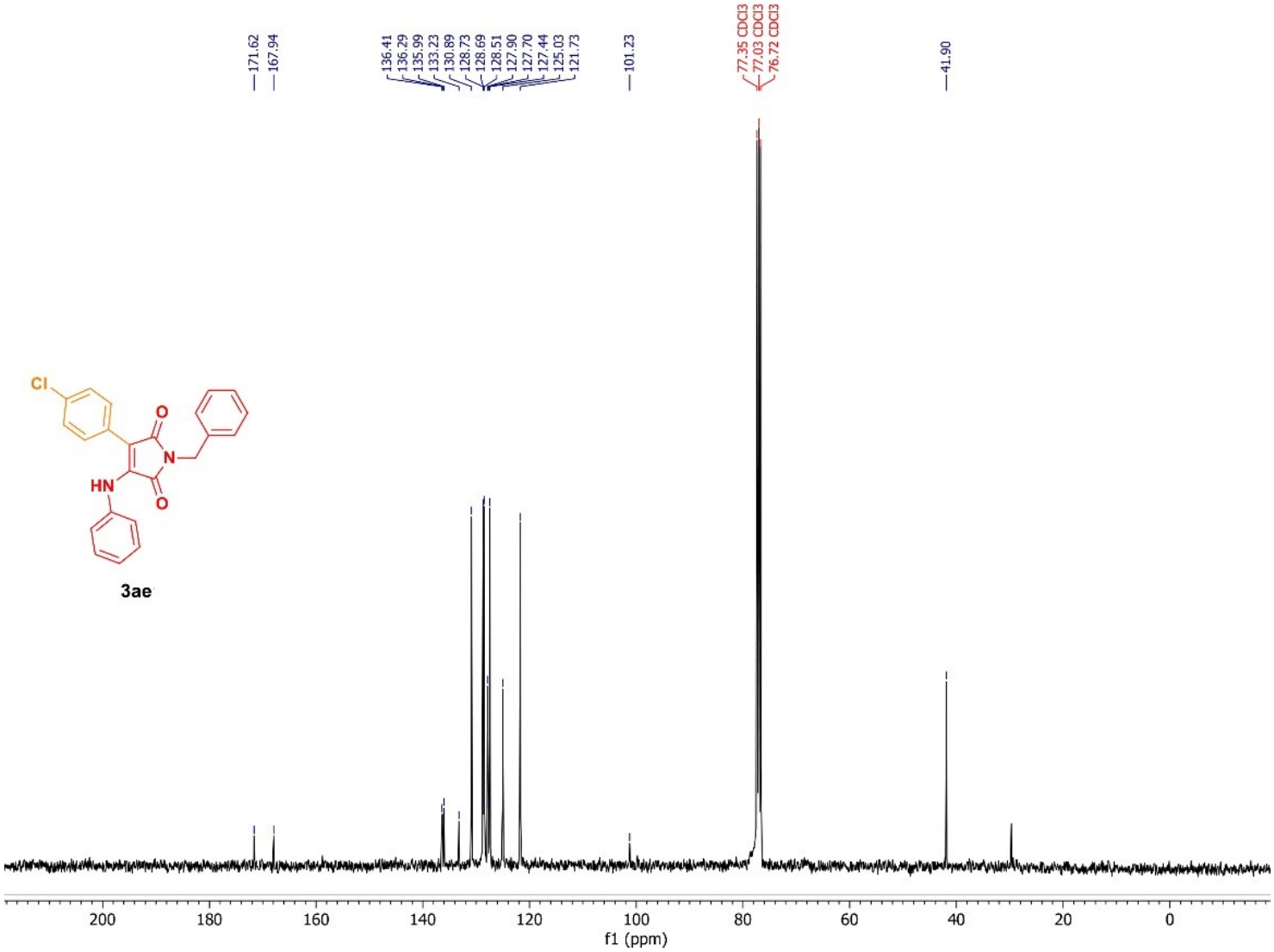
^{1}H NMR of compound **3ad** ($CDCl_3$, 400 MHz)



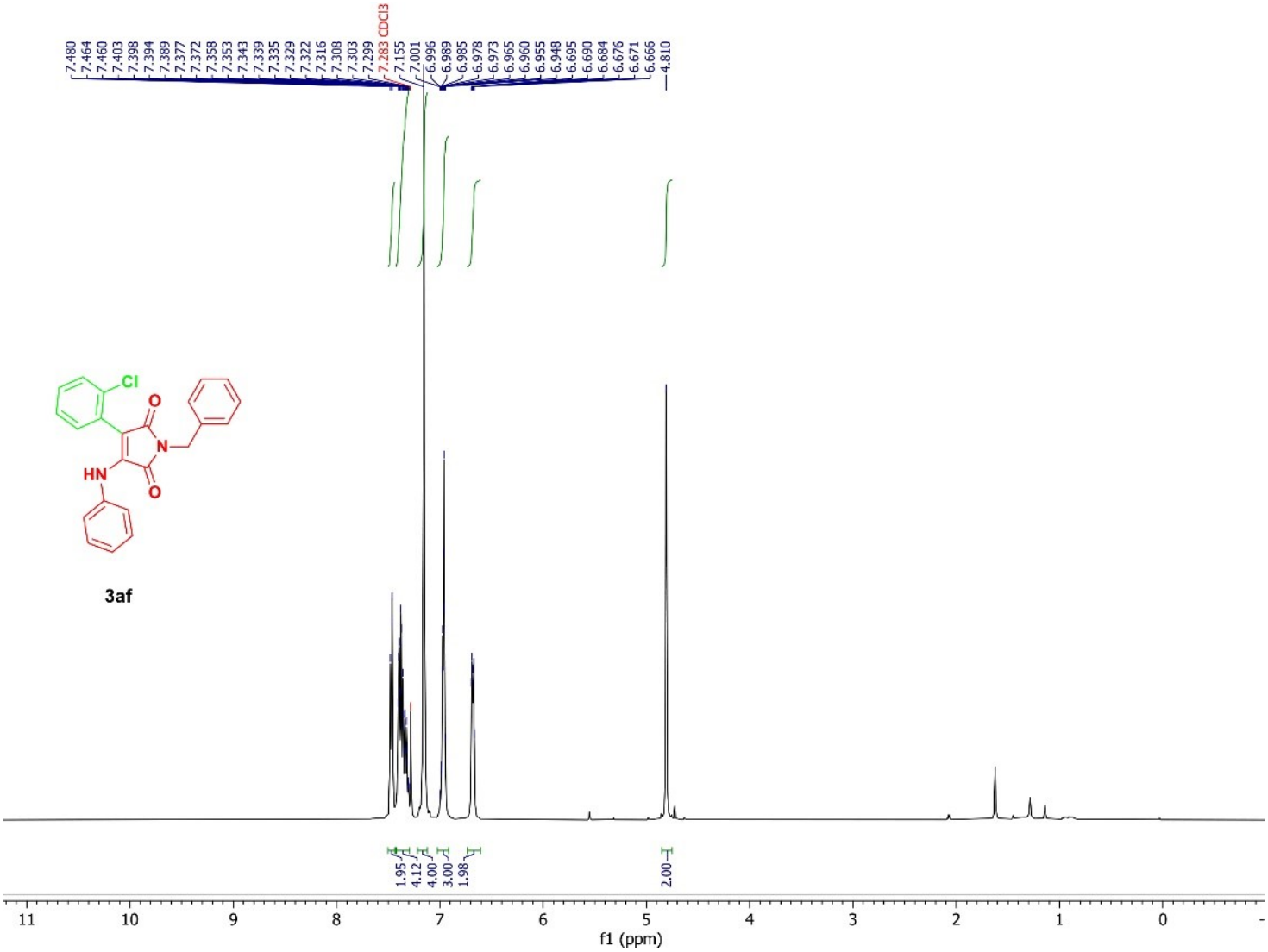
^{13}C NMR of compound **3ad** ($CDCl_3$, 100 MHz)



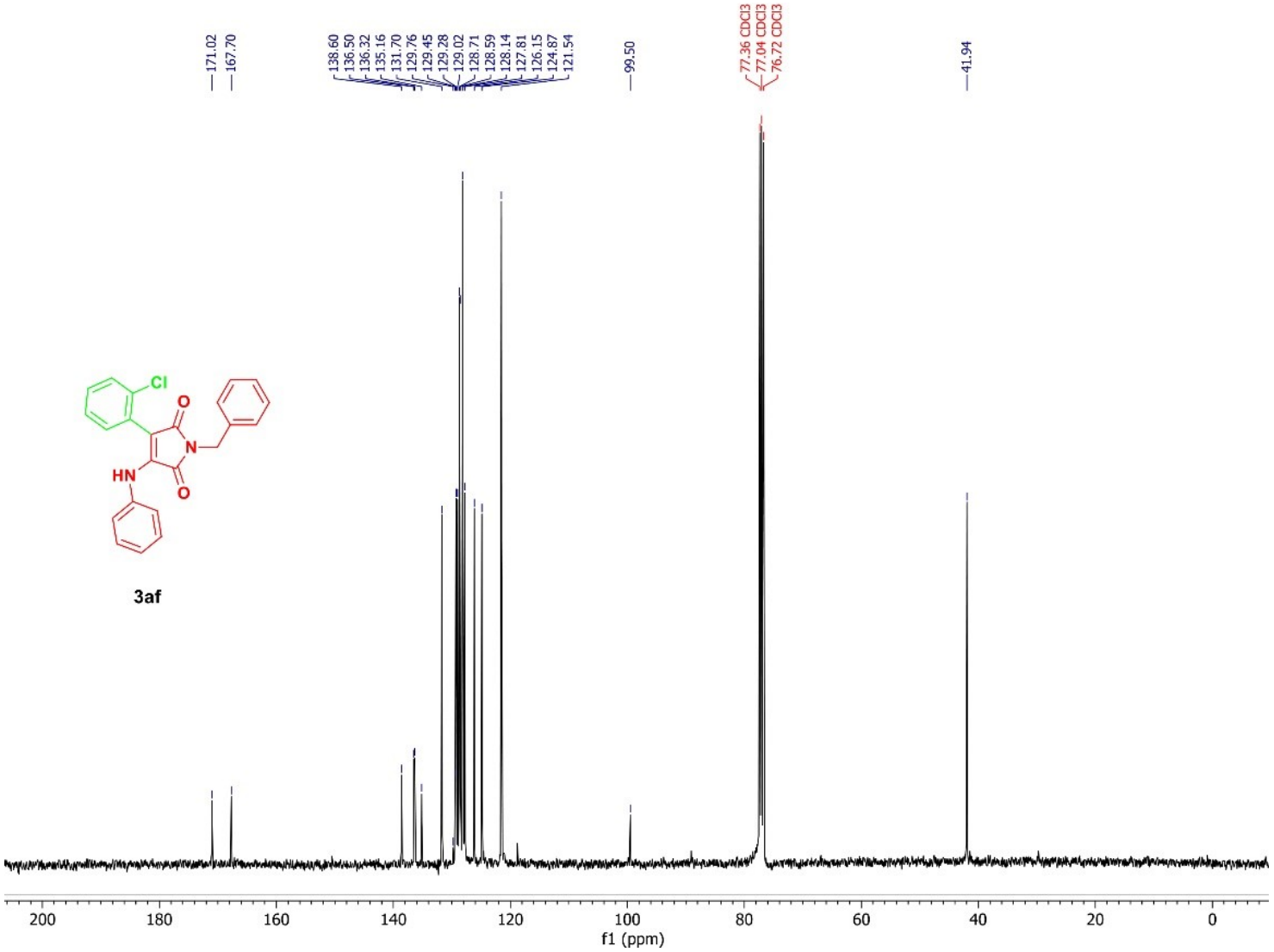
^{1}H NMR of compound **3ea** ($CDCl_3$, 400 MHz)



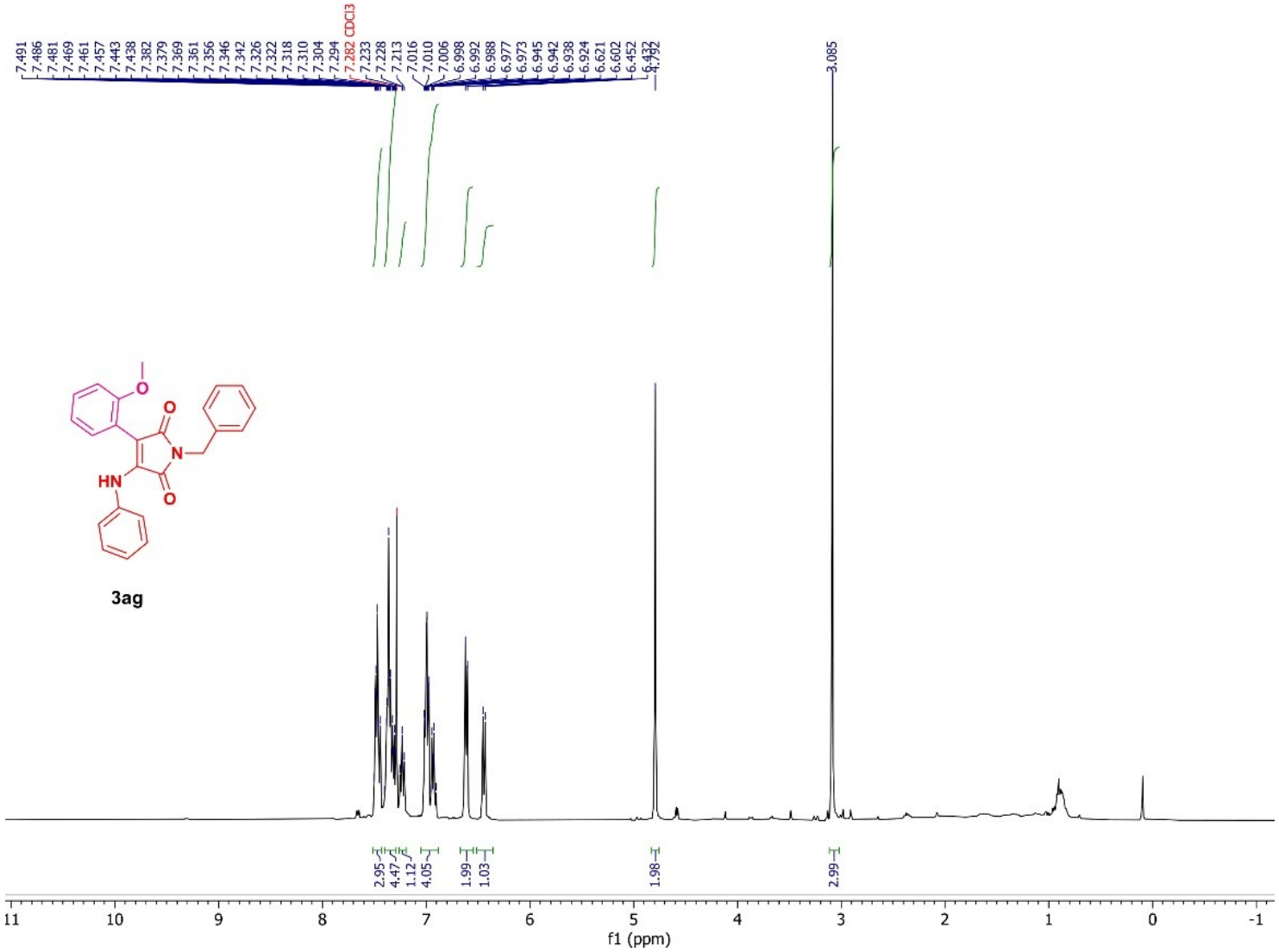
^{13}C NMR of compound **3ea** ($CDCl_3$, 100 MHz)



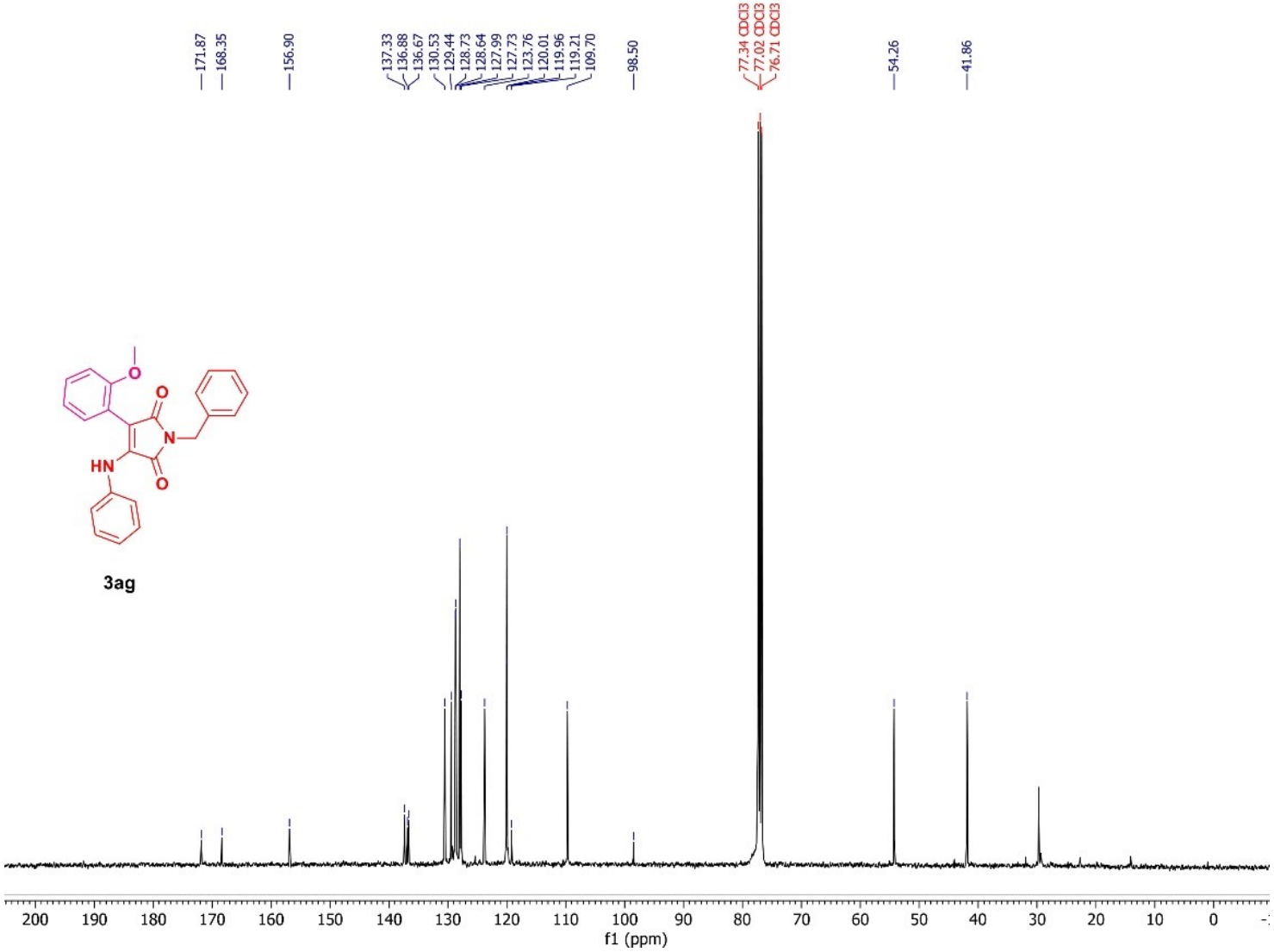
^{1}H NMR of compound **3af** ($CDCl_3$, 400 MHz)



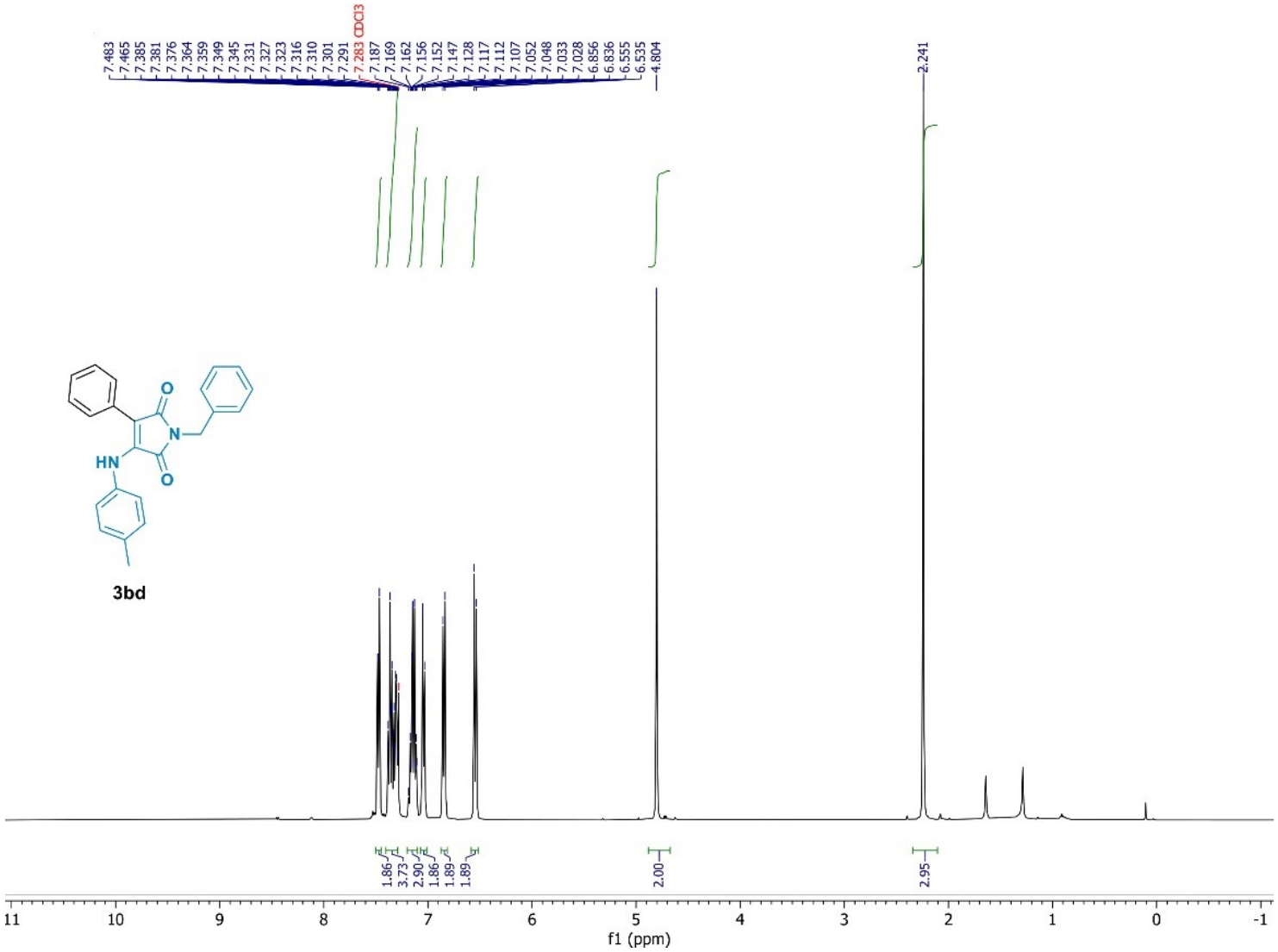
^{13}C NMR of compound **3af** ($CDCl_3$, 100 MHz)



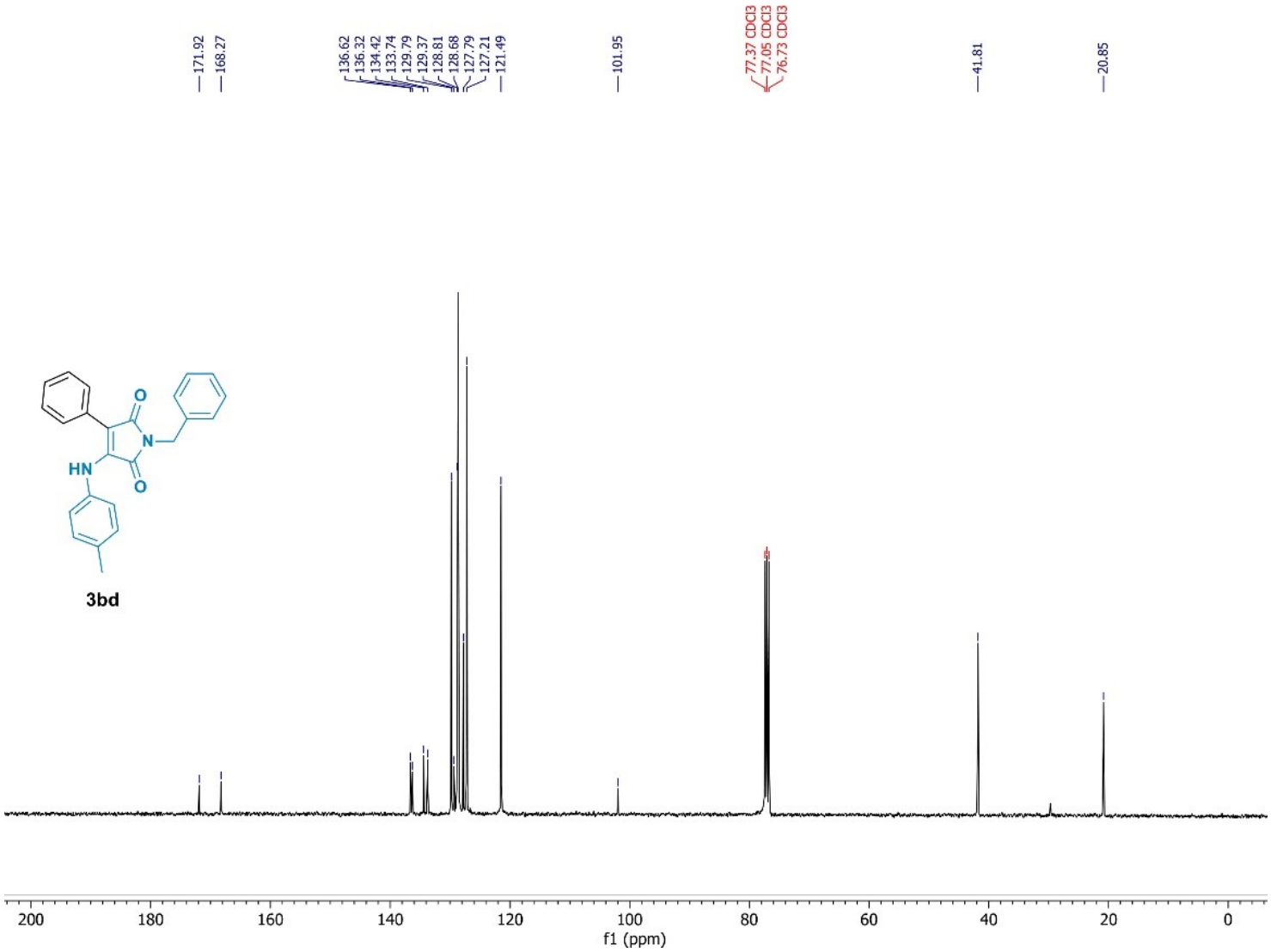
^{1}H NMR of compound **3ag** ($CDCl_3$, 400 MHz)



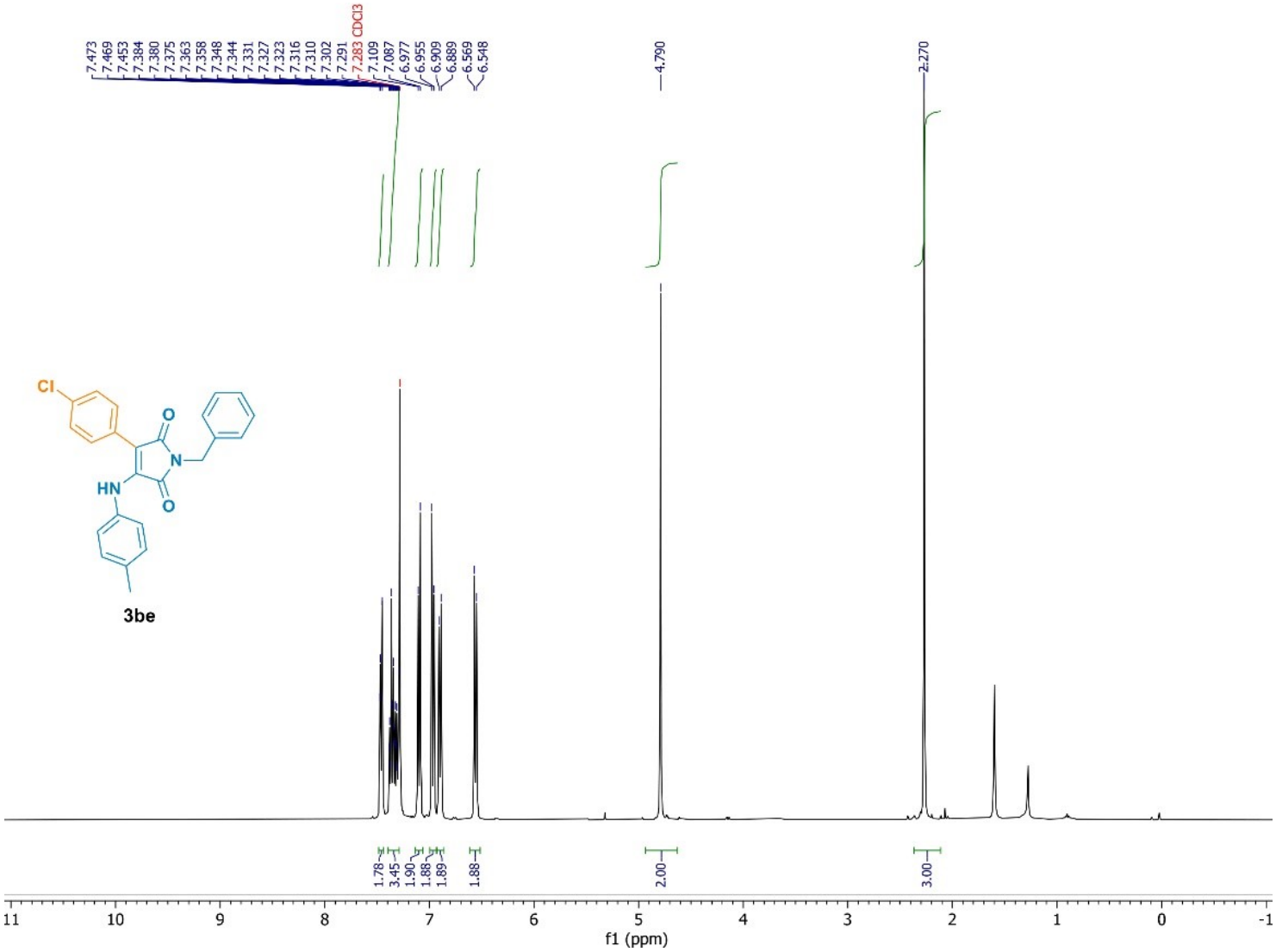
^{13}C NMR of compound **3ag** ($CDCl_3$, 100 MHz)



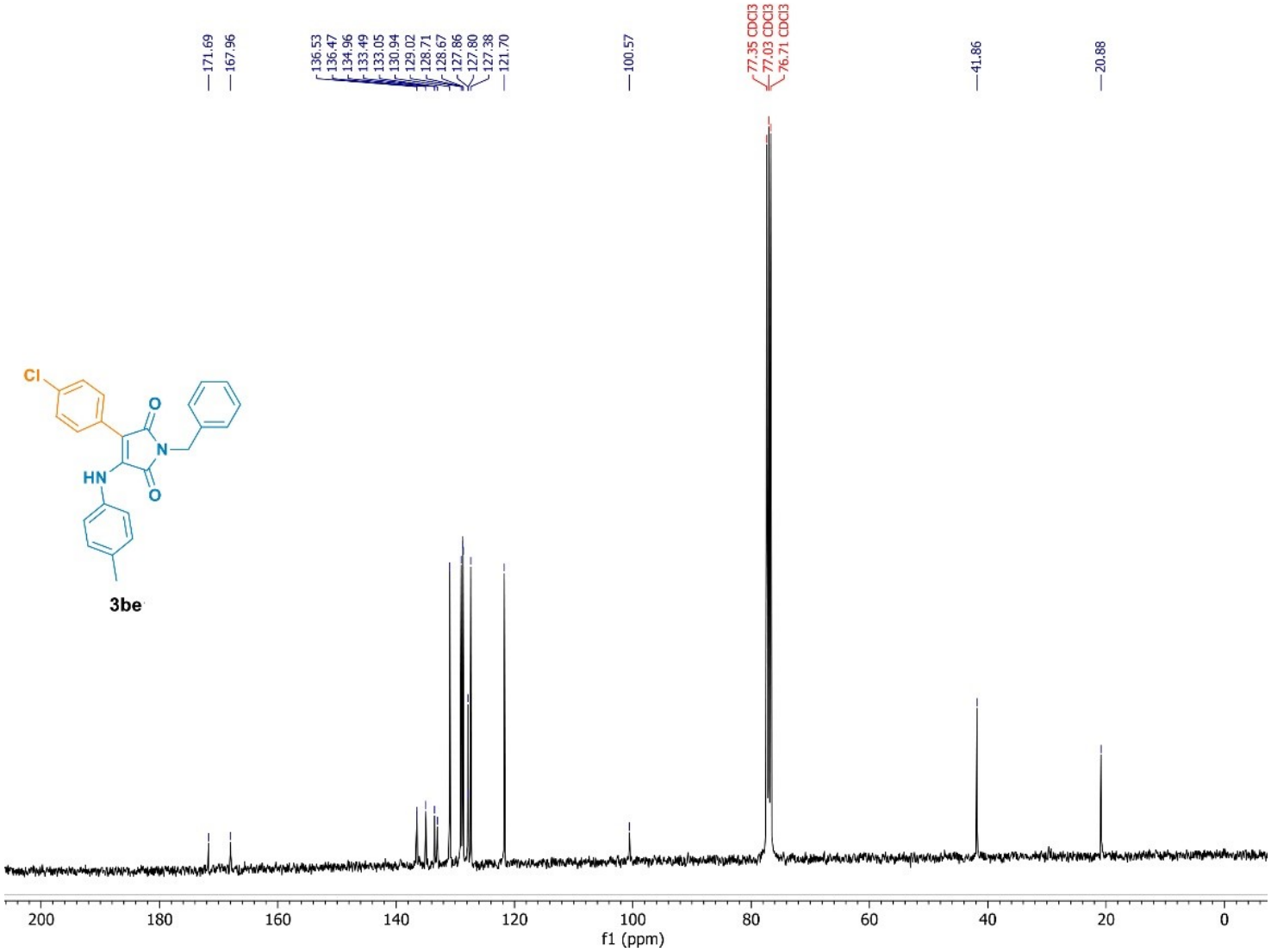
^{1}H NMR of compound **3bd** ($CDCl_3$, 400 MHz)



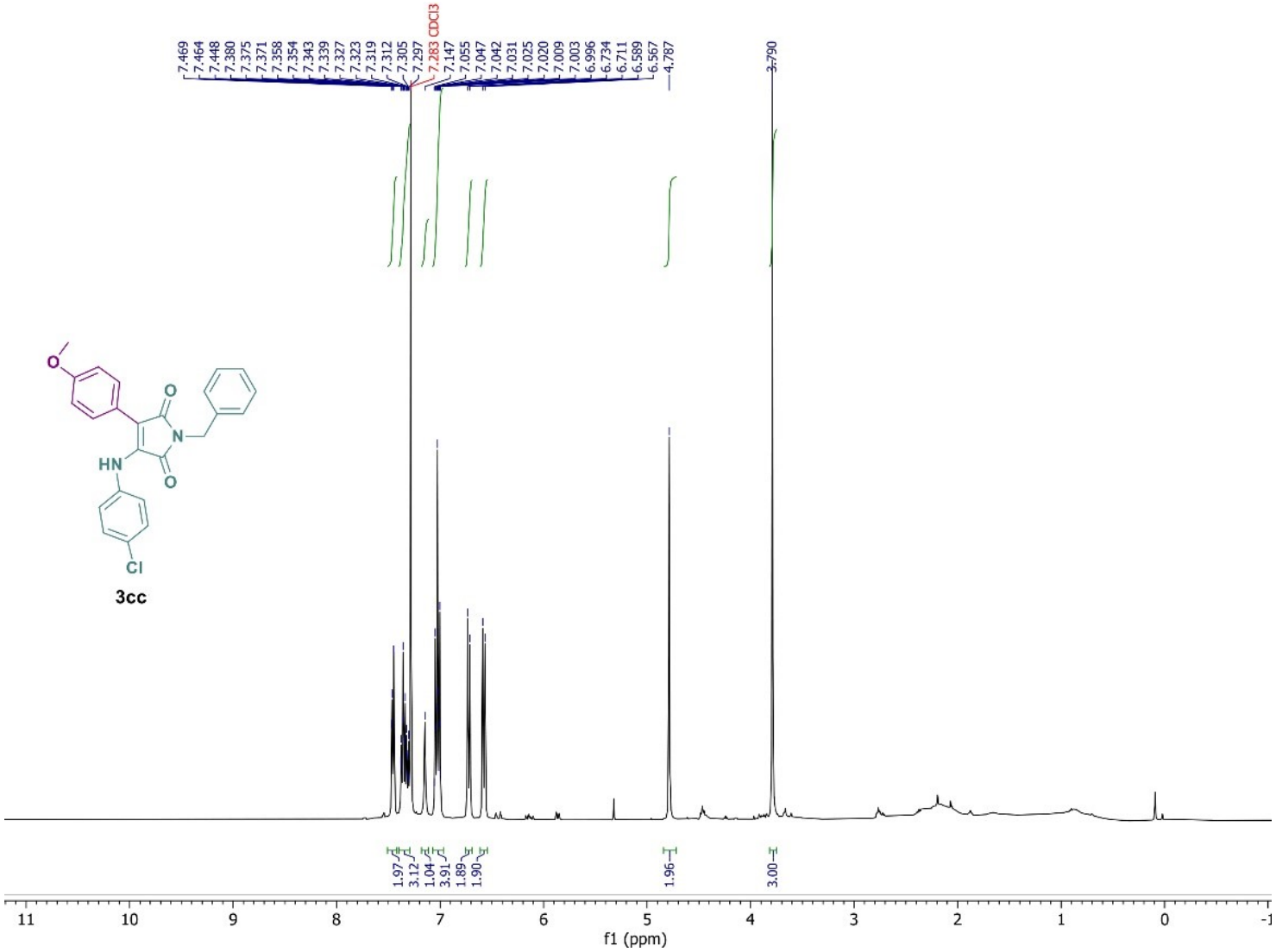
^{13}C NMR of compound **3bd** ($CDCl_3$, 100 MHz)



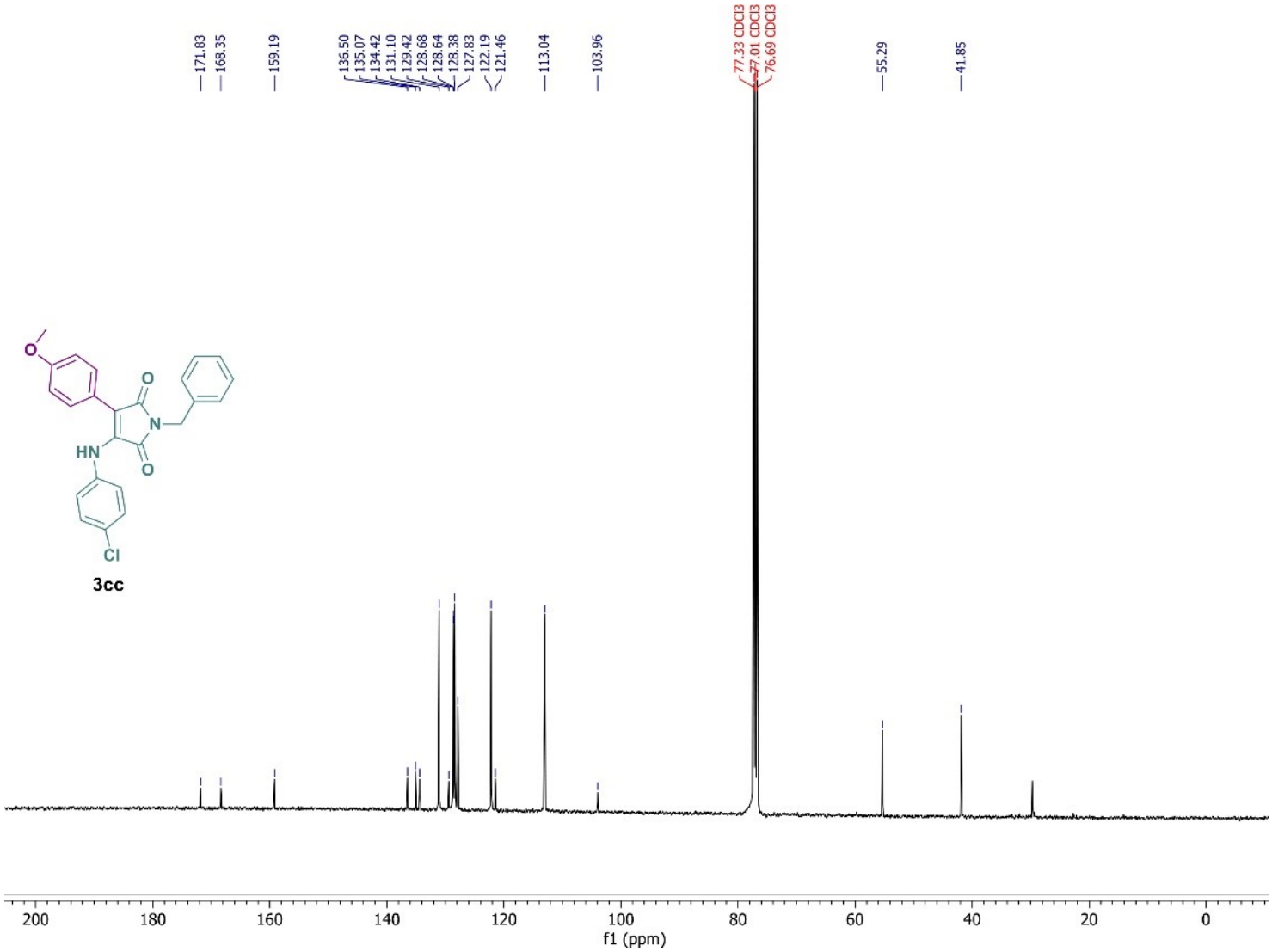
^{1}H NMR of compound **3be** ($CDCl_3$, 400 MHz)



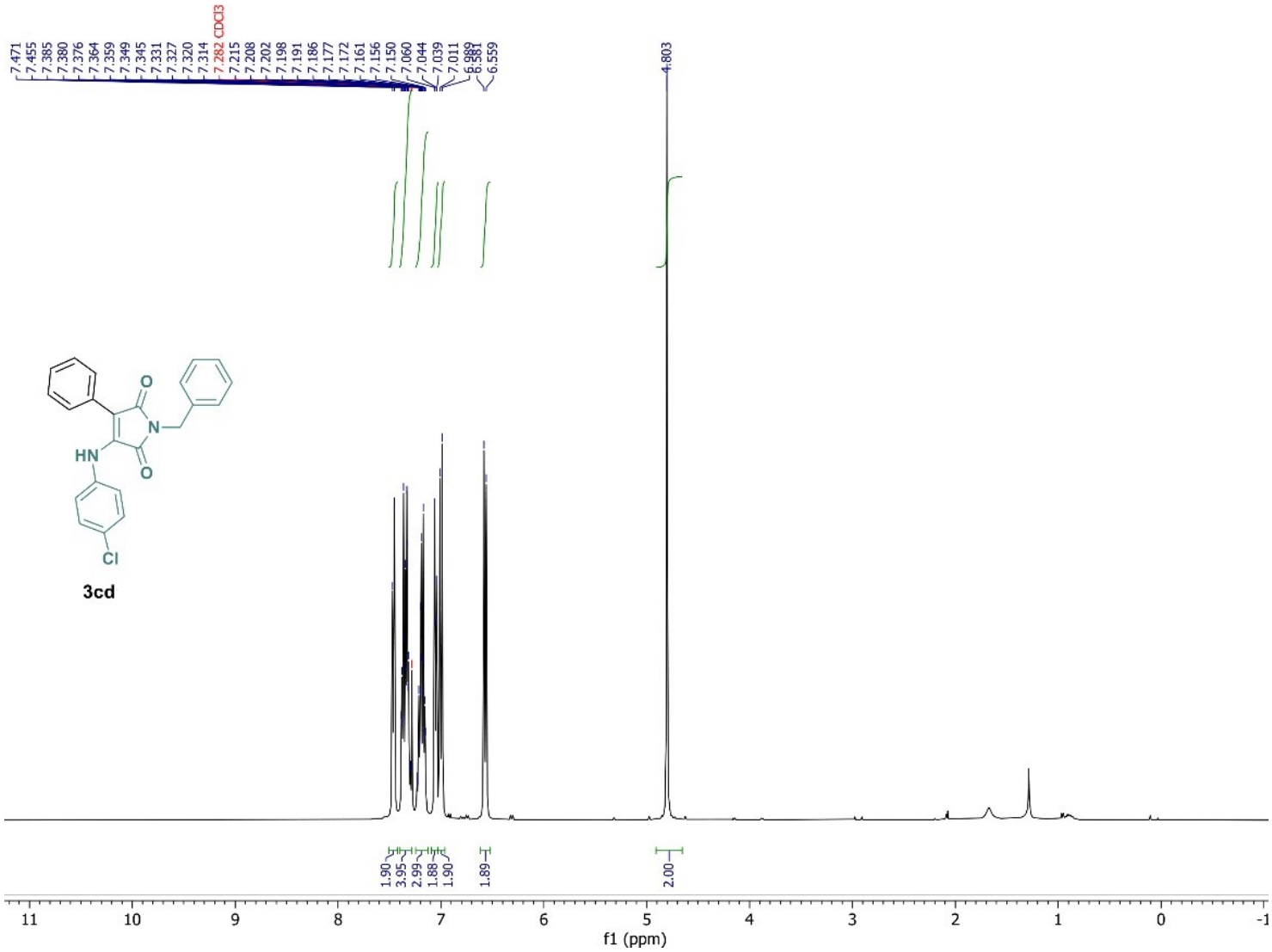
^{13}C NMR of compound **3be** ($CDCl_3$, 100 MHz)



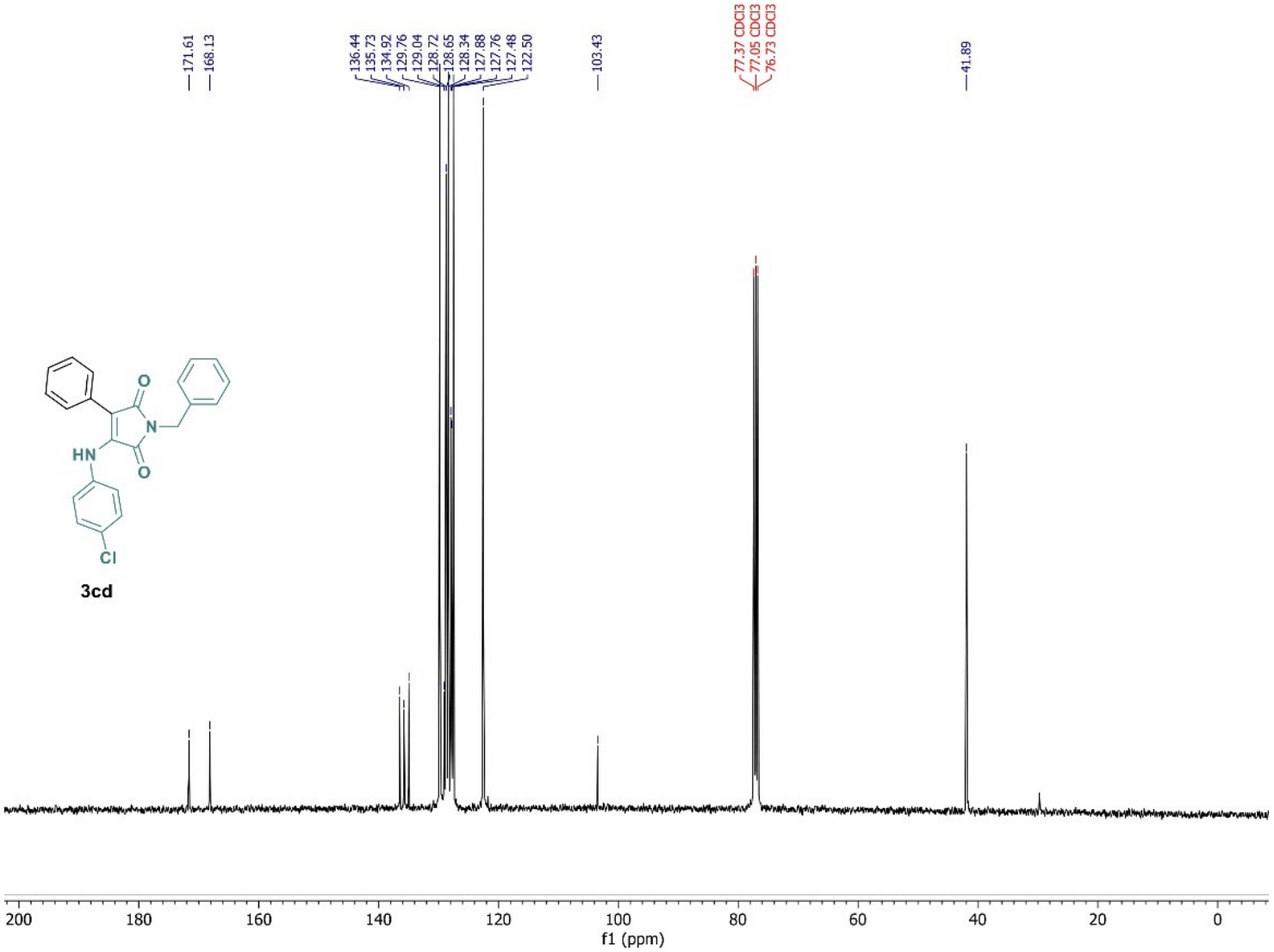
^{1}H NMR of compound **3cc** ($CDCl_3$, 400 MHz)



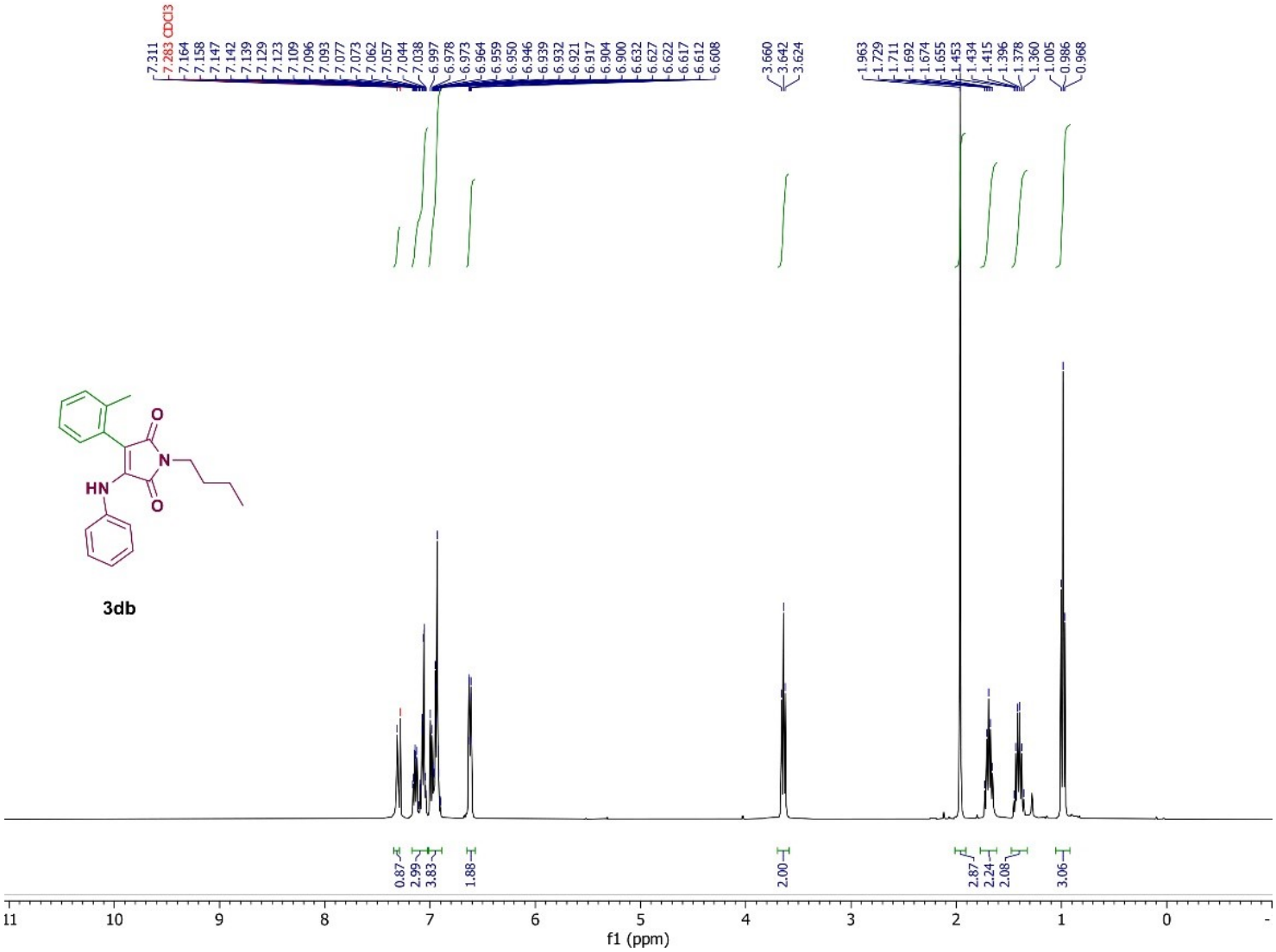
^{13}C NMR of compound **3cc** ($CDCl_3$, 100 MHz)



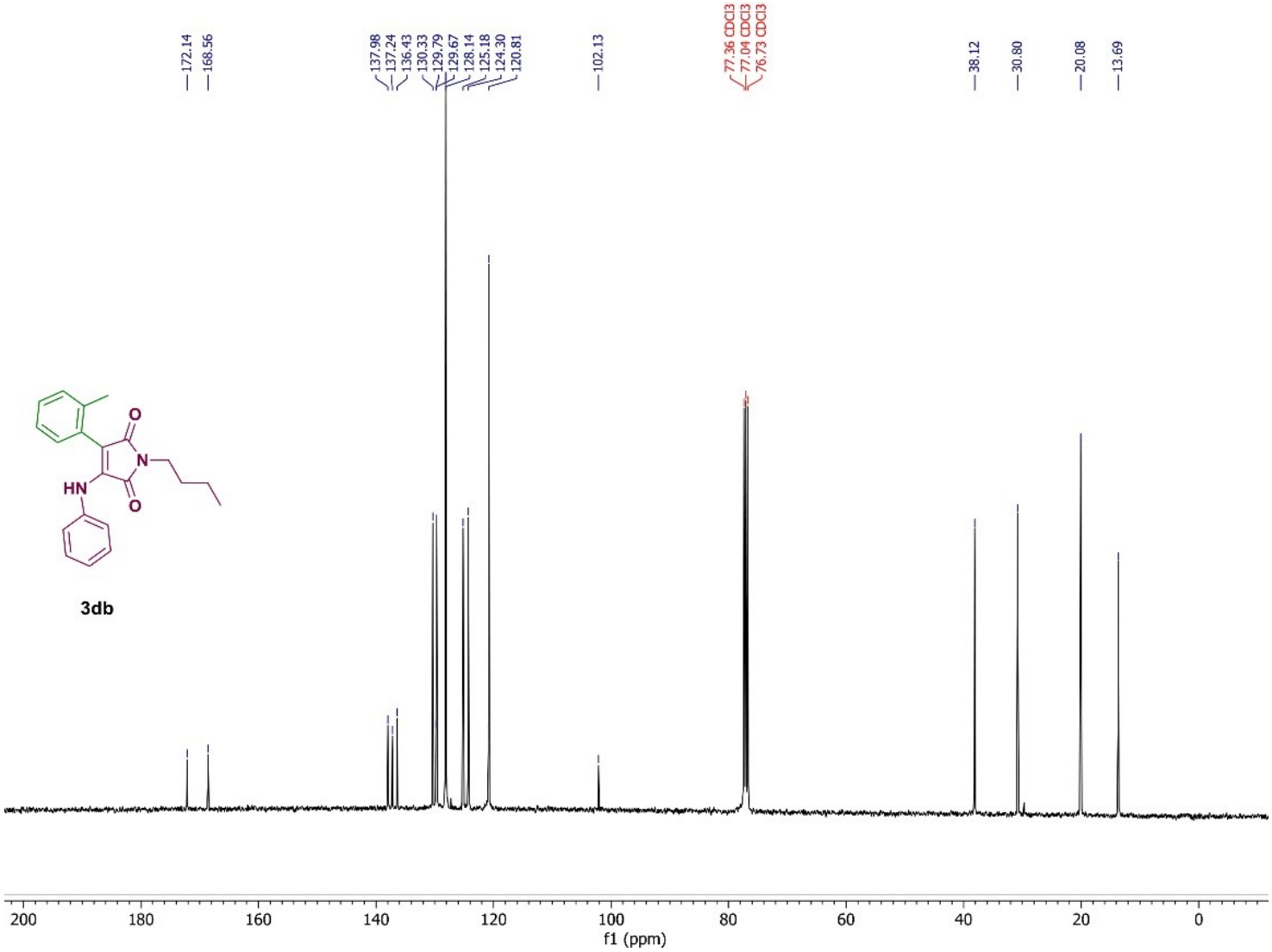
^{1}H NMR of compound **3cd** ($CDCl_3$, 400 MHz)



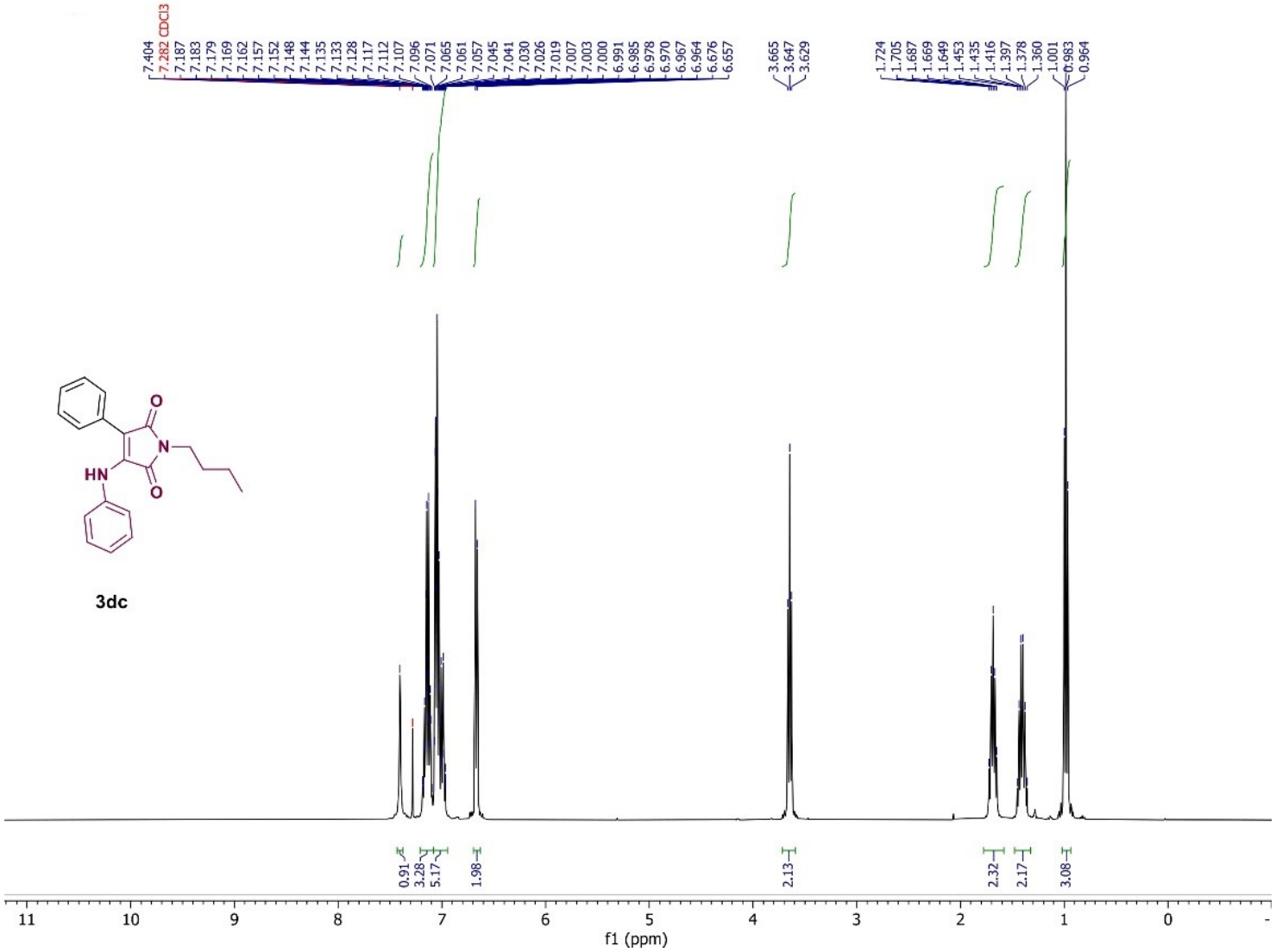
^{13}C NMR of compound **3cd** ($CDCl_3$, 100 MHz)



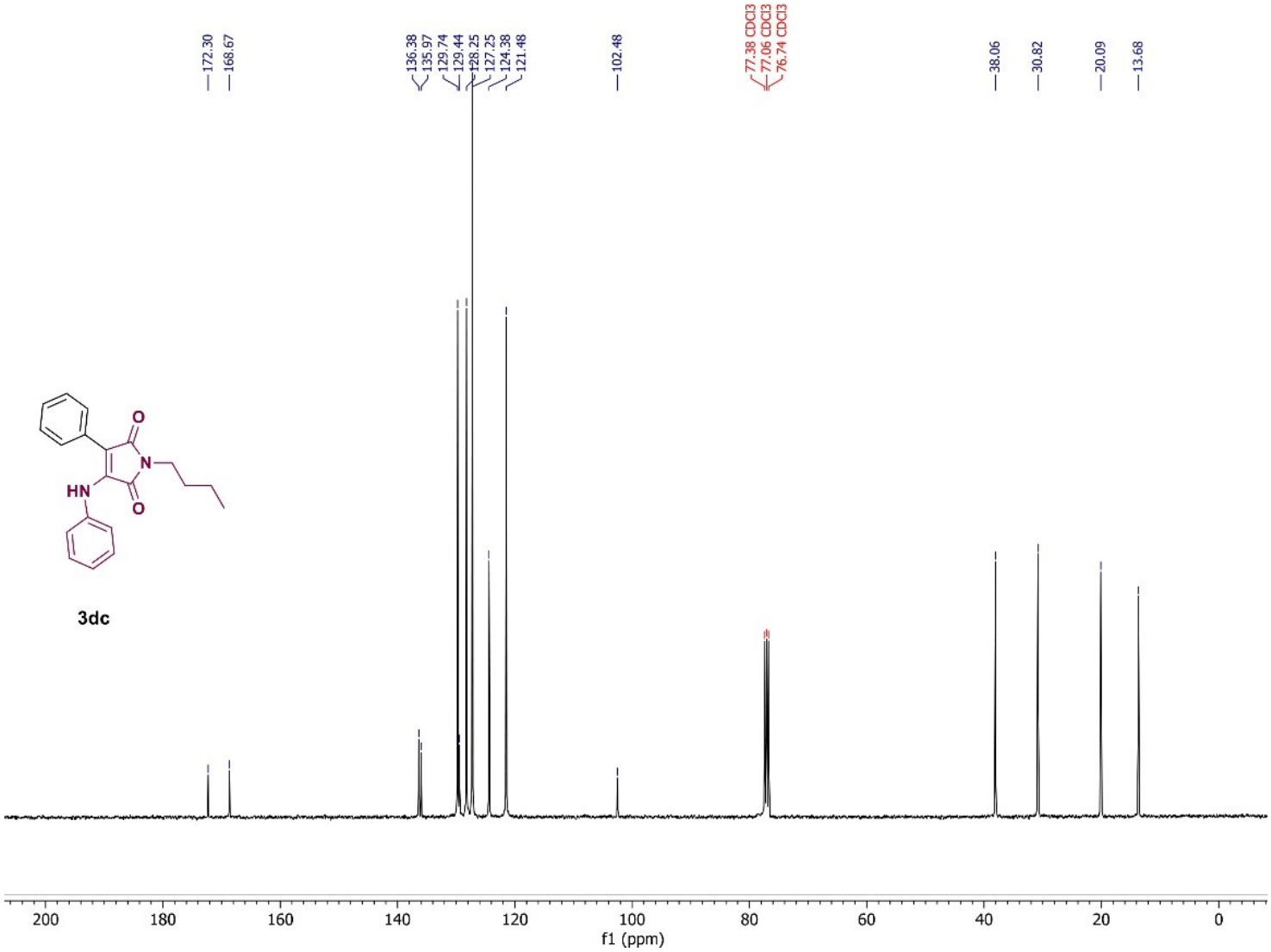
^{1}H NMR of compound **3db** ($CDCl_3$, 400 MHz)



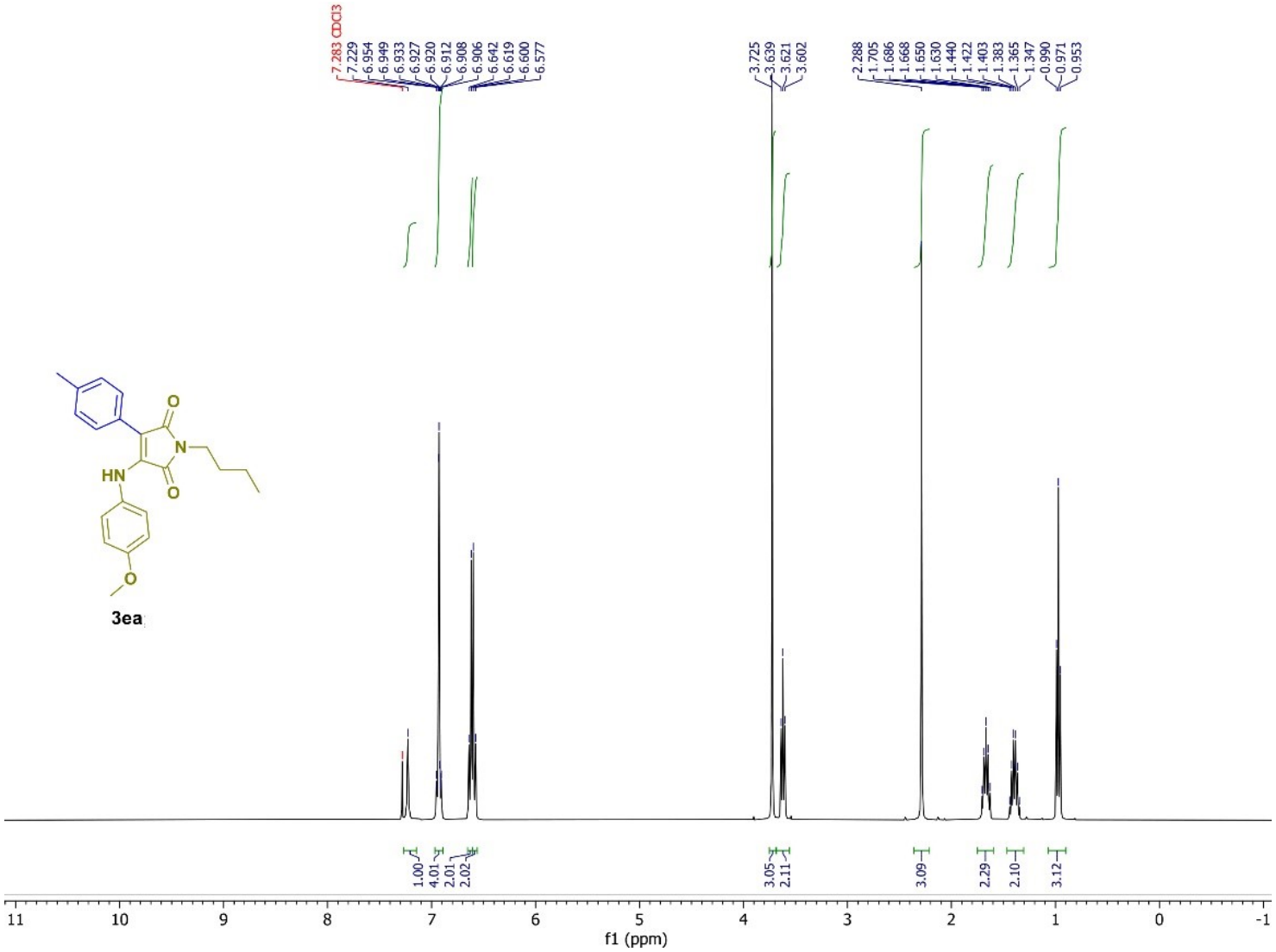
^{13}C NMR of compound **3db** ($CDCl_3$, 100 MHz)



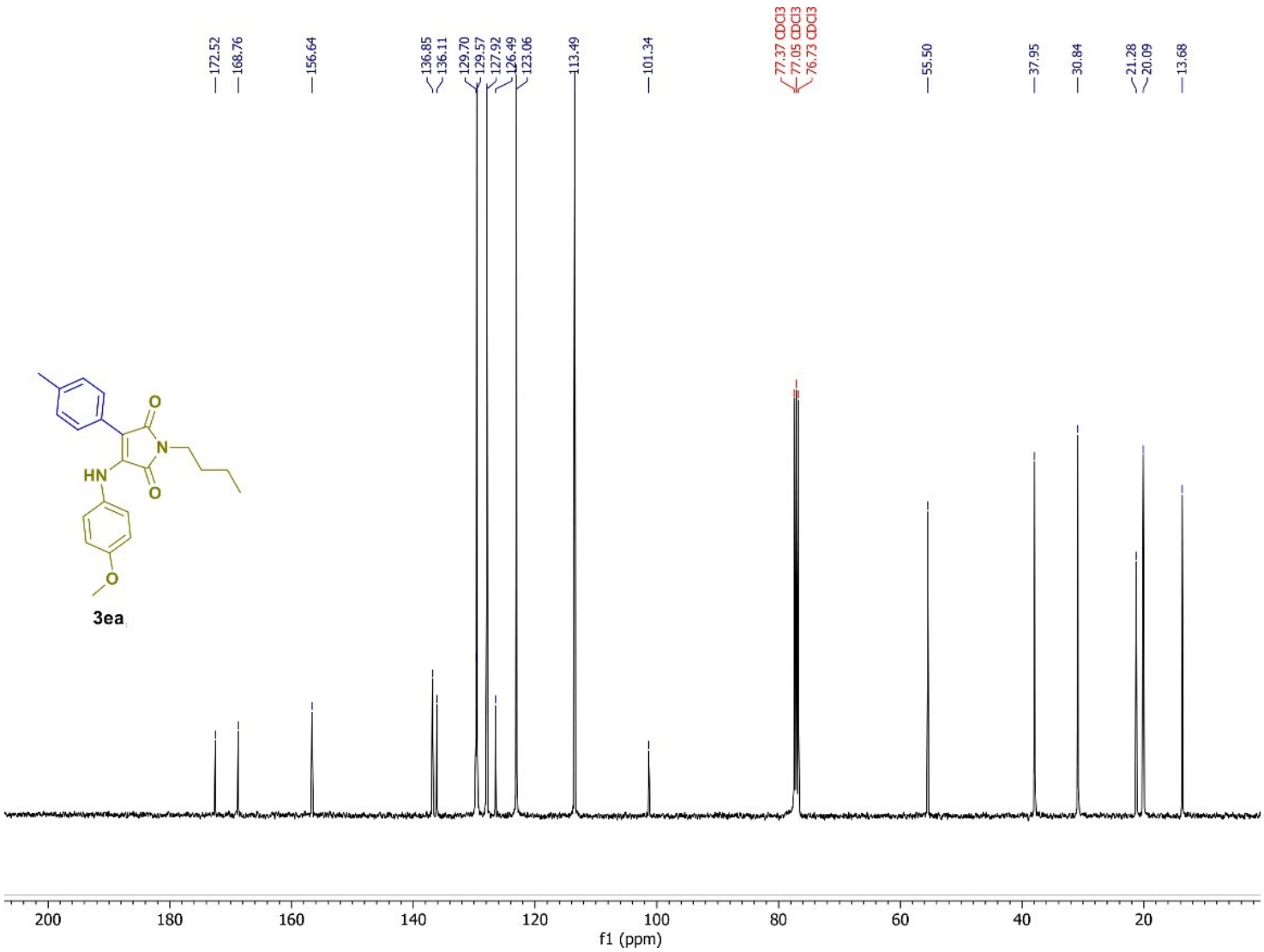
^{1}H NMR of compound **3dc** ($CDCl_3$, 400 MHz)



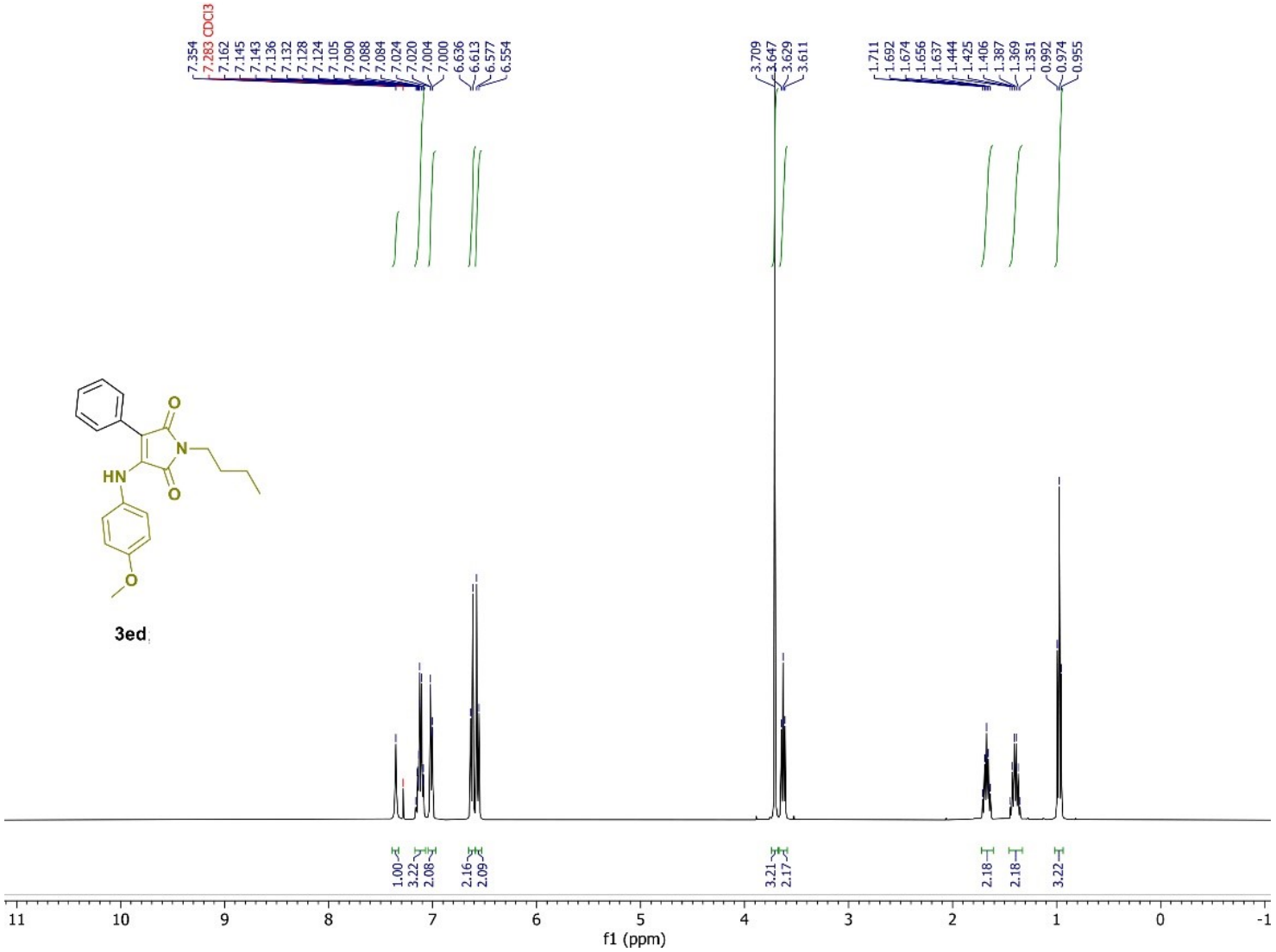
^{13}C NMR of compound **3dc** ($CDCl_3$, 100 MHz)



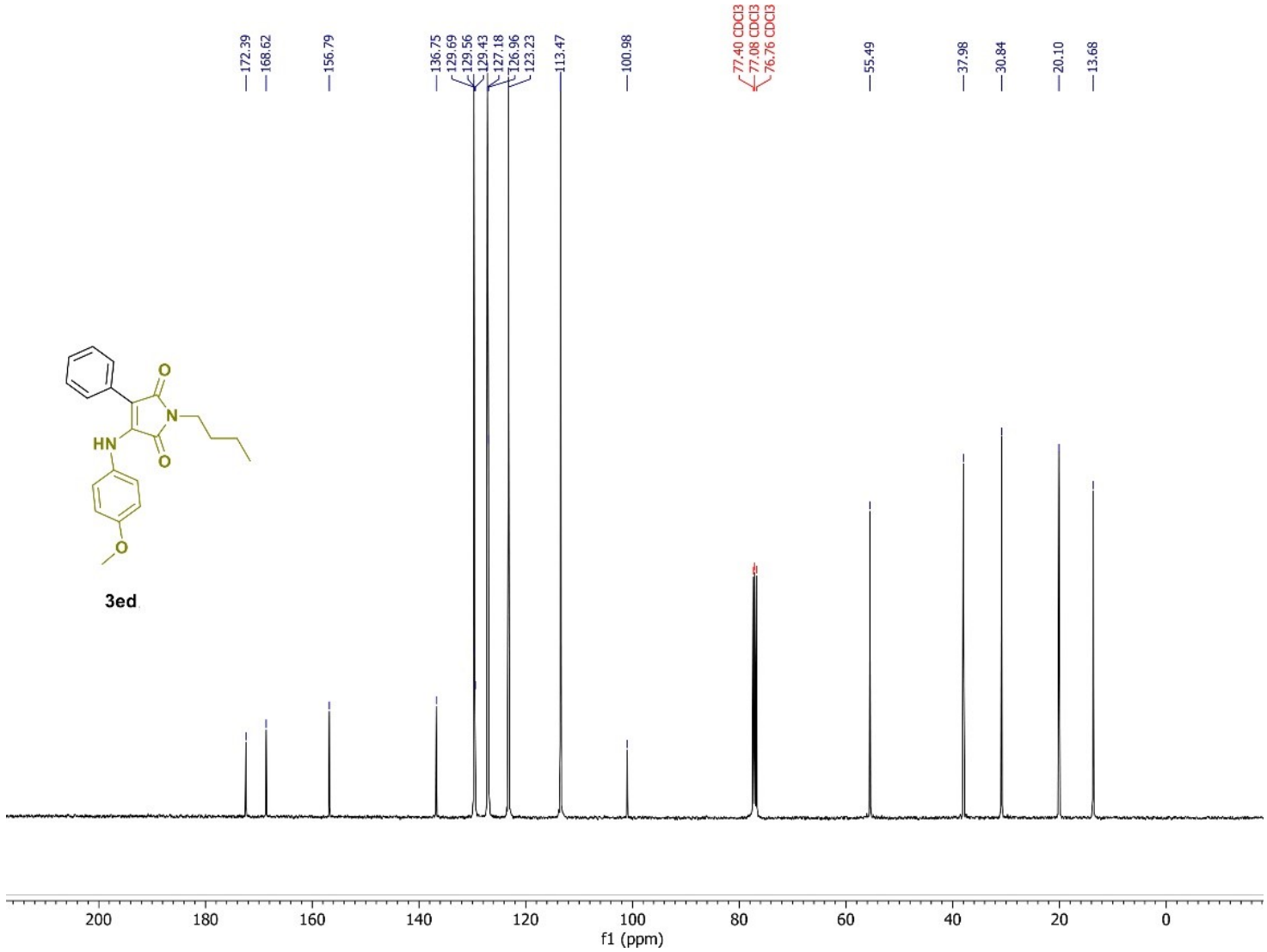
^{1}H NMR of compound **3ea** ($CDCl_3$, 400 MHz)



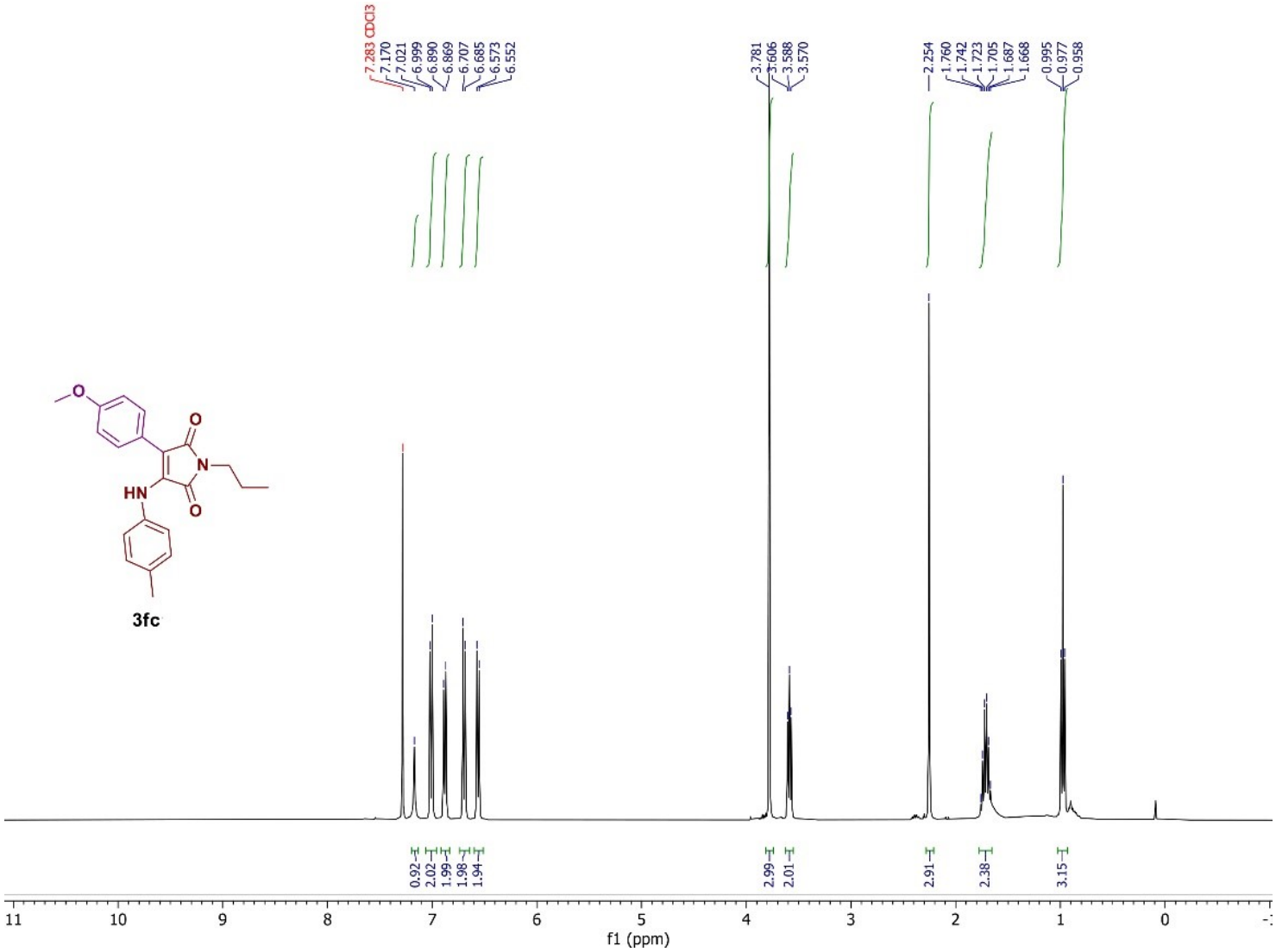
^{13}C NMR of compound **3ea** ($CDCl_3$, 100 MHz)



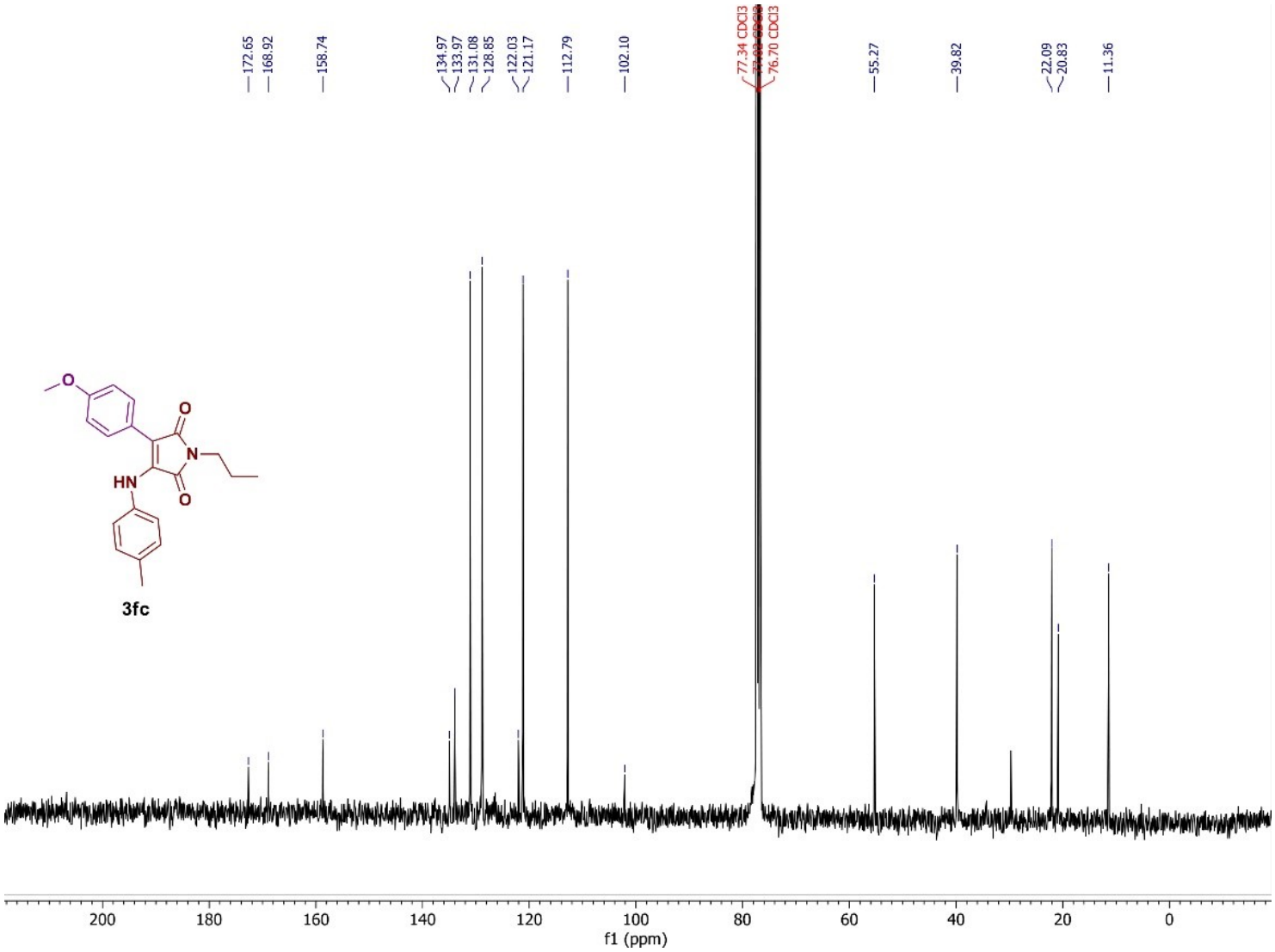
^{1}H NMR of compound **3ed** ($CDCl_3$, 400 MHz)



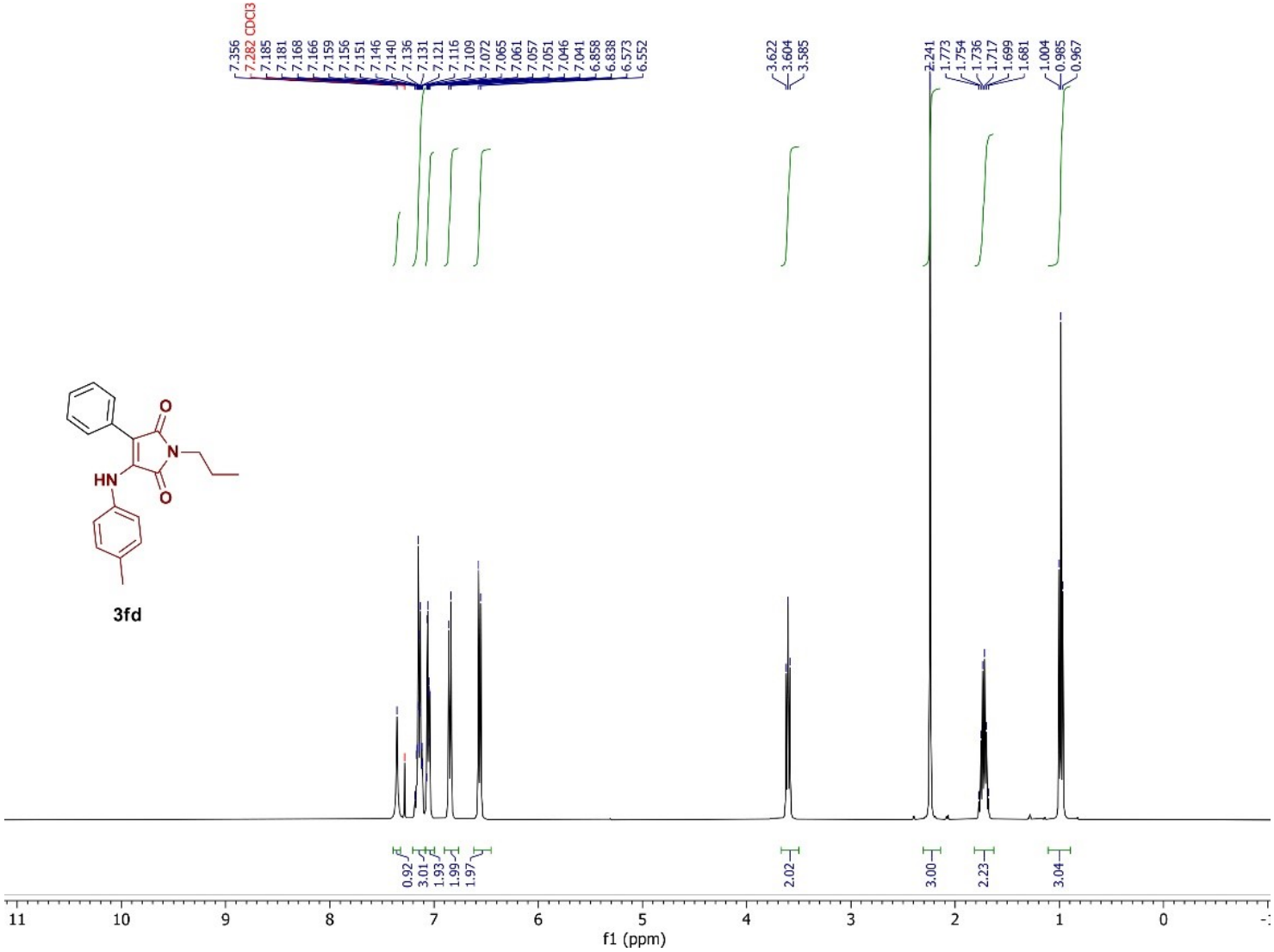
^{13}C NMR of compound **3ed** ($CDCl_3$, 100 MHz)



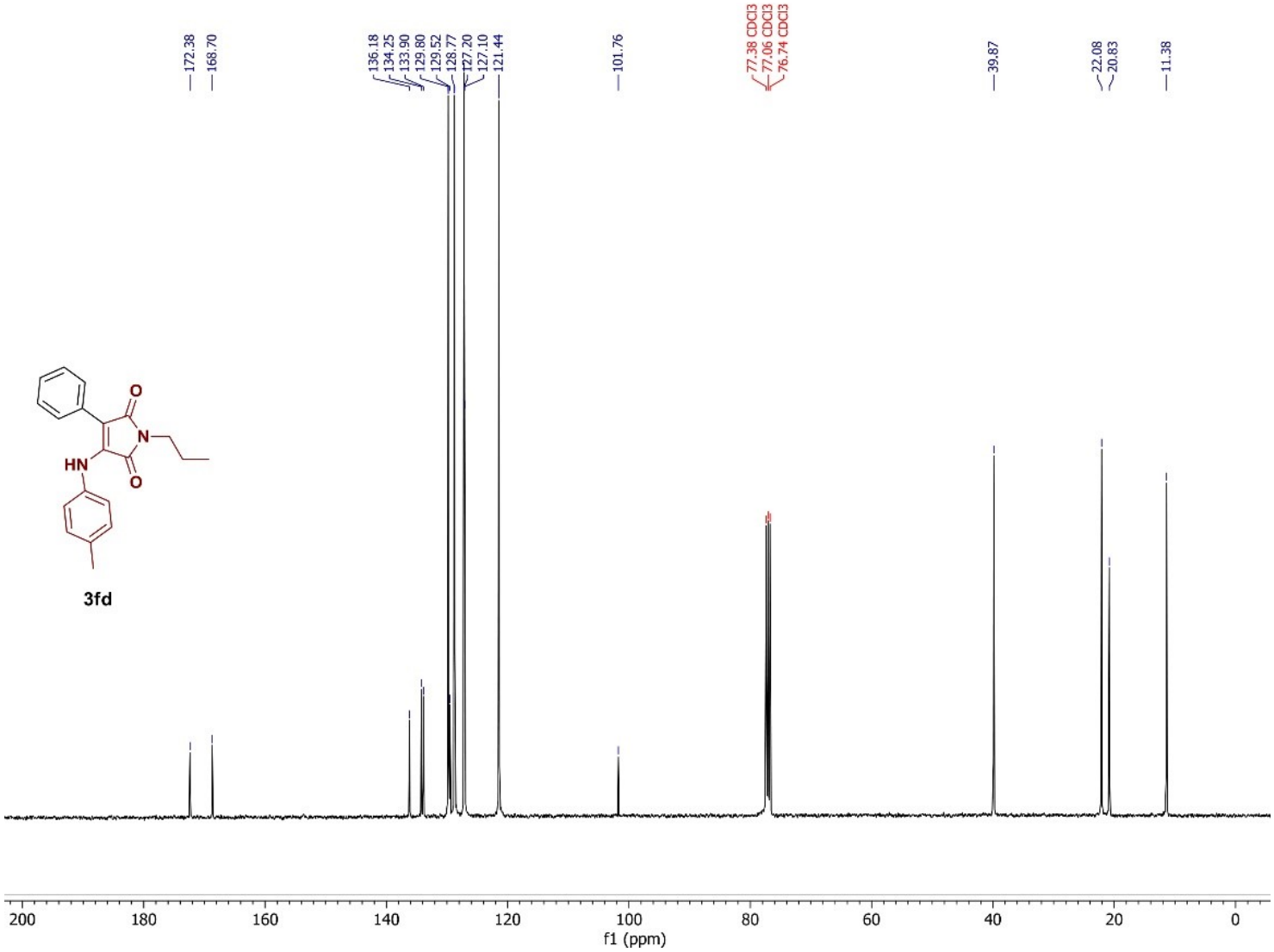
^{1}H NMR of compound **3fc** ($CDCl_3$, 400 MHz)



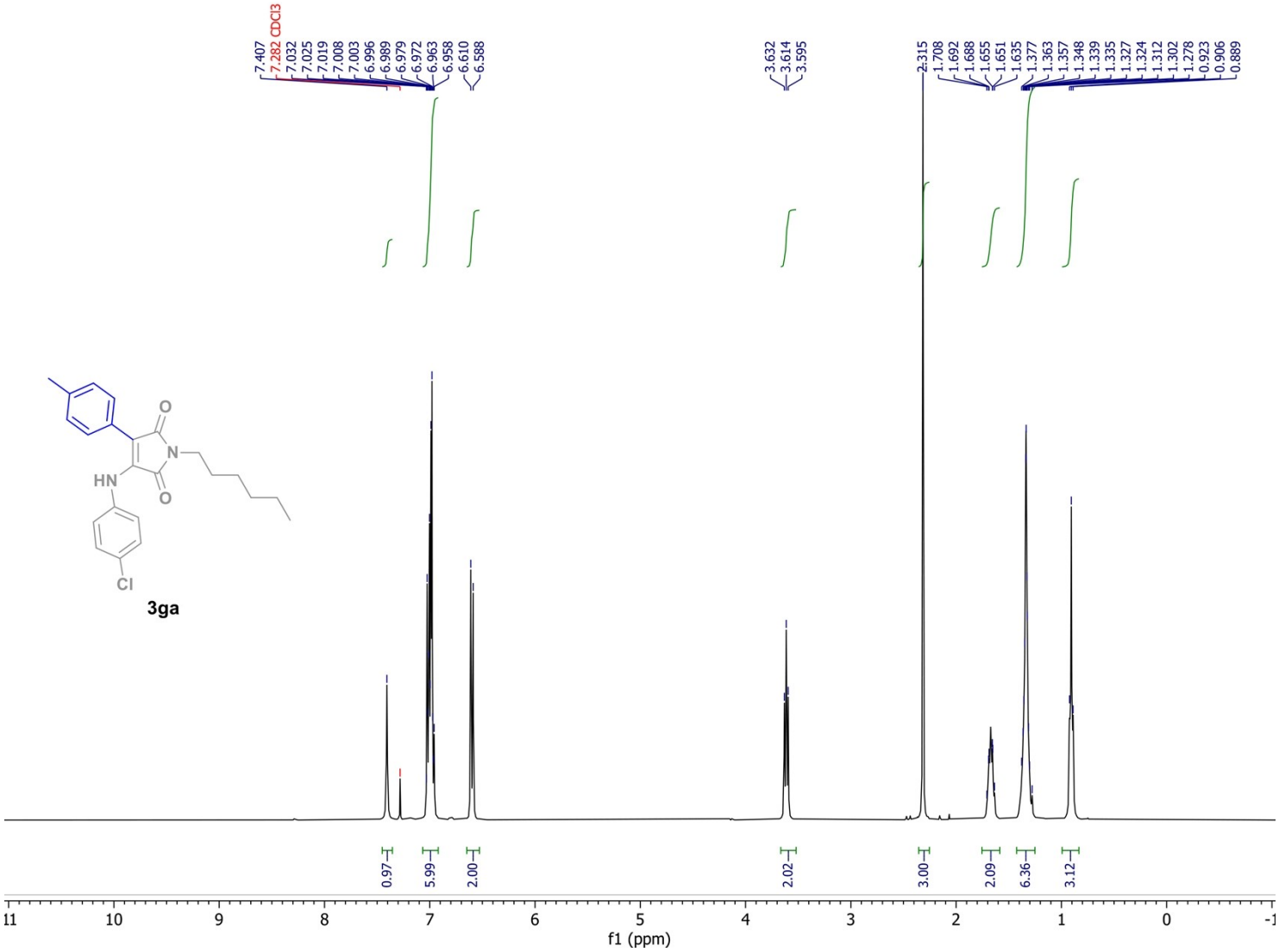
^{13}C NMR of compound **3fc** ($CDCl_3$, 100 MHz)



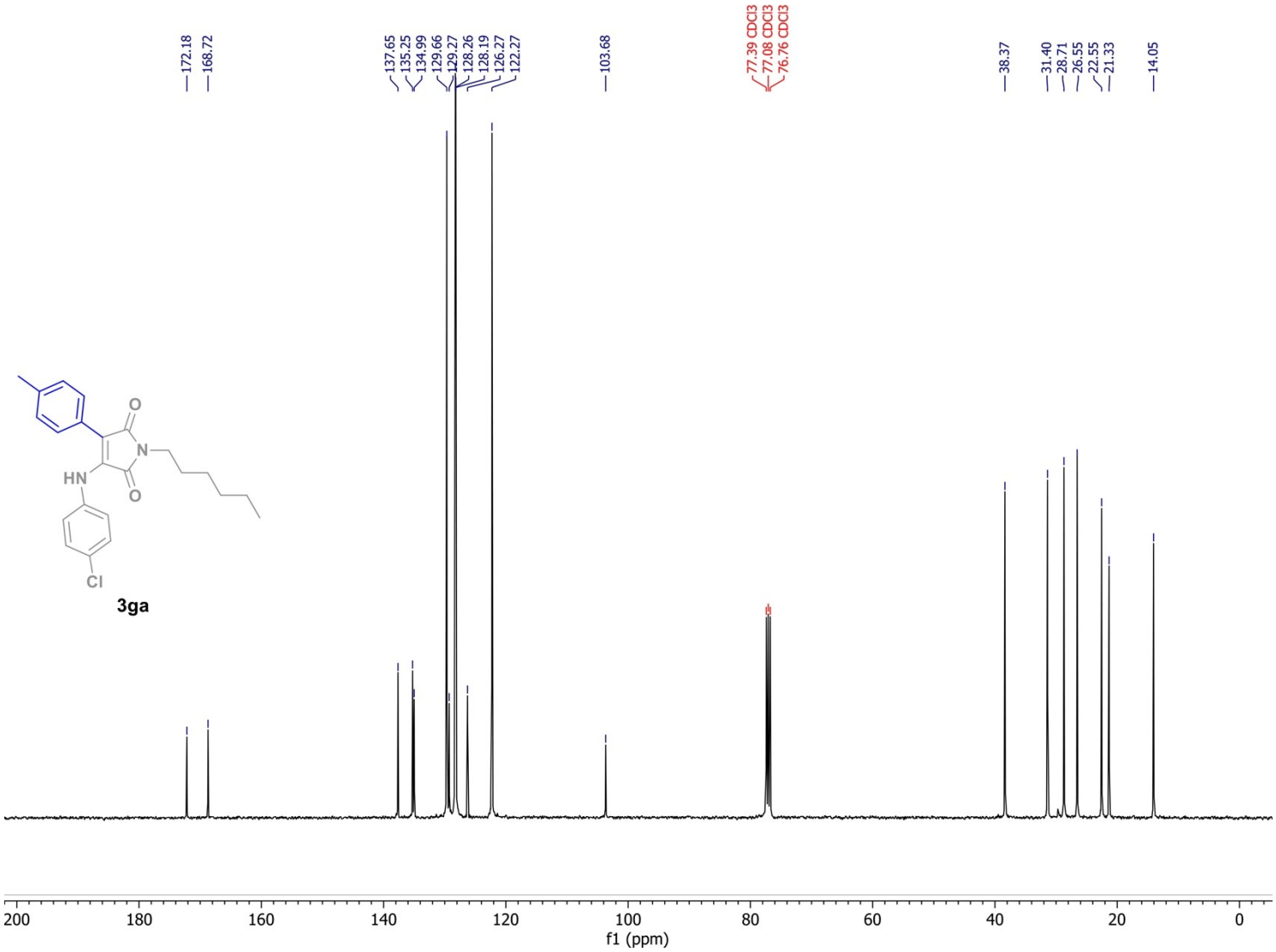
^{1}H NMR of compound **3fd** ($CDCl_3$, 400 MHz)



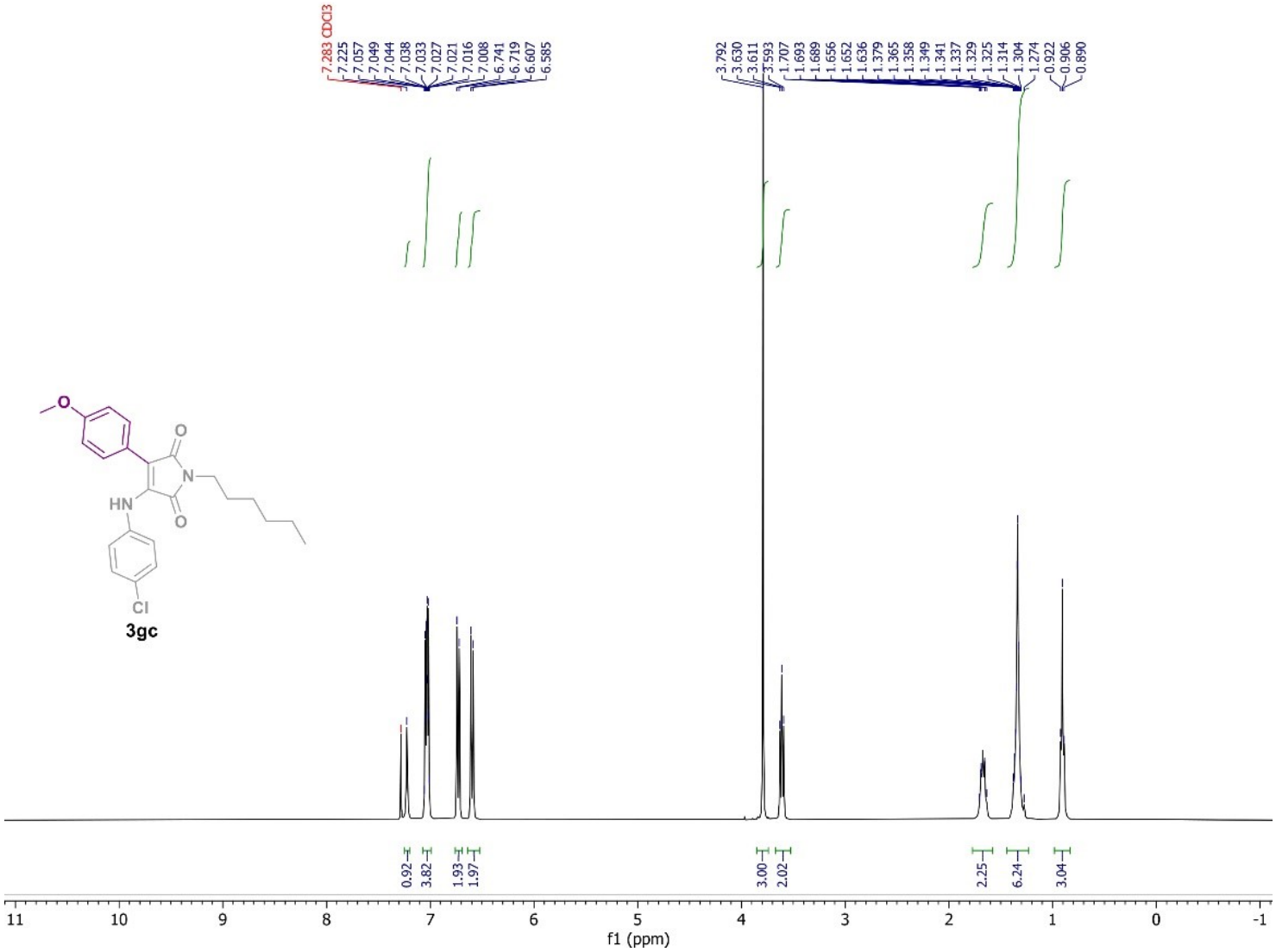
^{13}C NMR of compound **3fd** ($CDCl_3$, 100 MHz)



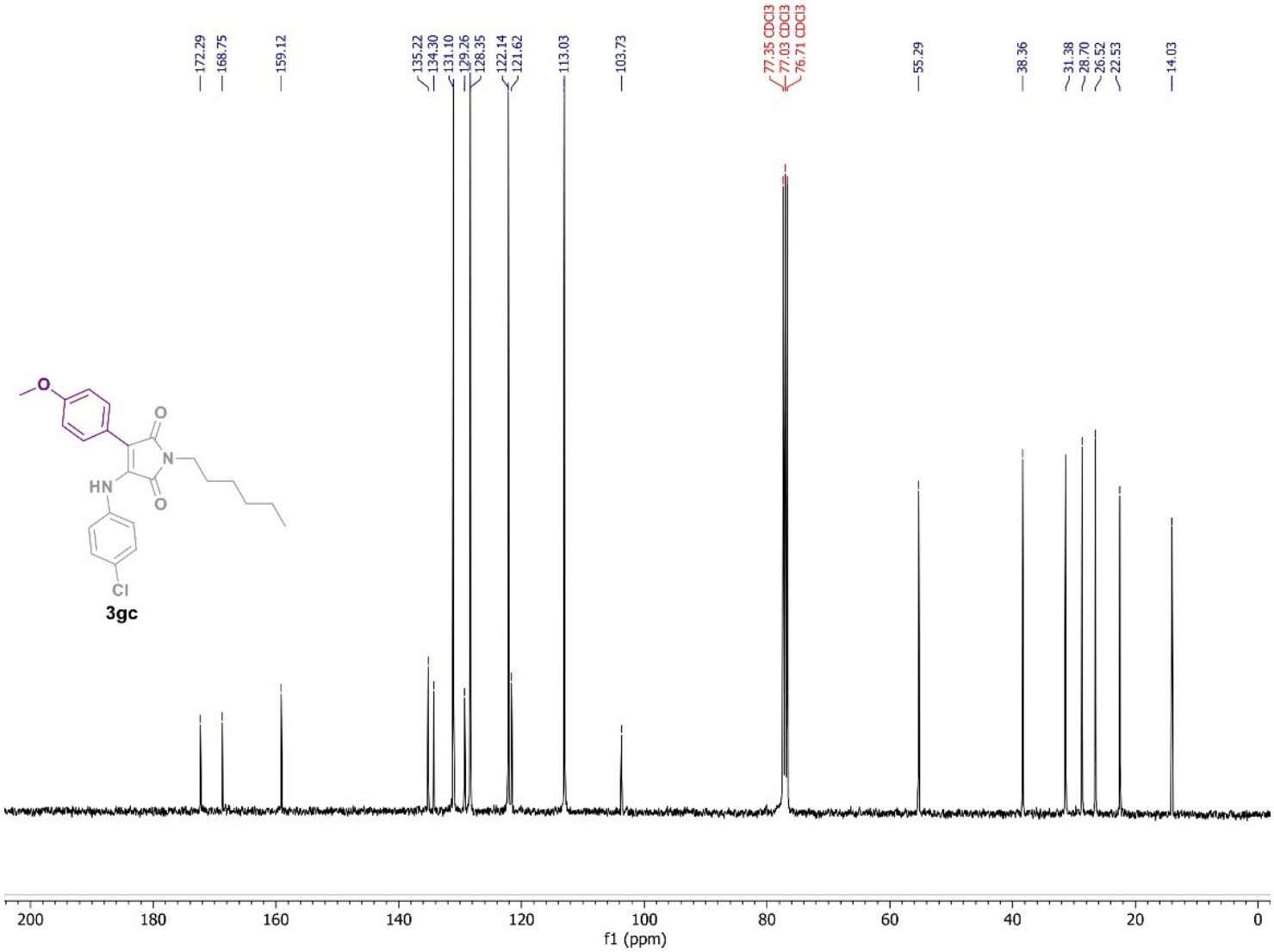
^{1}H NMR of compound **3ga** ($CDCl_3$, 400 MHz)



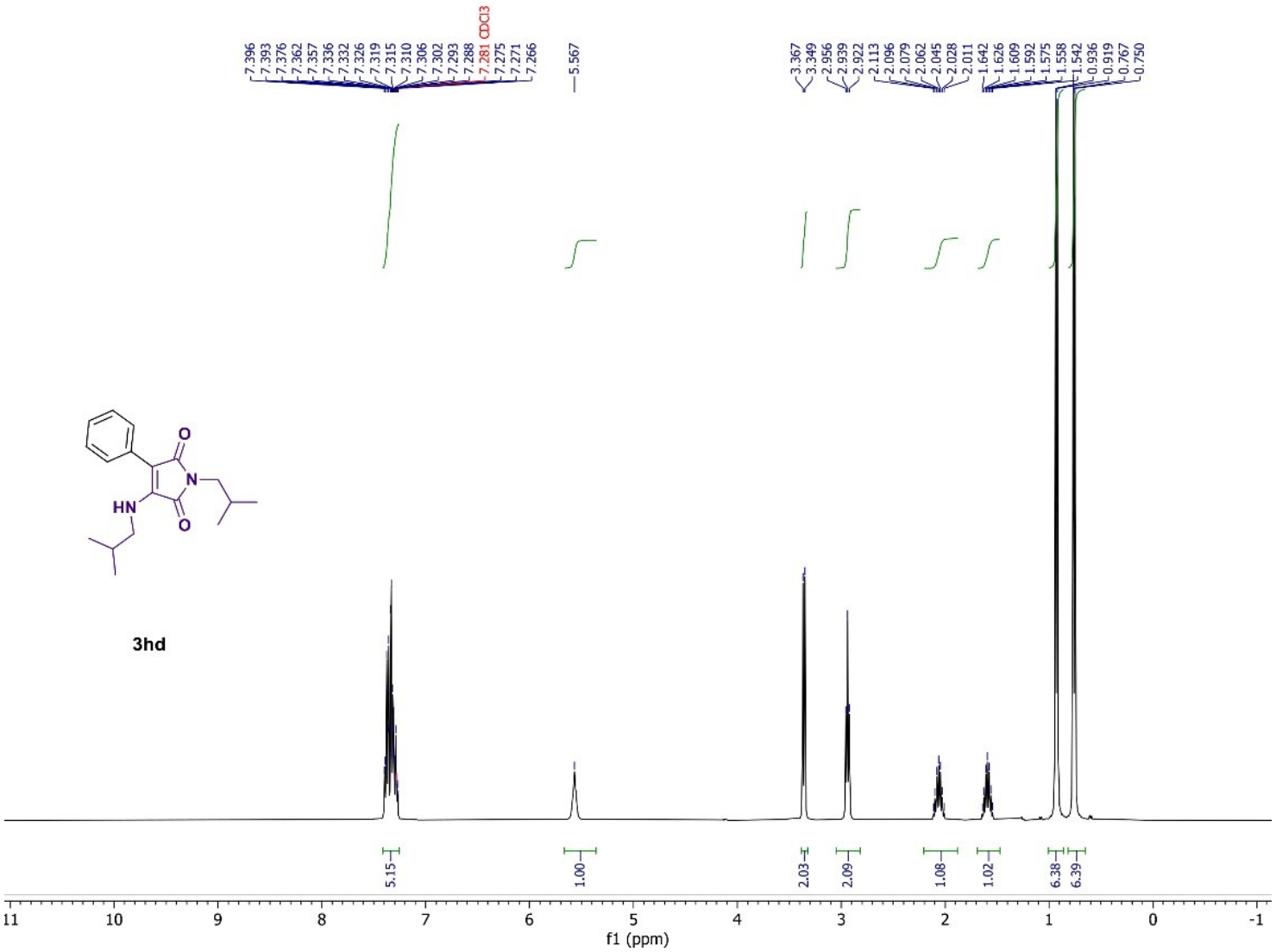
^{13}C NMR of compound **3ga** ($CDCl_3$, 100 MHz)



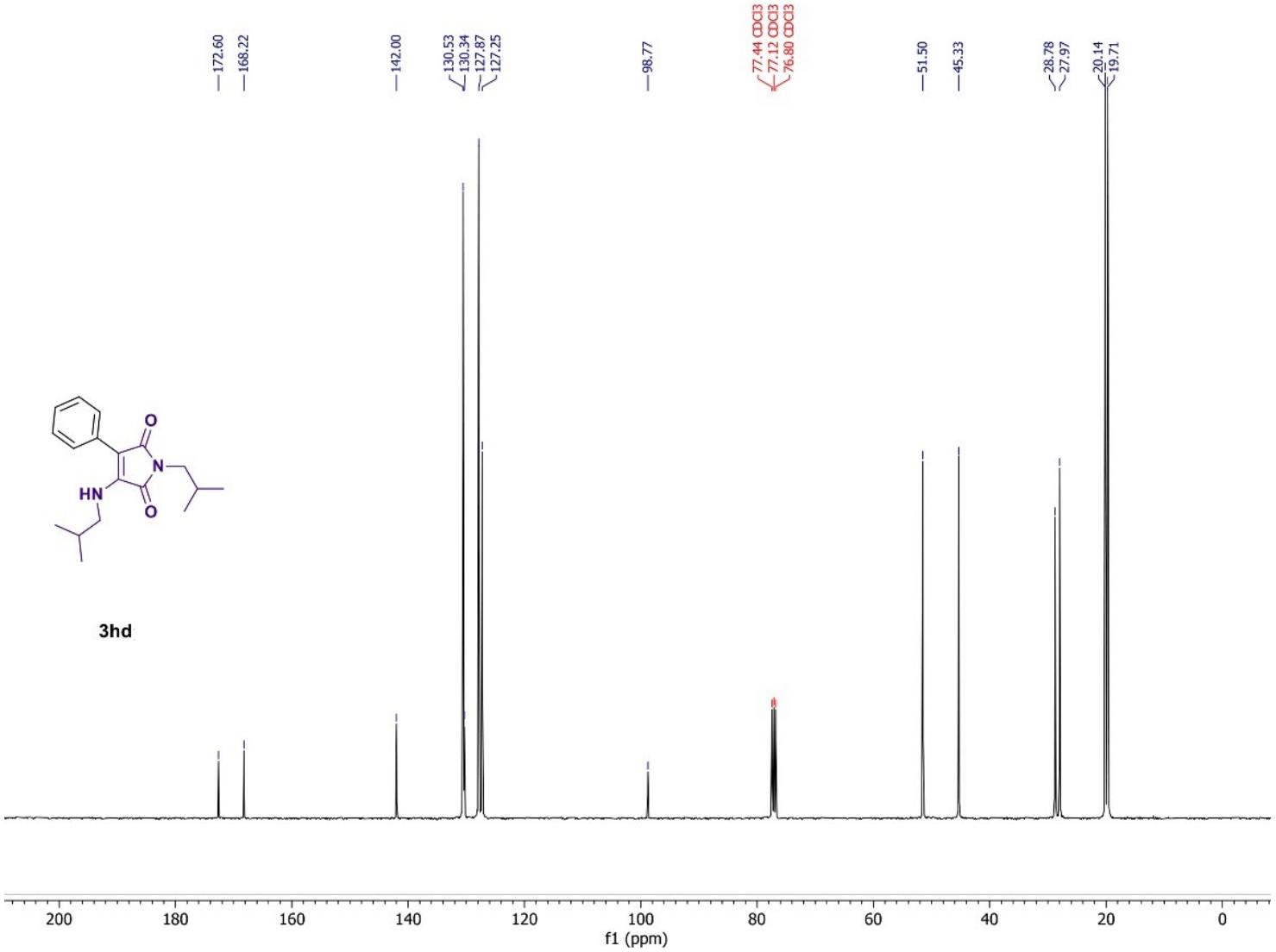
^{1}H NMR of compound **3gc** ($CDCl_3$, 400 MHz)



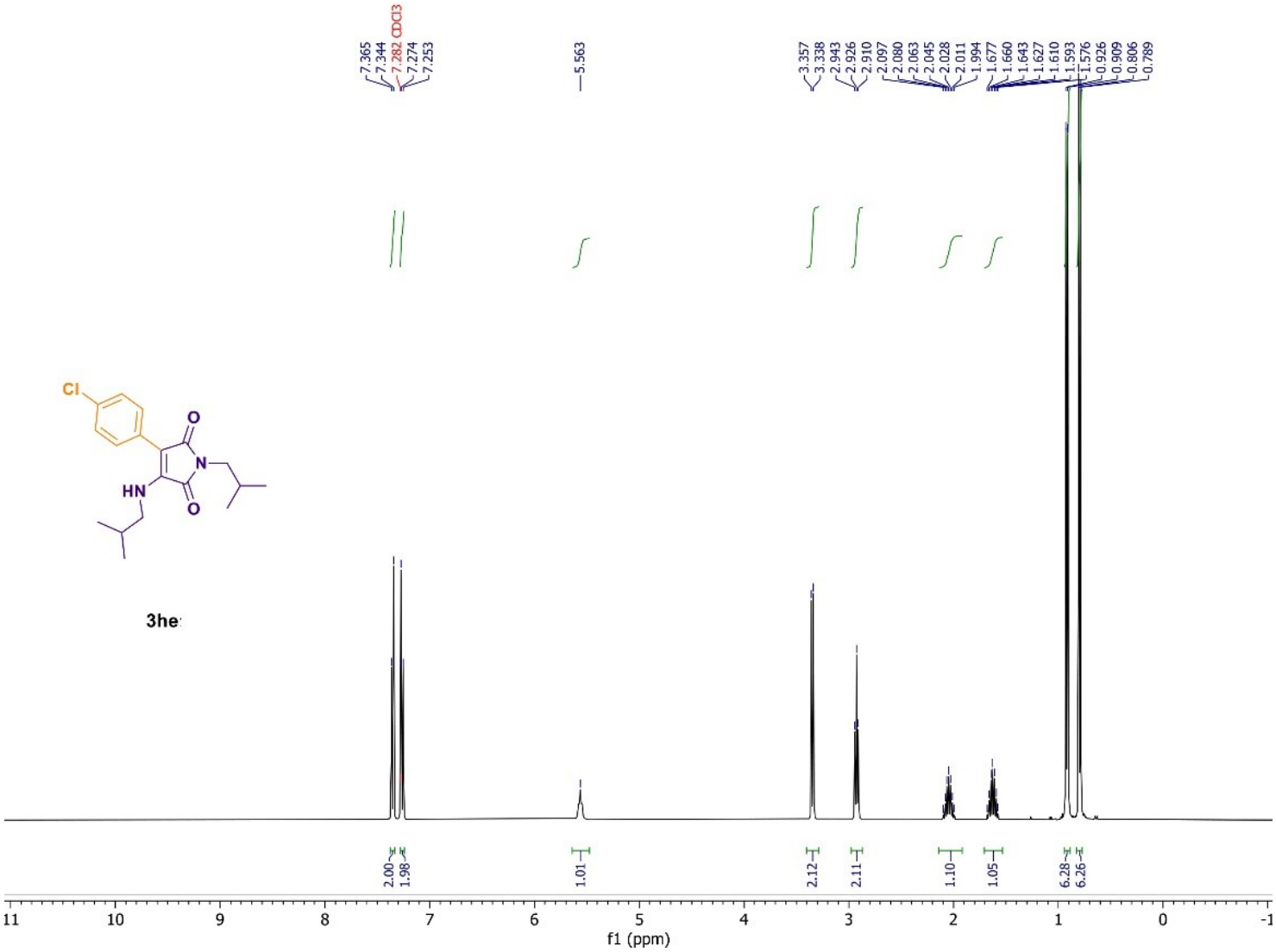
^{13}C NMR of compound **3gc** ($CDCl_3$, 100 MHz)



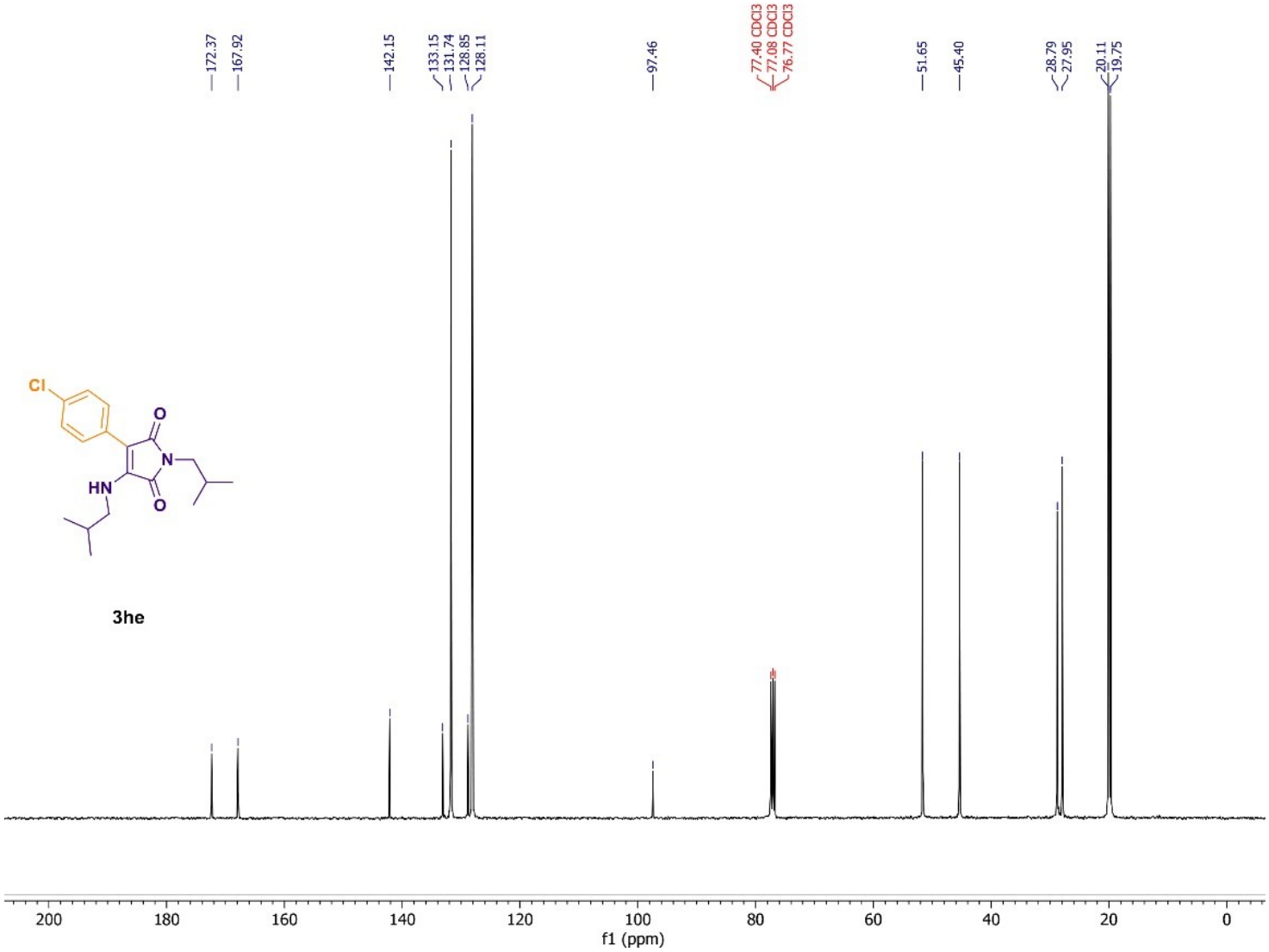
^{1}H NMR of compound **3hd** ($CDCl_3$, 400 MHz)



^{13}C NMR of compound **3hd** ($CDCl_3$, 100 MHz)



^{1}H NMR of compound **3he** ($CDCl_3$, 400 MHz)



^{13}C NMR of compound **3he** ($CDCl_3$, 100 MHz)