Iron catalyzed cascade one pot reaction between azlactones and O-acetyl oximes to afford 6*H*-pyrrolo[3,2-*d*]oxazole and pyrrol-2-one nucleus

Parth P. Patel [a] , Rajnikant N.Ghoghari[b], Kishor H. Chikhalia [*]

[a] Department of Chemistry, Veer Narmad South Gujarat University, Surat – 395007, Gujarat, India.

Email Address: chikhalia_kh@yahoo.com

The ^{1}H NMR & ^{13}C NMR spectra of the products ……

Experimental section

1. General Information

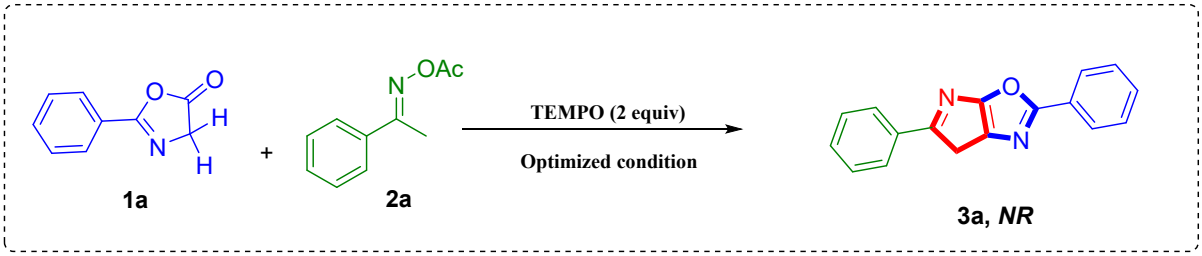
Unless otherwise noted, all commercial reagents, catalysts, oxidants, and solvents were acquired from commercial suppliers and used without being previously purified. Analytical thin layer chromatography (TLC) was used on Merck 60 F254 precoated silica gel (0.25 mm thickness) to monitor the progression of each reaction. The TLC plates were rendered visible with the application of visualization techniques including potassium permanganate and UV light (254 nm). The generated compounds were examined with ^{1}H NMR, ^{13}C NMR and mass spectral analysis. Melting points in open capillaries were measured using the Vego electronic device VMP-DS and they are uncorrected. HRMS was carried out on a Waters Xevo G2-XS QTOF mass spectrometer. A Bruker AM400 (400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR) instrument was used to record the ^{1}H and ^{13}C NMR spectra using DMSO-d_6 as the solvent and tetramethylsilane (TMS) as an internal standard. Parts per million were used to report chemical shifts for the ^{13}C NMR spectra, which were connected to the DMSO-d_6 centerline. The ^{1}H NMR spectra data set includes the following variables: chemical shift (δ shift), coupling constant (Hz), integration, multiplicity (s=singlet, d=doublet, t=triplet, q=quartet, m=multiplet).

2. General procedure for the synthesis of 2, 5-diphenyl-6*H*-pyrrolo[3,2-*d*]oxazole and 4-methoxy-N-(2-oxo-3, 5-diphenyl-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide

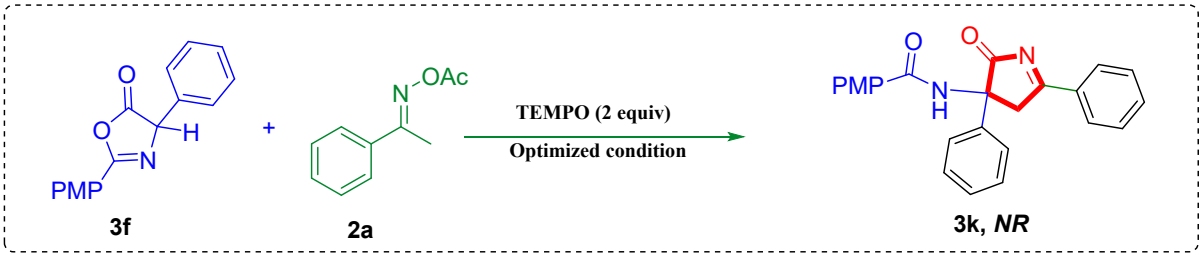
In an oven-dried flat-bottomed flask with a magnetic bar and condenser, 5 ml of chlorobenzene was used to dissolve 2-phenyloxazol-5(4*H*)-one (0.43 g, 1 equivalent)[64] and (*E*)-1-phenylethan-1-one O-acetyl oxime (0.44 g, 2.0 equivalent)[63]. Next, $FeCl_3$ (15.0 mol%), oxidant DTBP (3 equiv) and additive Cs_2CO_3 (1.7 equiv) were added. For 9 h, the charged flat-bottom flask was agitated at 110 ˚C in a N_2 environment. And progress of the reaction's was assessed by TLC using an ethyl acetate:hexane (3:4) eluent mixture. After the completion of reaction, the crude product was transferred to crushed ice and filtered. After that, 20 ml of ethyl acetate were used as a solvent to extract the reaction mixture. After being separated, the organic layer was dried over anhydrous $MgSO_4$ and concentrated at lower pressure. The crude product was further processed using column chromatography on silica gel (petroleum ether/ethyl acetate) in order to yield the desired product of 2, 5-diphenyl-6*H*-pyrrolo[3,2-*d*]oxazole **3a**. 2-(4-Methoxyphenyl)-4-phenyloxazol-5(4*H*)-one[54, 65] (0.47 g, 1 equivalent) and (*E*)-1-phenylethan-1-one O-acetyl oxime (0.44 g, 2.0 equivalent)[63] were reacted for 11 hours to produce 4-methoxy-N-(2-oxo-3, 5-diphenyl-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide **3k** using the same reaction procedure.

3. Radical trapping experiment by adding TEMPO

In an oven-dried flat-bottomed flask with a magnetic bar and condenser, 5 ml of chlorobenzene was used to dissolve 2-phenyloxazol-5(4*H*)-one (0.43 g, 1 equivalent)[64] **1a** and (*E*)-1-phenylethan-1-one O-acetyl oxime (0.44 g, 2.0 equivalent)[63] **2a.** Next, $FeCl_3$ (15.0 mol%), oxidant DTBP (3 equiv), TEMPO (2 equiv) and additive Cs_2CO_3 (1.7 equiv) were added. For 9 h, the charged flat-bottom flask was agitated at 110 ˚C in a N_2 environment. And progress of the reaction's was assessed by TLC using an ethyl acetate:hexane (3:4) eluent mixture. No desired product was observed.

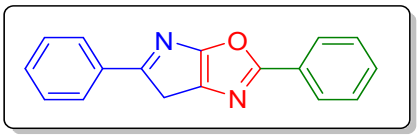


In order to yield the desired product of 4-methoxy-N-(2-oxo-3, 5-diphenyl-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide **3k**, 2-(4-Methoxyphenyl)-4-phenyloxazol-5(4*H*)-one[54, 65] (0.47 g, 1 equivalent) **1f** and (*E*)-1-phenylethan-1-one O-acetyl oxime (0.44 g, 2.0 equivalent)[63] **2a** in an oven-dried flat-bottomed flask with a magnetic bar and condenser, 5 ml of chlorobenzene, $FeCl_3$ (15.0 mol%), oxidant DTBP (3 equiv), TEMPO (2 equiv) and additive Cs_2CO_3 (1.7 equiv) were added were reacted for 11 hours using the same reaction procedure. No Desired product was produced.



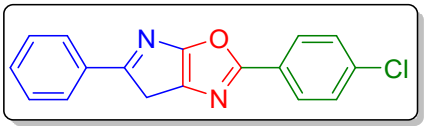
4. Characterization of products

1) 2, 5-Diphenyl-6*H*-pyrrolo[3,2-*d*]oxazole (3a).



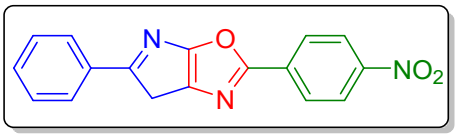
Yield: 74 %. Brown solid; mp: 135-137 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 7.75-7.78 (m, 4H), 7.33-7.44 (m, 6H), 2.93 (s, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 177.02, 172.13, 144.63, 137.16, 135.10, 131.82, 129.70, 129.00, 127.35, 126.30, 123.27, 122.83, 53.86. anal. calcd For $C_{17}H_{12}N_2O$: C, 78.44; H, 4.65; N, 10.76;. found: C, 78.53; H, 4.62; N, 10.81;. HRMS-ESI (*m/z*) calcd for $C_{17}H_{12}N_2O$ $[M + H]^+$ 261.065; found 260.059.

2) 2-(4-Chlorophenyl)-5-phenyl-6*H*-pyrrolo[3,2-*d*]oxazole (3b).



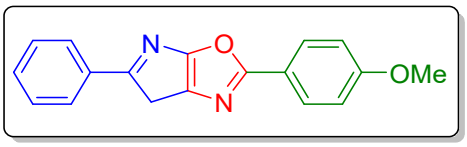
Yield: 75 %. Orange solid; mp: 140-142 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 8.03-8.05 (m, 2H), 7.58-7.59 (m, 2H), 7.24-7.35 (m, 5H), 2.95 (s, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 176.50, 172.65, 146.65, 134.10, 130.65, 130.10, 127.66, 126.00, 125.97, 125.54, 124.88, 122.11, 53.83. anal. calcd For $C_{17}H_{11}ClN_2O$: C: C, 69.28; H, 3.76; N, 9.50. found: C, 69.34; H, 3.79; N, 9.59. HRMS-ESI (*m/z*) calcd for $C_{17}H_{11}ClN_2O$ $[M + H]^+$ 294.7387, found 294.7380.

3) 2-(4-Nitrophenyl)-5-phenyl-6*H*-pyrrolo[3,2-*d*]oxazole (3c).



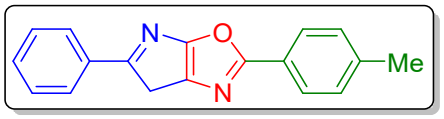
Yield: 77 %. Orange solid; mp: 141-143 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 8.17-8.18 (m, 2H), 7.61-7.62 (m, 2H), 7.23-7.31 (m, 5H), 3.02 (s, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 175.44, 171.55, 146.66, 134.71, 129.45, 126.62, 125.01, 123.58, 123.35, 123.32, 122.76, 122.23, 53.42. anal. calcd For $C_{17}H_{11}N_3O_3$: C, 66.88; H, 3.63; N, 13.76. found: C, 66.97; H, 3.67; N, 13.85. HRMS-ESI (*m/z*) calcd for $C_{17}H_{11}N_3O_3$ $[M + H]^+$ 305.2937, found 305.2930.

4) 2-(4-Methoxyphenyl)-5-phenyl-6*H*-pyrrolo[3,2-*d*]oxazole (3d).



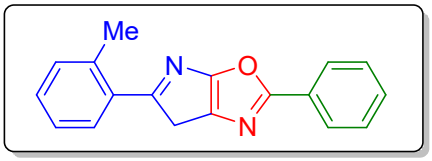
Yield: 65 %. Orange solid; mp: 144-146 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 7.97-7.98 (m, 2H), 7.22-7.38 (m, 5H), 7.06-7.08(m, 2H), 3.51(s, 3H) 2.97 (s, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 178.46, 170.68, 148.03, 135.83, 131.51, 127.87, 125.43, 124.28, 123.77, 123.05, 122.66, 122.34, 53.94, 31.21. anal. calcd For $C_{18}H_{14}N_2O_2$: C, 74.47; H, 4.86; N, 9.65. found: C, 74.52; H, 4.88; N, 9.71. HRMS-ESI (*m/z*) calcd for $C_{18}H_{14}N_2O_2$ $[M + H]^+$ 290.3232, found 290.3225.

5) 5-Phenyl-2-(p-tolyl)-6*H*-pyrrolo[3,2-*d*]oxazole (3e).



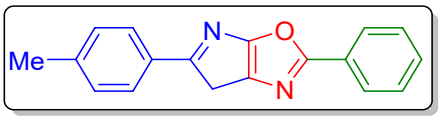
Yield: 69 %. Orange solid; mp: 134-136°C; ^{1}H NMR (400MHz, DMSO-d_6) δ ppm: δ 7.87 (m, 2H), 7.23-7.37 (m, 5H), 7.11-7.17 (m, 2H), 2.62 (s, 3H), 2.45 (s, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 177.05, 172.86, 144.78, 138.92, 138.72, 130.88, 128.44, 126.78, 126.75, 125.66, 125.43, 122.26, 56.21, 53.72. anal. calcd For $C_{18}H_{14}N_2O$: C, 78.81; H, 5.14; N, 10.21. found: C, 78.72; H, 5.17; N, 10.31. HRMS-ESI (*m/z*) calcd for $C_{18}H_{14}N_2O$ $[M + H]^+$ found 274.3241 found 274.3235.

6) 2-Phenyl-5-(o-tolyl)-6*H*-pyrrolo[3,2-*d*]oxazole (3f).



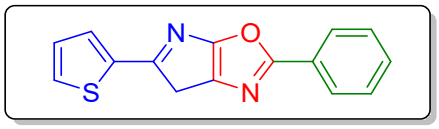
Yield: 63 %. Yellow solid; mp: 133-135°C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 7.82-7.83 (m, 2H), 7.24-7.47 (m, 5H), 6.72-6.75 (m, 2H), 2.82 (s, 2H), 2.64 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 178.21, 172.93, 147.76, 144.77, 140.73, 140.06, 135.51, 135.14, 130.28, 129.66,126.11, 125.57, 122.56, 119.96 54.04, 22.95. anal. calcd For $C_{18}H_{14}N_2O$: C, 78.81; H, 5.14; N, 10.21. found: C: C, 78.84; H, 5.12; N, 10.29. HRMS-ESI (*m/z*) calcd for $C_{18}H_{14}N_2O$ $[M + H]^+$ 274.3241, found 274.3233.

7) **2-Phenyl-5-(p-tolyl)-6*H*-pyrrolo[3,2-*d*]oxazole (3g).**



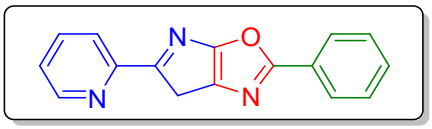
Yield: 61 %. Yellow semi solid; mp: 135-137 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 7.81-7.84 (m, 2H), 7.27-7.79 (m, 5H), 6.73-6.77 (m, 2H), 2.86 (s, 2H), 2.66 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 178.37, 173.00, 145.28, 139.07, 138.82, 133.94, 133.61, 130.56, 130.17, 127.60, 124.05, 122.66, 50.63, 26.31. anal. calcd For $C_{18}H_{14}N_2O$: C, 78.81; H, 5.14; N, 10.21. found: C, 78.72; H, 5.17; N, 10.28. HRMS-ESI (*m/z*) calcd for $C_{18}H_{14}N_2O$ $[M + H]^+$ 274.3241, found 274.3237.

8) **2-Phenyl-5-(thiophen-2-yl)-6*H*-pyrrolo[3,2-*d*]oxazole (3h).**



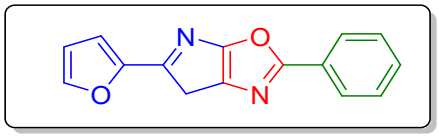
Yield: 70 %. Orange solid; mp: 125-127 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 8.04 (m, 2H), 7.32-7.41 (m, 5H), 7.21-7.23 (t, *J*=7.9Hz, 1H), 2.87 (s, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm:175.66, 171.74, 144.88, 144.53, 137.37, 137.17, 127.06, 124.39, 124.19, 123.60, 122.90,122.10, 48.70. anal. calcd For $C_{15}H_{10}N_2OS$: C, 67.65; H, 3.78; N, 10.52. found: C, 67.69; H, 3.81; N, 10.58. HRMS-ESI (*m/z*) calcd for $C_{15}H_{10}N_2OS$ $[M + H]^+$ 266.3194, found 266.3185.

9) **2-Phenyl-5-(pyridin-2-yl)-6*H*-pyrrolo[3,2-*d*]oxazole (3i)**



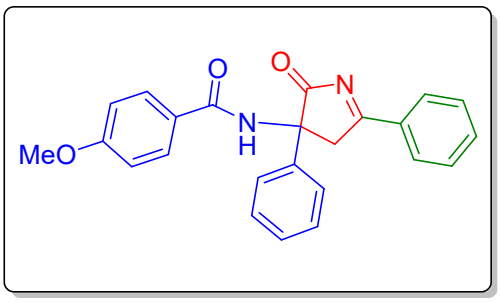
Yield: 66 %. Brown solid; mp: 130-132 °C; *^{1}H NMR* (400MHz, DMSO-d_6) δ ppm: δ 8.10 (m, 2H), 7.25-7.41 (m, 7H), 2.93 (s, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 177.21, 172.98, 148.81, 145.53, 134.81, 131.32, 127.65, 127.45, 127.25, 126.16,126.00, 122.10, 122.05, 53.25. anal. calcd For $C_{16}H_{11}N_3O$: C, 73.55; H, 4.24; N, 16.08;. found: C, 73.49; H, 4.26; N, 16.13;. HRMS-ESI (*m/z*) calcd for $C_{16}H_{11}N_3O$ $[M + H]^+$ 261.2853, found 261.2846.

10) 5-(Furan-2-yl)-2-phenyl-6*H*-pyrrolo[3,2-*d*]oxazole (3j).



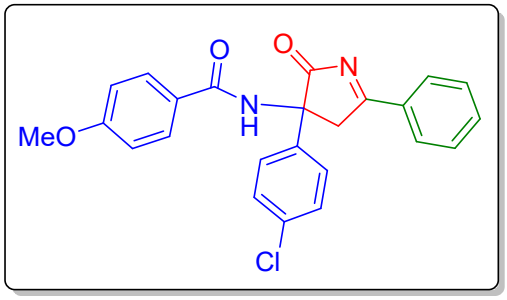
Yield: 68 %. Brown solid; mp: 115-117 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 7.92 (m, 2H), 7.29-7.45 (m, 5H), 7.21-7.23(t, *J*= 7.9Hz, 1H), 2.98 (s, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 177.14, 172.76, 145.73, 136.25, 127.50, 125.90, 125.52, 124.84, 124.64, 124.06, 123.35, 122.88, 50.21. anal. calcd For $C_{15}H_{10}N_2O_2$: C, 71.99; H, 4.03; N, 11.19. found: C, 72.06; H, 4.05; N, 11.08. HRMS-ESI (*m/z*) calcd for $C_{15}H_{10}N_2O_2$ $[M + H]^+$ 250.2580, found 250.2572.

11) 4-Methoxy-N-(2-oxo-3,5-diphenyl-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3k).



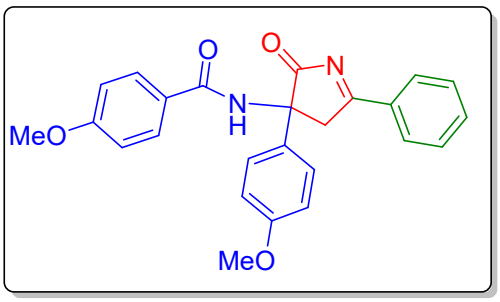
Yield: 71 %. Brown semi solid; mp: 121°C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 9.50 (s, 1H), 7.99 (m, 2H), 7.46-7.60 (m, 10H), 7.34 (m, 2H), 3.79 (s, 3H), 3.60-3.64 (d, *J*=16 Hz, 1H), 3.26-3.30 (d, *J*=16 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 177.10, 157.90, 157.21, 137.88, 135.81, 135.61, 131.68, 130.81, 129.54, 128.81, 127.96, 125.96, 125.03, 116.77, 112.27, 58.95, 53.45, 48.97. anal. calcd For $C_{24}H_{20}N_2O_3$: C, 74.98; H, 5.24; N, 7.29. found: C, 75.04; H, 5.27; N, 7.39. HRMS-ESI (*m/z*) calcd for $C_{24}H_{20}N_2O_3$ $[M + H]^+$ 384.1471; found 384.1466.

12) N-(3-(4-chlorophenyl)-2-oxo-5-phenyl-3,4-dihydro-2*H*-pyrrol-3-yl)-4-methoxybenzamide (3l).



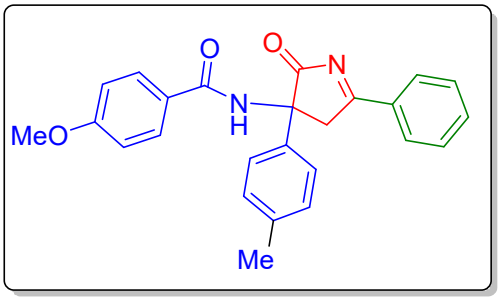
Yield: 73 %. Brown semi solid; mp: 129°C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 9.52 (s, 1H), 7.95 (s, 2H), 7.26-7.43 (m, 9 H), 7.15-7.16 (m, 2H), 3.96 (s, 3H), 3.67-3.70 (d, *J*=12 Hz, 1H), 3.45-3.48 (d, *J*=12 Hz, 1H).**^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 176.99, 158.90, 157.70, 143.85, 142.91, 138.79, 138.11, 134.66, 130.86, 130.00, 126.73, 126.12, 124.20, 116.87, 112.82, 57.62, 53.59, 49.13. anal. calcd For $C_{24}H_{19}ClN_2O_3$: C, 68.82; H, 4.57; N, 6.69;. found: C, 68.89; H, 4.58; N, 6.76;. HRMS-ESI (*m/z*) calcd for $C_{24}H_{19}ClN_2O_3$ $[M + H]^+$ 418.8781, found 418.8775.

13) 4-Methoxy-N-(3-(4-methoxyphenyl)-2-oxo-5-phenyl-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3m).



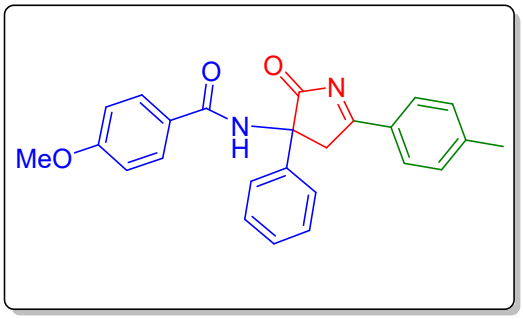
Yield: 67 %. Orange solid; mp: 120-122 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 9.41 (s, 1H), 7.72-7.74 (m, 2H), 7.57-7.59 (m, 2H), 7.38-7.49 (m, 9H), 3.69 (s, 6H), 3.49-3.52 (d, *J*=12 Hz, 1H), 3.22-3.25 (d, *J*=12 Hz, 1H).**^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 176.84, 158.25, 156.17, 149.01, 148.63,135.08, 134.69, 131.93, 131.11, 126.58, 126.17, 125.98, 125.78, 116.29, 112.82, 56.63, 53.83, 49.22. anal. calcd For $C_{25}H_{22}N_2O_4$: C, 72.45; H, 5.35; N, 6.76. found: C, 72.51; H, 5.34; N, 6.81 HRMS-ESI (*m/z*) calcd for $C_{25}H_{22}N_2O_4$ $[M + H]^+$ 414.4622, found 414.4615.

14) 4-Methoxy-N-(2-oxo-5-phenyl-3-(p-tolyl)-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3n).



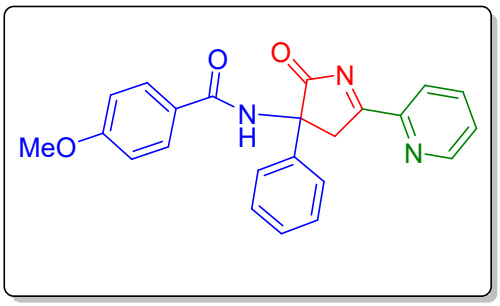
Yield: 63 %. Yellow solid; mp: 112°C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 9.57 (s, 1H), 7.62-7.92 (m, 6H), 7.54-7.56 (m, 2H), 7.36-7.47 (m, 4H), 7.16-7.18 (m, 1H) 3.75 (s, 3H), 3.59-3.62 (d, *J*=12 Hz, 1H), 3.38-3.41 (d, *J*=12 Hz, 1H), 2.22(s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 176.70, 157.27, 156.89, 149.27, 148.89, 133.80, 133.12, 128.99, 128.00, 127.88, 124.94, 124.90, 116.51, 113.35, 106.07, 57.33, 54.14, 49.46, 27.76. anal. calcd For $C_{25}H_{22}N_2O_3$: C, 75.36; H, 5.57; N, 7.03. found: C, 75.39; H, 5.56; N, 7.05. HRMS-ESI (*m/z*) calcd for $C_{25}H_{22}N_2O_3$ $[M + H]^+$ 398.4634, found 398.4623.

15) 4-Methoxy-N-(2-oxo-3-phenyl-5-(p-tolyl)-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3o).



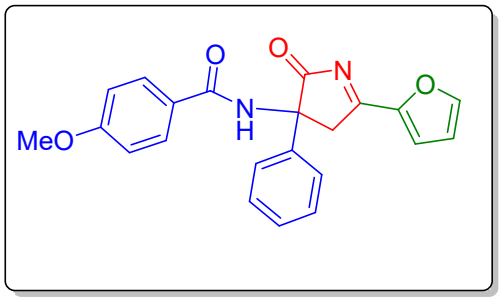
Yield: 60 %. Yellow solid; mp: 110-112 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 9.57 (s, 1H), 7.80-7.87 (m, 3H), 7.58-7.63 (m, 4H), 7.37-7.47 (m, 6H), 3.84 (s, 3H), 3.60-3.63 (d, *J*=12 Hz, 1H), 3.38-3.41 (d, *J*=12 Hz, 1H), 2.30(s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 177.07, 158.49, 157.24, 150.51, 149.95, 134.10, 129.15, 129.00, 128.49, 127.88, 124.90, 115.15, 113.35, 107.31, 58.34, 53.13, 50.40. 28.86 anal. calcd For $C_{25}H_{22}N_2O_3$: C, 75.36; H, 5.57; N, 7.03. found: C, 75.44; H, 5.58; N, 7.11. HRMS-ESI (*m/z*) calcd for $C_{25}H_{22}N_2O_3$ $[M + H]^+$ 398.4634, found 398.4625.

16) 4-Methoxy-N-(2-oxo-3-phenyl-5-(pyridin-2-yl)-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3p).



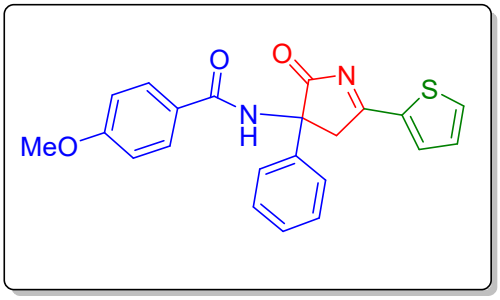
Yield: 65 %. Yellow solid; mp: 117-119 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 9.50 (s, 1H), 7.84-7.93(m, 2H), 7.57-7.60 (t, *J*=12Hz, 1H), 7.45-7.46(m, 2H), 7.28-7.31 (m, 5H), 7.20-7.21 (m, 2H), 7.05-7.07(t, *J*= 8 Hz, 1H) 4.12-4.15 (d, *J*= 12 Hz, 1H), 3.95 (s, 3H), 3.80-3.83 (d, *J*=12 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 176.02, 160.01, 158.91, 140.49, 138.99, 135.03, 134.98, 133.68, 131.82, 131.16, 127.70, 127.35, 123.27, 122.83, 116.61, 112.79, 58.69, 53.66, 50.06. anal. calcd For $C_{23}H_{19}N_3O_3$: C, 71.68; H, 4.97; N, 10.90. found: C, 71.62; H, 4.96; N, 10.99. HRMS-ESI (*m/z*) calcd for $C_{23}H_{19}N_3O_3$ $[M + H]^+$ 386.1428, found 386.1419.

17) N-(5-(furan-2-yl)-2-oxo-3-phenyl-3,4-dihydro-2*H*-pyrrol-3-yl)-4-methoxybenzamide (3q).



Yield: 69 %. Yellow solid; mp: 103-105°C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 9.94 (s, 1H), 7.42-7.46 (m, 2H), 7.26-7.27 (m, 2H), 7.09-7.13 (m, 7H), 7.05-7.06 (m, 1H) 6.58-6.61 (t, *J*=12 Hz 1H), 4.11-4.14 (d, *J*=12 Hz, 1H), 3.90 (s, 3H), 3.76-3.79 (d, *J*=12 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 177.25, 159.27, 157.80, 151.14, 149.34, 147.07, 138.79, 130.04, 129.15, 128.49, 127.50, 127.40, 126.79, 117.16, 113.34, 57.69, 53.74, 49.69 anal. calcd For $C_{22}H_{18}N_2O_4$: C, 67.68; H, 4.65; N, 7.17. found: C, 67.76; H, 4.66; N, 7.21. HRMS-ESI (*m/z*) calcd for $C_{22}H_{18}N_2O_4$ $[M + H]^+$ 374.3973, found 374.3962.

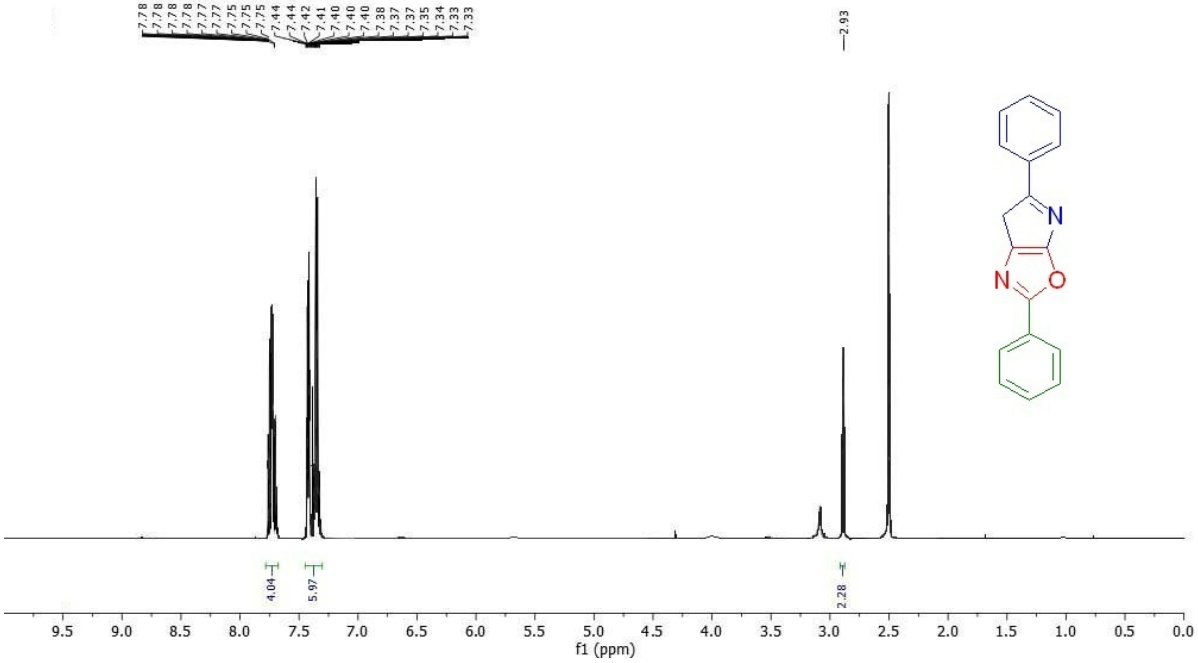
18)) 4-Methoxy-N-(2-oxo-3-phenyl-5-(thiophen-2-yl)-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3r).

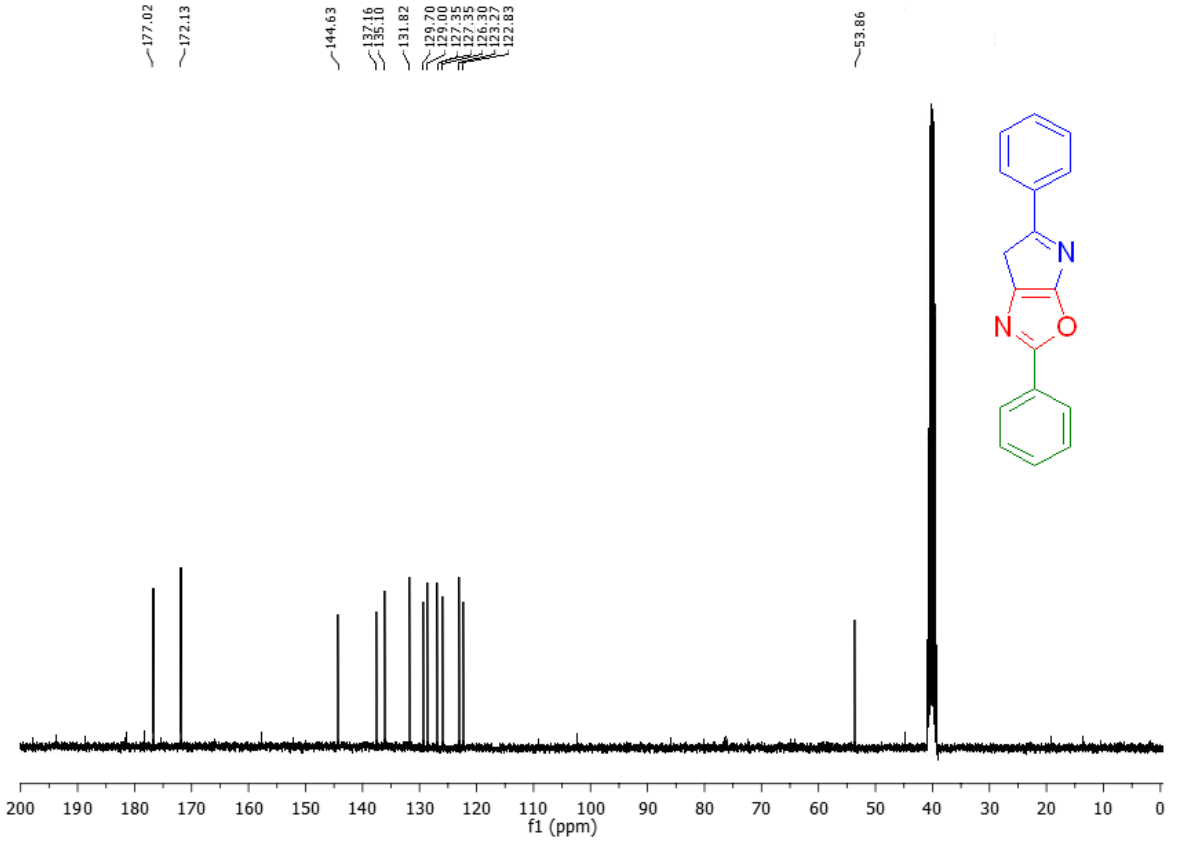


Yield: 67 %. Yellow solid; mp: 111 °C; **^{1}H NMR** (400MHz, DMSO-d_6) δ ppm: δ 9.46 (s, 1H), 7.49-7.54 (m, 3H), 7.17-7.32(m, 8H), 6.88-6.90 (t, *J*=7.9Hz, 1H), 3.76 (s, 3H), 3.66-3.69 (d, *J*=12 Hz, 1H), 3.42-3.45 (d, *J*=12 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 176.89, 160.43, 159.06, 150.19, 149.06, 147.00, 138.99, 130.04, 129.15, 128.49, 127.50, 126.79, 123.47, 117.00, 112.60, 58.14, 54.85, 50.32 anal. calcd For $C_{22}H_{18}N_2O_3S$ C, 70.58; H, 4.85; N, 7.48. found: C, 70.61; H, 4.84; N, 7.46. HRMS-ESI (*m/z*) calcd for $C_{22}H_{18}N_2O_3S$ $[M + H]^+$ 390.4572, found 390.4565.

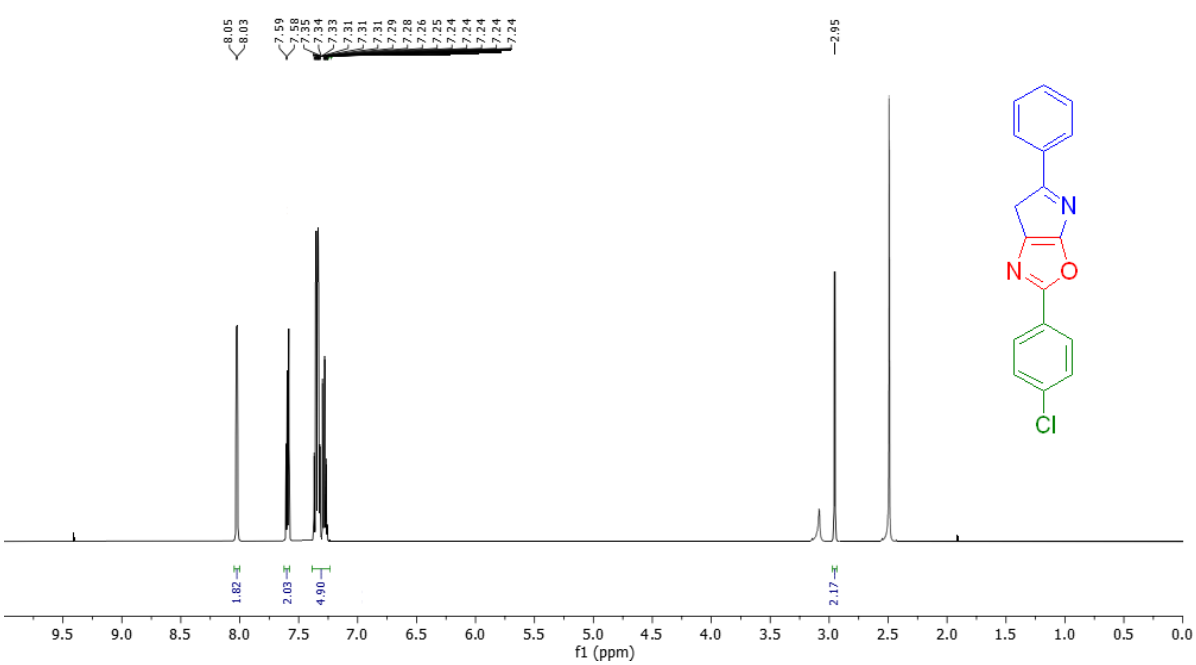
5. Spectra of ^{1}H NMR and ^{13}C NMR

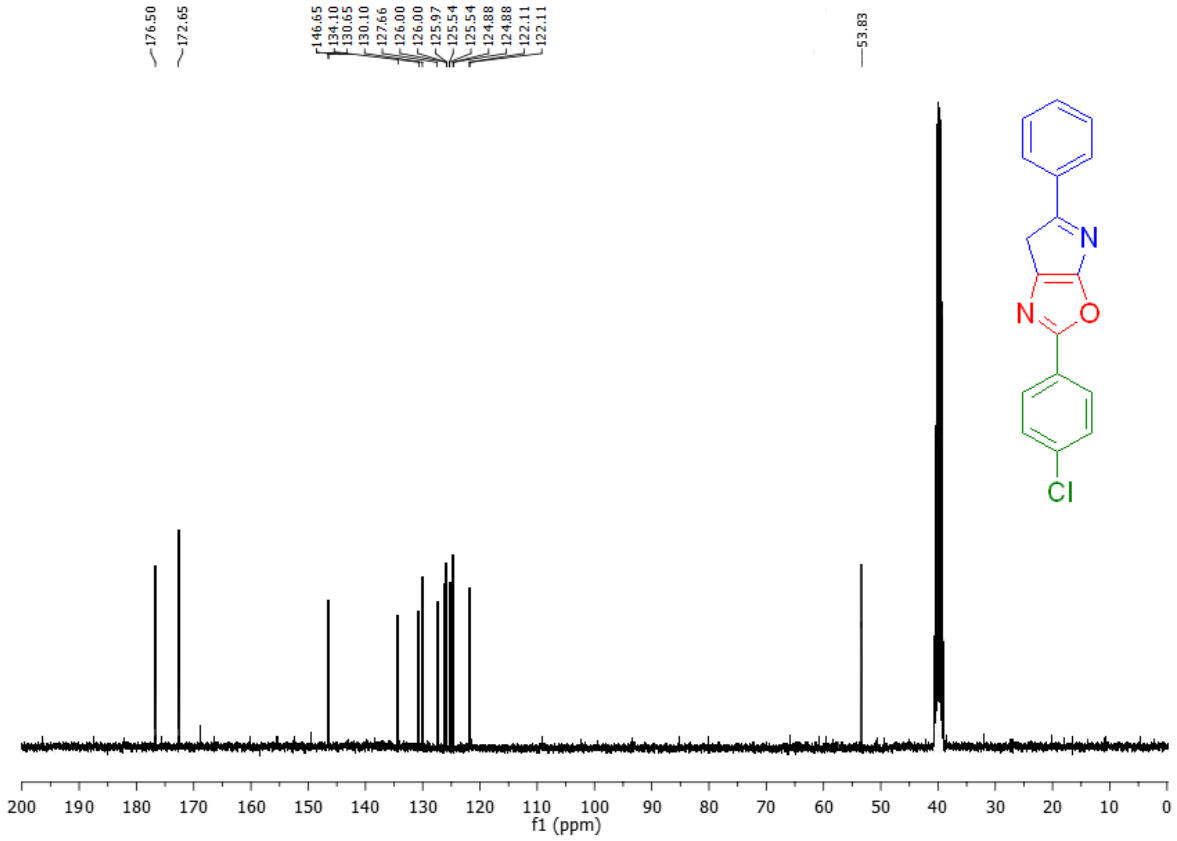
1) 2, 5-Diphenyl-6*H*-pyrrolo[3,2-*d*]oxazole (3a).



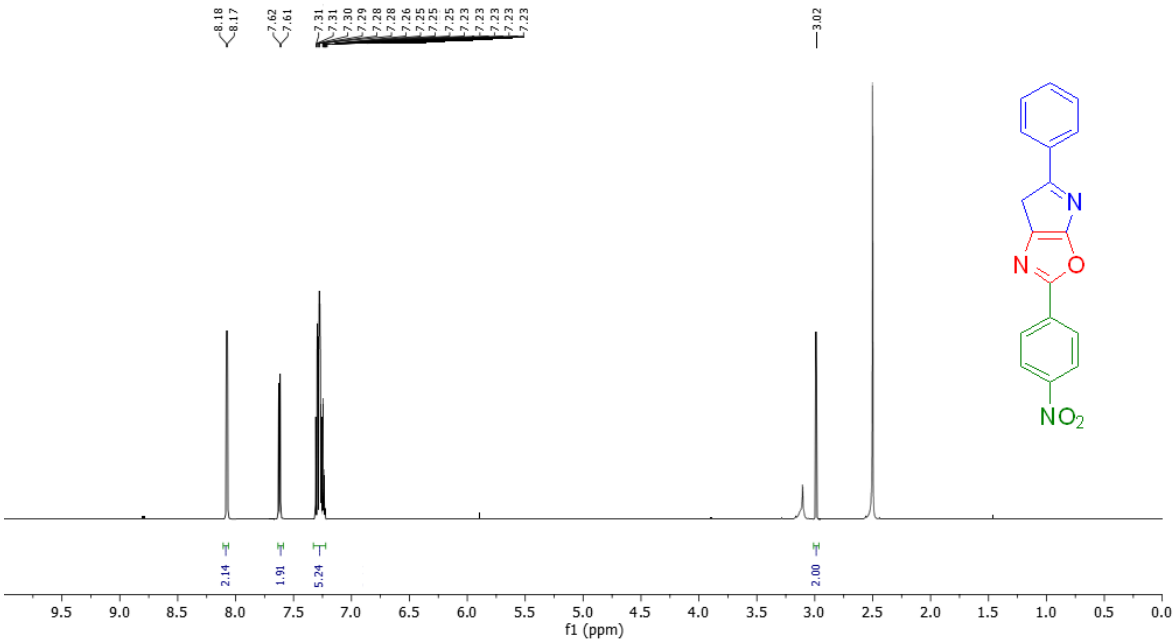


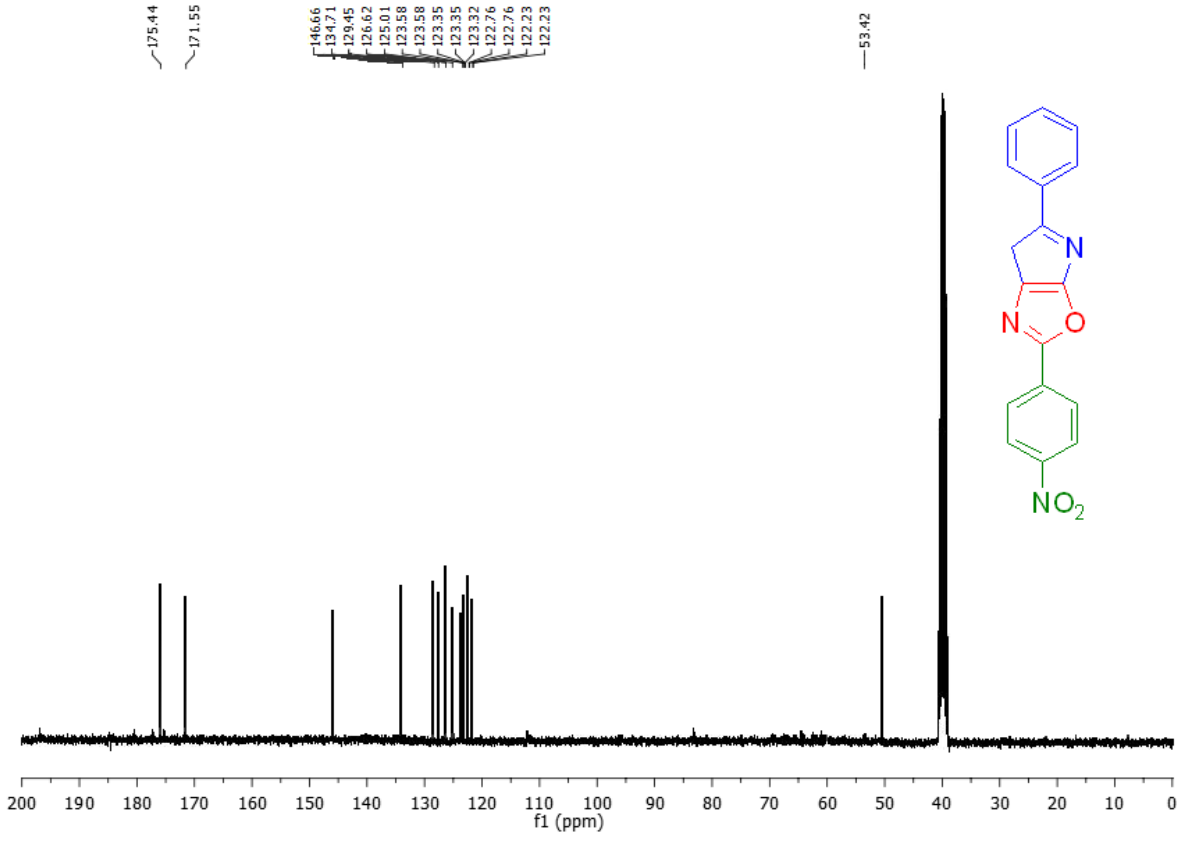
2) 2-(4-Chlorophenyl)-5-phenyl-6*H*-pyrrolo[3,2-*d*]oxazole (3b).



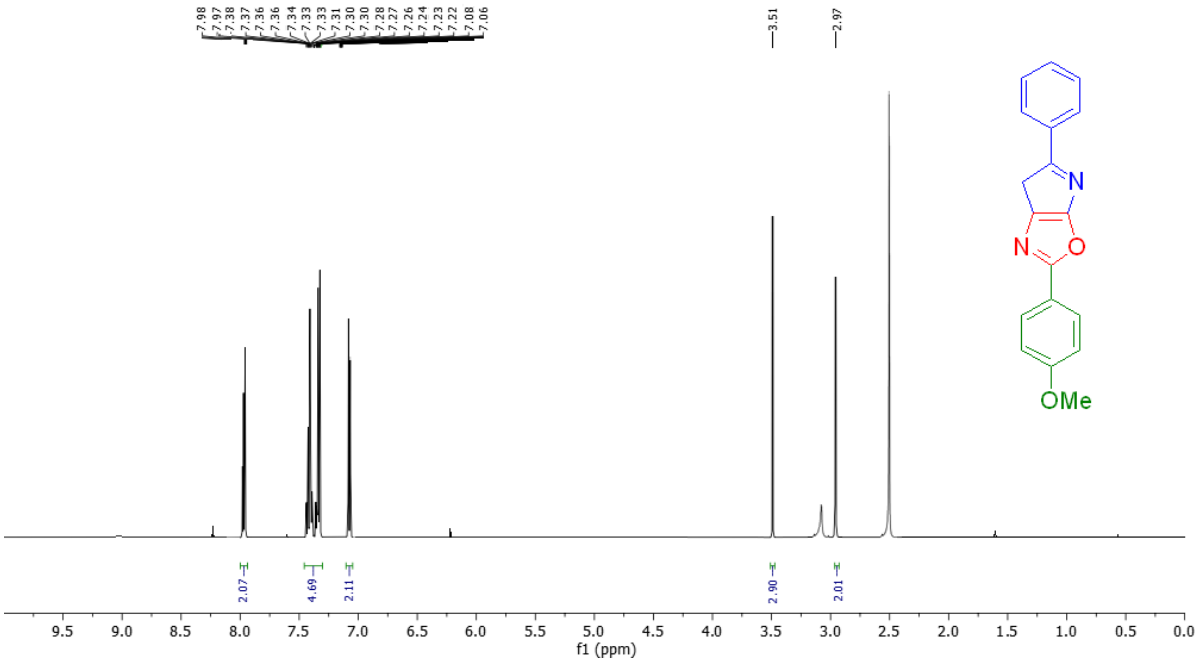


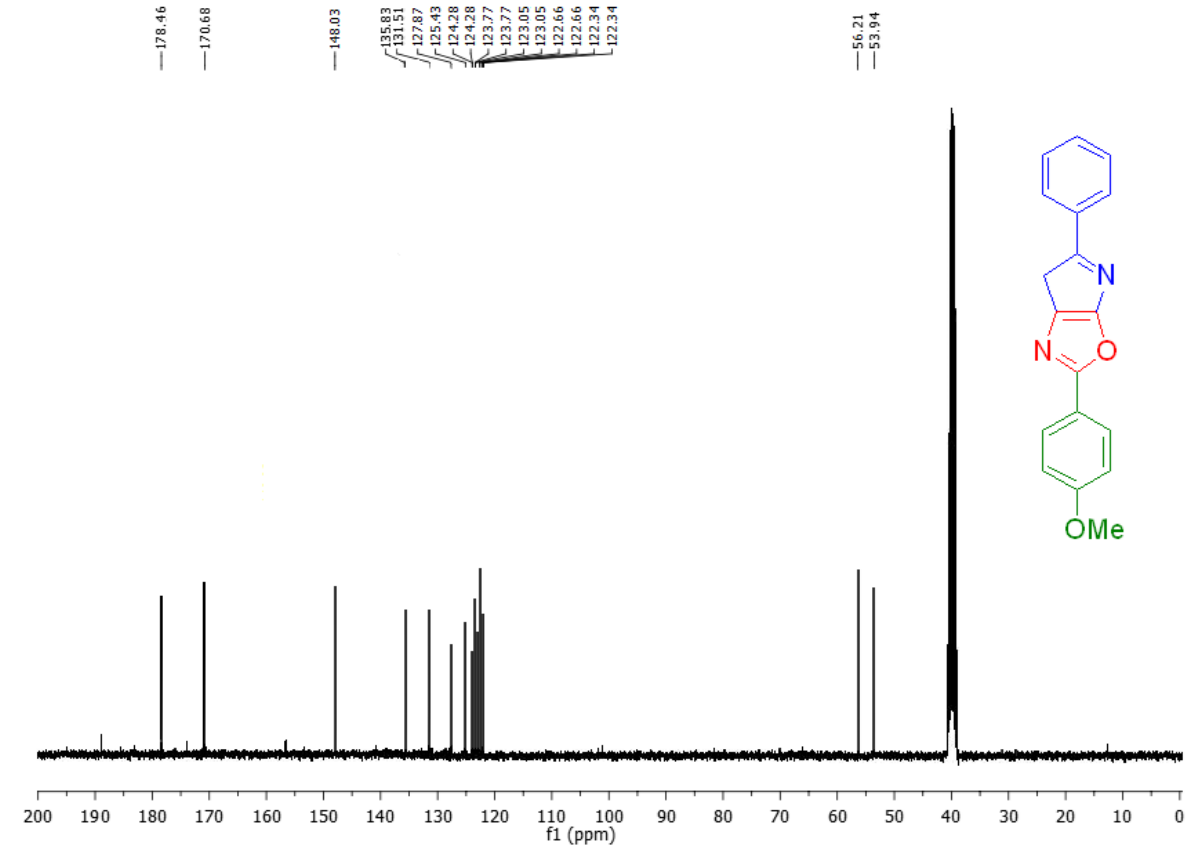
3) 2-(4-Nitrophenyl)-5-phenyl-6*H*-pyrrolo[3,2-*d*]oxazole (3c).



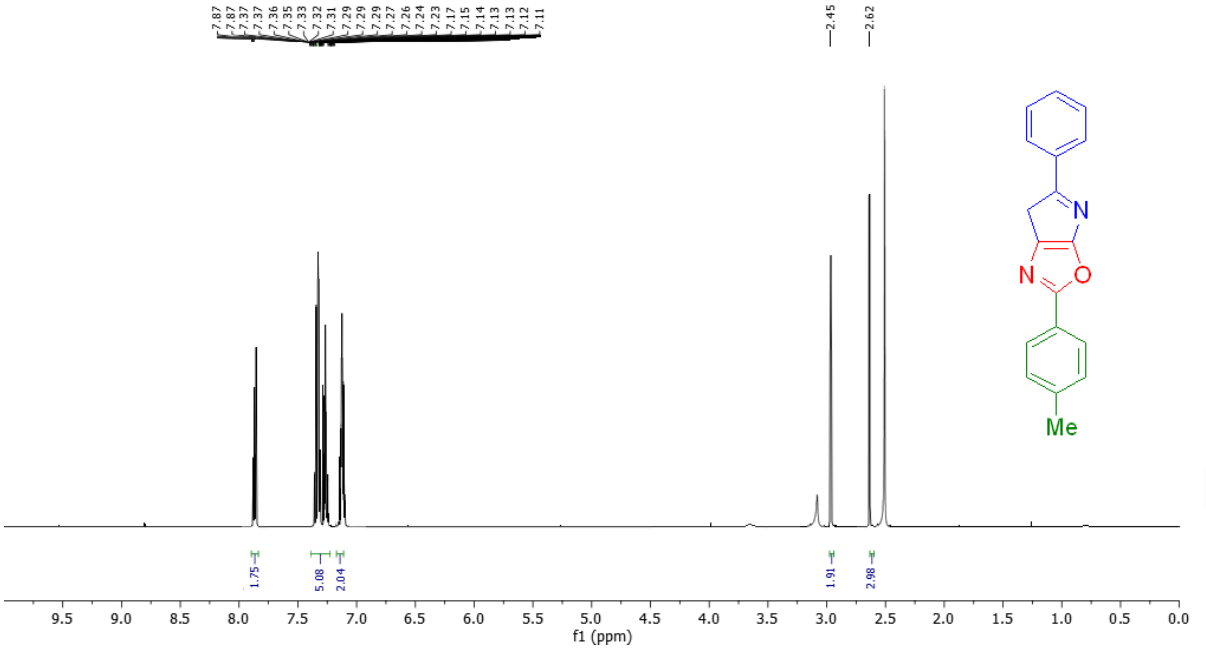


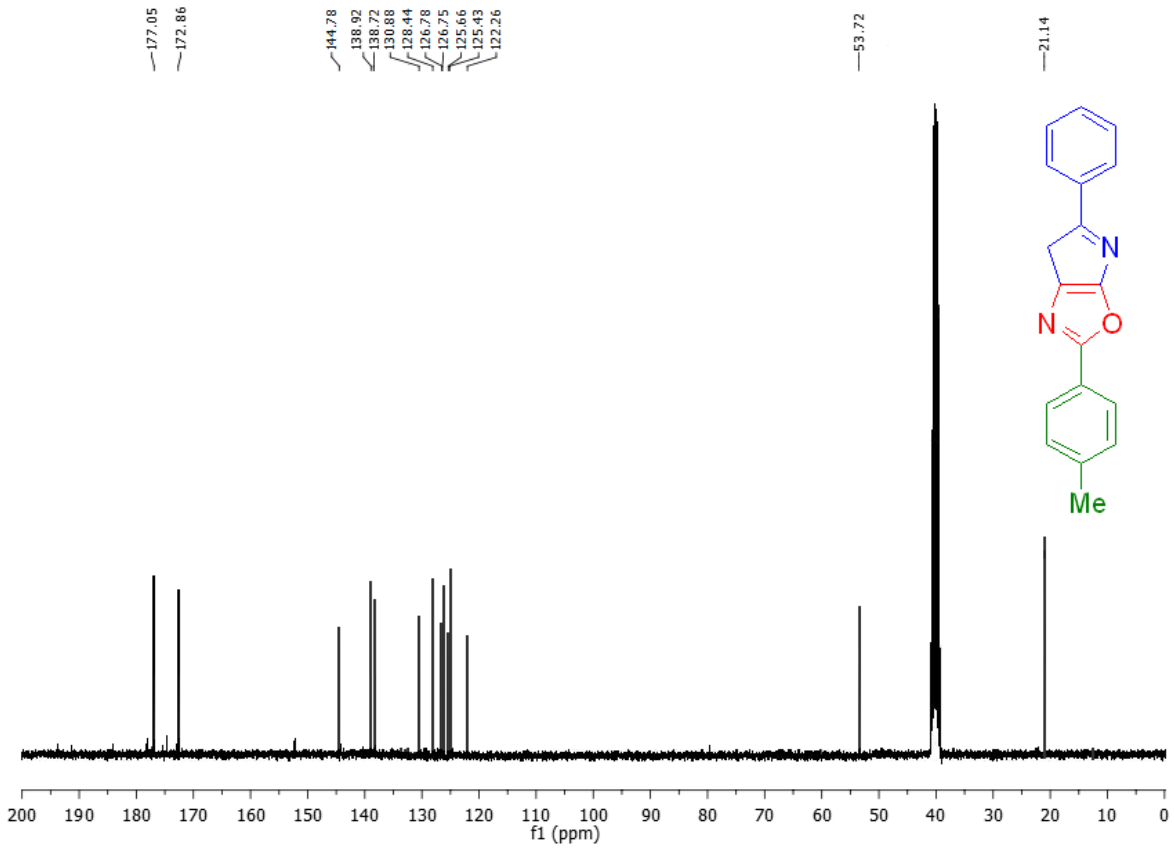
4) 2-(4-Methoxyphenyl)-5-phenyl-6*H*-pyrrolo[3,2-*d*]oxazole (3d).



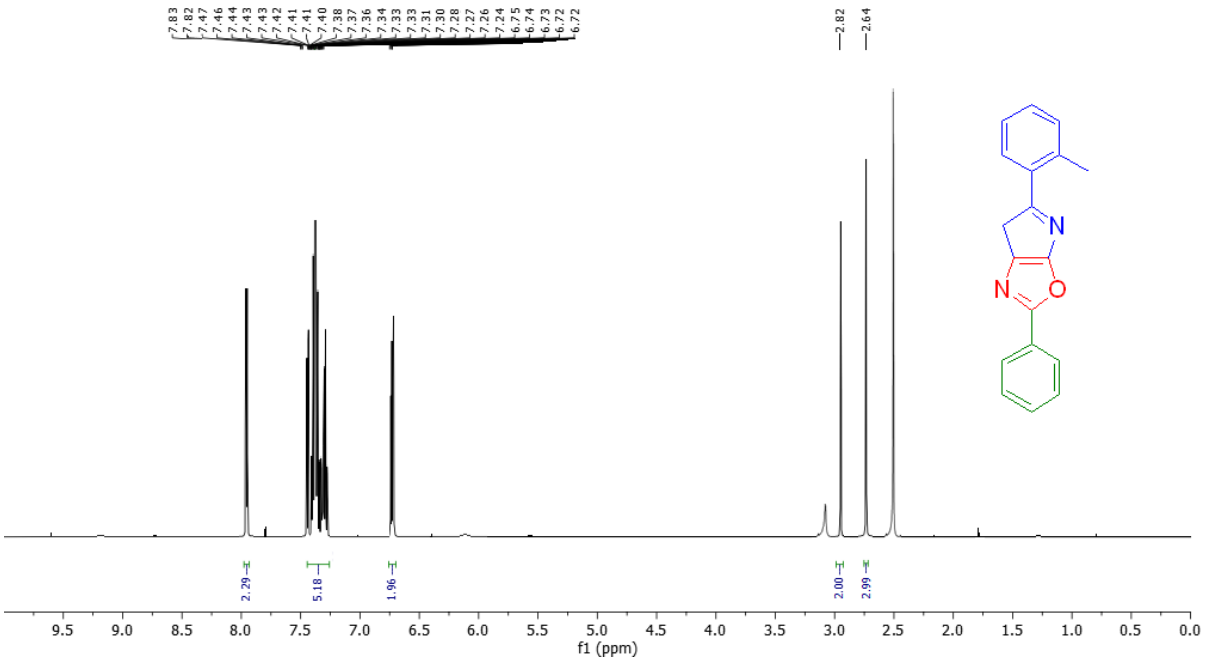


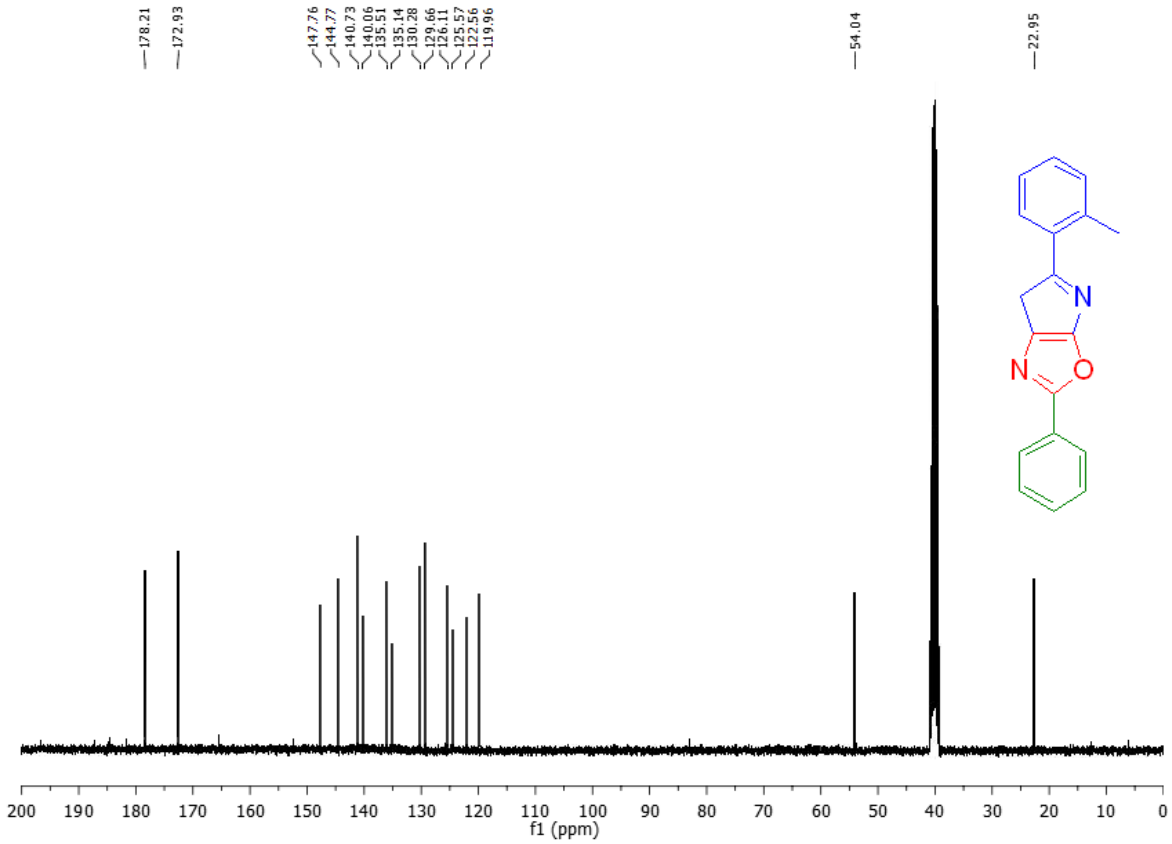
5) 5-Phenyl-2-(p-tolyl)-6*H*-pyrrolo[3,2-*d*]oxazole (3e).



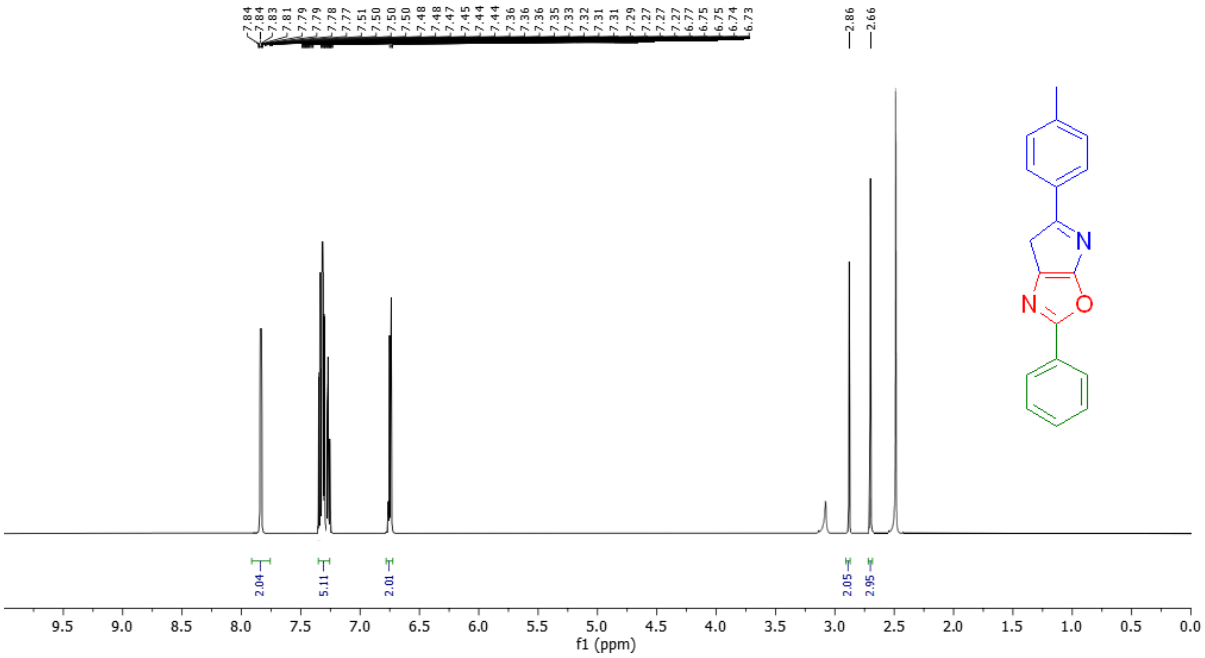


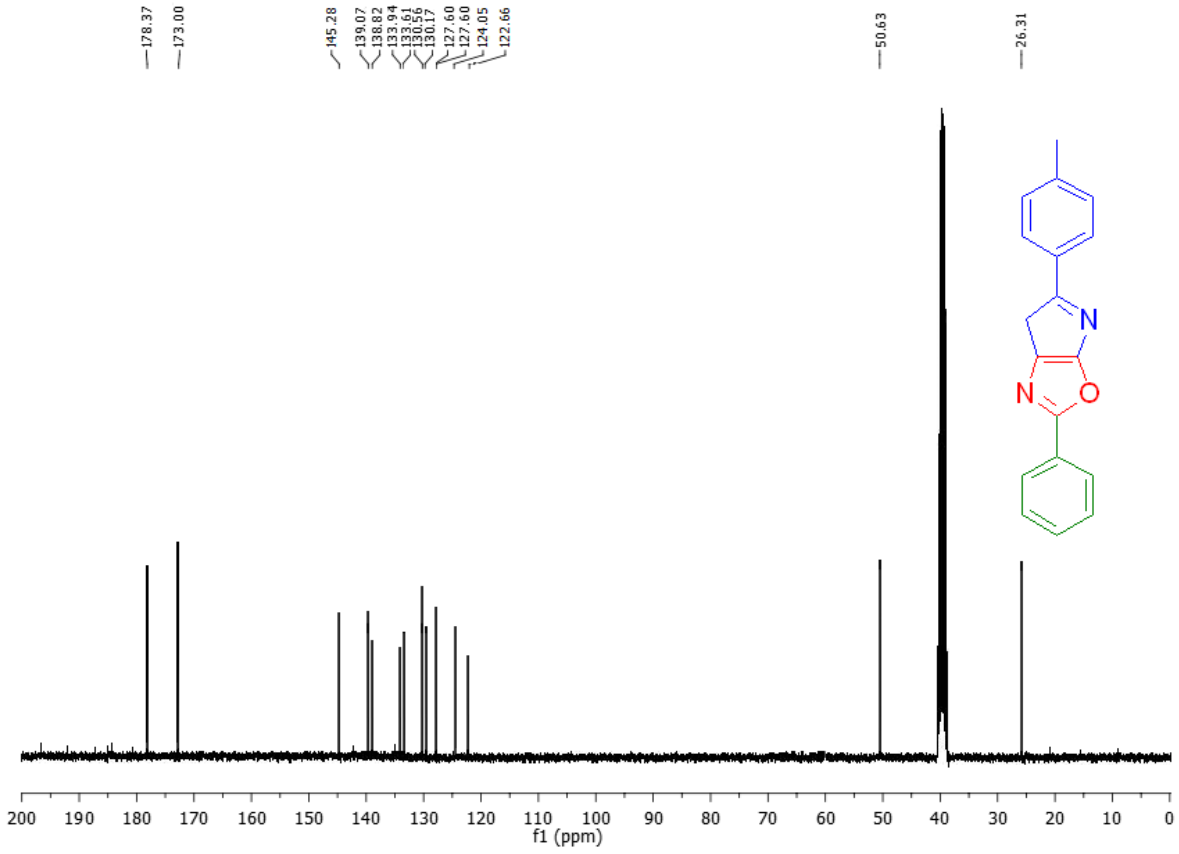
6) 2-Phenyl-5-(o-tolyl)-6*H*-pyrrolo[3,2-*d*]oxazole (3f).



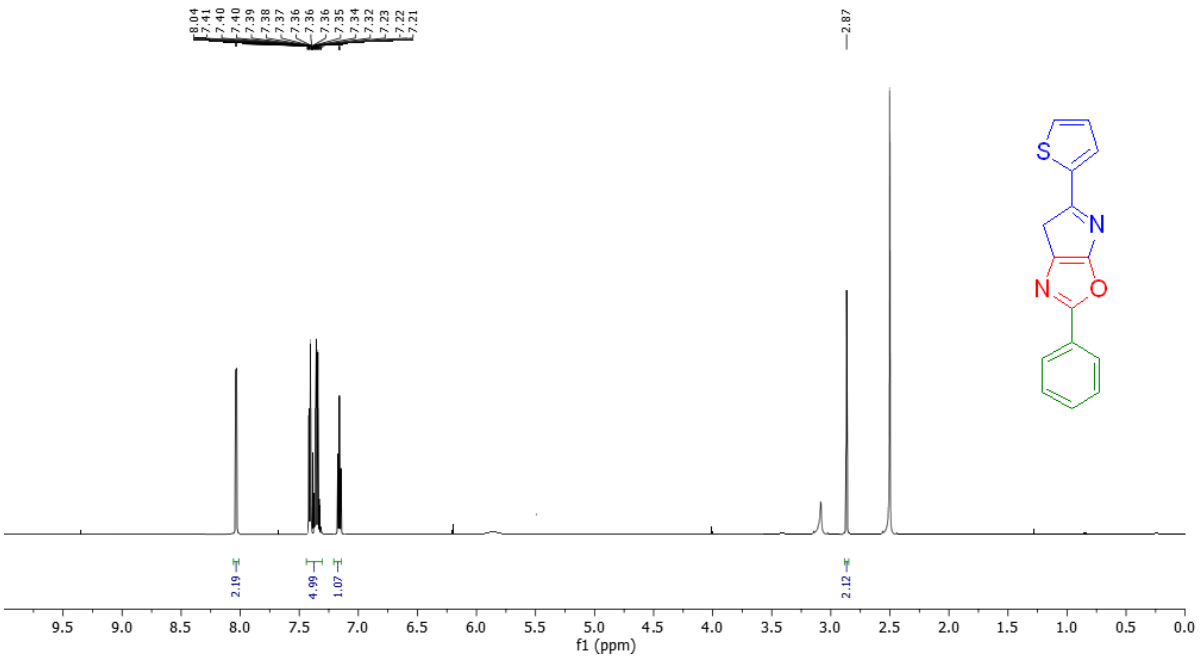


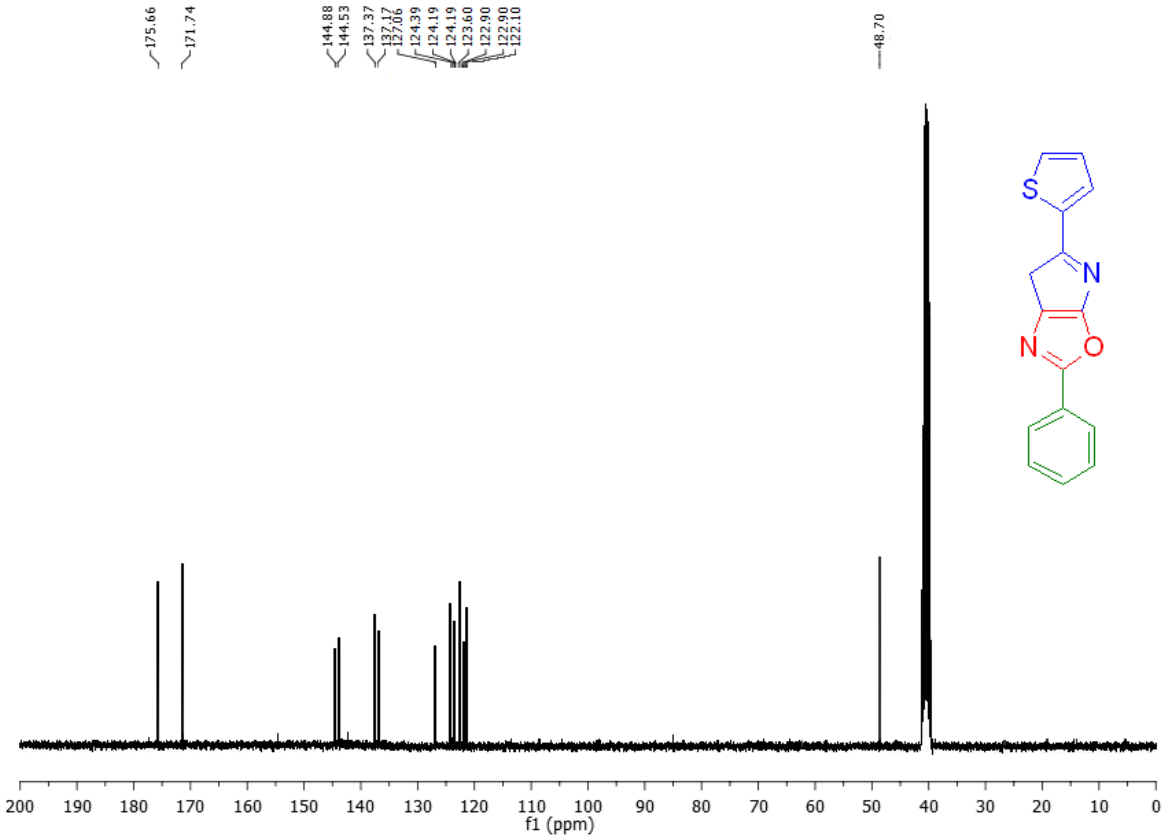
7) 2-Phenyl-5-(p-tolyl)-6*H*-pyrrolo[3,2-*d*]oxazole (3g).





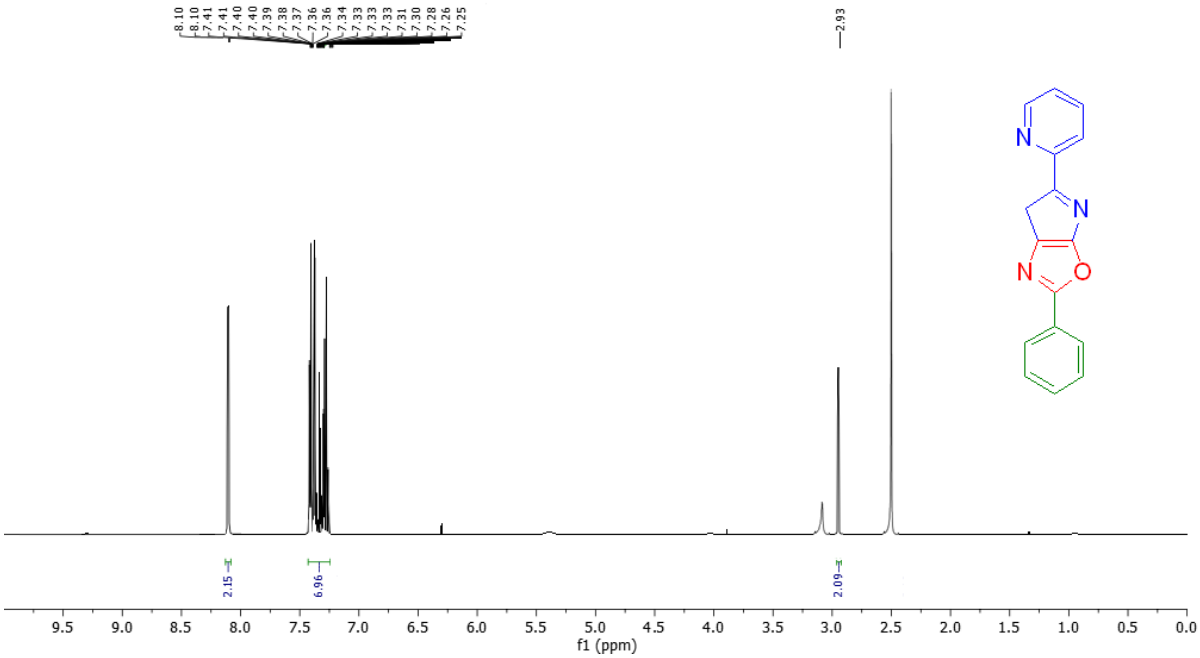
8) 2-Phenyl-5-(thiophen-2-yl)-6*H*-pyrrolo[3,2-*d*]oxazole (3h).

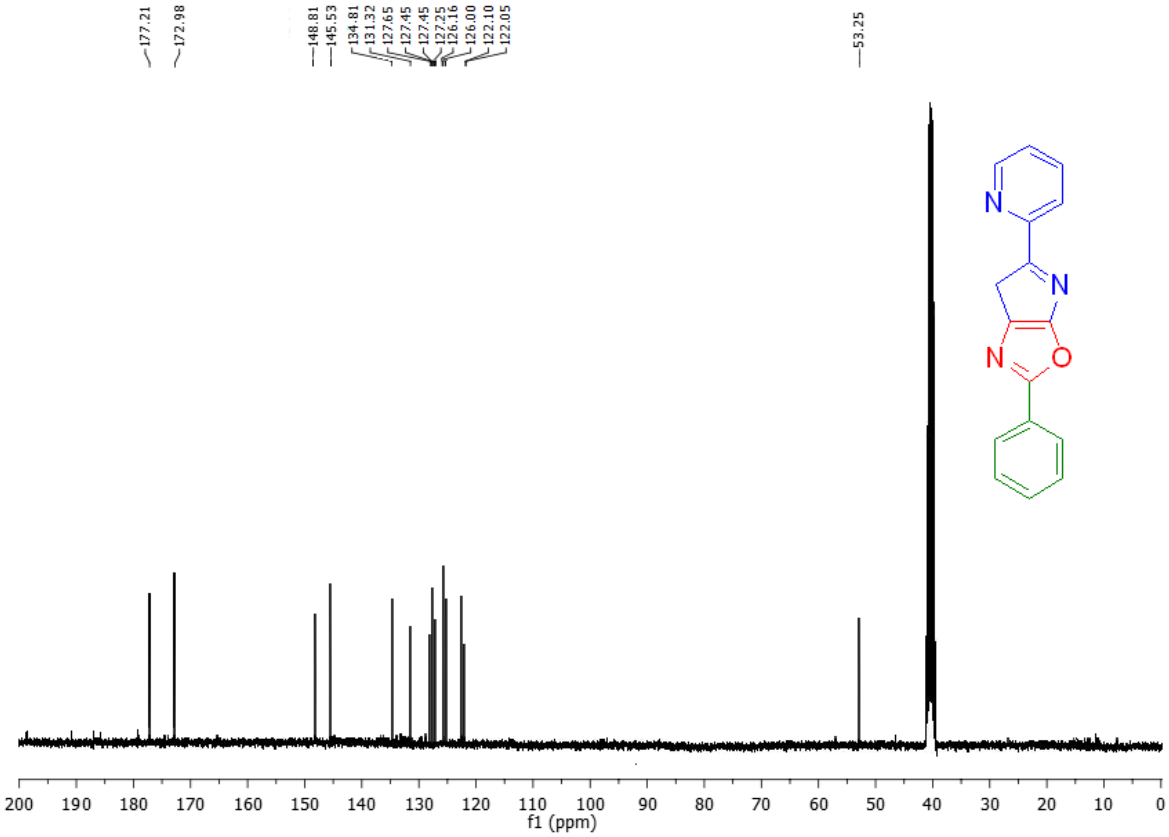




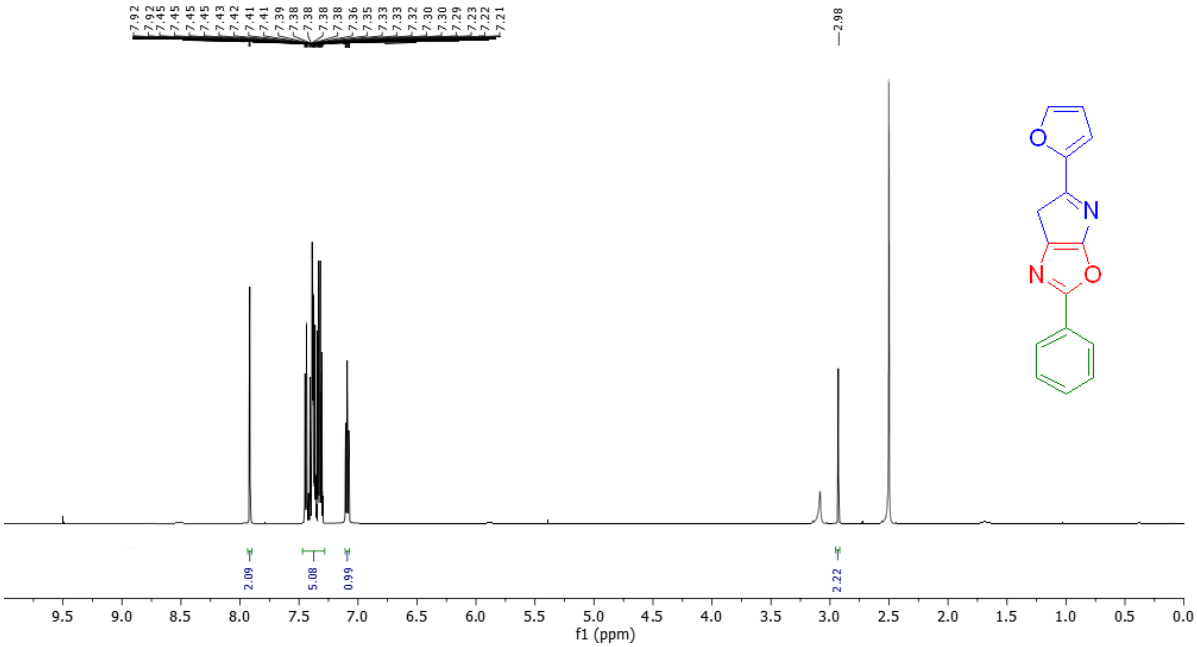
9) 2-Phenyl-5-(pyridin-2-yl)-6*H*-pyrrolo[3,2-*d*]oxazole (3i)

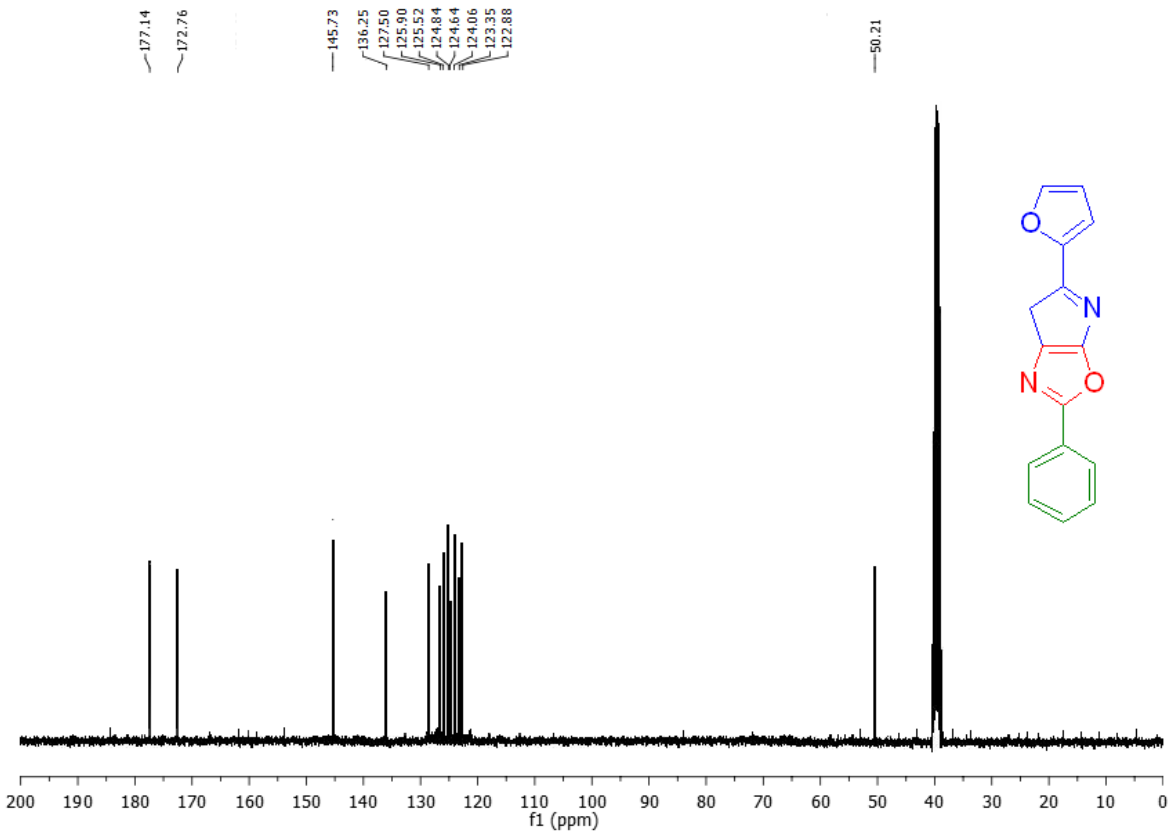
.



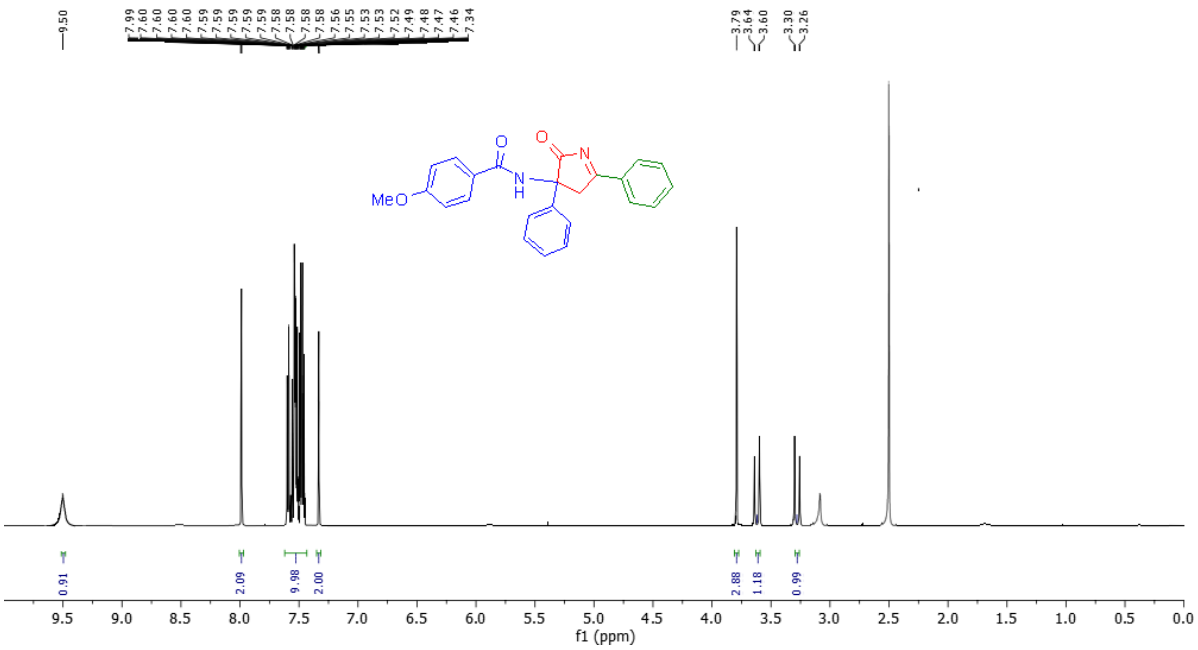


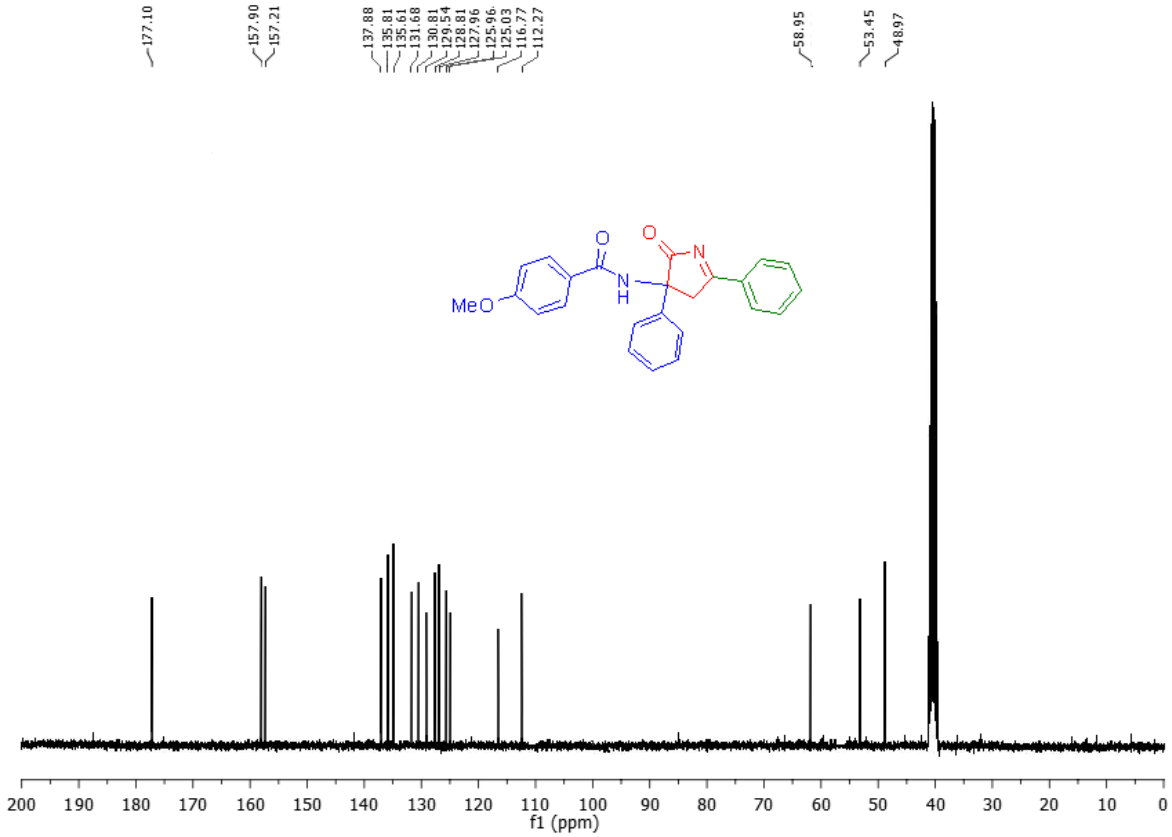
10) 5-(Furan-2-yl)-2-phenyl-6*H*-pyrrolo[3,2-*d*]oxazole (3j).



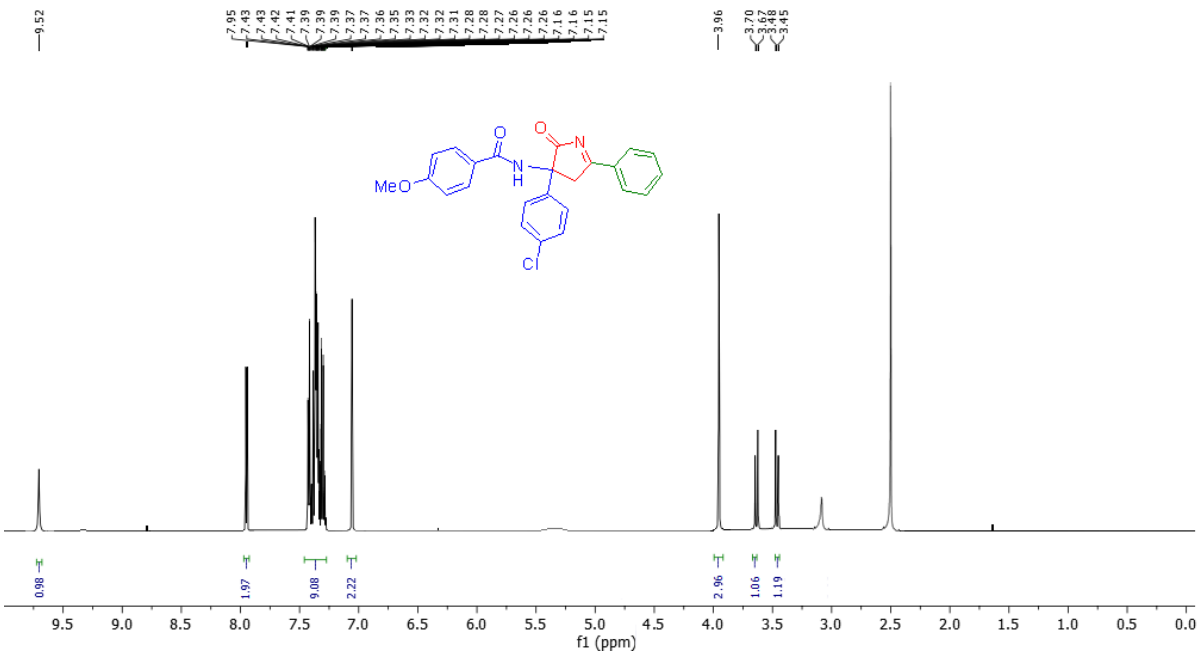


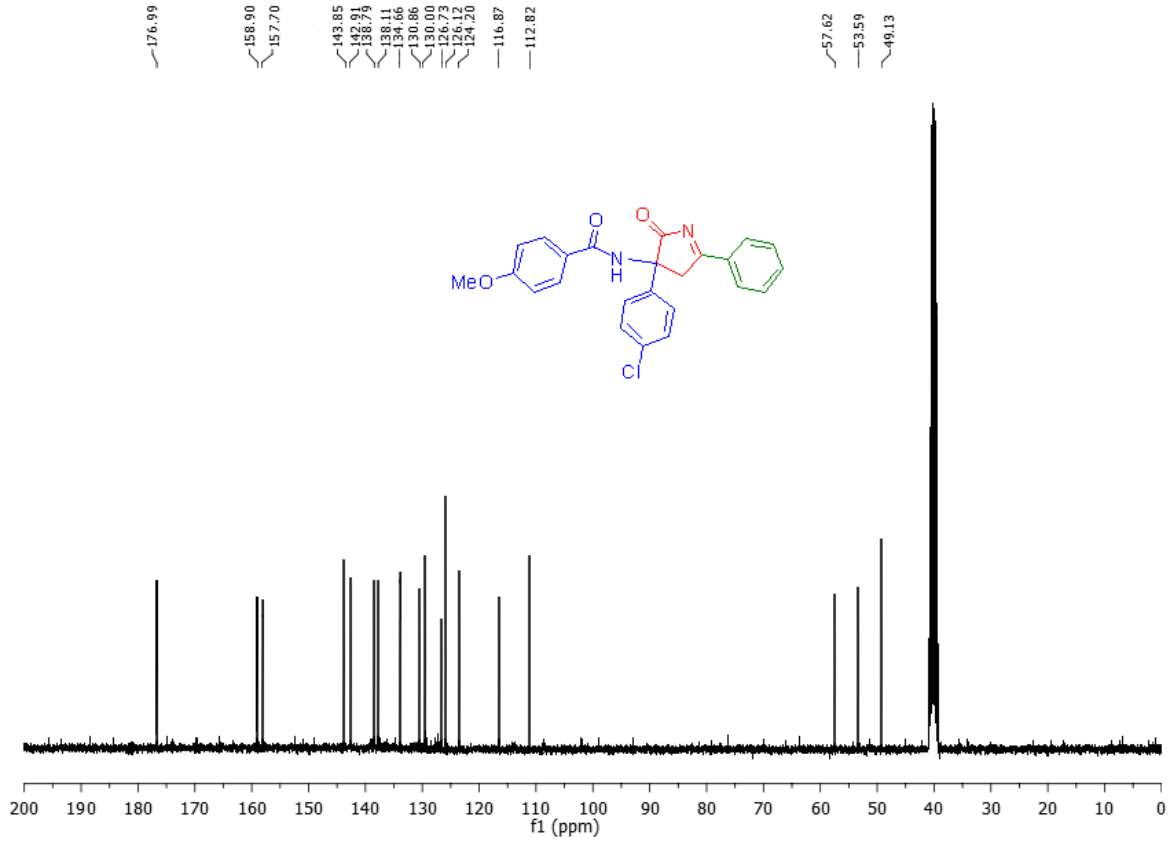
11) 4-Methoxy-N-(2-oxo-3,5-diphenyl-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3k).



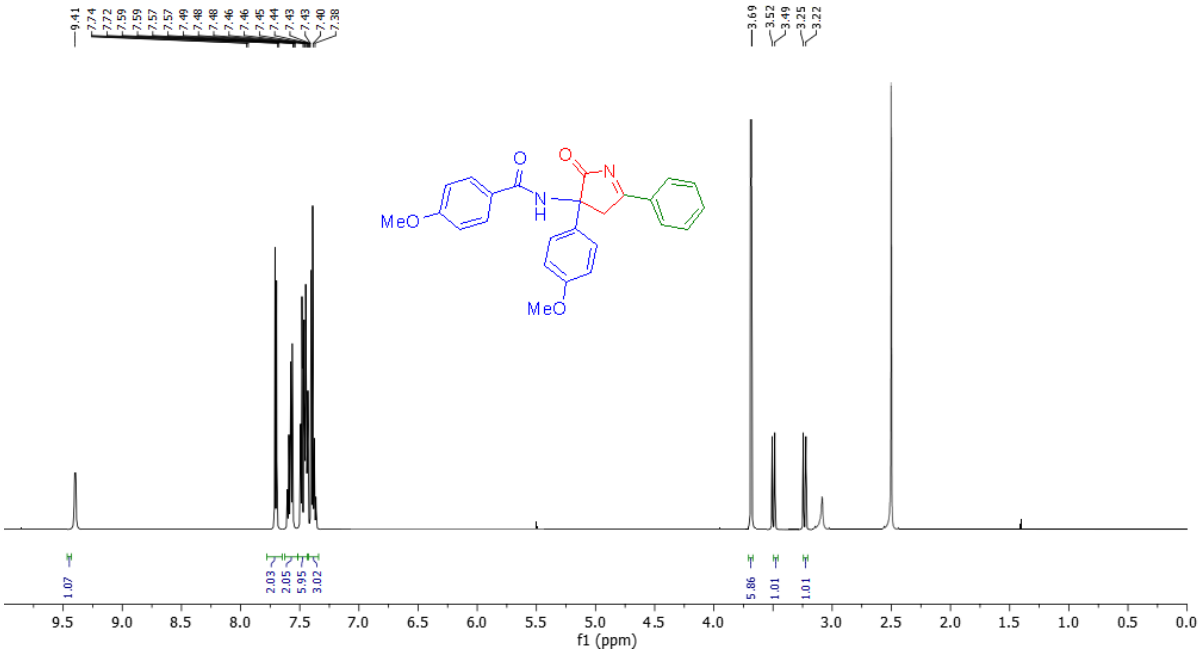


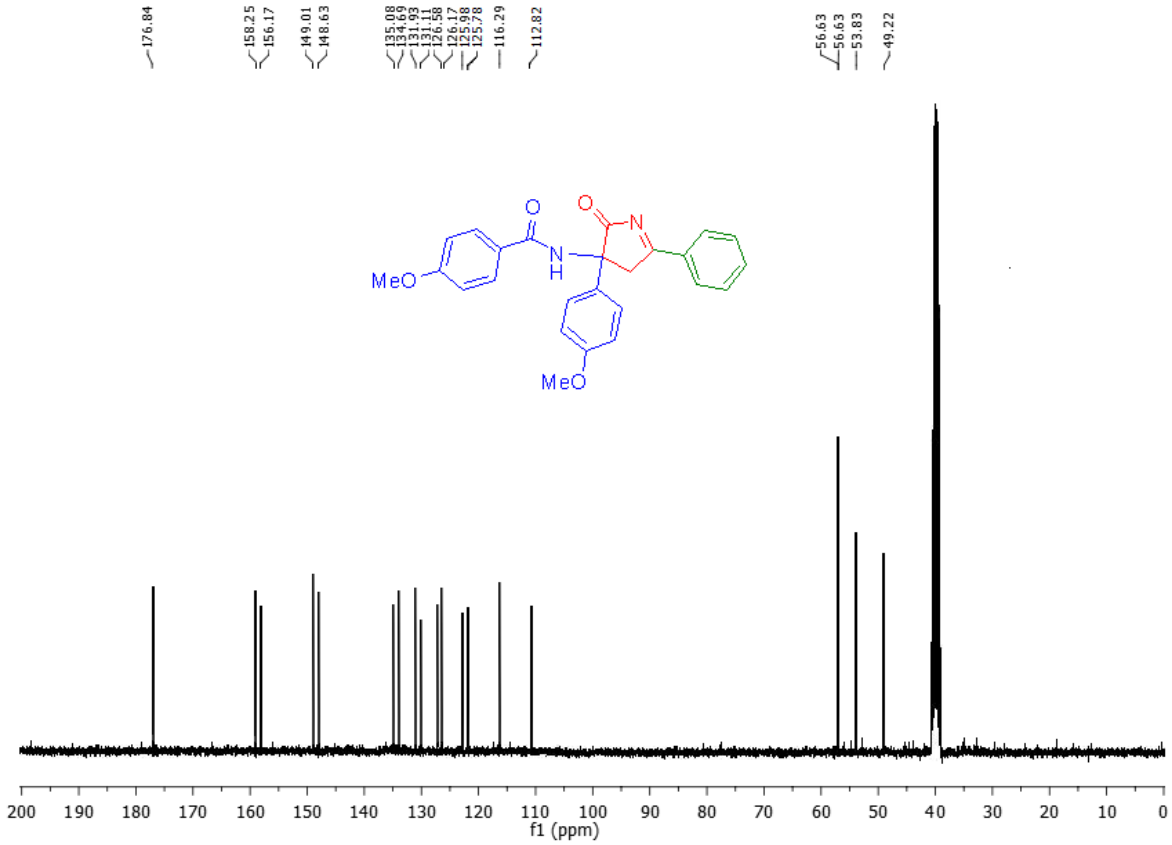
12) N-(3-(4-chlorophenyl)-2-oxo-5-phenyl-3,4-dihydro-2*H*-pyrrol-3-yl)-4-methoxybenzamide (3l).



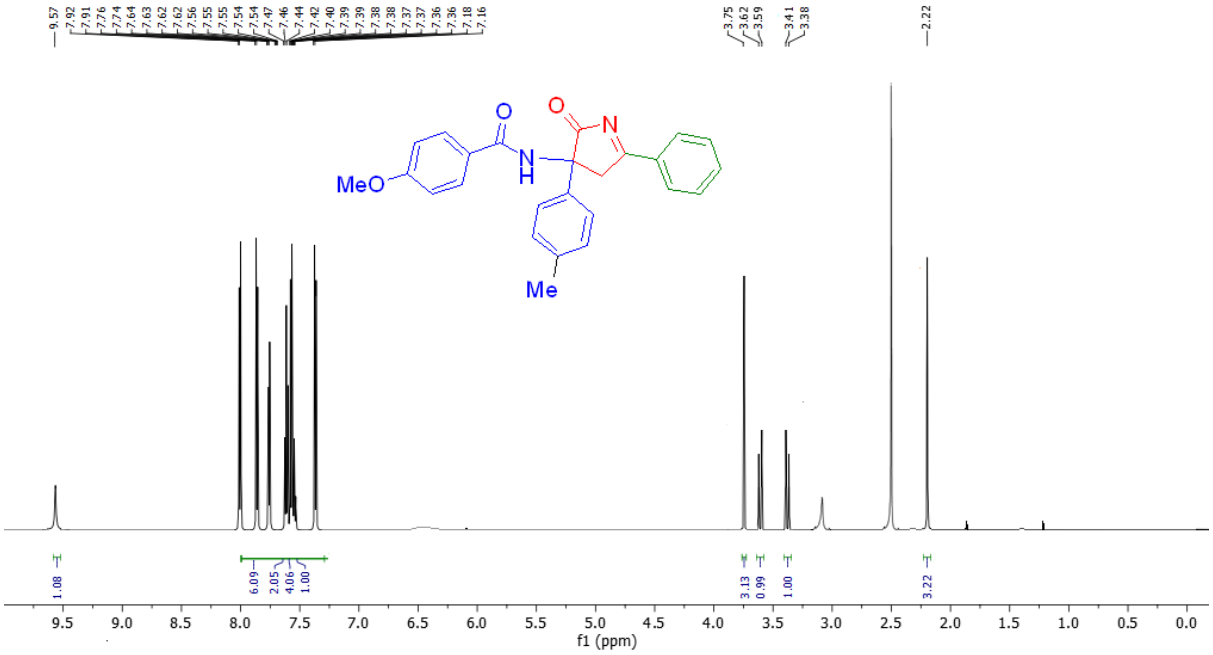


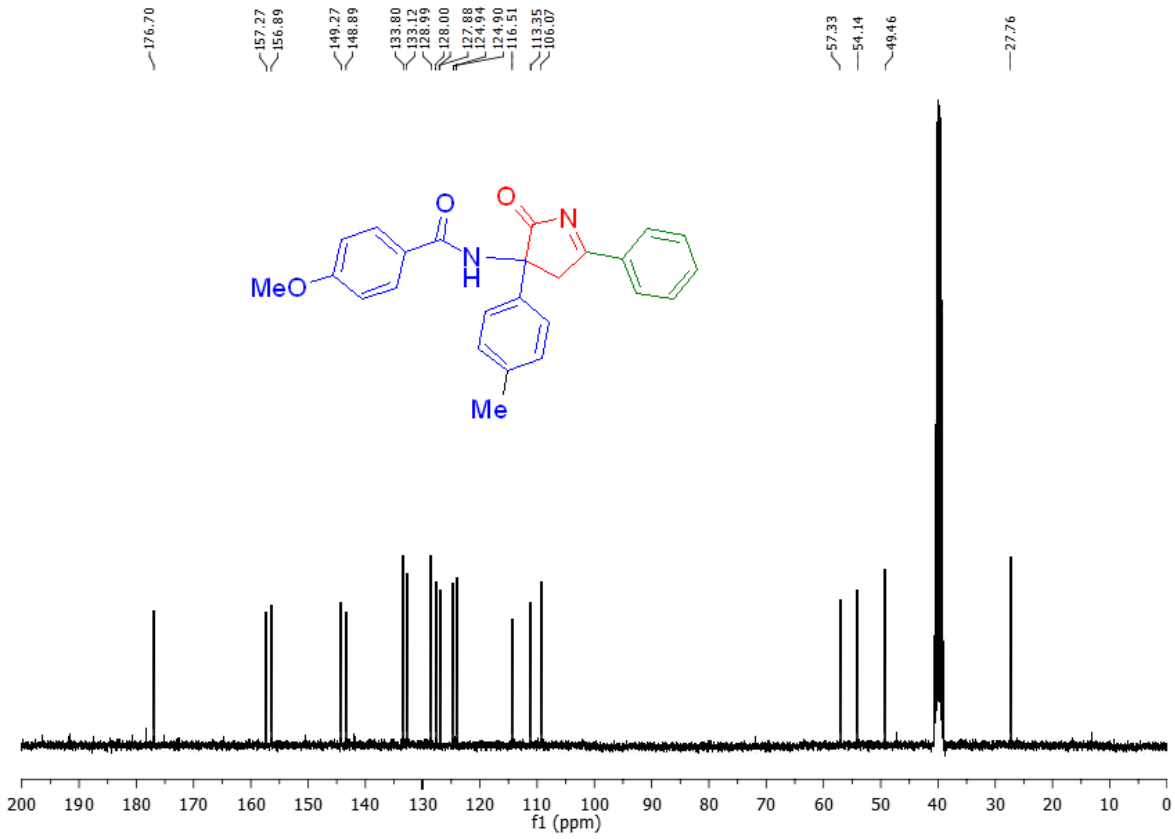
13) 4-Methoxy-N-(3-(4-methoxyphenyl)-2-oxo-5-phenyl-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3m).



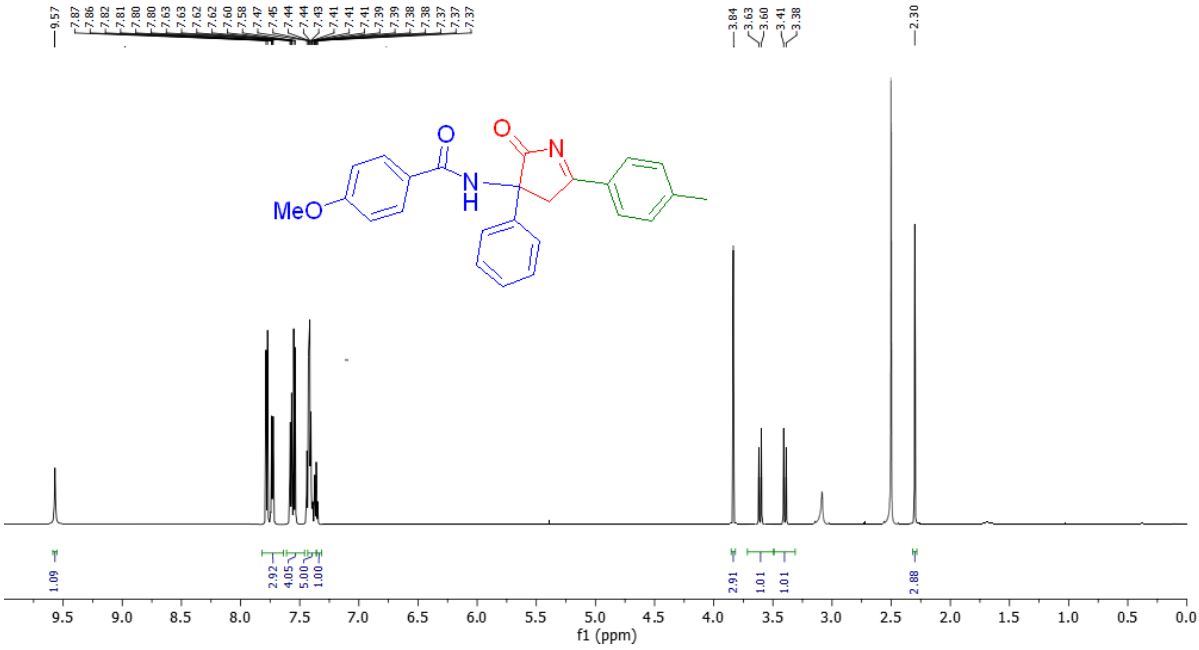


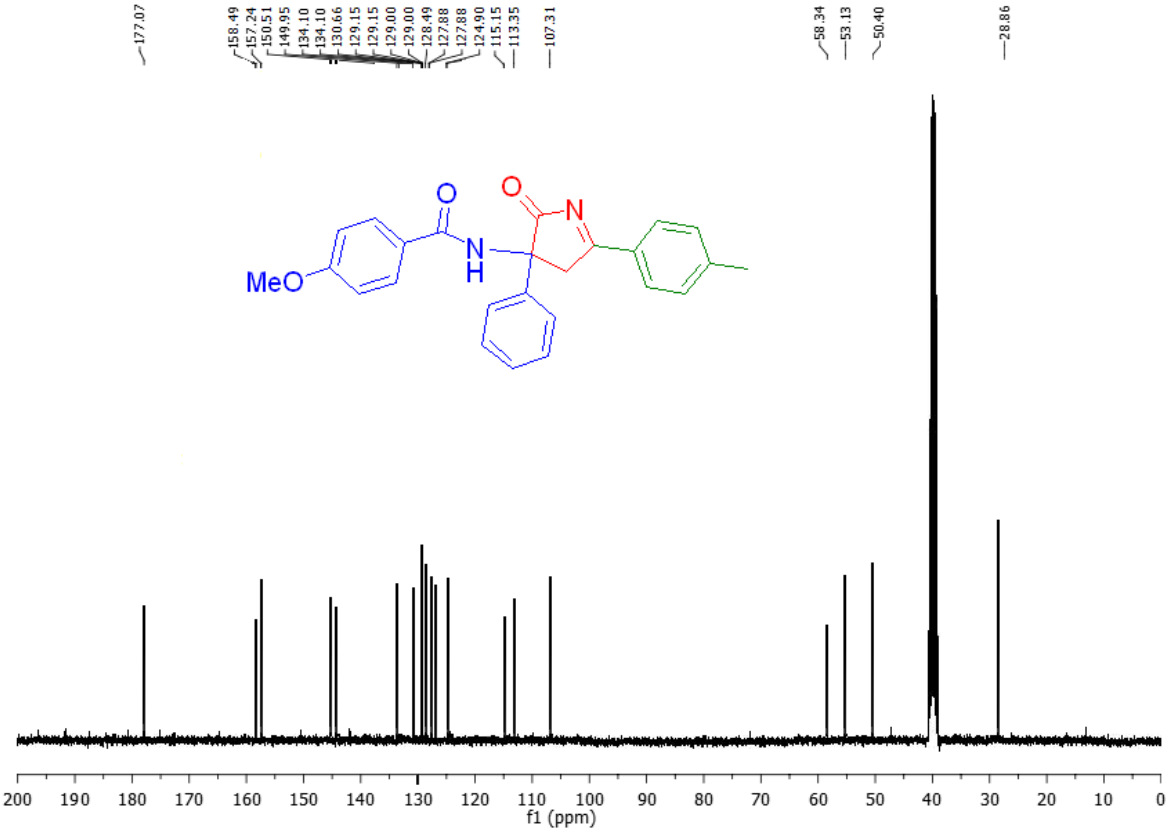
14) 4-Methoxy-N-(2-oxo-5-phenyl-3-(p-tolyl)-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3n).



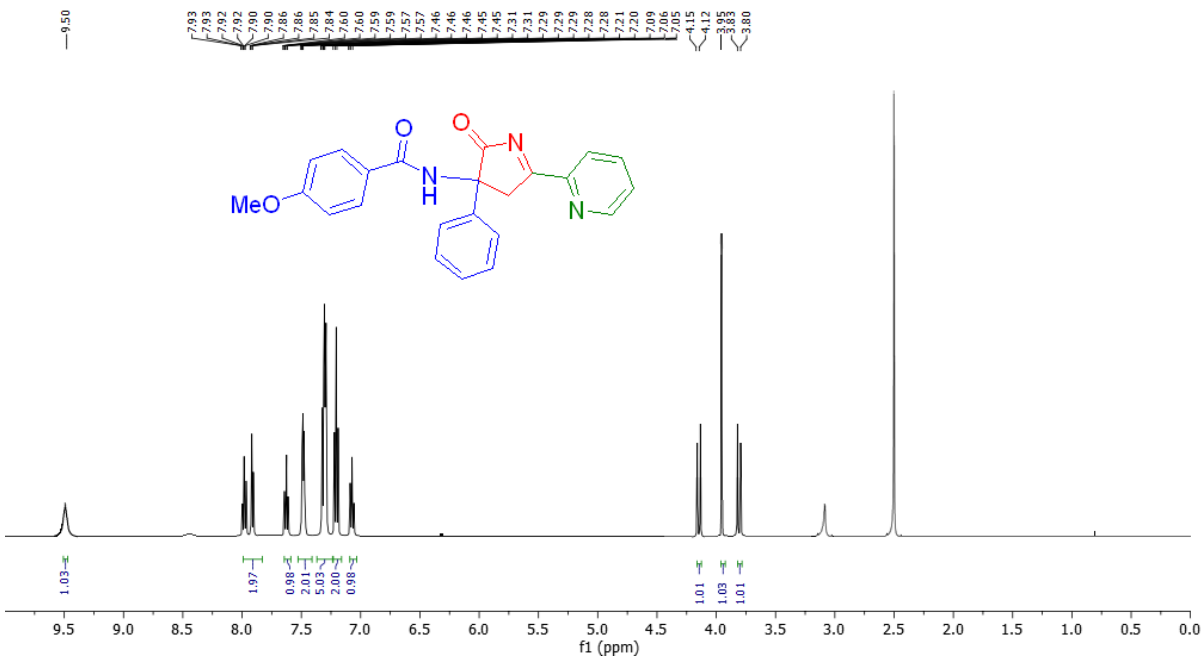


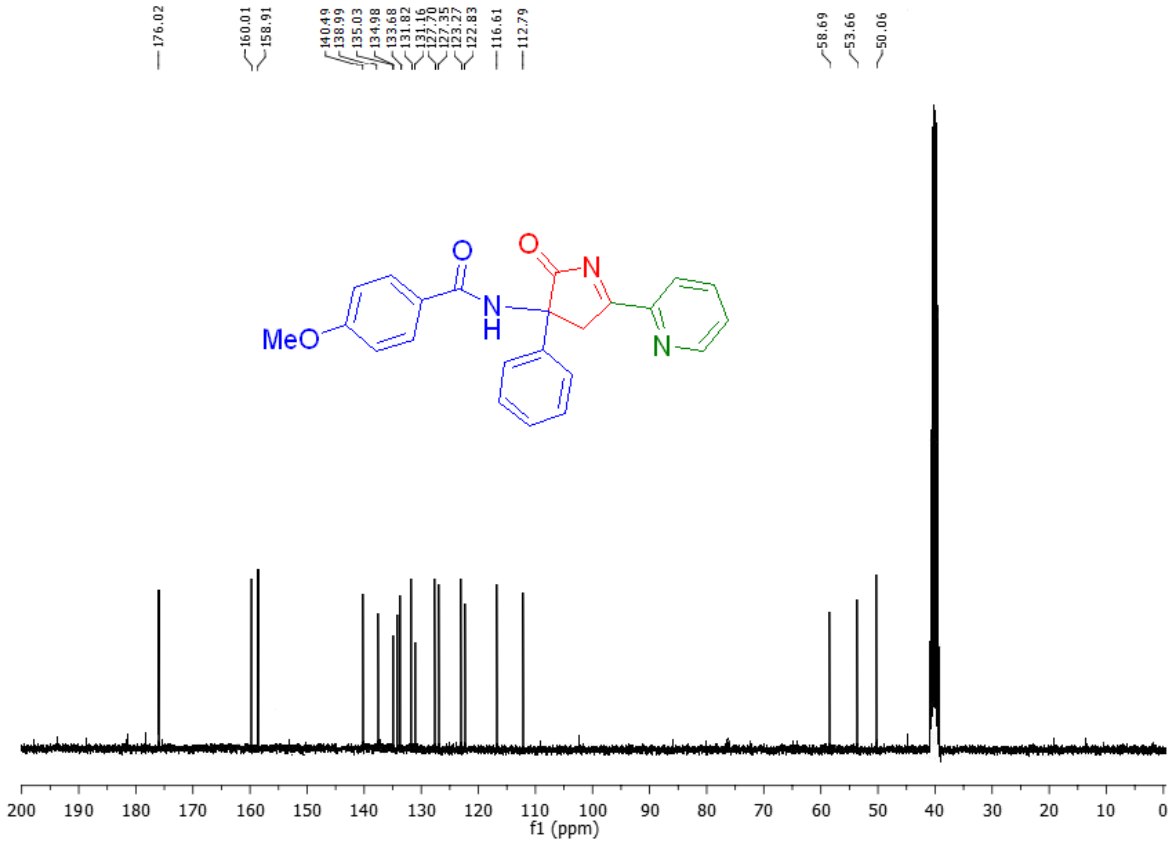
15) 4-Methoxy-N-(2-oxo-3-phenyl-5-(p-tolyl)-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3o).



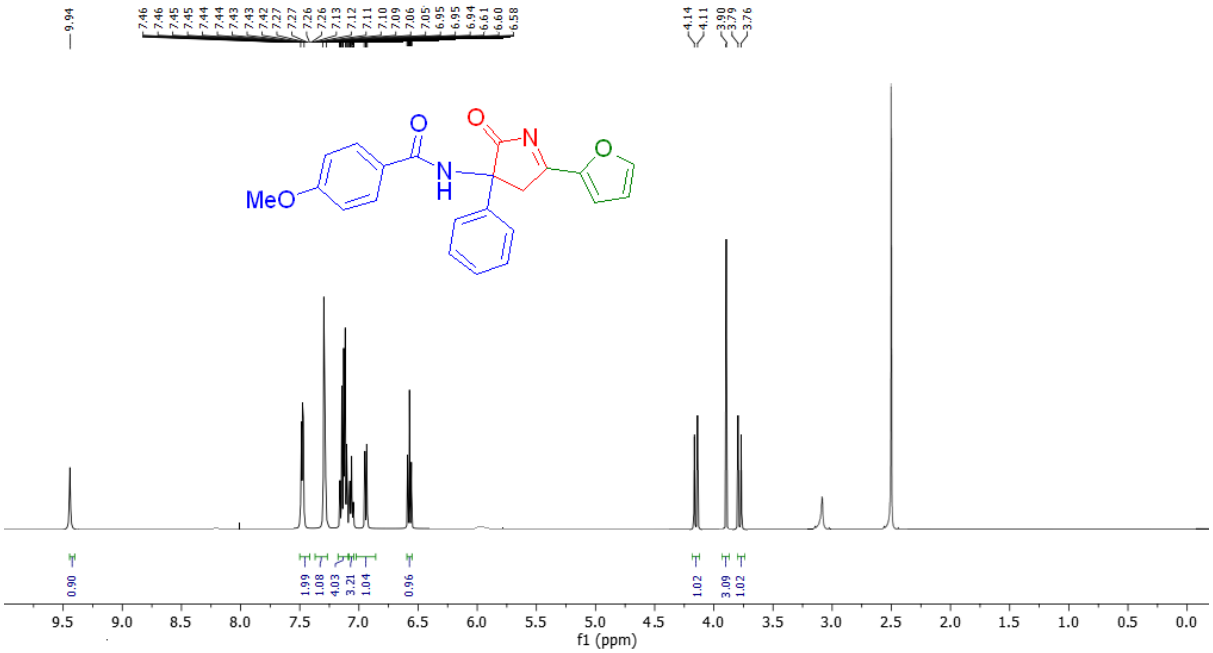


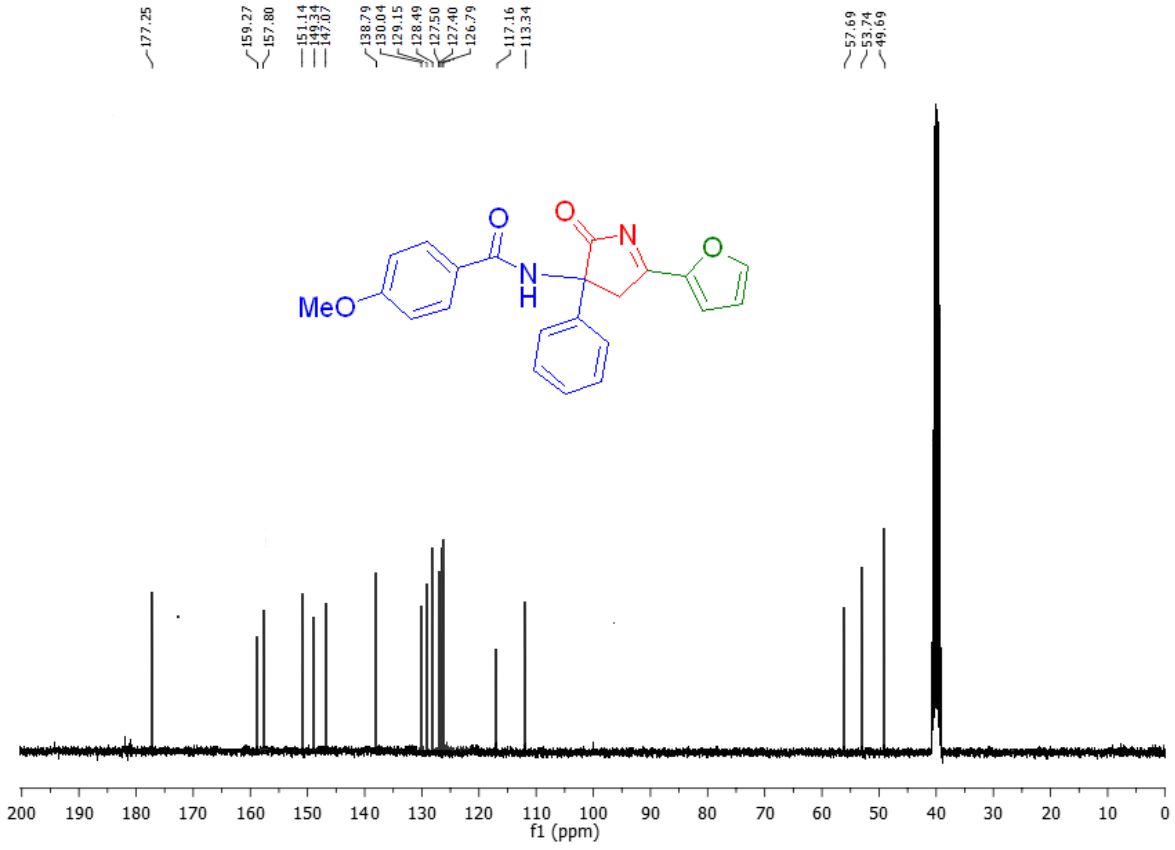
16) 4-Methoxy-N-(2-oxo-3-phenyl-5-(pyridin-2-yl)-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3p).





17) N-(5-(furan-2-yl)-2-oxo-3-phenyl-3,4-dihydro-2*H*-pyrrol-3-yl)-4-methoxybenzamide (3q).





18)) 4-Methoxy-N-(2-oxo-3-phenyl-5-(thiophen-2-yl)-3,4-dihydro-2*H*-pyrrol-3-yl)benzamide (3r).