

Supplementary Information

***N*-Arylation of (Hetero)arylamines Using Aryl Sulfamates and Carbamates *via* C–O Bond Activation Enabled by Reusable and Durable Nickel (0) Catalyst**

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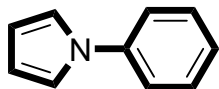
1. Experimental

1.1 General experimental methods

The products were characterized by comparison of their spectral and physical data such as NMR and CHNS with available literature data. ^1H and ^{13}C NMR spectra were recorded with Bruker Avance DPX 250MHz instruments with Me_4Si or solvent resonance as the internal standard. ^1H NMR spectroscopic data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, sept = septet, br. = broad, m = multiplet), coupling constants (Hz), and integration. ^{19}F NMR spectra were recorded with a Bruker DPX 400 MHz spectrometer in CDCl_3 that operating at 376 MHz for ^{19}F acquisitions. Elemental analysis was performed using Thermofinigan Flash EA-1112 CHNSO rapid elemental analyzer. Determination of the purity of the substrate and monitoring of the reaction were accomplished by thin-layer chromatography (TLC) on a silica-gel polygram SILG/UV 254 plates.

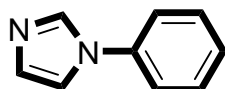
1.2 Chemicals

All starting materials and solvents were purchased from the Merck, Flucka and Aldrich Chemical Companies in high purity.



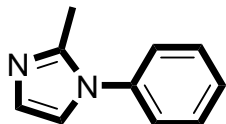
1-Phenyl-1H-pyrrole (C1):¹

Dark brown oil, ^1H NMR (250 MHz, CDCl_3): δ = 7.28-7.33 (m, 4H), 7.12-7.18 (m, 1H), 7.00 (t, J = 4.5 Hz, 2H), 6.27 (t, J = 4.5 Hz, 2H); ^{13}C NMR (63 MHz, CDCl_3): δ = 110.4, 119.3, 120.5, 125.6, 129.5, 140.8; Anal. Calcd for $\text{C}_{10}\text{H}_9\text{N}$: C, 83.88; H, 6.34; N, 9.78%. Found: C, 83.64; H, 6.43; N, 9.93%.



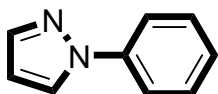
1-Phenyl-1H-imidazole (C2):¹

Dark brown oil, ^1H NMR (250 MHz, CDCl_3): δ = 7.80 (s, 1H), 7.14-7.45 (m, 7H); ^{13}C NMR (63 MHz, CDCl_3): δ = 118.2, 121.4, 127.5, 129.9, 130.4, 135.5, 137.4; Anal. Calcd for $\text{C}_9\text{H}_8\text{N}_2$: C, 74.98; H, 5.59; N, 19.43%. Found: C, 74.93; H, 5.56; N, 19.51%.



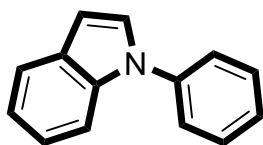
2-Methyl-1-phenyl-1H-imidazole (C3):¹

Dark brown oil, ¹H NMR (250 MHz, CDCl₃): δ= 7.51-7.35 (m, 3H), 7.26 (d, *J* = 7.0 Hz, 2H), 7.01 (s, 1H), 6.98 (s, 1H), 2.35(s, 3H); ¹³C NMR (63 MHz, CDCl₃): δ= 13.7, 120.6, 125.5, 127.5, 128.2, 129.5, 137.8, 144.6; Anal. Calcd for C₁₀H₁₀N₂: C, 75.92; H, 6.37; N, 17.71%. Found: C, 75.86; H, 6.35; N, 17.79%.



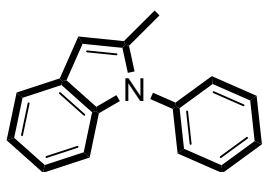
1-Phenyl-1H-pyrazole (C4):¹

Dark brown oil, ¹H NMR (250 MHz, CDCl₃): δ= 7.85 (d, *J* = 7.5 Hz, 1H), 7.74-7.62 (m, 3H), 7.46-7.40 (m, 2H), 7.33-7.27 (m, 2H), 6.45 (t, *J* = 7.5 Hz, 1H); ¹³C NMR (63 MHz, CDCl₃): δ= 107.7, 119.3, 126.1, 126.5, 129.9, 140.8, 141.8; Anal. Calcd for C₉H₈N₂: C, 74.98; H, 5.59; N, 19.43%. Found: C, 74.92; H, 5.54; N, 19.54%.



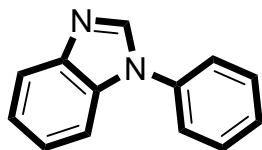
1-Phenyl-1H-indole (C5):²

Dark brown oil, ¹H NMR (250 MHz, CDCl₃): δ= 7.59-7.64 (m, 1H), 7.41-7.52 (m, 5H), 7.25-7.30 (m, 2H), 7.06-7.17 (m, 2H), 6.59-6.63 (m, 1H); ¹³C NMR (63 MHz, CDCl₃): δ= 103.6, 110.5, 120.4, 121.1, 122.4, 124.4, 126.4, 128.0, 129.3, 129.6, 135.8, 139.8; Anal. Calcd for C₁₄H₁₁N: C, 87.01; H, 5.75; N 7.25%. Found: C, 86.91; H, 5.86; N, 7.23%.



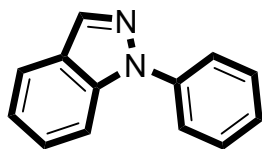
2-Methyl-1-phenyl-1H-indole (C6):³

Dark brown oil, ¹H NMR (250 MHz, CDCl₃): δ= 7.36-7.51 (m, 4H), 7.25-7.29 (m, 2H), 7.00-7.07 (m, 3H), 6.32 (s, 1H), 2.22 (s, 3H); ¹³C NMR (63 MHz, CDCl₃): δ= 13.4, 101.3, 110.0, 119.6, 120.0, 121.0, 127.7, 128.0, 128.2, 129.4, 137.0, 138.2; Anal. Calcd for C₁₅H₁₃N: C, 86.92; H, 6.32; N, 6.76%. Found: C, 86.72; H, 6.45; N, 6.83%.



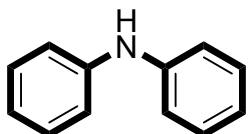
1-Phenyl-1H-benzimidazole (C7):¹

Brown oil, ¹H NMR (250 MHz, CDCl₃): δ= 8.17 (s, 1H), 7.89-7.90 (m, 1H), 7.44-7.61 (m, 6H), 7.32-7.36 (m, 2H); ¹³C NMR (63 MHz, CDCl₃): δ= 110.5, 120.6, 122.8, 123.7, 124.0, 128.0, 130.0, 136.3, 142.8, 144.2; Anal. Calcd for C₁₃H₁₀N₂: C, 80.39; H, 5.19; N, 14.42%. Found: C, 80.51; H, 5.01; N, 14.48%.



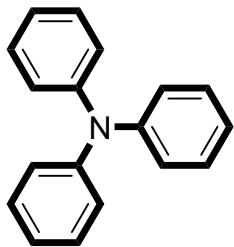
1-phenyl-1H-indazole (C8):⁴

Colorless crystals; mp = 76-77 °C; ¹H NMR (250 MHz, CDCl₃): δ= 8.19 (s, 1H), 7.85-7.65 (m, 4H), 7.51 (t, *J* = 7.0 Hz, 2H), 7.39 (t, *J* = 7.0 Hz, 1H), 7.33 (t, *J* = 7.0 Hz, 1H), 7.20 (t, *J* = 7.0 Hz, 1H); ¹³C NMR (63 MHz, CDCl₃): δ= 110.5, 121.4, 121.6, 122.8, 125.4, 126.7, 127.2, 129.5, 135.5, 138.8, 140.2; Anal. Calcd for C₁₃H₁₀N₂: C, 80.39; H, 5.19; N, 14.42%. Found: C, 80.51; H, 4.99; N, 14.50%.



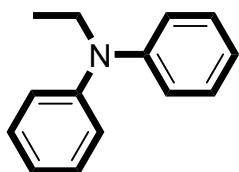
Diphenylamine (C9):⁵

Colorless crystals; mp = 52-54 °C; ¹H NMR (250 MHz, CDCl₃): δ= 7.39-7.34 (m, 4H), 7.22-7.15 (m, 4H), 7.89-7.83 (m, 2H), 5.81 (s, 1H, NH); ¹³C NMR (63 MHz, CDCl₃): δ= 116.9, 120.3, 129.0, 145.9; Anal. Calcd for C₁₂H₁₁N: C, 85.17; H, 6.55; N, 8.28%. Found: C, 85.13; H, 6.53; N, 8.34%.



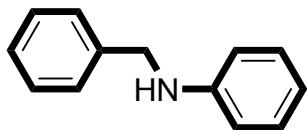
Triphenylamine (C10)

Colorless crystals; mp = 126-128 °C; ^1H NMR (250 MHz, CDCl_3): δ = 7.46-7.41 (m, 6H), 7.29-7.22 (m, 6H), 6.96-6.99 (m, 3H); ^{13}C NMR (63 MHz, CDCl_3): δ = 121.7, 123.1, 129.0, 149.0; Anal. Calcd for $\text{C}_{18}\text{H}_{15}\text{N}$: C, 88.13; H, 6.16; N, 5.71%. Found: C, 88.07; H, 6.10; N, 5.83%.



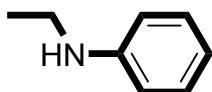
N-Ethyl-N-phenylaniline (C11)

Brown oil, ^1H NMR (250 MHz, CDCl_3): δ = 7.39-7.34 (m, 4H), 7.22-7.15 (m, 4H), 6.89-6.83 (m, 2H), 3.03 (q, J = 7.5 Hz, 2H), 1.17 (t, J = 7.5 Hz, 2H); ^{13}C NMR (63 MHz, CDCl_3): δ = 14.5, 40.7, 121.3, 124.7, 129.0, 141.8; Anal. Calcd for $\text{C}_{14}\text{H}_{15}\text{N}$: C, 85.24; H, 7.66; N, 7.10%. Found: C, 85.18; H, 7.61; N, 7.21%.



N-Benzylaniline (C12):⁵

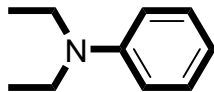
Colorless oil; ^1H NMR (250 MHz, CDCl_3): δ = 7.38-7.23 (m, 7H), 6.75-6.67 (m, 3H), 4.08 (s, 3H), 3.93 (s, 1H, NH); ^{13}C NMR (63 MHz, CDCl_3): δ = 48.8, 112.4, 117.5, 128.2, 128.5, 128.8, 129.0, 139.7, 148.5; Anal. Calcd for $\text{C}_{13}\text{H}_{13}\text{N}$: C, 85.21; H, 7.15; N, 7.64%. Found: C, 85.16; H, 7.13; N, 7.71%.



N-Ethylaniline (C13):⁵

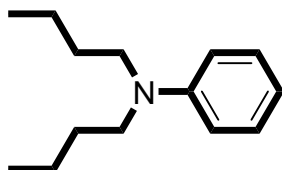
Colorless oil; ^1H NMR (250 MHz, CDCl_3): δ = 7.32-7.17 (m, 4H), 7.00-6.94 (m, 1H), 3.49 (s, 1H, NH), 3.13 (q, J = 7.5 Hz, 2H), 1.23 (d, J = 7.5 Hz, 3H); ^{13}C NMR (63 MHz, CDCl_3): δ = 15.8, 38.7,

112.8, 117.2, 129.2, 148.7; Anal. Calcd for C₈H₁₁N: C, 79.29; H, 9.15; N, 11.56%. Found: C, 79.22; H, 9.11; N, 11.67%.



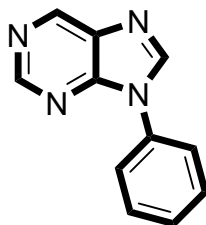
***N,N*-Diethylaniline (C14)**

Dark brown oil, ¹H NMR (250 MHz, CDCl₃): δ= 7.20-7.27 (m, 2H), 6.63-6.73 (m, 3H), 3.37 (q, *J* = 7.5 Hz, 4H), 1.18 (t, *J* = 7.5 Hz, 6H); ¹³C NMR (63 MHz, CDCl₃): δ= 12.6, 44.3, 111.8, 115.3, 129.3, 147.8; Anal. Calcd for C₁₀H₁₅N: C, 80.48; H, 10.13; N, 9.39%. Found: C, 80.25; H, 10.03; N, 9.72%.



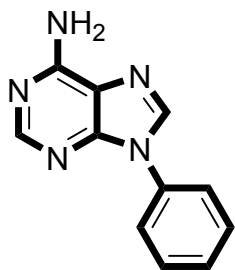
***N,N*-Dibutylaniline (C15)**

Black oil, ¹H NMR (250 MHz, CDCl₃): δ= 7.09-7.17 (m, 2H), 6.54-6.58 (m, 3H), 3.18 (t, *J* = 7.5 Hz, 4H), 1.46-1.55 (m, 4H), 1.20-1.32 (m, 4H), 0.88 (t, *J* = 7.5 Hz, 6H); ¹³C NMR (63 MHz, CDCl₃): δ= 14.0, 20.4, 29.4, 50.8, 111.6, 115.0, 129.2, 148.2; Anal. Calcd for C₁₄H₂₃N: C, 81.89; H, 11.29; N, 6.82%. Found: C, 81.84; H, 11.25; N, 6.91%.



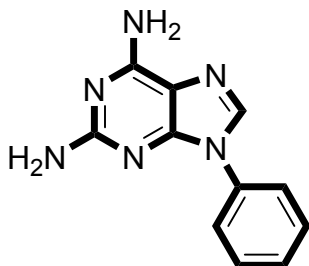
9-Phenylpurine (C16):

Colorless crystals; mp = 160-162 °C; ¹H NMR (250 MHz, CDCl₃): δ= 9.21 (s, 1H), 9.06 (s, 1H), 8.34 (s, 1H), 7.84-7.76 (m, 2H), 7.69-7.61 (m, 2H), 7.30-7.22 (m, 1H); ¹³C NMR (63 MHz, CDCl₃): δ= 153.3, 151.4, 149.4, 144.6, 135.0, 134.3, 130.2, 128.8, 123.7; Anal. Calcd for C₁₁H₈N₄: C, 67.34; H, 4.11; N, 28.55%. Found: C, 74.45; H, 5.22; N, 28.69%.



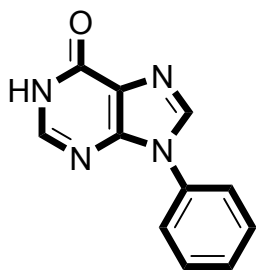
9-Phenyladenine (C17):

Colorless crystals; mp = 245-247 °C; ¹H NMR (250 MHz, DMSO-*d*₆): δ= 8.59 (s, 1H), 8.22 (s, 1H), 7.87-7.84 (m, 2H), 7.62-7.57 (m, 2H), 7.45-7.39 (m, 1H), 7.34 (s, 2H); ¹³C NMR (63 MHz, DMSO-*d*₆): δ= 156.3, 152.9, 149.2, 139.6, 135.2, 129.7, 127.3, 122.5, 119.8; Anal. Calcd for C₁₁H₉N₅: C, 62.55; H, 4.29; N, 33.16%. Found: C, 62.45; H, 4.24; N, 33.31%.



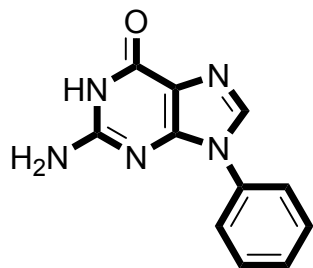
9-Phenylpurine-2,6-diamine (C18):

Colorless crystals; mp = 285-286 °C; ¹H NMR (250 MHz, DMSO-*d*₆): δ= 8.20 (s, 1H), 7.92-7.84 (m, 2H), 7.63-7.54 (m, 2H), 7.38-7.31 (m, 1H), 6.81 (s, 2H), 5.91 (s, 2H); ¹³C NMR (63 MHz, DMSO-*d*₆): δ= 160.8, 156.2, 151.5, 136.1, 135.9, 129.4, 126.1, 122.8, 113.3; Anal. Calcd for C₁₁H₁₀N₆: C, 58.40; H, 4.46; N, 37.15%. Found: C, 58.31; H, 4.42; N, 37.28%.



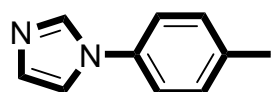
9-Phenylhypoxanthine (C19):

Colorless crystals; mp = 317-319 °C; ¹H NMR (250 MHz, DMSO-*d*₆): δ= 12.47 (br, 1H), 8.47 (s, 1H), 8.09 (s, 1H), 7.79-7.76 (m, 2H), 7.61-7.58 (m, 2H), 7.49-7.44 (m, 1H); ¹³C NMR (63 MHz, DMSO-*d*₆): δ= 156.8, 147.8, 146.1, 139.4, 134.5, 129.6, 128.1, 124.9, 123.9; Anal. Calcd for C₁₁H₈N₄O: C, 62.26; H, 3.80; N, 26.40%. Found: C, 62.23; H, 3.76; N, 26.49%.



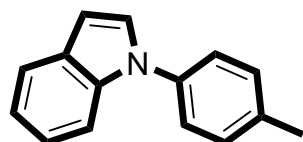
9-Phenylguanine (C20):

Colorless crystals; mp = 341-343 °C; ¹H NMR (250 MHz, DMSO-*d*₆): δ= 10.76 (br, 1H), 8.04 (s, 1H), 7.78-7.73 (m, 2H), 7.55-7.52 (m, 2H), 7.43-7.40 (m, 1H), 6.51 (br, 2H); ¹³C NMR (63 MHz, DMSO-*d*₆): δ= 156.7, 153.9, 150.9, 136.6, 135.1, 129.7, 127.6, 123.8, 117.8; Anal. Calcd for C₁₁H₉N₅O: C, 58.14; H, 3.99; N, 30.82%. Found: C, 58.07; H, 4.39; N, 30.93%.



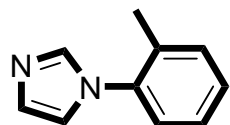
1-(*p*-Tolyl)-1H-imidazole (C22):³

Colorless crystals; mp = 61-63 °C; ¹H NMR (250 MHz, CDCl₃): δ= 7.88 (s, 1H), 7.39-7.34 (m, 5H), 7.19-7.14 (m, 1H), 2.30 (s, 3H); ¹³C NMR (63 MHz, CDCl₃): δ= 20.1, 118.8, 120.5, 130.0, 131.1, 135.5, 135.9, 137.9; Anal. Calcd for C₁₀H₁₀N₂: C, 75.92; H, 6.37; N, 17.71%. Found: C, 75.85; H, 6.31; N, 17.84%.



1-(*p*-Tolyl)-1H-indole (C23):²

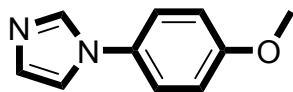
Dark brown oil, ¹H NMR (250 MHz, CDCl₃): δ= 7.58-7.62 (m, 1H), 7.43-7.47 (m, 1H), 7.04-7.32 (m, 7H), 6.58 (dd, *J*= 4.2 Hz, 1H), 2.35 (s, 3H); ¹³C NMR (63 MHz, CDCl₃): δ= 21.1, 103.2, 110.5, 120.1, 121.1, 122.2, 124.3, 128.1, 129.2, 130.1, 136.3, 137.3; Anal. Calcd for C₁₅H₁₃N: C, 86.92; H, 6.32; N, 6.76%. Found: C, 86.57; H, 6.55; N, 6.88%.



1-(*o*-Tolyl)-1H-imidazole (C24)

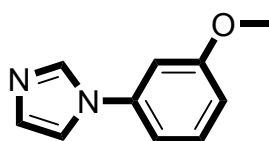
Pale yellow oil; ¹H NMR (250 MHz, CDCl₃): δ= 7.68 (s, 1H), 7.45-7.33 (m, 5H), 7.18-7.13 (m, 1H), 2.04 (s, 3H); ¹³C NMR (63 MHz, CDCl₃): δ= 17.5, 120.6, 125.2, 125.8, 128.5, 128.7, 131.2, 134.0,

136.3, 137.7; Anal. Calcd for C₁₀H₁₀N₂: C, 75.92; H, 6.37; N, 17.71%. Found: C, 75.83; H, 6.30; N, 17.87%.



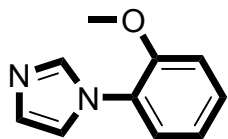
1-(4-Methoxyphenyl)-1H-imidazole (C25):¹

Colorless crystals; mp = 59-60 °C; ¹H NMR (250 MHz, CDCl₃): δ= 7.54 (s, 1H), 7.37-7.32 (m, 2H), 7.19-7.14 (m, 2H), 7.00-6.92 (m, 2H), 3.83 (s, 3H); ¹³C NMR (63MHz, CDCl₃): δ= 55.8, 114.2, 118.3, 123.4, 129.2, 130.2, 135.3, 158.6; Anal. Calcd for C₁₀H₁₀N₂O: C, 68.95; H, 5.79; N, 16.08%. Found: C, 68.88; H, 5.75; N, 16.19%.



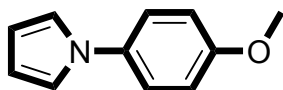
1-(3-Methoxyphenyl)-1H-imidazole (C26):⁶

Pale yellow oil; ¹H NMR (250 MHz, CDCl₃): δ= 7.84 (s, 1H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.26 (s, 1H), 7.18 (s, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.93-6.84 (m, 2H), 3.83 (s, 3H); ¹³C NMR (63MHz, CDCl₃): δ= 55.7, 107.6, 112.6, 113.5, 118.2, 130.2, 130.6, 135.5, 138.4, 160.6; Anal. Calcd for C₁₀H₁₀N₂O: C, 68.95; H, 5.79; N, 16.08%. Found: C, 68.87; H, 5.75; N, 16.20%.



1-(2-Methoxyphenyl)-1H-imidazole (C27):⁴

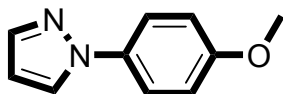
Pale yellow oil; ¹H NMR (250 MHz, CDCl₃): δ= 7.77 (s, 1H), 7.33 (t, *J* = 8.0 Hz, 1H), 7.23 (dd, *J*₁ = 7.0 Hz, *J*₂ = 1.2 Hz, 1H), 7.18 (s, 1H), 7.14 (s, 1H), 7.09-6.95 (m, 2H), 3.79 (s, 3H); ¹³C NMR (63MHz, CDCl₃): δ= 55.7, 112.3, 120.2, 121.0, 125.4, 126.3, 128.6, 128.9, 137.7, 152.5; Anal. Calcd for C₁₀H₁₀N₂O: C, 68.95; H, 5.79; N, 16.08%. Found: C, 68.86; H, 5.74; N, 16.22%.



1-(4-Methoxyphenyl)-1H-pyrrole (C28):²

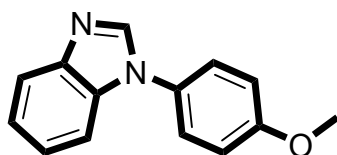
Colorless crystals; mp = 111-113 °C; ¹H NMR (250 MHz, CDCl₃): δ= 7.32 (d, *J* = 7.0 Hz, 2H), 7.03-7.00 (m, 2H), 6.96 (d, *J* = 7.0 Hz, 2H), 6.37-6.33 (m, 2H), 3.85 (s, 3H); ¹³C NMR (63MHz, CDCl₃):

δ = 55.5, 109.8, 114.6, 119.7, 122.2, 134.5, 157.6; Anal. Calcd for C₁₁H₁₁NO: C, 76.28; H, 6.40; N, 8.06%. Found: C, 76.28; H, 6.37; N, 8.15%.



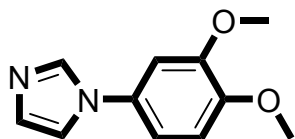
1-(4-methoxyphenyl)-1H-pyrazole (C29):²

Colorless crystals; mp = 43-44 °C; ¹H NMR (250 MHz, CDCl₃): δ = 7.80 (d, *J* = 2.0 Hz, 1H), 7.69 (d, *J* = 1.0 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.41 (t, *J* = 2.0 Hz, 1H), 3.81 (s, 3H); ¹³C NMR (63MHz, CDCl₃): δ = 55.5, 107.2, 114.5, 120.8, 126.8, 134.0, 140.6, 158.2; Anal. Calcd for C₁₀H₁₀N₂O: C, 68.95; H, 5.79; N, 16.08%. Found: C, 68.87; H, 5.74; N, 16.21%.



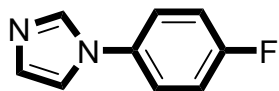
1-(4-Methoxyphenyl)-1H-benzoimidazole (C30):³

Colorless crystals; mp = 94-96 °C; ¹H NMR (250 MHz, CDCl₃): δ = 7.97 (s, 1H), 7.79-7.76 (m, 1H), 7.39-7.17 (m, 5H), 7.01-6.96 (m, 2H), 3.81 (s, 3H); ¹³C NMR (63MHz, CDCl₃): δ = 55.5, 107.3, 109.8, 114.6, 115.9, 119.7, 122.2, 136.0, 163.2; Anal. Calcd for C₁₄H₁₂N₂O: C, 74.98; H, 5.39; N, 12.49%. Found: C, 74.94; H, 5.36; N, 12.55%.



1-(3,4-Dimethoxyphenyl)-1H-imidazole (C31)

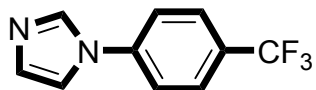
Colorless crystals; mp = 73-75 °C; ¹H NMR (250 MHz, CDCl₃): δ = 7.91 (s, 1H), 7.58-7.53 (m, 2H), 7.09-7.04 (m, 2H), 6.53 (s, 1H), 4.02 (s, 3H), 4.01 (s, 3H); ¹³C NMR (63MHz, CDCl₃): δ = 53.4, 54.7, 113.1, 118.6, 122.3, 124.4, 126.5, 129.1, 134.7, 155.1, 155.5; Anal. Calcd for C₁₁H₁₂N₂O₂: C, 64.69; H, 5.92; N, 13.72%. Found: C, 64.62; H, 5.87; N, 13.81%.



1-(4-Fluorophenyl)-1H-imidazole (C32):⁶

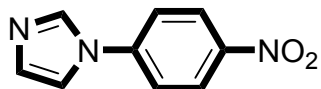
Pale yellow oil; ¹H NMR (250 MHz, CDCl₃): δ = 7.94 (s, 1H), 7.44-7.40 (m, 2H), 7.28-7.12 (m, 4H); ¹³C NMR (63MHz, CDCl₃): δ = 116.6 (d, *J* = 22.7 Hz), 118.5, 123.4 (d, *J* = 8.2 Hz), 130.3, 133.5 (d,

$J = 2.2$ Hz), 135.6, 161.5 (d, $J = 246.7$ Hz); ^{19}F NMR (376 MHz, CDCl_3): $\delta = -117.3$. Anal. Calcd for $\text{C}_9\text{H}_7\text{FN}_2$: C, 66.66; H, 4.35; N, 17.27%. Found: C, 66.62; H, 4.31; N, 17.39%.



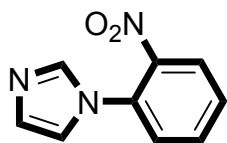
1-(4-(triFluoromethyl)phenyl)-1H-imidazole (C33):⁷

Colorless crystals; mp = 66-68 °C; ^1H NMR (250 MHz, CDCl_3): $\delta = 7.99$ (s, 1H), 7.83 (d, $J = 8.0$ Hz, 2H), 7.54 (d, $J = 8.0$ Hz, 2H), 7.40 (s, 1H), 7.23 (s, 1H); ^{13}C NMR (63 MHz, CDCl_3): $\delta = 117.7$, 121.5, 122.4, 125.2, 127.4 (d, $J = 14.8$ Hz), 127.7, 129.9, 131.9, 135.3, 141.1; ^{19}F NMR (376 MHz, CDCl_3): $\delta = -62.3$. Anal. Calcd for $\text{C}_{10}\text{H}_7\text{F}_3\text{N}_2$: C, 56.61; H, 3.33; N, 13.20%. Found: C, 56.54; H, 3.31; N, 13.29%.



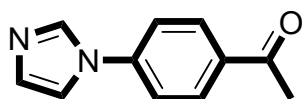
1-(4-Nitrophenyl)-1H-imidazole (C34):¹

Yellow crystals; mp = 207-209 °C; ^1H NMR (250 MHz, CDCl_3): $\delta = 8.39$ (d, $J = 7.5$ Hz, 2H), 8.02 (s, 1H), 7.49 (d, $J = 7.5$ Hz, 2H), 7.33 (s, 1H), 7.07 (s, 2H); ^{13}C NMR (63 MHz, CDCl_3): $\delta = 117.7$, 121.7, 125.2, 130.9, 136.3, 142.9, 147.0; Anal. Calcd for $\text{C}_9\text{H}_7\text{N}_3\text{O}_2$: C, 57.14; H, 3.73; N, 22.21%. Found: C, 57.08; H, 3.67; N, 22.32%.



1-(2-Nitrophenyl)-1H-imidazole (C35)

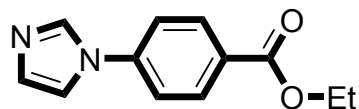
Yellow crystals; mp = 108-110 °C; ^1H NMR (250 MHz, CDCl_3): $\delta = 7.81$ -7.73 (m, 2H), 7.61-7.50 (m, 1H), 7.44-7.32 (m, 3H), 6.51 (s, 1H); ^{13}C NMR (63 MHz, CDCl_3): $\delta = 108.4$, 125.8, 126.8, 128.7, 129.9, 232.9, 133.6, 142.5; Anal. Calcd for $\text{C}_9\text{H}_7\text{N}_3\text{O}_2$: C, 57.14; H, 3.73; N, 22.21%. Found: C, 57.07; H, 3.64; N, 22.34%.



1-(4-(1H-imidazol-1-yl)phenyl)ethan-1-one (C36):¹

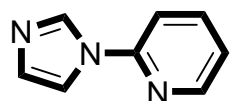
Yellow crystals; mp = 110-112 °C; ^1H NMR (250 MHz, CDCl_3): $\delta = 8.09$ (d, $J = 8.0$ Hz, 2H), 7.97 (s, 1H), 7.51 (d, $J = 8.0$ Hz, 2H), 7.38 (s, 1H), 7.24 (s, 1H), 2.64 (s, 3H); ^{13}C NMR (63 MHz, CDCl_3):

δ = 26.6, 117.7, 120.6, 130.3, 131.1, 135.3, 135.7, 140.7, 196.5; Anal. Calcd for C₁₁H₁₀N₂O: C, 70.95; H, 5.41; N, 15.04%. Found: 70.90; H, 5.38; N, 15.12%.



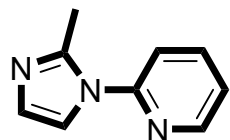
Ethyl 4-(1*H*-imidazol-1-yl)benzoate (C37):⁶

Yellow crystals; mp = 102-104 °C; ¹H NMR (250 MHz, CDCl₃): δ = 8.17 (d, *J* = 8.0 Hz, 2H), 7.97 (s, 1H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.37 (s, 1H), 7.25 (s, 1H), 4.41 (q, *J* = 7.0 Hz, 2H), 1.42 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (63 MHz, CDCl₃): δ = 14.3, 61.3, 117.8, 120.5, 129.3, 131.0, 131.4, 135.4, 140.6, 165.5; Anal. Calcd for C₁₂H₁₂N₂O₂: C, 66.65; H, 5.59; N, 12.96%. Found: C, 66.61; H, 5.56; N, 13.06%.



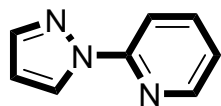
2-Imidazol-1-ylpyridine (C38):¹

Dark brown oil, ¹H NMR (250 MHz, CDCl₃): δ = 8.41-8.43 (m, 1H), 8.28 (s, 1H), 7.73-7.80 (m, 1H), 7.58 (s, 1H), 7.25-7.34 (m, 1H), 7.28-7.34 (m, 1H), 7.14-7.20 (m, 2H); ¹³C NMR (63 MHz, CDCl₃): δ = 112.3, 116.7, 122.0, 130.6, 132.2, 134.9, 139.0, 149.1; Anal. Calcd for C₈H₇N₃: C, 66.19; H, 4.86; N, 28.95%. Found: C, 65.89; H, 4.97; N, 29.14%.



2-Methyl-1-phenyl-1*H*-imidazole (C39):⁶

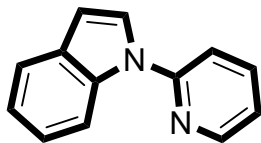
Yellow crystals; mp = 91-93 °C; ¹H NMR (250 MHz, CDCl₃): δ = 7.51-7.35 (m, 3H), 7.26 (d, *J* = 7.0 Hz, 2H), 7.01 (s, 1H), 6.98 (s, 1H), 2.35 (s, 3H); ¹³C NMR (63 MHz, CDCl₃): δ = 13.6, 120.5, 125.4, 127.5, 128.1, 129.4, 137.9, 144.5; Anal. Calcd for C₉H₉N₃: C, 67.90; H, 5.70; N, 26.40%. Found: C, 67.84; H, 5.67; N, 26.49%.



2-(1*H*-Pyrazol-1-yl)pyridine (C40):⁷

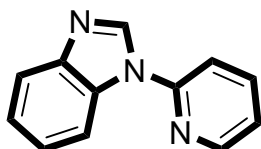
Dark brown oil, ¹H NMR (250 MHz, CDCl₃): δ = 8.57 (d, *J* = 2.1 Hz, 1H), 8.38 (d, *J* = 4.0 Hz, 1H), 7.97 (d, *J* = 7.5 Hz, 1H), 7.83-7.67 (m, 2H), 7.14 (d, *J* = 6.5 Hz, 1H), 6.45 (t, *J* = 1.5 Hz, 1H); ¹³C

NMR (63 MHz, CDCl₃): δ = 107.8, 112.4, 121.3, 127.0, 138.6, 142.0, 148.0, 151.6; Anal. Calcd for C₈H₇N₃: C, 66.19; H, 4.86; N, 28.95%. Found: C, 66.10; H, 4.80; N, 29.11%.



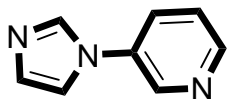
1-Pyridin-2-yl-1H-indole (C41):³

Dark brown oil, ¹H NMR (250 MHz, CDCl₃): δ = 8.36-8.39 (m, 1H), 8.09 (d, J = 8.2 Hz, 1H), 7.49-7.56 (m, 3H), 7.00-7.25 (m, 3H), 6.97 (t, J = 6.0 Hz, 1H), 6.56 (d, J = 3.5 Hz, 1H); ¹³C NMR (63 MHz, CDCl₃): δ = 105.7, 113.3, 114.6, 120.2, 121.2, 121.5, 123.3, 126.1, 130.6, 135.2, 138.5, 149.0, 152.5; Anal. Calcd for C₁₃H₁₀N₂: C, 80.39; H, 5.19; N, 14.42%. Found: C, 80.57; H, 5.09; N, 14.34%.



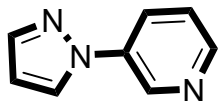
1-Pyridin-2-yl-1H-benzimidazole (C42):³

Brown oil, ¹H NMR (250 MHz, CDCl₃): δ = 8.58-8.62 (m, 2H), 8.06 (d, J = 7.8 Hz, 1H), 7.86-7.93 (m, 2H), 7.58 (d, J = 8.2 Hz, 1H), 7.26-7.39 (m, 3H); ¹³C NMR (63 MHz, CDCl₃): δ = 112.6, 114.3, 120.6, 121.8, 123.3, 124.2, 132.1, 138.9, 141.3, 144.7, 149.5, 149.9; Anal. Calcd for C₁₂H₉N₃: C, 73.83; H, 4.65; N, 21.52%. Found: C, 73.62; H, 4.76; N, 21.62%.



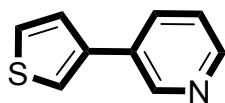
3-(1H-Imidazol-1-yl)pyridine (C43):⁶

Yellow crystals; mp = 57-58 °C; ¹H NMR (250 MHz, CDCl₃): δ = 8.76 (d, J = 2.3 Hz, 1H), 8.64 (d, J = 6.5 Hz, 1H), 7.92 (s, 1H), 7.82-7.72 (m, 1H), 7.47 (d, J = 7.5 Hz, 1H), 7.34 (s, 1H), 7.26 (s, 1H); ¹³C NMR (63 MHz, CDCl₃): δ = 118.1, 124.3, 128.9, 130.9, 133.8, 135.4, 142.7, 148.7; Anal. Calcd for C₈H₇N₃: C, 66.19; H, 4.86; N, 28.95%. Found: C, 66.11; H, 4.81; N, 29.08%.



3-(1H-Pyrazol-1-yl)pyridine (C44):⁶

Yellow crystals; mp = 48-49 °C; ¹H NMR (250 MHz, CDCl₃): δ= 8.99 (d, *J* = 1.5 Hz, 1H), 8.54 (d, *J* = 4.0 Hz, 1H), 8.12-8.03 (m, 1H), 7.97 (d, *J* = 2.0 Hz, 2H), 7.77 (d, *J* = 1.0 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 1H), 6.52 (d, *J* = 1.5 Hz, 1H); ¹³C NMR (63 MHz, CDCl₃): δ= 108.4, 123.9, 126.5, 126.8, 136.5, 140.5, 141.9, 147.5; Anal. Calcd for C₈H₇N₃: C, 66.19; H, 4.86; N, 28.95%. Found: C, 66.12; H, 4.82; N, 29.06%.



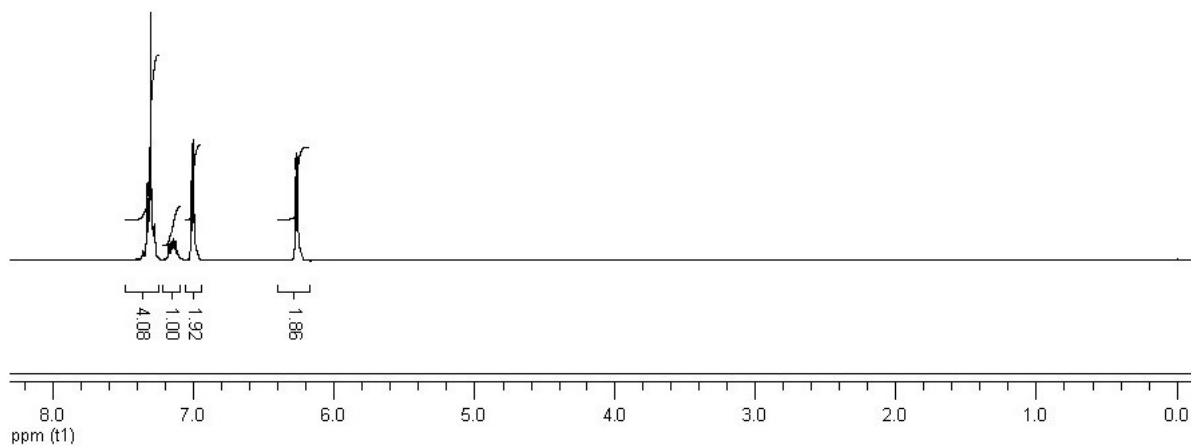
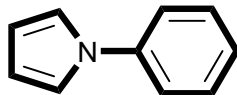
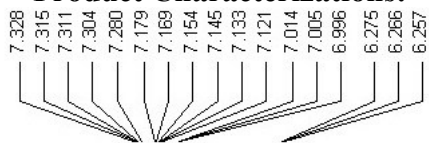
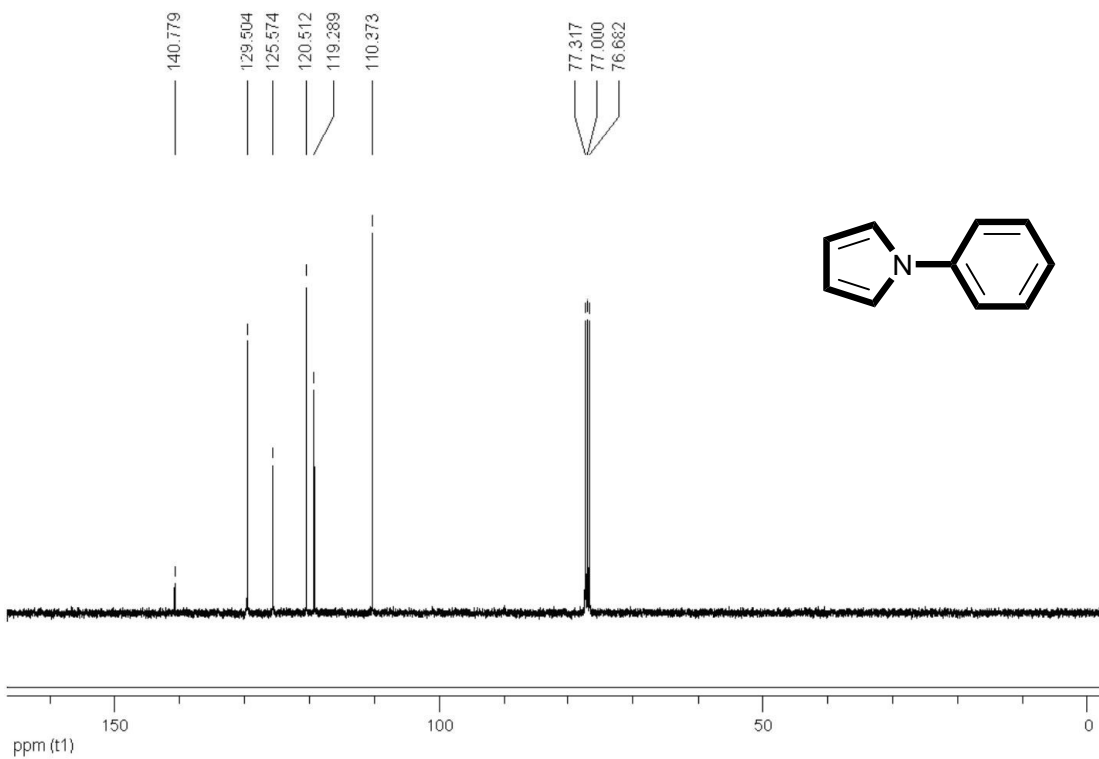
1-(Thiophen-3-yl)-1H-imidazole (C45):⁶

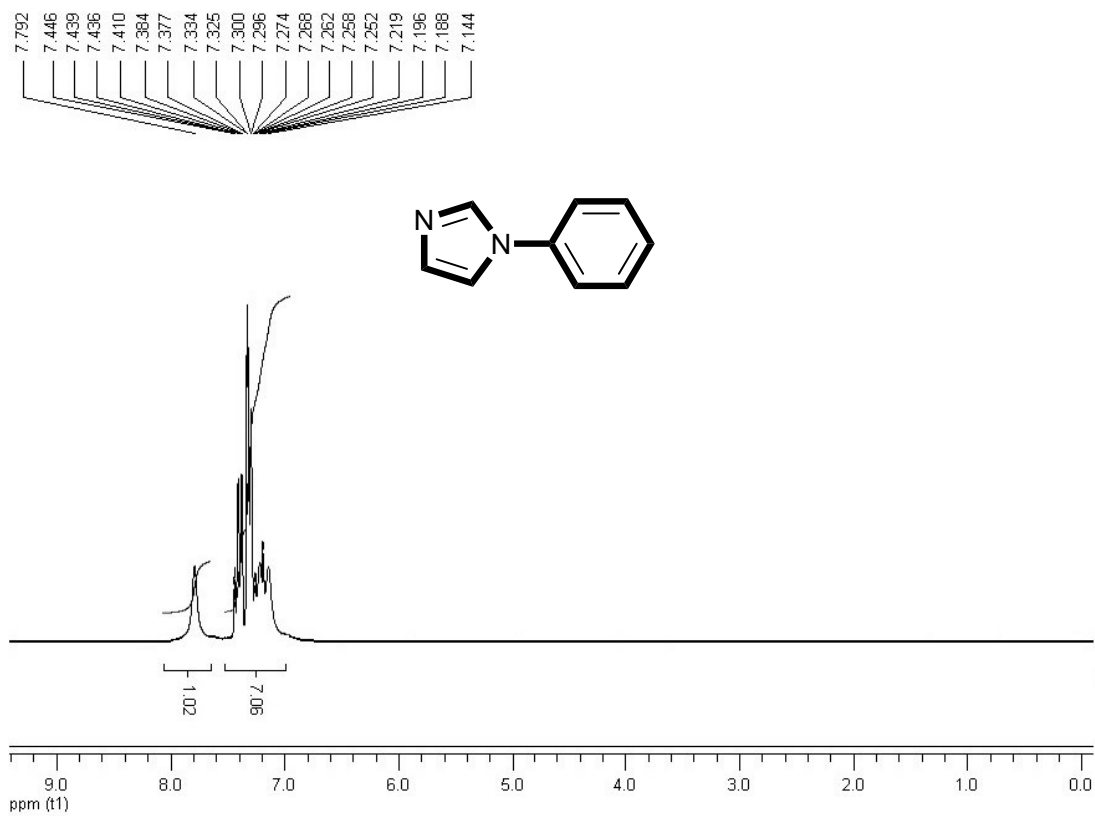
Yellow crystals; mp = 73-75 °C; ¹H NMR (250 MHz, CDCl₃): δ= 7.81 (s, 1H), 7.42 (d, *J* = 5.0 Hz, 1H), 7.23 (s, 1H), 7.23-7.13 (m, 3H); ¹³C NMR (63 MHz, CDCl₃): δ= 113.2, 118.5, 121.4, 127.2, 130.0, 135.8, 136.3; Anal. Calcd for C₉H₇NS: C, 67.35; H, 4.38; N, 8.69; S, 19.89%. Found: C, 67.31; H, 4.35; N, 8.72; S, 19.94%.

Notes and references

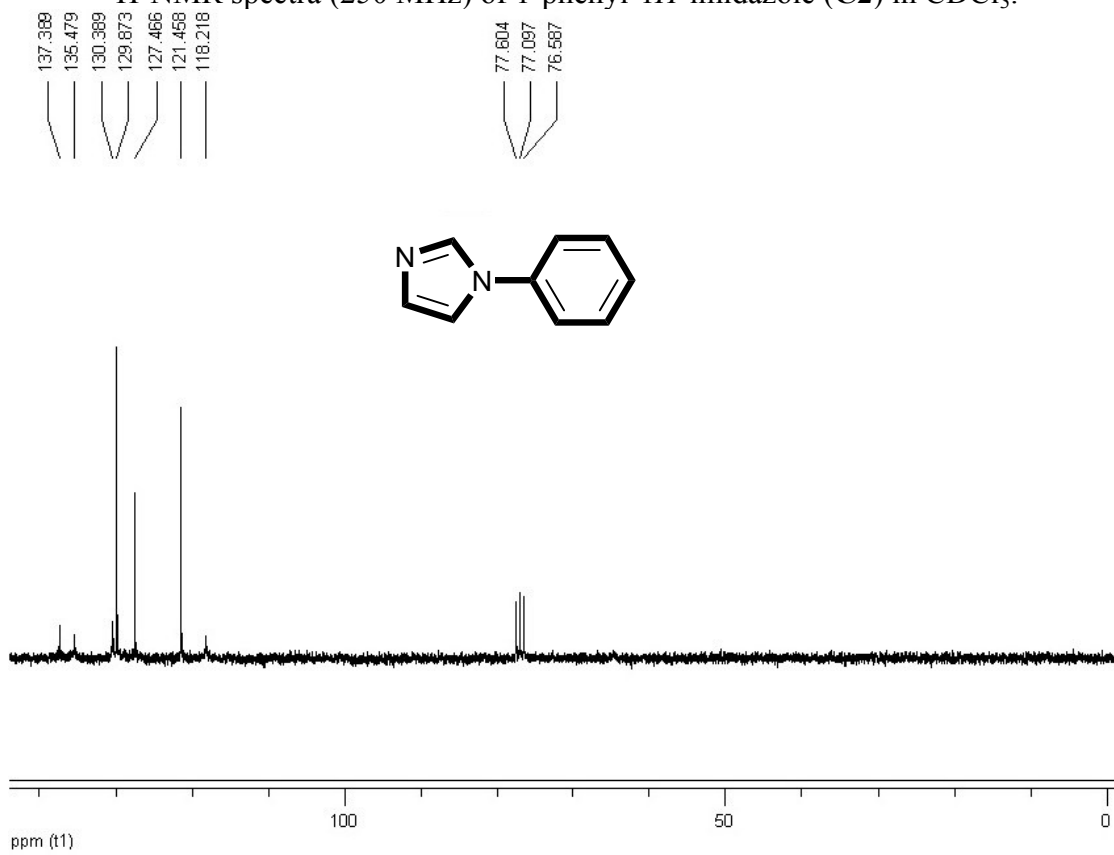
- 1 Q. Yang, Y. Wang, L. Yang, M. Zhang, *Tetrahedron*, 2013, **69**, 6230-6233.
- 2 D. Nandi, S. Siwal, K. Mallick, *New J. Chem.*, 2017, **41**, 3082-3088.
- 3 S. Zahmatkesh, M. Esmailpour, A. Mollaiy Poli, *Inorg. Nano-Met. Chem.*, 2019, **49**, 323-334.
- 4 G. Pai, A. P. Chattopadhyay, *Tetrahedron Lett.*, 2016, **57**, 3140-3145.
- 5 X. Zhu, L. Su, L. Huang, G. Chen, J. Wang, H. Song, Y. Wan, *Eur. J. Org. Chem.*, 2009, 635-642.
- 6 Y. Wang, Y. Zhang, B. Yang, A. Zhang, Q. Yao, *Org. Biomol. Chem.*, 2015, **13**, 4101-4114.
- 7 L. Li, L. Zhu, D. Chen, X. Hu, R. Wang, *Eur. J. Org. Chem.*, 2011, 2692-2696.

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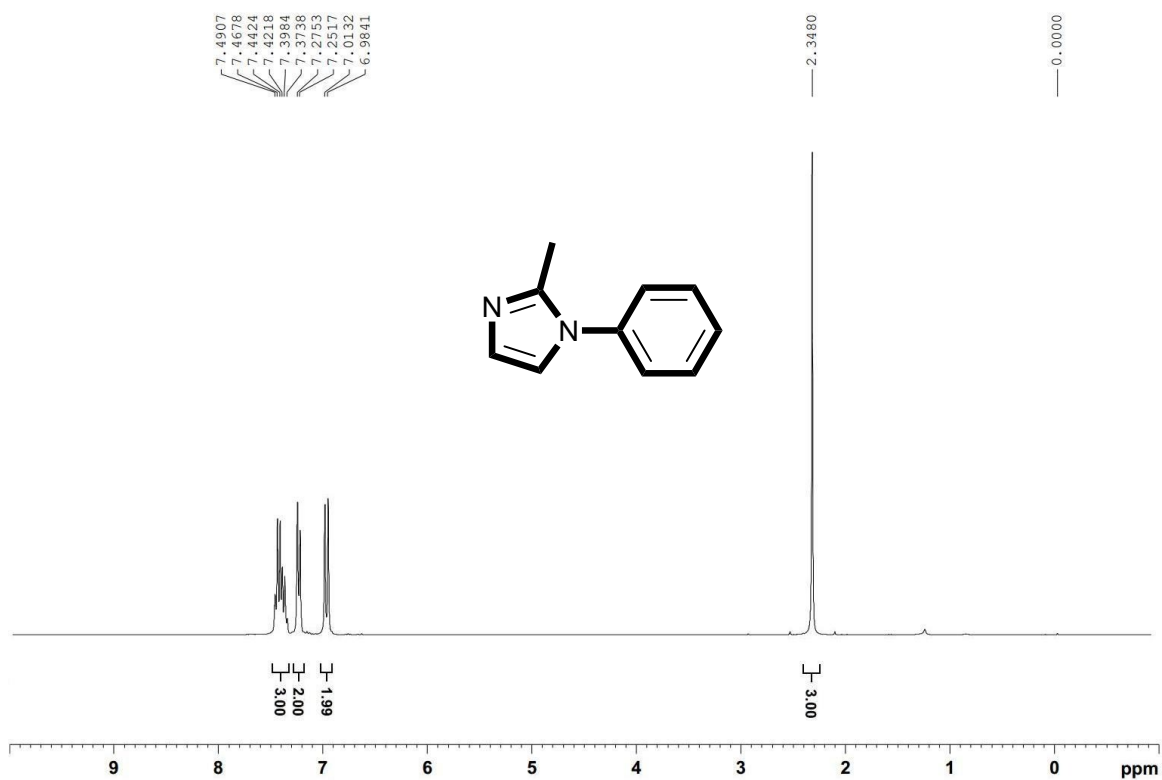
Product Characterizations:¹H-NMR spectra (250 MHz) of 1-phenyl-1*H*-pyrrole (**C1**) in CDCl₃.¹³C-NMR spectra (63 MHz) of 1-phenyl-1*H*-pyrrole (**C1**) in CDCl₃.



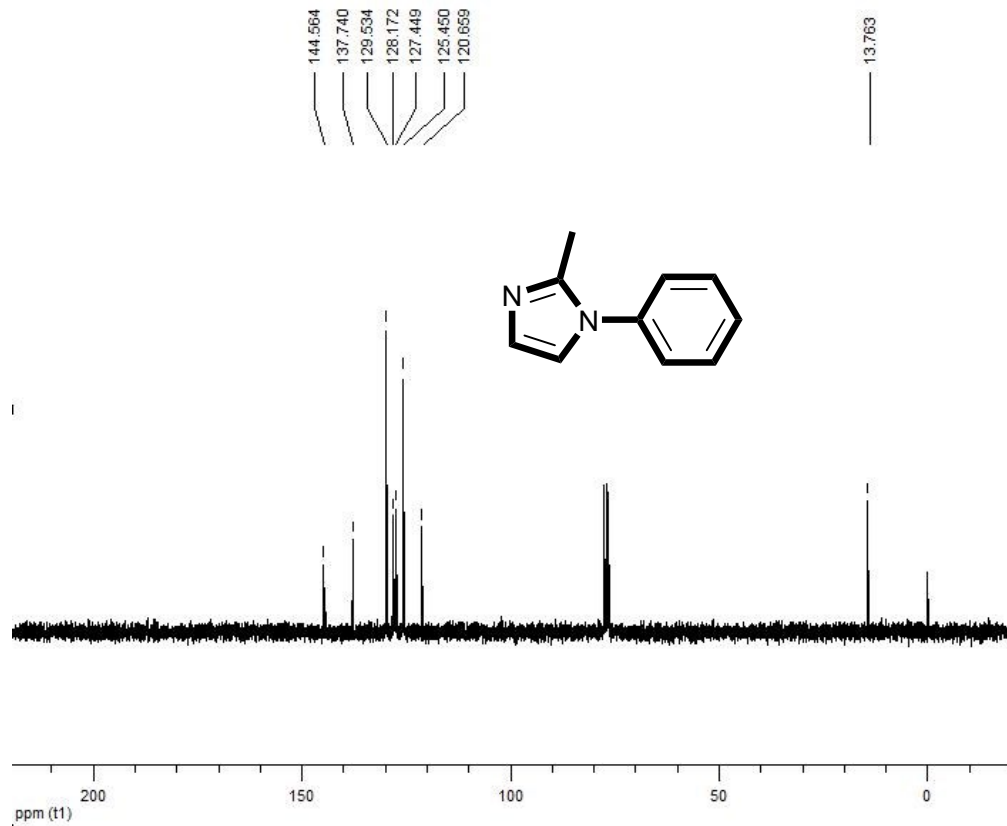
¹H-NMR spectra (250 MHz) of 1-phenyl-1*H*-imidazole (**C2**) in CDCl₃.



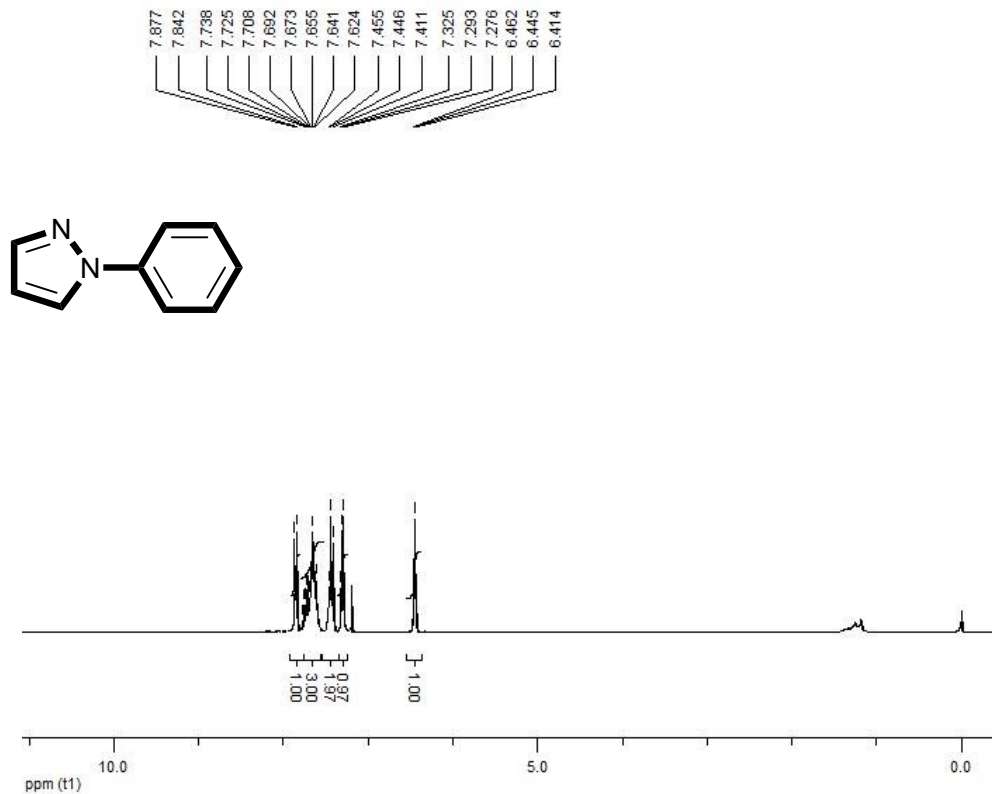
¹³C-NMR spectra (63 MHz) of 1-phenyl-1*H*-imidazole (**C2**) in CDCl₃.



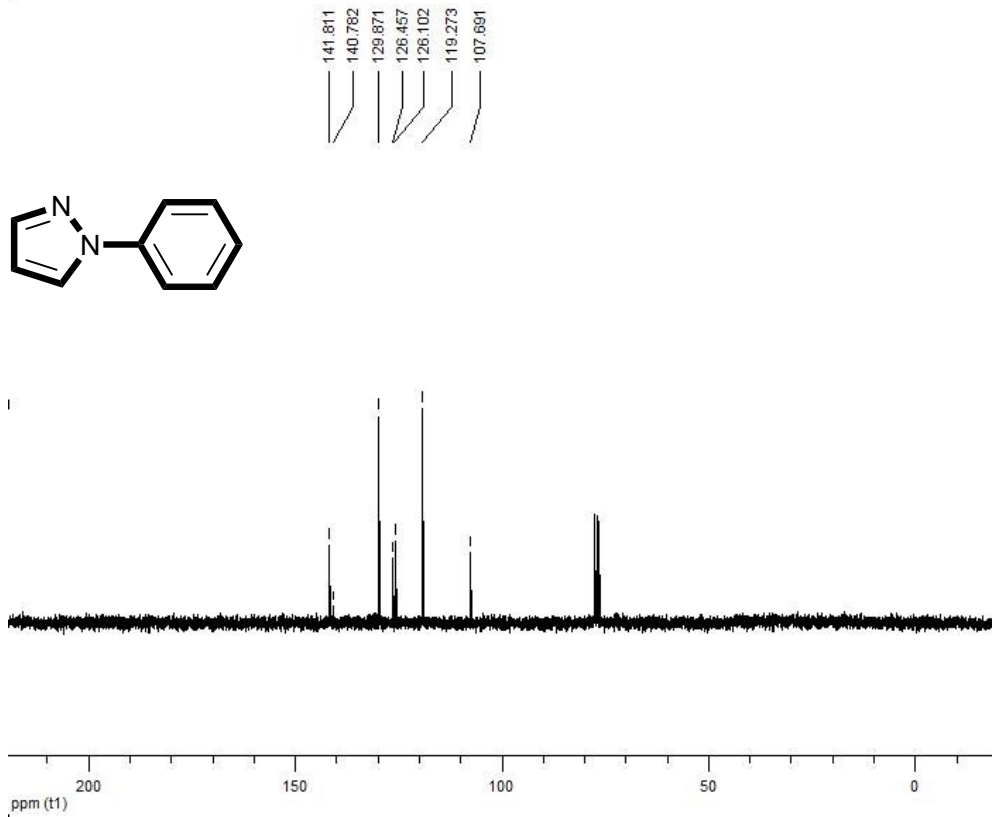
¹H-NMR spectra (250 MHz) of 2-methyl-1-phenyl-1*H*-imidazole (**C3**) in CDCl₃.



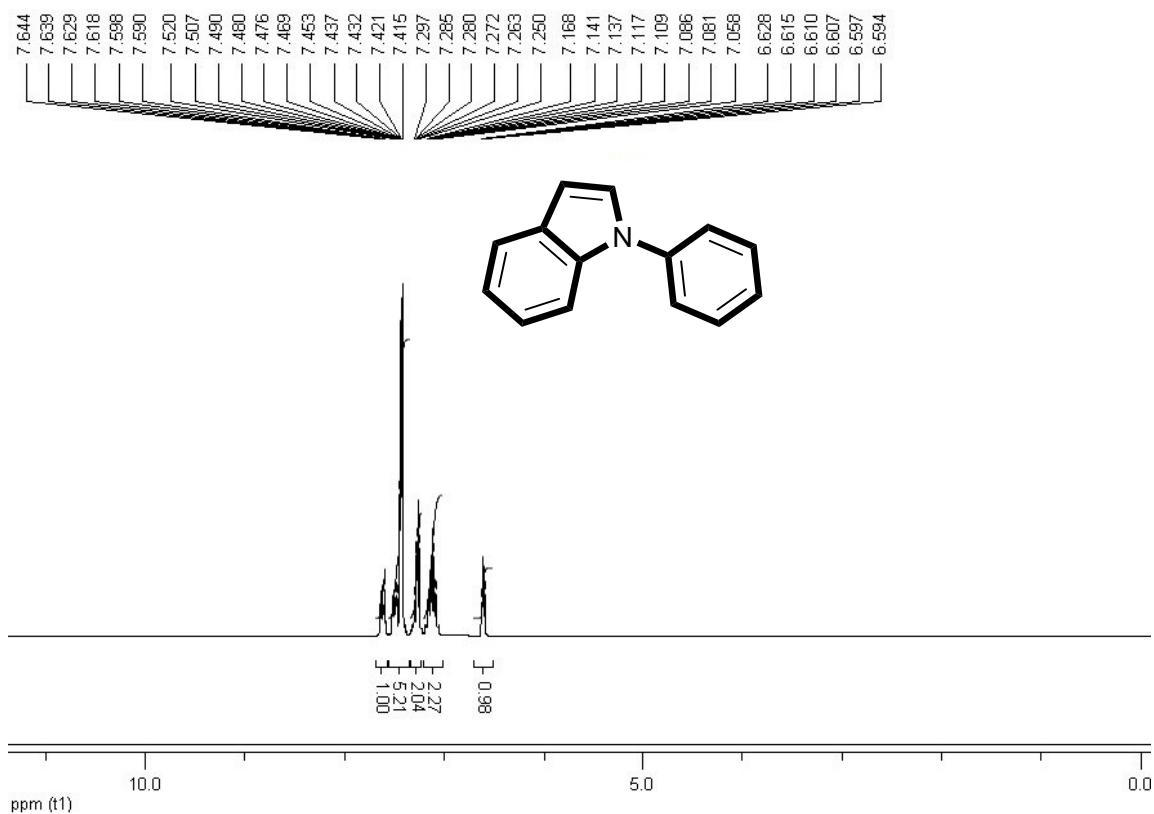
¹³C-NMR spectra (63 MHz) of 2-methyl-1-phenyl-1*H*-imidazole (**C3**) in CDCl₃.



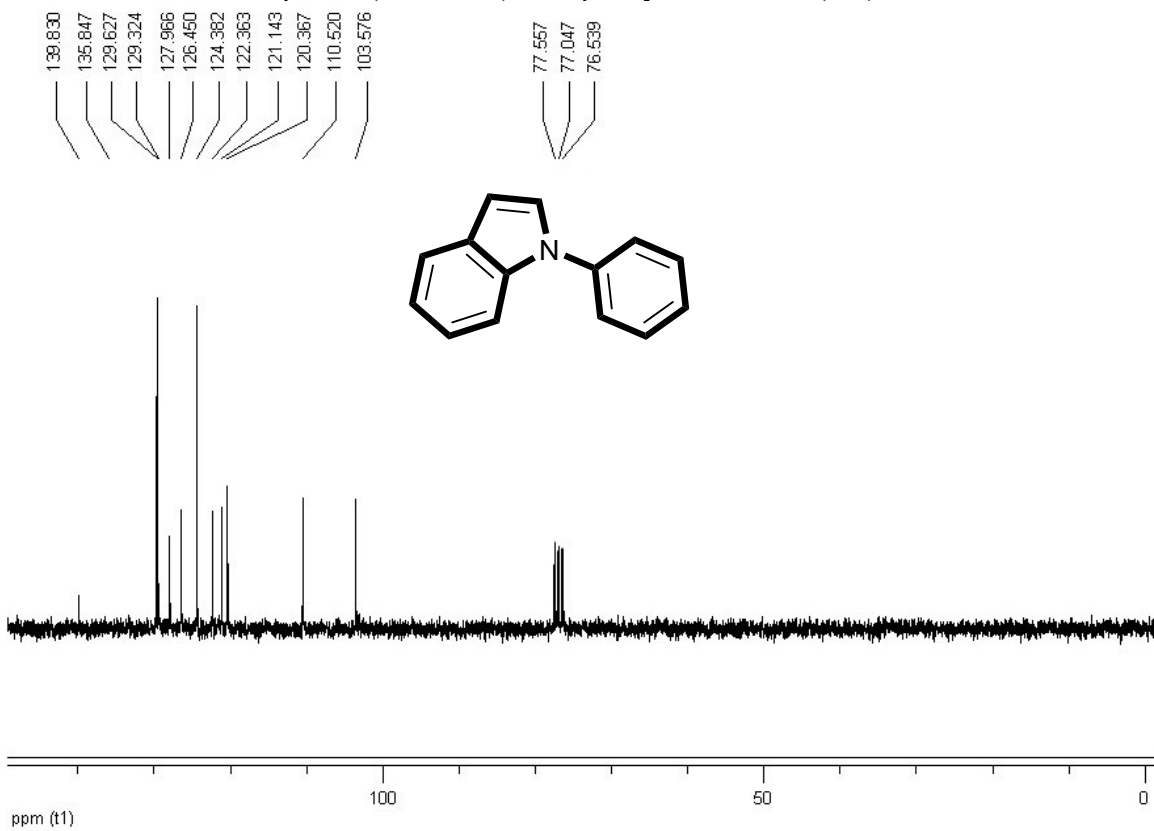
¹H-NMR spectra (250 MHz) of 1-phenyl-1*H*-pyrazole (C4) in CDCl₃.



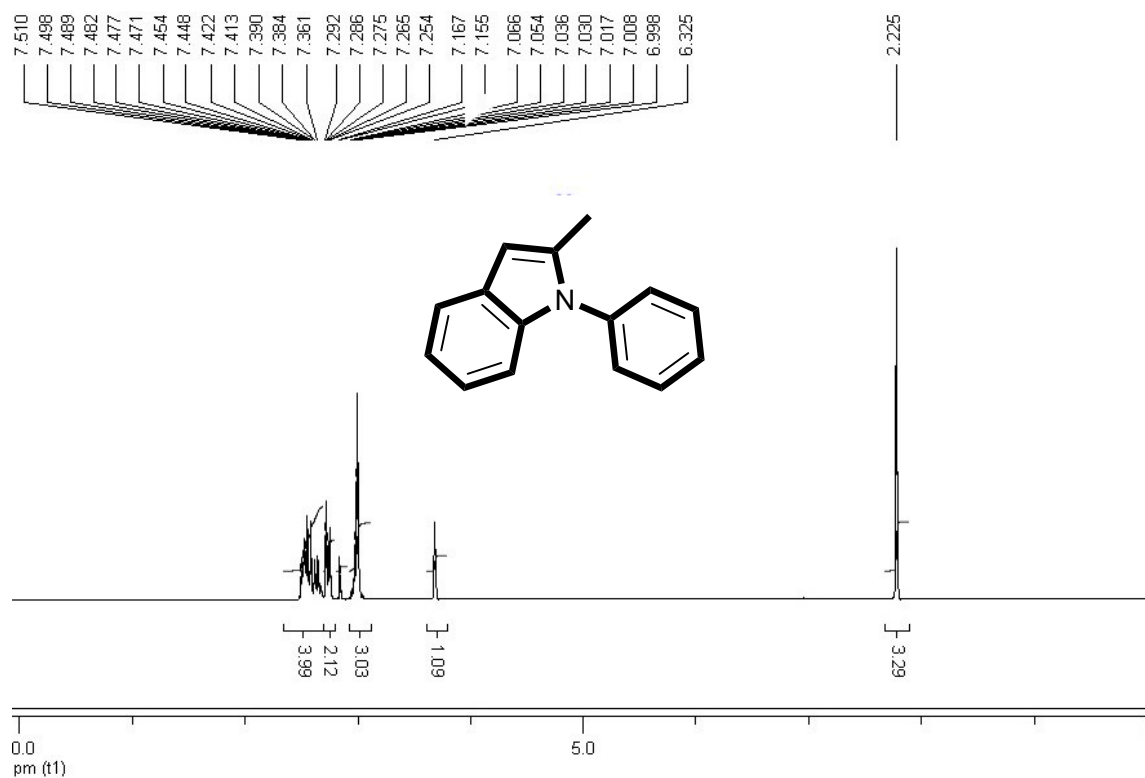
¹³C-NMR spectra (63 MHz) of 1-phenyl-1*H*-pyrazole (C4) in CDCl₃.



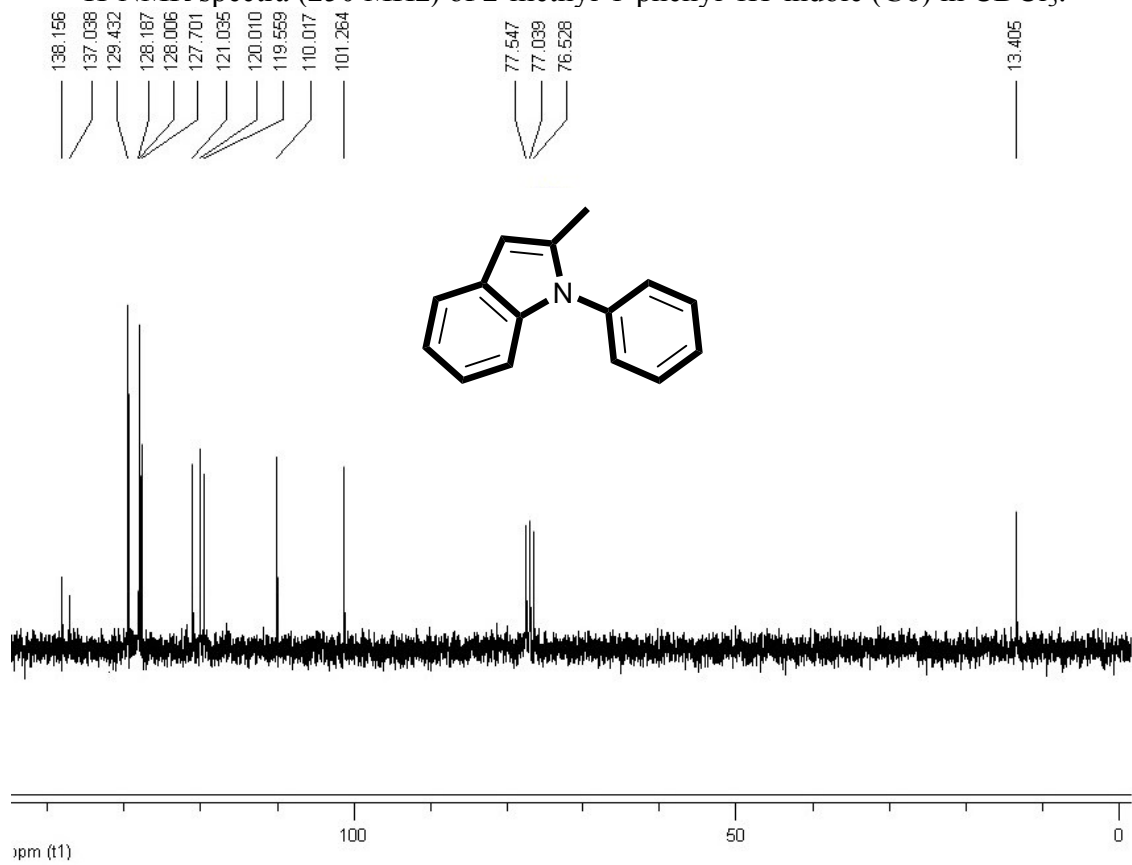
¹H-NMR spectra (250 MHz) of 1-phenyl-1*H*-indole (C5) in CDCl₃.



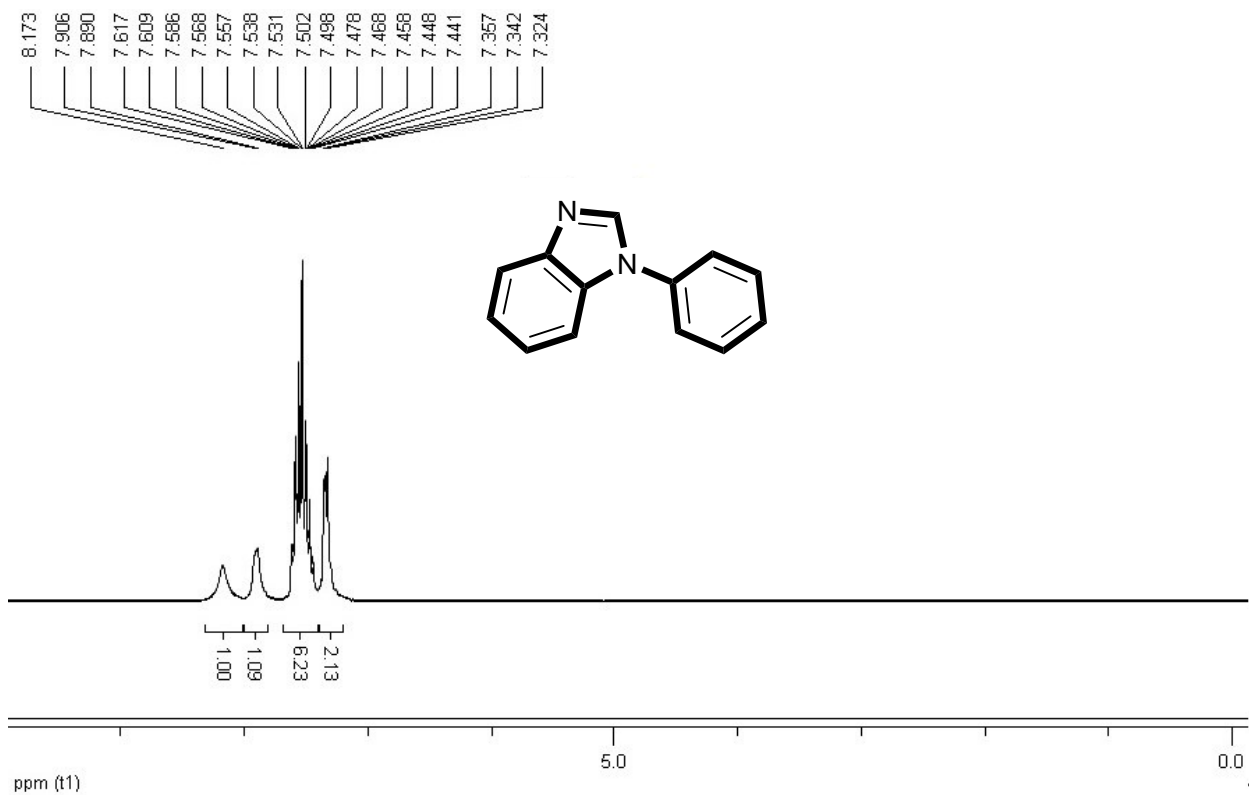
¹³C-NMR spectra (63 MHz) of 1-phenyl-1*H*-indole (C5) in CDCl₃.



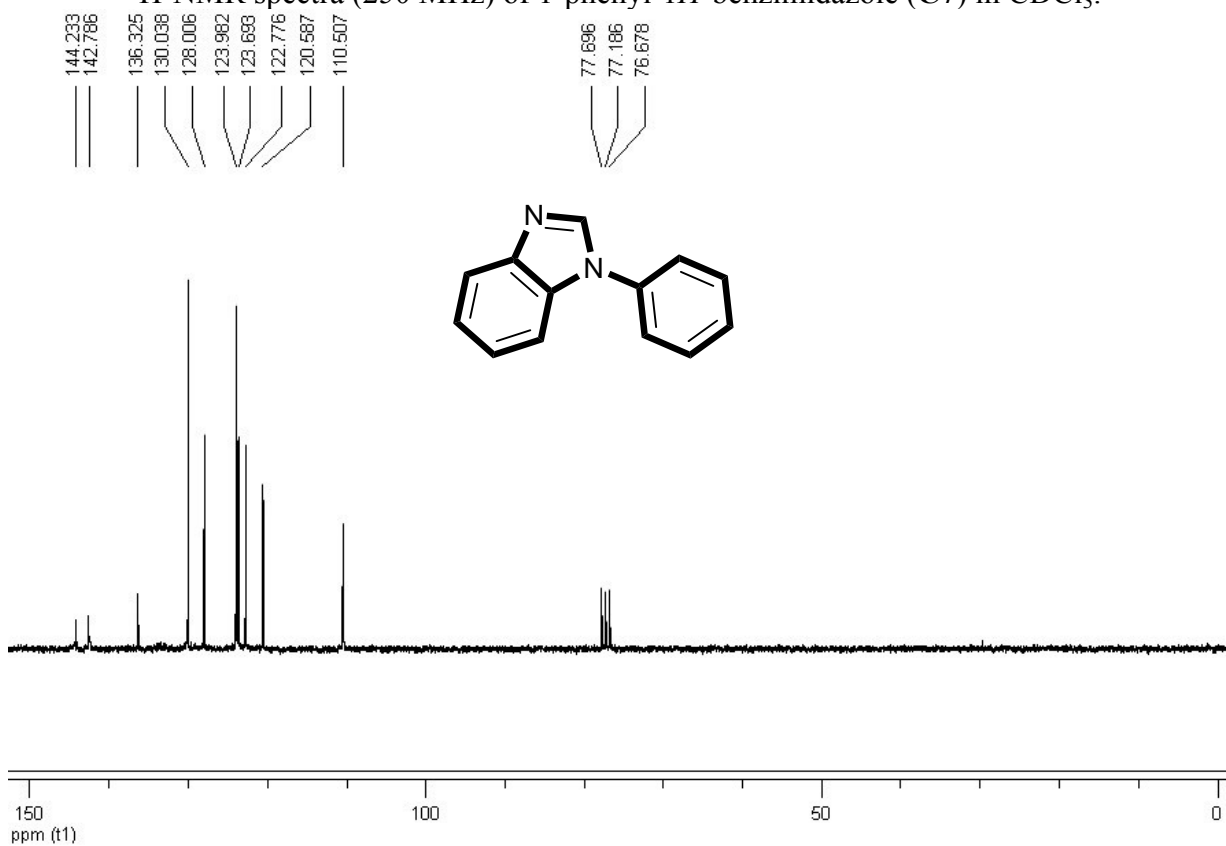
¹H-NMR spectra (250 MHz) of 2-methyl-1-phenyl-1H-indole (C6) in CDCl₃.



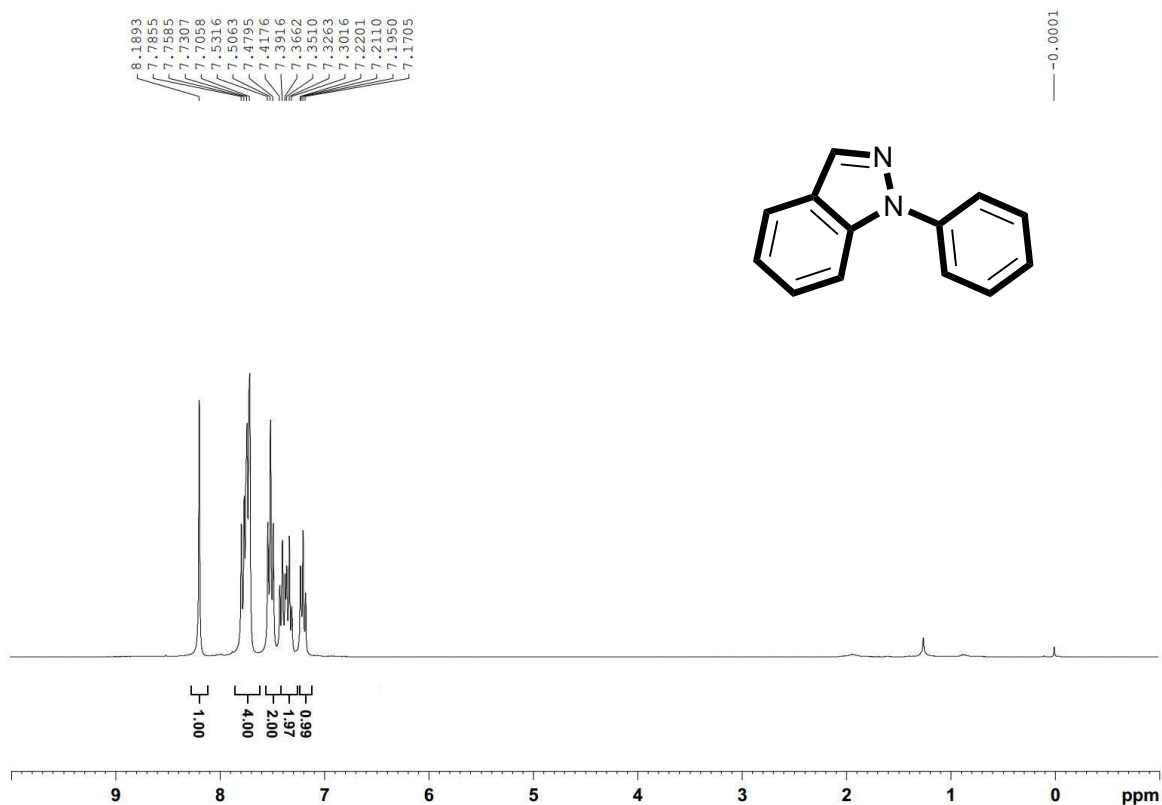
¹³C-NMR spectra (63 MHz) of 2-methyl-1-phenyl-1H-indole (C6) in CDCl₃.



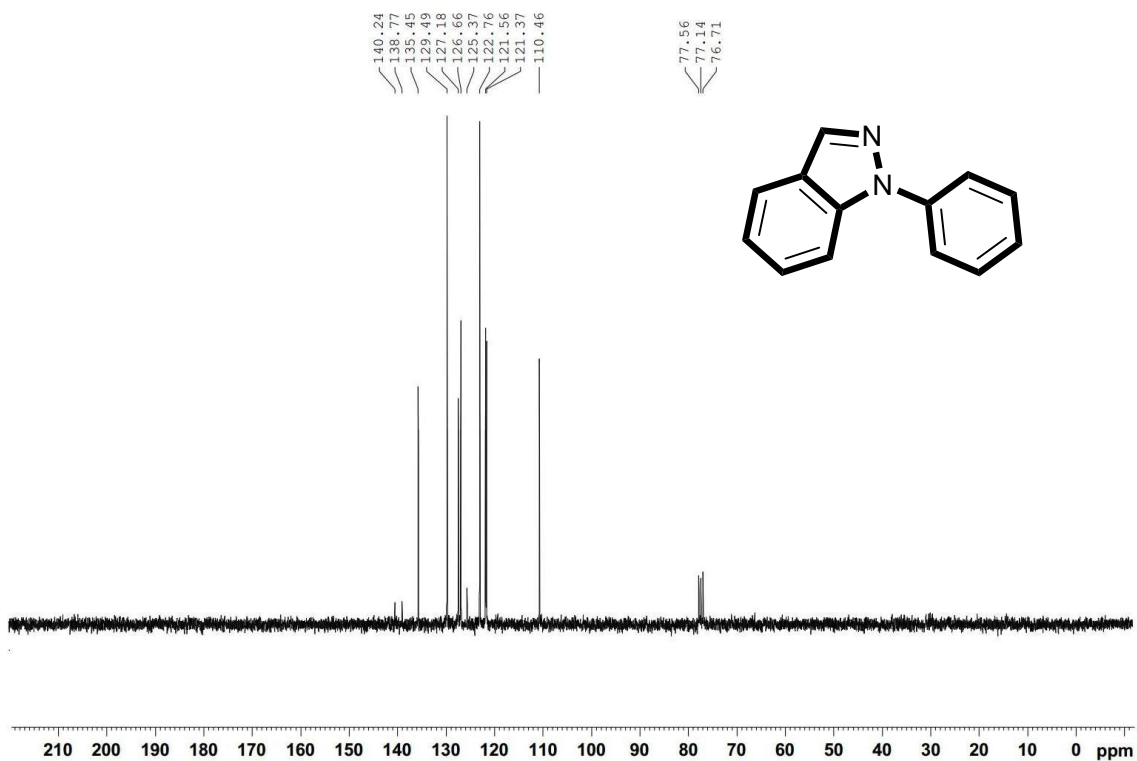
¹H-NMR spectra (250 MHz) of 1-phenyl-1*H*-benzimidazole (C7) in CDCl₃.



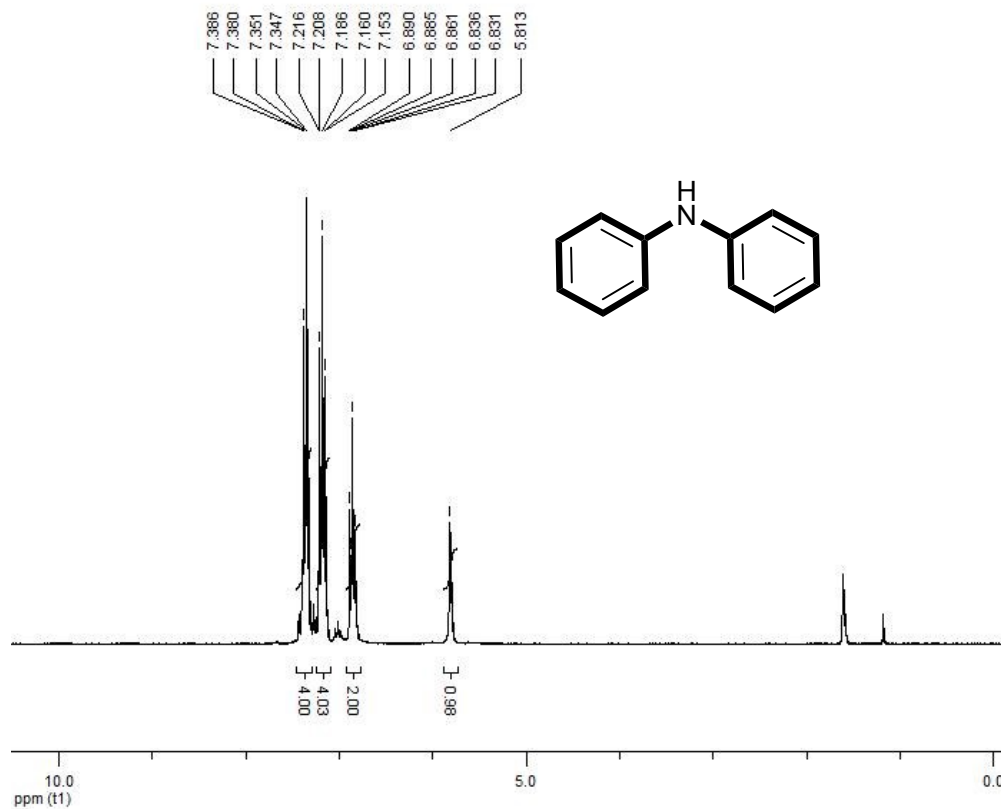
¹³C-NMR spectra (63 MHz) of 1-phenyl-1*H*-benzimidazole (C7) in CDCl₃.



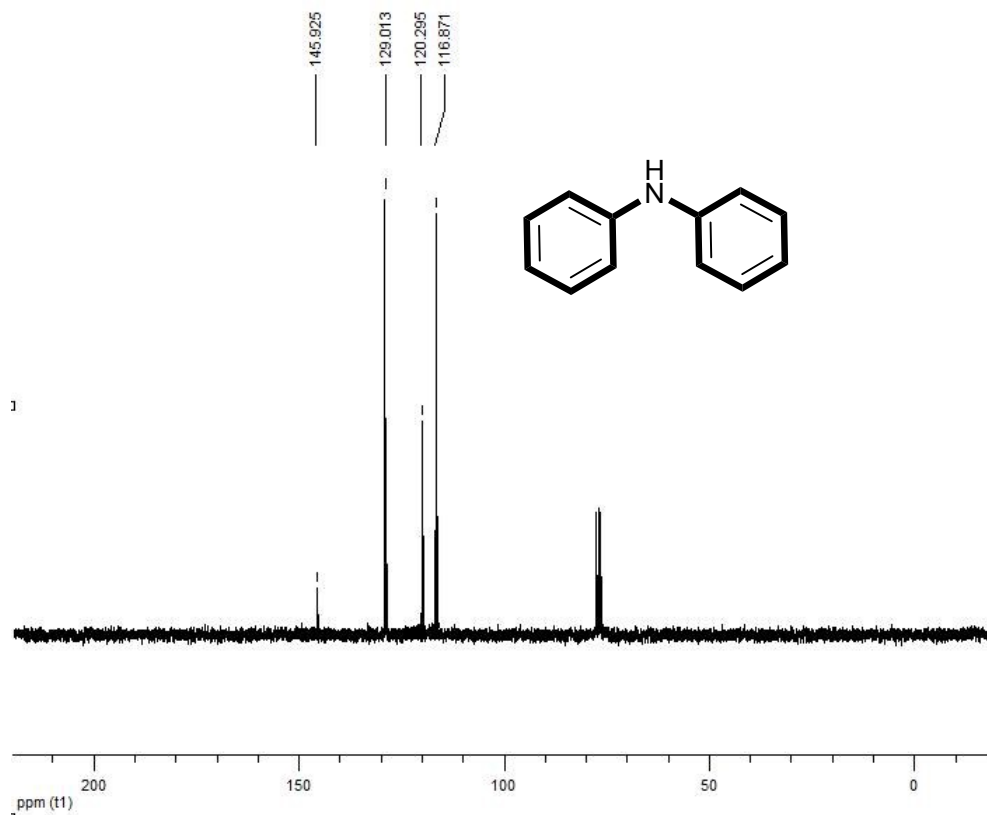
¹H-NMR spectra (250 MHz) of 1-phenyl-1*H*-indazole (C8) in CDCl₃.



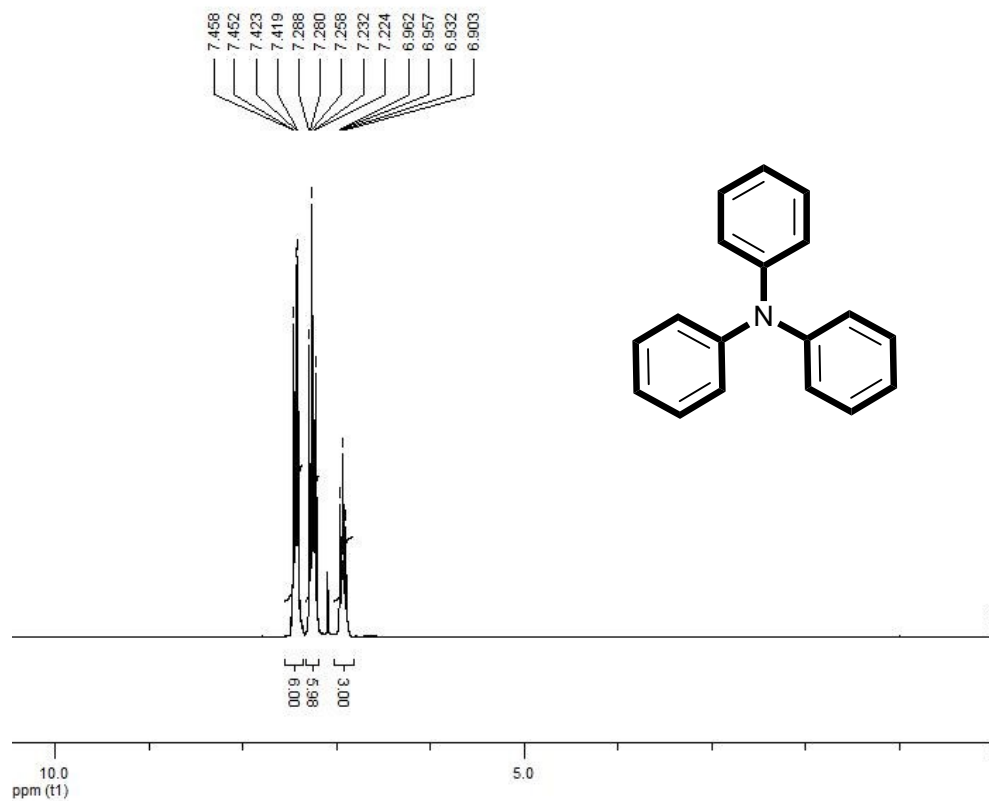
¹³C-NMR spectra (63 MHz) of 1-phenyl-1*H*-indazole (C8) in CDCl₃.



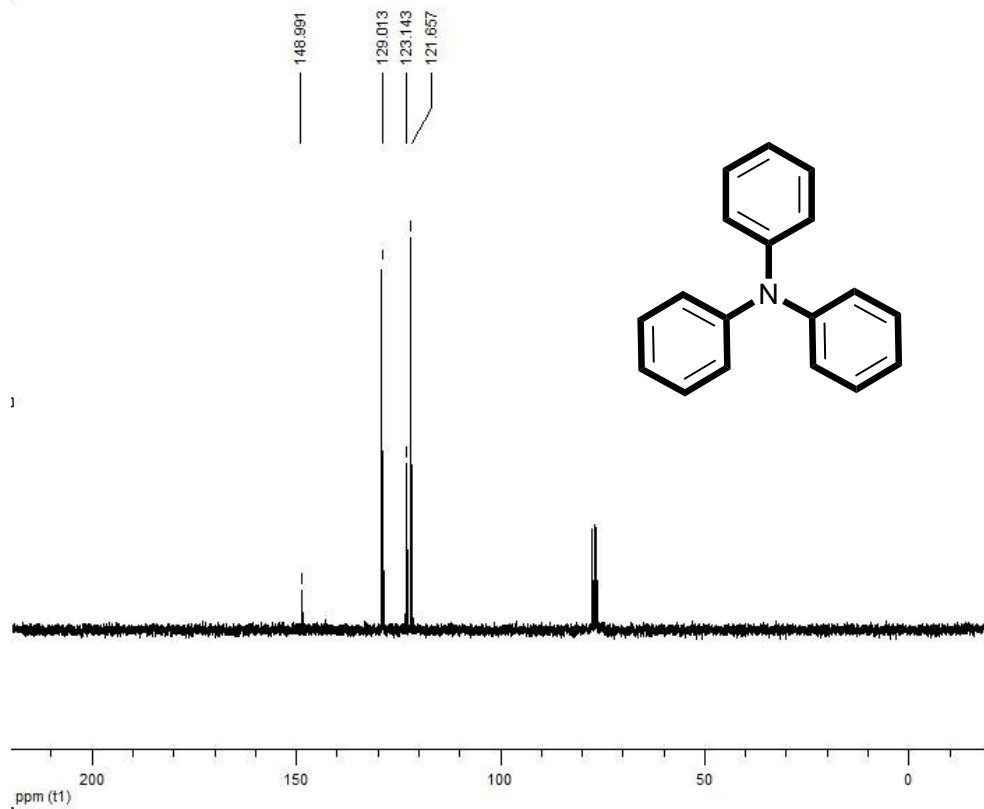
¹H-NMR spectra (250 MHz) of diphenylamine (C9) in CDCl₃.



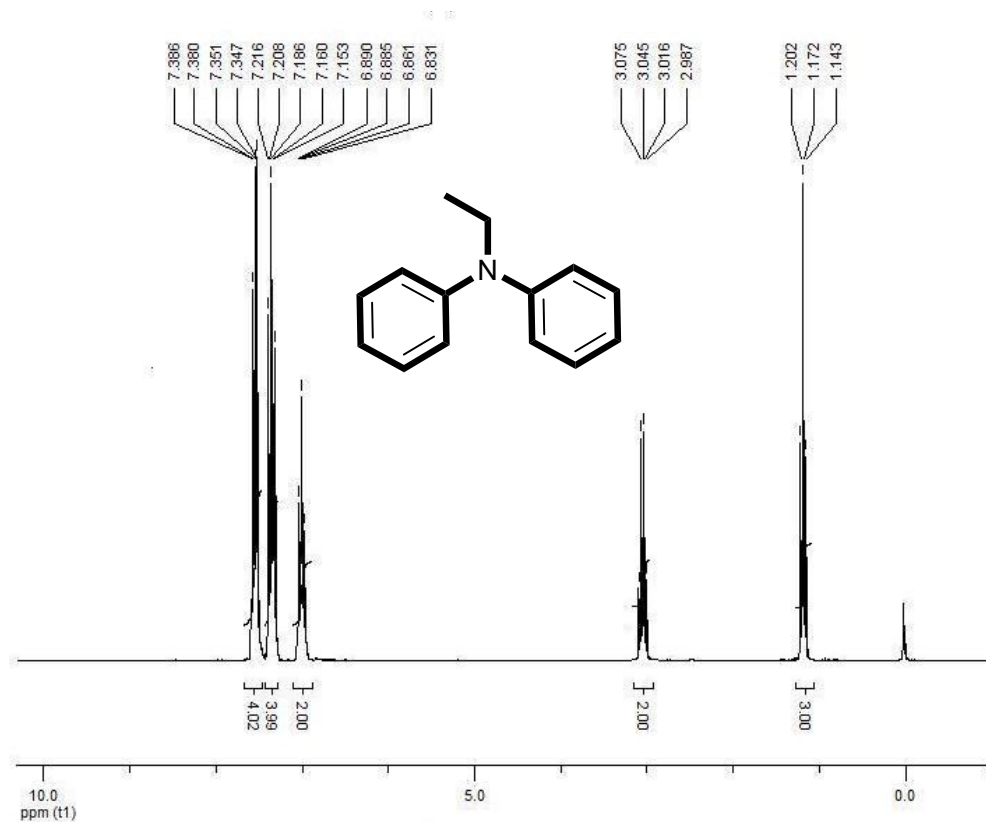
¹³C-NMR spectra (63 MHz) of diphenylamine (C9) in CDCl₃.



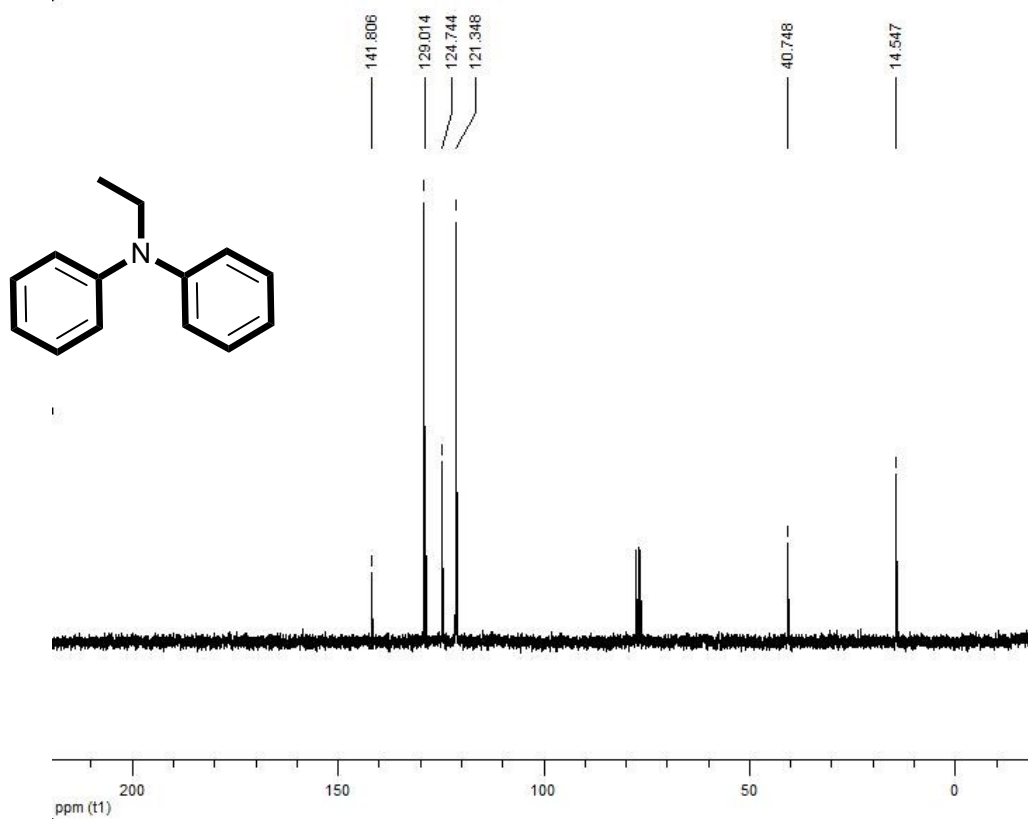
¹H-NMR spectra (250 MHz) of triphenylamine (C10) in CDCl₃.



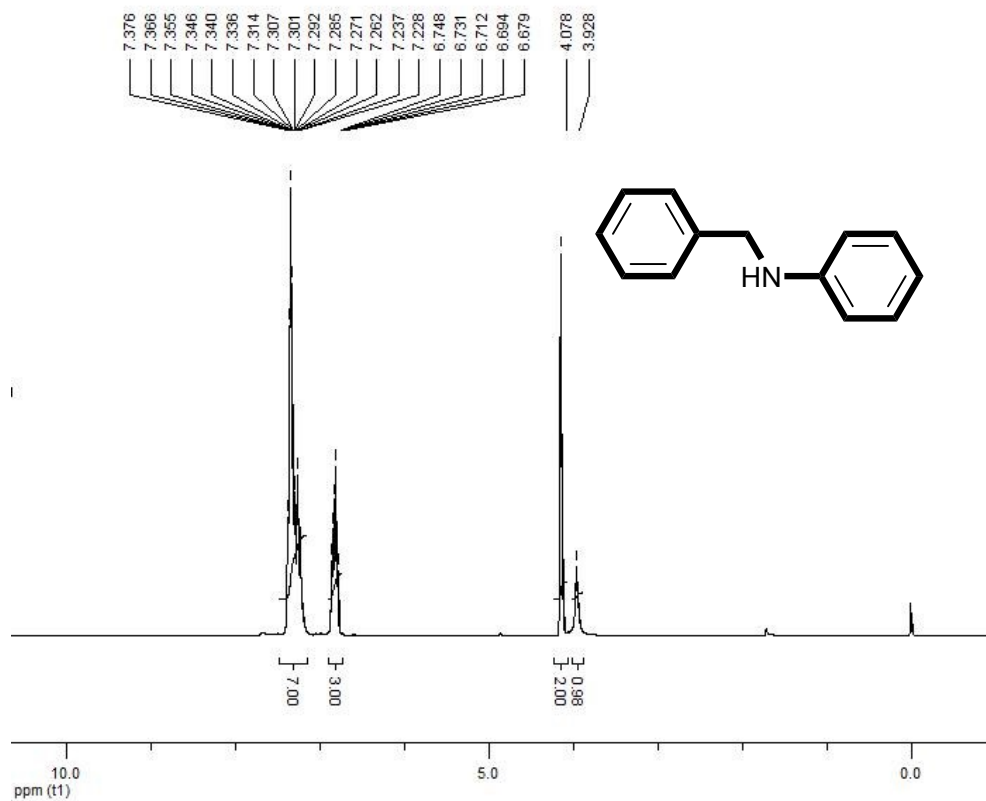
¹³C-NMR spectra (63 MHz) of triphenylamine (C10) in CDCl₃.



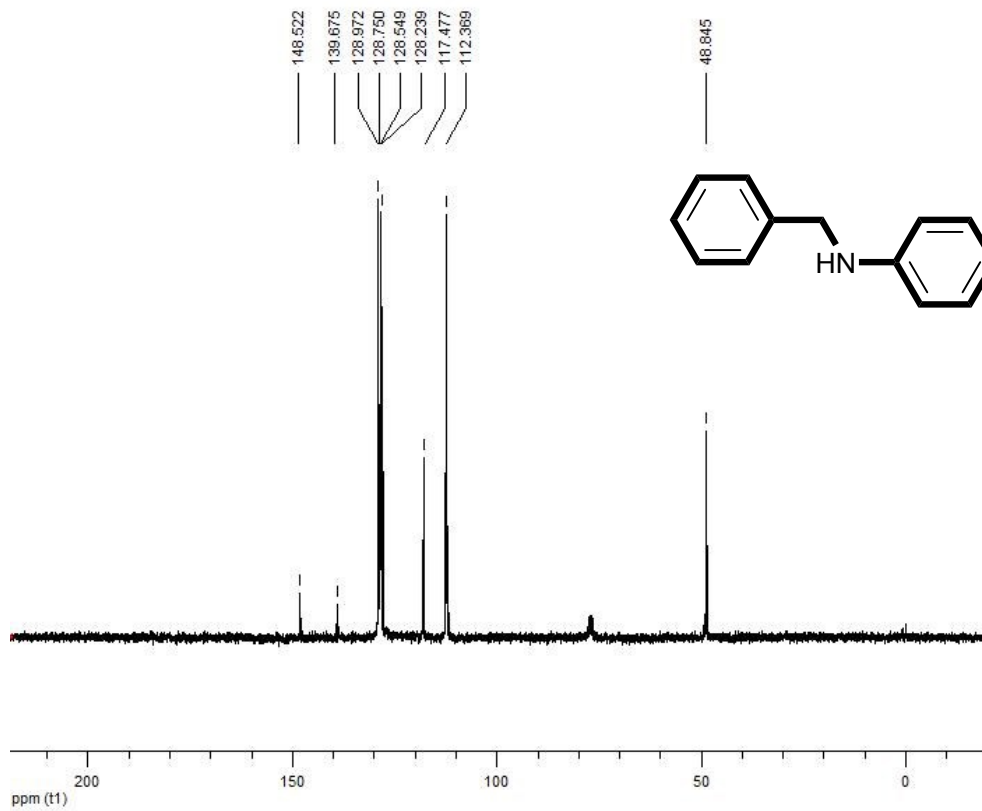
¹H-NMR spectra (250 MHz) of *N*-ethyl-*N*-phenylaniline (C11) in CDCl₃.



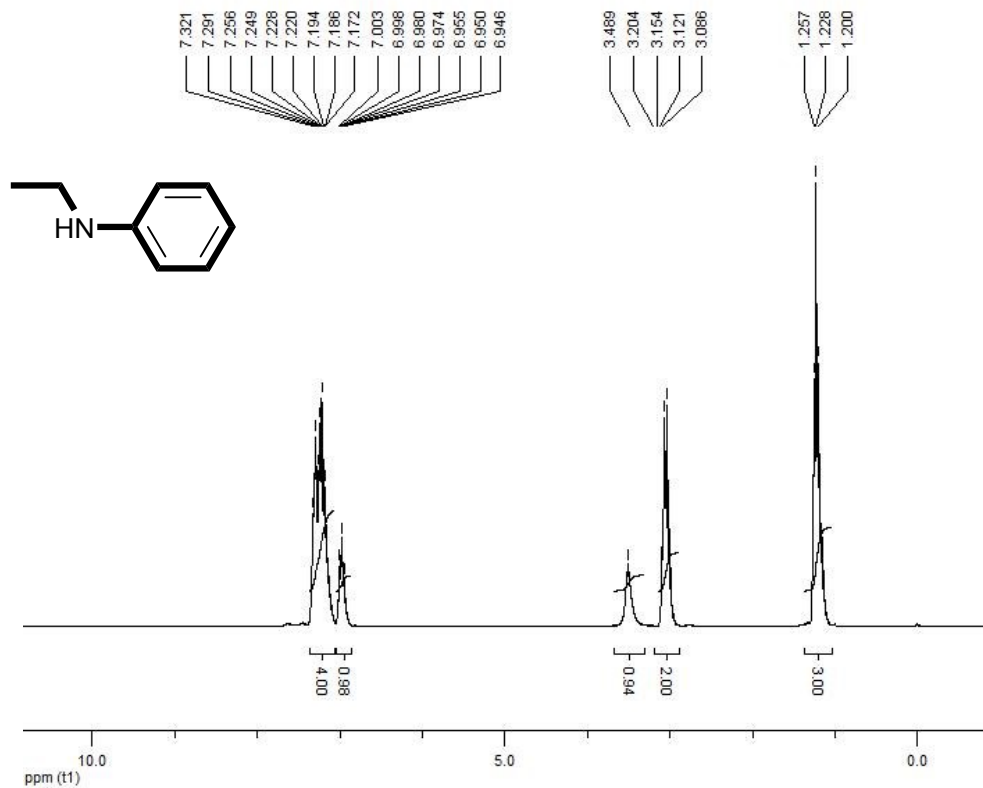
¹³C-NMR spectra (63 MHz) of *N*-ethyl-*N*-phenylaniline (C11) in CDCl₃.



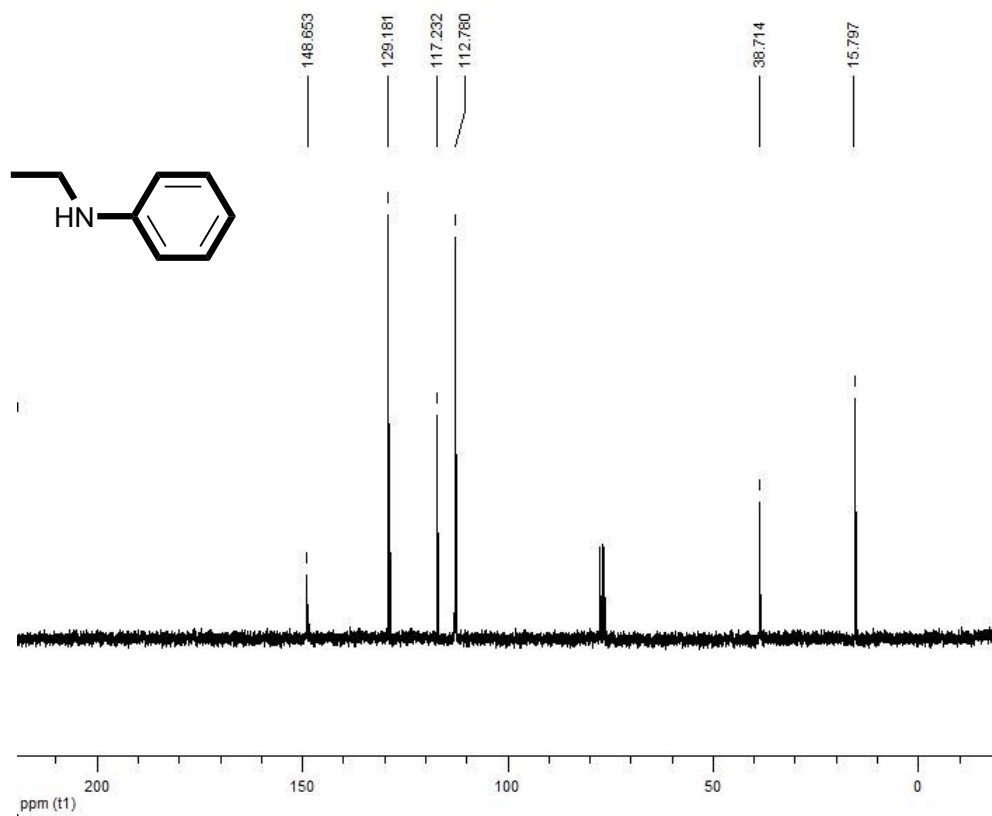
¹H-NMR spectra (250 MHz) of *N*-benzylaniline (C12) in CDCl₃.



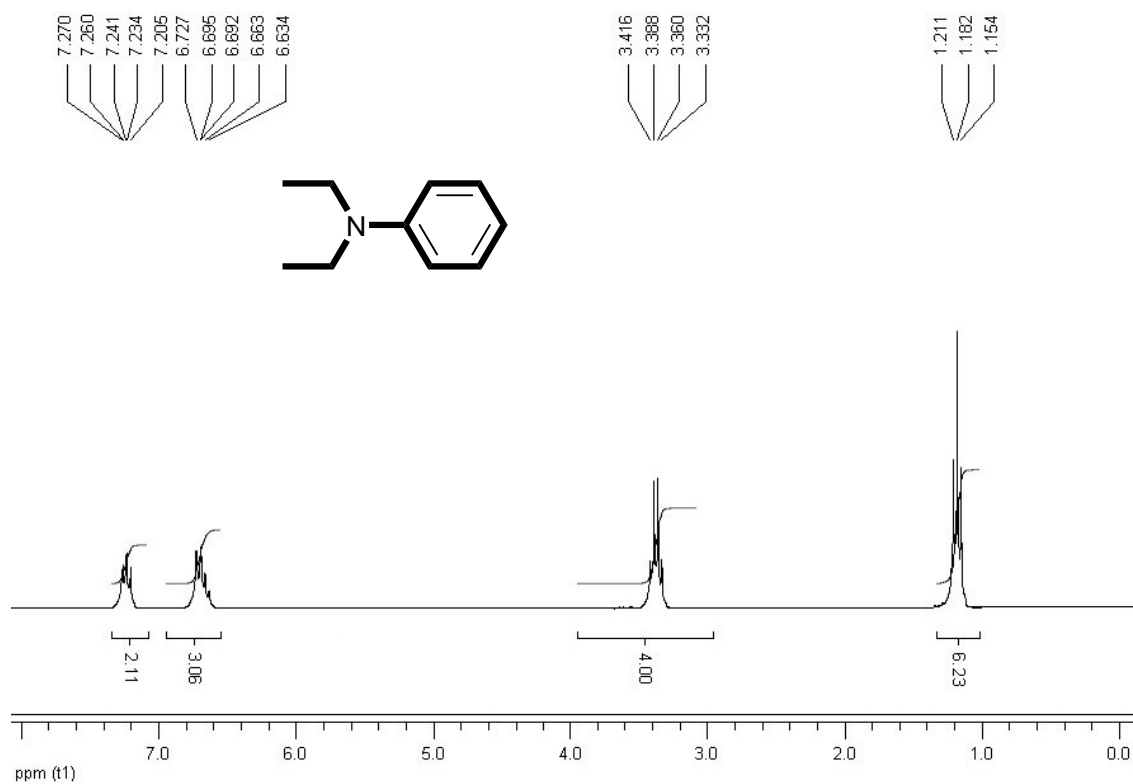
¹³C-NMR spectra (63 MHz) of *N*-benzylaniline (C12) in CDCl₃.



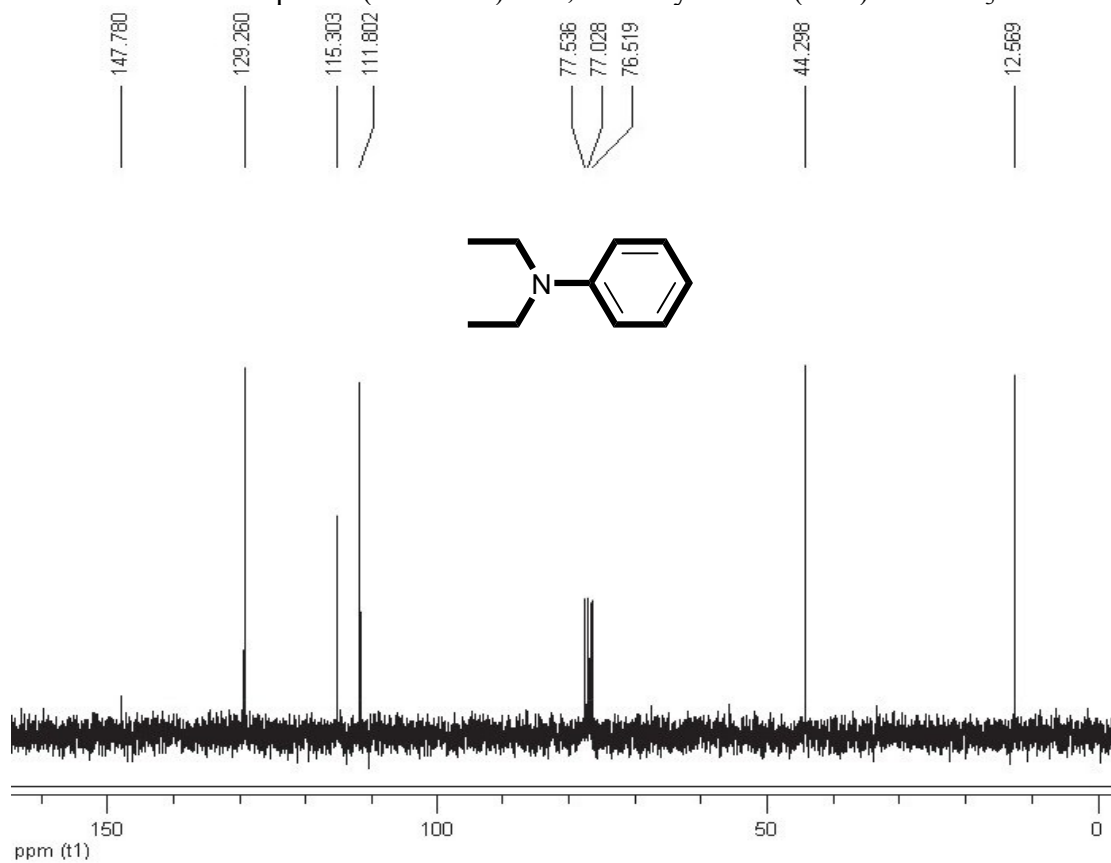
¹H-NMR spectra (250 MHz) of *N*-ethylaniline (**C13**) in CDCl₃.



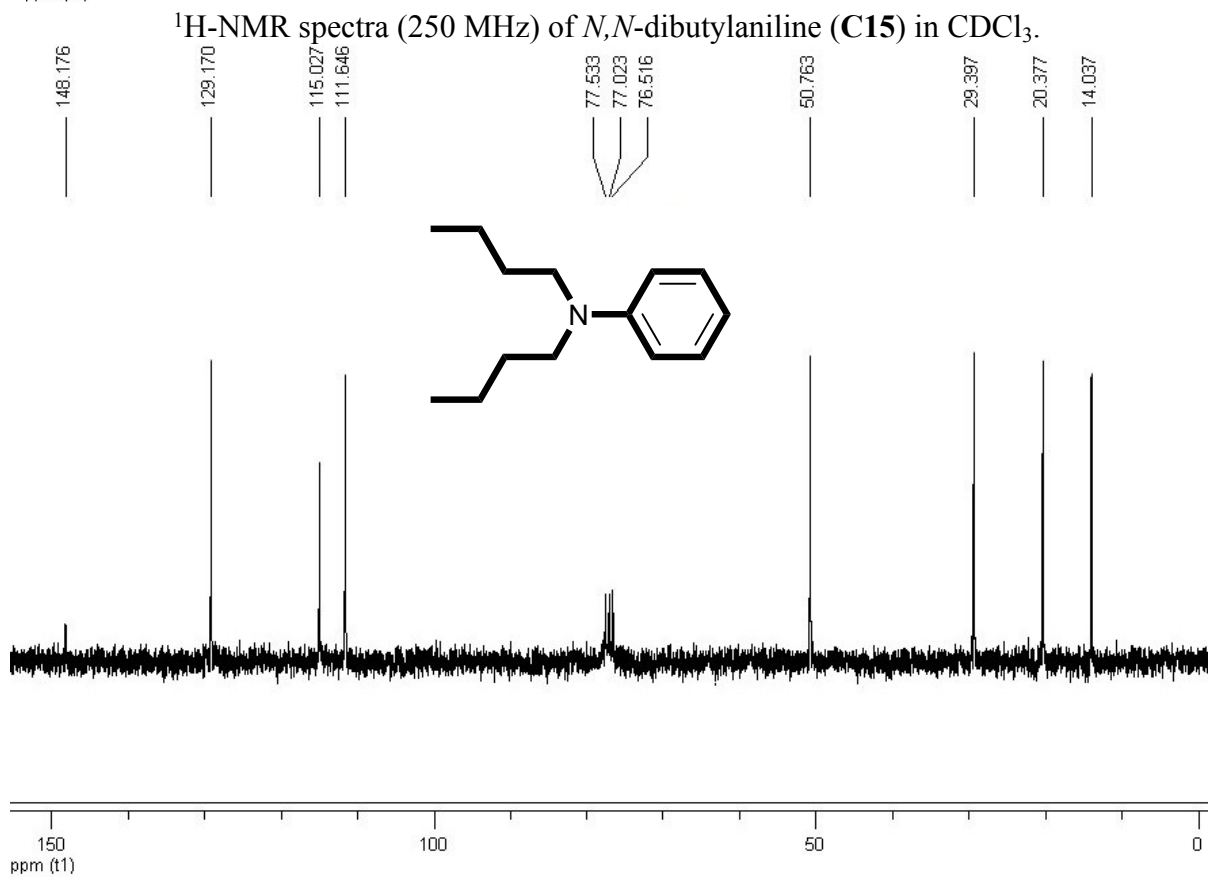
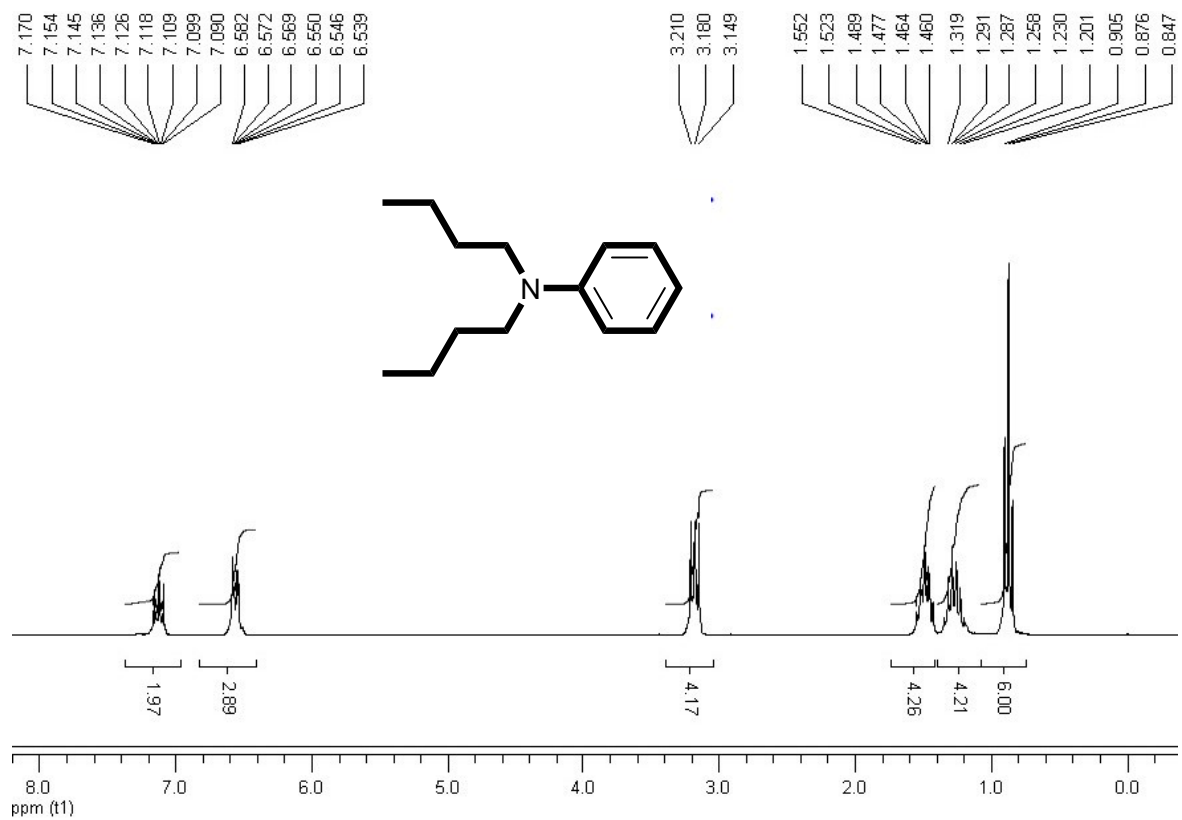
¹³C-NMR spectra (63 MHz) of *N*-ethylaniline (**C13**) in CDCl₃.

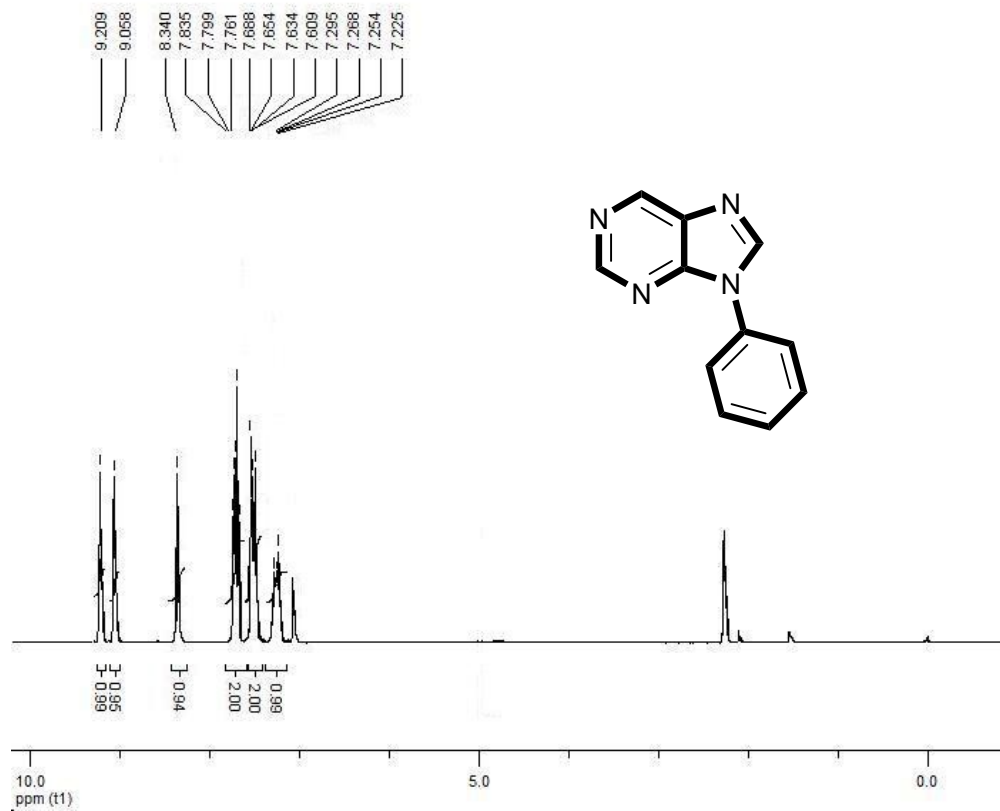


¹H-NMR spectra (250 MHz) of *N,N*-diethylaniline (**C14**) in CDCl₃.

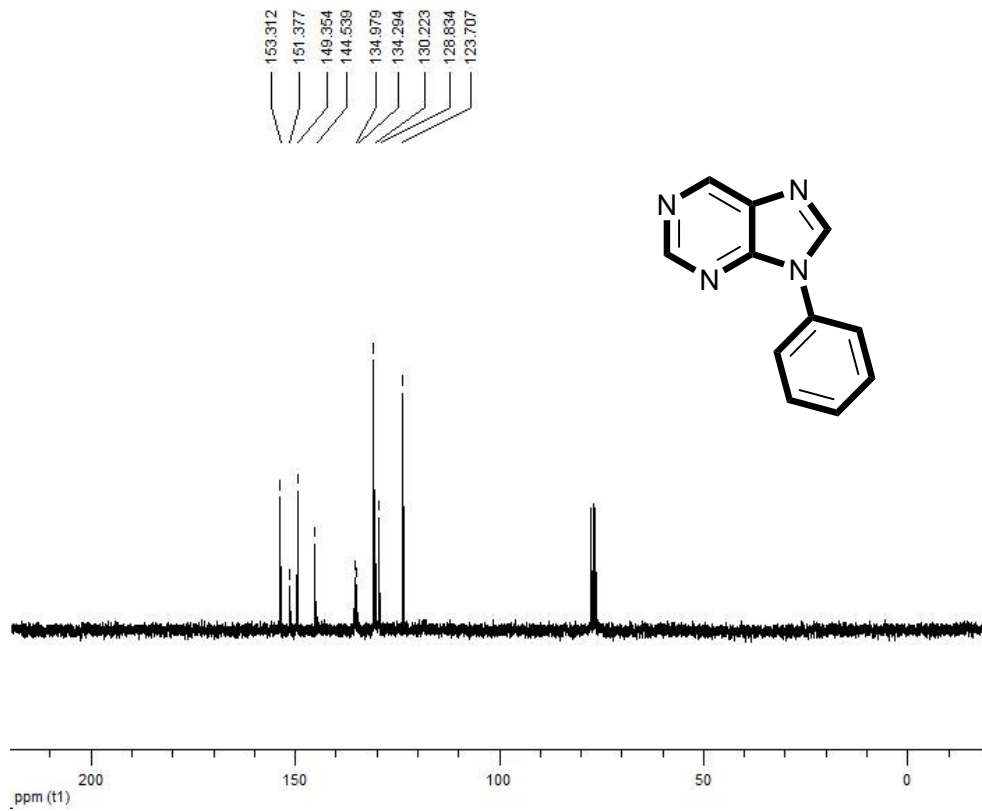


¹³C-NMR spectra (63 MHz) of *N,N*-diethylaniline (**C14**) in CDCl₃.

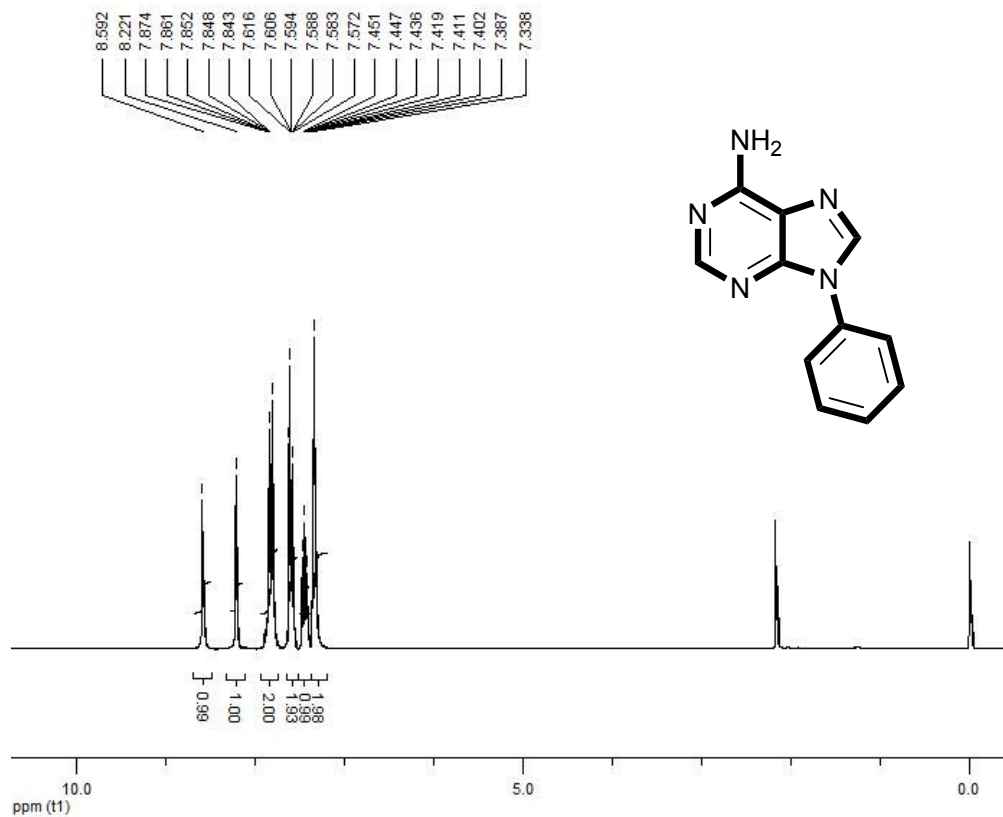




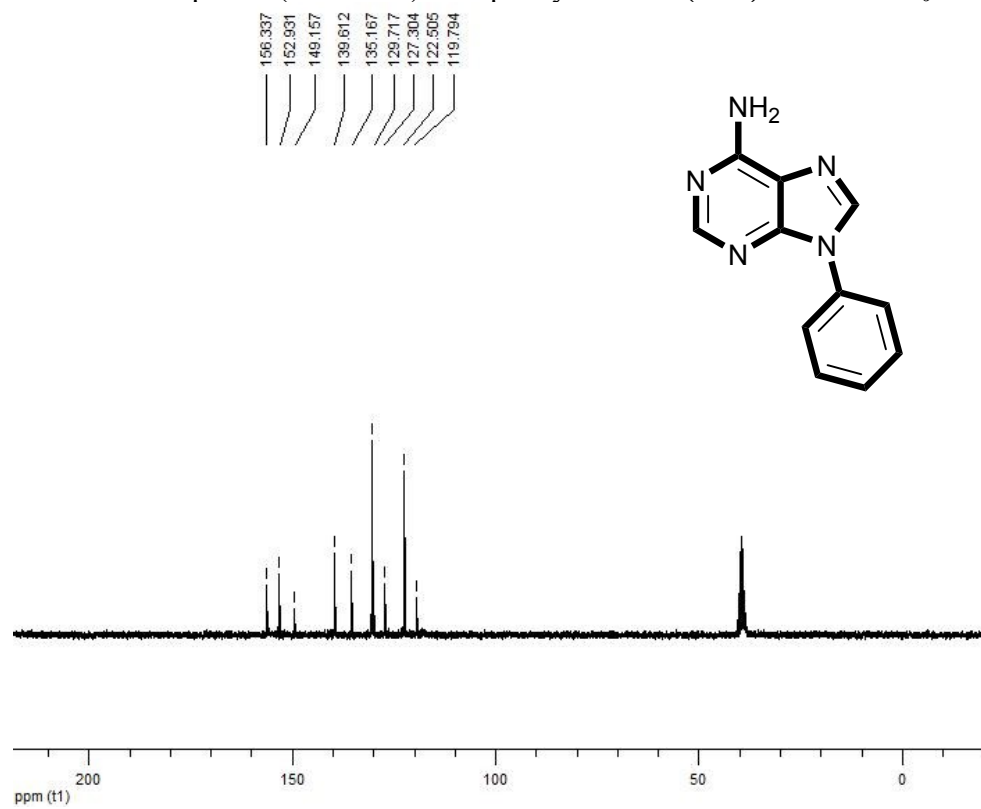
¹H-NMR spectra (250 MHz) of 9-phenylpurine (C16) in CDCl₃.



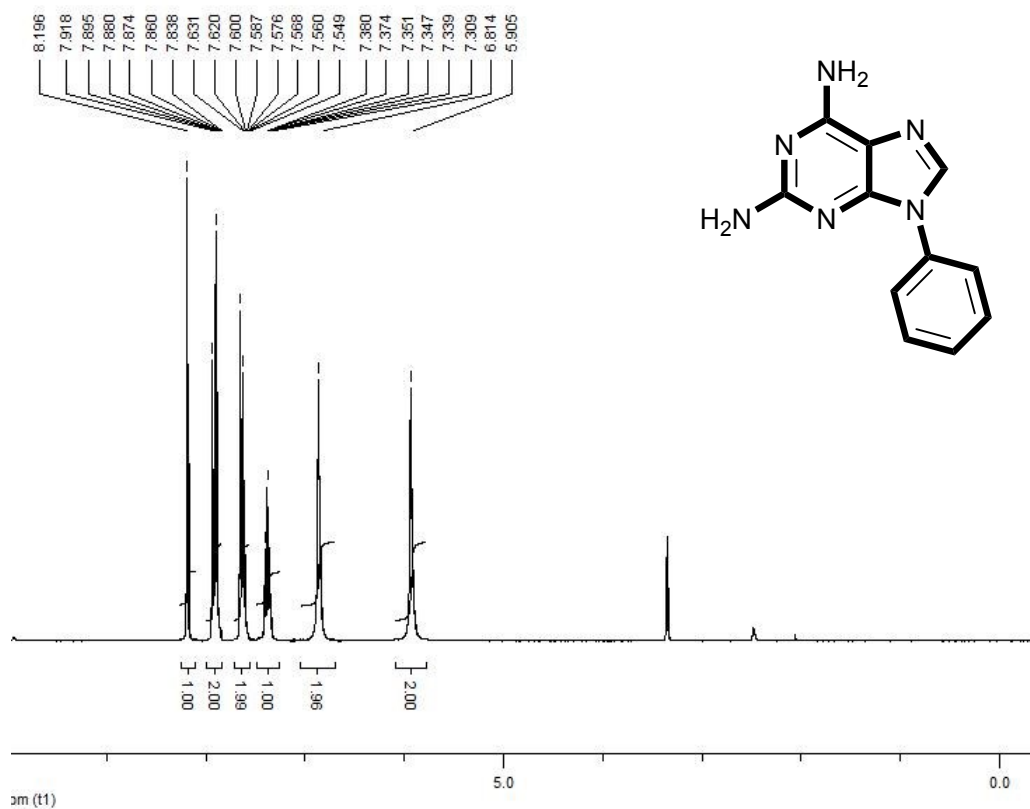
¹³C-NMR spectra (63 MHz) of 9-phenylpurine (C16) in CDCl₃.



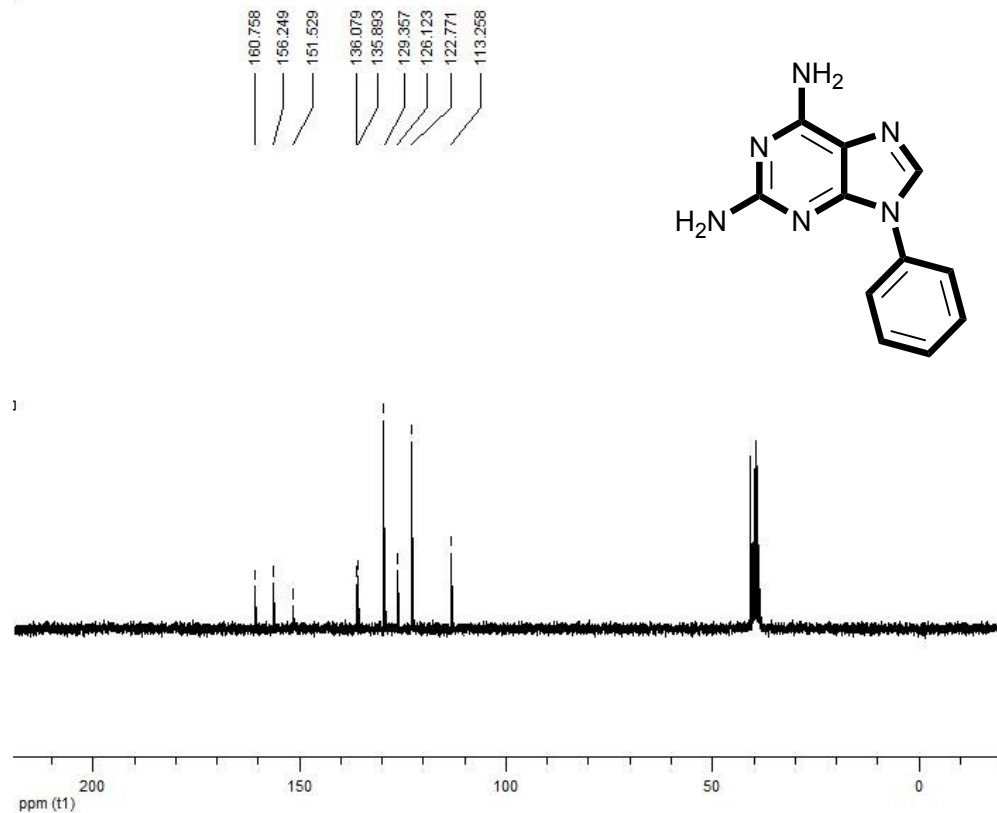
¹H-NMR spectra (250 MHz) of 9-phenyladenine (C17) in DMSO-*d*₆.



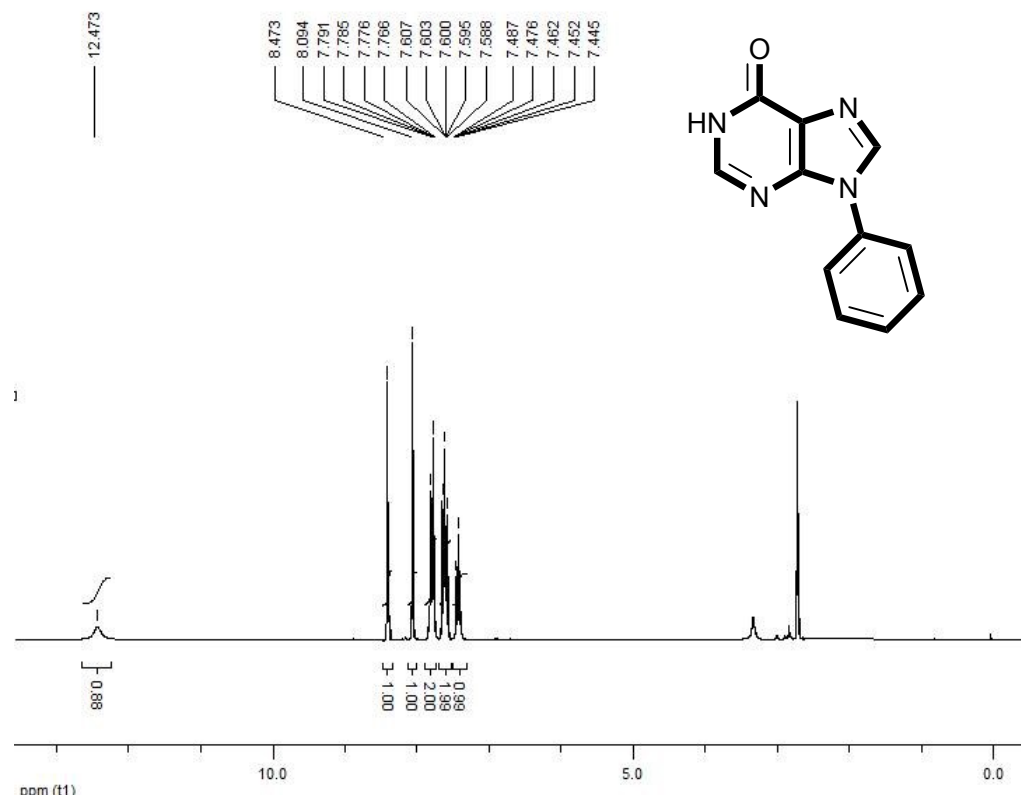
¹³C-NMR spectra (63 MHz) of 9-phenyladenine (C17) in DMSO-*d*₆.



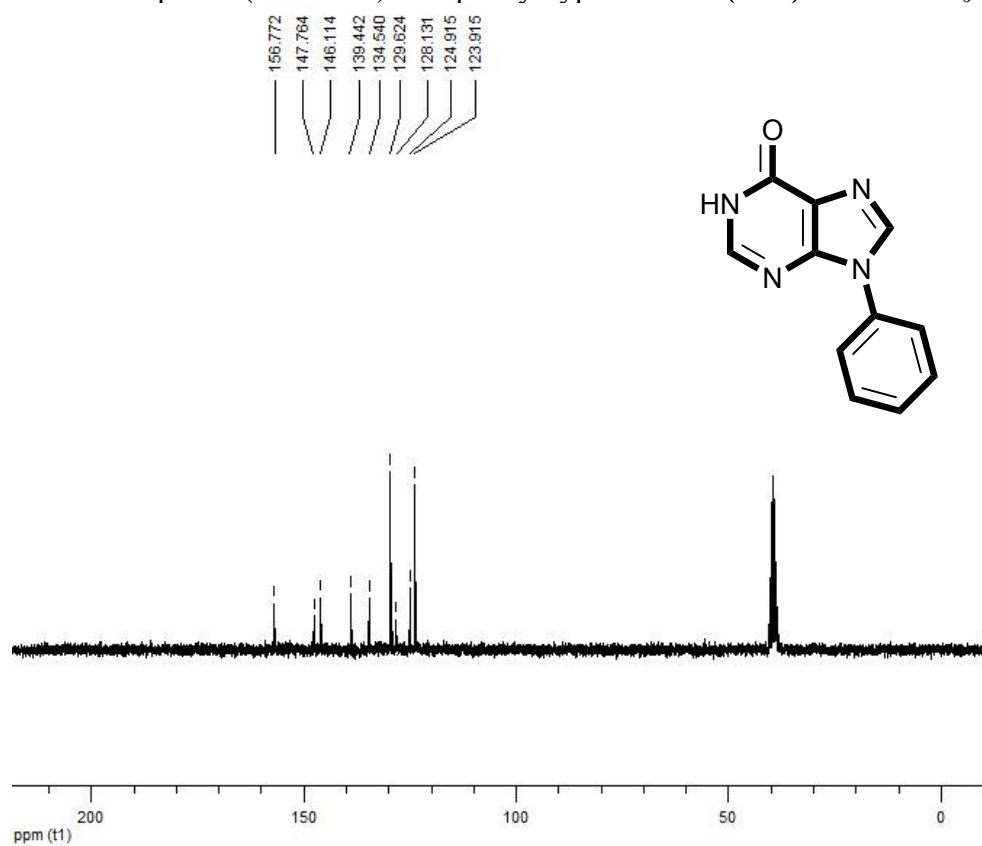
¹H-NMR spectra (250 MHz) of 9-phenylpurine-2,6-diamine (C18) in DMSO-*d*₆.



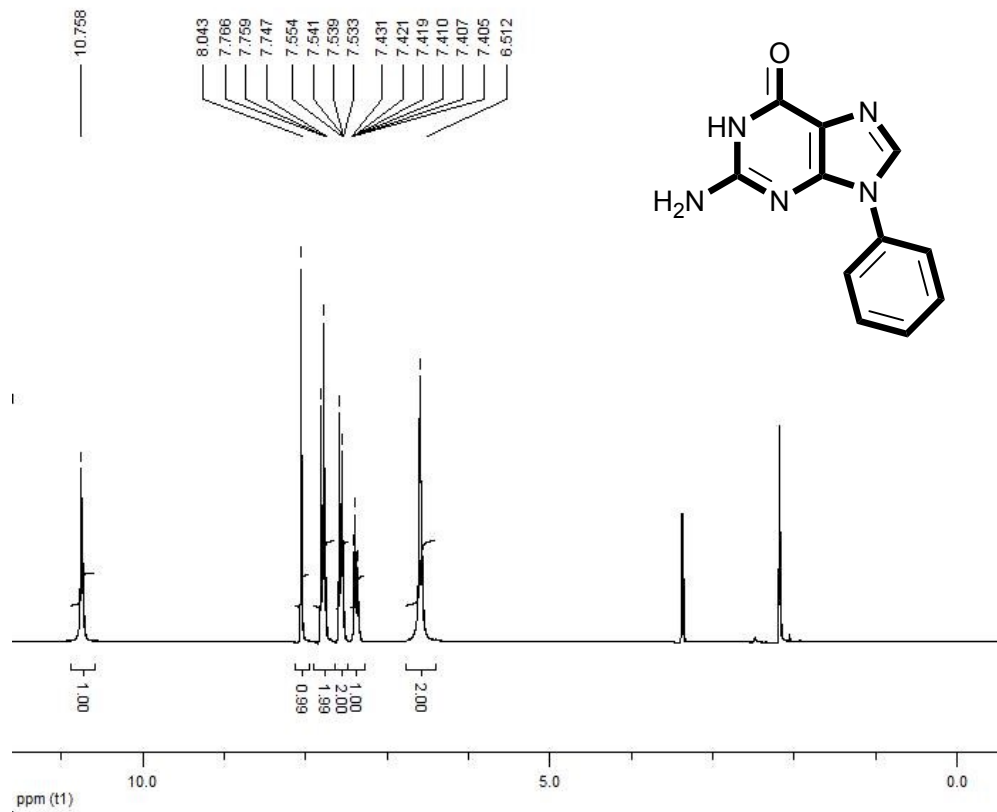
¹³C-NMR spectra (63 MHz) of 9-phenylpurine-2,6-diamine (C18) in DMSO-*d*₆.



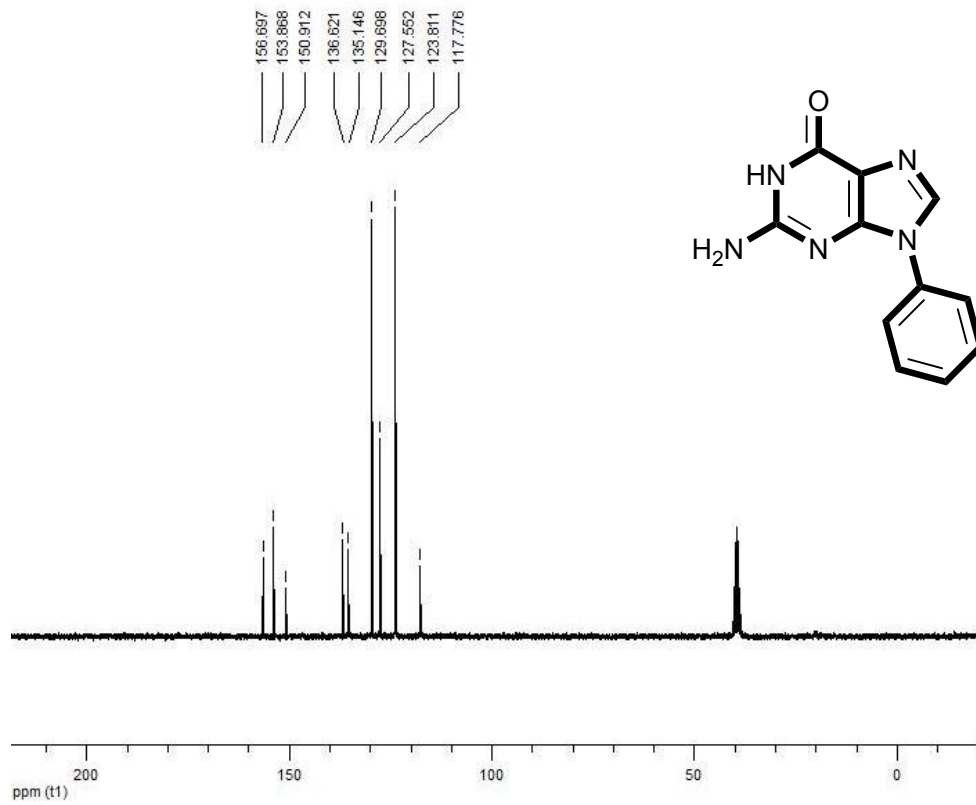
¹H-NMR spectra (250 MHz) of 9-phenylhypoxanthine (C19) in DMSO-*d*₆.



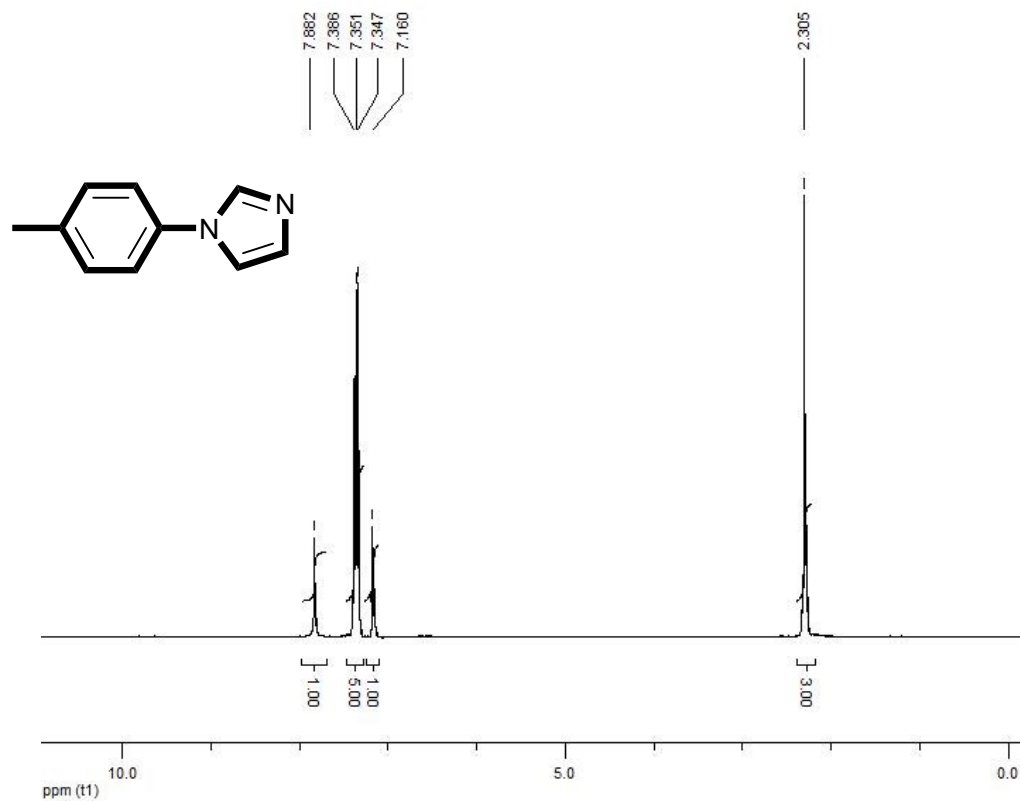
¹³C-NMR spectra (63 MHz) of 9-phenylhypoxanthine (C19) in DMSO-*d*₆.



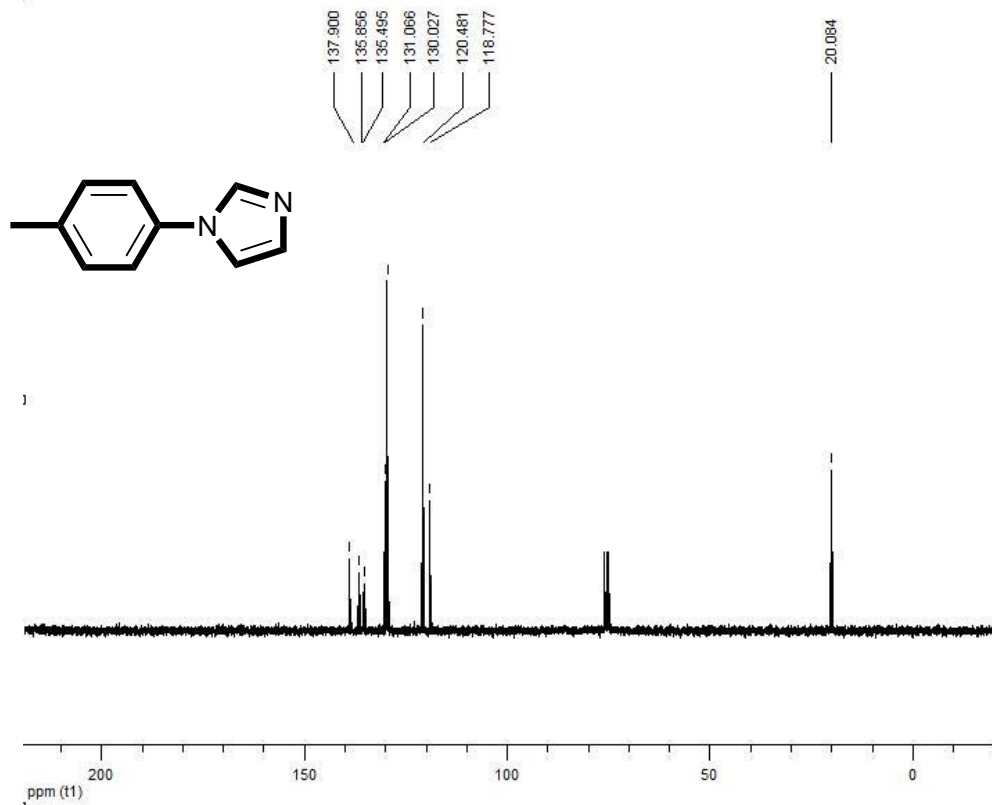
$^1\text{H-NMR}$ spectra (250 MHz) of 9-phenylguanine (C20) in $\text{DMSO-}d_6$.



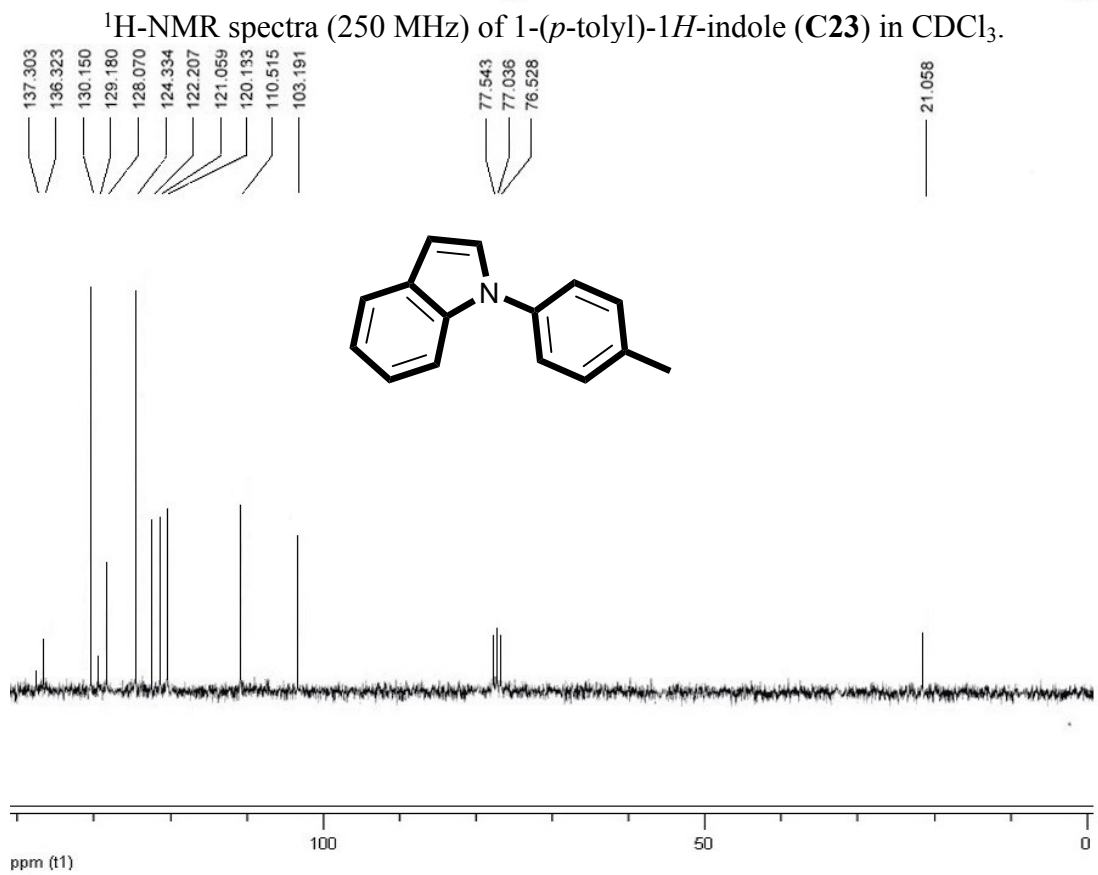
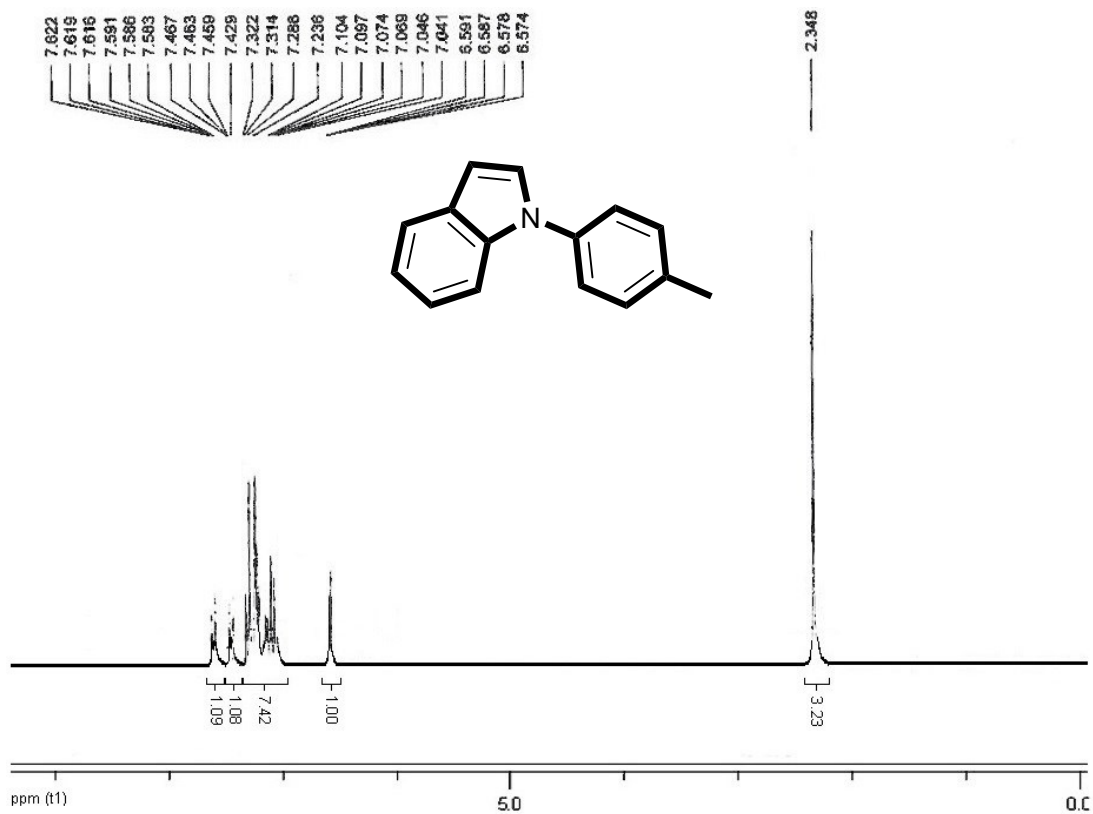
$^{13}\text{C-NMR}$ spectra (63 MHz) of 9-phenylguanine (C20) in $\text{DMSO-}d_6$.

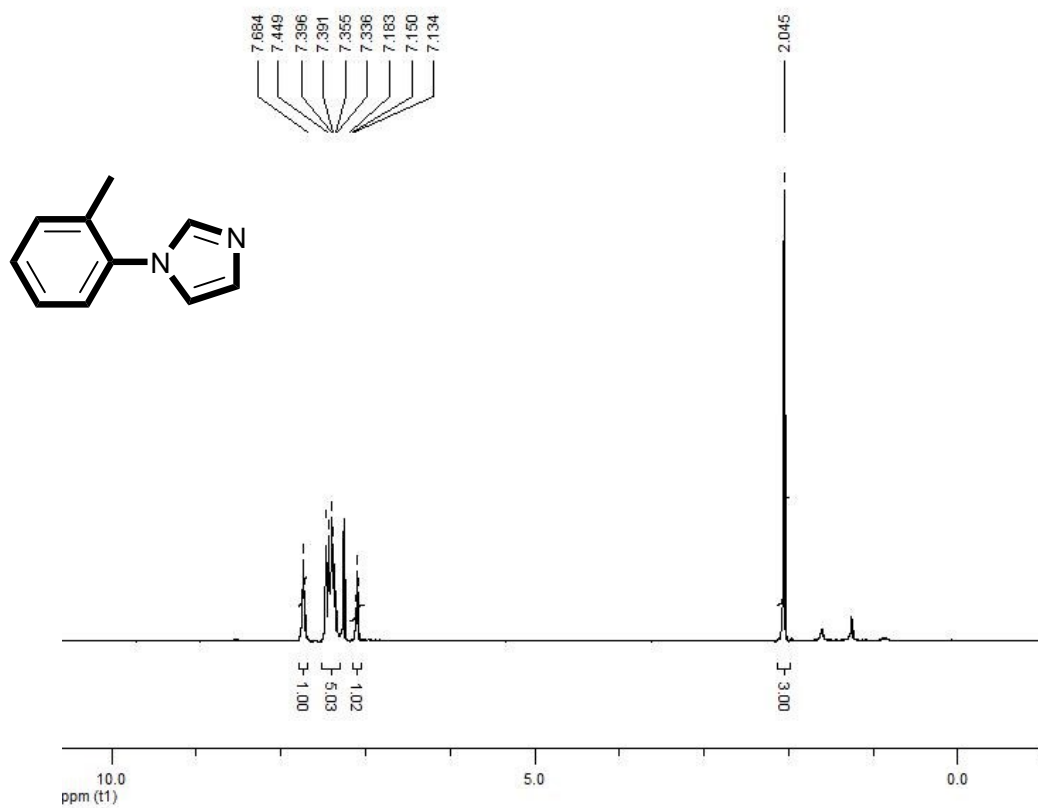


¹H-NMR spectra (250 MHz) of 1-(*p*-tolyl)-1*H*-imidazole (**C22**) in CDCl₃.

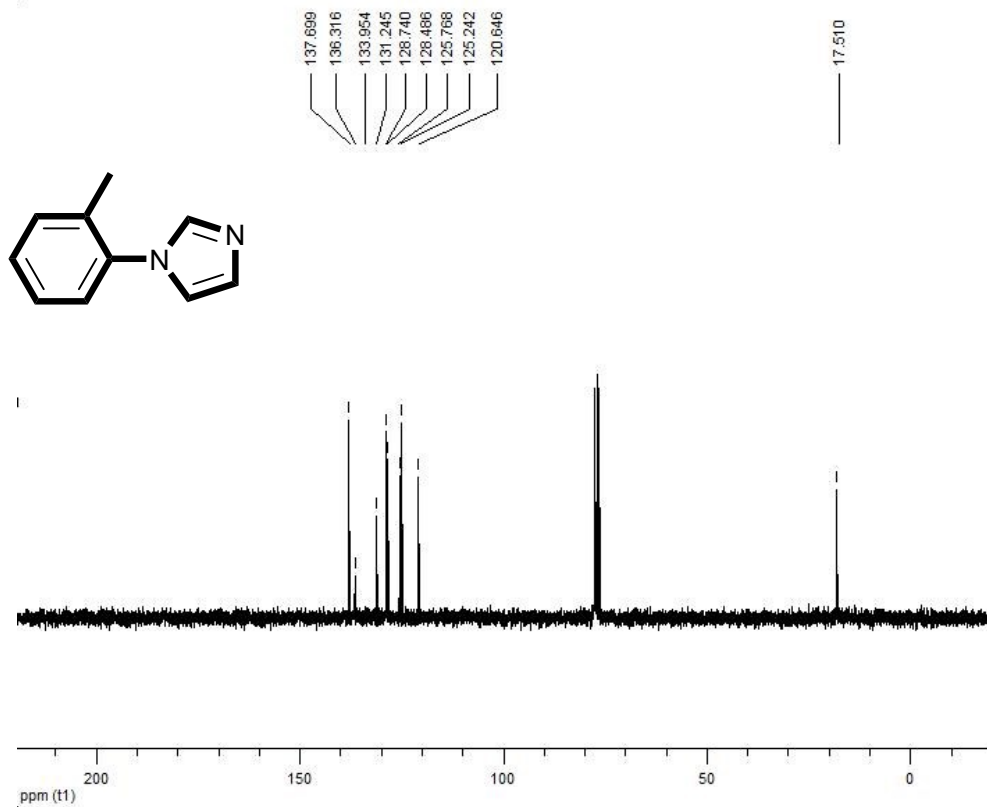


¹³C-NMR spectra (63 MHz) of 1-(*p*-tolyl)-1*H*-imidazole (**C22**) in CDCl₃.

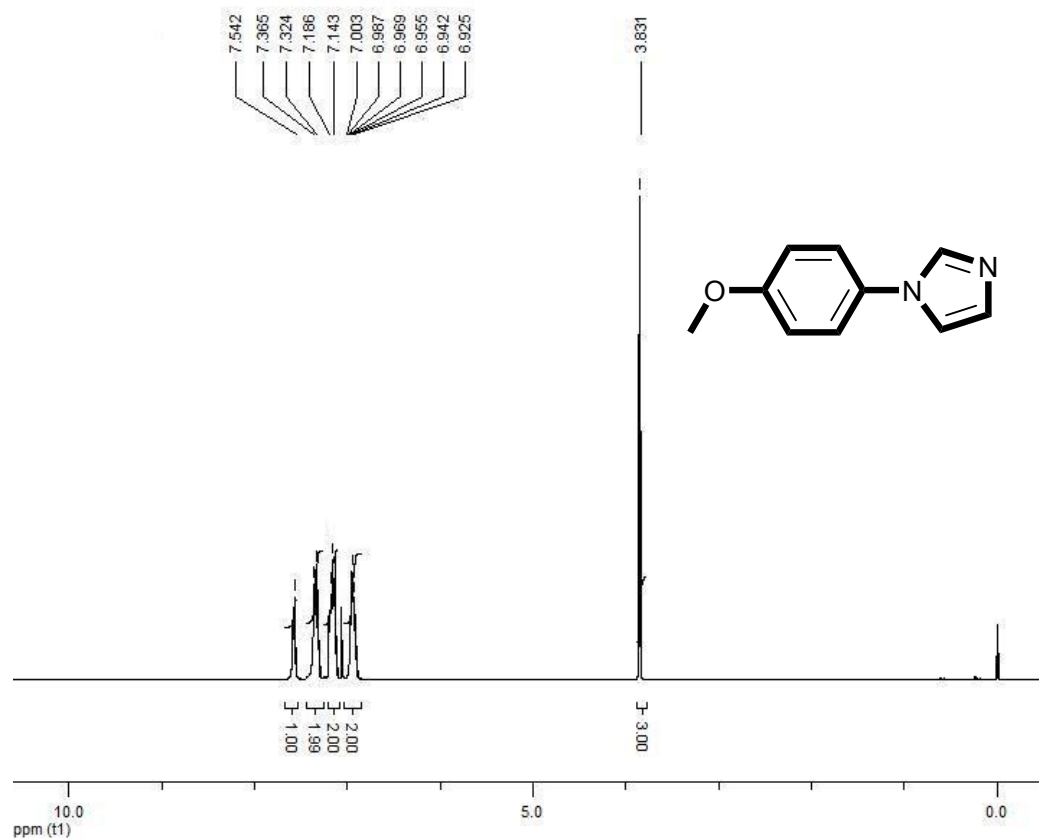




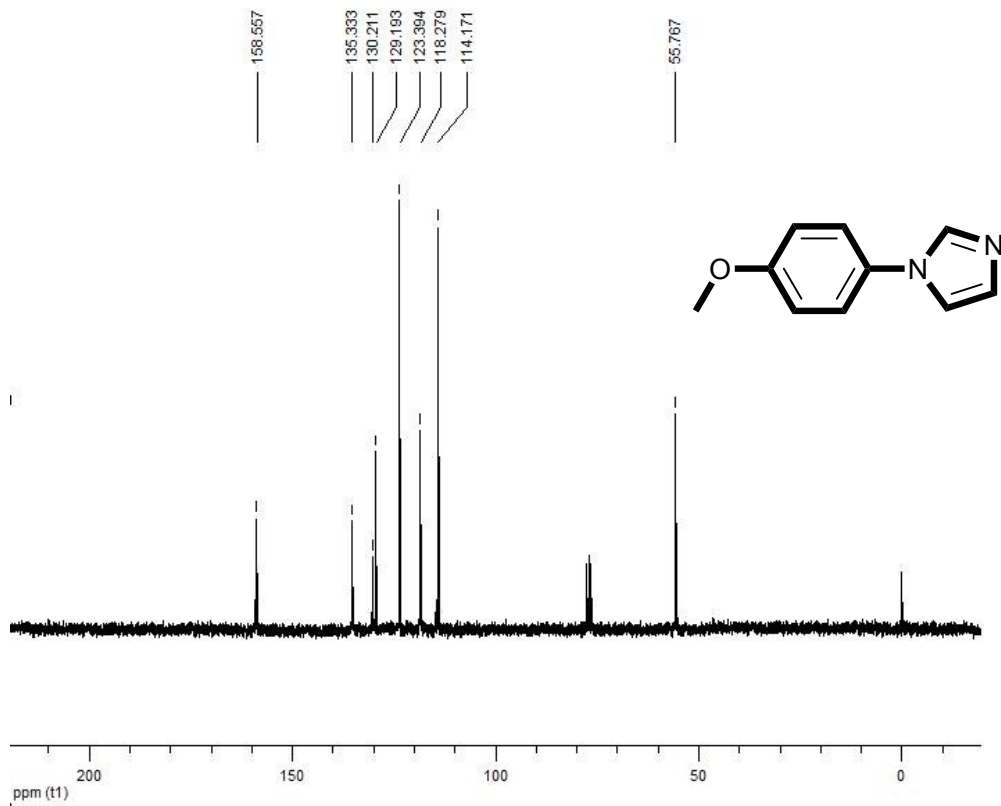
¹H-NMR spectra (250 MHz) of 1-(*o*-tolyl)-1*H*-imidazole (**C24**) in CDCl₃.



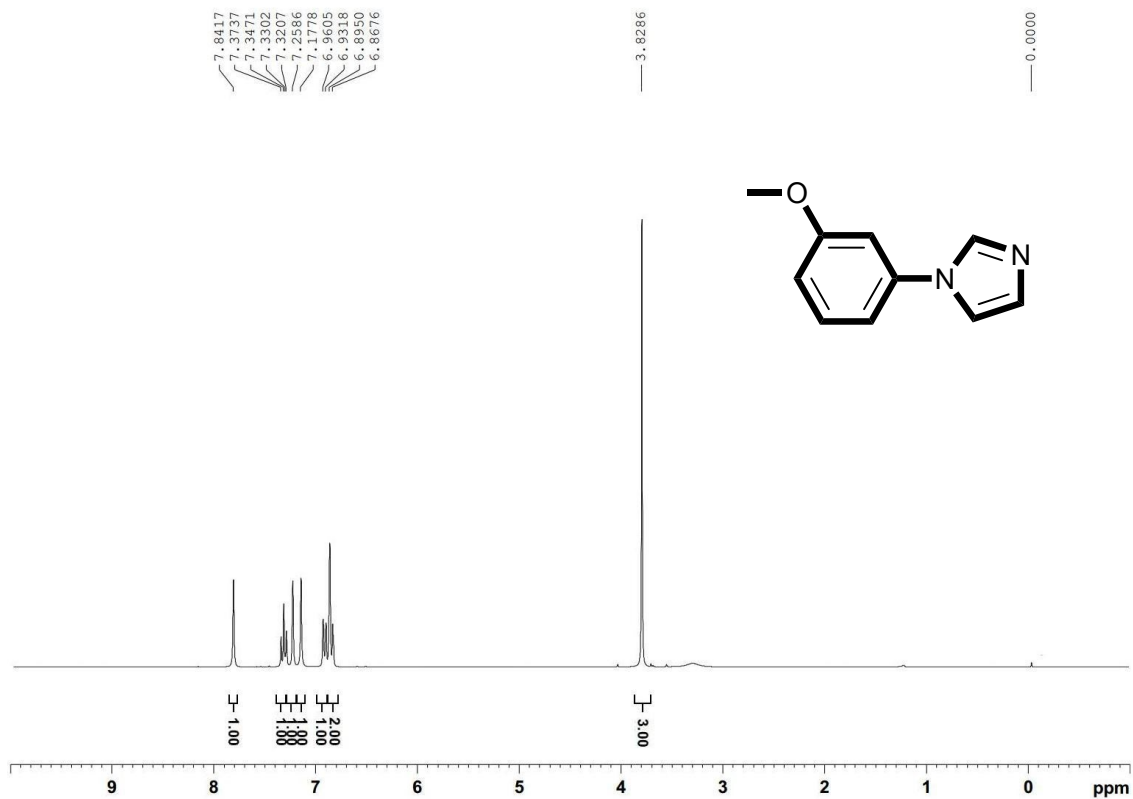
¹³C-NMR spectra (63 MHz) of 1-(*o*-tolyl)-1*H*-imidazole (**C24**) in CDCl₃.



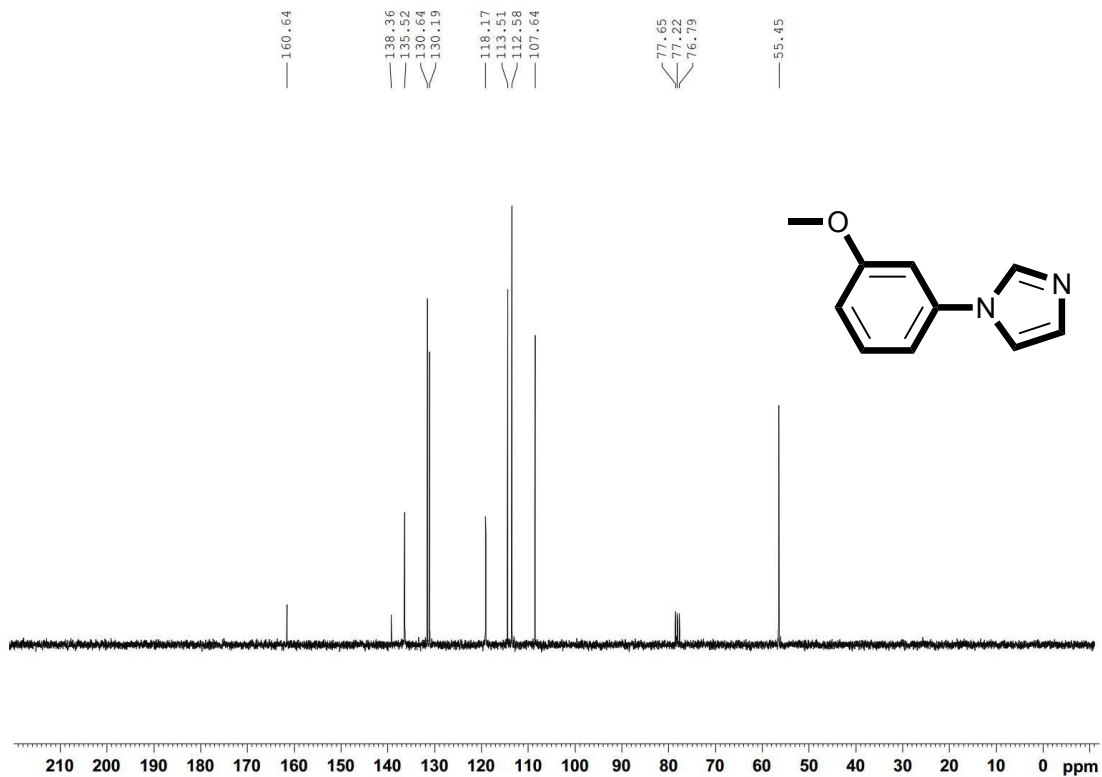
¹H-NMR spectra (250 MHz) of 1-(4-methoxyphenyl)-1*H*-imidazole (**C25**) in CDCl₃.



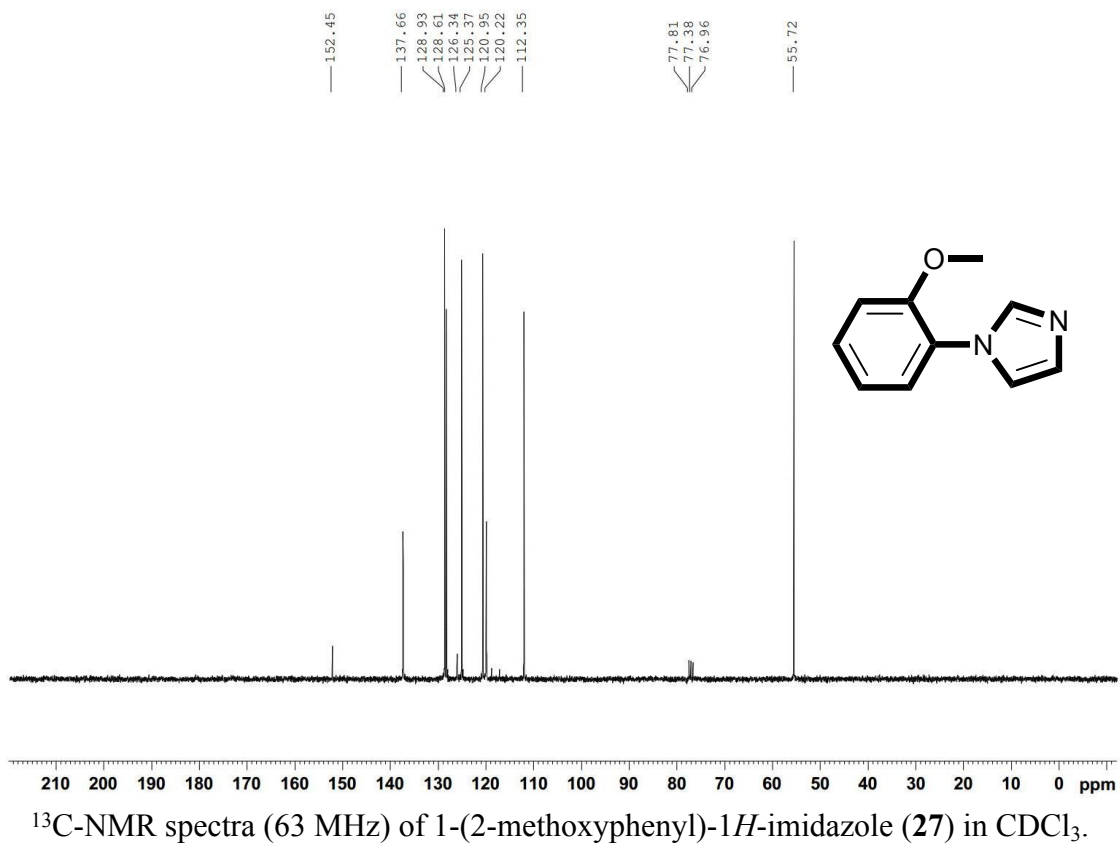
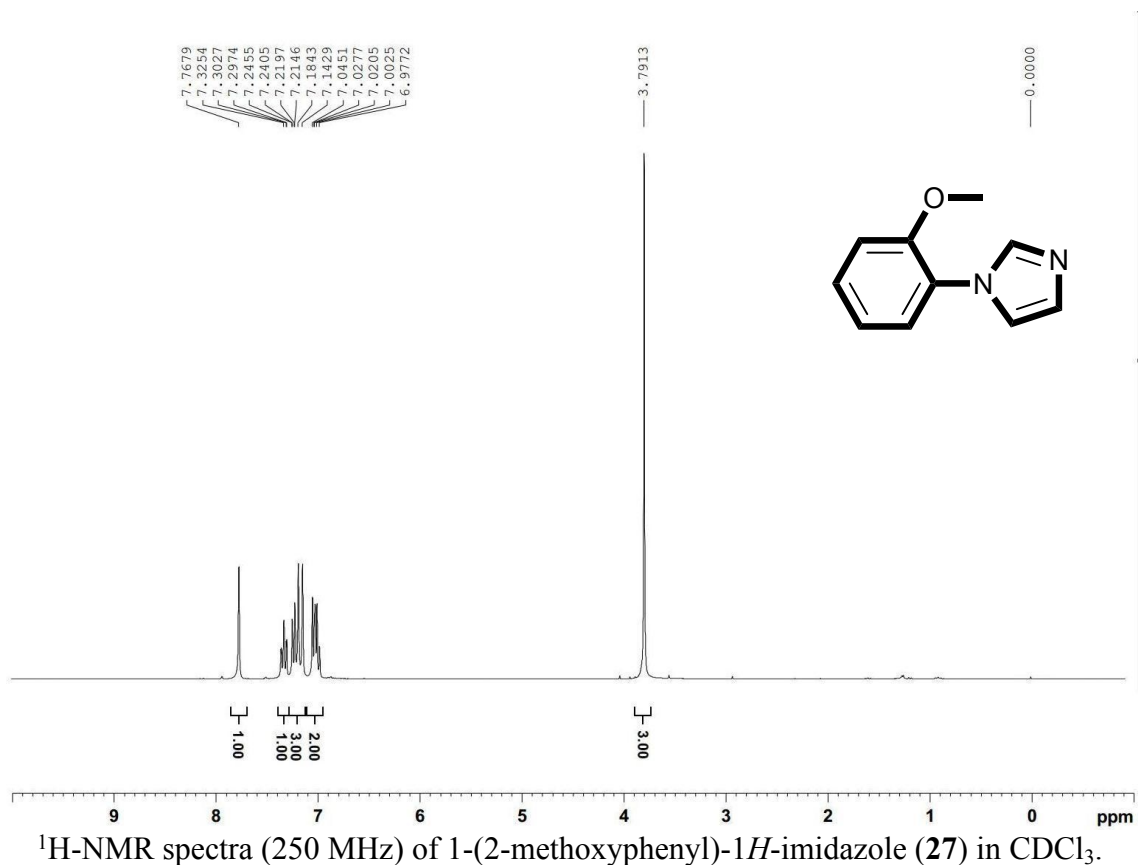
¹³C-NMR spectra (63 MHz) of 1-(4-methoxyphenyl)-1*H*-imidazole (**C25**) in CDCl₃.

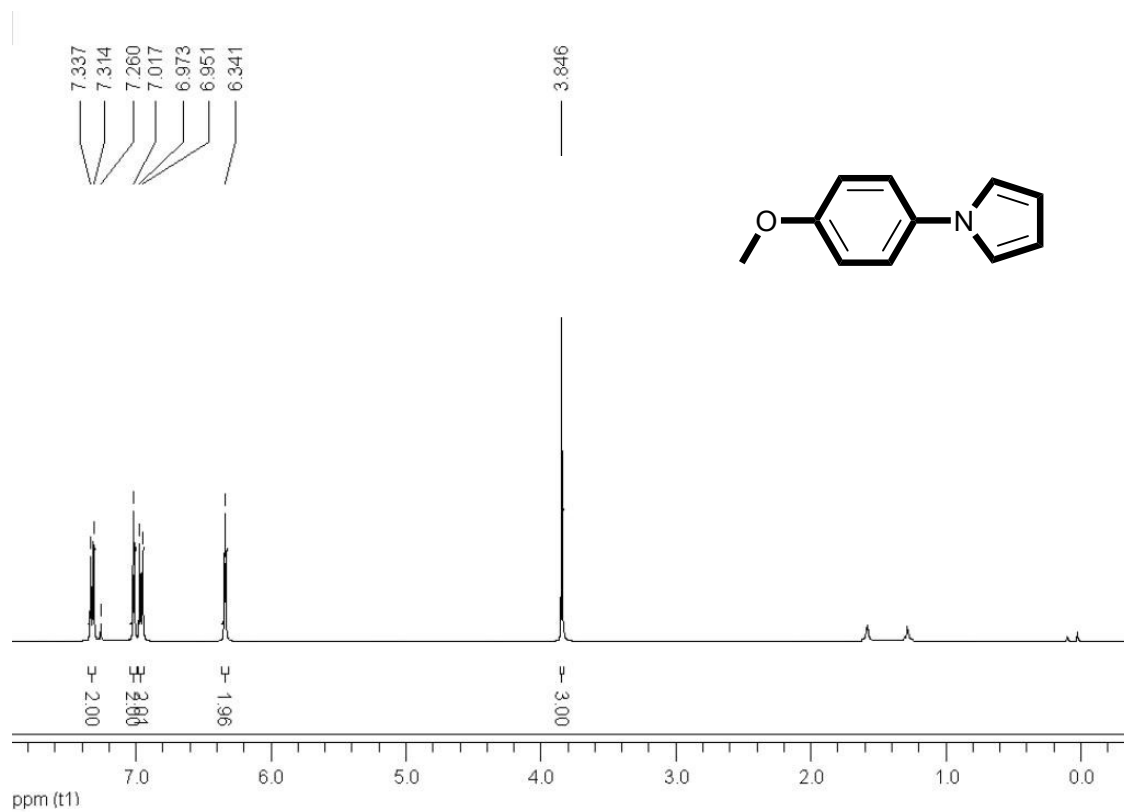


¹H-NMR spectra (250 MHz) of 1-(3-methoxyphenyl)-1H-imidazole (26) in CDCl₃.

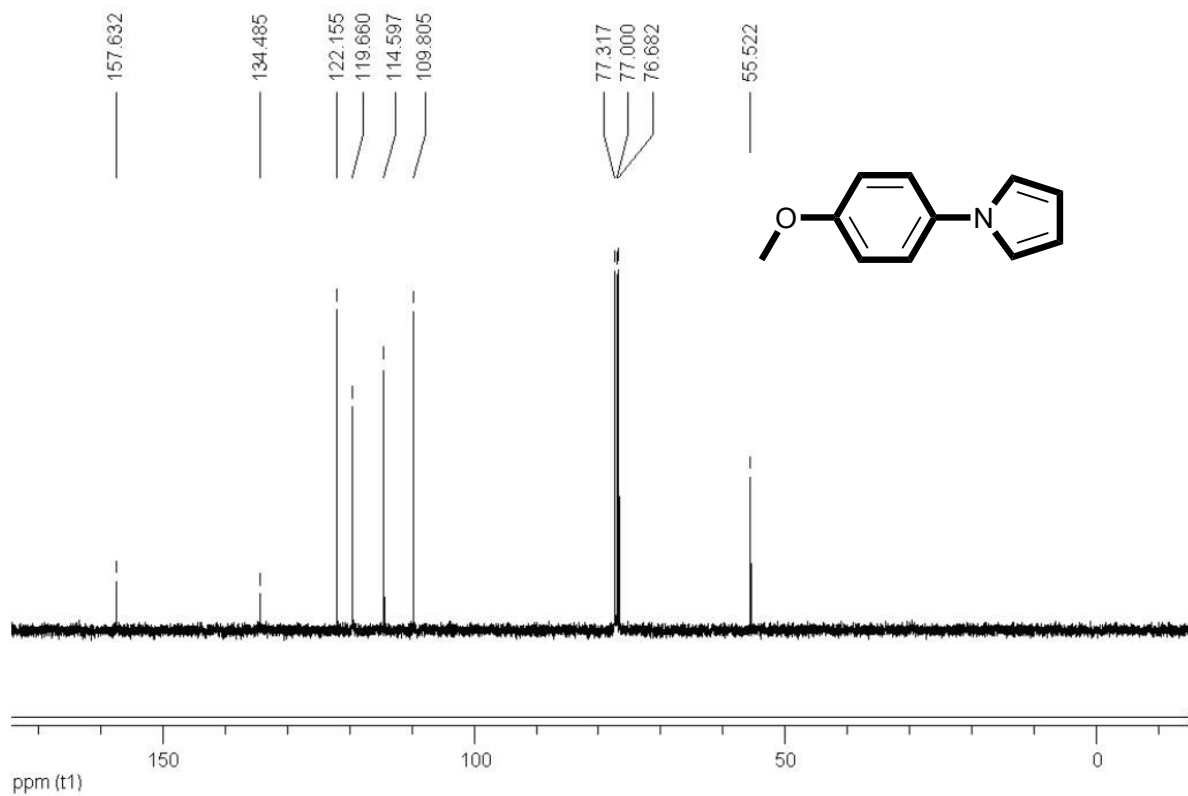


¹³C-NMR spectra (63 MHz) of 1-(3-methoxyphenyl)-1H-imidazole (26) in CDCl₃.

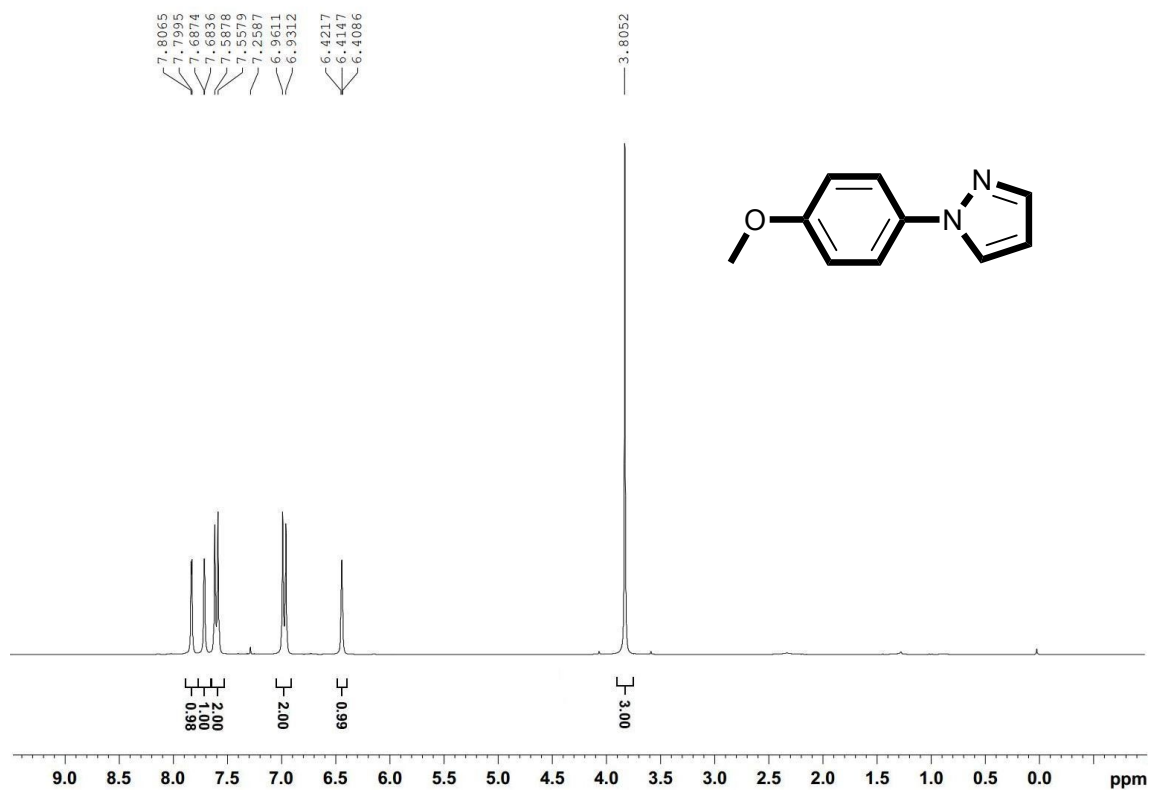




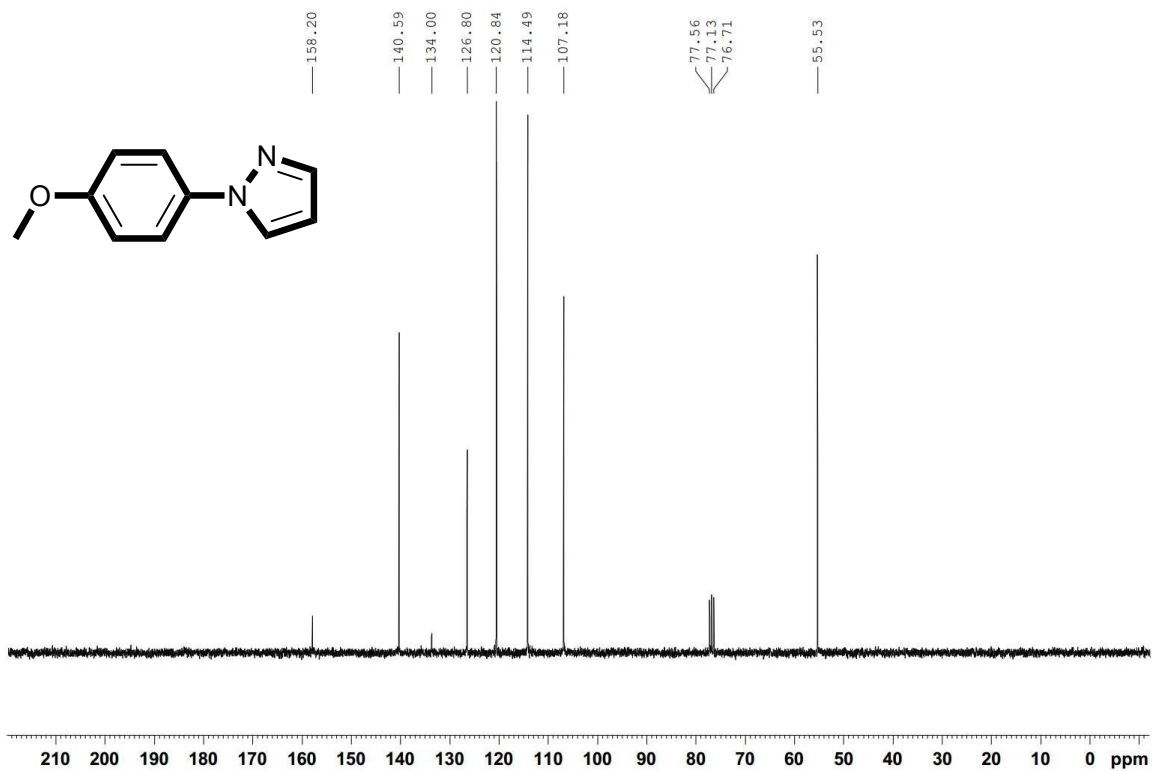
¹H-NMR spectra (250 MHz) of 1-(4-methoxyphenyl)-1H-pyrrole (**28**) in CDCl₃.



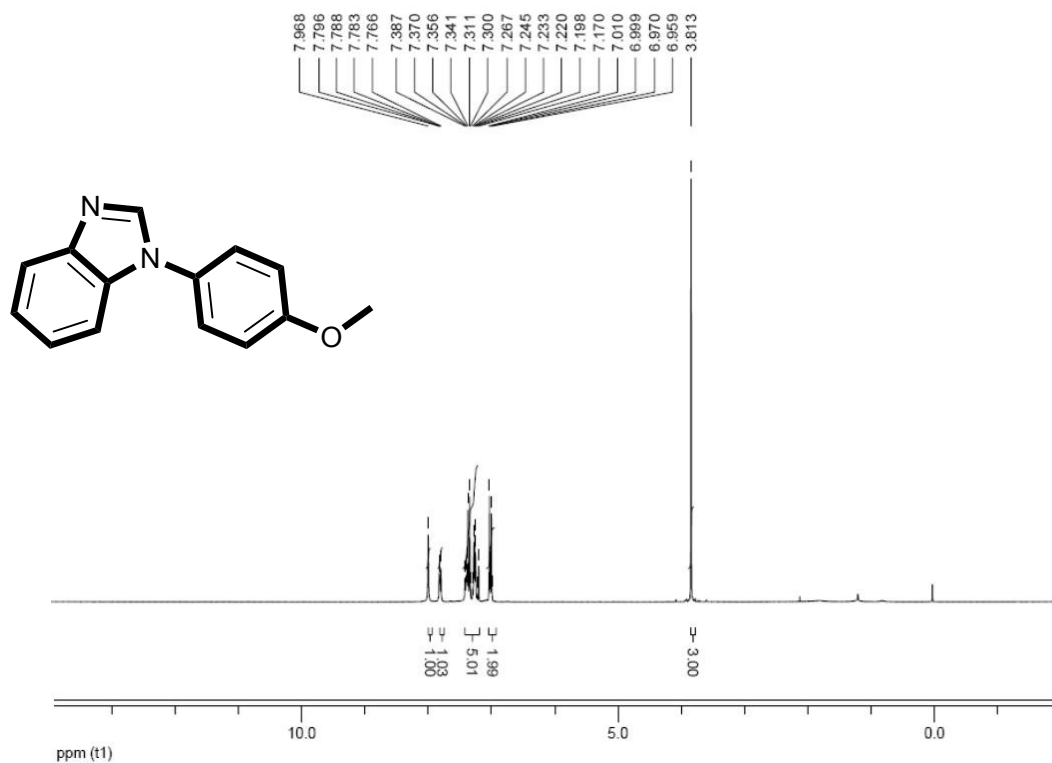
¹³C-NMR spectra (63 MHz) of 1-(4-methoxyphenyl)-1H-pyrrole (**28**) in CDCl₃.



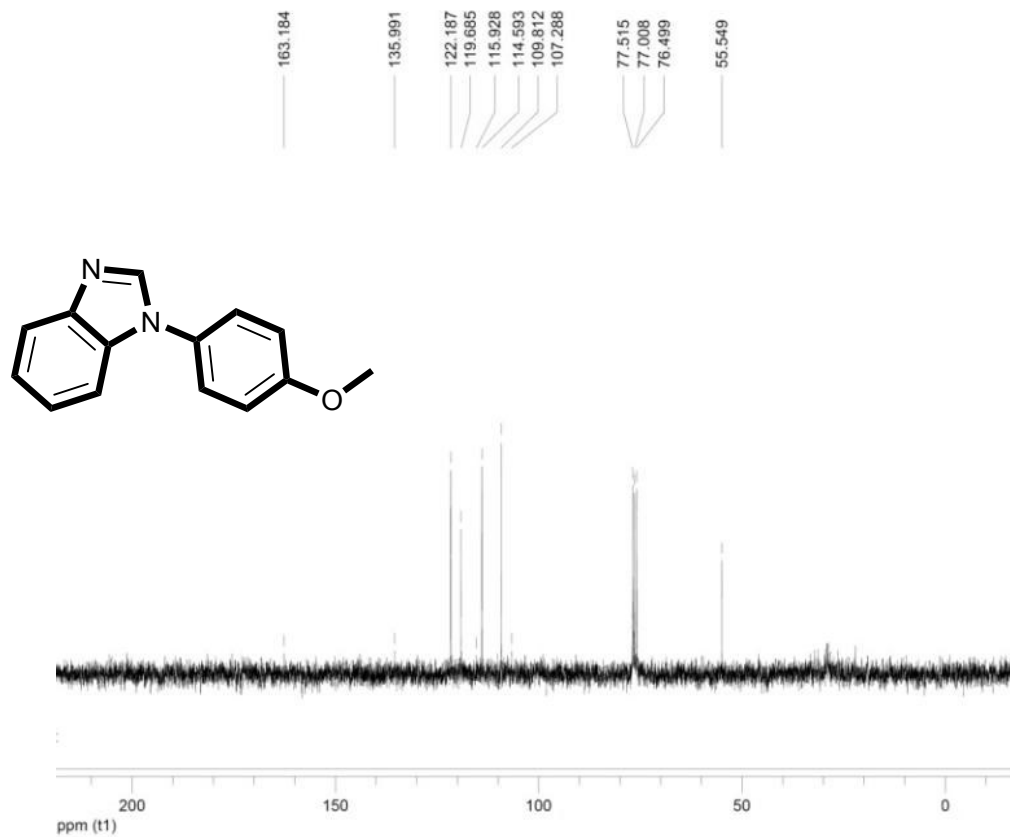
¹H-NMR spectra (250 MHz) of 1-(4-methoxyphenyl)-1H-pyrazole (29) in CDCl₃.



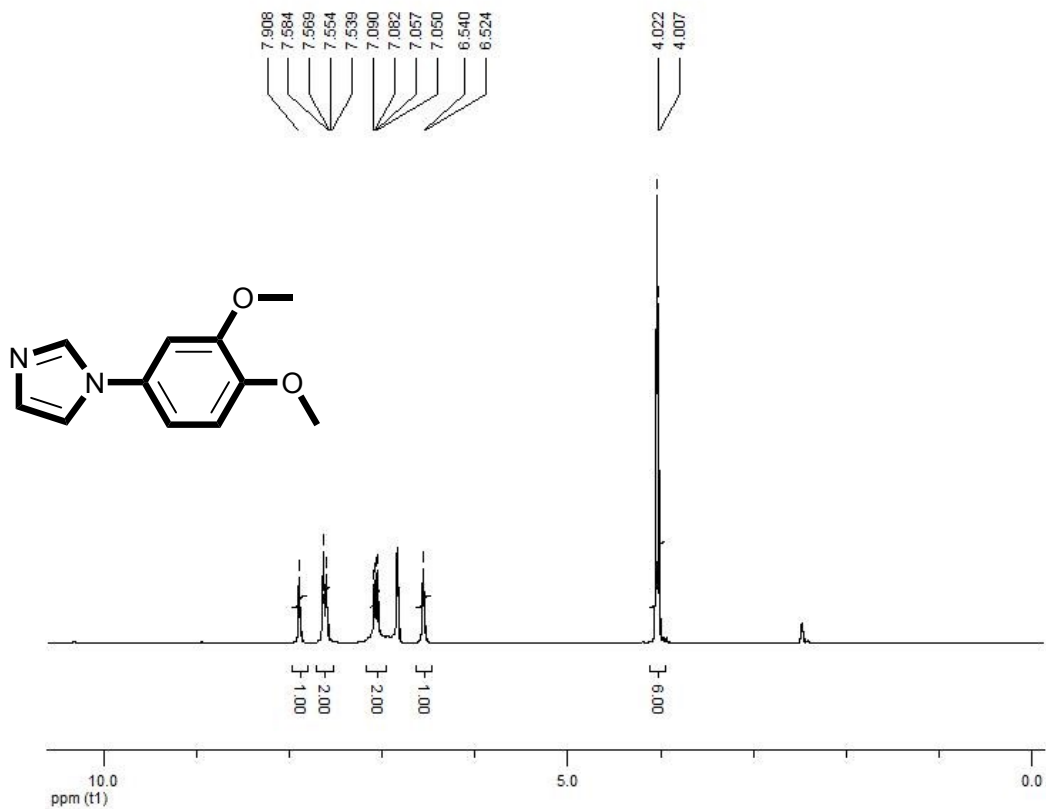
¹³C-NMR spectra (63 MHz) of 1-(4-methoxyphenyl)-1H-pyrazole (29) in CDCl₃.



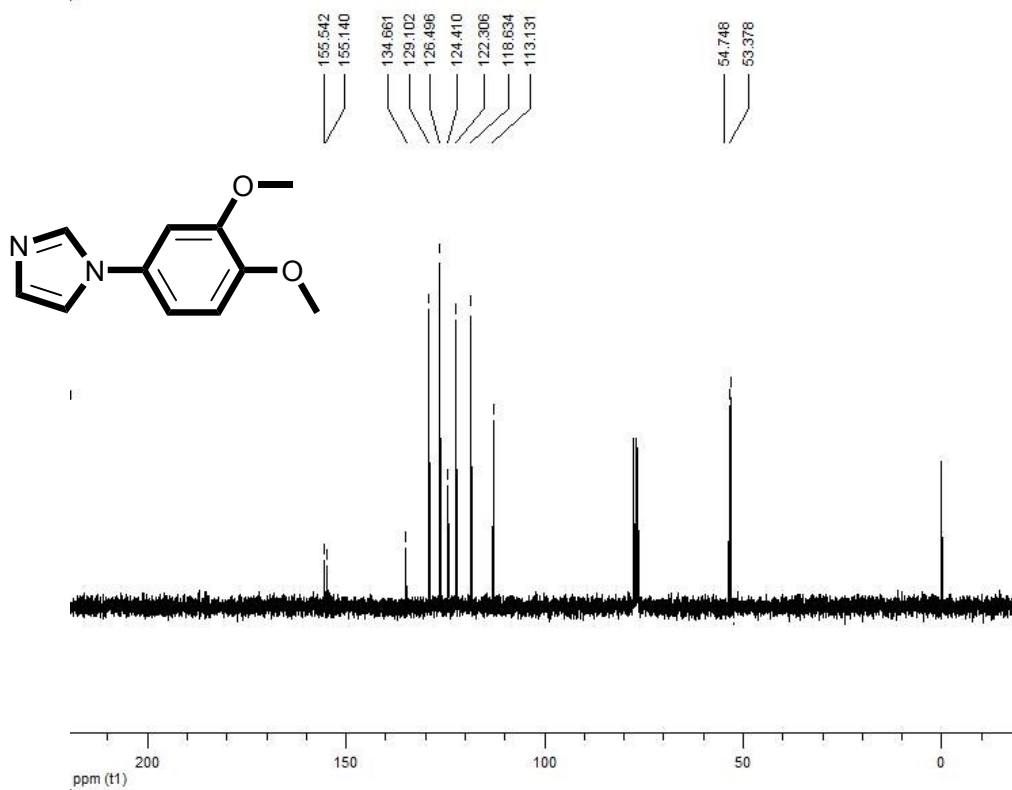
¹H-NMR spectra (250 MHz) of 1-(4-methoxyphenyl)-1*H*-benzimidazole (**C30**) in CDCl₃.



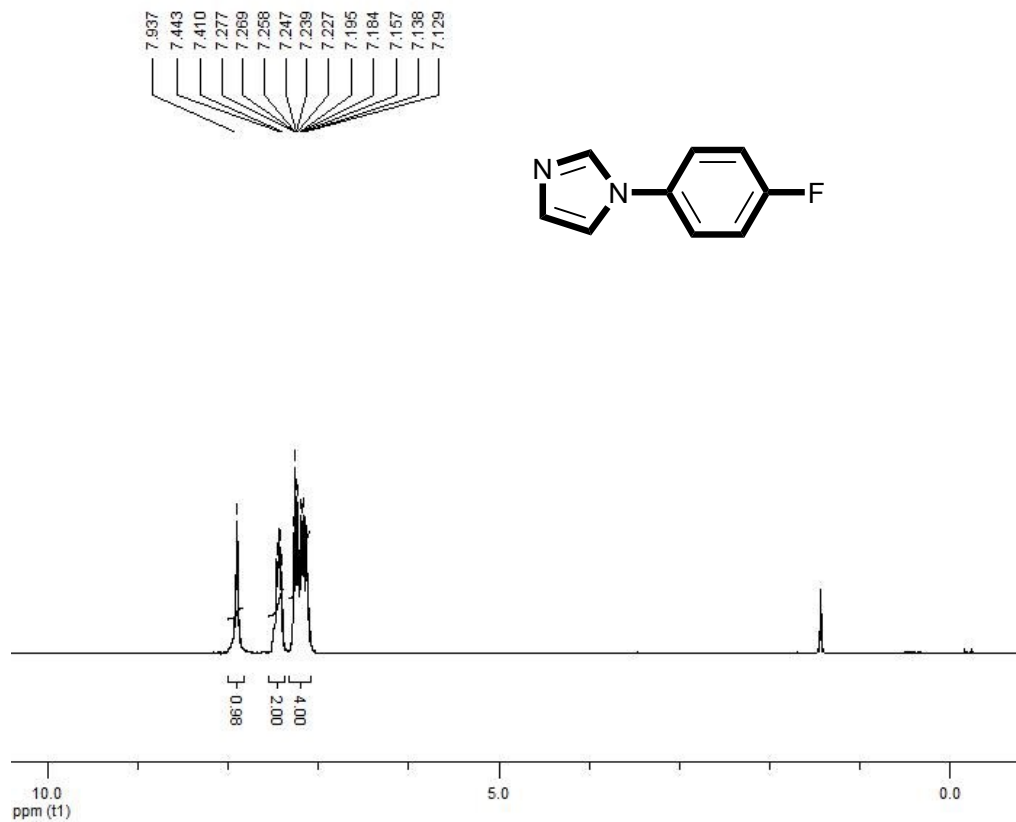
¹³C-NMR spectra (63 MHz) of 1-(4-methoxyphenyl)-1*H*-benzimidazole (**C30**) in CDCl₃.



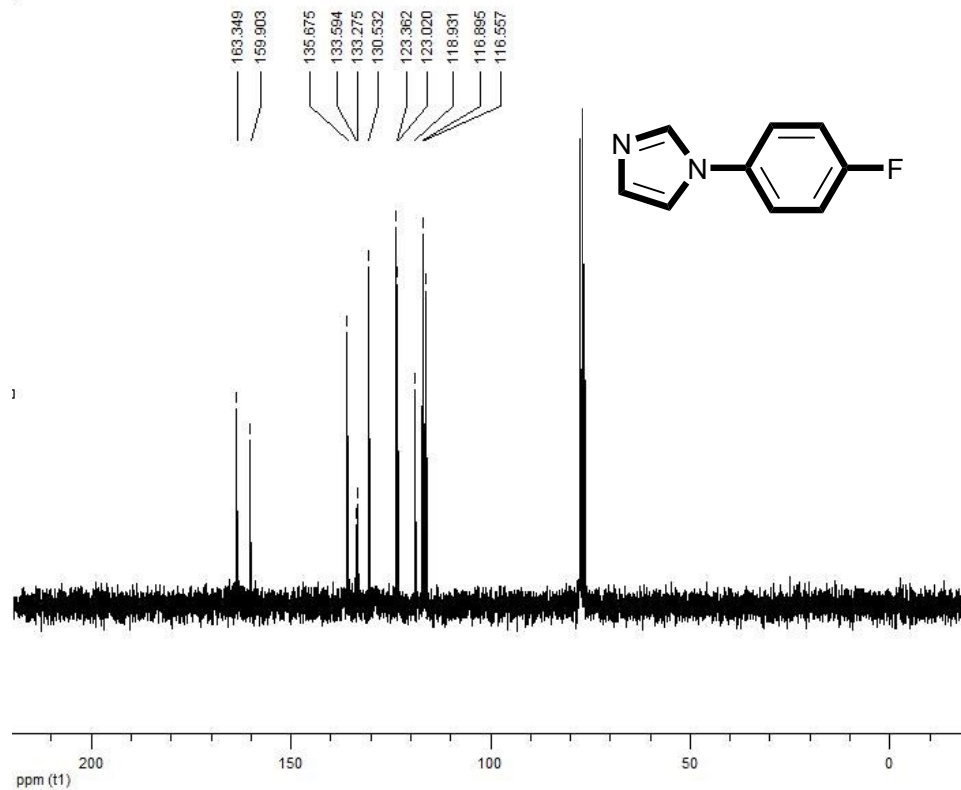
¹H-NMR spectra (250 MHz) of 1-(3,4-dimethoxyphenyl)-1H-imidazole (C31) in CDCl₃.



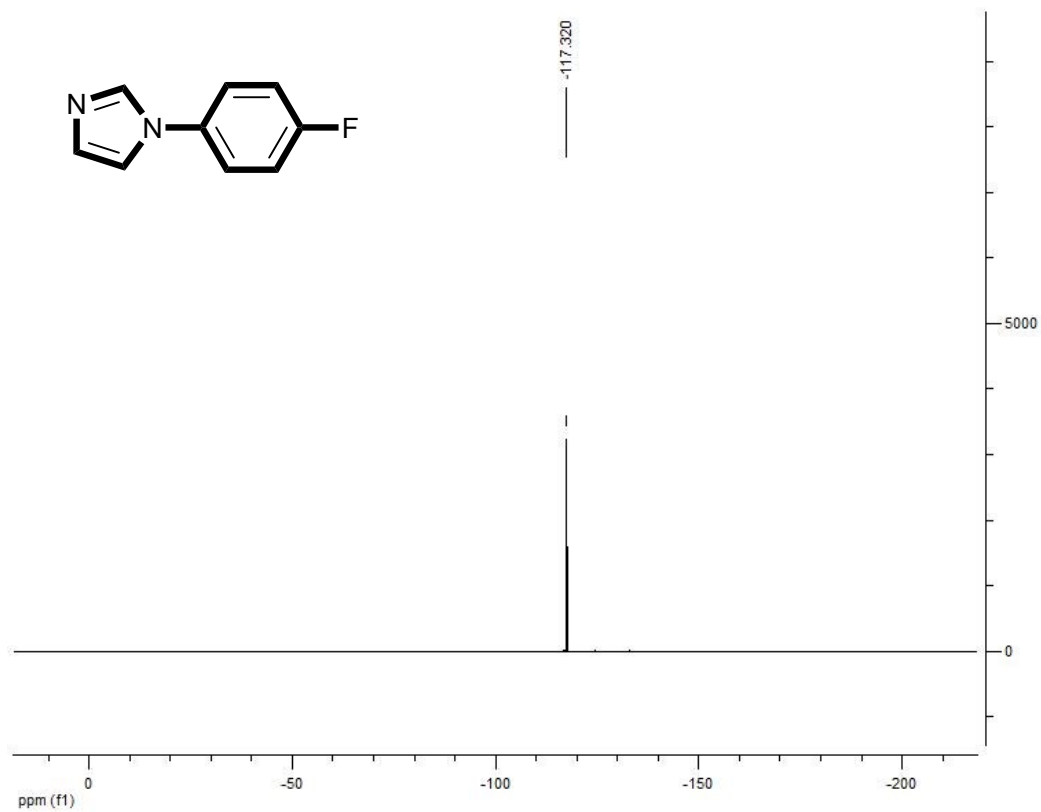
¹³C-NMR spectra (63 MHz) of 1-(3,4-dimethoxyphenyl)-1H-imidazole (C31) in CDCl₃.



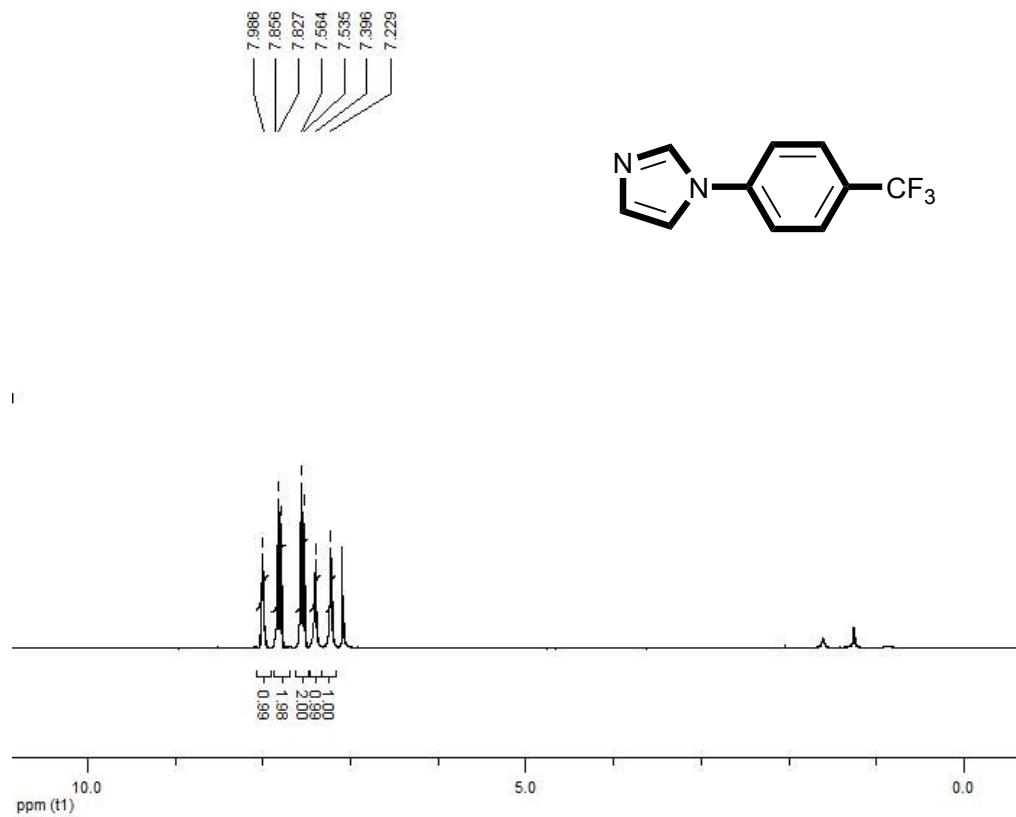
¹H-NMR spectra (250 MHz) of 1-(4-fluorophenyl)-1H-imidazole (C32) in CDCl₃.



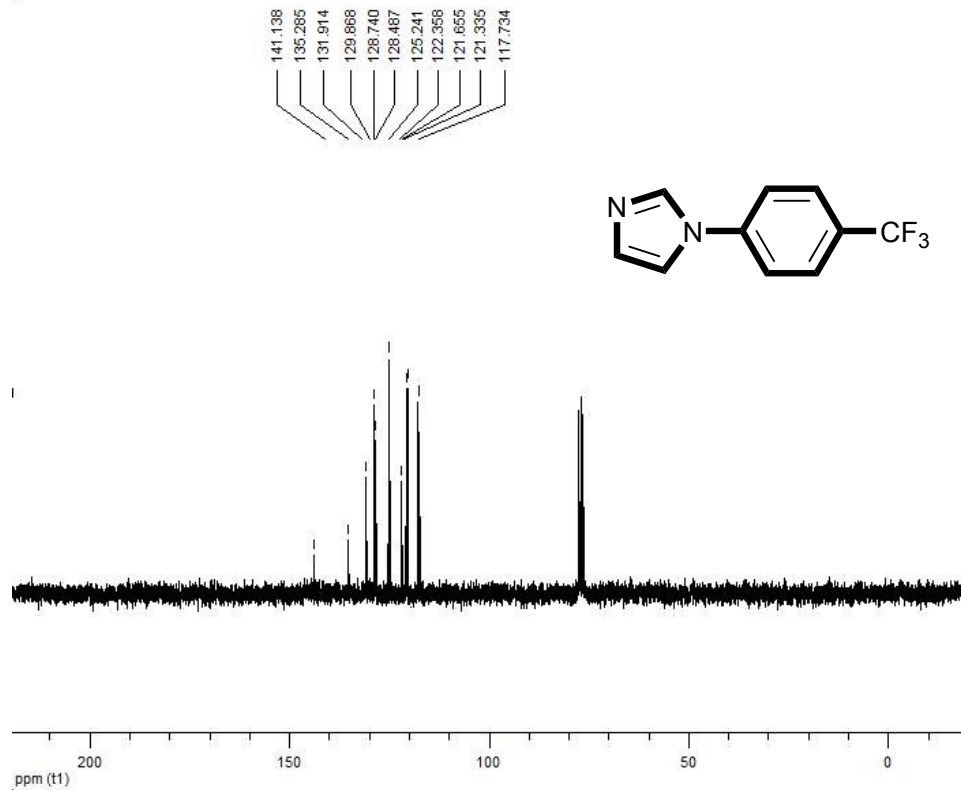
¹³C-NMR spectra (63 MHz) of 1-(4-fluorophenyl)-1H-imidazole (C32) in CDCl₃.



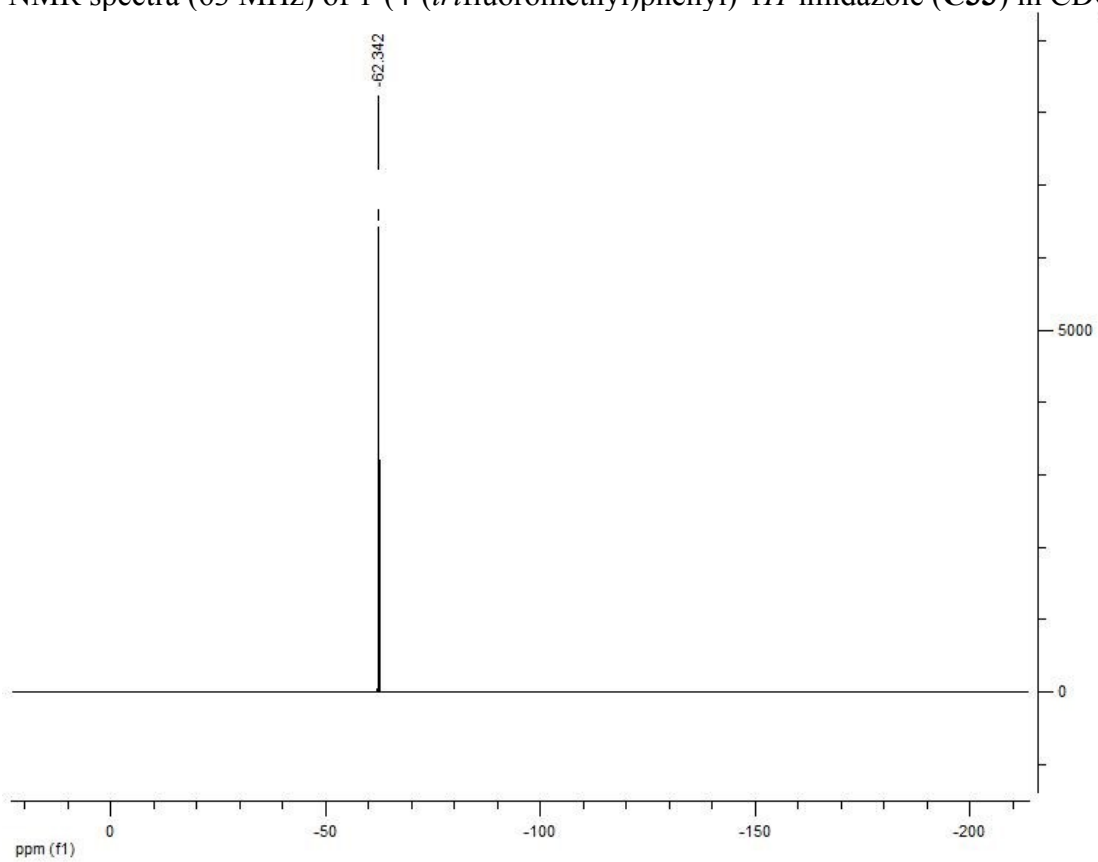
^{19}F -NMR spectra (376 MHz) of 1-(4-fluorophenyl)-1*H*-imidazole (**C32**) in CDCl_3 .



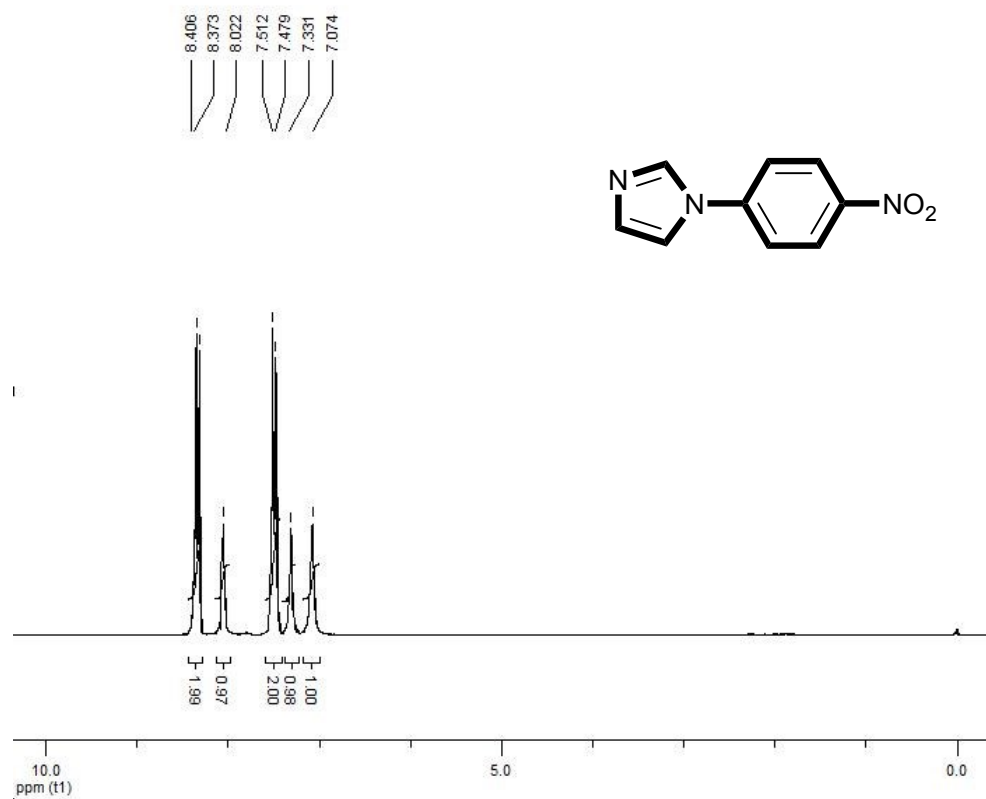
^1H -NMR spectra (250 MHz) of 1-(4-(trifluoromethyl)phenyl)-1*H*-imidazole (**C33**) in CDCl_3 .



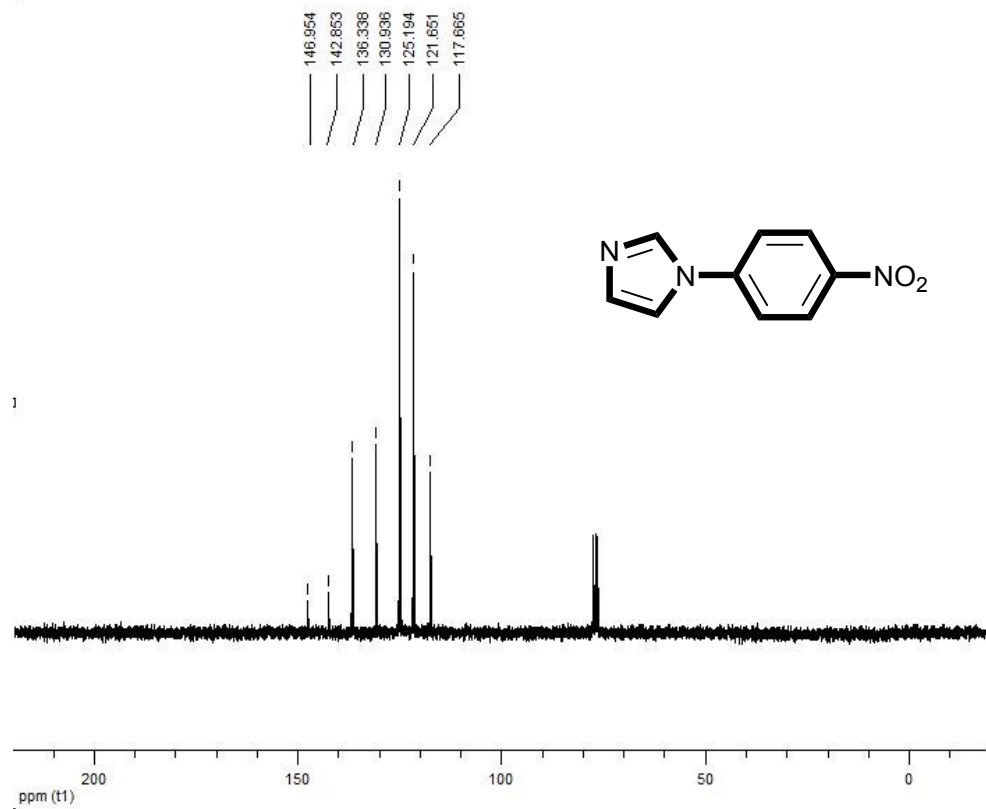
¹³C-NMR spectra (63 MHz) of 1-(4-(trifluoromethyl)phenyl)-1H-imidazole (C33) in CDCl₃.



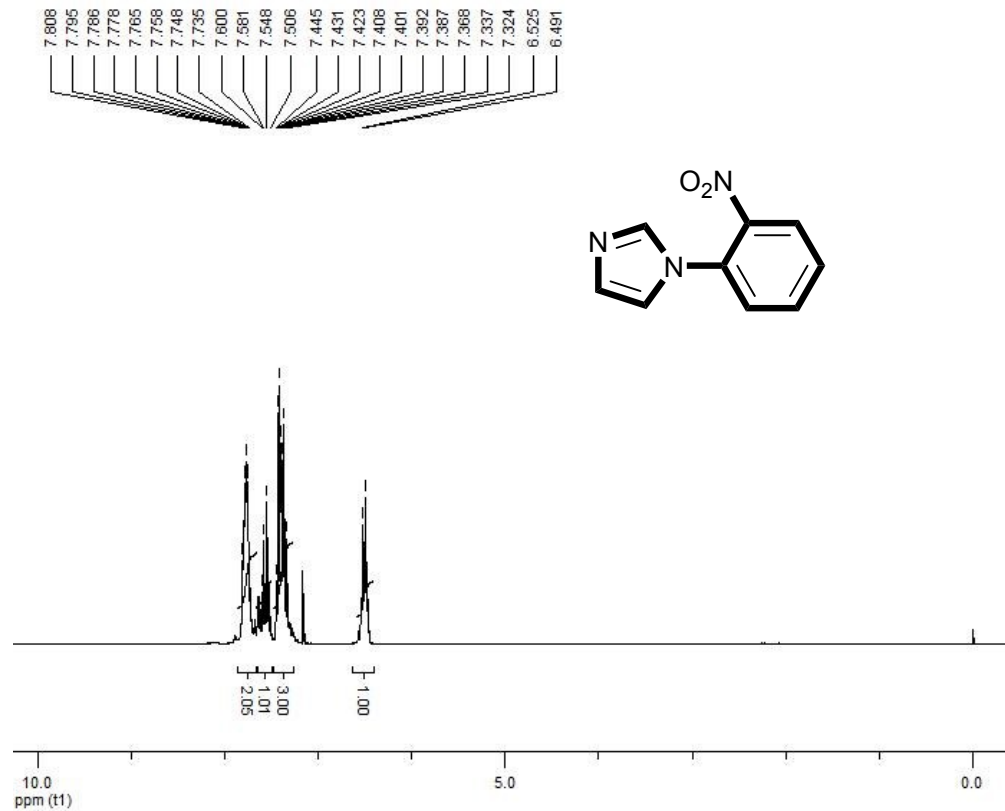
¹⁹F-NMR spectra (376 MHz) of 1-(4-(trifluoromethyl)phenyl)-1H-imidazole (C33) in CDCl₃.



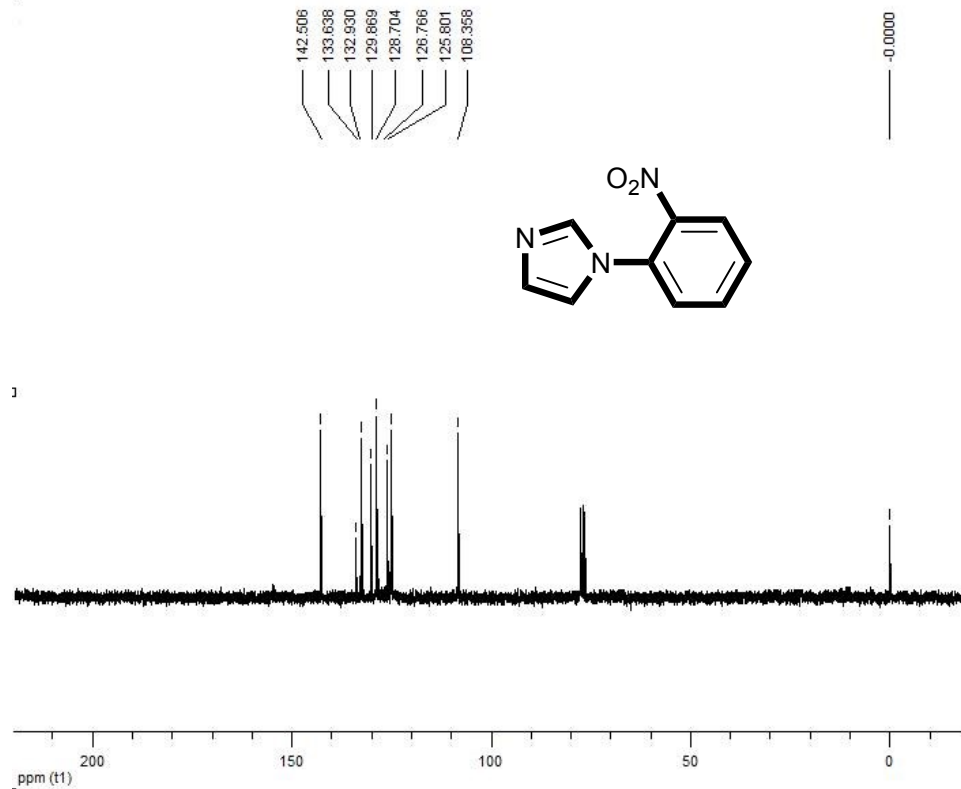
¹H-NMR spectra (250 MHz) of 1-(4-nitrophenyl)-1H-imidazole (C34) in CDCl₃.



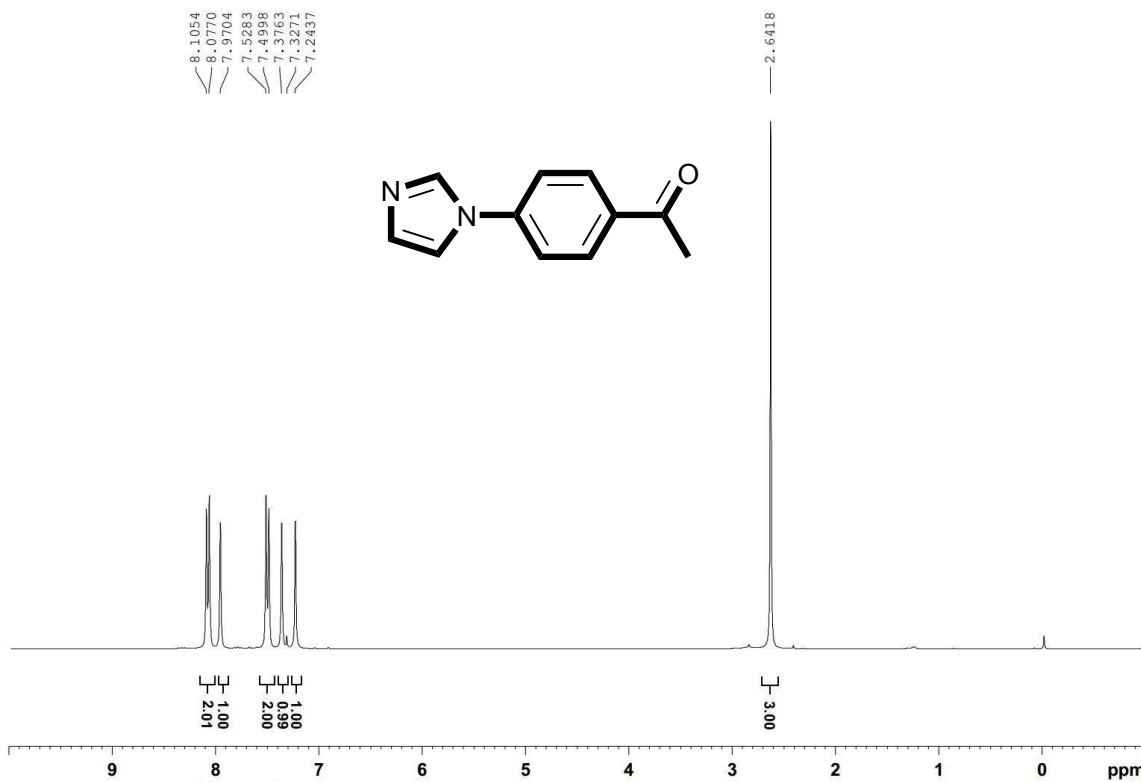
¹³C-NMR spectra (63 MHz) of 1-(4-nitrophenyl)-1H-imidazole (C34) in CDCl₃.



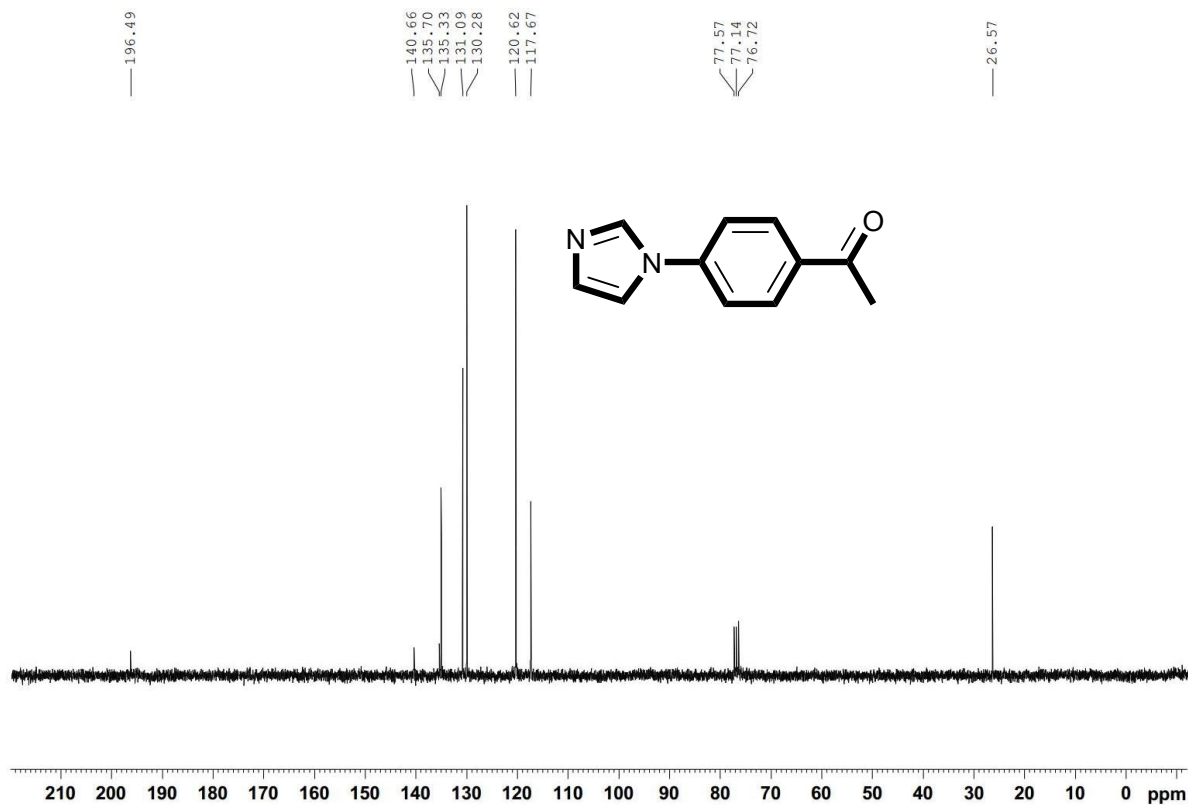
¹H-NMR spectra (250 MHz) of 1-(2-nitrophenyl)-1H-imidazole (C35) in CDCl₃.



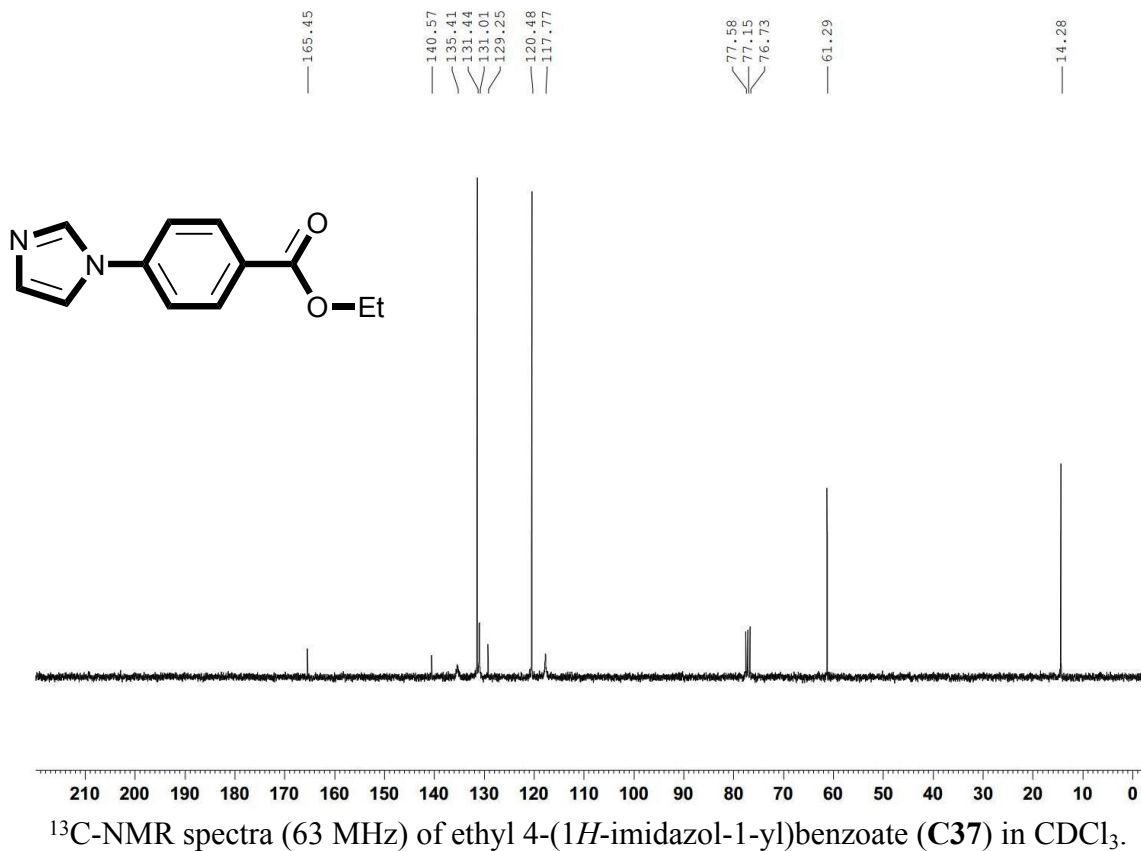
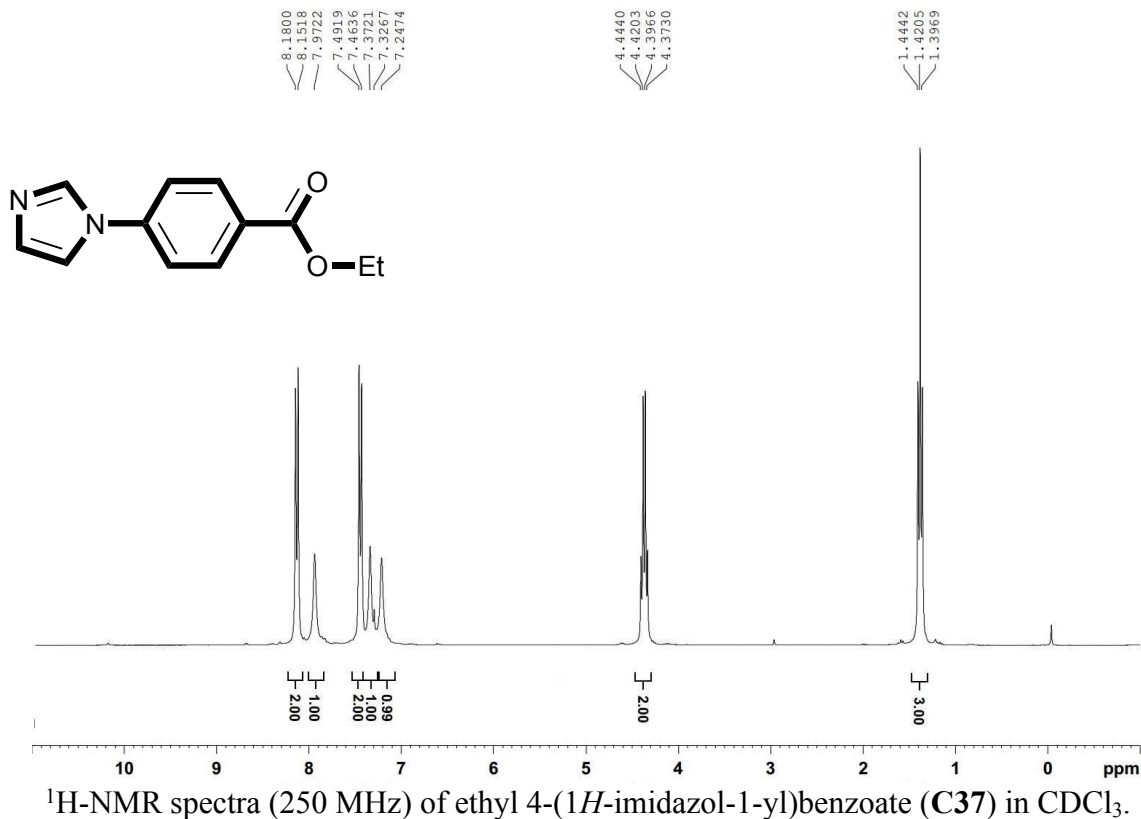
¹³C-NMR spectra (63 MHz) of 1-(2-nitrophenyl)-1H-imidazole (C35) in CDCl₃.

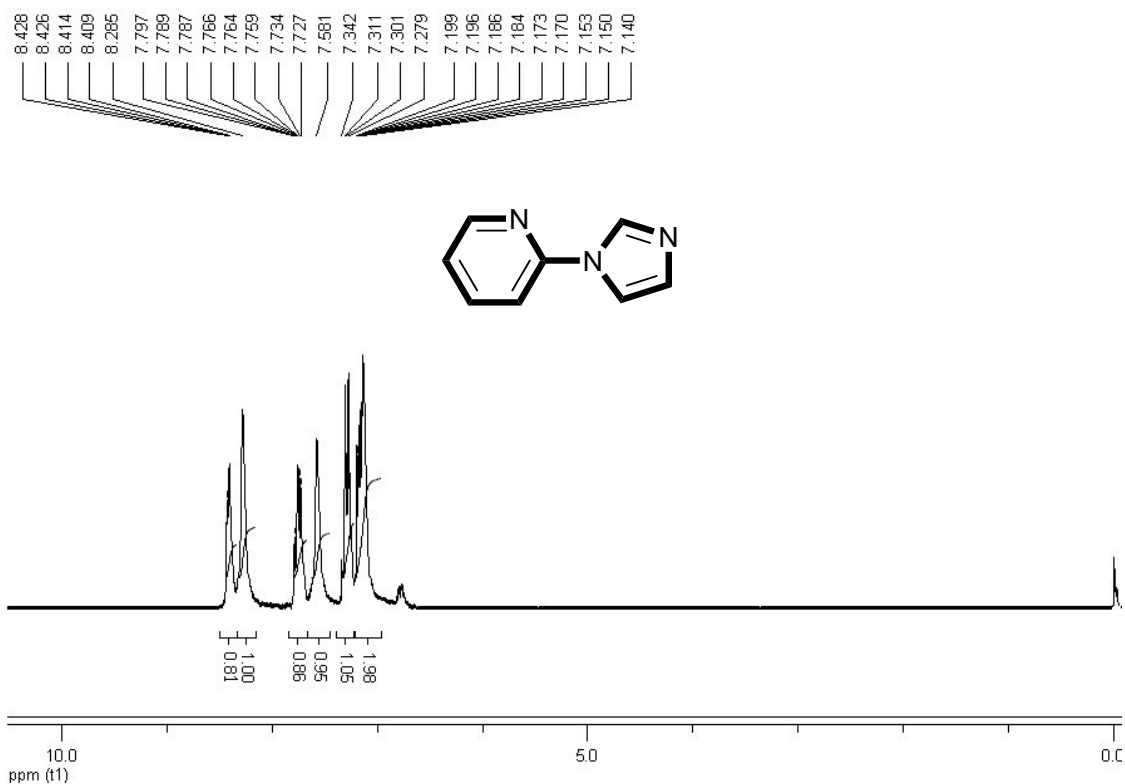


¹H-NMR spectra (250 MHz) of 1-(4-(1H-imidazol-1-yl)phenyl)ethan-1-one (C36) in CDCl₃.

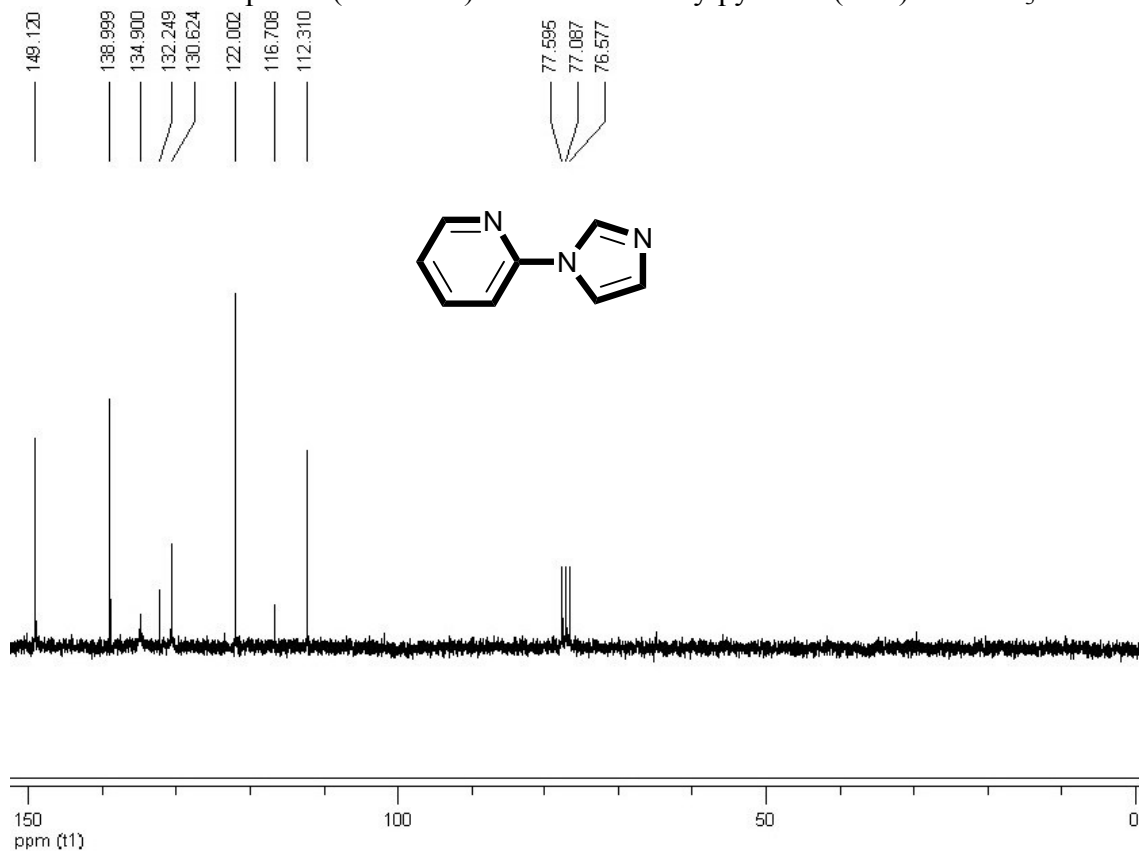


¹³C-NMR spectra (63 MHz) of 1-(4-(1H-imidazol-1-yl)phenyl)ethan-1-one (C36) in CDCl₃.

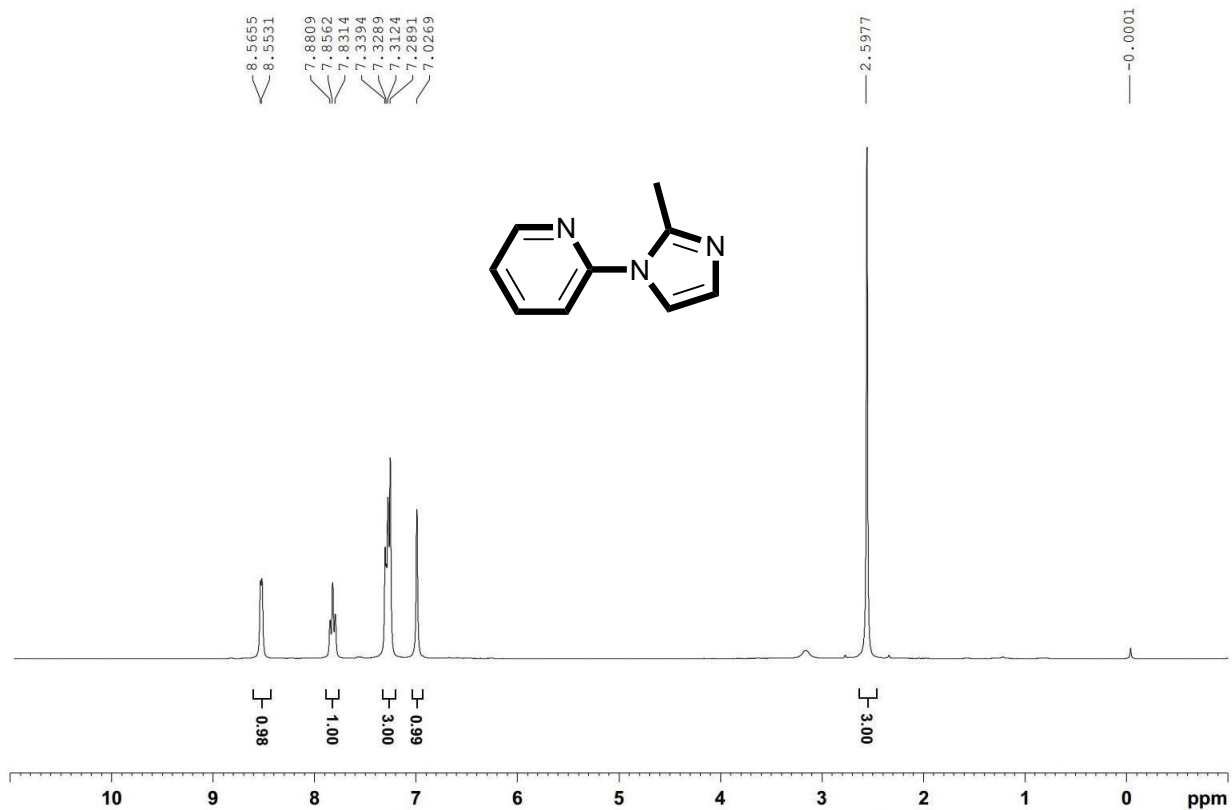




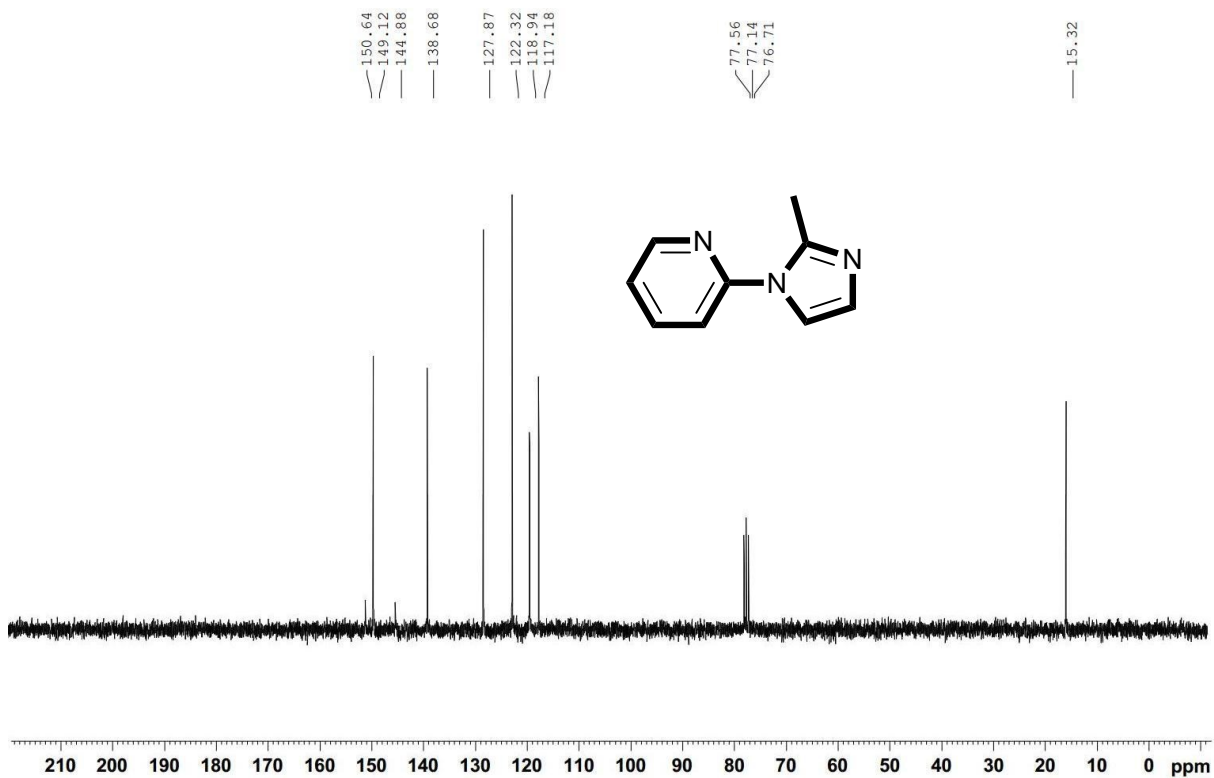
¹H-NMR spectra (250 MHz) of 2-imidazol-1-ylpyridine (C38) in CDCl₃.



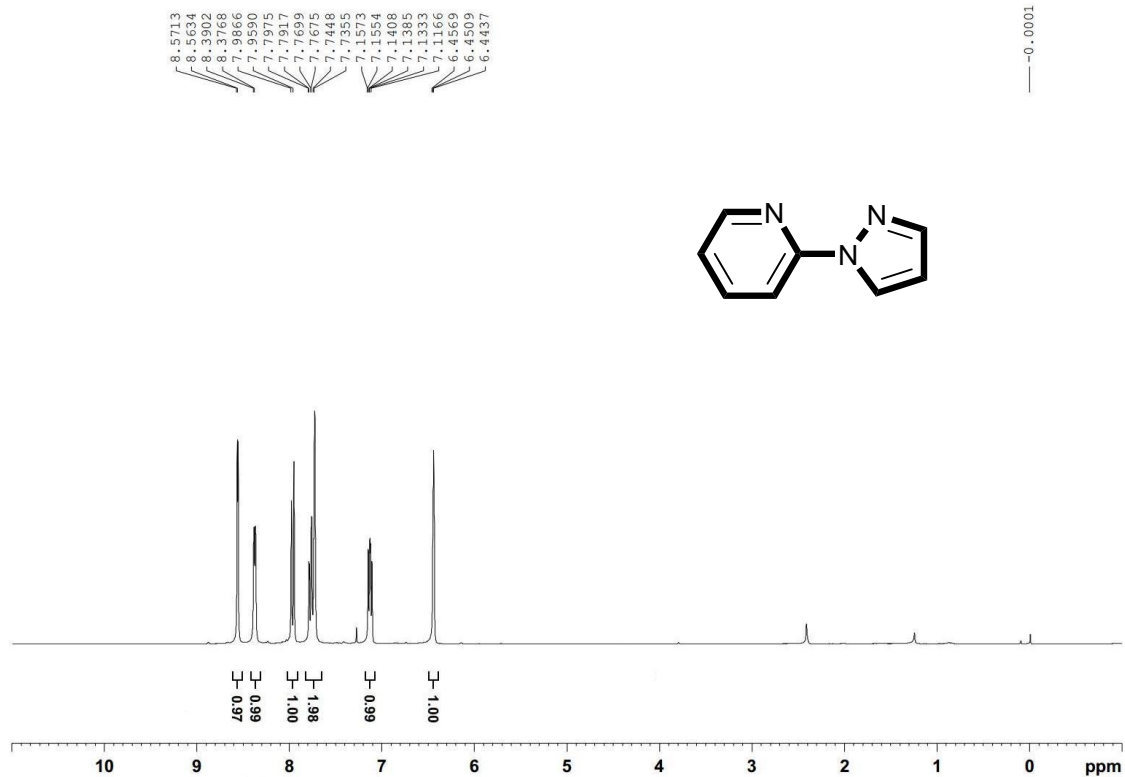
¹³C-NMR spectra (63 MHz) of 2-imidazol-1-ylpyridine (C38) in CDCl₃.



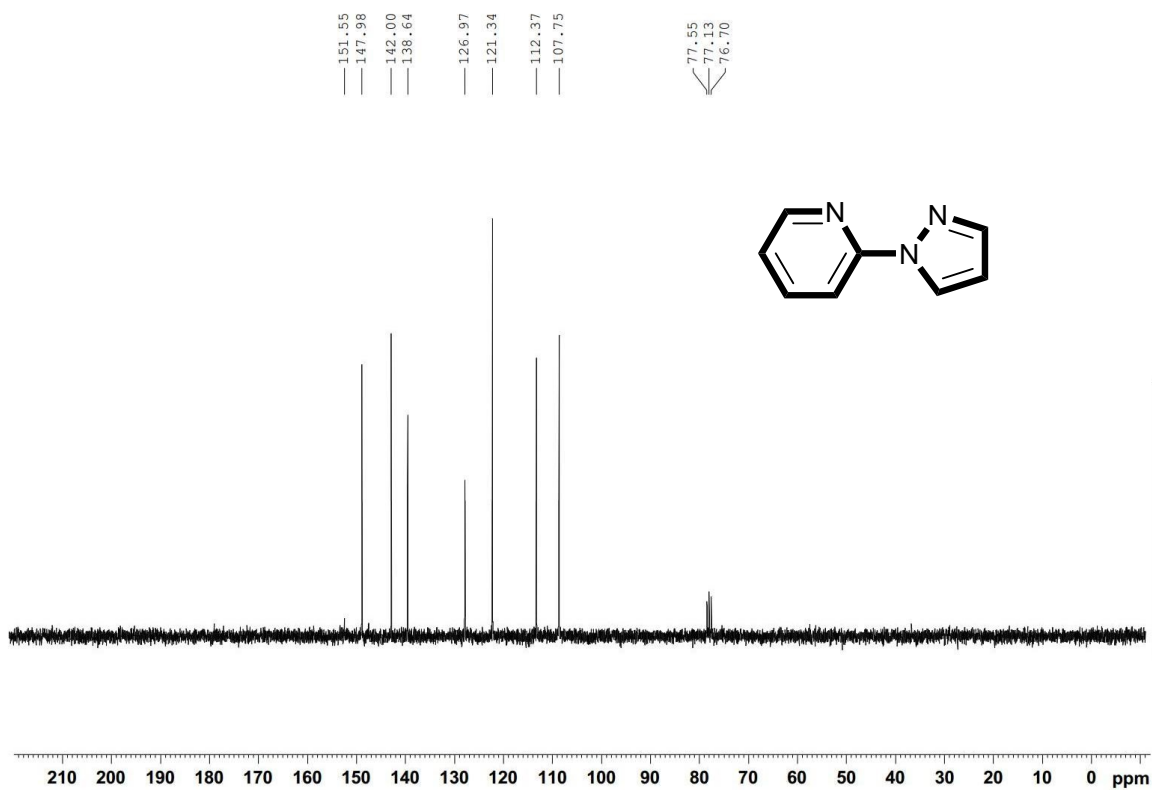
¹H-NMR spectra (250 MHz) of 2-(2-methyl-1H-imidazol-1-yl)pyridine (C39) in CDCl₃.



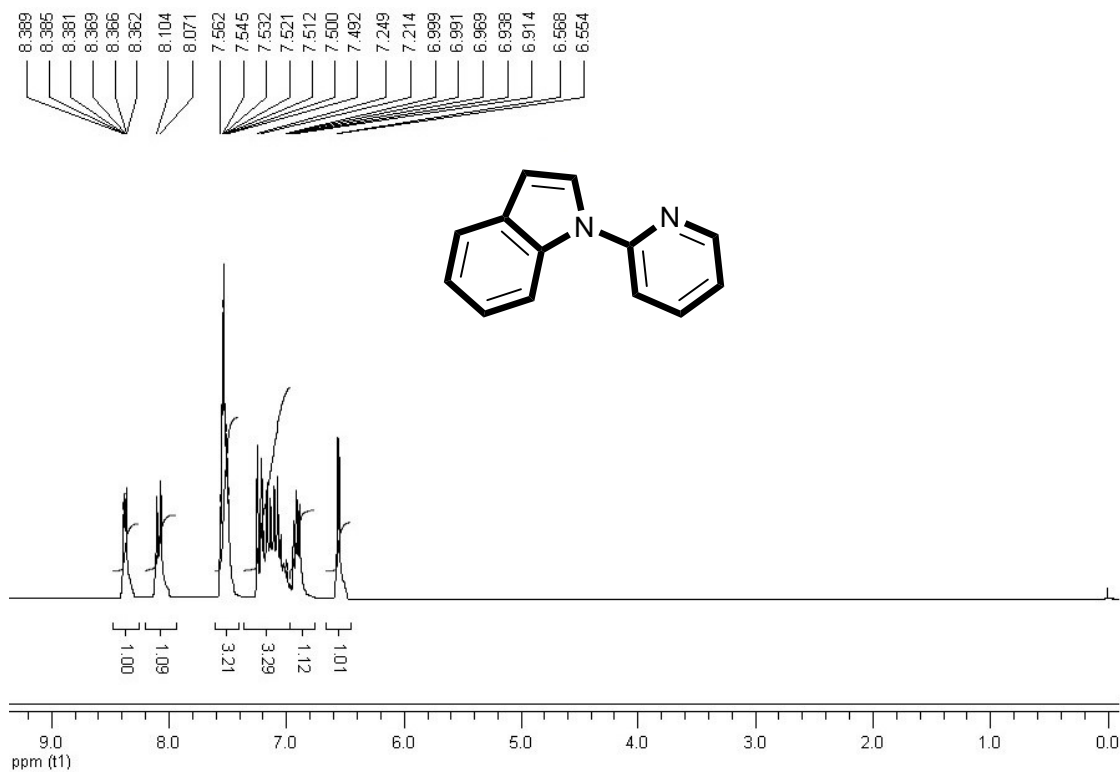
¹³C-NMR spectra (63 MHz) of 2-(2-methyl-1H-imidazol-1-yl)pyridine (C39) in CDCl₃.



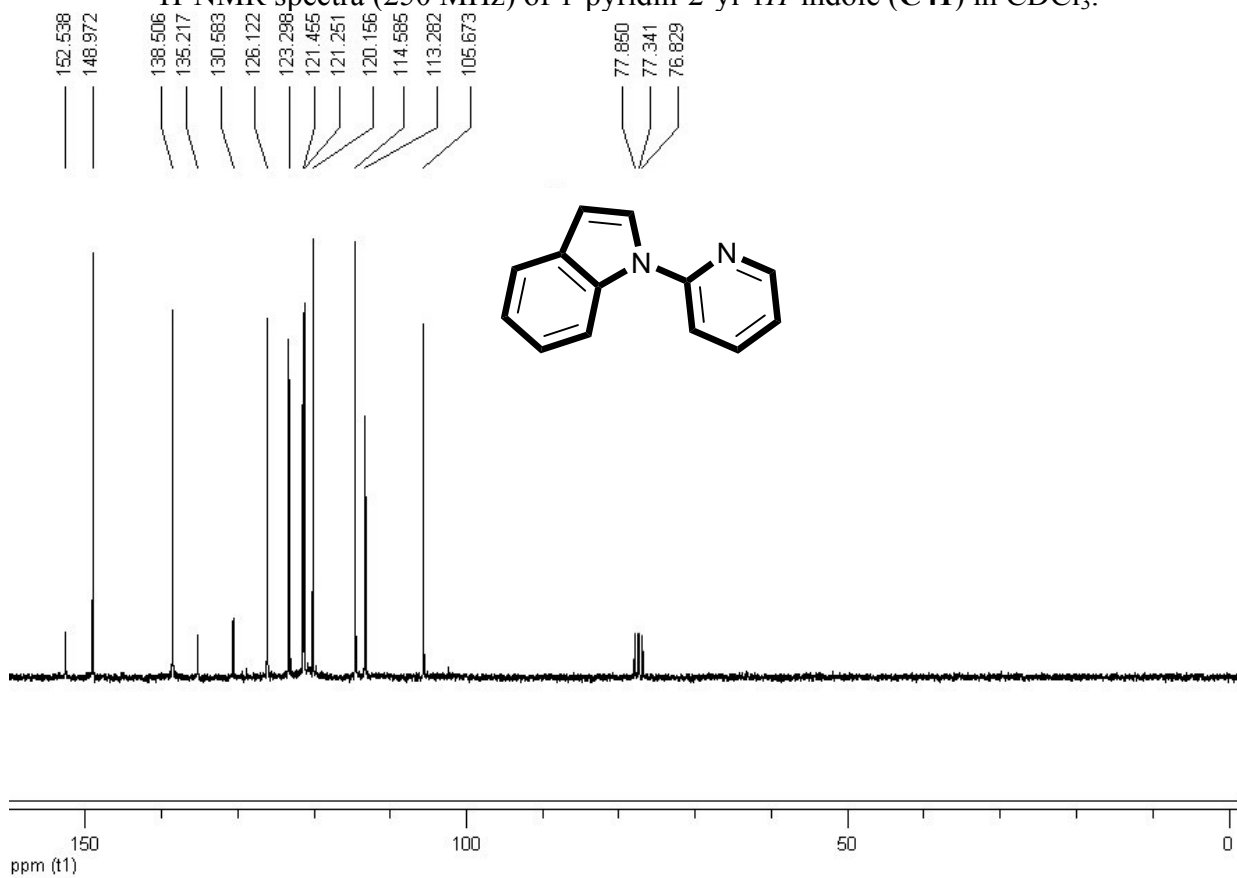
$^1\text{H-NMR}$ spectra (250 MHz) of 2-(1*H*-pyrazol-1-yl)pyridine (C40) in CDCl_3 .



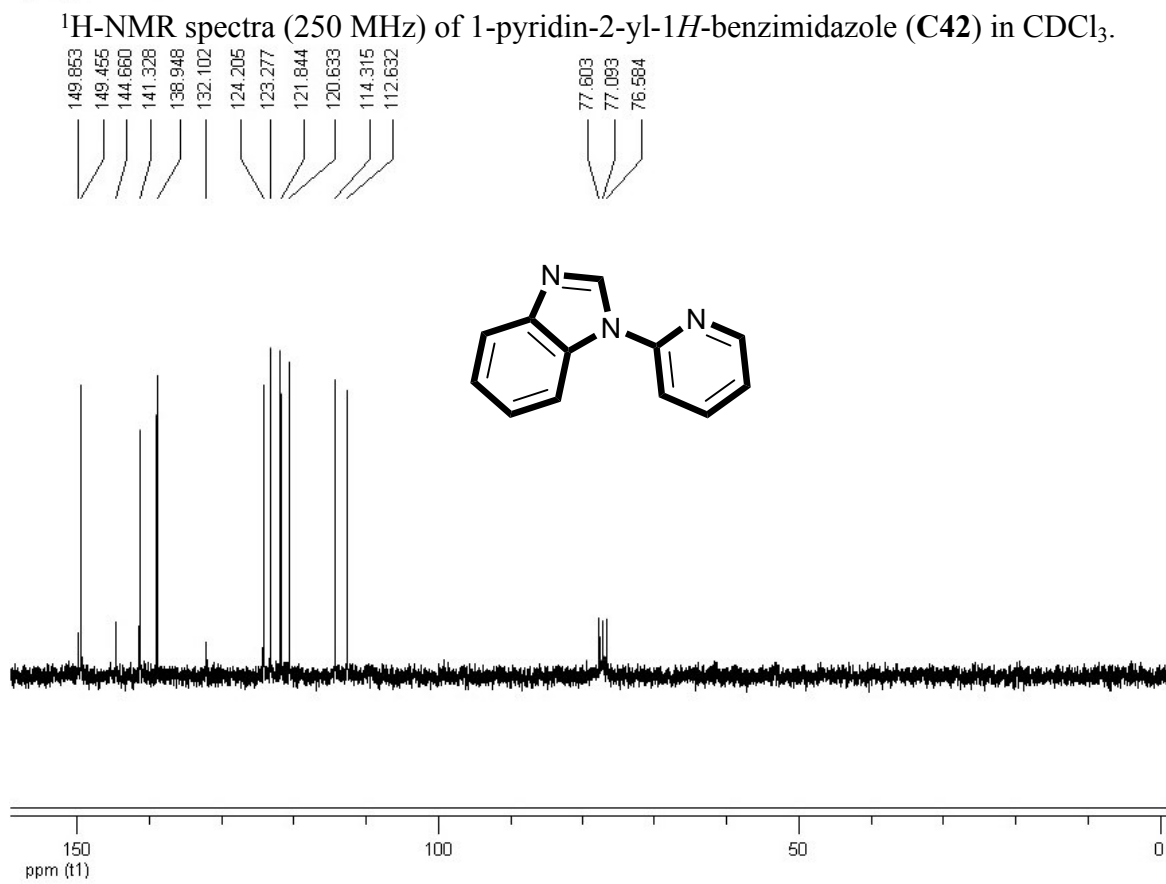
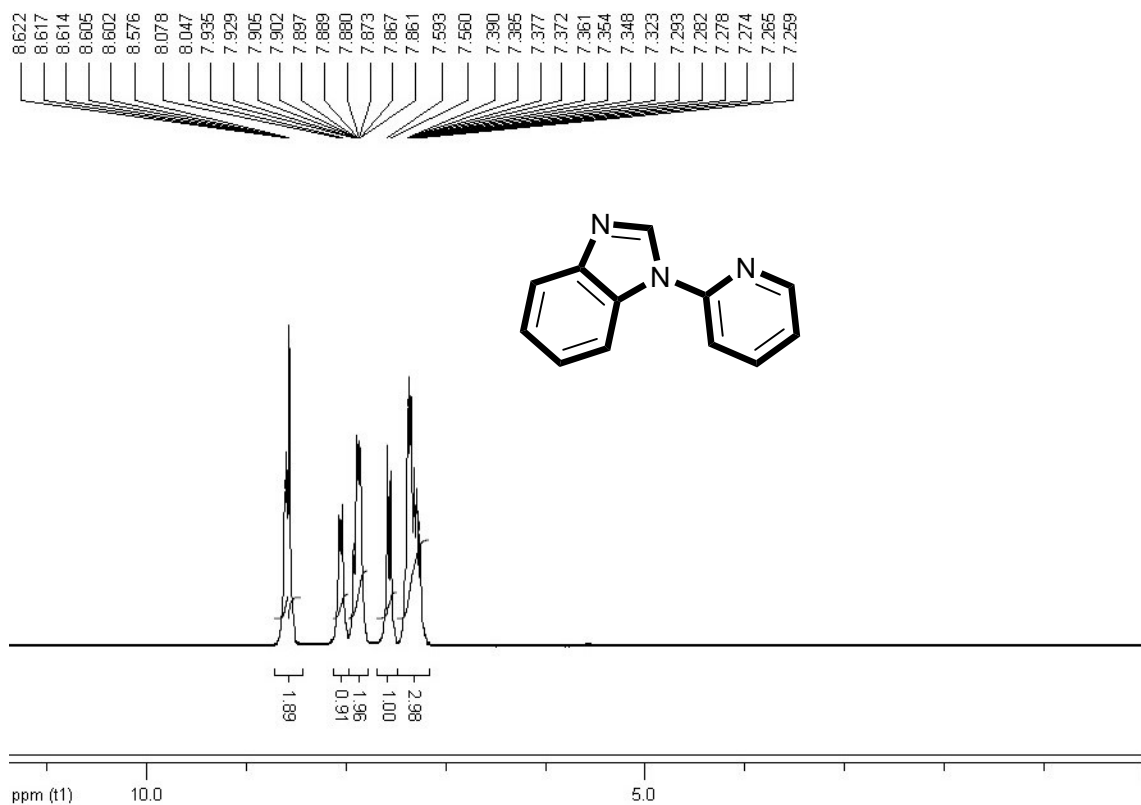
$^{13}\text{C-NMR}$ spectra (63 MHz) of 2-(1*H*-pyrazol-1-yl)pyridine (C40) in CDCl_3 .

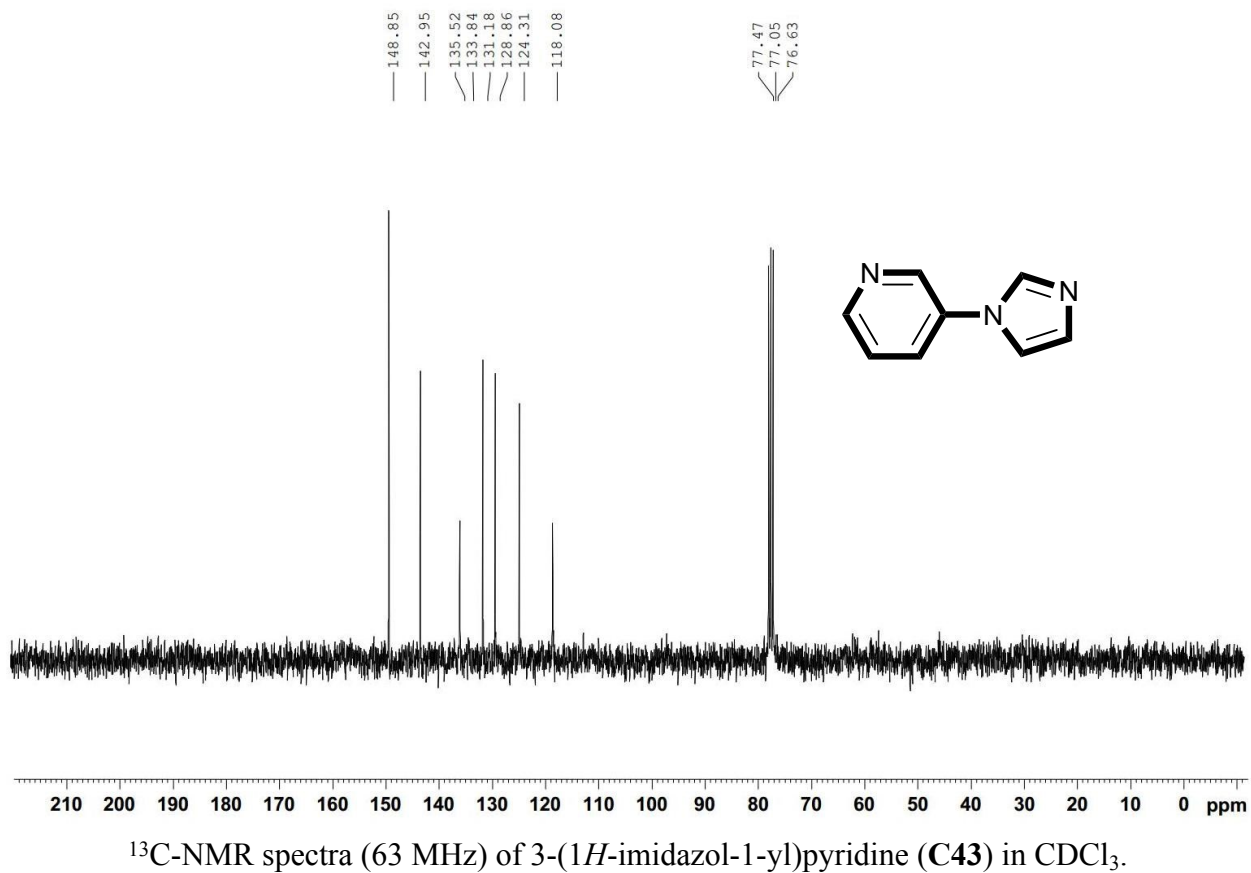
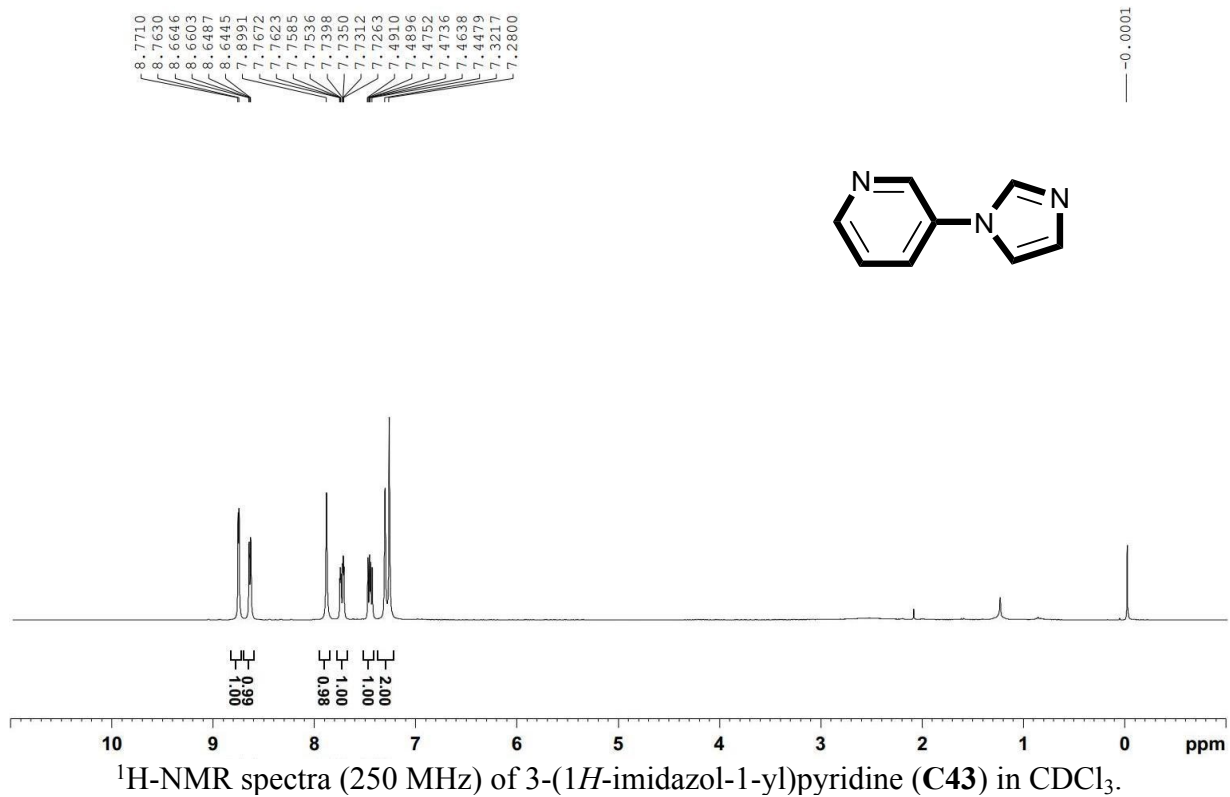


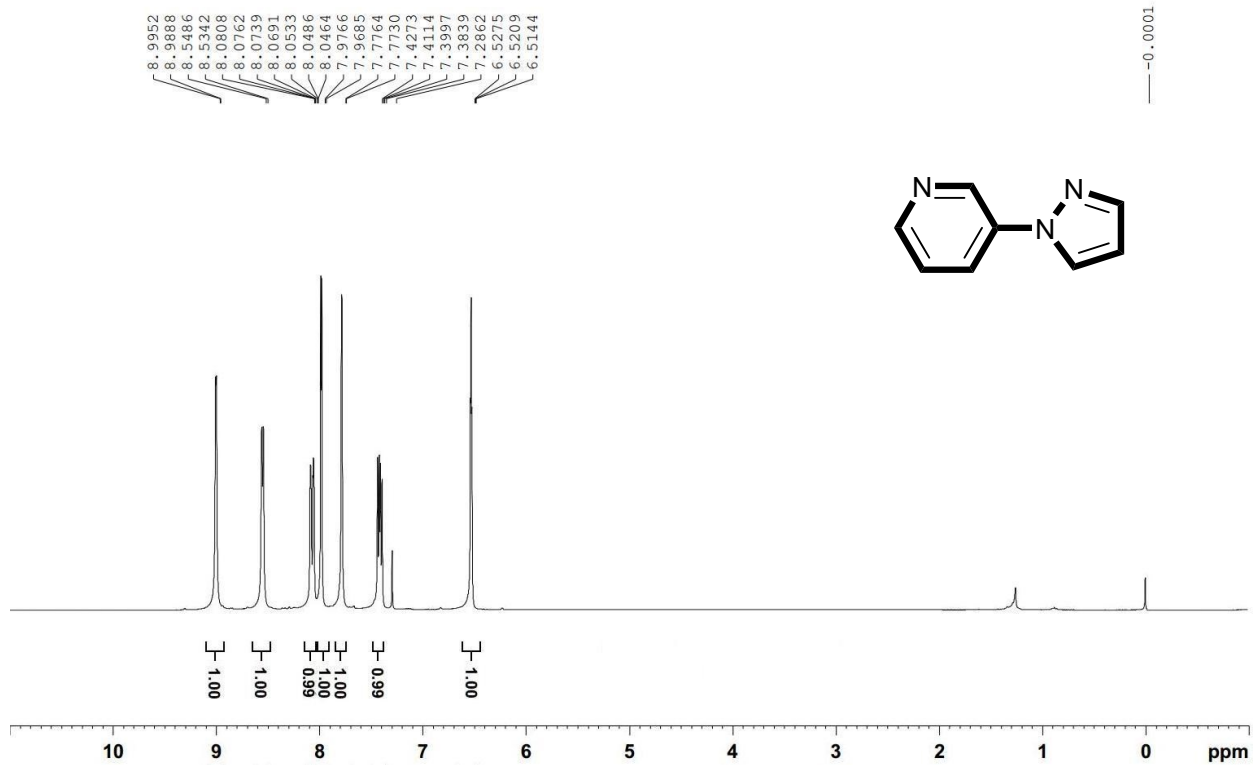
¹H-NMR spectra (250 MHz) of 1-pyridin-2-yl-1H-indole (C41) in CDCl₃.



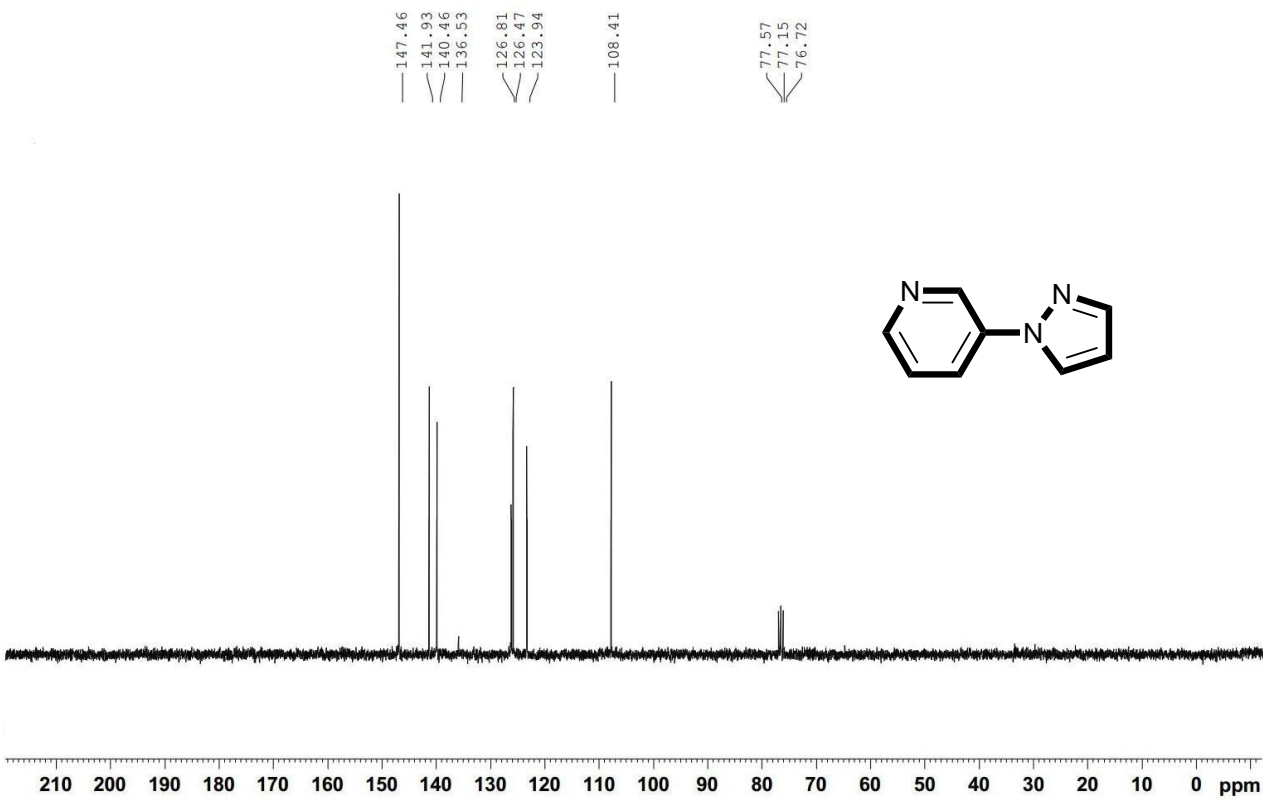
¹³C-NMR spectra (63 MHz) of 1-pyridin-2-yl-1H-indole (C41) in CDCl₃.



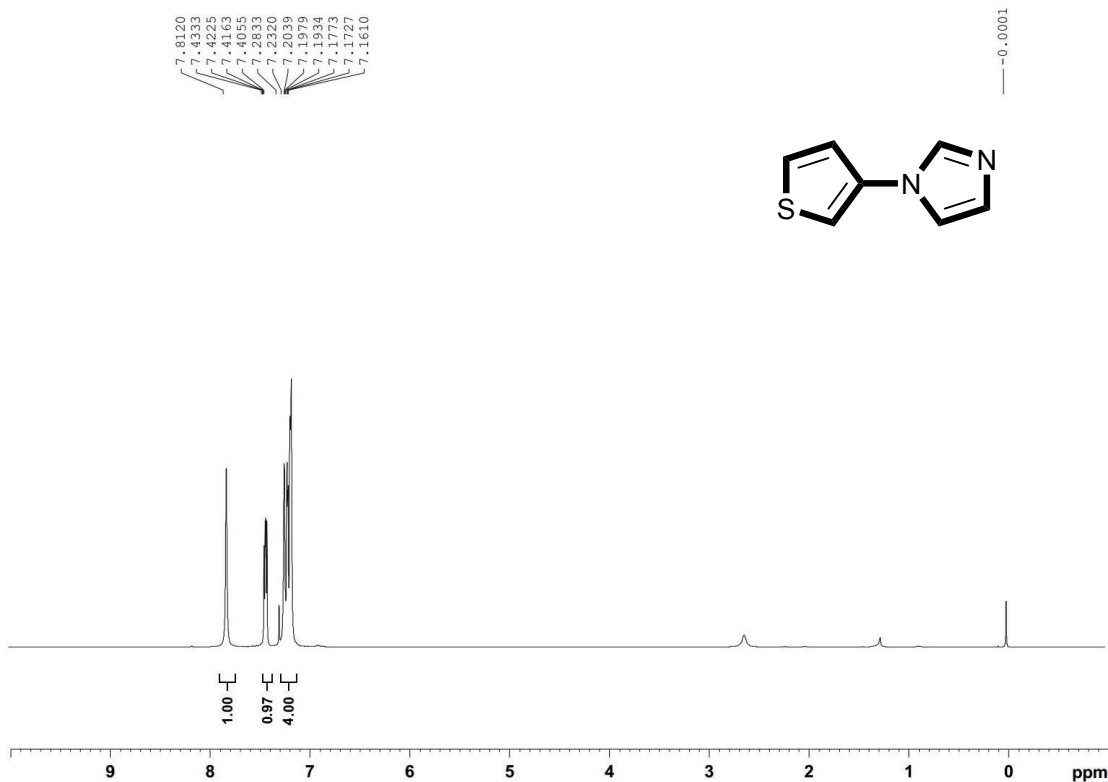




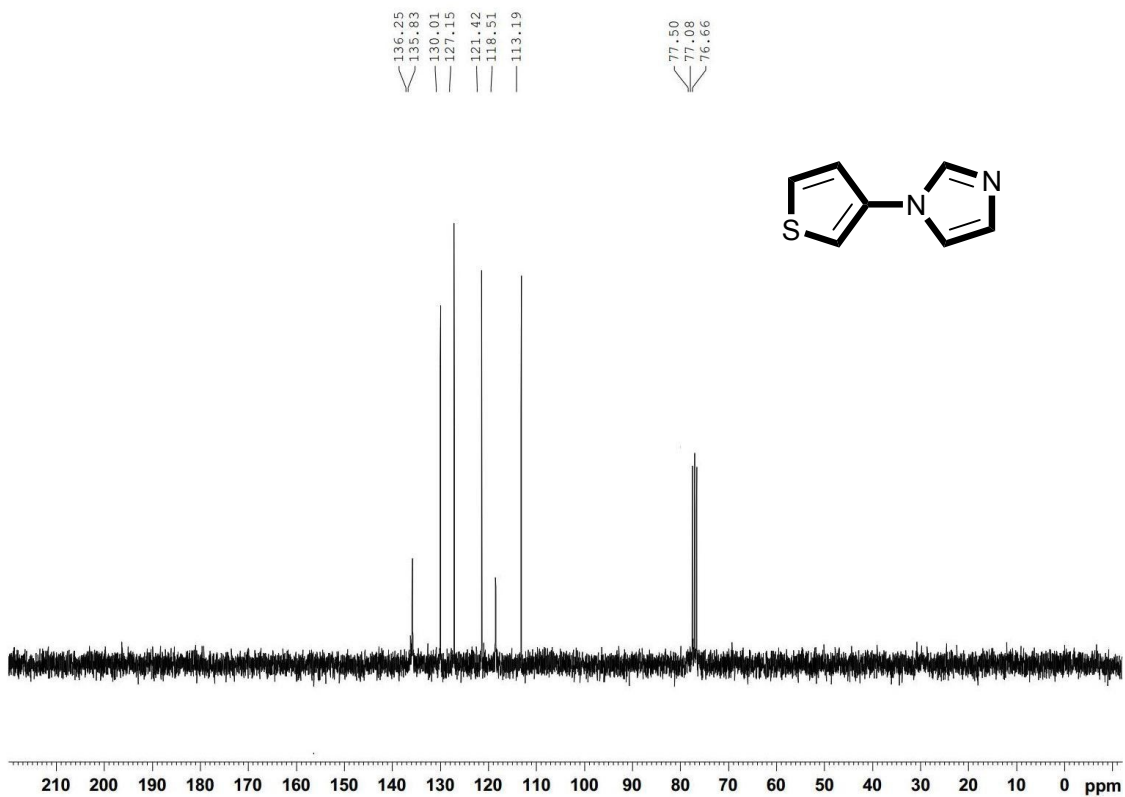
¹H-NMR spectra (250 MHz) of 3-(1*H*-pyrazol-1-yl)pyridine (C44) in CDCl₃.



¹³C-NMR spectra (63 MHz) of 3-(1*H*-pyrazol-1-yl)pyridine (C44) in CDCl₃.



¹H-NMR spectra (250 MHz) of 1-(thiophen-3-yl)-1*H*-imidazole (**C45**) in CDCl₃.



¹³C-NMR spectra (63 MHz) of 1-(thiophen-3-yl)-1*H*-imidazole (**C45**) in CDCl₃.