SUPPORTING INFORMATION

Metal-free C-H functionalization of 2*H*-imidazole 1-oxides with pyrrolyl fragments in the design of novel azaheterocyclic ensembles

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General Experimental Methods

The ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded using TMS as the internal standard and DMSO-d_6 as a deuterated solvent. The X-ray diffraction analysis was performed on a diffractometer, equipped with CDD detector (Mo KR graphite-monochromated radiation, λ = 1.54184 Å, ω-scanning technique, the scanning step was 1° and the exposure time per frame was 10 s at 295(2) K. Analytical absorption correction was used in the reflection intensity integration.[1] The structure was solved by the direct method and refined applying full matrix least-squares versus F^2_{hkl} with anisotropic displacement parameters for all non-hydrogen atoms using the SHELX97 program package.[2] All hydrogen atoms were located in different electron density maps and refined using a riding model with fixed thermal parameters. The mass spectra were recorded on a mass spectrometer with sample ionization by electron impact (EI). The IR spectra were recorded using a Fourier-transforminfrared spectrometer equipped with a diffuse reflection attachment. The elemental analysis was carried out on a CHNS/O analyzer. The course of the reactions was monitored by TCL on 0.25 mm silica gel plates (60F 254). Column chromatography was performed on silica gel (60, 0.035-0.070 mm (220-440 mesh)).

2,2-dimethyl-4-phenyl-2*H*-imidazole 1-oxide **1a**, 3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene 1-oxide **1c**,[3] 2-Ethyl-2-methyl-4-phenyl-2*H*-imidazole **1b**,[4] were prepared according to the published procedures. Pyrrole **2a**, 1-methylpyrrole **2b**, 2-phenyl-1*H*-pyrrole **2c**, 4,5,6,7-tetrahydro-1*H*-indole **2d** were purchased.

Experimental Procedure and Characterization Data for (1*H*-Pyrrol-2-yl)-2*H*-imidazole hydrochlorides (3a−m)HCl

To a stirring solution of the corresponding nitrone **1a−c** (1 mmol) and pyrrole **2a−d** (1 mmol) in benzene (15 mL), AcCl (0.07 mL, 1 mmol) was added dropwise at 5 °C. After 10 min, the reaction mixture was warmed to room temperature. The precipitate of hydrochloride **(4a-c, e-g, i, l)HCl** was formed, in order to initiate a precipitation heptane (5 mL) in case of **(4d, h, k, m)HCl**. The formed precipitate was filtered off, washed with benzene, and dried in air for 24 h.

2,2-Dimethyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3aHCl). Yield: 218 mg (80 %), mp = 142-145 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.71 (s, 6H); 6.34-6.29 (m, 2H); 7.71-7.54 (m, 6H); 12.95 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 24.0 (CH_3); 96.47 (C); 112.5 (CH); 119.6 (C); 122.6 (CH); 128.3 (CH); 128.8 (CH); 130.6 (CH); 131.9 (C); 132.0 (CH); 153.0 (C); 163.5 (C) ppm. IR (DRA): ν 3085, 2976, 2841, 2536, 1630, 1607, 1584, 1526, 1444, 1400,

1363, 1153, 1054, 851, 697, 591 cm^{-1}. MS (EI): *m/z* 237 $[M]^+$. Anal. Calcd for $C_{15}H_{16}ClN_3$: C, 65.81; H, 5.89; N, 15.35. Found: C, 65.44; H, 6.26; N, 14.98.

2,2-Dimethyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole hydrochloride (3bHCl). Yield: 264 mg (92 %), mp = 37-40 □C. R_f 0.1 (hexane/EtOAc, 6:4). ^1H NMR (DMSO-d_6): δ 1.63 (s, 6H); 3.98 (s, 3H); 5.99-5.97 (m, 1H); 6.08-6.04 (m, 1H); 7.26 (s, 1H); 7.52-7.45 (m, 2H); 7.59-7.53 (m, 3H); ppm. ^{13}C NMR (DMSO-d_6): δ 24.1 (CH_3); 36.5 (CH_3); 99.8 (C); 108.4 (CH); 118.8 (CH); 122.8 (C); 128.1 (CH); 128.7 (CH); 130.3 (CH); 131.7 (CH); 132.5 (C); 153.9 (C); 164.3 (C) ppm. IR (DRA): ν 3070, 2985, 2501, 1626, 1604, 1583, 1490, 1422, 1401, 1427, 1084, 1071, 961, 760, 700, 607 cm^{-1}. MS (EI): *m/z* 251 $[M]^+$. Anal. Calcd for $C_{16}H_{18}ClN_3$: C, 66.78; H, 6.30; Cl, 12.32; N, 14.60. Found: C, 66.60; H, 6.51; N, 14.38.

2,2-Dimethyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3cHCl). Yield: 268 mg (77 %), mp = 172-175 □C. R_f 0.1 (hexane/EtOAc, 6:4). ^1H NMR (DMSO-d_6): δ 1.76 (s, 6H); 6.44-6.40 (m, 1H); 6.94-6.91 (m, 1H); 7.54-7.42 (m, 3H); 7.68-7.56 (m, 3H); 7.75-7.70 (m, 2H); 8.11-8.07 (m, 2H); 13.57 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 24.1 (CH_3); 95.66 (C); 111.2 (CH); 120.0 (C); 126.0 (CH); 127.2 (CH); 128.3 (CH); 128.3 (CH); 128.8 (CH); 129.0 (C); 129.1 (CH); 129.8 (CH); 130.7 (CH); 131.7 (C); 145.1 (C); 151.7 (C); 163.4 (C) ppm. IR (DRA): ν 3043, 2979, 2932, 2349, 1558, 1446, 1407, 1366, 1299, 1194, 1159, 1130, 1015, 740, 696, 661 cm^{-1}. MS (EI): *m/z* 317 $[M]^+$. Anal. Calcd for $C_{21}H_{20}ClN_3O$: C, 72.09; H, 5.76; N, 12.01. Found: C, 72.25; H, 5.91; N, 12.09.

2-(2,2-Dimethyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole hydrochloride (3dHCl). Yield: 222 mg (68 %), mp = 137-140 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^1H NMR (DMSO-d_6): δ 1.74-1.58 (m, 10H); 2.31(t, 2H, J = 5.88); 2.69 (t, 2H, J = 6.02); 6.14 (s, 1H); 7.70-7.53 (m, 5H); 13.06 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 21.7 (CH_2); 21.8 (CH_2); 22.4 (CH_2); 22.9 (CH_2); 24.4 (CH_3); 94.8 (C); 117.3 (C); 122.8 (CH); 123.5 (C); 128.4 (CH); 128.7 (CH); 130.8 (CH); 131.7 (C); 146.4 (C); 150.6 (C); 163.4 (C) ppm. IR (DRA): ν 2990, 2932, 1635, 1548 1464, 1375, 1279, 1188, 1082, 1070, 1005, 844, 750, 662, 599 cm^{-1}. MS (EI): *m/z* 291 $[M]^+$. Anal. Calcd for $C_{19}H_{22}ClN_3$: C, 69.61; H, 6.76; N, 12.82. Found: C, 69.58; H, 7.03; N, 12.44.

2-Ethyl-2-methyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3eHCl). Yield: 226 mg (79 %), mp = 177-180 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^1H NMR (DMSO-d_6): δ 0.94 (t, 3H, J = 7.38); 1.69 (s, 3H); 2.15-2.00 (m, 2H); 6.37-6.31 (m, 2H); 7.72-7.53 (m, 6H); 13.09 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 8.3 (CH_3); 21.8 (CH_3); 30.7 (CH_2); 99.2 (C); 112.7 (CH); 119.5 (C); 123.0 (CH); 128.4 (CH); 128.8 (CH); 130.7 (CH); 131.9 (C); 132.4 (CH); 153.2 (C); 163.9 (C) ppm. IR (DRA): ν 3087, 2972, 2876, 2637, 2478, 1626, 1583, 1489, 1444, 1363, 1296, 1159, 930, 850, 780, 696 cm^{-1}. MS (EI): *m/z* 251 $[M]^+$. Anal. Calcd for $C_{16}H_{18}ClN_3$: C, 66.78; H, 6.30; N, 14.60. Found: C, 66.52; H, 6.30; N, 14.48.

2-Ethyl-2-methyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole hydrochloride (3fHCl). Yield: 273 mg (91 %), mp = 112-115 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 0.74 (t, 3H, J = 7.36); 1.60 (s, 3H); 2.15-2.04 (m, 2H); 3.96 (s, 3H); 5.98-5.96 (m, 1H); 6.07-6.04 (m, 1H); 7.23 (s, 1H); 7.60-7.44 (m, 5H) ppm. ^{13}C NMR (DMSO-d_6): δ 8.1 (CH_3); 22.6 (CH_3); 30.6 (CH_2); 36.6 (CH_3); 102.4 (C); 108.4 (CH); 118.5 (CH); 122.9 (C); 128.2 (CH); 128.7 (CH); 130.3 (CH); 131.7 (CH); 132.6 (C); 154.5 (C); 165.0 (C) ppm. IR (DRA): ν 3058, 2967, 2933, 1618, 1580, 1488, 1444, 1401, 1341, 1243, 1160, 1064, 1015, 961, 813, 711, 646 cm^{-1}. MS (EI): *m/z* 265 $[M]^+$. Anal. Calcd for $C_{17}H_{20}ClN_3$: C, 67.65; H, 6.68; N, 13.92. Found: C, 67.64; H, 6.74; N, 13.80.

2-Ethyl-2-methyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3gHCl). Yield: 286 mg (79 %), mp = 67-70 °C. R_f 0.1 (hexane/EtOAc, 7:3). ^{1}H NMR (DMSO-d_6): δ 0. 99 (t, 3H, J = 7.38); 1.73 (s, 3H); 2.18-2.02 (m, 2H); 6.42 (d, 1H; J = 2.12); 6.96-6.92 (m, 1H); 7.55-7.40 (m, 3H); 7.75-7.57 (m, 5H); 8.08 (d, 2H, J = 7.32); 13.58 (m, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 8.3 (CH_3); 21.9 (CH_3); 30.9 (CH_2); 95.3 (C); 98.8 (C); 111.3 (CH); 120.1 (CH); 126.0 (CH); 128.3 (CH); 128.5 (CH); 128.8 (CH); 129.1 (C); 129.2 (CH); 129.8 (CH); 130.8 (CH); 131.8 (C); 152.0 (C); 163.9 (C) ppm. IR (DRA): ν 3098, 2937, 2839, 2455, 2343 1625, 1550, 1399, 1295, 1165, 997, 861, 805, 764, 693, 602 cm^{-1}. MS (EI): *m/z* 327 $[M]^+$. Anal. Calcd for $C_{22}H_{22}ClN_3$: C, 72.62; H, 6.09; N, 11.55. Found: C, 72.46; H, 6.13; N, 11.40.

2-(2-Ethyl-2-methyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole hydrochloride (3hHCl). Yield: 231 mg (68 %), mp = 135-138 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 0.92 (t, 3H, J = 7.38); 1.76-1.56 (m, 7H); 2.14-1.97 (m, 2H); 2.31 (t, 2H, J = 5.94); 2.70 (t, 2H, J = 6.1); 6.15 (s, 1H); 7.61-7.54 (m, 2H); 7.69-7.61 (m, 3H); 13.18 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 8.0 (CH_3); 21.7 (CH_2); 21.8 (CH_2); 22.3 (CH_3); 22.4 (CH_2); 22.9 (CH_2); 31.1 (CH_2); 97.6 (C); 117.2 (C); 123.0 (CH); 123.7 (C); 128.5 (CH); 128.7 (CH); 130.8 (CH); 131.7 (C); 146.8 (C); 150.8 (C); 163.9 (C) ppm. IR (DRA): ν 3103, 2929, 2865, 2780, 2569, 1630, 1585, 1442, 1373, 1278, 1145, 1058, 996, 844, 700 cm^{-1}. MS (EI): *m/z* 305 $[M]^+$. Anal. Calcd for $C_{20}H_{24}ClN_3$: C, 70.26; H, 7.08; N, 12.29. Found: C, 70.15; H, 7.23; N, 12.24.

2-Phenyl-3-(1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3iHCl). Yield: 244 mg (78 %), mp = 188-190 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 2.07-1.49 (m, 10H); 6.38-6.30 (d, 2H); 7.47-7.52 (m, 6H); 13.36 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 22.3 (CH_2); 24.1 (CH_2); 34.0 (CH_2); 99.1 (CH); 99.4 (C); 111.9 (CH); 119.9 (C); 121.8 (CH); 128.0 (CH); 128.4 (CH); 130.1 (CH); 132.0 (C); 152.8 (C); 163.2 (C) ppm. IR (DRA): ν 3020, 2934, 2851, 2681, 1632, 1586, 1491, 1397, 1337, 1152, 1057, 952, 824, 769, 702 cm^{-1}. MS (EI): *m/z* 277 $[M]^+$. Anal. Calcd for $C_{18}H_{20}ClN_3$: C, 68.89; H, 6.42; N, 13.39. Found: C, 68.56; H, 6.50; N, 13.28.

(1-methyl-1*H*-pyrrol-2-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3kHCl). Yield: 261 mg (80 %), mp = 137-140 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6):

δ 1.65 (s, 2H); 1.88-1.74 (m, 8H); 3.94 (s, 3H); 5.98-5.95 (m, 1H); 6.04-6.01 (m, 1H); 7.35 (s, 1H); 7.51-7.44 (m, 2H); 7.58-7.51 (m, 3H) ppm. ^{13}C NMR (DMSO-d_6): δ 23.5 (CH_2); 24.9 (CH_2); 34.4 (CH_2); 36.4 (CH_3); 102.4 (C); 108.0 (CH); 117.4 (CH); 123.3 (C); 128.0 (CH); 128.6 (CH); 130.1 (CH); 130.8 (CH); 132.8 (C); 154.1 (C); 164.4 (C) ppm. IR (DRA): ν 2940, 2857, 1746, 1617, 1568, 1471, 1418, 1361, 1237, 1158, 986, 785, 744, 706, 584, 556 cm^{-1}. MS (EI): *m/z* 291 $[M]^+$. Anal. Calcd for $C_{19}H_{22}ClN_3$: C, 69.61; H, 6.76; N, 12.82. Found: C, 69.35; H, 6.94; N, 12.51.

2-Phenyl-3-(5-phenyl-1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3lHCl). Yield: 342 mg (88 %), mp = 212-215 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.61-1.49 (m, 1H), 1.78-1.68 (m, 1H); 1.94-1.79 (m, 4H); 2.13-1.97 (m, 4H); 6.46-6.40 (m, 1H); 6.97-6.92 (m, 1H); 7.48-7.42 (m, 1H); 7.54-7.48 (m, 2H); 7.63-7.56 (m, 2H); 7.69-7.63 (m, 1H); 7.75-7.69 (m, 2H); 8.12 (d, 2H, J = 7.32); 13.87 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 22.3 (CH_2); 24.3 (CH_2); 34.0 (CH_2); 98.6 (C); 111.4 (CH); 120.1 (C); 126.1 (CH); 128.2 (CH); 128.4 (CH); 128.9 (CH); 129.0 (C); 129.2 (CH); 129.9 (CH); 130.7 (CH); 131.9 (CH); 145.6 (C); 151.7 (C); 163.5 (C) ppm. IR (DRA): ν 2942, 2892, 2741, 1624, 1602, 1576, 1553, 1445, 1306, 1293, 1057, 954, 854, 765, 690 cm^{-1}. MS (EI): *m/z* 353 $[M]^+$. Anal. Calcd for $C_{24}H_{24}ClN_3$: C, 73.93; H, 6.20; N, 10.78. Found: C, 73.89; H, 6.30; N, 10.60.

2-Phenyl-3-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3mHCl). Yield: 256 mg (70 %), mp = 206-210 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.89-1.47 (m, 12H); 2.1-1.9 (m, 2H); 2.32 (t, 2H, J = 5.96); 2.71 (t, 2H, J = 6.1); 6.14 (s, 1H); 7.60-7.53(m, 2H); 7.69-7.61 (m, 3H); 13.38 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 21.7 (CH_2); 21.8 (CH_2); 22.3 (CH_2); 22.4 (CH_2); 22.9 (CH_2); 24.2 (CH_2); 34.3 (CH_2); 97.8 (C); 99.5 (C); 117.5 (C); 123.1 (CH); 123.6 (C); 128.4 (CH); 128.8 (CH); 130.7 (CH); 131.9 (C); 150.6 (C); 163.4 (C) ppm. IR (DRA): ν 3099, 2999, 2927, 1631, 1585, 1529, 1439, 1421, 1343, 1280, 1251, 1146, 956, 846, 699 cm^{-1}. MS (EI): *m/z* 331 $[M]^+$. Anal. Calcd for $C_{22}H_{26}ClN_3$: C, 71.82; H, 7.12; N, 11.42. Yield: C, 71.57; H, 7.32; N, 11.12.

Experimental Procedure and Characterization Data for (1*H*-Pyrrol-2-yl)-2*H*-imidazoles 3a-m

In order to convert hydrochlorides **(4a−m)HCl** to the corresponding bases **4a−m**, $NaHCO_3$ (2.5 mL, 2 mmol) was added to **(4a−m)HCl** in aq EtOH (30 mL), and the mixture was heated under reflux for 40 min. Finally, the reaction mixture was cooled and filtered through silica gel and then concentrated in vacuo. The residue was additionally purified by recrystallization from the heptane/benzene mixture, 1:1 mixture.

2,2-Dimethyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole (3a). Yield: 182 mg (77 %), mp = 115-118 °C. R_f 0.2 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.51 (s, 6H); 5.82-5.89 (m, 1H); 5.95-6.03 (m, 1H); 6.89-6.97 (m, 1H); 7.45-7.61 (m, 5H); 11.74 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 24.6 (CH_3); 100.9 (C); 108.9 (CH); 113.3 (CH); 123.1 (CH); 123.1(C); 128.1(CH); 128.2(CH); 129.6(CH); 134.1(C); 155.1(C); 163.8(C) ppm. IR (DRA): ν 3850, 3243, 3188, 3167, 3141, 2978, 1602, 1579, 1519, 1442, 1133, 917, 735, 696, 580 cm^{-1}. MS (EI): *m/z* 237 $[M]^+$. Anal. Calcd for $C_{15}H_{15}N_3$: C, 75.92; H, 6.37; N, 17.71. Found: C, 76.15; H, 6.20; N, 17.65.

2,2-Dimethyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole (3b). Yield: 225 mg (90 %), mp = 47-50 °C. R_f 0.2 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.51 (s, 6H); 3.87 (s, 3H); 5.82-5.81 (m, 1H); 5.96-5.94 (m, 1H); 7.00 (t, 1H, J = 2.1); 7.51-7.45 (m, 5H) ppm. ^{13}C NMR (DMSO-d_6): δ 24.4 (CH_3); 36.4 (CH_3); 101.4 (C); 107.1 (CH); 114.9 (CH); 124.3 (C); 127.9 (CH); 128.2 (CH); 128.3 (CH); 129.6 (CH); 133.9 (C); 155.2 (C); 164.3(C) ppm. IR (DRA): ν 2975, 2930, 1726, 1558, 1419, 1241, 1215, 1171, 1078, 1061, 958, 898, 695, 679, 574 cm^{-1}. MS (EI): *m/z* 251 $[M]^+$. Anal. Calcd for $C_{16}H_{17}N_3$: C, 76.46; H, 6.82; N, 16.72. Found: C, 76.26; H, 7.23; N, 16.51.

2,2-Dimethyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole (3c). Yield: 234 mg (75 %), mp = 72-75 °C. R_f 0.3 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.55 (s, 6H); 5.90 (d, 1H, J = 1.14); 6.49 (t, 1H, J = 1.74); 7.22 (t, 1H, J = 7.36); 7.37-7.30 (m, 2H); 7.58-7.48 (m, 5H); 7.85 (t, 2H, J = 4.18), 11.99 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 24.6 (CH_3); 101.1 (C); 107.2 (CH); 115.0 (CH); 124.9 (CH); 125.5 (C); 126.7 (CH); 128.0 (CH); 128.2 (CH); 128.4 (CH); 129.4 (CH); 131.5 (C); 134.1 (C); 136.2 (C); 154.8 (C); 163.8 (C) ppm. IR (DRA): ν 2977, 2838, 2493, 1624, 1550, 1487, 1447, 1303, 1174, 1059, 913, 861, 764, 597, 566 cm^{-1}. MS (EI): *m/z* 313 $[M]^+$. Anal. Calcd for $C_{21}H_{19}N_3$: C, 80.48; H, 6.11; N, 13.41. Found: C, 80.03; H, 6.30; N, 13.67.

2-(2,2-Dimethyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole (3d). Yield: 183 mg (63 %), mp = 87-90 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.69-1.39 (m, 12H); 2.32-2.15 (m, 2H); 5.57 (s, 1H); 7.62-7.43 (m, 5H); 11.19 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 22.2 (CH_2); 22.4 (CH_2); 22.6 (CH_2); 23.2 (CH_2); 24.8 (CH); 100.5 (C); 112.4 (CH); 117.2 (C); 122.0 (C); 128.0 (CH); 128.2 (CH); 129.5 (CH); 133.0 (C); 154.9 (C); 164.0 (C) ppm. IR (DRA): ν 3288, 3212, 2927, 2854, 1705, 1660, 1603, 1538, 1490, 1443, 1402, 1184, 934, 694, 578 cm^{-1}. MS (EI): m/z 291 [M]+. Anal. Calcd for $C_{19}H_{21}N_3$: C, 78.32; H, 7.26; N, 14.42. Found: C, 78.48; H, 7.21; N, 14.31.

2-Ethyl-2-methyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole (3e). Yield: 185 mg (74 %), mp = 80-83 °C. R_f 0.2 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 0.71 (t, 3H, J = 7.14); 1.49 (s, 3H); 2.08-1.94(m, 2H); 5.85 (s, 1H); 5.94 (s, 1H); 6.92 (s, 1H); 7.58-7.45 (m, 5H); 11.71 (s, 1H); ^{13}C NMR (DMSO-d_6): δ 8.2 (CH_3); 23.1 (CH_3); 30.8 (CH_2); 103.2 (C); 108.9 (CH_2); 113.2 (CH_2); 123.0 (CH_2); 123.1 (C); 128.1 (CH_2); 128.2 (CH_2); 129.6 (CH_2); 134.2 (C); 155.6 (C); 164.5 (C). IR (DRA): ν 3256, 3168, 3146, 3115, 2974, 2933, 1601, 1579, 1519, 1418, 1120, 1042, 931, 736, 696 cm^{-1}. MS

(EI): *m/z* 251 $[M]^+$. Anal. Calcd for $C_{16}H_{17}N_3$: C, 76.46; H, 6.82; N, 16.72. Found: C, 76.68; H, 6.42; N, 16.90.

2-Ethyl-2-methyl-5-(1-methyl-1*H*-pyrrol-2-yl)-4-phenyl-2*H*-imidazole (3f). Yield: 230 mg (87 %), mp =97-100 °C. R_f 0.3 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 0.72 (t, 3H, J = 7.36); 1.49 (s, 3H); 2.03-1.95 (m, 2H); 3.87 (s, 3H); 5.82-5.79 (m, 1H); 5.96-5.93 (m, 1H); 7.01 (t, 1H, J = 2.04); 7.52-7.42 (m, 5H) ppm. ^{13}C NMR (DMSO-d_6): 8.2(CH_3); 22.9 (CH_3); 30.6 (CH_2); 36.4 (CH_3); 103.7 (C); 107.1 (CH); 114.9 (CH); 124.3 (C); 128.0 (CH); 128.3 (CH); 128.3 (CH); 129.6 (CH); 133.9 (C); 155.7 (C); 164.9 (C) δ ppm. IR (DRA): ν 2974, 2933, 1600, 1570, 1514, 1459, 1423, 1240, 1067, 961, 726, 696, 607, 569, 524 cm^{-1}. MS (EI): *m/z* 265 $[M]^+$. Anal. Calcd for $C_{17}H_{19}N_3$: C, 76.95; H, 7.22; N, 15.84. Found: C, 76.73; H, 7.59; N, 15.68.

2-Ethyl-2-methyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole (3g). Yield: 241 mg (74 %), mp = 80-82 °C. R_f 0.2 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 0.73 (t, 3H, J = 7.02); 1.5 (s, 3H); 2.16-1.93 (m, 2H); 5.91 (d, 1H, J = 4.00); 6.48 (d, 1H, J = 4.00); 7.22 (t, 1H, J = 8.00); 7.35 (t, 2H, J = 8.00); 7.53 (t, 5H, J = 7.55); 7.83 (d, 2H, J = 7.52); 11.94 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): 8.1 (CH_3); 23.2 (CH_3); 30.8 (CH_2); 103.4 (C); 107.3 (CH); 115.1 (C); 124.9 (CH); 125.5 (C); 126.8 (CH); 128.1(CH); 128.2 (CH); 128.5 (CH); 129.6 (CH); 131.5 (C); 136.2 (C); 155.3 (C); 164.6 (C) δ ppm. IR (DRA): ν 3383, 3295, 3063, 2965, 2923, 1725, 1600, 1572, 1538, 1488, 1456, 1288, 1273, 1052, 754, 692 cm^{-1}. MS (EI): *m/z* 327 $[M]^+$. Anal. Calcd for $C_{22}H_{21}N_3$: C, 80.70; H, 6.46; N, 12.83. Found: C, 80.36; H, 6.85; N, 12.79.

2-(2-Ethyl-2-methyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole (3h). Yield: 192 mg (63 %), mp = 127-130 °C. R_f 0.2 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 0.72 (t, 3H, J = 7.34); 1.48 (s, 3H); 1.76-1.60 (t, 4H); 2.08-1.88 (m, 2H); 2.29 (t, 2H, J = 5.78); 2.56 (t, 2H, J = 5.92); 5.56 (d, 1H, J = 2.00); 7.56-7.41 (d, 5H); 10.87 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): 8.1 (CH_3); 22.2 (CH_2); 22.4 (CH_2); 22.6 (CH_2); 23.2 (CH_2); 23.4 (CH_3); 30.8 (CH_2); 102.7 (C); 112.3 (CH); 117.2 (C); 122.0 (C); 128.0 (CH); 128.1 (CH); 129.5 (CH); 132.9 (C); 134.4 (C); 155.4 (C); 164.7 (C) δ ppm. IR (DRA): ν 3330, 3274, 3213, 3180, 2968, 2855, 1641, 1603, 1537, 1443, 1372, 1180, 1143, 941, 694 cm^{-1}. MS (EI): *m/z* 305 $[M]^+$. Anal. Calcd for $C_{20}H_{23}N_3$: C, 78.65; H, 7.59; N, 13.76. Found: C, 78.63; H, 7.83; N, 13.54.

2-Phenyl-3-(1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene (3i). Yield: 210 mg (76 %), mp = 122-125 °C. R_f 0.3 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.91-1.48 (m, 10H); 5.86 (s, 1H); 5.99 (s, 1H); 6.92 (s, 1H); 7.57-7.43 (m, 5H); 11.61 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 23.7 (CH_2); 25.2 (CH_2); 34.8 (CH_2); 103.1 (C); 108.8 (CH); 113.1 (CH); 122.9 (CH); 124.1 (C); 128.0 (CH); 128.3 (CH); 129.5 (CH); 134.3 (C); 154.9 (C); 163.9 (C) ppm. IR (DRA): ν 3169, 3123, 3085, 3028, 2941, 2922, 2849, 1604, 1580, 1523, 1418, 1097, 736, 693, 562 cm^{-1}. MS (EI): *m/z* 277 $[M]^+$. Anal. Calcd for $C_{18}H_{19}N_3$: C, 77.95; H, 6.90; N, 15.15. Found: C, 77.93; H, 6.78; N, 15.29.

2-(1-Methyl-1*H*-pyrrol-2-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene (3k). Yield: 221 mg (76 %), mp = 102-105 °C. R_f 0.2 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.91-1.48 (m, 10H); 3.88 (s, 3H); 5.82 (s, 1H); 5.94 (s, 1H); 7.00 (s, 1H); 7.54-7.39 (m, 5H) ppm. ^{13}C NMR (DMSO-d_6): δ 23.8 (CH_2); 25.2 (CH_2); 34.7 (CH_2); 36.4 (CH_3); 103.6 (C); 107.0 (CH); 114.7 (CH); 124.5 (C); 128.0 (CH); 128.2 (CH); 128.3 (CH); 129.5 (CH); 134.1 (C); 155.1 (C); 164.3 (C) ppm. IR (DRA): ν 3350, 3098, 2932, 2844, 1598, 1564, 1443, 1418, 1243, 1103, 976, 958, 736, 697, 676, 566 cm^{-1}. MS (EI): *m/z* 291 $[M]^+$. Anal. Calcd for $C_{19}H_{21}N_3$: C, 78.32; H, 7.26; N, 14.42. Found: C, 78.21; H, 7.64; N, 14.15.

2-Phenyl-3-(5-phenyl-1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene (3l). Yield: 292 mg (83 %), mp = 107-110 °C. R_f 0.2 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.94-1.48 (m, 10H); 5.92 (d, 1H, J = 3.4); 6.48 (d, 1H, J = 3.32); 7.22 (t, 1H, J = 7.24); 7.35 (t, 2H, J = 7.58); 7.61-7.46 (m, 5H); 7.83 (d, 2H, J = 7.64); 11.86 (s, 1H) ppm. ^{13}C NMR (DMSO-d_6): δ 23.7 (CH_2); 25.2 (CH_2); 34.9 (CH_2); 103.3 (C); 107.4 (CH); 115.1 (CH); 125.0(CH); 125.6 (C); 126.8 (CH); 128.1 (CH); 128.3 (CH); 128.5 (CH); 129.5 (CH); 131.5 (C); 134.3 (C); 136.2 (C); 154.7 (C); 163.9 (C) ppm. IR (DRA): ν 3449, 2927, 2847, 1601, 1572, 1535, 1487, 1443, 1269, 955, 752, 690, 646, 565 cm^{-1}. MS (EI): *m/z* 353 $[M]^+$. Anal. Calcd for $C_{24}H_{23}N_3$: C, 81.55; H, 6.56; N, 11.89. Found: C, 81.79; H, 6.59; N, 11.62.

2-Phenyl-3-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene (3m). Yield: 208 mg (63 %), mp = 117-120 °C. R_f 0.1 (hexane/EtOAc, 6:4). ^{1}H NMR (DMSO-d_6): δ 1.91-1.46 (m, 14H); 2.27-2.19 (t, 2H, J = 5.62); 2.56-2.50 (m, 2H); 5.59-5.57 (m, 1H); 7.56-7.44 (m, 5H); 11.08 (s, 1H). ^{13}C NMR (DMSO-d_6): δ 22.2 (CH_2); 22.5 (CH_2); 22.6 (CH_2); 23.2 (CH_2); 23.7 (CH_2); 25.2 (CH_2); 35.1 (CH_2); 102.6 (C); 112.2 (CH); 117.2 (C); 122.2 (C); 128.0 (CH); 128.2 (CH); 129.4 (CH); 132.8 (C); 134.6 (C); 154.8 (C); 164.1 (C) ppm. IR (DRA): ν 2924, 2851, 1601, 1538, 1489, 1442, 1336, 1267, 1233, 1184, 1009, 971, 954, 698, 566 cm^{-1}. MS (EI): *m/z* 331 $[M]^+$. Anal. Calcd for $C_{22}H_{25}N_3$: C, 79.72; H, 7.60; N, 12.68. Yield: C, 79.84; H, 7.87; N, 12.29.

^{1}H and ^{13}C NMR Spectra

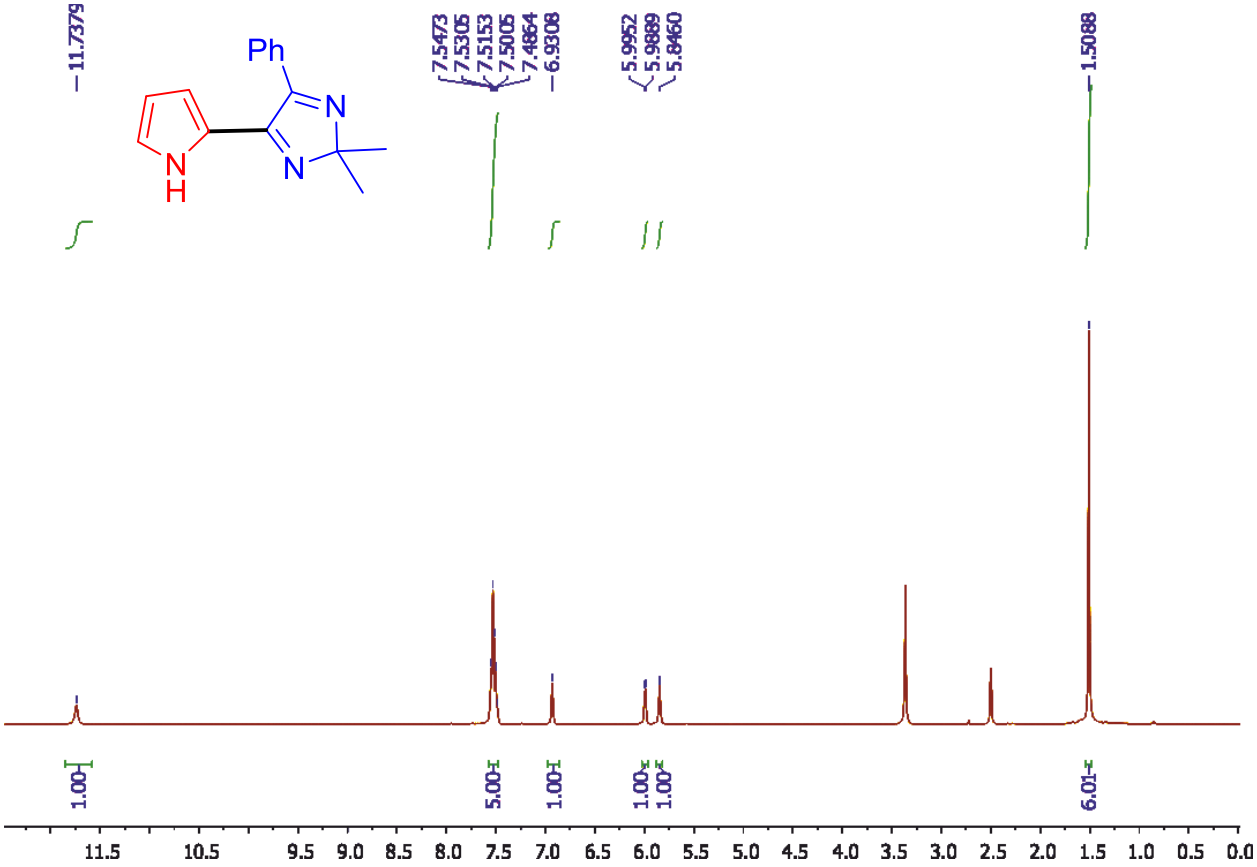

Figure S1 ^{1}H NMR Spectrum of 2,2-dimethyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole (3a)

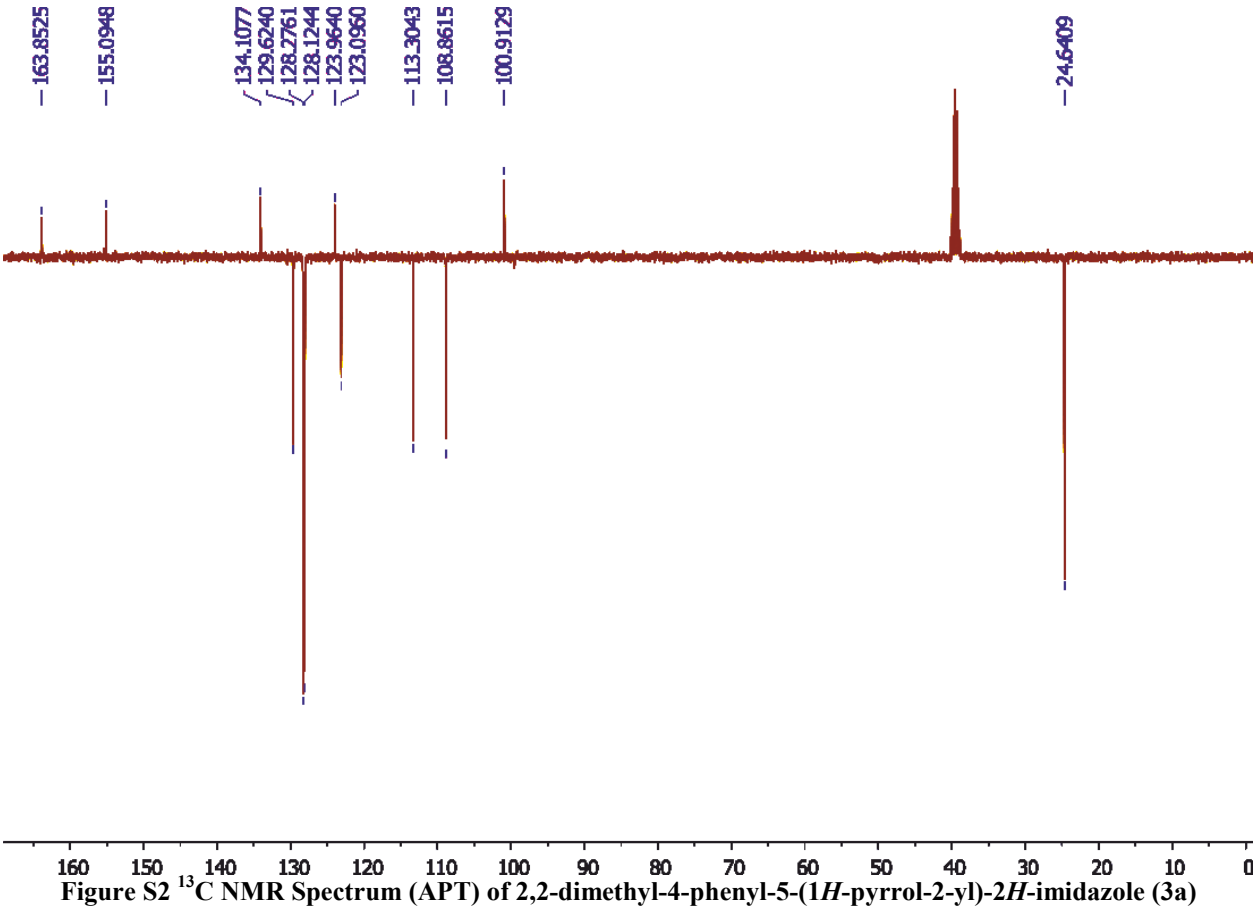

Figure S2 ^{13}C NMR Spectrum (APT) of 2,2-dimethyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole (3a)

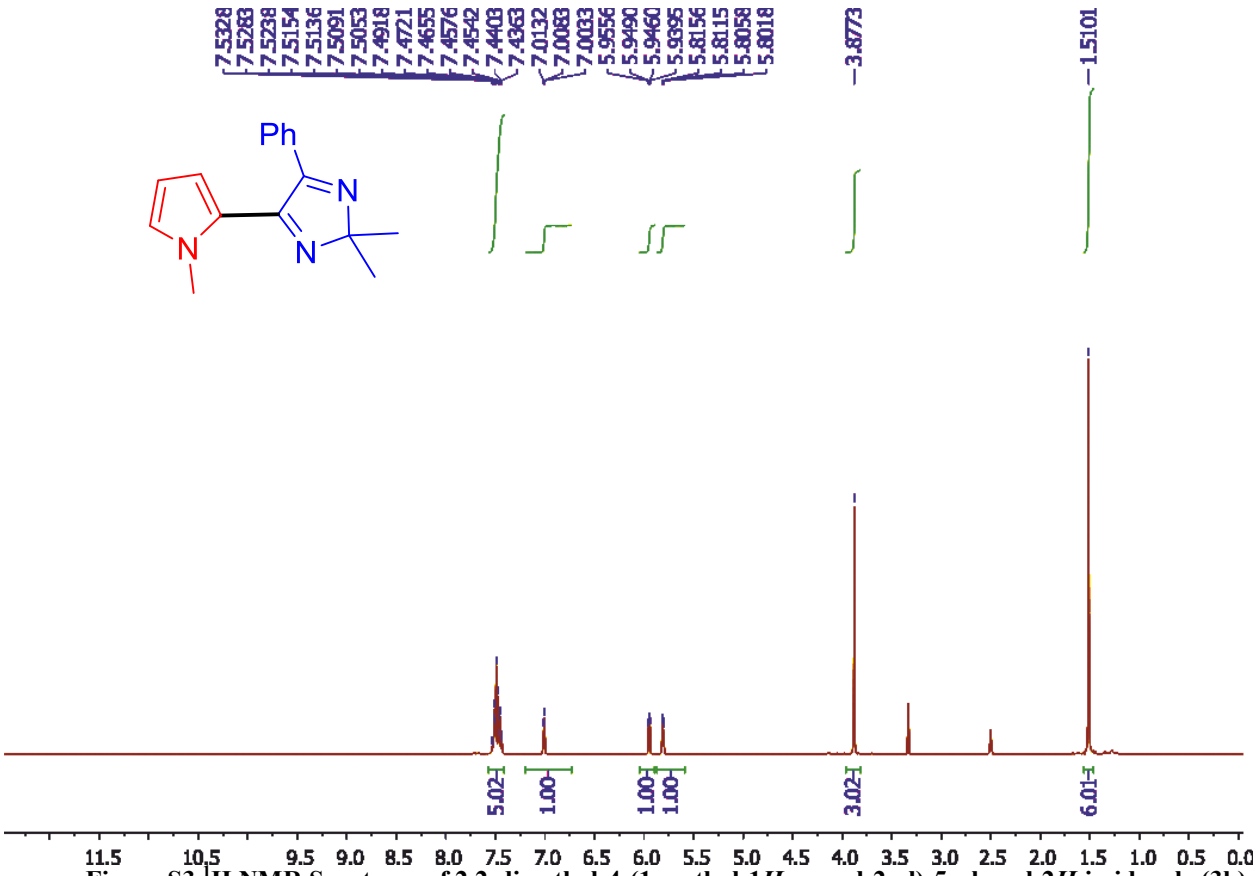

Figure S3 ^{1}H NMR Spectrum of 2,2-dimethyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole (3b)

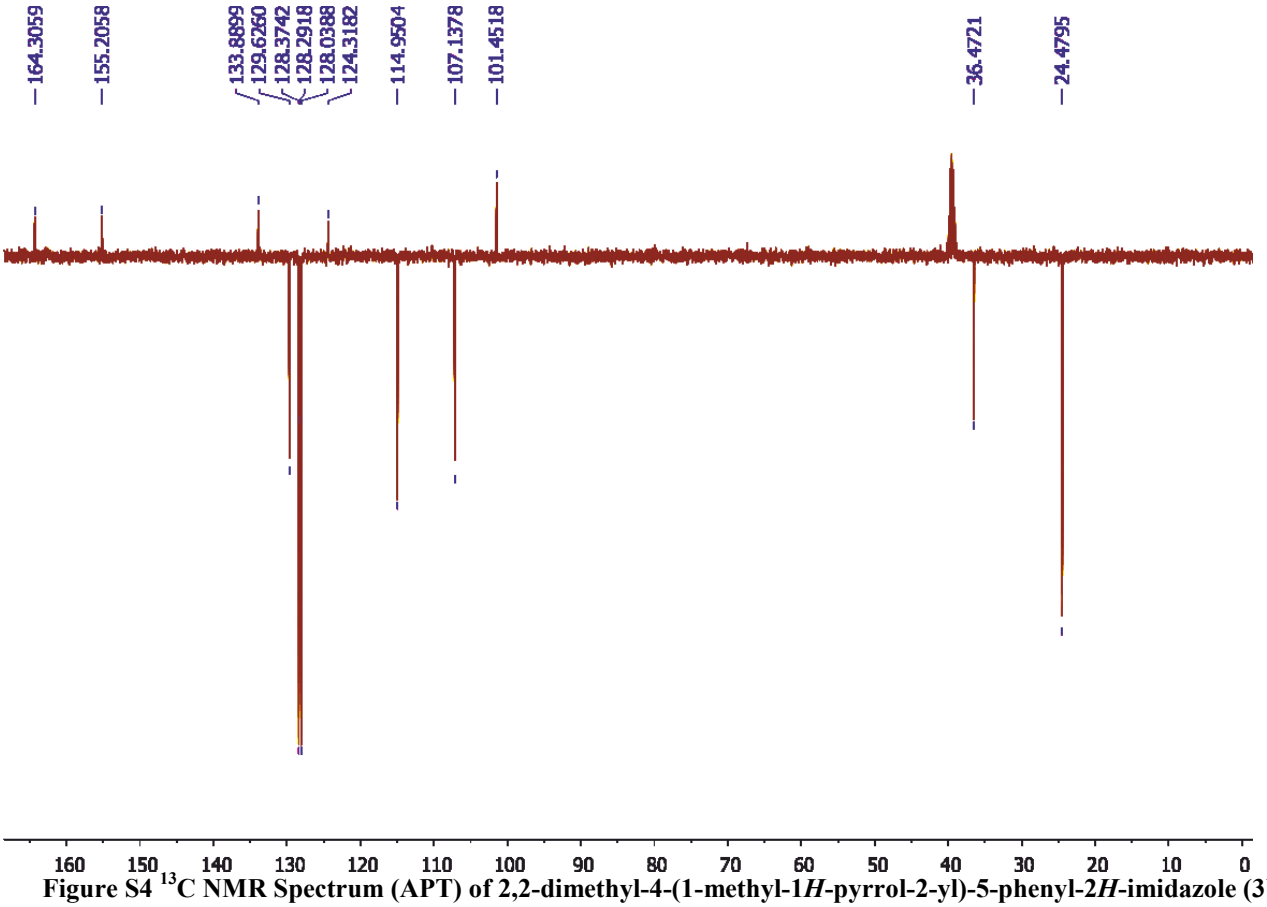

Figure S4 ^{13}C NMR Spectrum (APT) of 2,2-dimethyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole (3b)

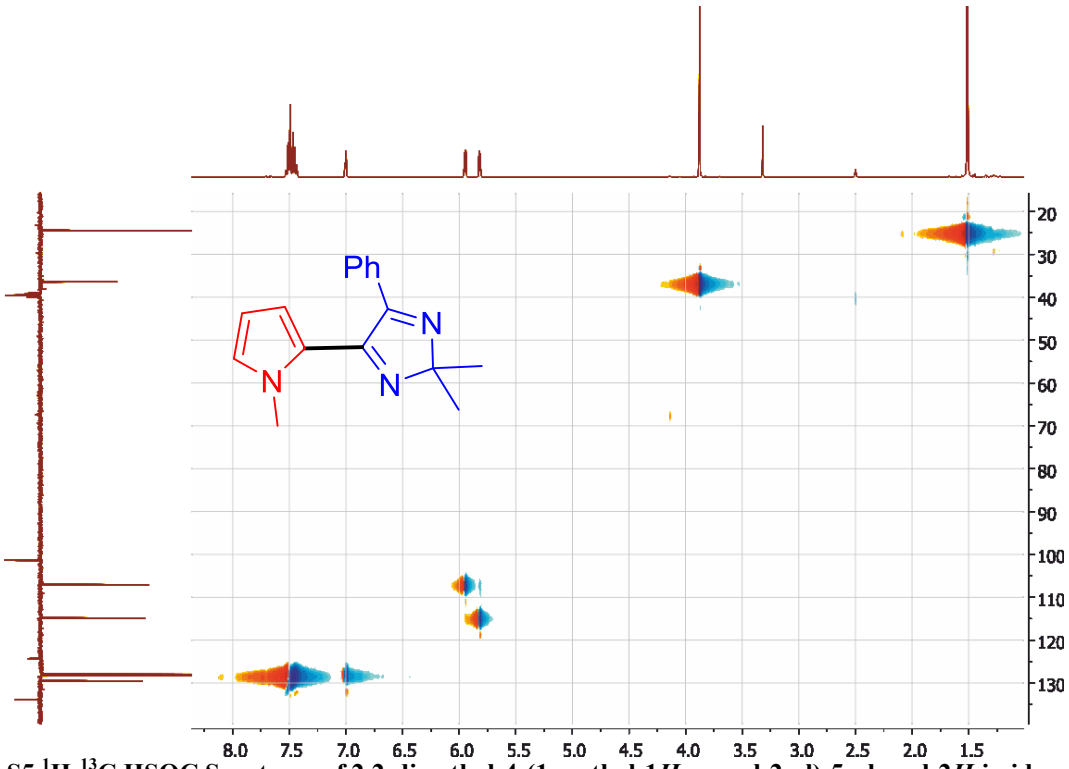

Figure S5 ^{1}H-^{13}C HSQC Spectrum of 2,2-dimethyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole (3b)

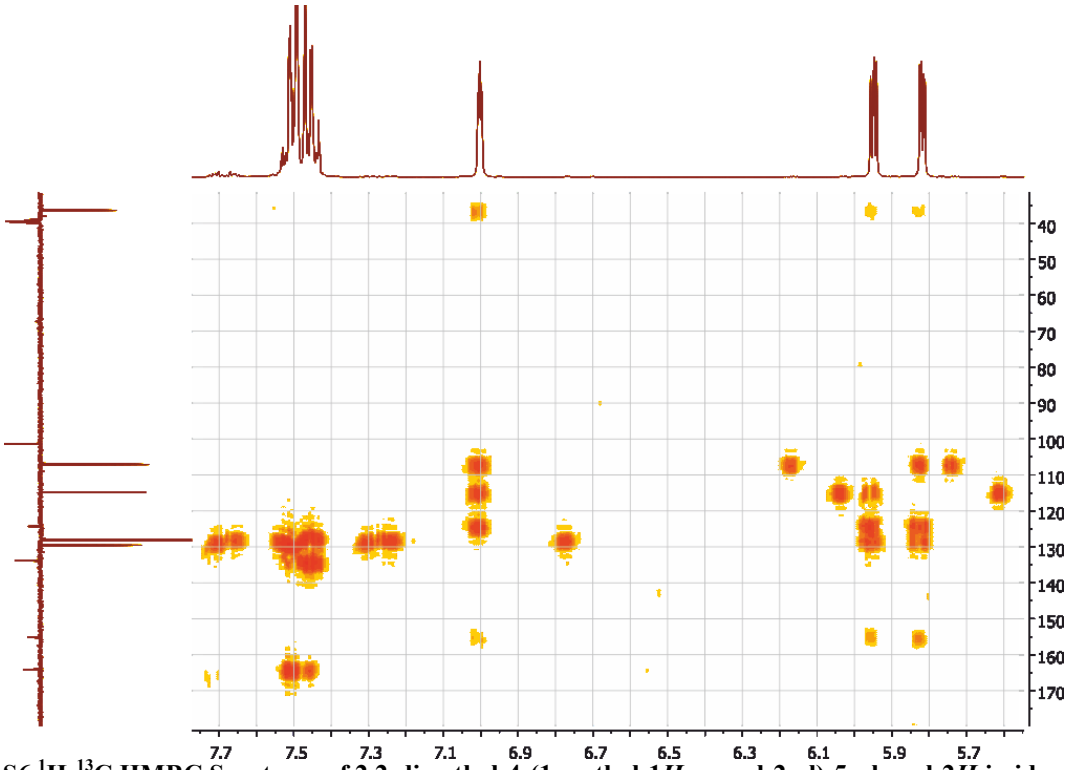

Figure S6 ^{1}H-^{13}C HMBC Spectrum of 2,2-dimethyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole (3b)

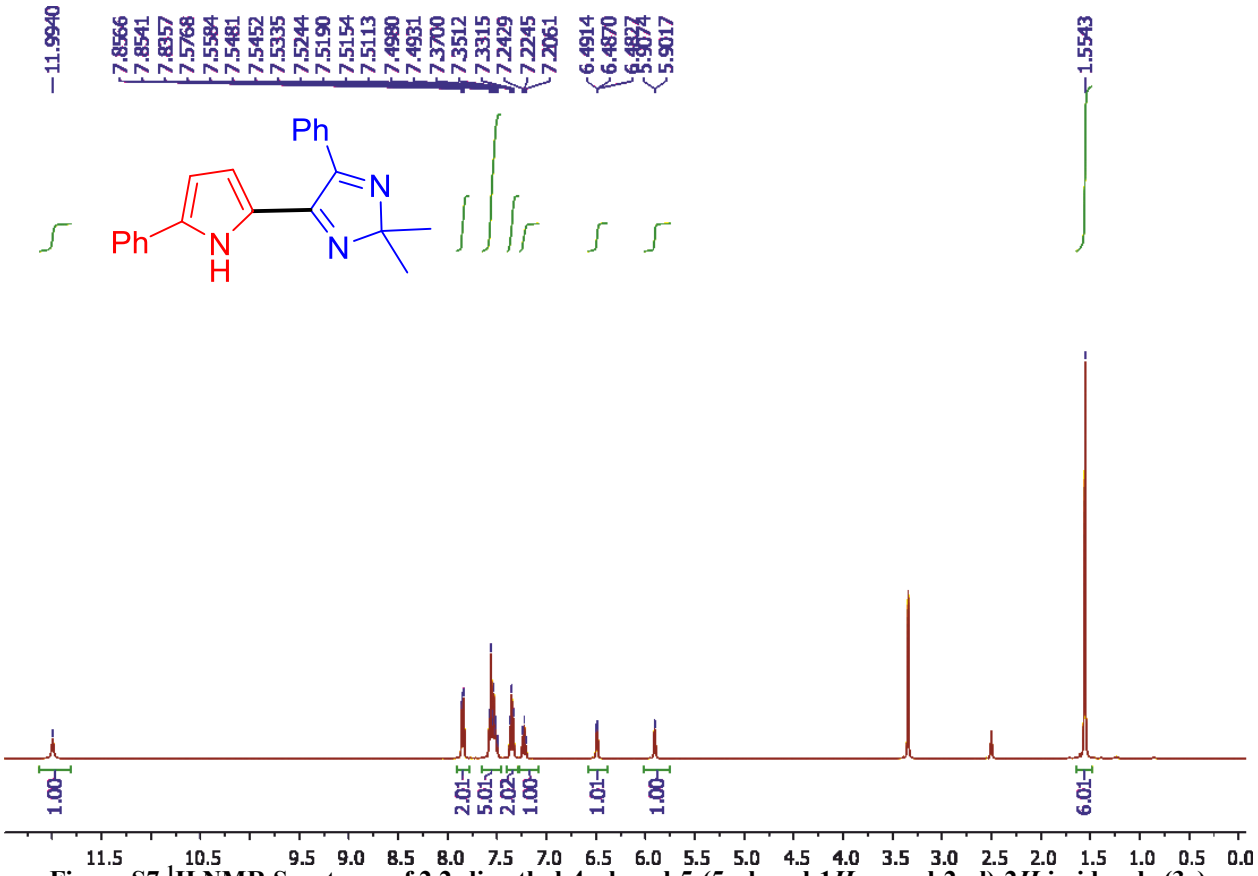

Figure S7 ^{1}H NMR Spectrum of 2,2-dimethyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole (3c)

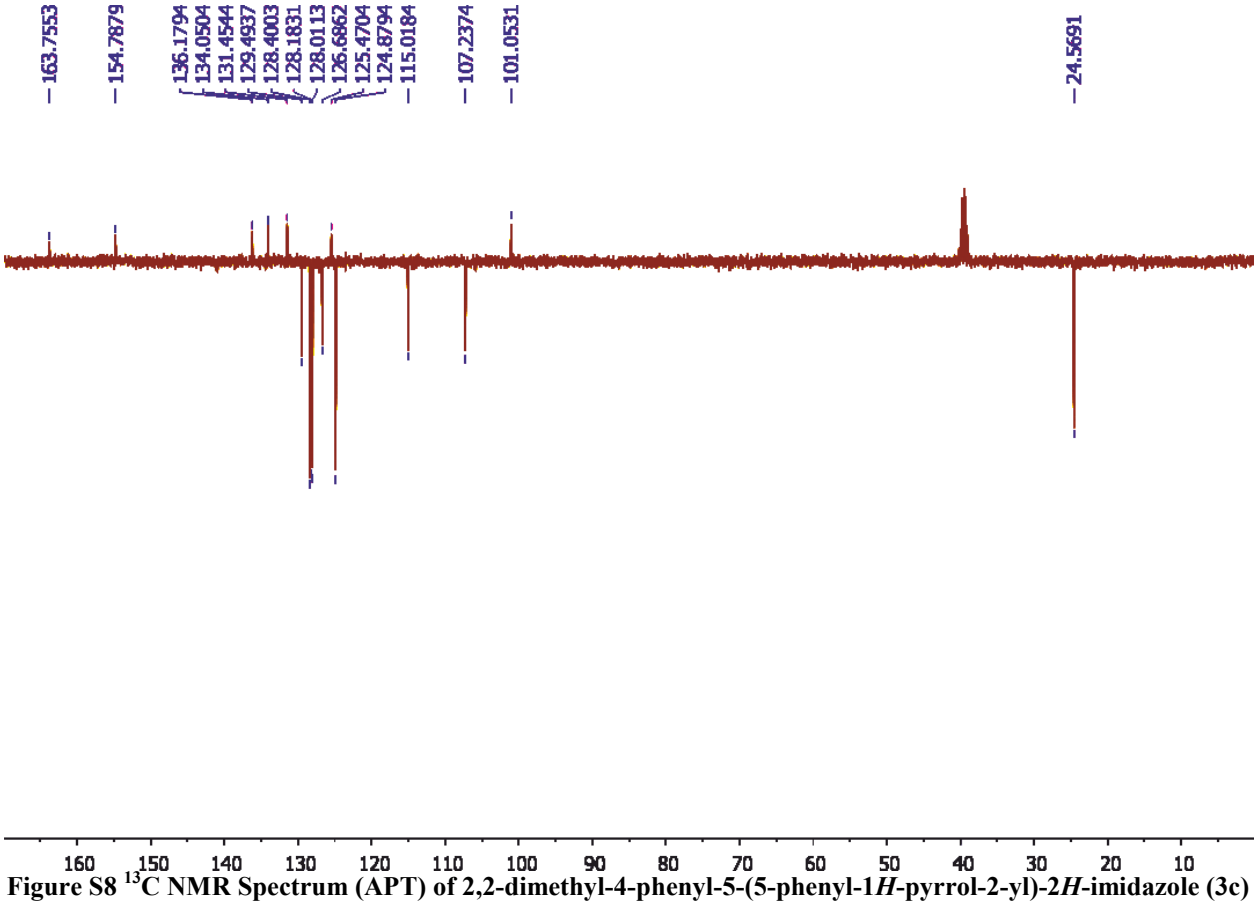

Figure S8 ^{13}C NMR Spectrum (APT) of 2,2-dimethyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole (3c)

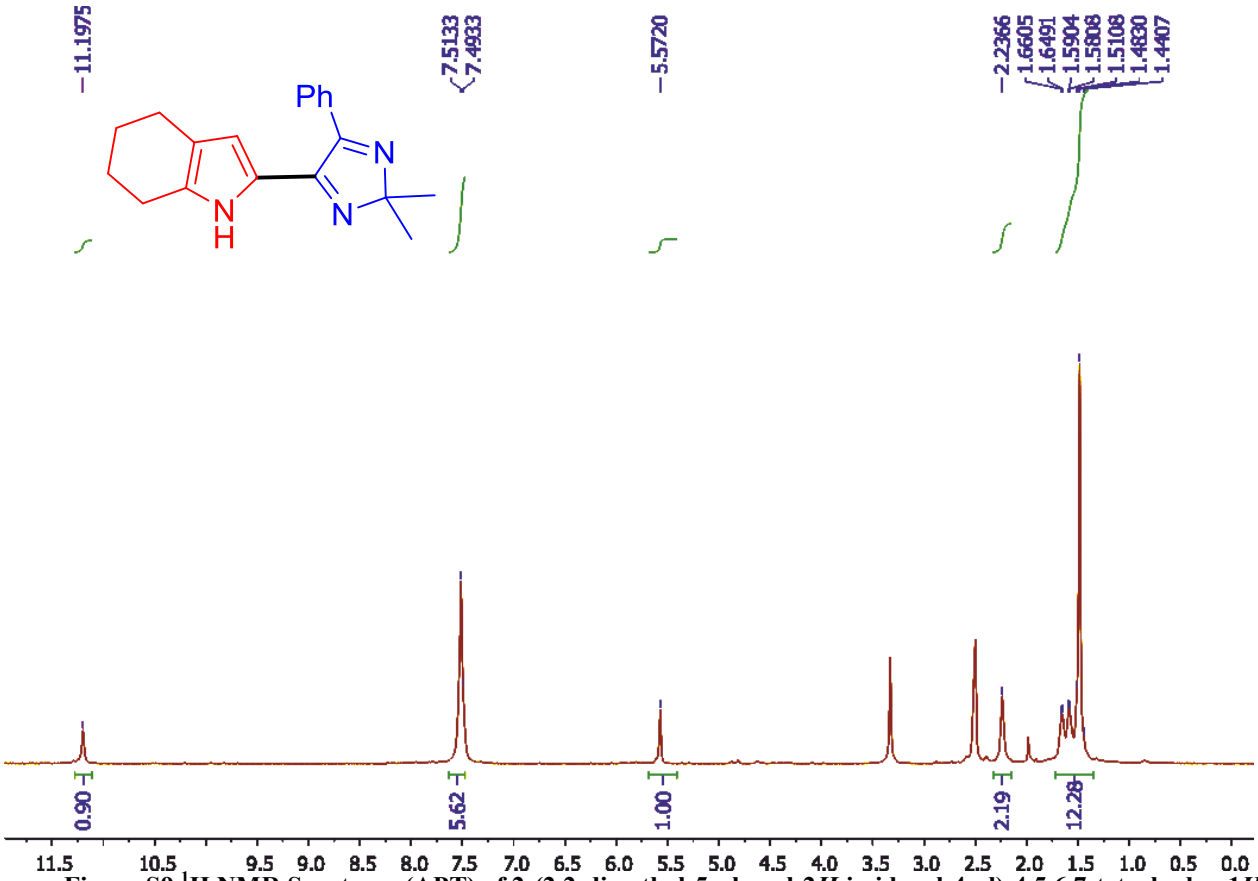

Figure S9 ^{1}**H NMR Spectrum (APT) of 2-(2,2-dimethyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole (3d)**

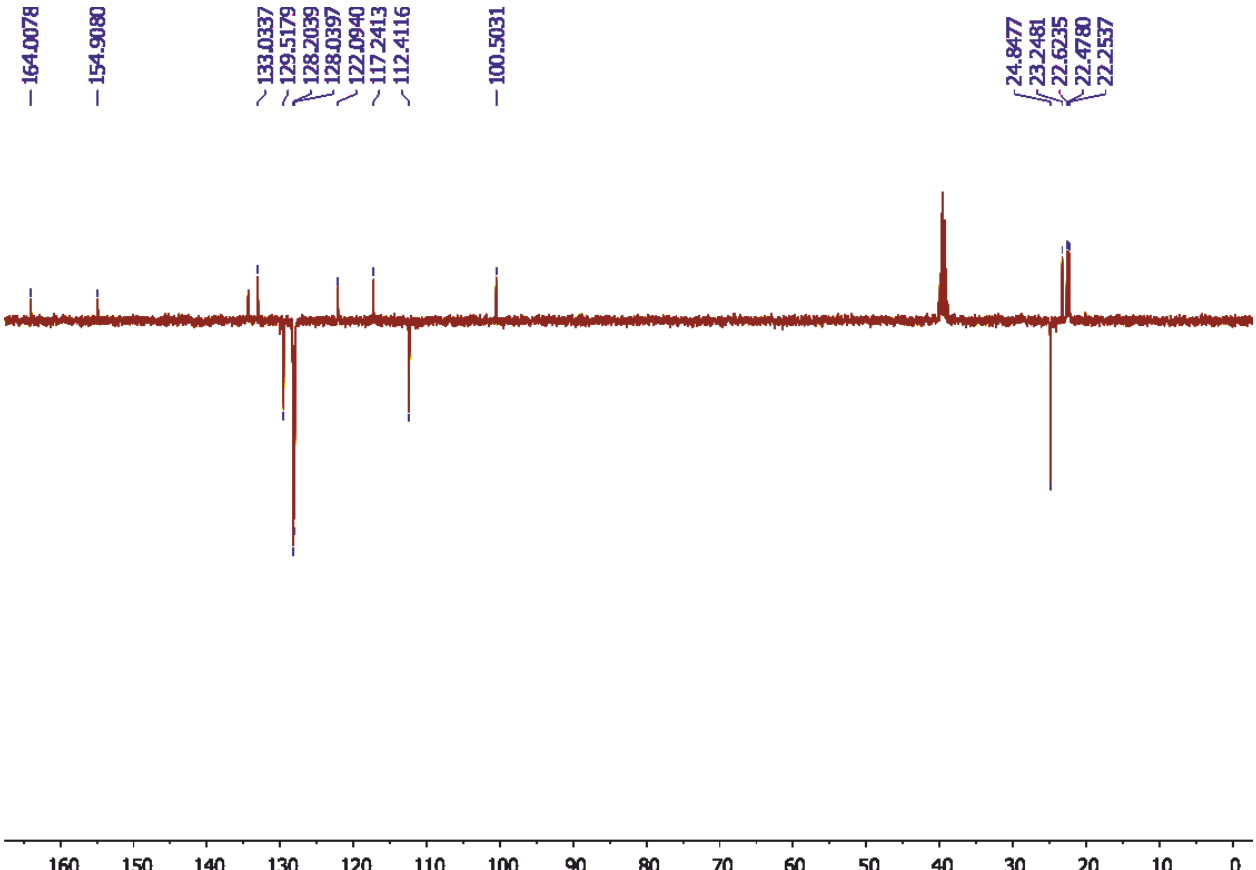

Figure S10 ^{13}**C NMR Spectrum (APT) of 2-(2,2-dimethyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole (3d)**

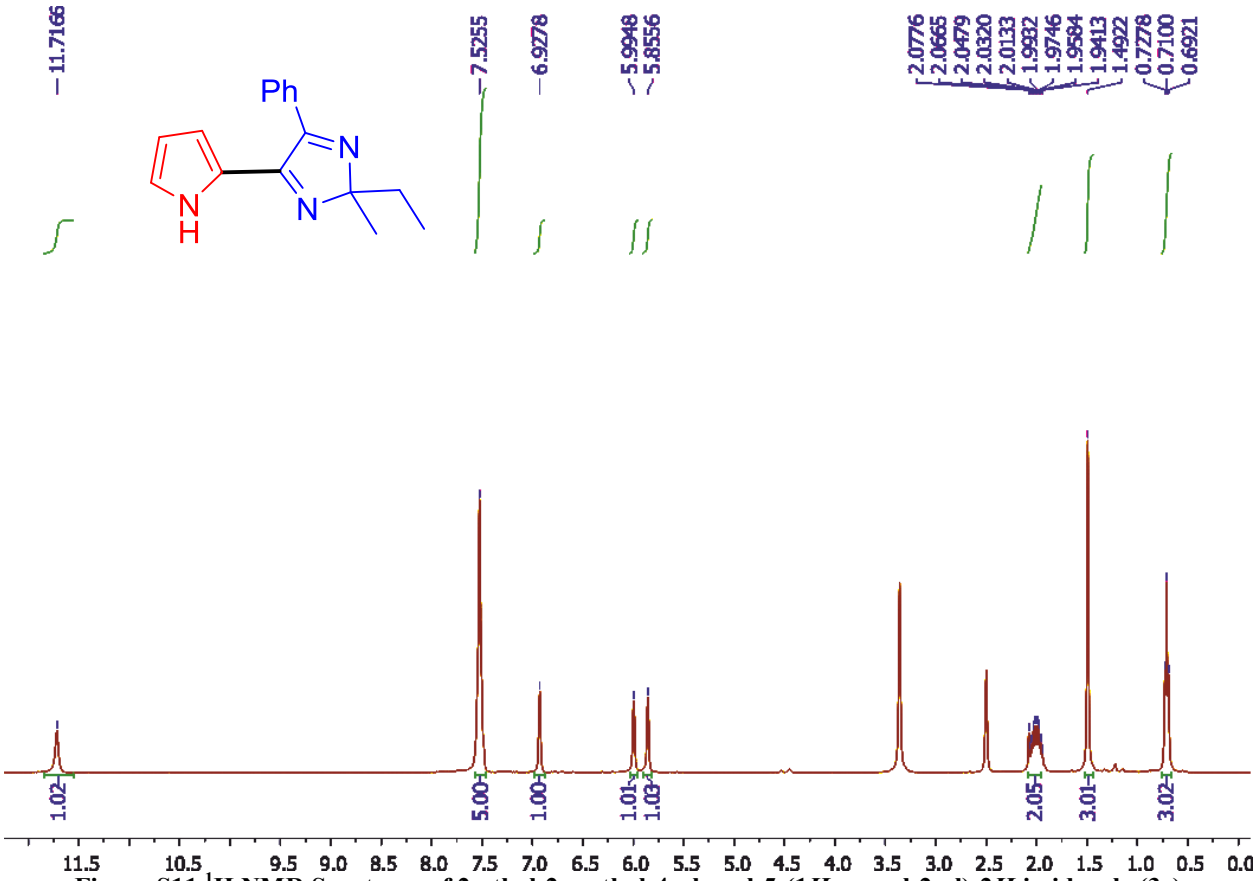

Figure S11 ^{1}H NMR Spectrum of 2-ethyl-2-methyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole (3e)

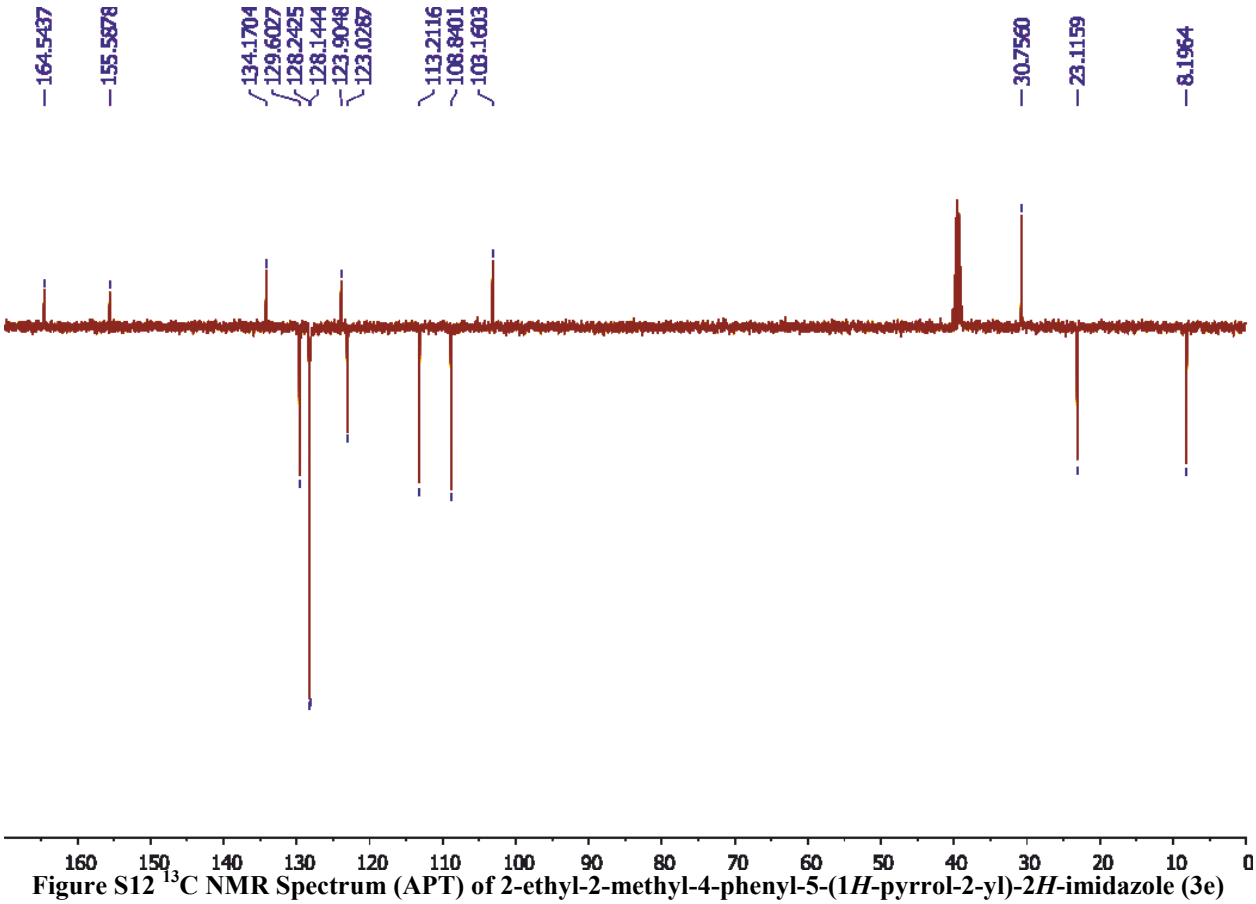

Figure S12 ^{13}C NMR Spectrum (APT) of 2-ethyl-2-methyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole (3e)

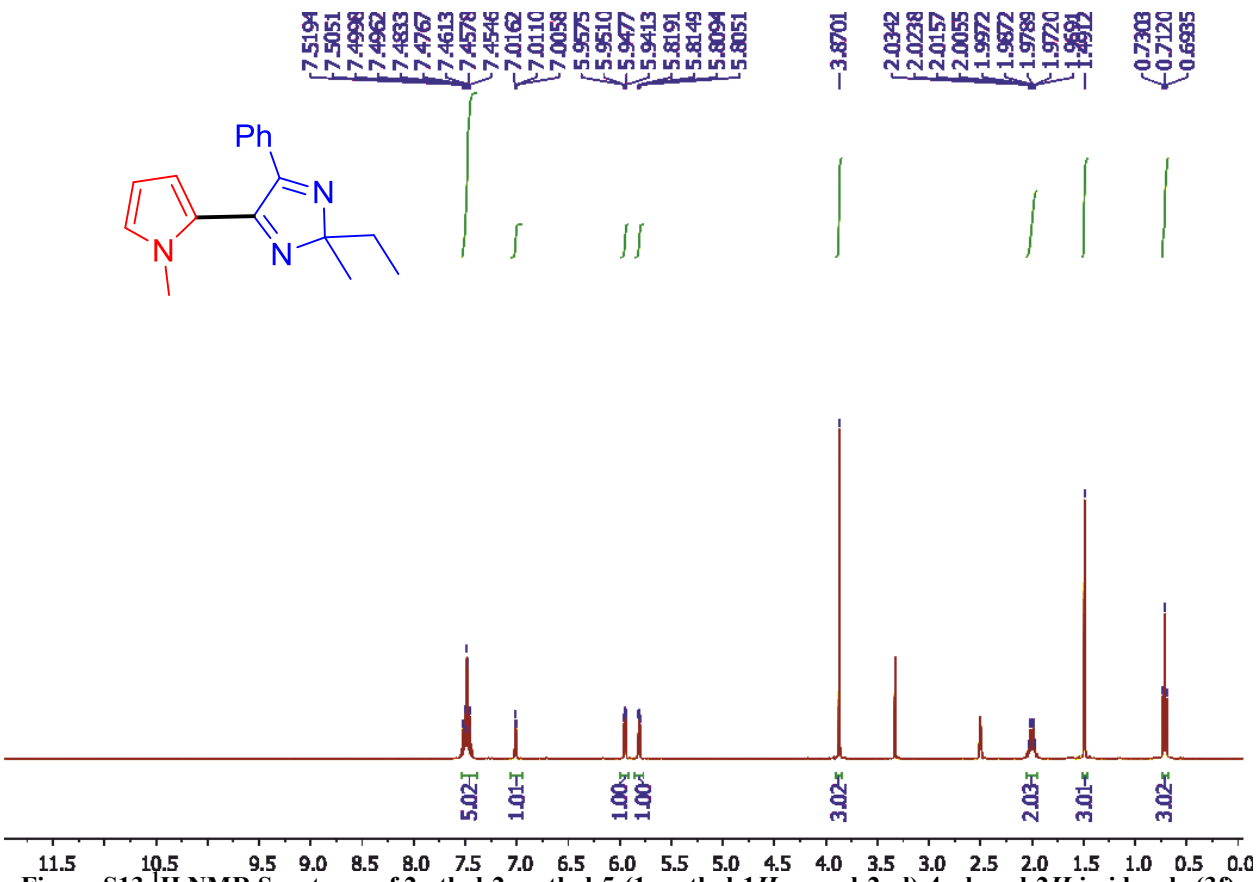

Figure S13 ^{1}H NMR Spectrum of 2-ethyl-2-methyl-5-(1-methyl-1*H*-pyrrol-2-yl)-4-phenyl-2*H*-imidazole (3f)

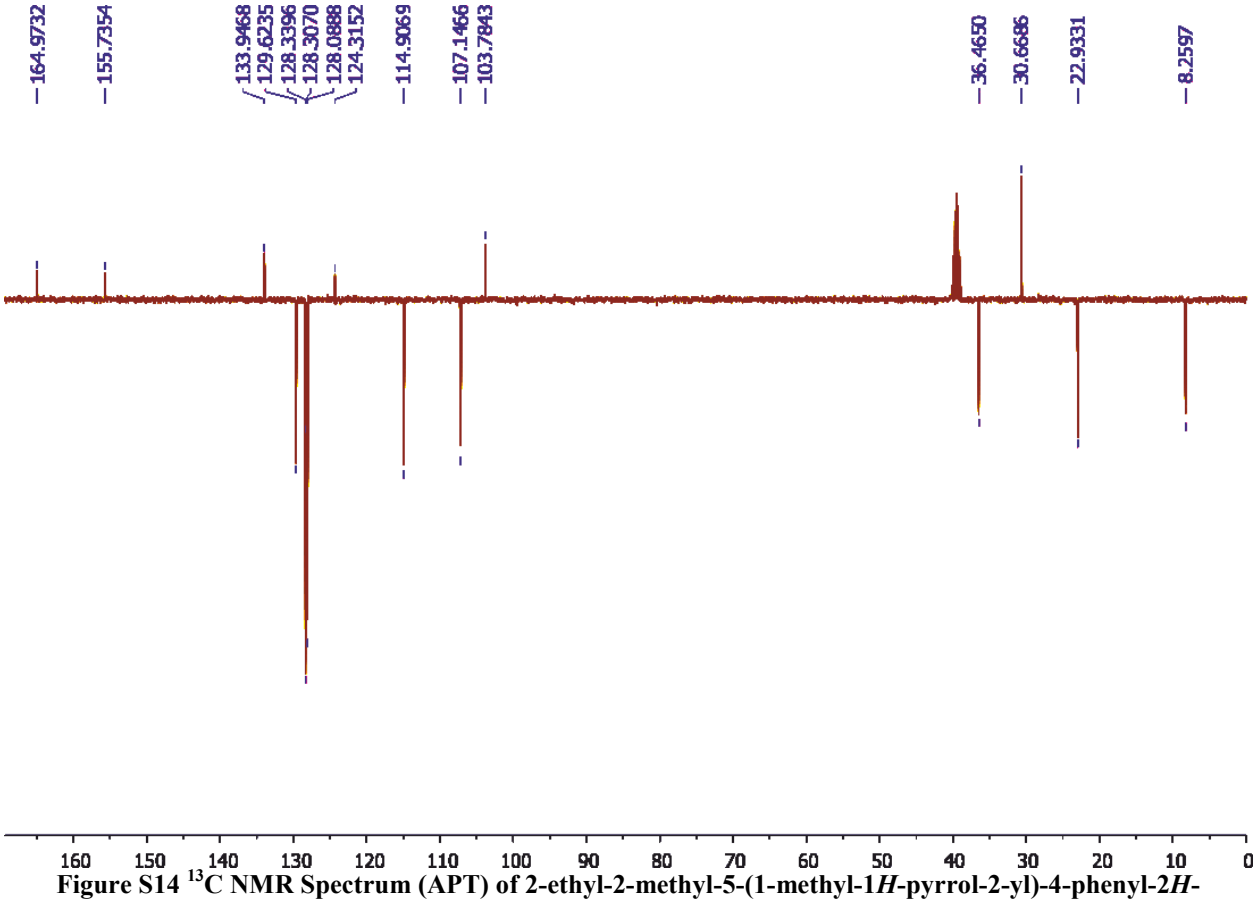

Figure S14 ^{13}C NMR Spectrum (APT) of 2-ethyl-2-methyl-5-(1-methyl-1*H*-pyrrol-2-yl)-4-phenyl-2*H*-imidazole (3f)

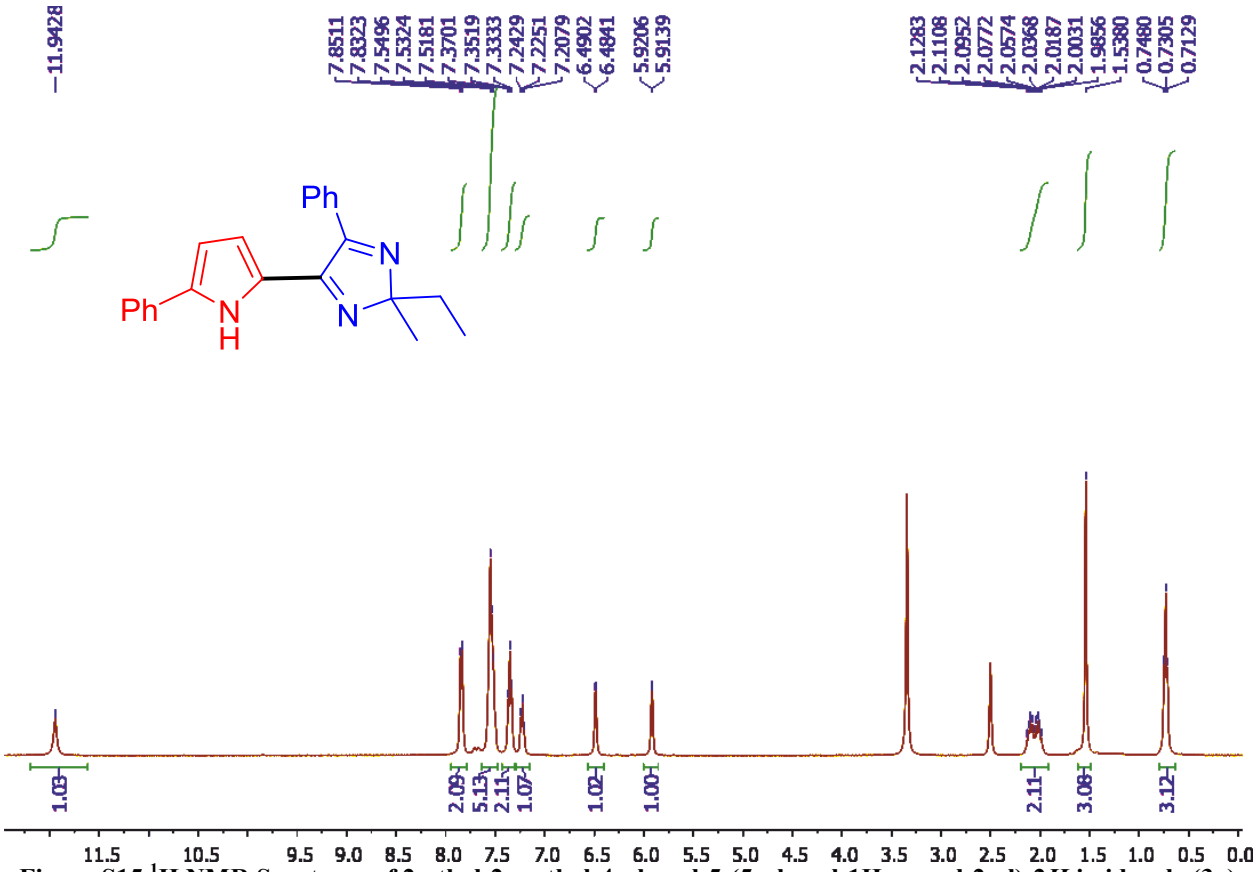

Figure S15 ^{1}H NMR Spectrum of 2-ethyl-2-methyl-4-phenyl-5-(5-phenyl-1H-pyrrol-2-yl)-2*H*-imidazole (3g)

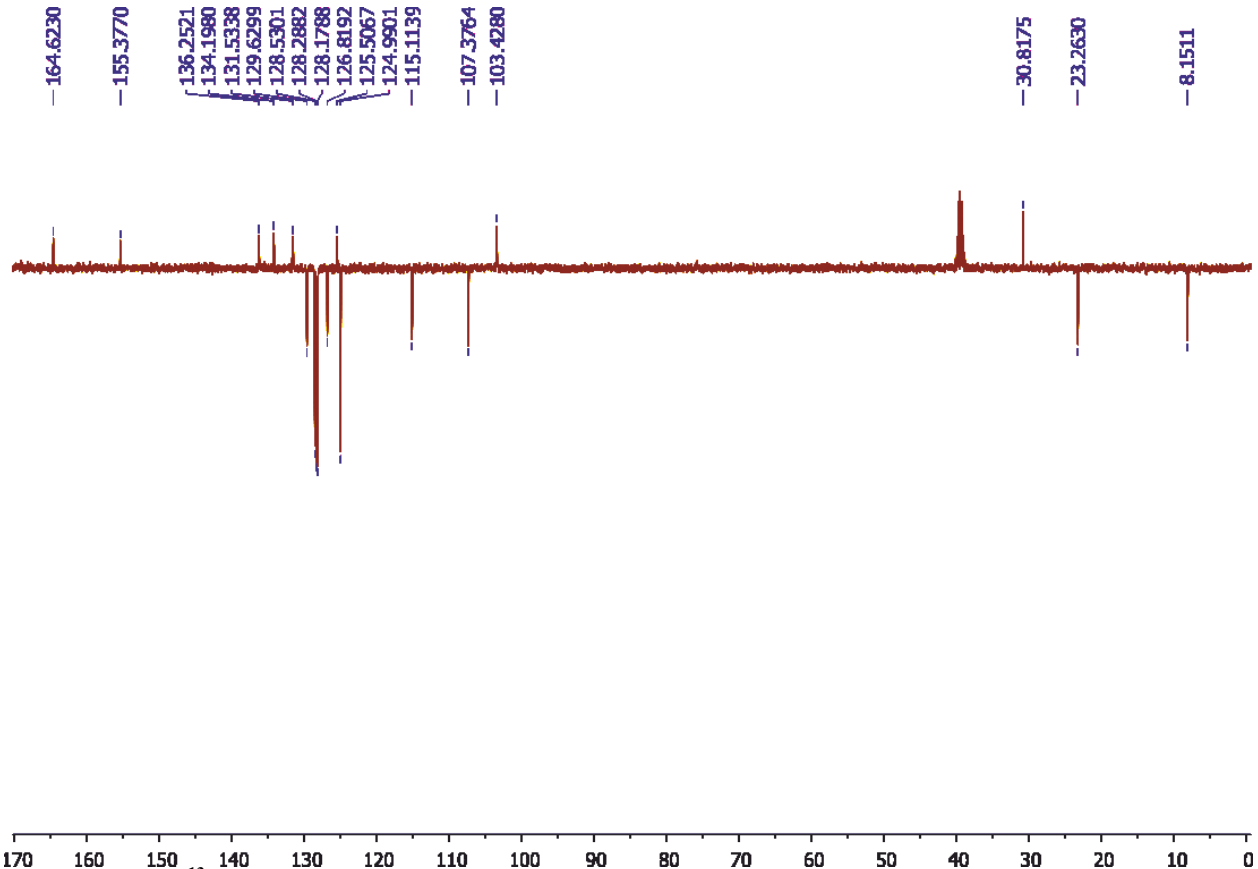

Figure S16 ^{13}C NMR Spectrum (APT) of 2-ethyl-2-methyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole (3g)

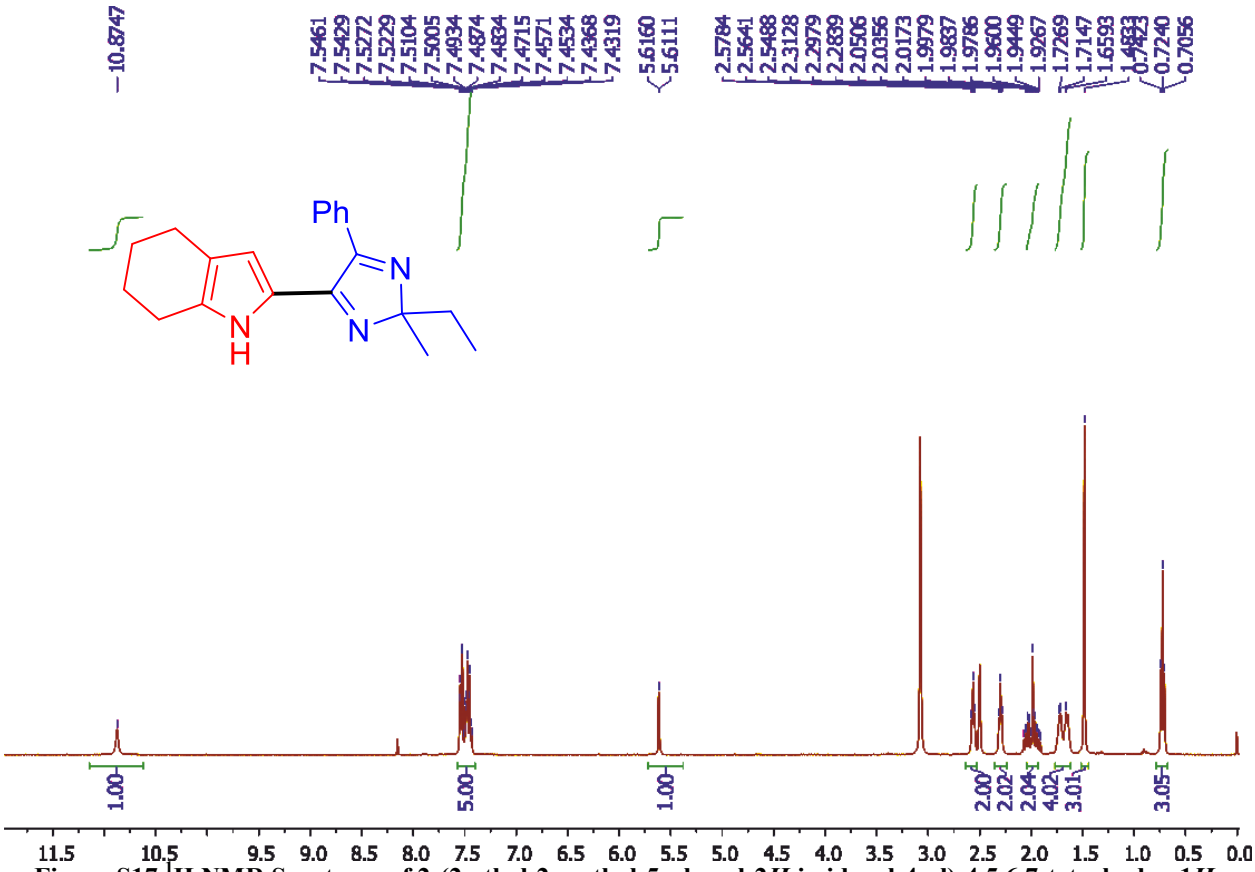

Figure S17 ^{1}H NMR Spectrum of 2-(2-ethyl-2-methyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole (3h)

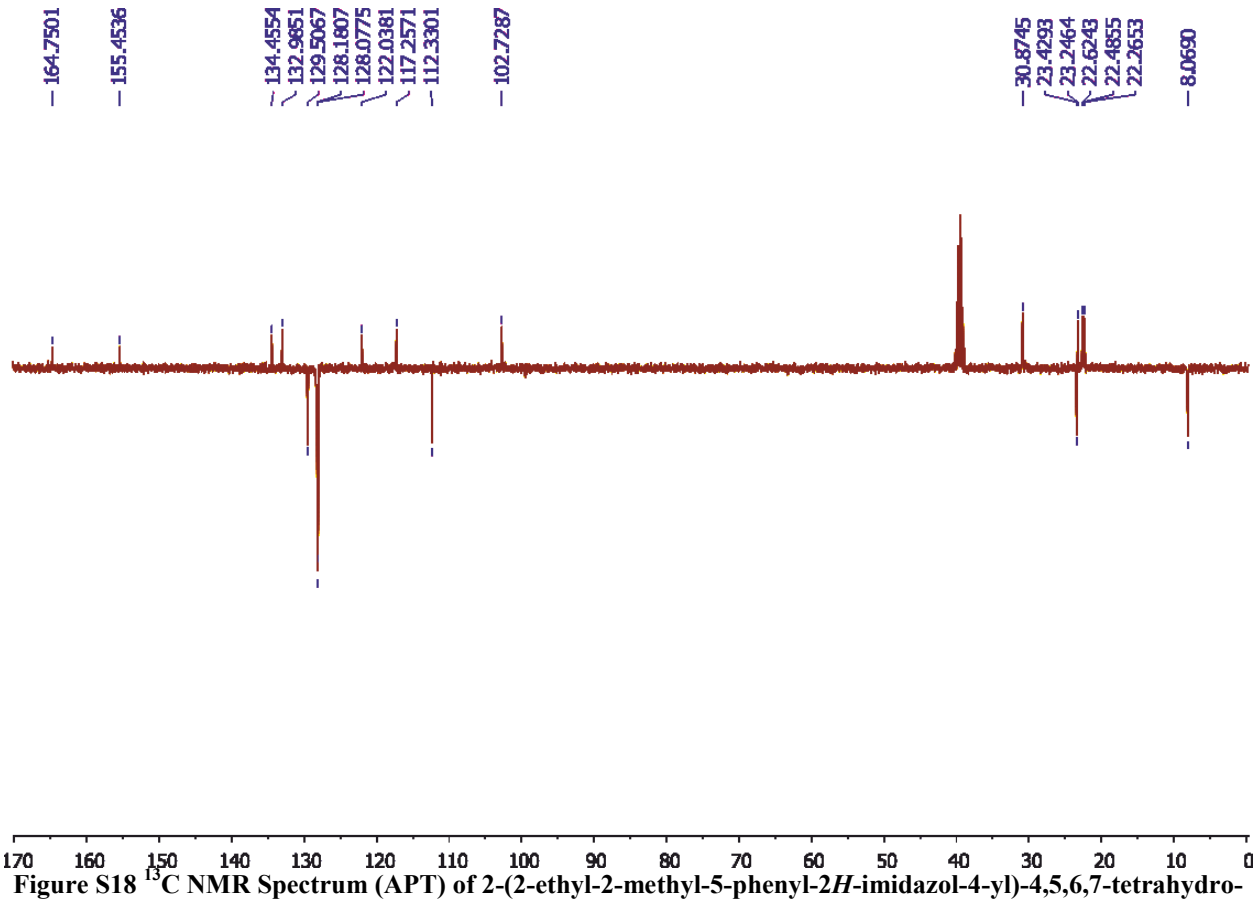

Figure S18 ^{13}C NMR Spectrum (APT) of 2-(2-ethyl-2-methyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole (3h)

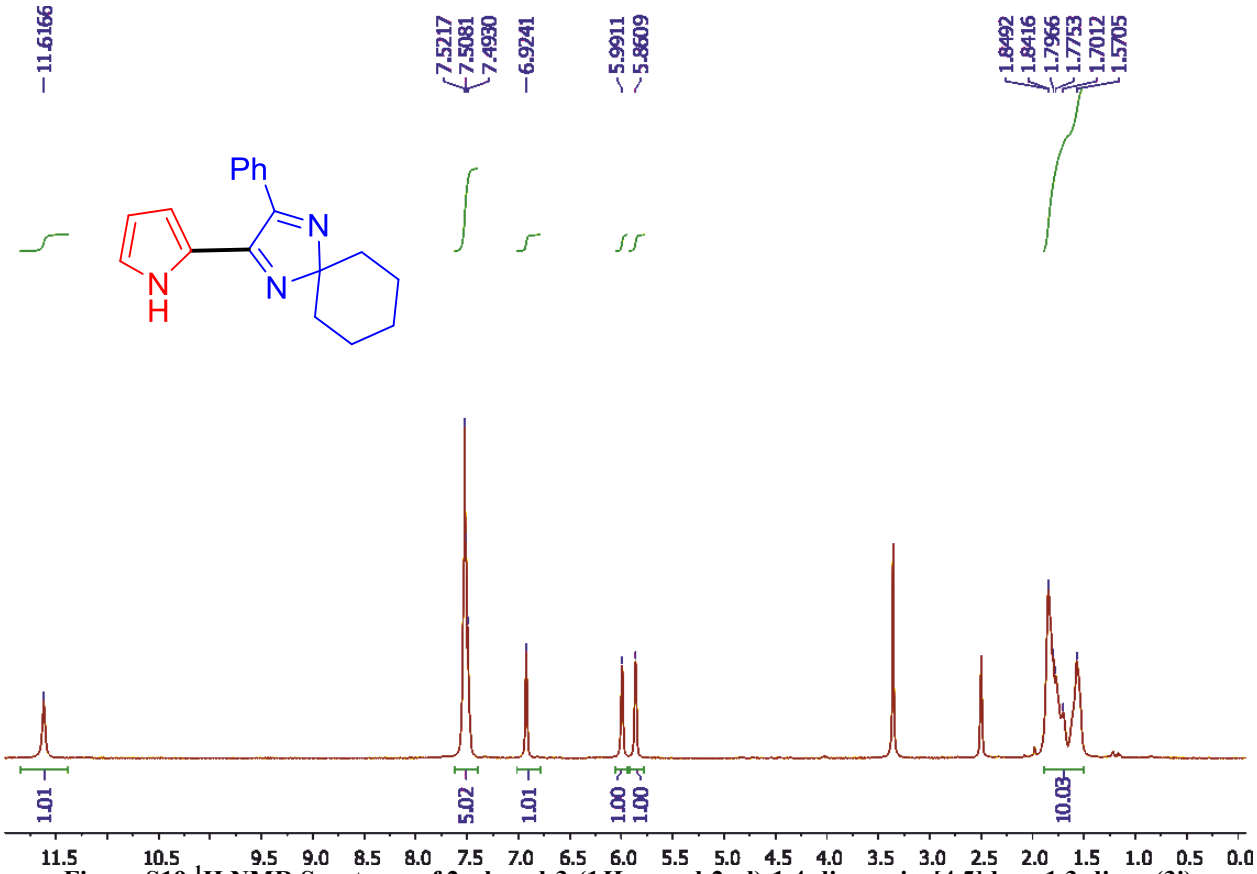

Figure S19 ^{1}H NMR Spectrum of 2-phenyl-3-(1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene (3i)

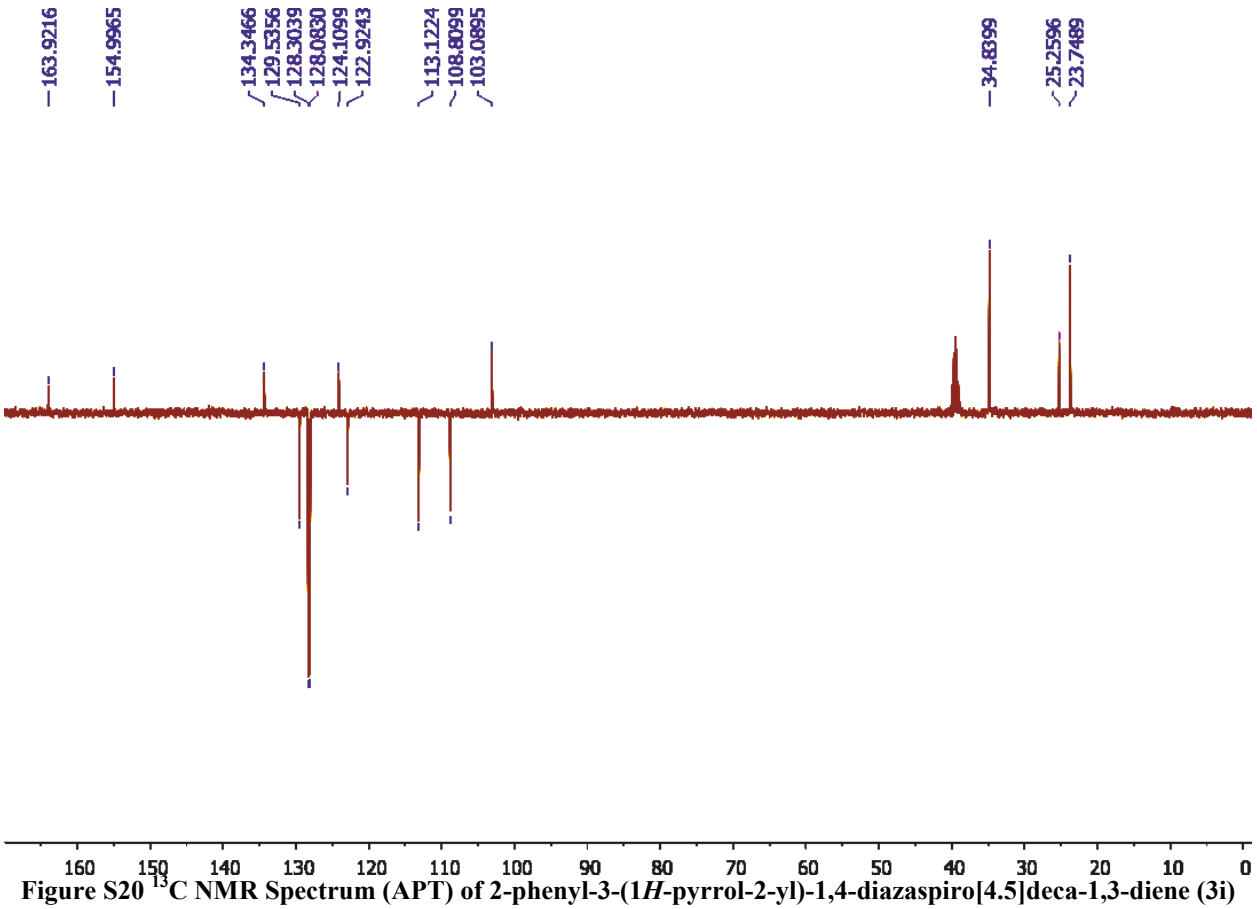

Figure S20 ^{13}C NMR Spectrum (APT) of 2-phenyl-3-(1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene (3i)

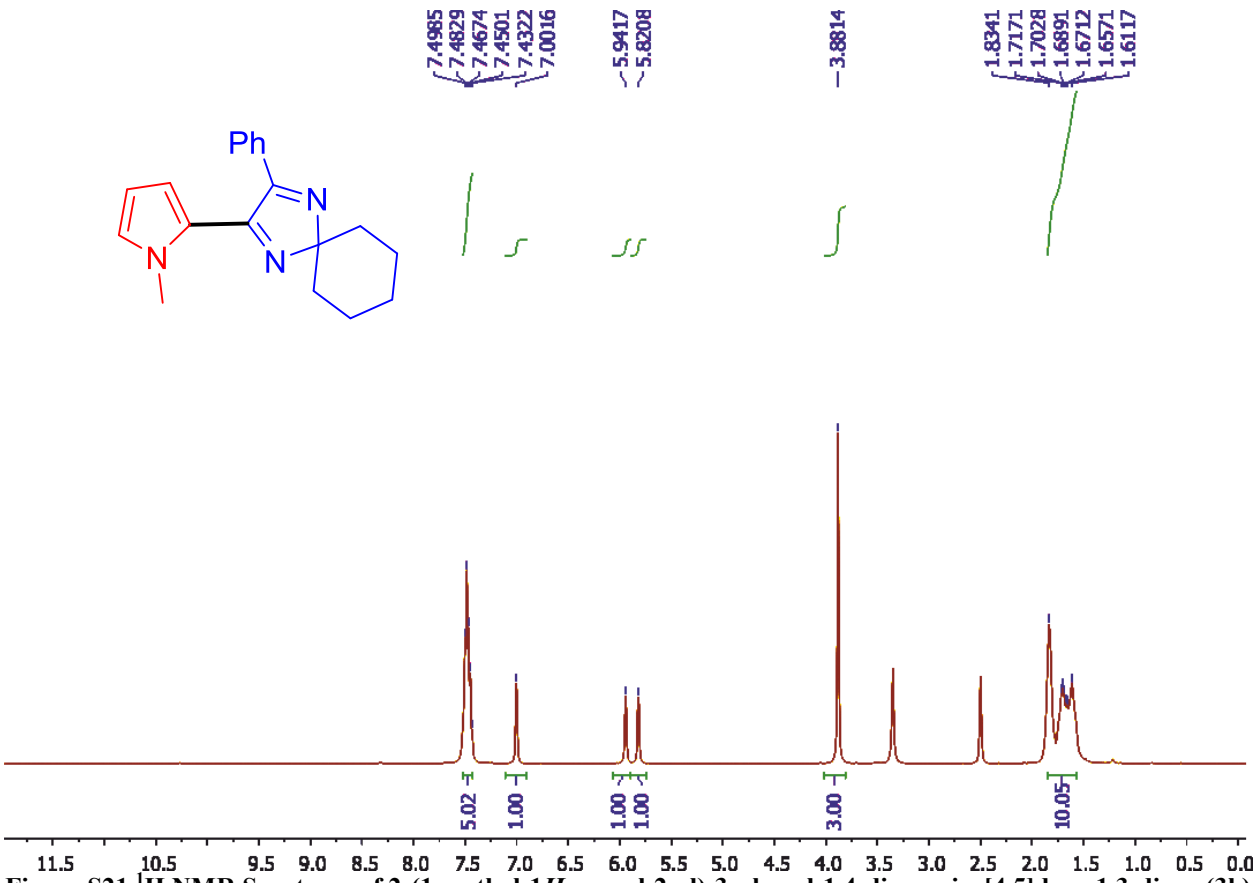

Figure S21 ^{1}H NMR Spectrum of 2-(1-methyl-1*H*-pyrrol-2-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene (3k)

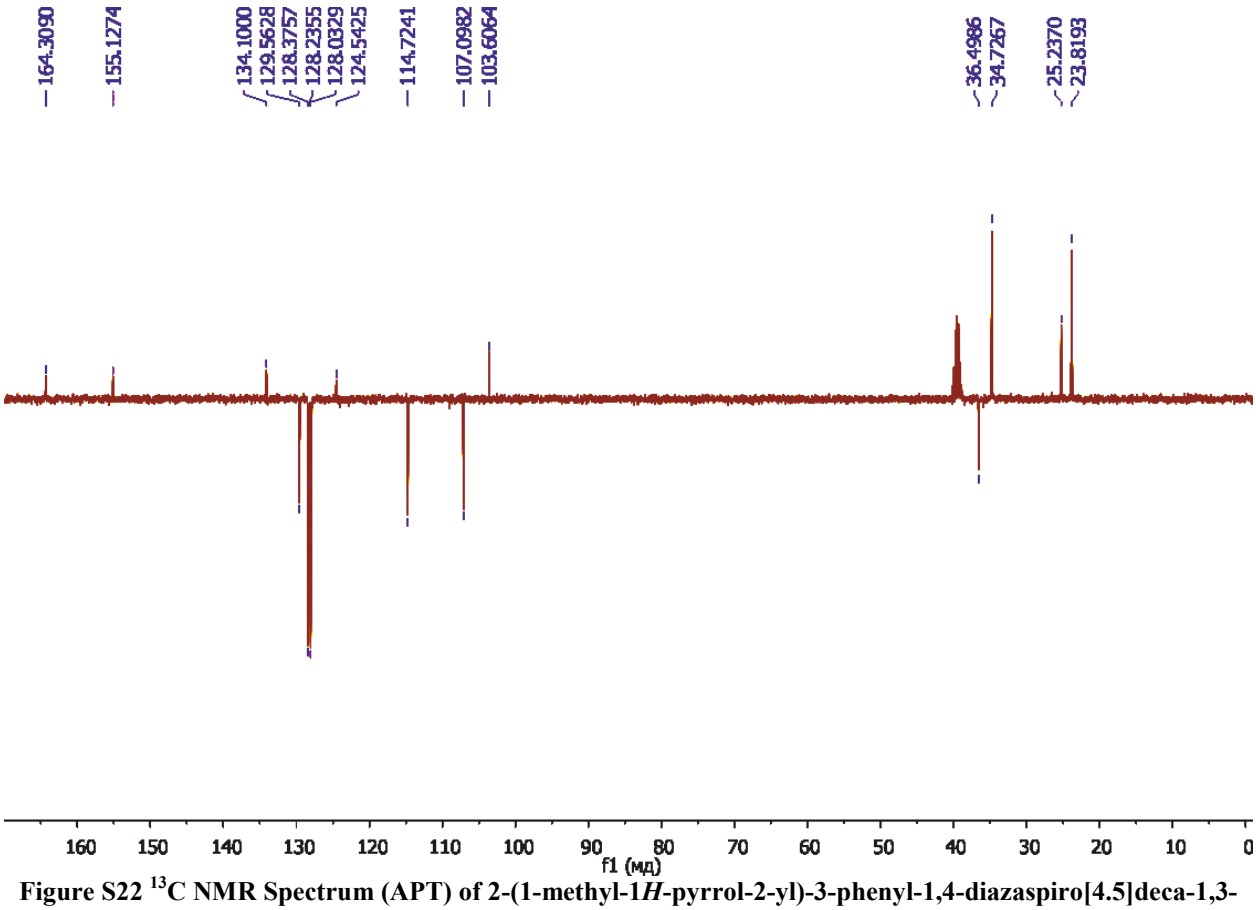

Figure S22 ^{13}C NMR Spectrum (APT) of 2-(1-methyl-1*H*-pyrrol-2-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene (3k)

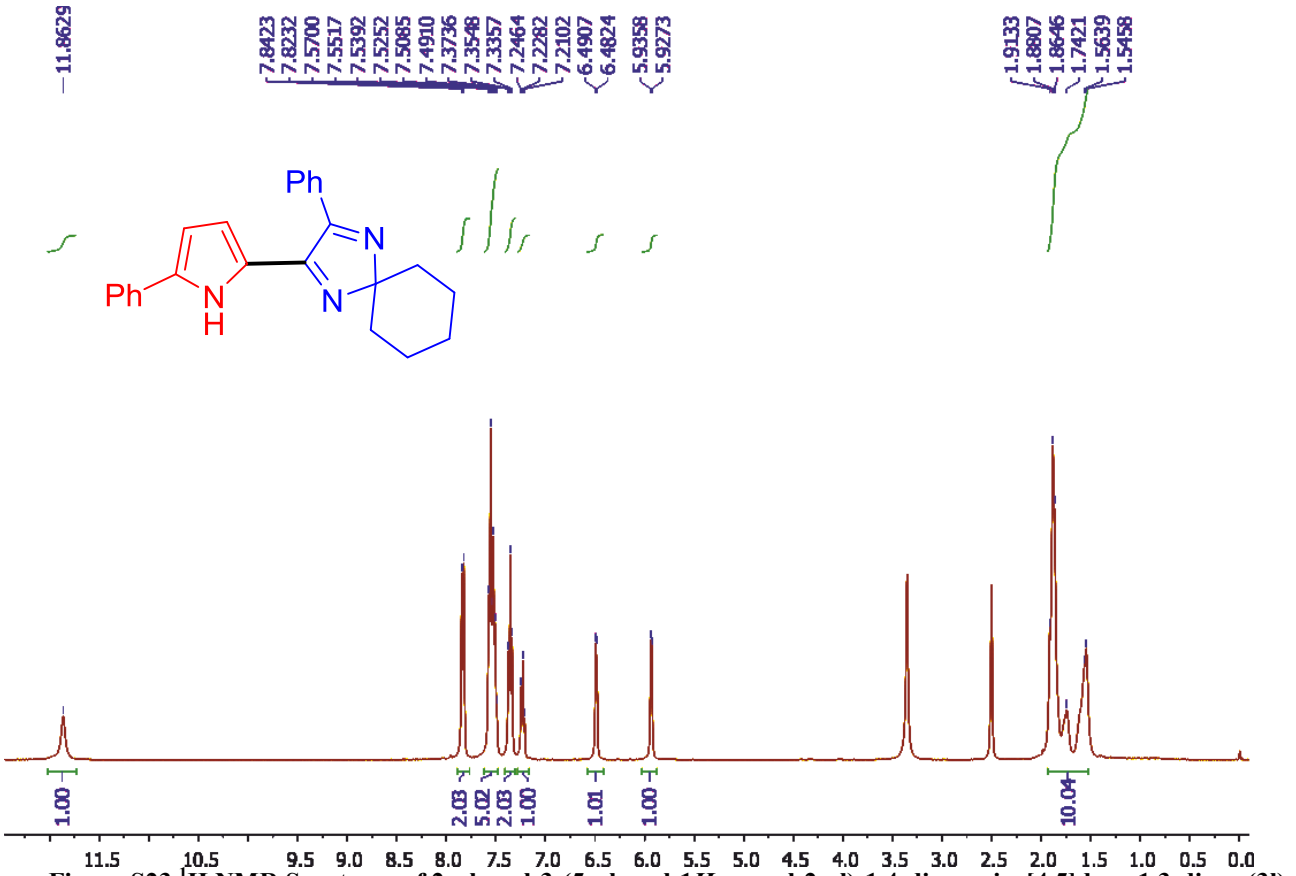

Figure S23 ^{1}H NMR Spectrum of 2-phenyl-3-(5-phenyl-1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene (3l)

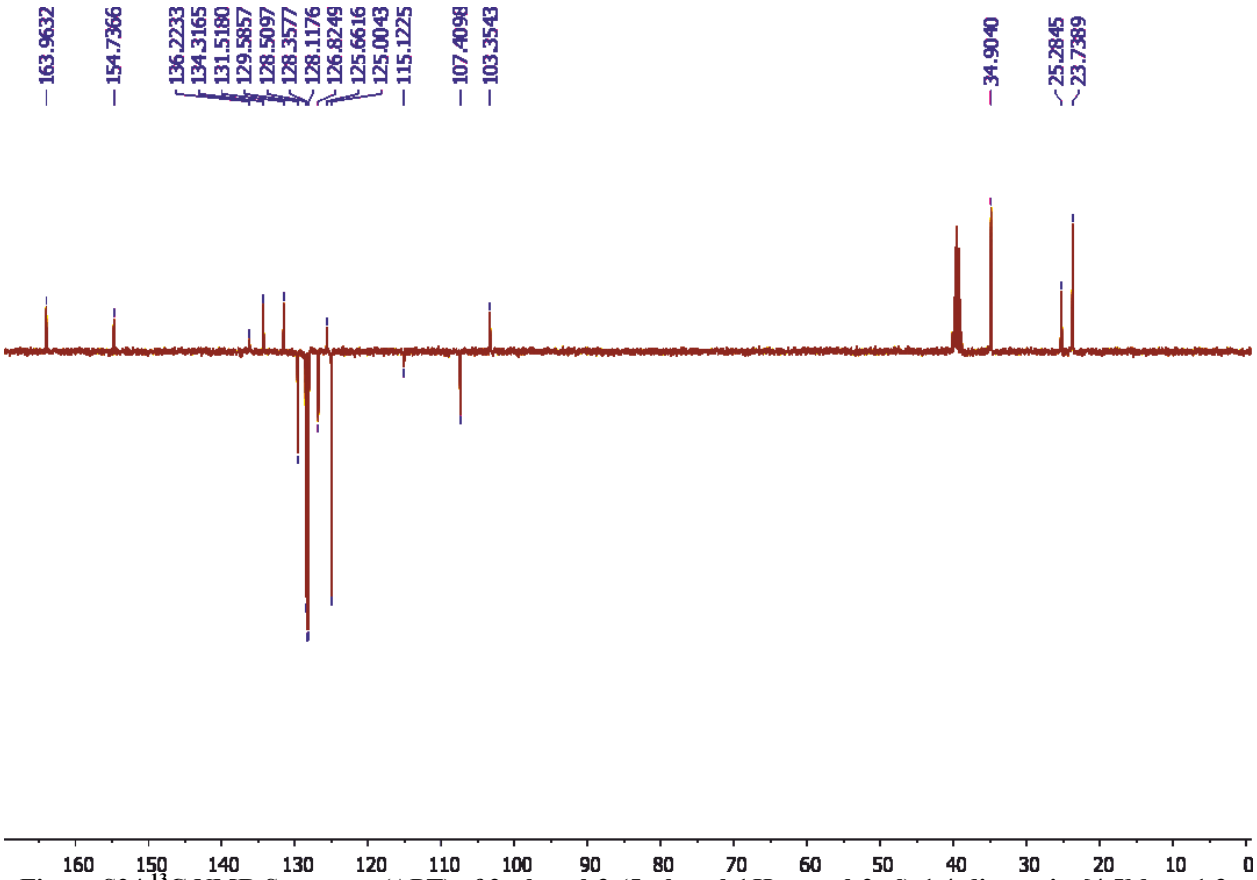

Figure S24 ^{13}C NMR Spectrum (APT) of 2-phenyl-3-(5-phenyl-1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene (3l)

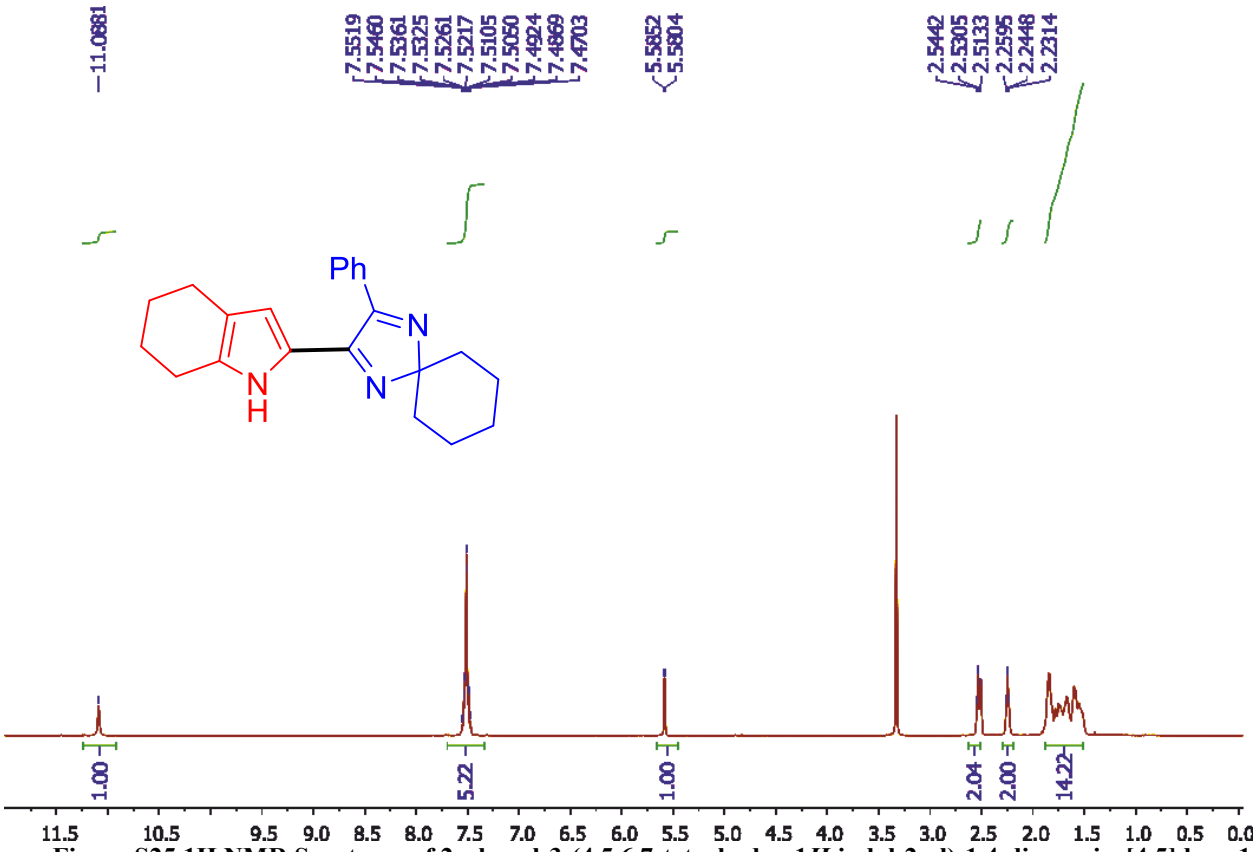

Figure S25 1H NMR Spectrum of 2-phenyl-3-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene (3m)

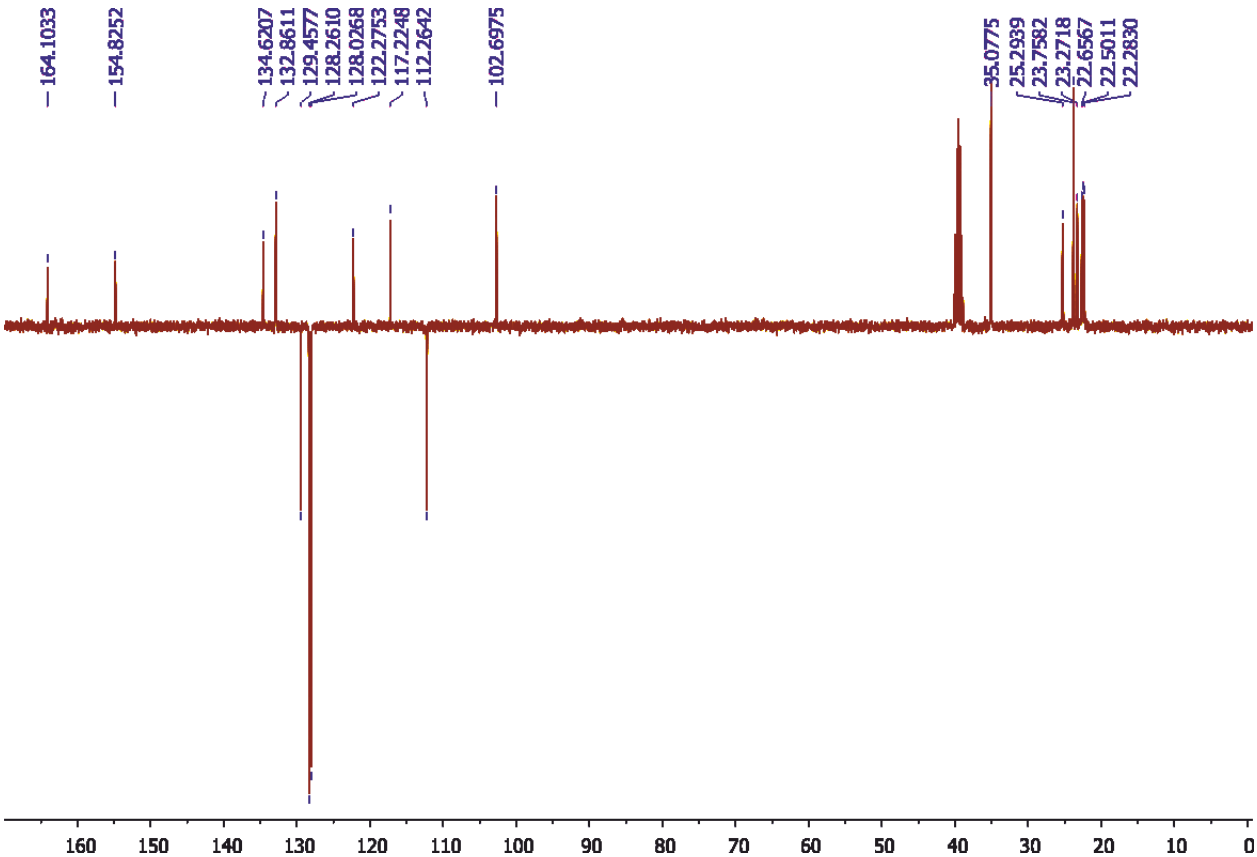

Figure S26 13C NMR Spectrum (APT) of 2-phenyl-3-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene (3m)

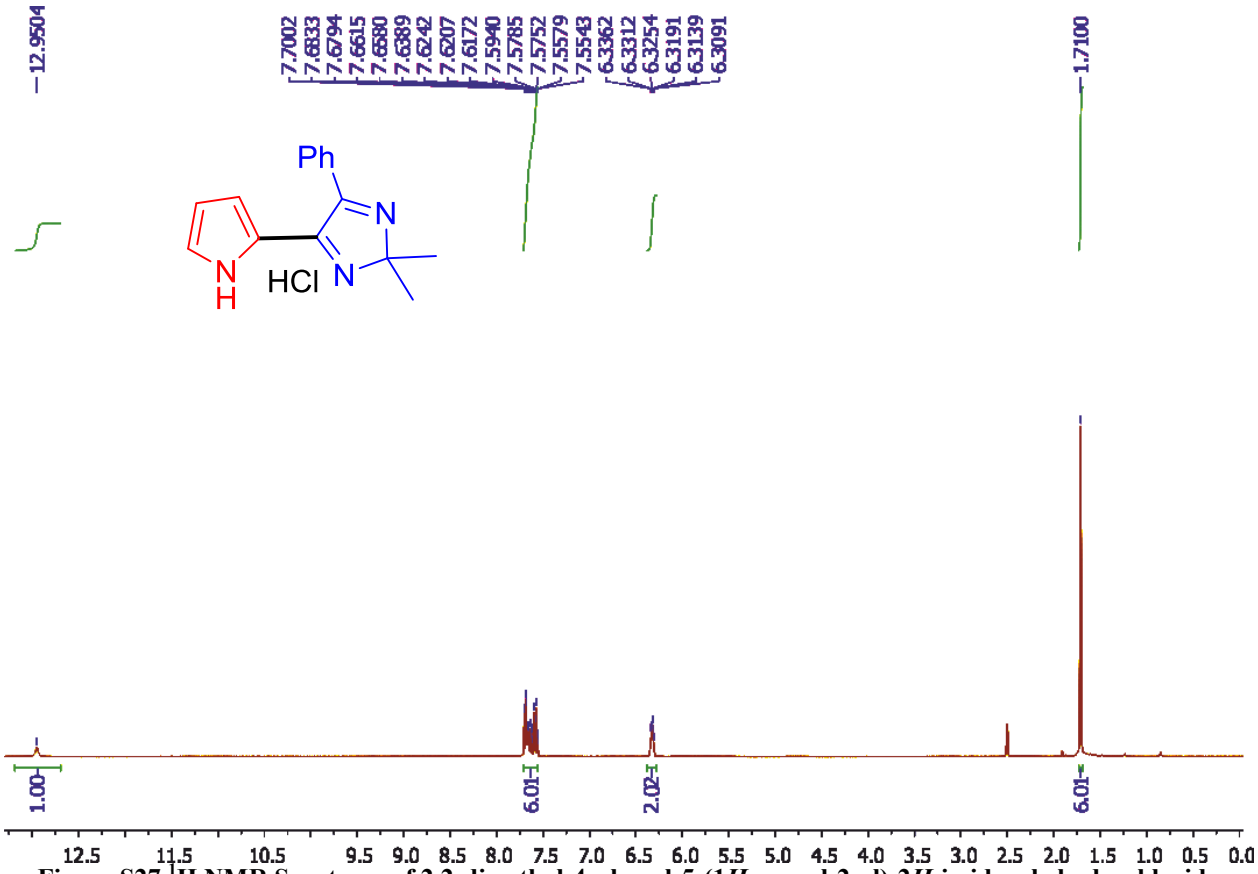

Figure S27 ^{1}H NMR Spectrum of 2,2-dimethyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3aHCl)

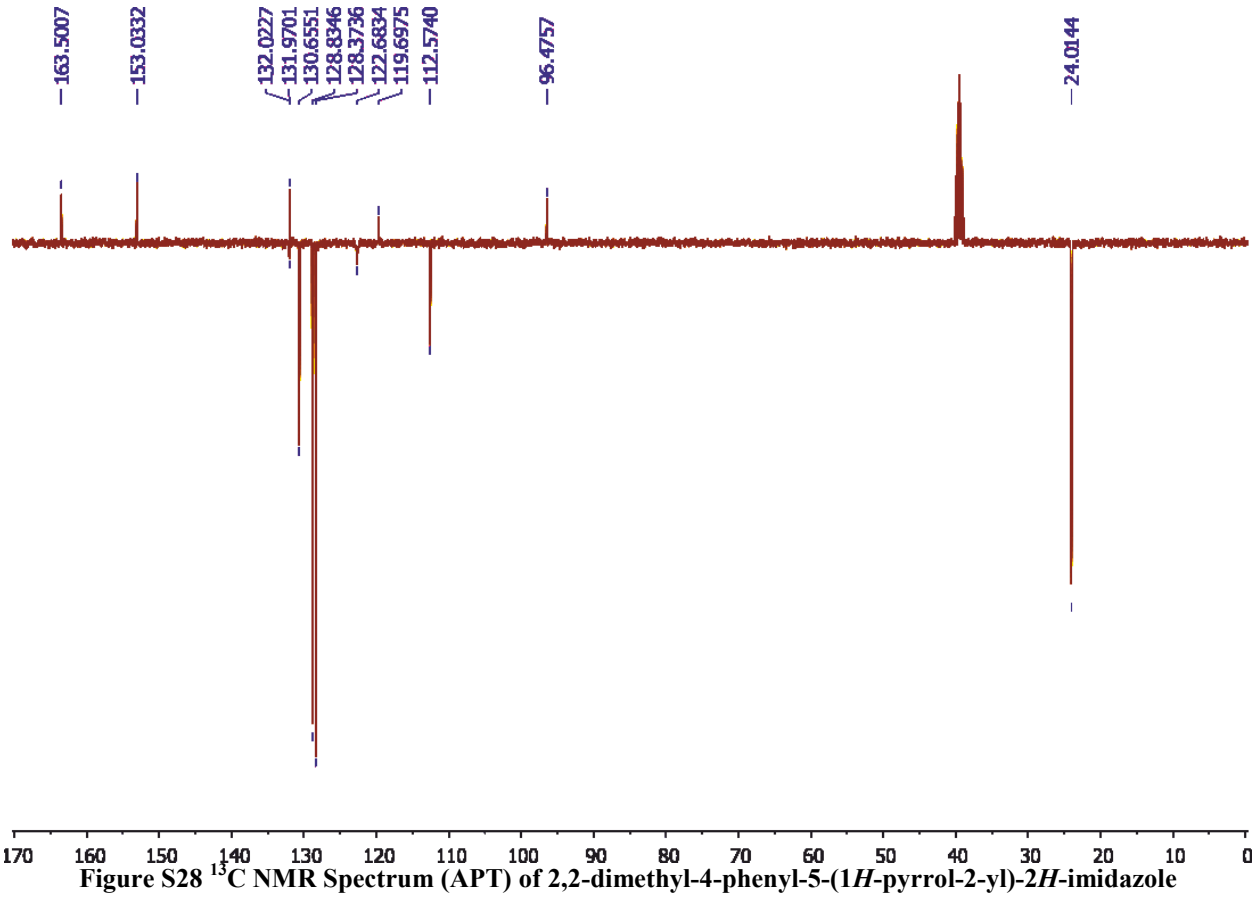

Figure S28 ^{13}C NMR Spectrum (APT) of 2,2-dimethyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3aHCl)

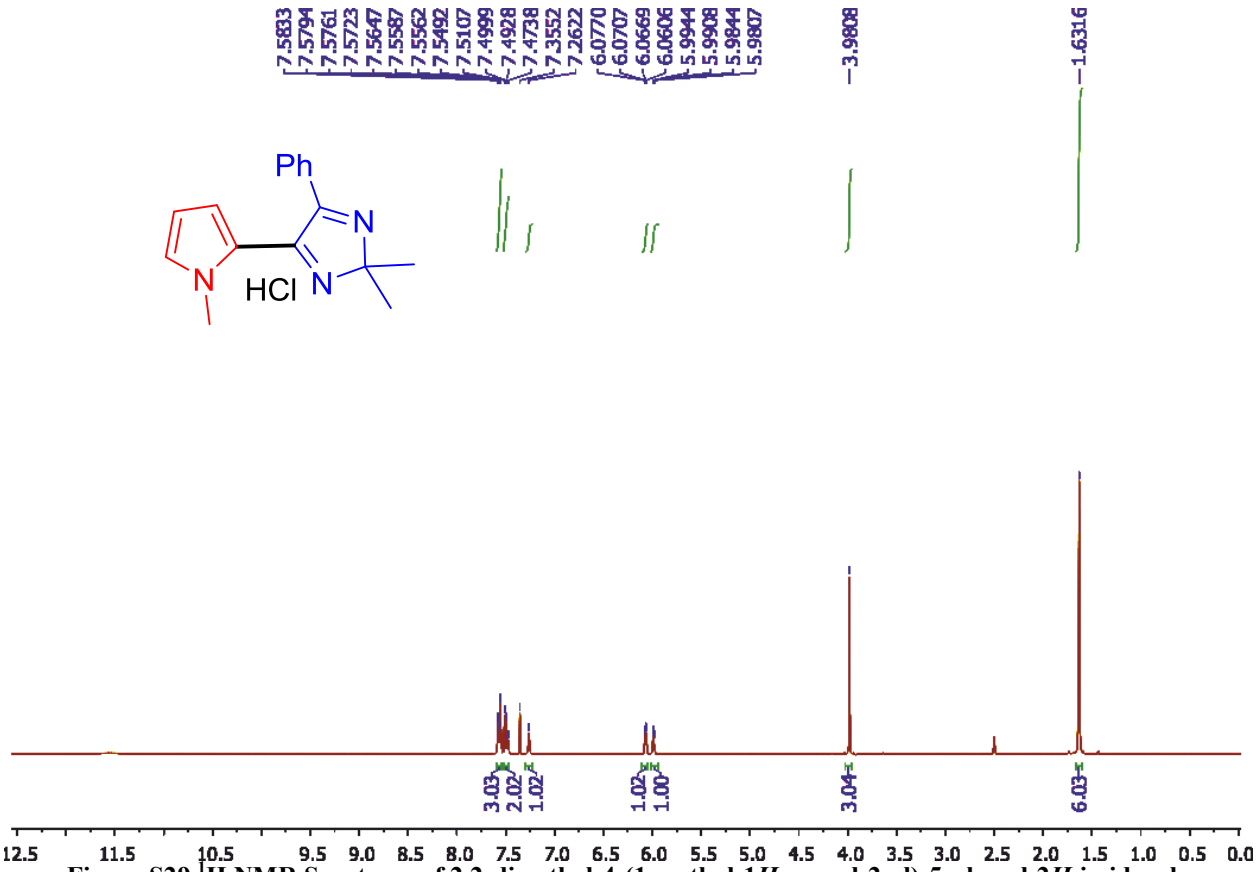

Figure S29 ^{1}**H NMR Spectrum of 2,2-dimethyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole hydrochloride (3bHCl)**

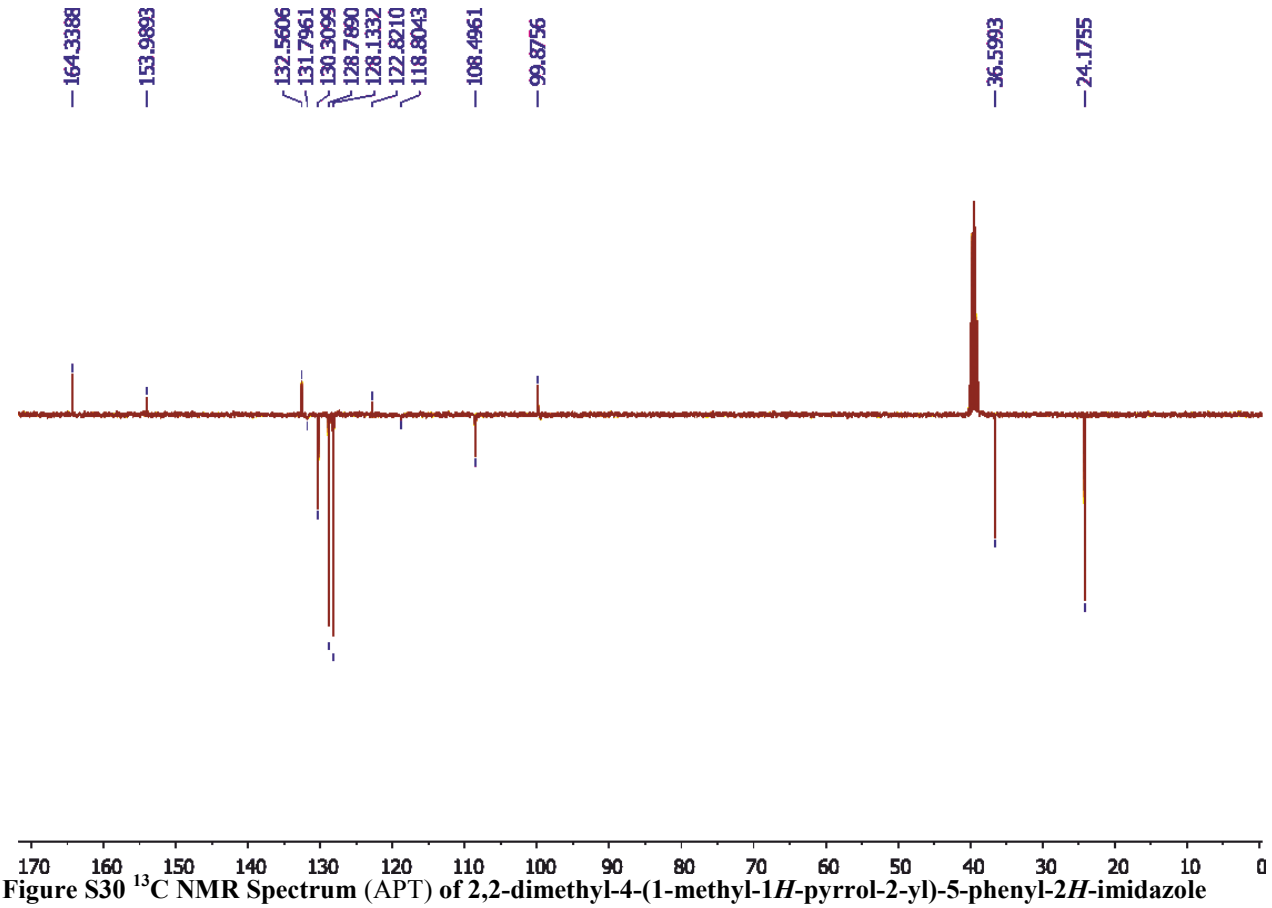

Figure S30 ^{13}**C NMR Spectrum** (APT) **of 2,2-dimethyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole hydrochloride (3bHCl)**

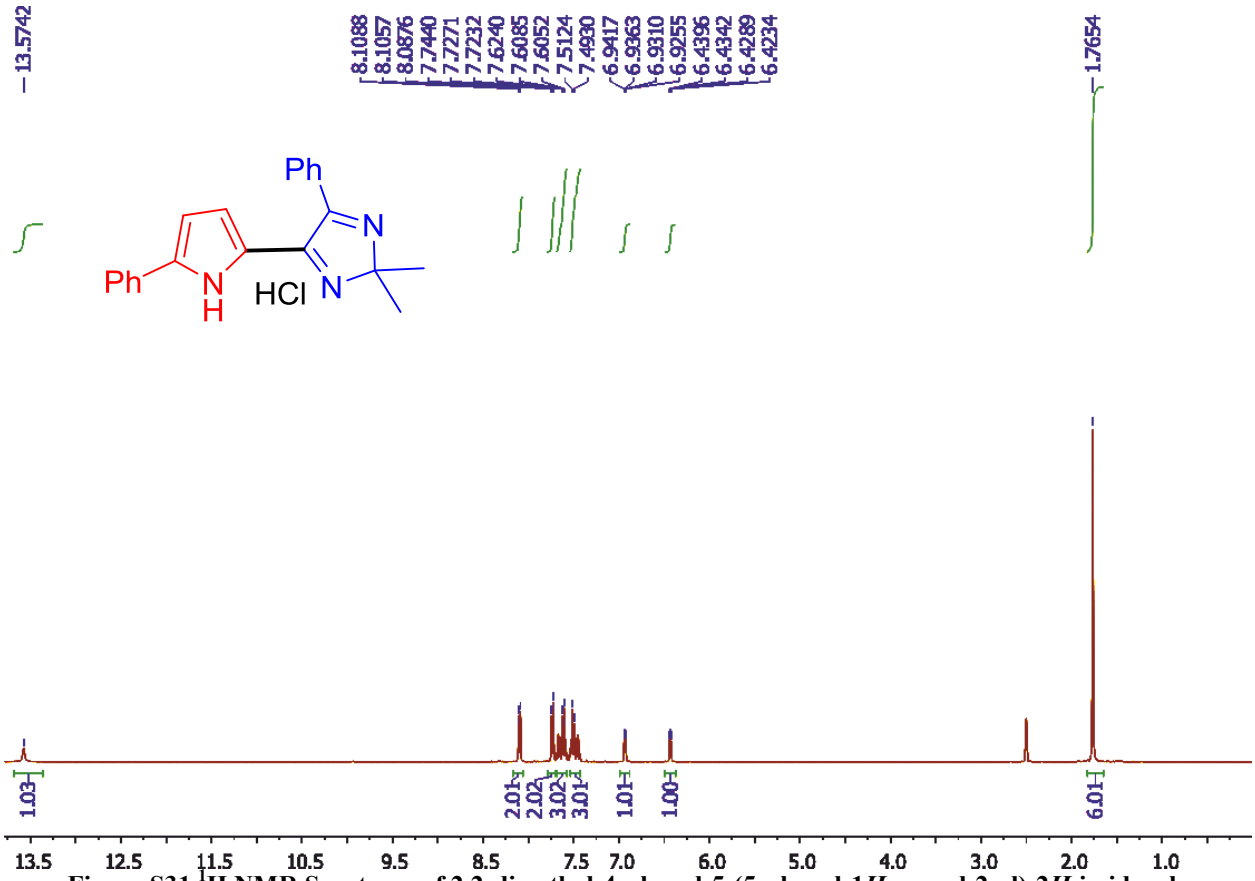

Figure S31 ^{1}H NMR Spectrum of 2,2-dimethyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3cHCl)

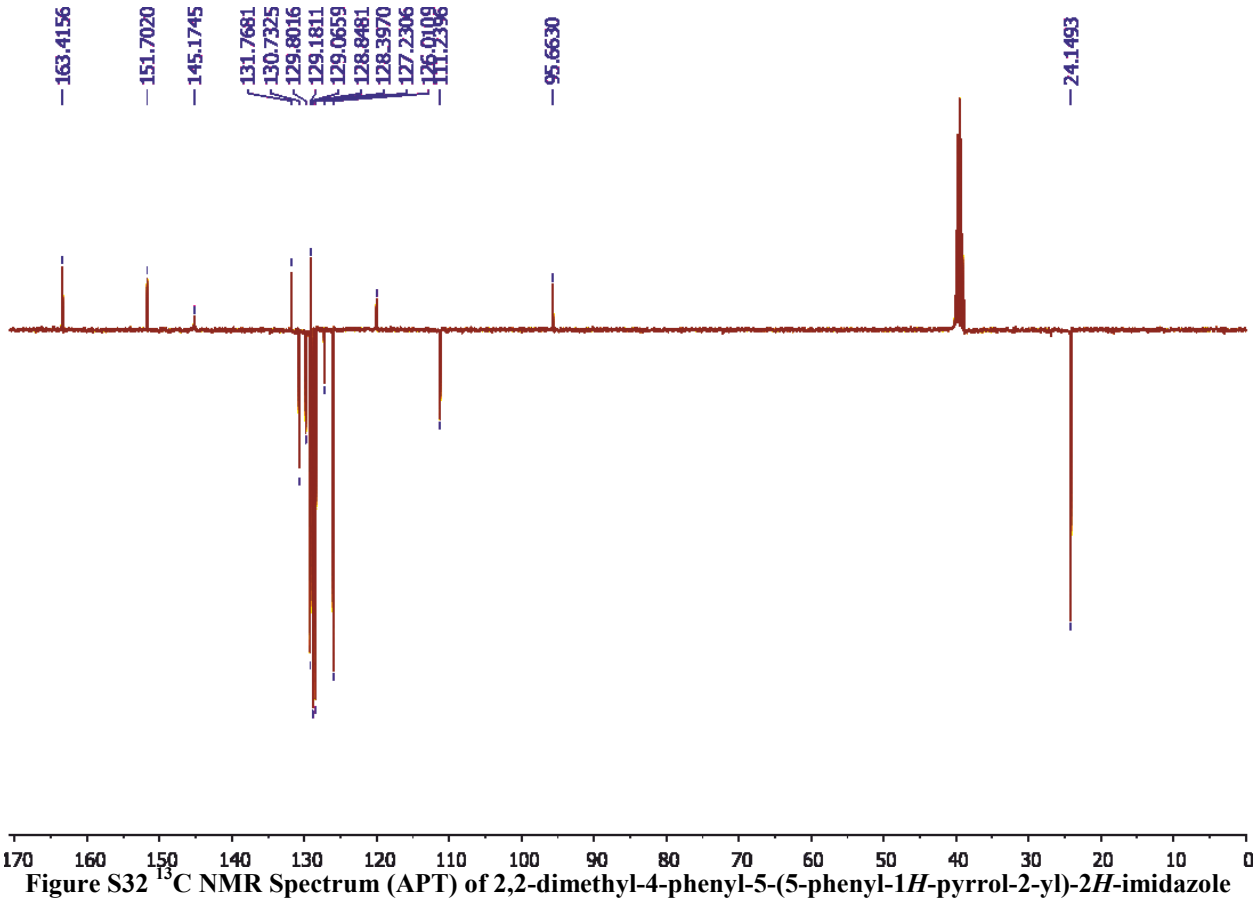

Figure S32 ^{13}C NMR Spectrum (APT) of 2,2-dimethyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3cHCl)

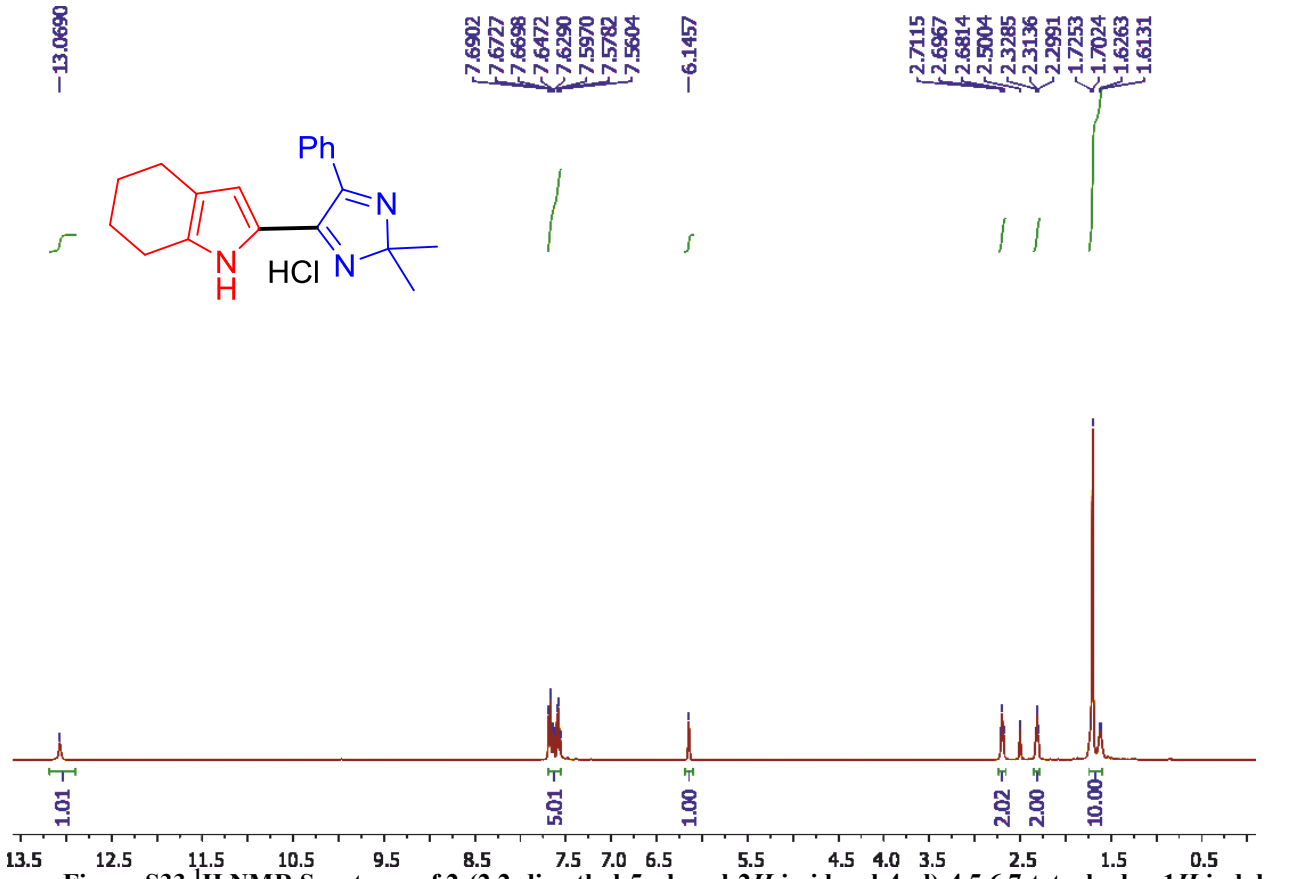

Figure S33 ^{1}**H NMR Spectrum of 2-(2,2-dimethyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole hydrochloride (3dHCl)**

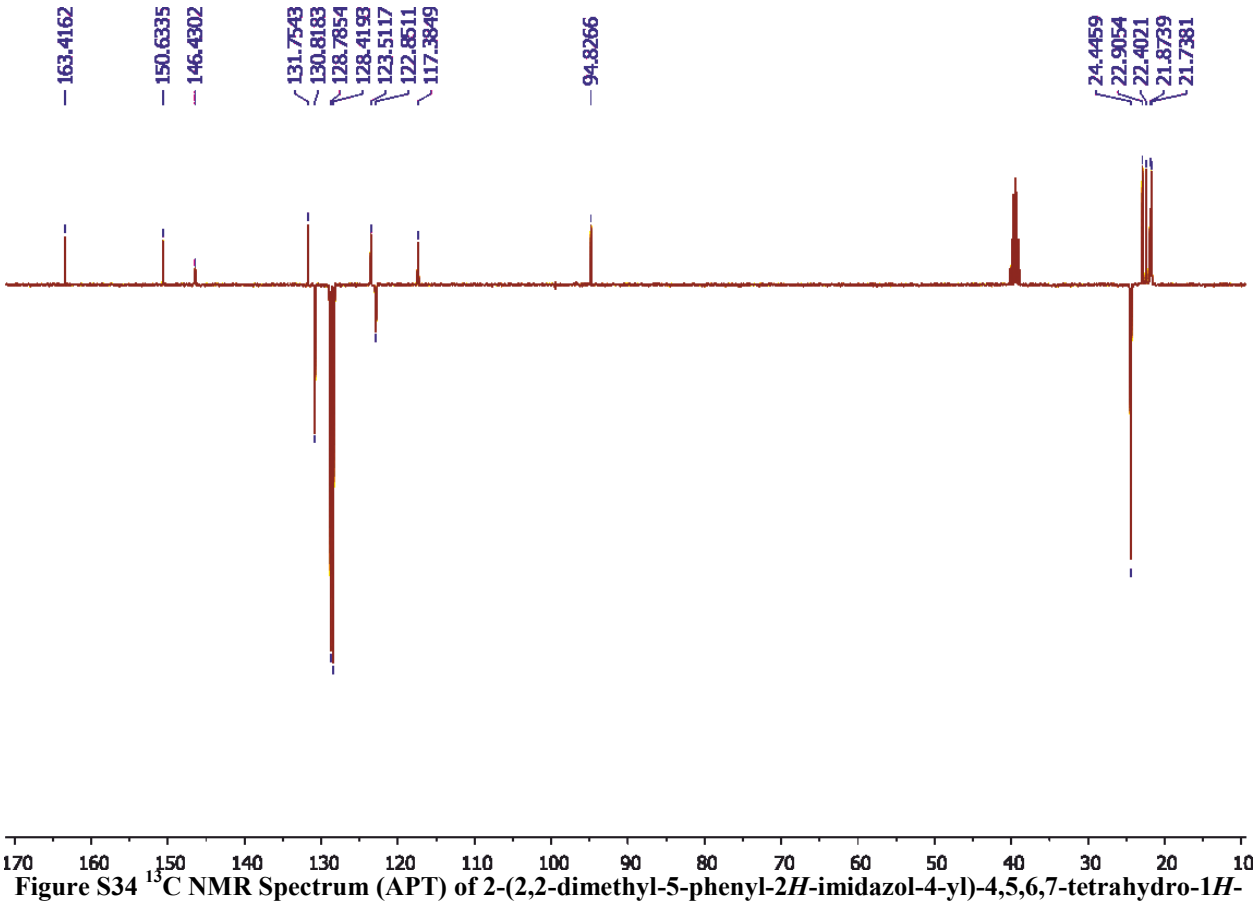

Figure S34 ^{13}**C NMR Spectrum (APT) of 2-(2,2-dimethyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole hydrochloride (3dHCl)**

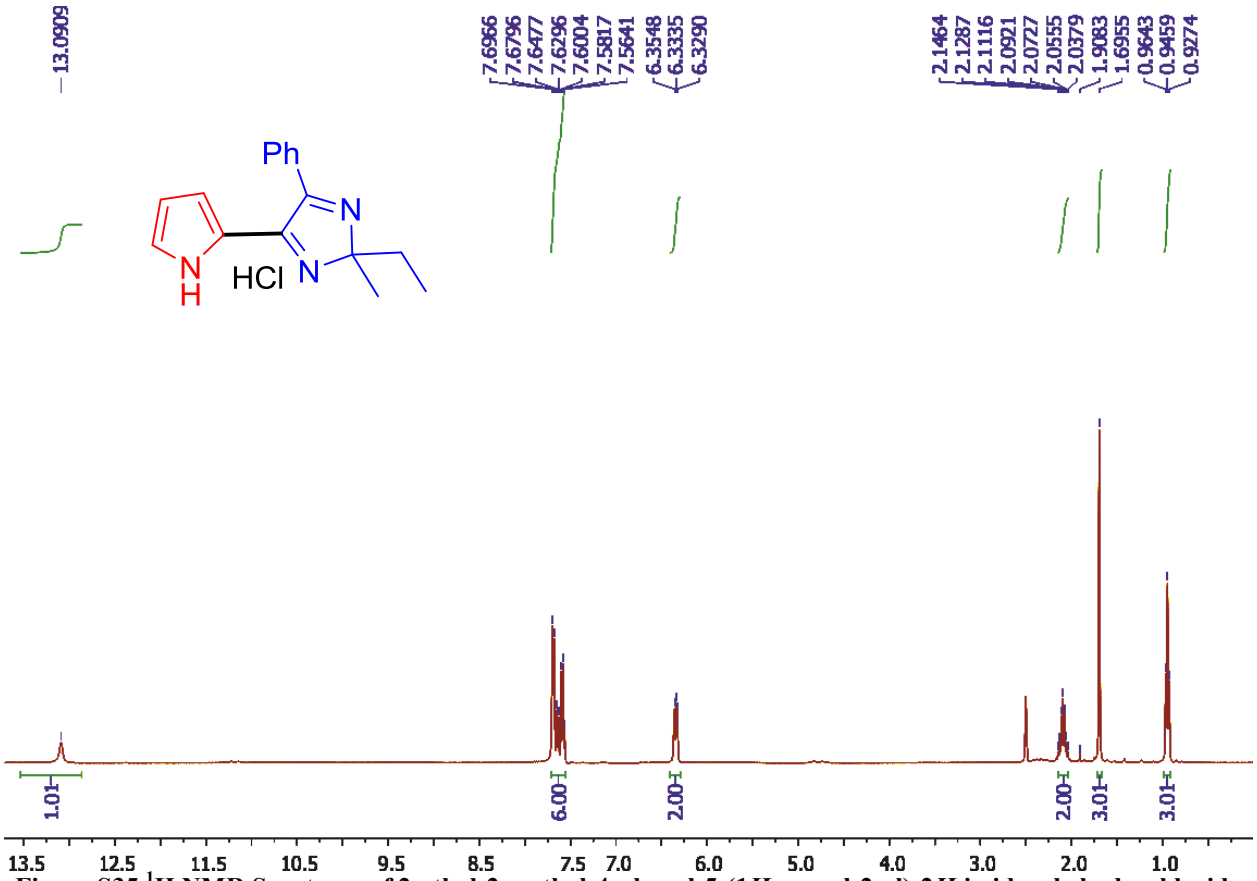

Figure S35 ^{1}H NMR Spectrum of 2-ethyl-2-methyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3eHCl)

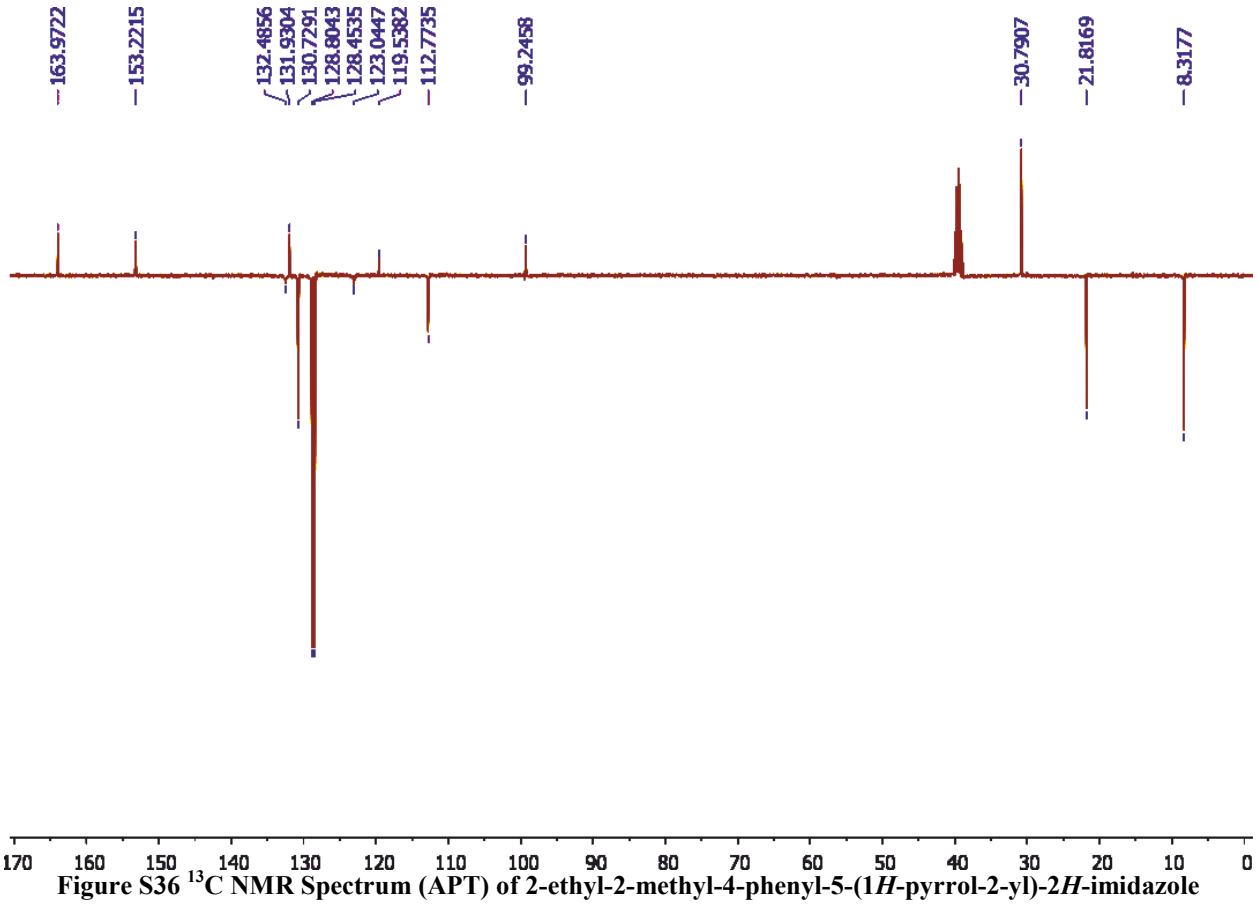

Figure S36 ^{13}C NMR Spectrum (APT) of 2-ethyl-2-methyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3eHCl)

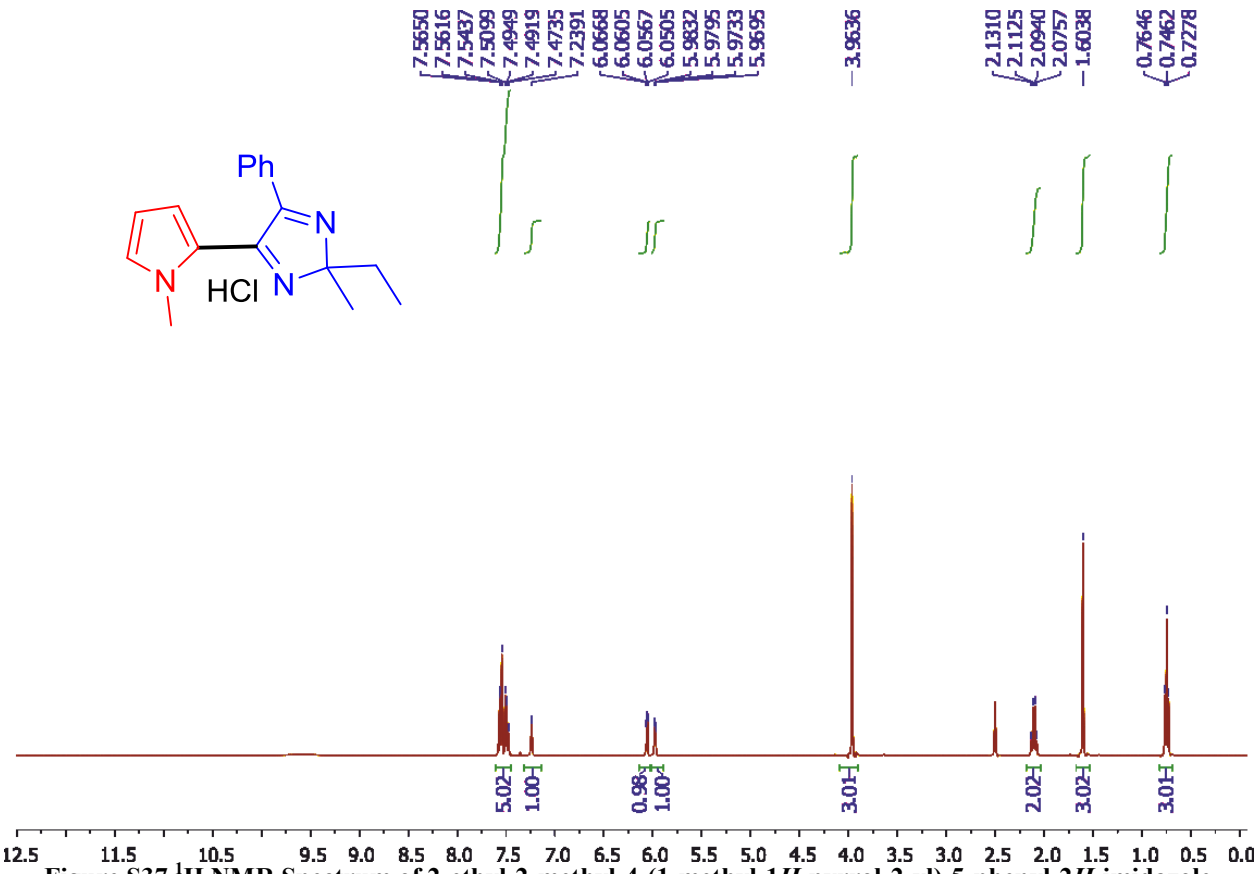

Figure S37 ^{1}H NMR Spectrum of 2-ethyl-2-methyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole hydrochloride (3fHCl)

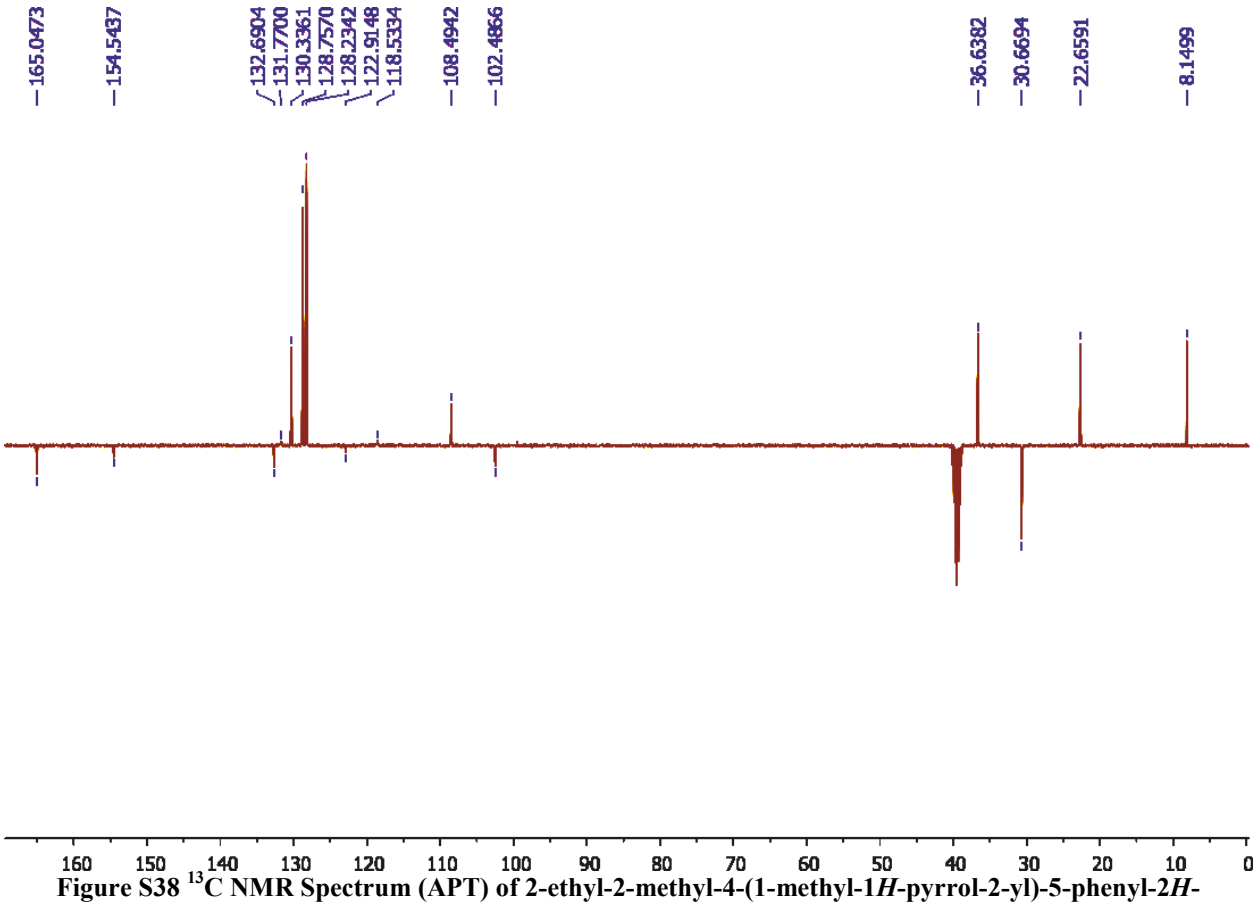

Figure S38 ^{13}C NMR Spectrum (APT) of 2-ethyl-2-methyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5-phenyl-2*H*-imidazole hydrochloride (3fHCl)

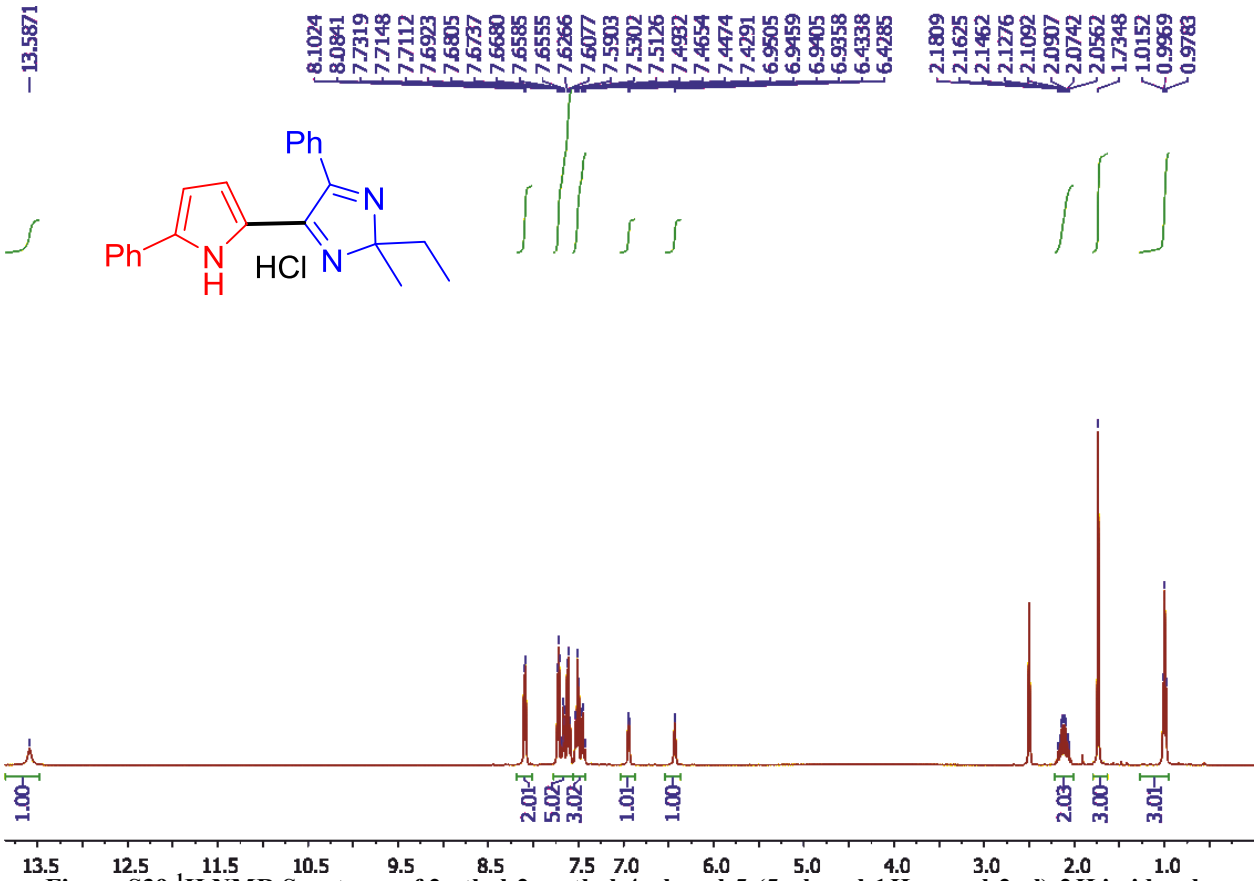

Figure S39 ^{1}H NMR Spectrum of 2-ethyl-2-methyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3gHCl)

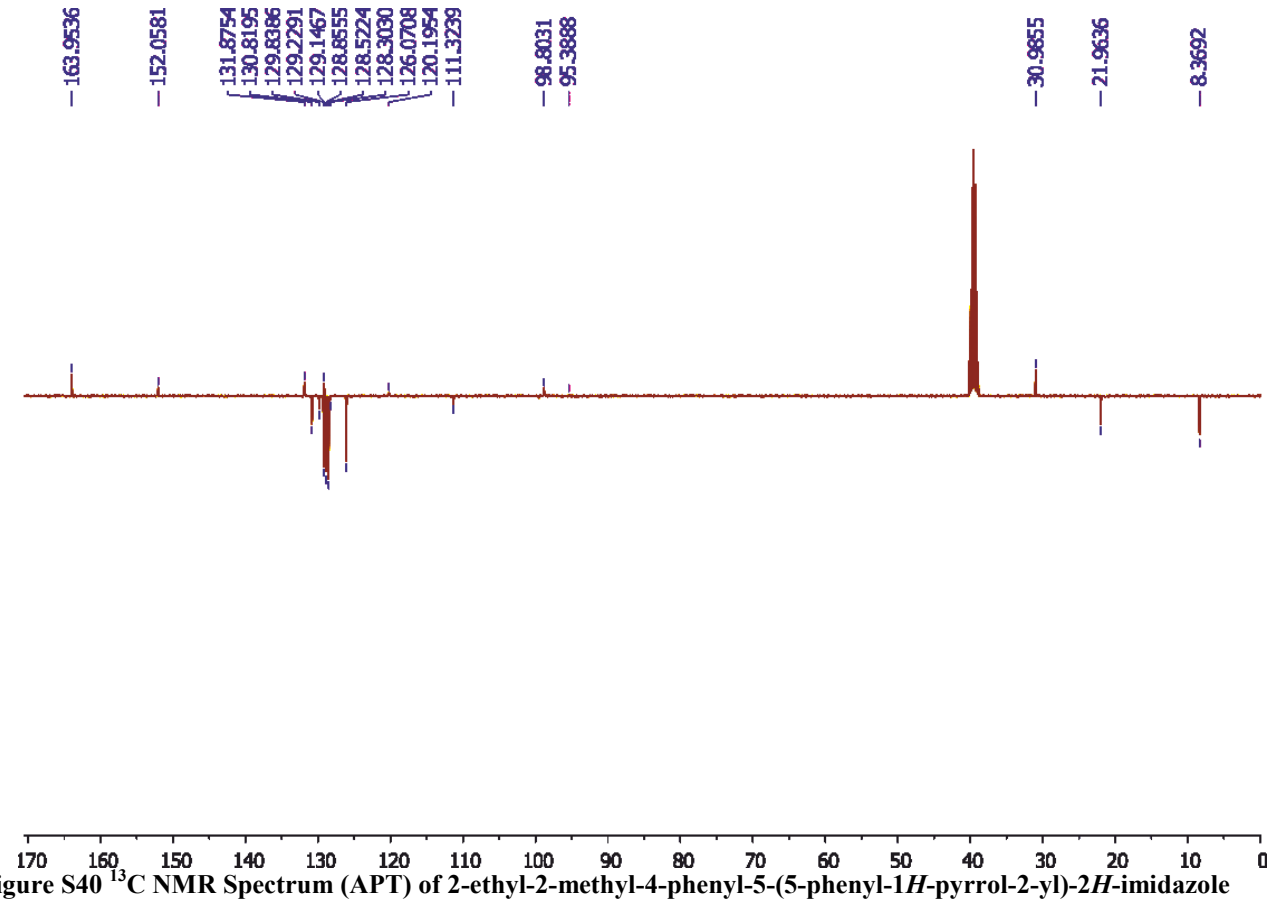

Figure S40 ^{13}C NMR Spectrum (APT) of 2-ethyl-2-methyl-4-phenyl-5-(5-phenyl-1*H*-pyrrol-2-yl)-2*H*-imidazole hydrochloride (3gHCl)

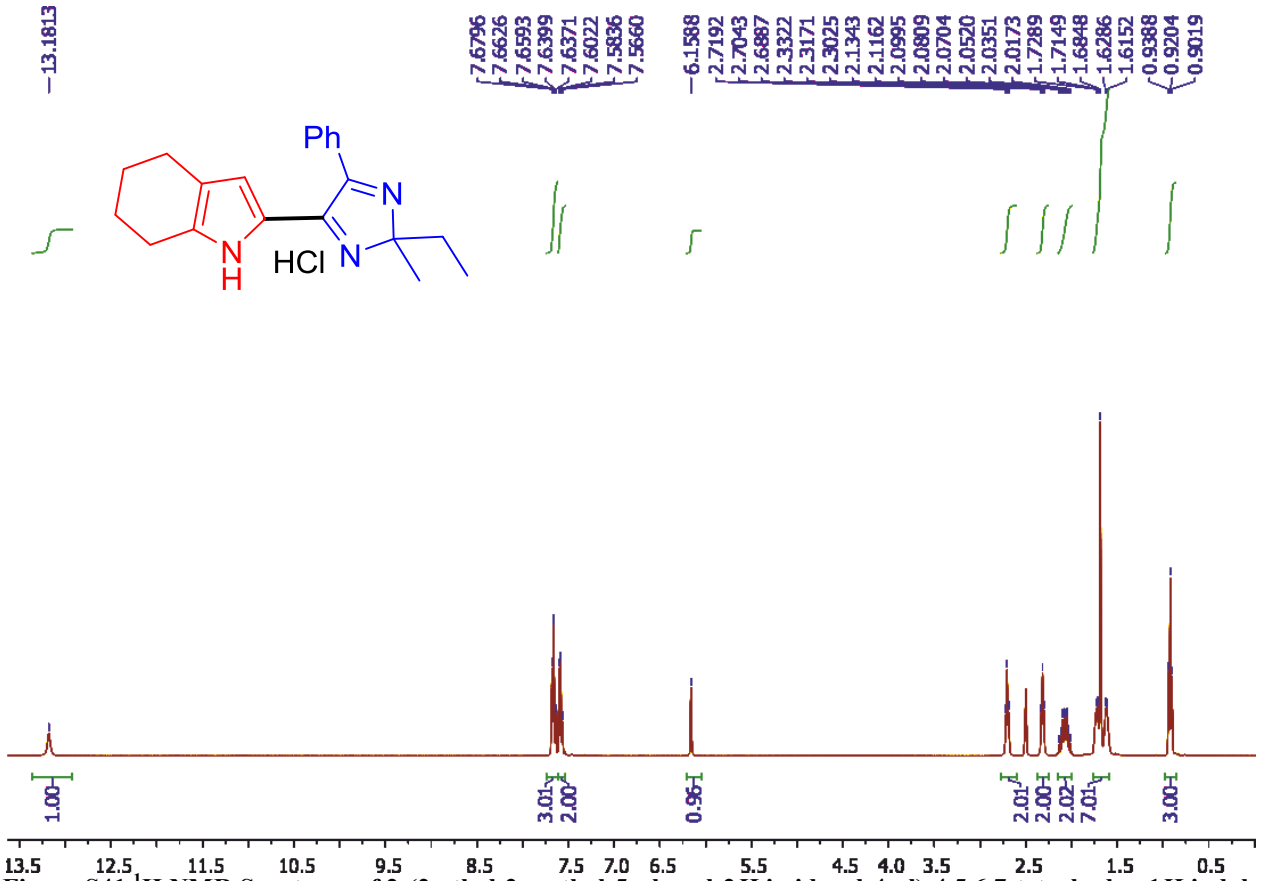

Figure S41 ^{1}H NMR Spectrum of 2-(2-ethyl-2-methyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole hydrochloride (3hHCl)

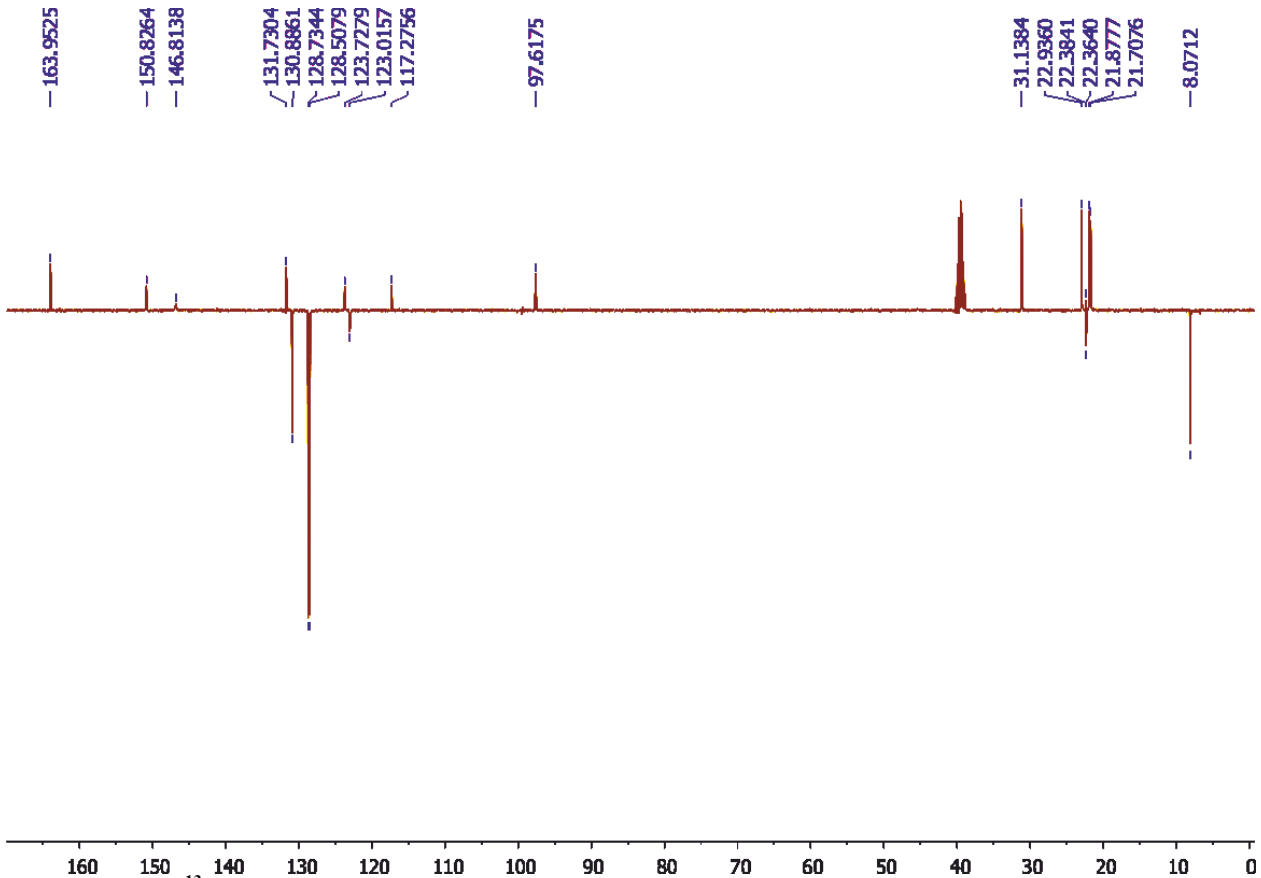

Figure S42 ^{13}C NMR Spectrum (APT) of 2-(2-ethyl-2-methyl-5-phenyl-2*H*-imidazol-4-yl)-4,5,6,7-tetrahydro-1*H*-indole hydrochloride (3hHCl)

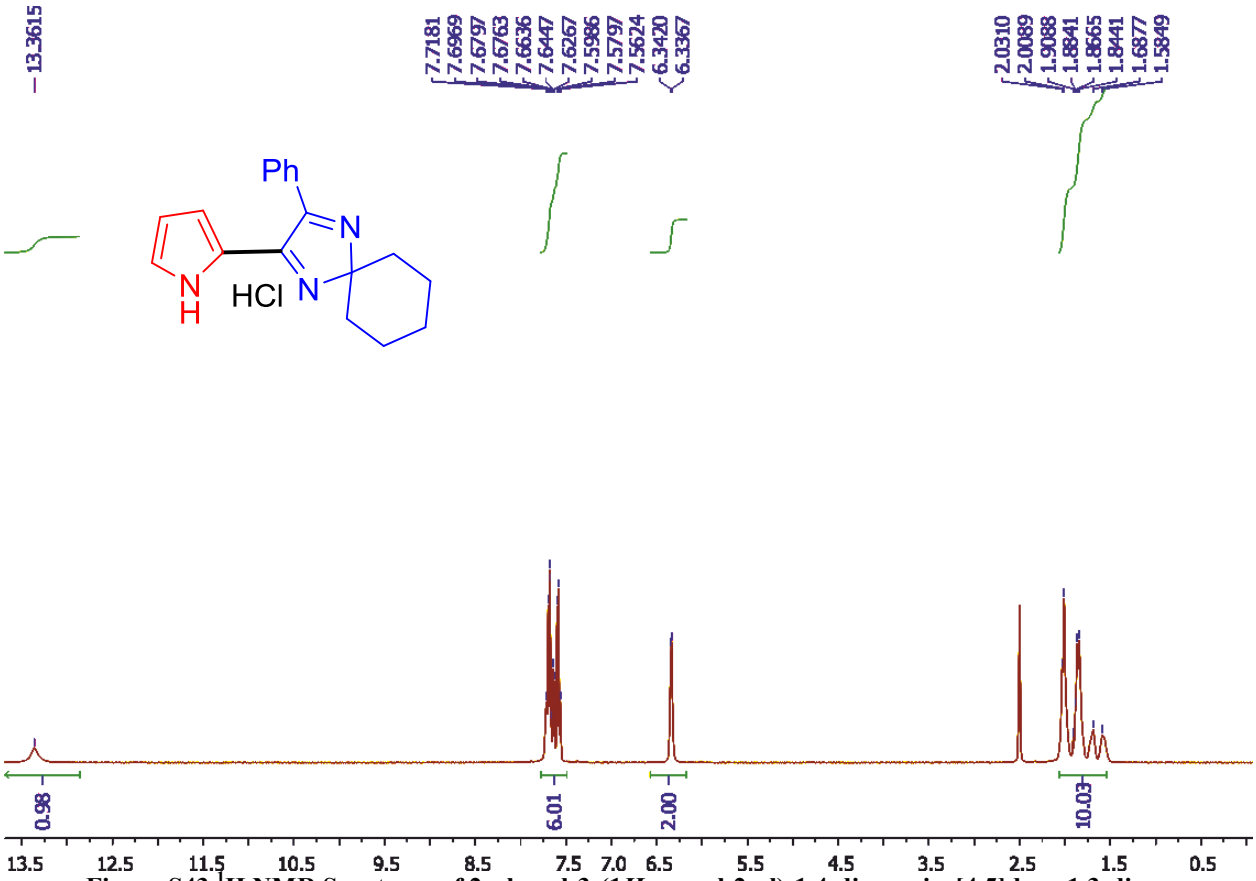

Figure S43 ^{1}H NMR Spectrum of 2-phenyl-3-(1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3iHCl)

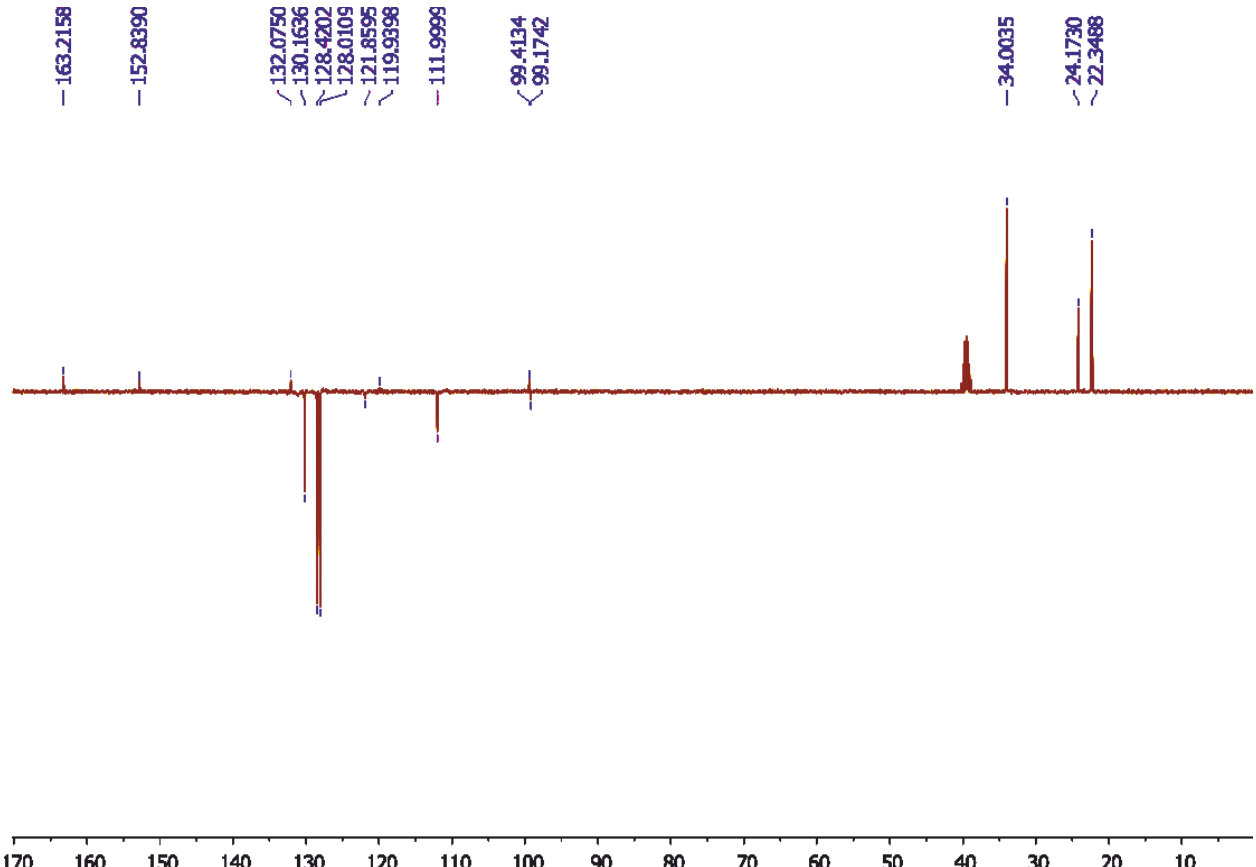

Figure S44 ^{13}C NMR Spectrum (APT) of 2-phenyl-3-(1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3iHCl)

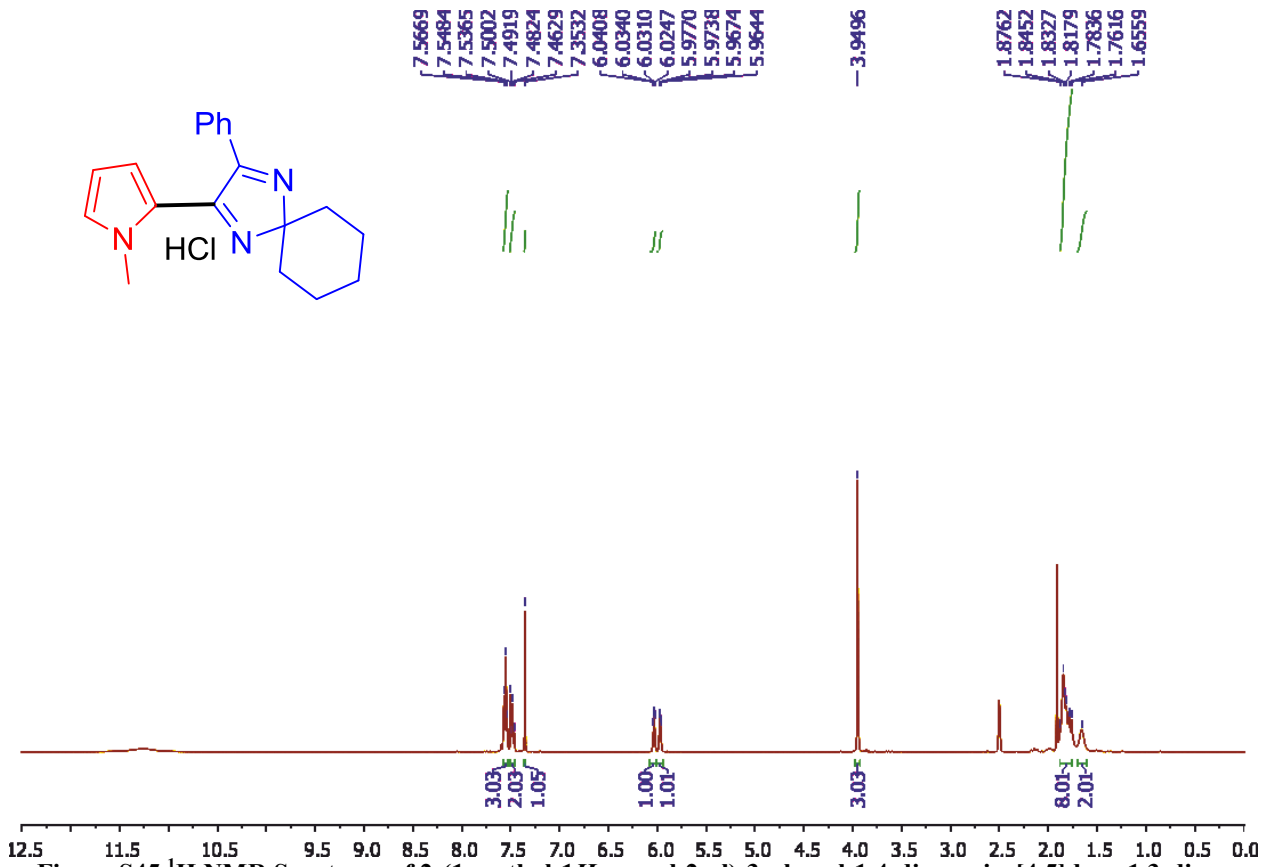

Figure S45 ^{1}H NMR Spectrum of 2-(1-methyl-1*H*-pyrrol-2-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3kHCl)

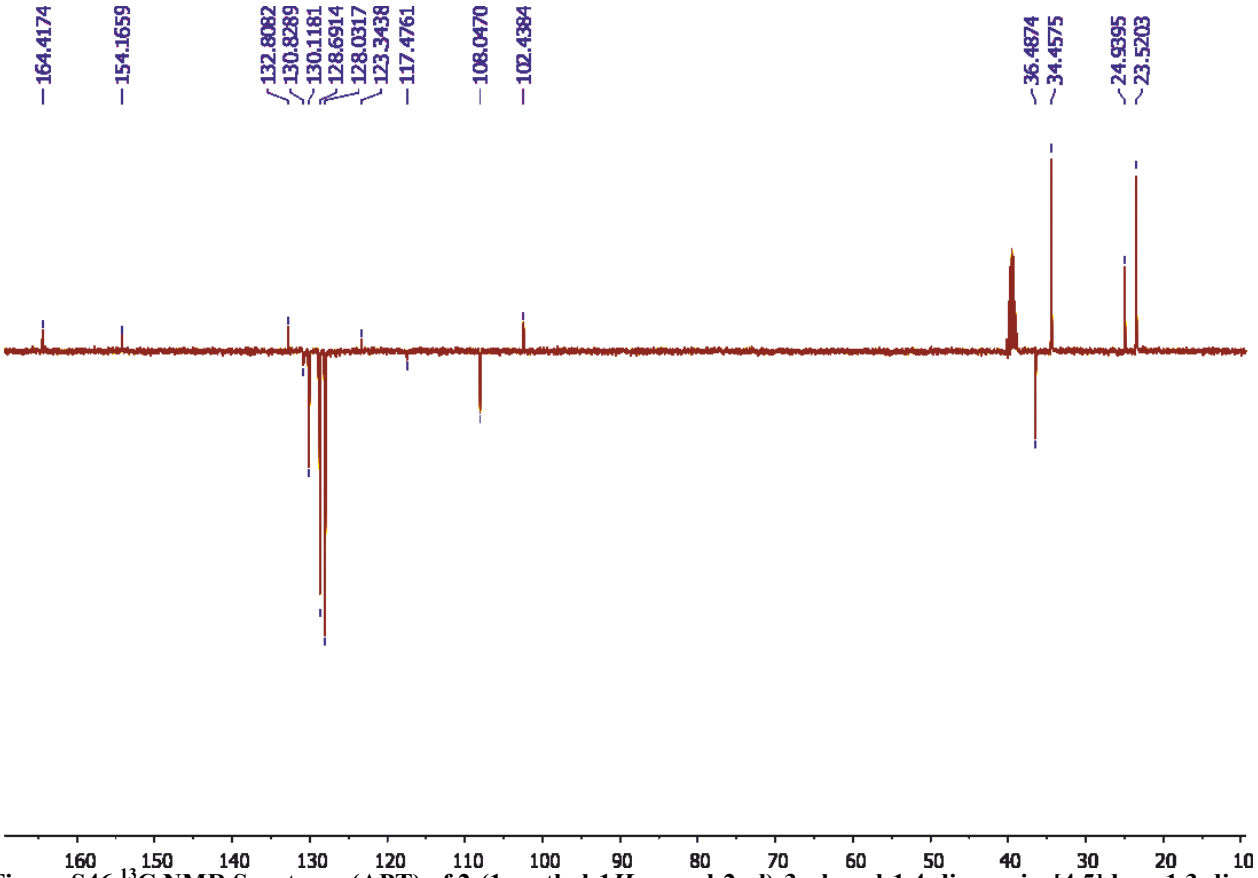

Figure S46 ^{13}C NMR Spectrum (APT) of 2-(1-methyl-1*H*-pyrrol-2-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3kHCl)

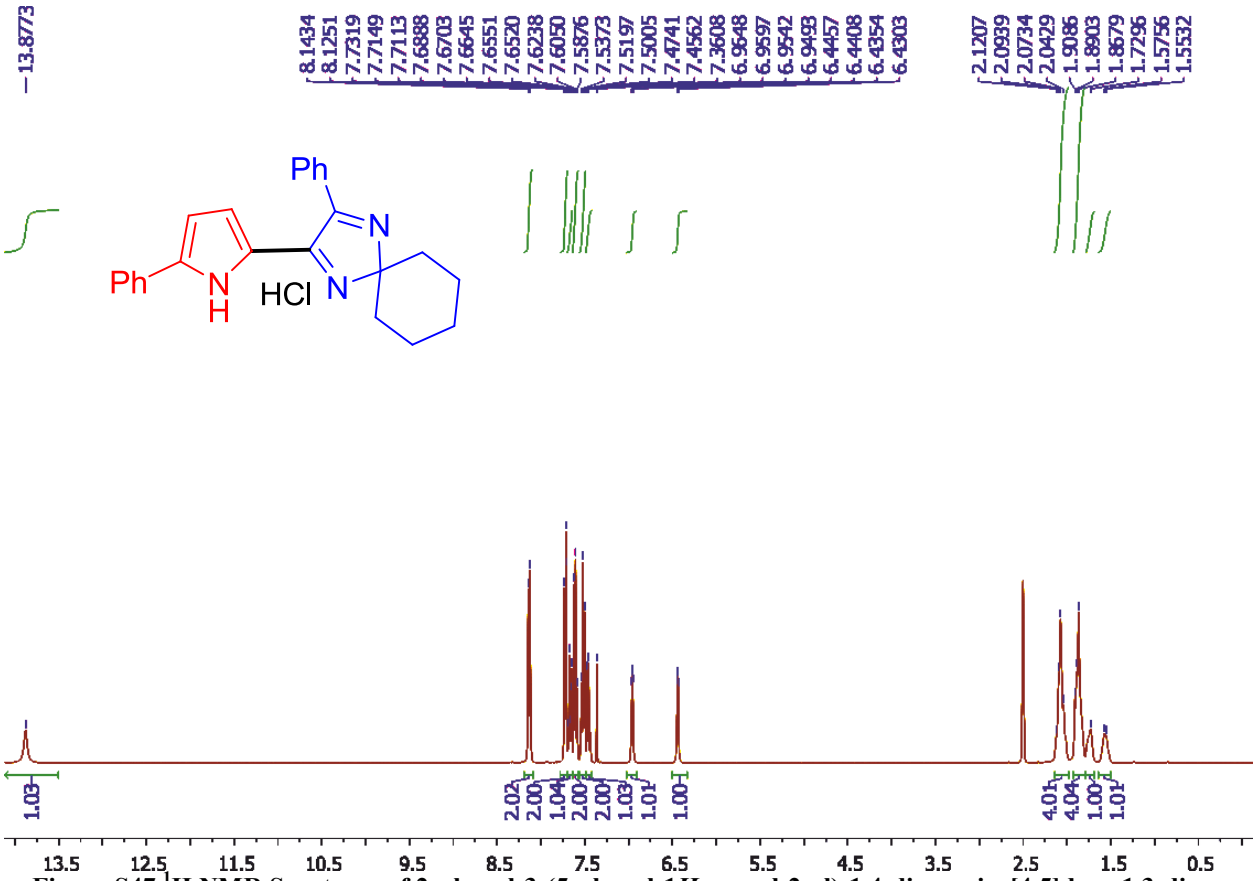

Figure S47 ^{1}H NMR Spectrum of 2-phenyl-3-(5-phenyl-1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3lHCl)

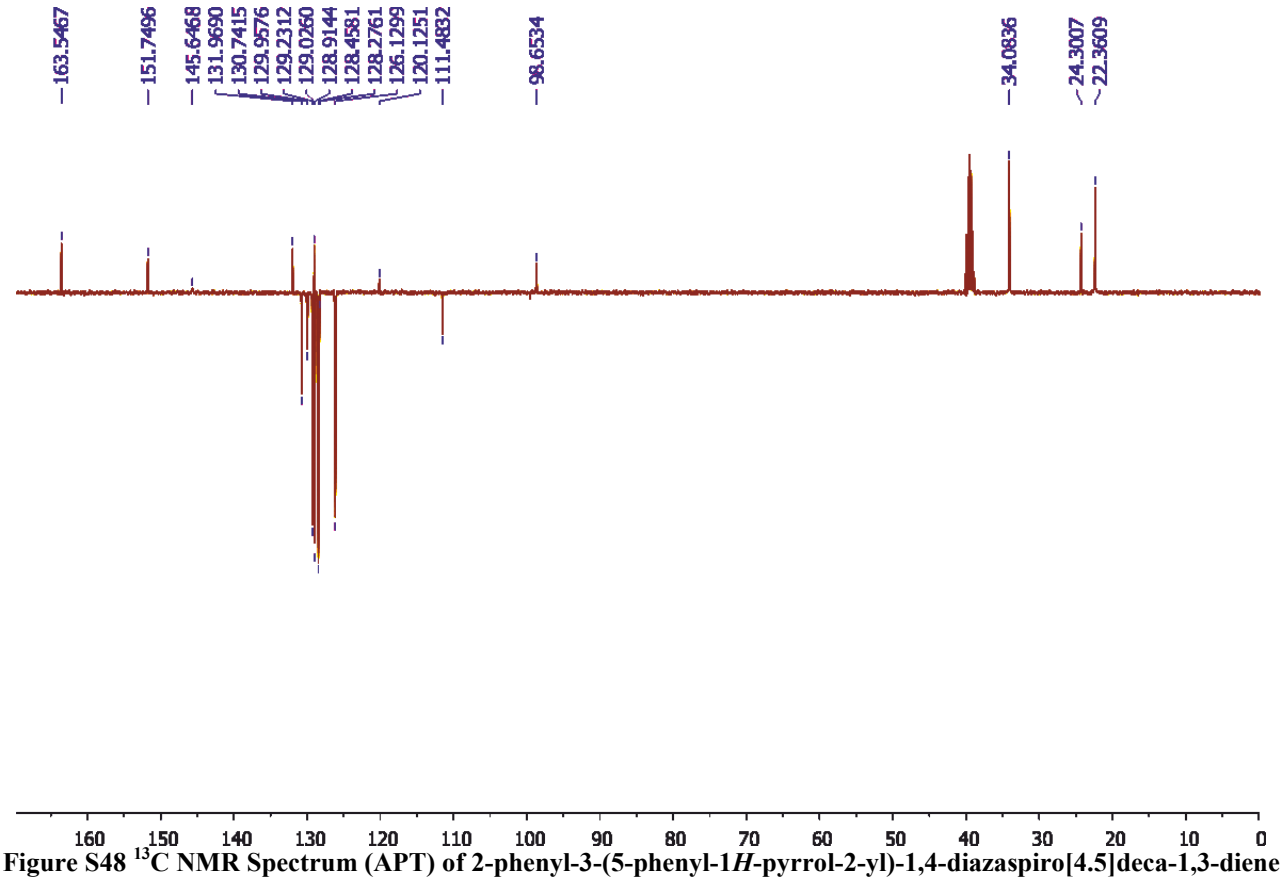

Figure S48 ^{13}C NMR Spectrum (APT) of 2-phenyl-3-(5-phenyl-1*H*-pyrrol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3lHCl)

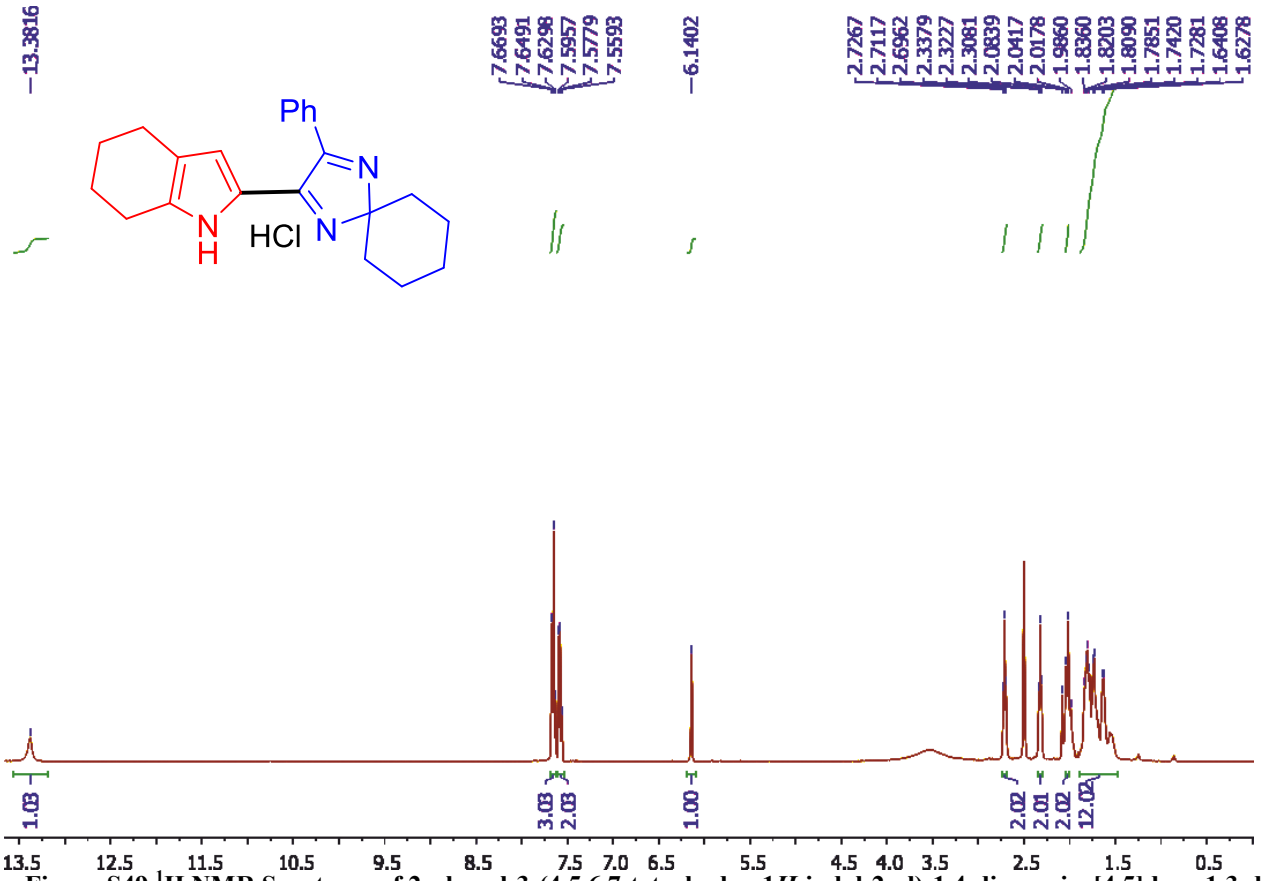

Figure S49 ^{1}H NMR Spectrum of 2-phenyl-3-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3mHCl)

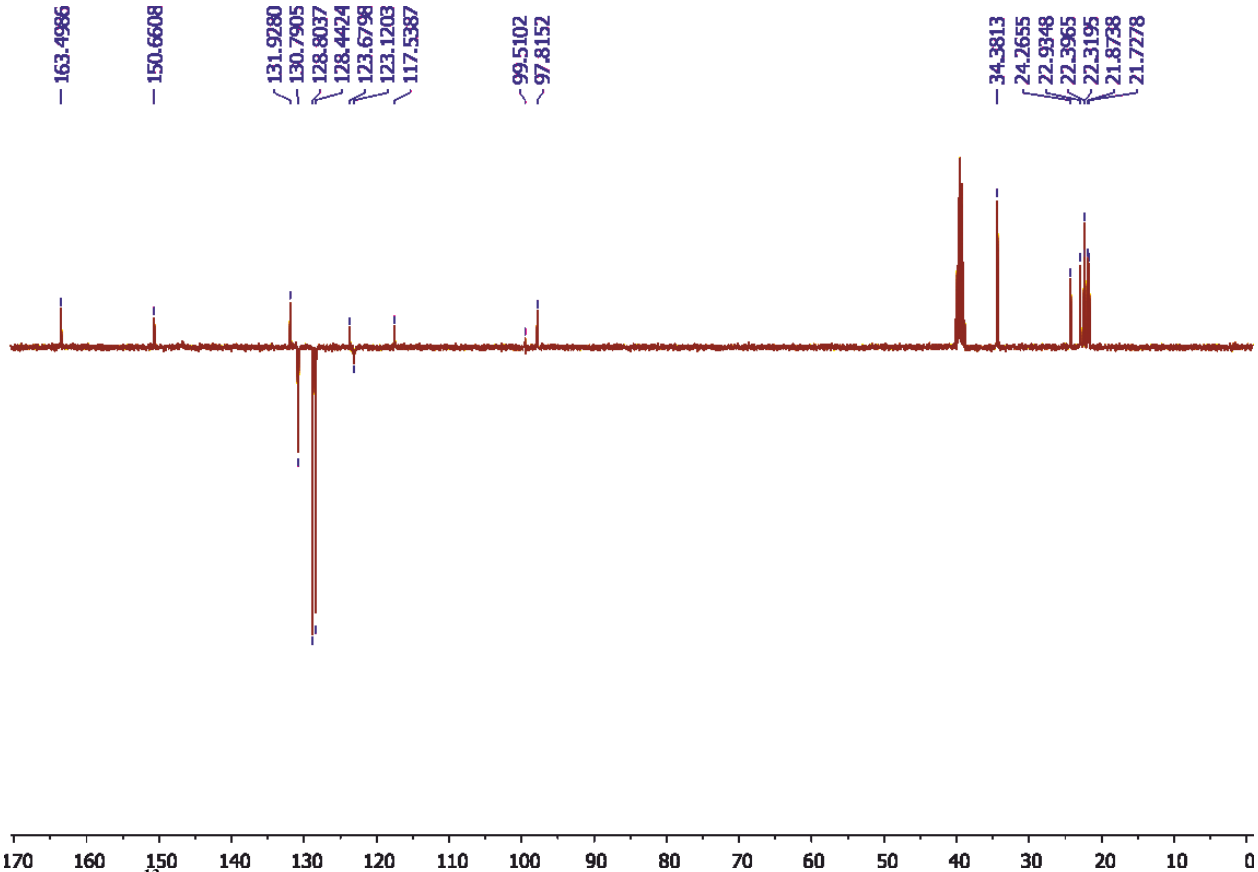

Figure S50 ^{13}C NMR Spectrum (APT) of 2-phenyl-3-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-1,4-diazaspiro[4.5]deca-1,3-diene hydrochloride (3mHCl)

X-ray Analysis Data

The crystallographic data and basic refinement parameters for 2-ethyl-2-methyl-4-phenyl-5-(1*H*-pyrrol-2-yl)-2*H*-imidazole **3e** are shown in Table S1.

Table S1. X-ray analysis data and basic refinement parameters for **3e**

Parameter	**4e**
Molecular formula	$C_{21}H_{21}N_3O$
Molecular weight	331.41
T/K	295.(2)
λ/Å	1.54184
Syngony	monoclinic
Space group	$P2_1/c$
a/Å	6.098(3)
b/Å	27.444(14)
c/Å	11.214(3)
α/deg	90.00
β/deg	103.50(3)
γ/deg	90.00
V, Å^3	1824.8(13)
Z	4
d_{calc}/g·cm^{-3}	1.206
μ/mm^{-1}	0.597
F(000)	704
Crystal size/mm	0.45x0.18x0.03
2θ-Scan range/deg	3.201-65.46
Completeness based on $2\theta_{max}$	0.982
Completeness based on 2θ= 52^o	0.982
hkl ranges	-7 < h < 7 -32 < k < 31 -13 < l < 13
Total number of reflections	16506
Number of independent reflections	3134
Number of reflections with $I > 2\sigma(I)$	2442
Number of refined parameters	248
Absorption correction	multi-scan
GOOF (based on F^2)	1.003
R factors (based on reflections with $I > 2\sigma(I)$)	
R_1	0.0434
wR_2	0.0895
R factors (based on all reflections)	
R_1	0.0696
wR_2	0.0922
$\Delta\rho_{max}$/ $\Delta\rho_{min}$, eÅ^{-3}	0.158 /-0.162

Crystallographic data (excluding structure factors) for the structure **3e** in this paper has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication nos. CCDC 1567078. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44 (0)1223 336033 or e-mail: deposit@ccdc.cam.ac.uk).

References

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2. R. C. Clark, J. S. Reid, *Acta Crystallogr., Sect. A: Found. Crystallogr.,* 1995, **51**, 887−897.

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