Supporting Information

***Bioorg. Med. Chem. Rep.* 4:1 (2021) 1-9**

Antibacterial activity of some 1,2,3,4-tetrasubstituted pyrrole derivatives and molecular docking studies

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Table of Contents	Page

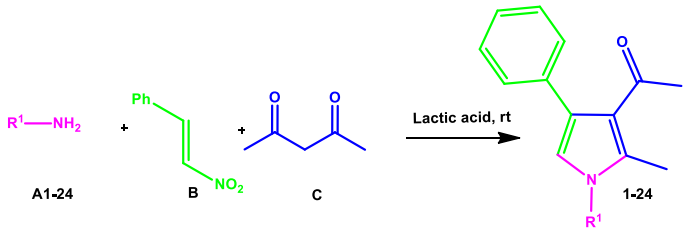
Chemistry experimental procedure:

General. Unless noted otherwise, all compounds were used as provided without further purification. Chemical names were generated using Cambridgesoft ChemBioDraw Ultra 10.0. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ

scale. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ or $DMSO_4$-d_6 [using the solvent peak as internal reference ($CDCl_3$: δ H 7.24; δ C 77.23, $DMSO_4$-d_6 : δ H 2.50; δ C 39.51) on a Bruker 300 MHz Ultrashield TM spectrometer operating at 300 MHz and 75 MHz, respectively or a Bruker Avance III 400 MHz spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constant quoted in Hz. IR spectra were recorded on a Perkin-Elmer 55148 spectrometer. Melting points were determined using an Electrothermal 9100 instrument. Elemental analyses were measured on a Thermo Flash 2000 Organic Elemental Analyzer.

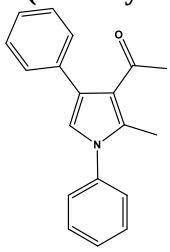
General procedure for preparation of compounds 1-24[8]

A mixture of primary amines **A1-24** (5 mmol), trans-β-nitrostyrene **B** (5 mmol) and acetylacetone **C** (5 mmol) in 5 mL lactic acid was stirred at room temperature for 1-6 h. After completion of reaction, as indicated by thin-layer chromatography (TLC; petroleum ether:ethylacetate is 4:1), the crude product was precipitated by adding a minimum amount of water. The solid was recrystallized in aqueous ethanol to afford the pure products **1-24**.



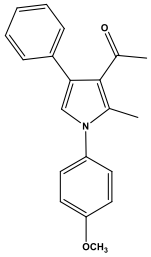
R[1]: C_6H_5, 4-OCH_3-C_6H_4, 4-OH-C_6H_4, 4-COOH-C_6H_4, 4-OC_2H_5-C_6H_4, 4-NO_2-C_6H_4, 4-CH_3-C_6H_4, 4-F-C_6H_4, 4-Cl-C_6H_4, 4-Br-C_6H_4, 3-NO_2-C_6H_4, 3-CF_3-C_6H_4, 3-Cl-C_6H_4, 3-F-C_6H_4, 3-Br-C_6H_4, 2-OH-C_6H_4, 2-CH_3-C_6H_4, 2-F-C_6H_4, C_6H_5-CH_2, 4-CH_3-C_6H_4-CH_2, 4-OCH_3-C_6H_4-CH_2, cyclohexyl, 2-furfuryl, 2-naphthyl

1-(2-methyl-1,4-diphenyl-1*H*-pyrrol-3-yl)ethanone (1)[1]



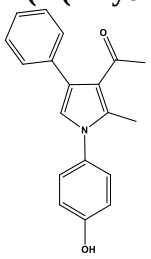
Light brown solid; yield 99%; m.p: 105-106 °C; ^{1}H NMR (300 MHz, $CDCl_3$)δ: 7.48-7.30 (m, 10H, Ar-H), 6.66 (s, 1H, Ar-H), 2.41 (s, 3H, -$COCH_3$), 2.08 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $CDCl_3$)δ: 197.64, 138.79, 136.06, 135.31, 129.38, 129.36, 128.31, 128.14, 126.85, 126.35, 126.27, 122.62, 120.64, 31.14, 12.94; IR (υ_{max}, cm^{-1}): 3120-3058, 2910, 1640, 1596, 1375; Anal. Calcd. for $C_{19}H_{17}NO$: C, 82.88; H, 6.22; N, 5.09. Found: C, 82.99; H, 6.19; N, 5.05.

1-(1-(4-methoxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (2)[1]



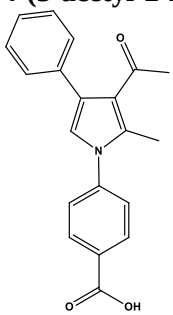
Light brown solid; yield 99%; m.p: 92-93ºC; ^{1}H NMR (300 MHz, $DMSO_4$-d_6) δ:7.41-7.34 (m, 7 H, Ar-H), 7.08 (d, *J*=9 Hz, 2H, Ar-H), 6.90 (s, 1H, Ar-H), 3.82 (s, 3H, -OCH_3), 2.89 (s, 3H, -$COCH_3$), 2.01 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $DMSO_4$-d_6) δ: 195.58, 158.79, 137.72, 134.43, 131.00, 128.94, 128.20, 127.36, 126.49, 125.03, 121.60, 121.05, 114.51, 55.45, 30.79, 12.52; IR (υ_{max}, cm^{-1}): 3106, 2958-2931-2828, 1651, 1514, 1387, 1247, 1035, 773; Anal. Calcd. for $C_{20}H_{19}NO_2$: C, 78.66; H, 6.27; N, 4.59. Found: C, 78.78; H, 6.24; N, 4.55.

1-(1-(4-hydroxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (3)[2]



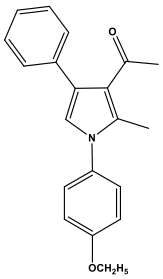
Pale pink solid; yield 75%; m.p: 162-163ºC; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 7.38-7.35 (m, 4 H, Ar-H), 7.33-7.29 (m, 1H, Ar-H), 7.15 (dd, J_1= 8.8 Hz, J_2=2.2 Hz, 2H, Ar-H), 6.99 (dd, J_1= 8.8 Hz, J_2=2.2 Hz, 2H, Ar-H), 6.62 (s, 1H, Ar-H), 4.99 (s, 1H, -OH), 2.39 (s, 3H, -$COCH_3$), 2.12 (s, 3H, -CH_3); ^{13}C NMR (100 MHz, $CDCl_3$)δ: 198.85, 156.61, 136.54, 136.03, 130.94, 129.42, 128.32, 127.57, 126.90, 126.29, 121.86, 121.36, 116.16, 30.92, 13.05; IR (υ_{max}, cm^{-1}): 3123, 3029, 2811, 1624, 1494, 1388, 1223; Anal. Calcd. for $C_{19}H_{17}NO_2$: C, 78.33; H, 5.88; N, 4.81. Found: C, 78.44; H, 5.84; N, 4.78.

4-(3-acetyl-2-methyl-4-phenyl-1*H*-pyrrol-1-yl)benzoic acid (4)[8]



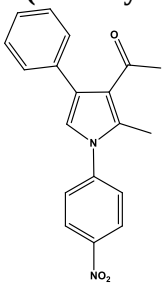
Light brown solid; yield 52%; m.p: decomposed; ^{1}H NMR (300 MHz, $DMSO_4$-d_6)δ: 13.09 (s, 1H,-COOH), 8.09 (d, *J*= 8.4 Hz, 2H, Ar-H), 7.86 (dd, J_1= 8.4 Hz, $J_{2=}$ 1.5 Hz, 1H, Ar-H), 7.63 (d, *J*= 8.4 Hz, 2H, Ar-H), 7.40-7.33 (m, 4H, Ar-H), 7.06 (s, 1H, Ar-H), 2.36 (s, 3H, -$COCH_3$), 2.02 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $DMSO_4$-d_6)δ: 195.84, 166.56, 141.71, 138.04, 135.35, 130.49, 129.15, 128.88, 128.27, 126.68, 125.89, 125.72, 122.65, 120.68, 30.87, 12.70; IR (υ_{max}, cm^{-1}): 3129-2539, 3129, 2990-2880, 1685, 1605, 1352; Anal. Calcd. for $C_{20}H_{17}NO_3$: C, 75.21; H, 5.37; N, 4.39. Found: C, 75.33; H, 5.33; N, 4.36.

1-(1-(4-ethoxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (5)[1]



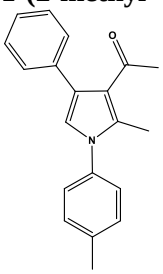
White solid; yield 97%; **m.p:** 89-90°C; **^{1}H NMR** (300 MHz, $DMSO_4$-d_6)δ: 7.39-7.30 (m, 7 H, Ar-H), 7.06 (d, *J*= 9 Hz, 2H, Ar-H), 6.89 (s, 1H, Ar-H), 4.08 (q, *J*= 6.9 Hz, 2H, -CH_2-), 2.28 (s, 3H, -$COCH_3$), 2.00 (s, 3H, -CH_3), 1.36 (t, J=6.9 Hz, 3H, -CH_3); **^{13}C NMR** (75 MHz, $DMSO_4$-d_6)δ: 195.57, 158.01, 135.72, 134.43, 130.85, 128.94, 128.20, 127.35, 126.48, 125.01, 121.58, 121.04, 114.91, 63.42, 30.79, 14.60, 12.52; **IR** (υ_{max}, cm^{-1}): 3115, 2980-2926, 1648, 1500, 1389, 1250, 1042, 768; **Anal. Calcd.** for $C_{21}H_{21}NO_2$: C, 78.96; H, 6.63; N, 4.39. Found: C, 79.07; H, 6.59; N, 4.36.

1-(2-methyl-1-(4-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone (6)[1]



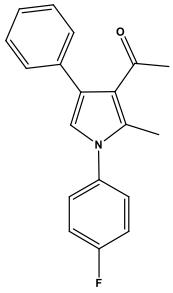
Yellow solid; yield 99%; m.p:171-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.38 (dd, J_1= 8.8 Hz, $J_{2=}$ 2 Hz, 2H, Ar-H), 7.54 (d, *J*= 8.8 Hz, 2H, Ar-H), 7.40-7.36 (m, 5H, Ar-H), 6.73 (s, 1H, Ar-H), 2.47 (s, 3H, -$COCH_3$), 2.09 (s, 3H, -CH_3); ^{13}C NMR (100 MHz, $CDCl_3$)δ: 197.87, 151.17, 139.45, 139.39, 136.19, 135.25, 134.76, 129.64, 129.24, 126.32, 126.21, 125.03, 112.55, 31.20, 13.12; IR (υ_{max}, cm^{-1}): 3111-3083-3029, 2914, 1645, 1497, 1342, 853, 1519, 1342; Anal. Calcd. for $C_{19}H_{16}N_2O_3$: C, 71.25; H, 5.03; N, 8.74. Found: C, 71.37; H, 4.99; N, 8.71.

1-(2-methyl-4-phenyl-1-(p-tolyl)-1*H*-pyrrol-3-yl)ethanone (7)[1]



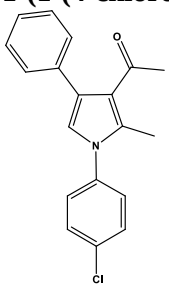
White solid; yield 92%; m.p: 109-110°C; ^{1}H NMR (300 MHz, $DMSO_4$-d_6)δ: 7.42-7.30 (m, 9H, Ar-H), 6.92 (s, 1H, Ar-H), 2.38 (s, 3H, -$COCH_3$), 2.31 (s, 3H, -CH_3), 2.01 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $DMSO_4$-d_6)δ: 195.62, 137.60, 135.67, 134.17, 129.87, 128.94, 128.21, 126.52, 125.81, 125.20, 121.84, 120.85, 30.81, 20.58, 11.95; IR (υ_{max}, cm^{-1}): 3106-3070-3028, 2919, 1638, 1501, 1387; Anal. Calcd. for $C_{20}H_{19}NO$: C, 83.01; H, 6.62; N, 4.84. Found: C, 83.12; H, 6.58; N, 4.81.

1-(1-(4-fluorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (8)[1]



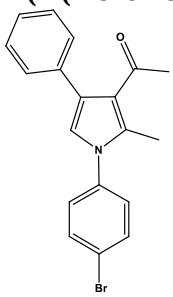
Light brown solid; yield 99%; m.p: 128-129ºC; ^{1}H NMR (300 MHz, $DMSO_4$-d_6)δ: 7.58-7.53 (m, 2H, Ar-H), 7.42-7.31 (m, 7H, Ar-H), 6.97 (s, 1H, Ar-H), 2.30 (s, 3H, -$COCH_3$), 2.01(s, 3H, -CH_3); ^{13}C NMR (75 MHz, $DMSO_4$-d_6)δ: 195.70, 159.73, 135.53, 134.29, 128.91, 128.35, 128.24, 126.58, 125.24, 121.92, 121.01, 116.40, 116.10, 30.82, 12.47; IR (υ_{max}, cm^{-1}): 3111-3074, 2984, 1646, 1504, 1388, 1218; Anal. Calcd. for $C_{19}H_{16}FNO$: C, 77.80; H, 5.50; F, 6.48; N, 4.77. Found: C, 77.97; H, 5.46; F, 6.43; N, 4.73.

1-(1-(4-chlorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (9)[1]



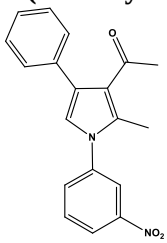
Yellow solid; yield 99%; m.p: 127-128 ºC; ^{1}H NMR (300 MHz, $CDCl_3$)δ: 7.47-7.26 (m, 9H, Ar-H), 6.64 (s, 1H, Ar-H), 2.40 (s, 3H, -$COCH_3$), 2.06 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $CDCl_3$)δ: 197.58, 137.29, 135.80, 135.15, 134.08, 129.62, 129.31, 128.35, 127.50, 126.98, 126.63, 122.90, 120.42, 31.13, 12.86; IR (υ_{max}, cm^{-1}): 3111-3081-3037, 2943, 1645, 1495, 1387, 1092; Anal. Calcd. for $C_{19}H_{16}ClNO$: C, 73.67; H, 5.21; Cl, 11.44; N, 4.52. Found: C, 73.84; H, 5.17; Cl, 11.39; N, 4.48.

1-(1-(4-bromophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (10)[1]



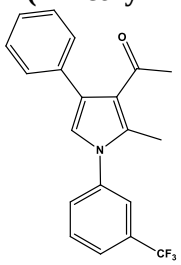
Light brown solid; yield 99%; m.p: 142-143ºC; ^{1}H NMR (300 MHz, $CDCl_3$)δ: 7.62 (dd, J_1= 8.7 Hz, J_2=2.1 Hz, 2H, Ar-H), 7.39-7.32 (m, 5H, Ar-H), 7.22 (dd, J_1= 8.7 Hz, J_2=2.1 Hz, 2H, Ar-H), 6.64 (s, 1H, Ar-H), 2.40 (s, 3H, -$COCH_3$), 2.07 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $CDCl_3$)δ: 197.67, 137.77, 135.76, 135.10, 132.61, 129.30, 128.37, 127.80, 126.99, 126.67, 122.93, 122.01, 120.35, 31.15, 12.91; IR (υ_{max}, cm^{-1}): 3078, 2922, 1658, 1492, 1322, 1068; Anal. Calcd. for $C_{19}H_{16}BrNO$: C, 64.42; H, 4.55; Br, 22.56; N, 3.95. Found: C, 64.59; H, 4.51; Br, 22.51; N, 3.91.

1-(2-methyl-1-(3-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone (11)[3]



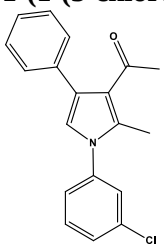
Yellow solid; yield 68%; m.p: 128-129°C; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.32-8.29 (m, 1H, Ar-H), 8.26-8.25 (m, 1H, Ar-H), 7.72-7.71 (m, 2H, Ar-H), 7.41-7.34 (m, 5 H, Ar-H), 6.72 (s, 1H, Ar-H), 2.45 (s, 3H, -$COCH_3$), 2.08 (s, 3H, -CH_3); ^{13}C NMR (100 MHz, $CDCl_3$)δ: 197.57, 148.82, 139.89, 135.39, 134.84, 131.98, 130.39, 129.28, 128.43, 127.30, 127.20, 123.60, 122.84, 121.26, 120.16, 31.13, 12.85; IR (υ_{max}, cm^{-1}): 3113-3088-3024, 2926-2872, 1650, 1529, 1506, 1343, 872; Anal. Calcd. for $C_{19}H_{16}N_2O_3$: C, 71.25; H, 5.03; N, 8.74. Found: C, 71.36; H, 4.99; N, 8.71.

1-(2-methyl-4-phenyl-1-(3-(trifluoromethyl)phenyl)-1*H*-pyrrol-3-yl)ethanone (12)[8]



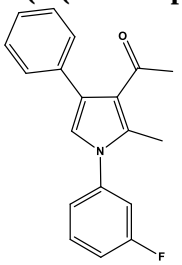
Orange solid; yield 99%; m.p: 146-147°C; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 7.70 (d, *J*= 7.6 Hz, 1H, Ar-H), 7.66-7.62 (m, 2H, Ar-H), 7.56 (d, *J*= 7.6 Hz, 1H, Ar-H), 7.38-7.31 (m, 6H, Ar-H), 6.69 (s, 1H, Ar-H), 2.42 (s, 3H, -$COCH_3$), 2.08 (s, 3H, -CH_3); ^{13}C NMR (100 MHz, $CDCl_3$)δ: 197.63, 139.36, 135.64, 135.03, 130.10, 129.55, 129.31, 128.37, 127.07, 126.95, 124.92, 124.88, 123.24, 123.21, 120.35, 31.11, 12.80; IR (υ_{max}, cm^{-1}): 3086-3066-3029, 2930, 1667, 1516, 1335, 1126; Anal. Calcd. for $C_{20}H_{16}F_3NO$: C, 69.96; H, 4.70; F, 16.60, N, 4.08. Found: C, 70.13; H, 4.66; F, 16.55; N, 4.04.

1-(1-(3-chlorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (13)[4]



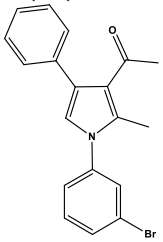
White solid; yield 93%; m.p: 88-89°C; ^{1}H NMR (300 MHz, $DMSO_4$-d_6)δ: 7.67-7.31 (m, 9H, Ar-H), 7.04 (s, 1H, Ar-H), 2.34 (s, 3H, -$COCH_3$), 2.02 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $DMSO_4$-d_6)δ: 195.78, 139.45, 135.40, 134.09, 133.68, 130.96, 128.88, 128.25, 128.05, 126.62, 125.97, 125.46, 124.86, 122.30, 120.88, 30.85, 12.54; IR (υ_{max}, cm^{-1}): 3098-3074, 2951, 1648, 1500, 1393, 1228; Anal. Calcd. for $C_{19}H_{16}ClNO$: C, 73.67; H, 5.21; Cl, 11.44; N, 4.52. Found: C, 73.84; H, 5.17; Cl, 11.39; N, 4.48.

1-(1-(3-fluorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (14)[1]



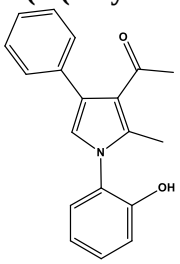
Light brown solid; yield 92%; m.p: 81-82°C; ^{1}H NMR (300 MHz, $DMSO_4$-d_6)δ: 7.67-7.31 (m, 9H, Ar-H), 7.04 (s, 1H, Ar-H), 2.34 (s, 3H, -$COCH_3$), 2.02 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $DMSO_4$-d_6)δ: 195.79, 163.72, 139.69, 135.41, 134.06, 131.14, 128.89, 128.26, 126.63, 125.45, 120.84, 115.09, 114.81, 113.66, 113.35, 30.84, 12.55; IR (υ_{max}, cm^{-1}): 3115-3082, 2974, 1644, 1493, 1354, 1246; Anal. Calcd. for $C_{19}H_{16}FNO$: C, 77.80; H, 5.50; F, 6.48; N, 4.77. Found: C, 77.97; H, 5.46; F, 6.43; N, 4.73.

1-(1-(3-bromophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (15)[3]



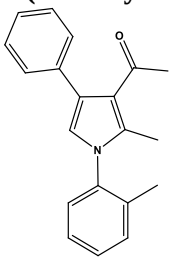
Light brown solid; yield 97%; m.p: 103-104°C; ^{1}H NMR (300 MHz, $CDCl_3$)δ: 7.58-7.52 (m, 2H, Ar-H), 7.39-7.26 (m, 7H, Ar-H), 6.65 (s, 1H, Ar-H), 2.41 (s, 3H, -$COCH_3$), 2.07 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $CDCl_3$)δ: 197.69, 139.96, 135.71, 135.13, 131.29, 130.63, 129.42, 129.30, 128.37, 127.01, 126.70, 124.95, 122.95, 122.82, 120.39, 31.17, 12.93; IR (υ_{max}, cm^{-1}): 3090-3061, 2967, 1647, 1498, 1351, 1065; Anal. Calcd. for $C_{19}H_{16}BrNO$: C, 64.42; H, 4.55; Br, 22.56; N, 3.95. Found: C, 64.59; H, 4.51; Br, 22.51; N, 3.91.

1-(1-(2-hydroxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (16)[8]



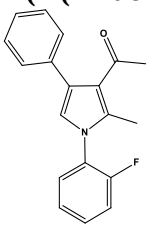
White solid; yield 83%; m.p: 148-149°C; ^{1}H NMR (300 MHz, $CDCl_3$)δ: 7.35-7.25 (m, 6H, Ar-H), 7.20-7.17 (m, 1H, Ar-H), 7.13-7.10 (m, 1H, Ar-H), 7.00-6.94 (m, 1H, Ar-H), 6.58 (s, 1H, Ar-H), 5.22 (s, 1H, -OH), 2.31 (s, 3H, -$COCH_3$), 2.08 (s, 3H,-CH_3); ^{13}C NMR (75 MHz, $CDCl_3$)δ: 198.88, 152.09, 137.56, 135.80, 130.34, 129.37, 128.43, 128.30, 126.88, 126.78, 125.48, 122.00, 120.92, 120.52, 117.05, 30.95, 12.49; IR (υ_{max}, cm^{-1}): 3135, 3053-3024, 2963, 1623, 1506, 1378, 1240; Anal. Calcd. for $C_{19}H_{17}NO_2$: C, 78.33; H, 5.88; N, 4.81. Found: C, 78.44; H, 5.84; N, 4.78.

1-(2-methyl-4-phenyl-1-(o-tolyl)-1*H*-pyrrol-3-yl)ethanone (17)[5]



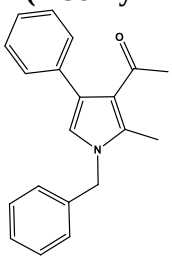
Pale pink solid; yield 95%; m.p: 89-90°C; ^{1}H NMR (300 MHz, $CDCl_3$)δ: 6.24-6.06 (m, 9H, Ar-H), 5.36 (s, 1H, Ar-H), 1.07 (s, 3H, -CH_3), 0.92 (s, 3H, -$COCH_3$), 0.91 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $CDCl_3$)δ: 197.54, 137.78, 136.25, 136.12, 135.86, 131.01, 129.46, 129.07, 128.26, 127.95, 126.81, 126.76, 126.19, 121.60, 120.28, 31.12, 17.38, 12.35; IR (υ_{max}, cm^{-1}): 3131-3057, 2916, 1641, 1496, 1387; Anal. Calcd. for $C_{20}H_{19}NO$: C, 83.01; H, 6.62; N, 4.84. Found: C, 83.12; H, 6.58; N, 4.81.

1-(1-(2-fluorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (18)[8]



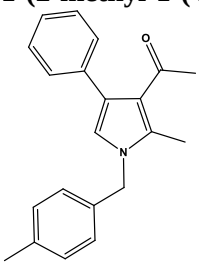
Light brown solid; yield 94%; m.p: 122-123°C; ^{1}H NMR (300 MHz, $DMSO_4$-d_6)δ: 7.62-7.31 (m, 9H, Ar-H), 6.96 (s, 1H, Ar-H), 2.23 (s, 3H, -$COCH_3$), 2.03 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $DMSO_4$-d_6)δ: 195.60, 158.15, 135.38, 135.12, 130.93, 130.83, 129.45, 128.96, 128.24, 126.64, 125.44, 121.68, 121.24, 116.87, 116.61, 30.80, 11.95; IR (υ_{max}, cm^{-1}): 3115, 2922, 1638, 1508, 1385, 1246; Anal. Calcd. for $C_{19}H_{16}FNO$: C, 77.80; H, 5.50; F, 6.48; N, 4.77. Found: C, 77.97; H, 5.46; F, 6.43; N, 4.73.

1-(1-benzyl-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (19)[4]



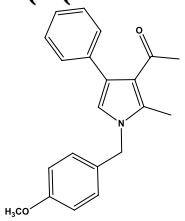
White solid; yield 97%; m.p: 87-88 °C; ^{1}H NMR (300 MHz, $CDCl_3$)δ: 7.38-7.24 (m, 8H, Ar-H), 7.08 (d, *J*= 6.9 Hz, 2H, Ar-H), 6.53 (s, 1H, Ar-H), 5.05 (s, 2H, -CH_2-), 2.43 (s, 3H, -$COCH_3$), 2.03 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $CDCl_3$)δ: 197.56, 136.61, 136.34, 135.14, 129.39, 128.97, 128.23, 127.87, 126.72, 126.70, 125.93, 122.11, 120.14, 50.34, 31.12, 11.60; IR (υ_{max}, cm^{-1}): 3115-3021, 2922, 1641, 1603, 1356; Anal. Calcd. for $C_{20}H_{19}NO$: C, 83.01; H, 6.62; N, 4.84. Found: C, 83.12; H, 6.58; N, 4.81.

1-(2-methyl-1-(4-methylbenzyl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone (20)[6]



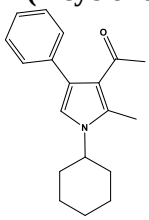
Orange solid; yield 68%; m.p: 102-103°C; ^{1}H NMR (300 MHz, $DMSO_4$-d_6)δ: 7.36-7.09 (m, 9H, Ar-H), 6.88 (s, 1H, Ar-H), 5.12 (s, 2H, -CH_2-), 2.33 (s, 3H, -$COCH_3$), 2.28 (s, 3H, -CH_3), 1.94 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $DMSO_4$-d_6)δ: 195.34, 136.68, 136.12, 134.37, 134.22, 129.25, 128.92, 128.14, 126.98, 126.30, 124.44, 121.10, 120.73, 49.20, 30.75, 20.65, 11.37; IR (υ_{max}, cm^{-1}): 3115-3033, 2942-2914, 1636, 1507, 1345; Anal. Calcd. for $C_{21}H_{21}NO$: C, 83.13; H, 6.98; N, 4.62. Found: C, 83.24; H, 7.02; N, 4.59.

1-(1-(4-methoxybenzyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (21)[7]



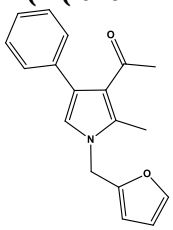
Light orange solid; yield 63%; m.p: 80-81°C; ^{1}H NMR (300 MHz, $DMSO_4$-d_6)δ: 7.36-7.26 (m, 5H, Ar-H), 7.15 (d, *J*= 8.7 Hz, 2H, Ar-H), 6.93 (d, *J*= 8.7 Hz, 2H, Ar-H), 6.88 (s, 1H), 5.09 (s, 2H, -CH_2-), 3.73 (s, 3H, -OCH_3), 2.34 (s, 3H, -$COCH_3$), 1.94 (s, 3H, -CH_3); ^{13}C NMR (75 MHz, $DMSO_4$-d_6)δ: 195.35, 158.62, 136.14, 134.14, 129.23, 128.91, 128.51, 128.14, 126.30, 124.42, 121.09, 120.59, 114.08, 55.06, 48.89, 30.74, 11.39; IR (υ_{max}, cm^{-1}): 3049, 2935-2906, 1636, 1513, 1350, 1251, 1029, 753; Anal. Calcd. for $C_{21}H_{21}NO_2$: C, 78.96; H, 6.63; N, 4.39. Found: C, 79.07; H, 6.59; N, 4.36.

1-(1-cyclohexyl-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (22)[7]



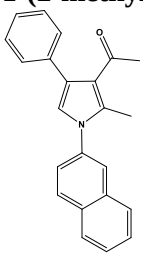
White solid; yield 61%; m.p: 151-152°C; ^{1}H NMR (300 MHz, $CDCl_3$)δ: 7.36-7.26 (m, 5H, Ar-H), 6.59 (s, 1H, Ar-H), 3.90 (tt, J_1= 11.7 Hz, J_2=3.6 Hz, 1H, cyclohexyl-H), 2.50 (s, 3H, -$COCH_3$), 2.02 (s, 3H, -CH_3), 1.94-1,24 (m, 10H, cyclohexyl-H); ^{13}C NMR (75 MHz, $CDCl_3$)δ: 197.81, 136.77, 134.16, 129.3, 128.2, 127.96, 126.50, 121.34, 115.77, 55.06, 33.94, 31.14, 30.49, 29.60, 25.84, 25.39, 11.33; IR (υ_{max}, cm^{-1}): 3045, 2929-2856, 1643, 1513, 1353; Anal. Calcd. for $C_{19}H_{23}NO$: C, 81.09; H, 8.24; N, 4.98. Found: C, 81.20; H, 8.20; N, 4.95.

1-(1-(furan-2-ylmethyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (23)[4]



White solid; yield 75%; m.p: 74-75°C; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 7.39-7.26 (m, 6H, Ar-H), 6.54 (s, 1H, Ar-H), 6.34 (dd, J_1= 5.2 Hz, J_2= 2 Hz, 1H, Ar-H), 6.25 (d, *J*= 5.2 Hz, 1H, Ar-H), 4.98 (s, 2H, -CH_2-), 2.55 (s, 3H, -$COCH_3$), 2.01 (s, 3H, -CH_3); ^{13}C NMR (100 MHz, $CDCl_3$)δ: 197.55, 149.49, 142.97, 136.29, 134.86, 129.36, 128.20, 127.97, 126.69, 122.03, 119.55, 110.56, 108.64, 43.27, 31.02, 11.40; IR (υ_{max}, cm^{-1}): 3115-3086, 2958, 1637, 1500, 1346, 1224, 1071; Anal. Calcd. for $C_{18}H_{17}NO_2$: C, 77.41; H, 6.13; N, 5.01. Found: C, 77.52; H, 6.09; N, 4.98.

1-(2-methyl-1-(naphthalen-2-yl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone (24)



Brown solid; yield 88%; m.p: 143-144^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 7.96 (t, *J*= 8.2 Hz, 2H, Ar-H), 7.58-7.25 (m, 10H, Ar-H), 6.71 (s, 1H, Ar-H), 2.22 (s, 3H, -$COCH_3$), 2.15 (s, 3H, -CH_3); ^{13}C NMR (100 MHz, $CDCl_3$)δ: 197.76, 137.18, 136.16, 135.35, 134.19, 130.67, 129.48, 128.31, 127.63, 126.94, 126.84, 126.22, 125.35, 125.25, 122.93, 121.80, 31.14, 12.45; IR (υ_{max}, cm^{-1}): 3111-3070, 2975, 1645, 1506, 1374; Anal. Calcd. for $C_{23}H_{19}NO$: C, 84.89; H, 5.89; N, 4.30. Found: C, 85.00; H, 5.85; N, 4.27.

Copies of ^{1}H and ^{13}C NMR spectra of the all compounds

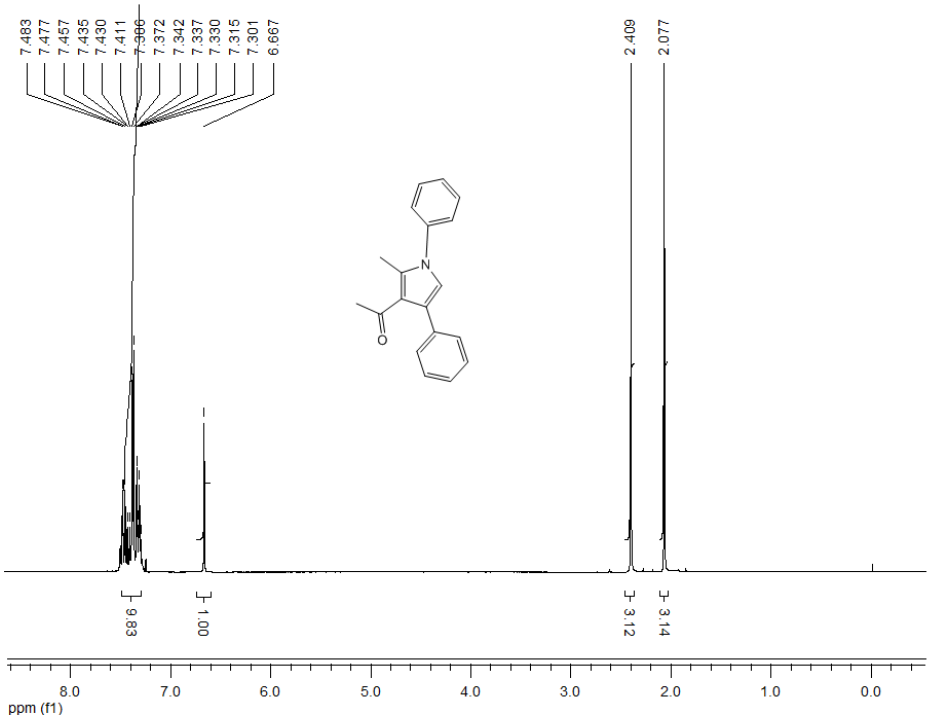


Figure S1: ^{1}H NMR spectrum of 1-(2-methyl-1,4-diphenyl-1*H*-pyrrol-3-yl)ethanone **(1)**

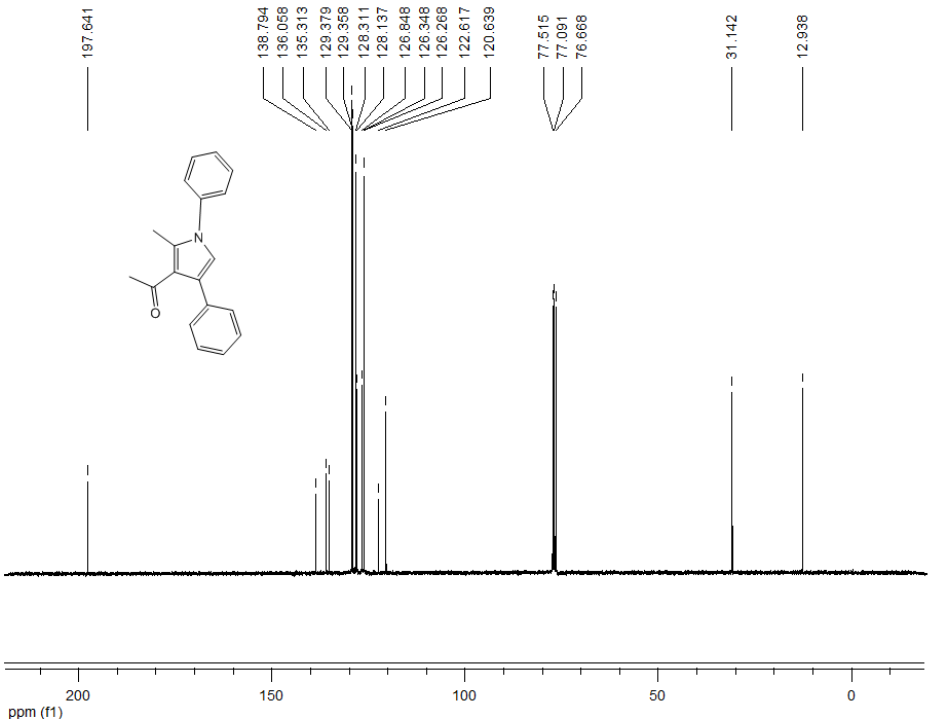


Figure S2: ^{13}C NMR spectrum of 1-(2-methyl-1,4-diphenyl-1*H*-pyrrol-3-yl)ethanone **(1)**

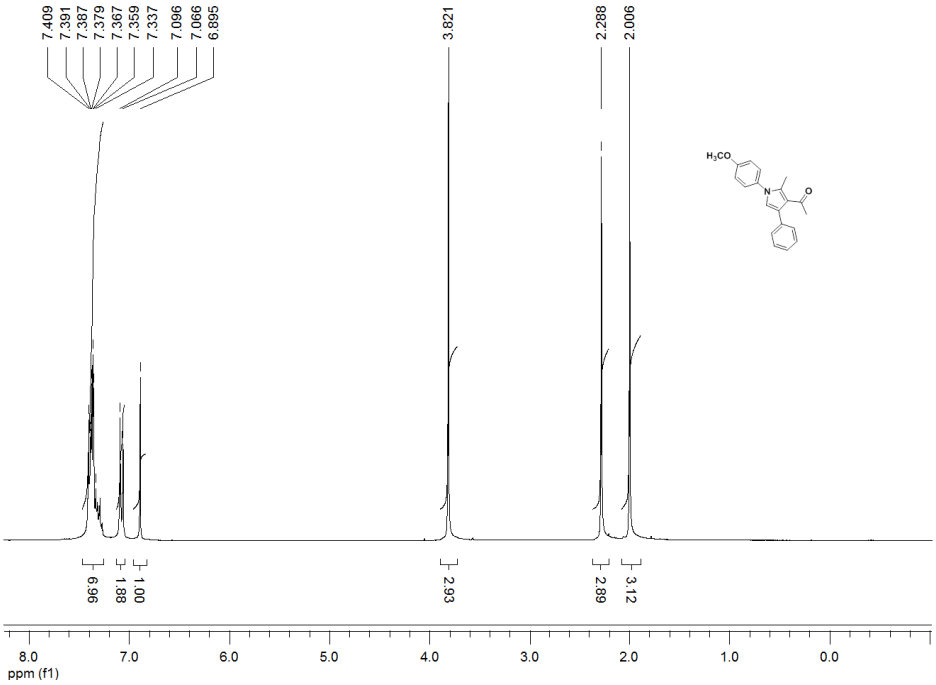


Figure S3: ^{1}H NMR spectrum of 1-(1-(4-methoxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(2)**

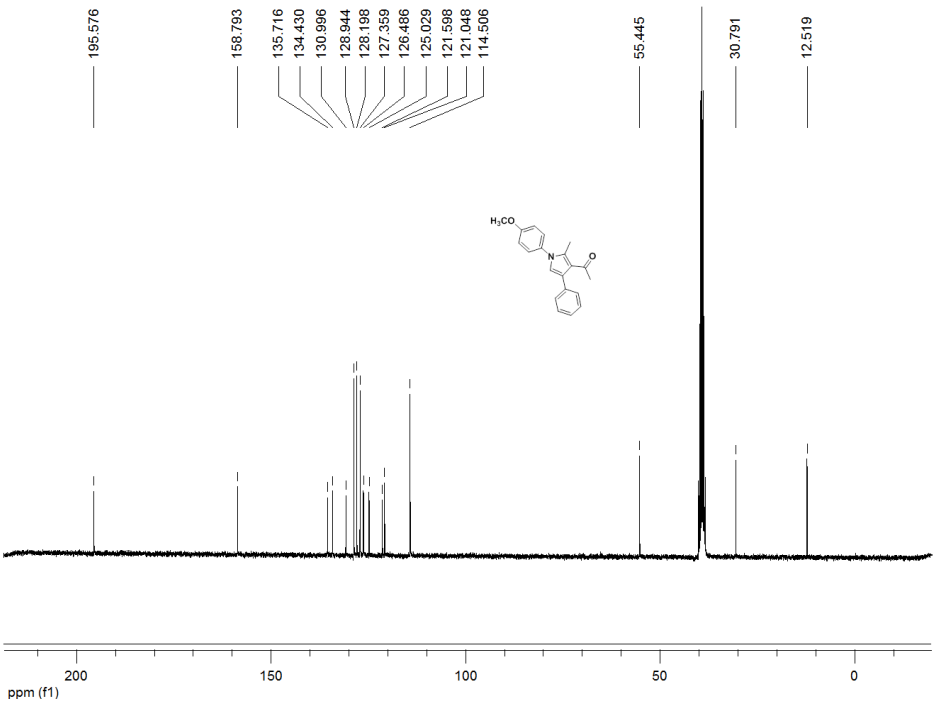


Figure S4: ^{13}C NMR spectrum of 1-(1-(4-methoxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(2)**

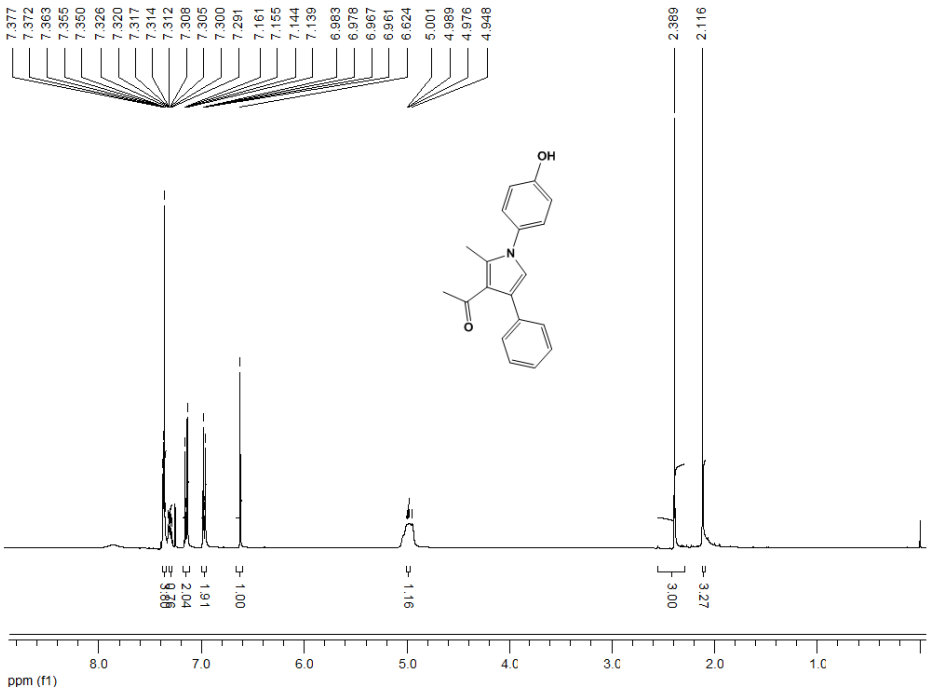


Figure S5: ^{1}H NMR spectrum of 1-(1-(4-hydroxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(3)**

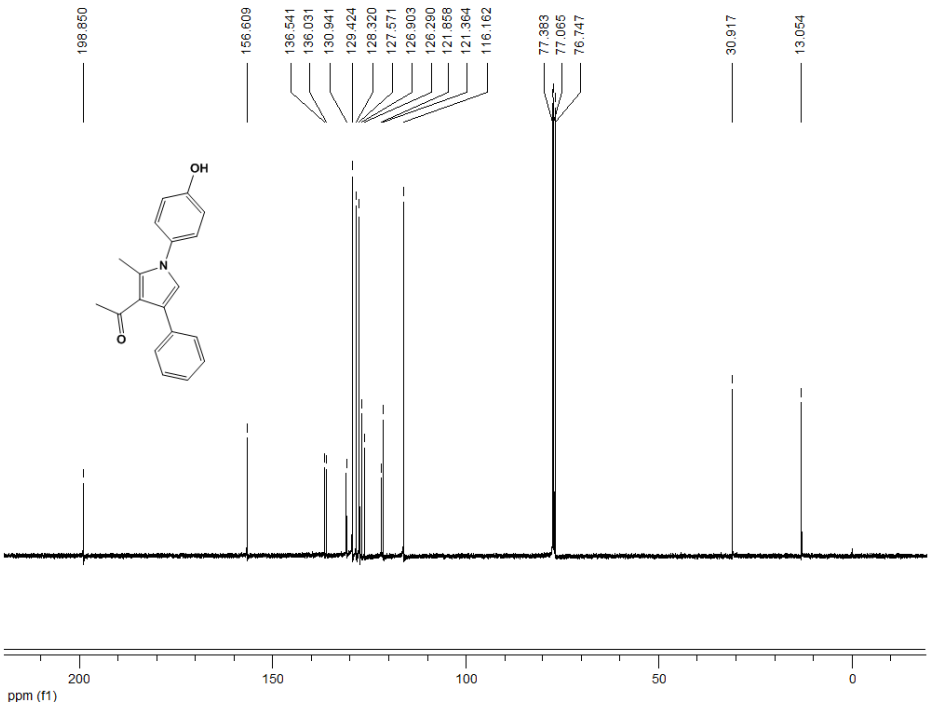


Figure S6: ^{13}C NMR spectrum of 1-(1-(4-hydroxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(3)**

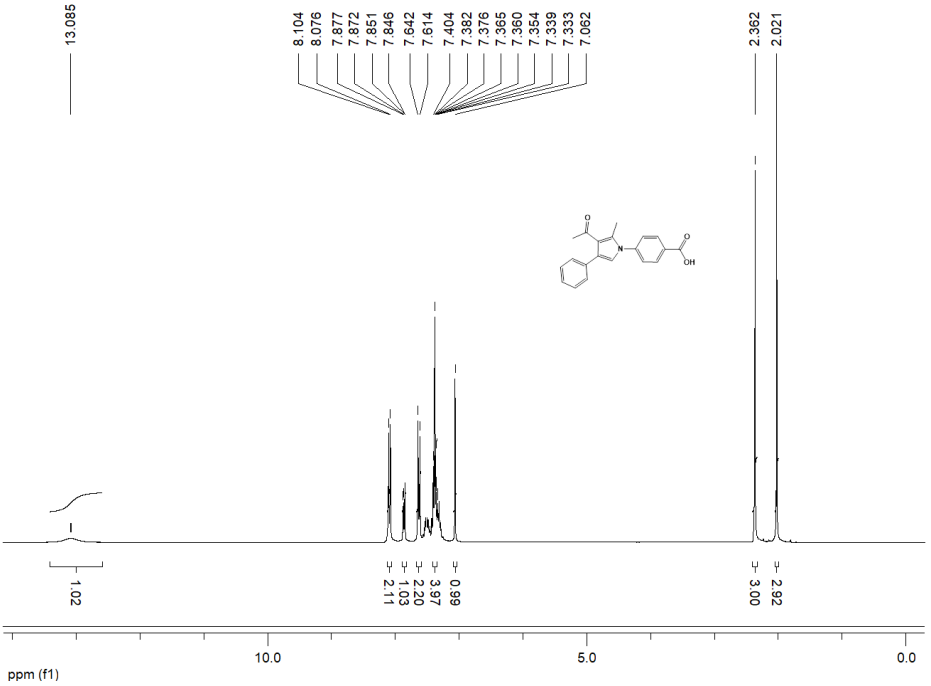


Figure S7: ^{1}H NMR spectrum of 4-(3-acetyl-2-methyl-4-phenyl-1*H*-pyrrol-1-yl)benzoic acid **(4)**

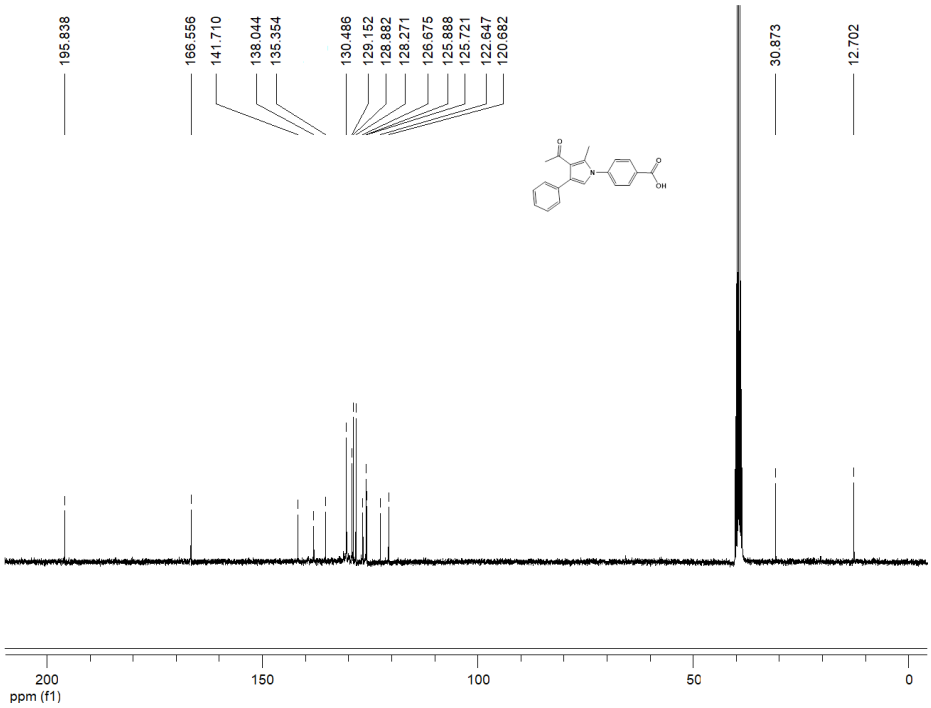


Figure S8: ^{13}C NMR spectrum of 4-(3-acetyl-2-methyl-4-phenyl-1*H*-pyrrol-1-yl)benzoic acid **(4)**

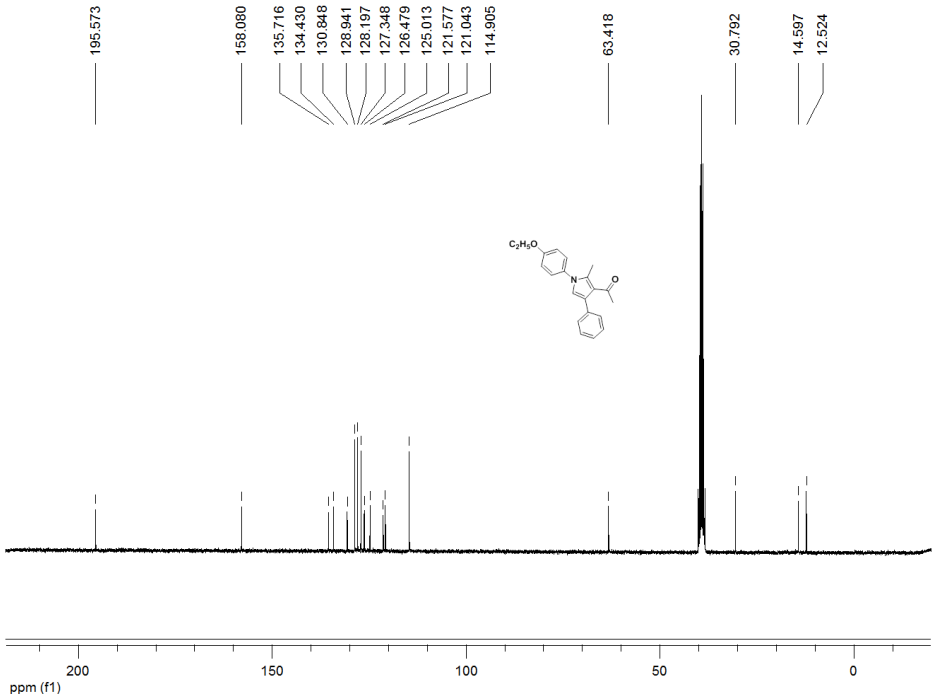


Figure S9: ^{1}H NMR spectrum of 1-(1-(4-ethoxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(5)**

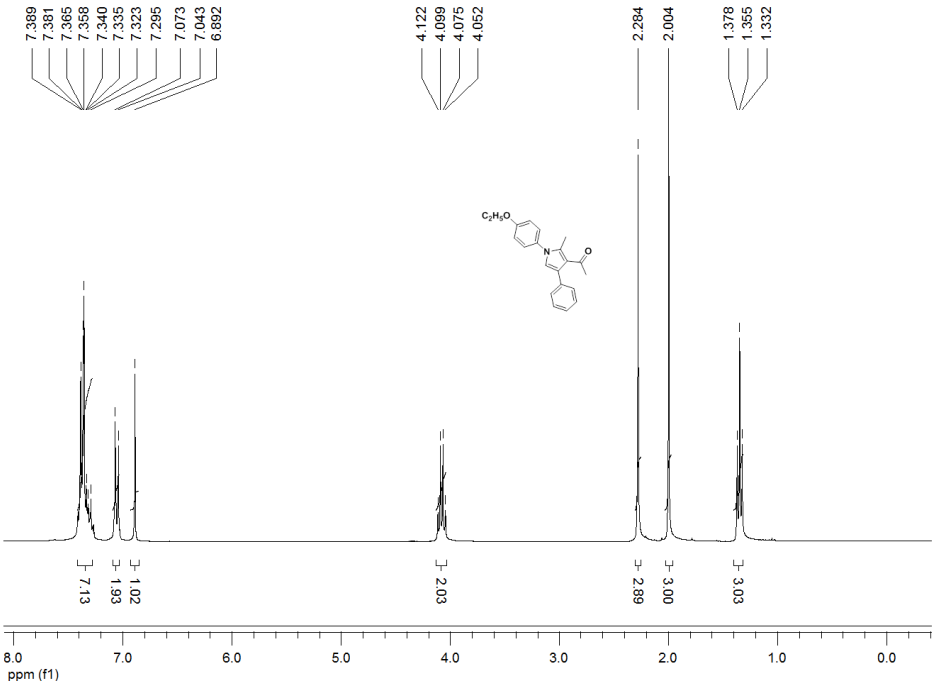


Figure S10: ^{13}C NMR spectrum of 1-(1-(4-ethoxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(5)**

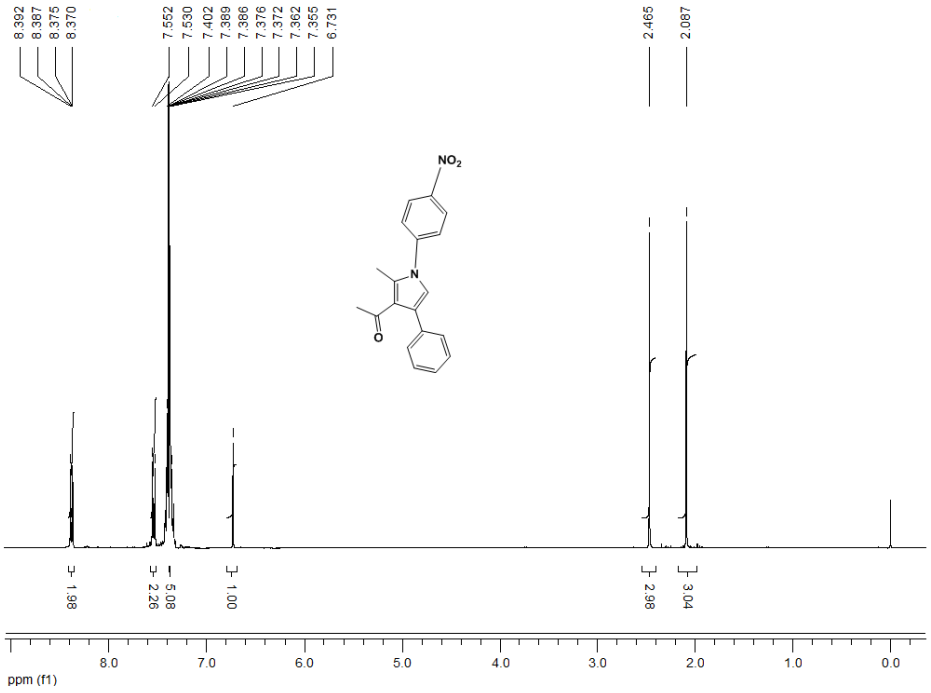


Figure S11: ^{1}H NMR spectrum of 1-(2-methyl-1-(4-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(6)**

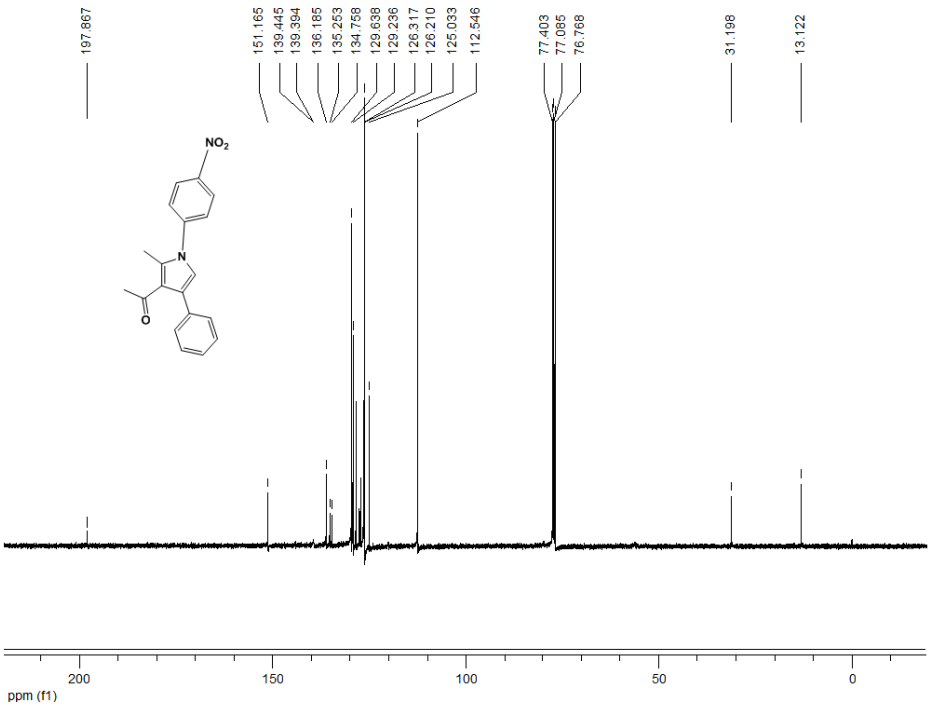


Figure S12: ^{13}C NMR spectrum of 1-(2-methyl-1-(4-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(6)**

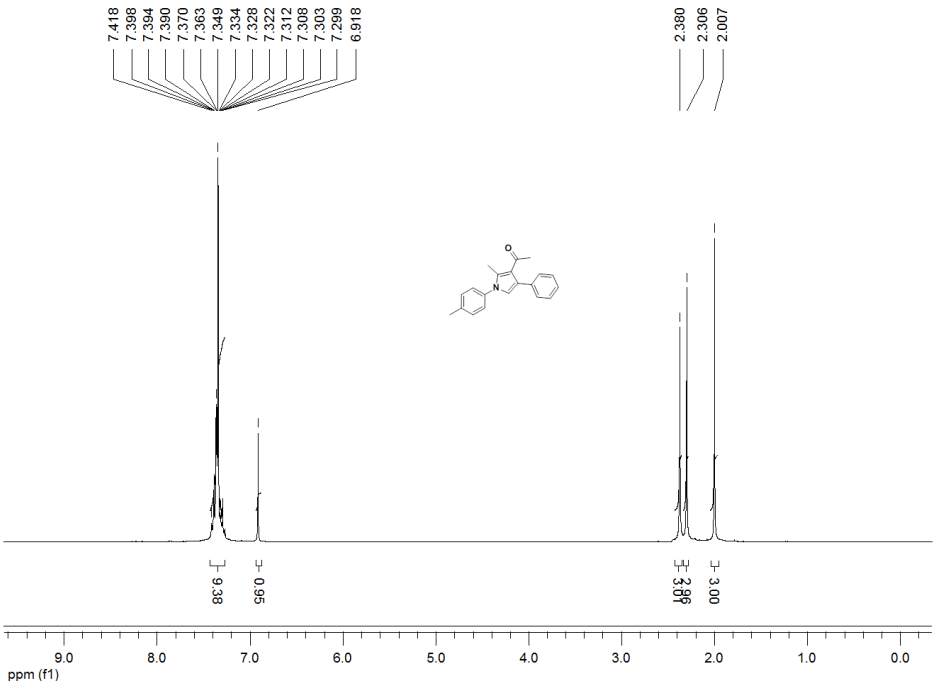


Figure S13: ^{1}H NMR spectrum of 1-(2-methyl-4-phenyl-1-(p-tolyl)-1*H*-pyrrol-3-yl)ethanone **(7)**

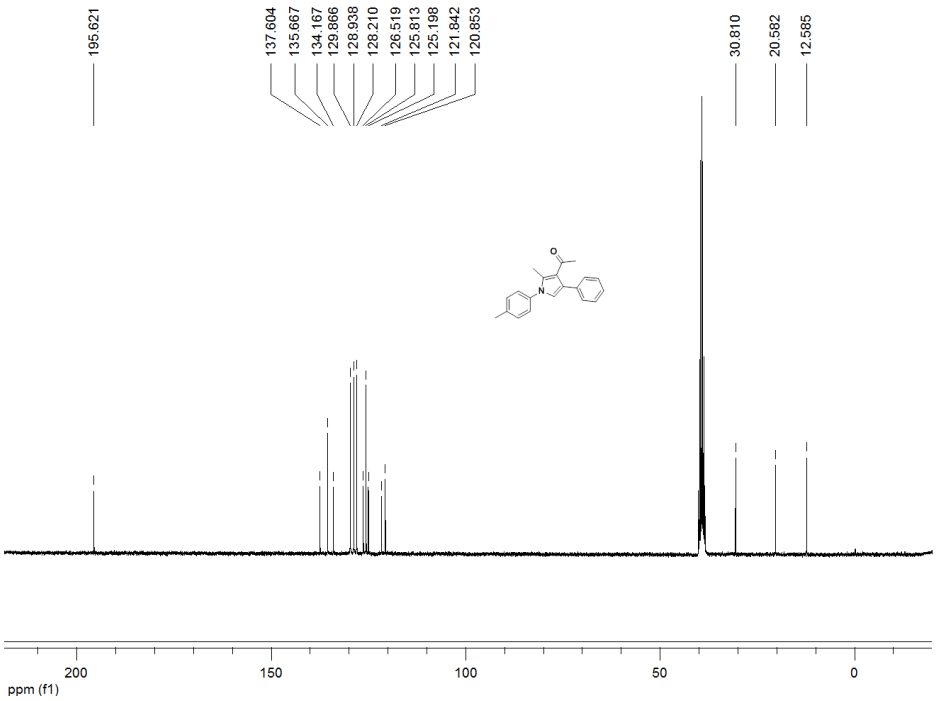


Figure S14: ^{13}C NMR spectrum of 1-(2-methyl-4-phenyl-1-(p-tolyl)-1*H*-pyrrol-3-yl)ethanone **(7)**

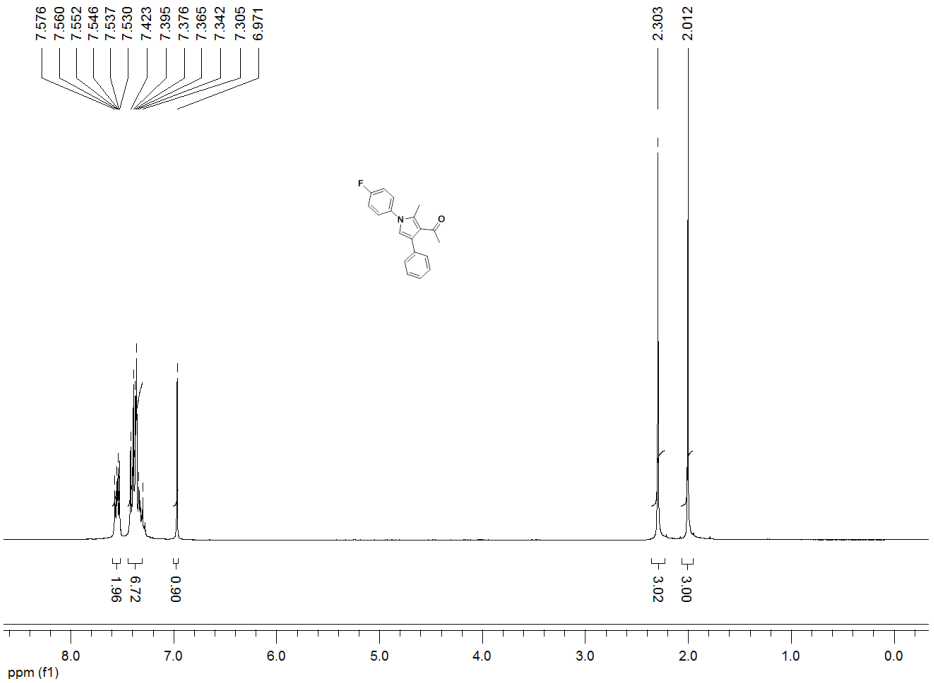


Figure S15: ^{1}H NMR spectrum of 1-(1-(4-fluorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(8)**

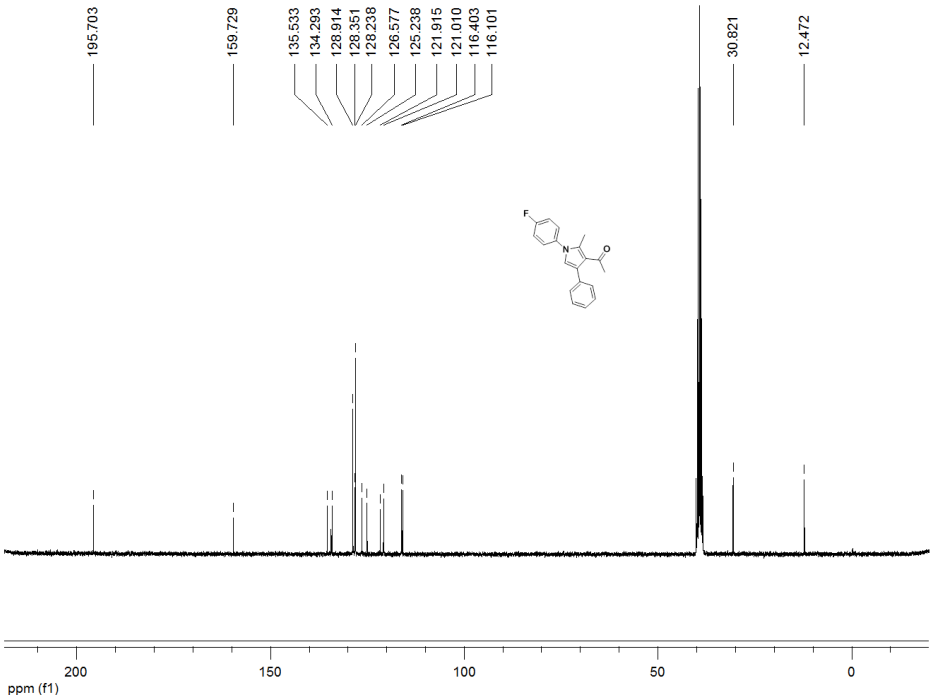


Figure S16: ^{13}C NMR spectrum of 1-(1-(4-fluorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(8)**

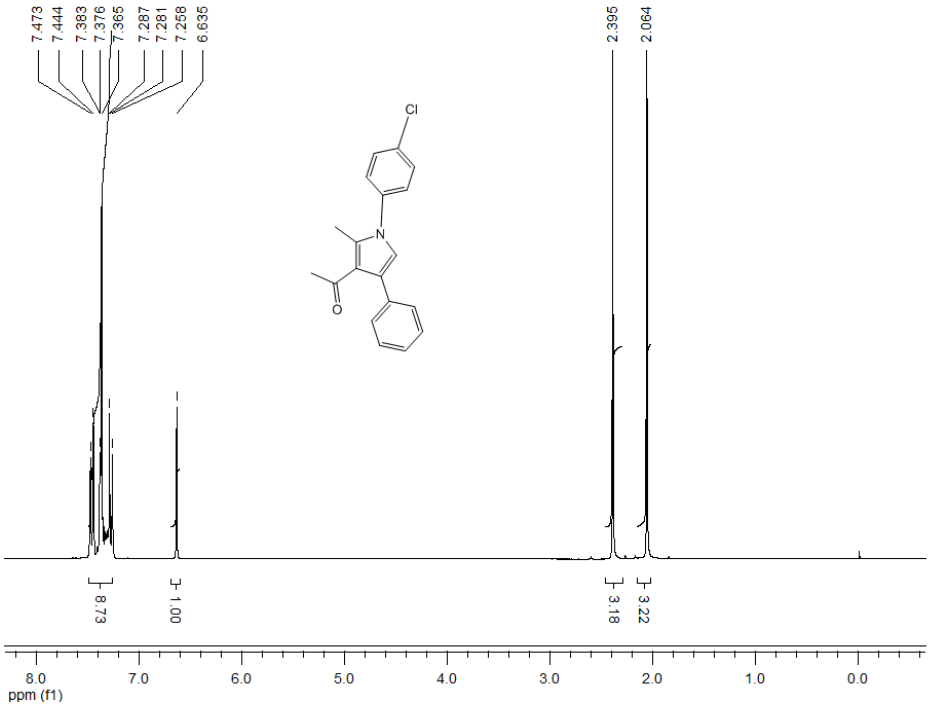


Figure S17: ^{1}H NMR spectrum of 1-(1-(4-chlorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(9)**

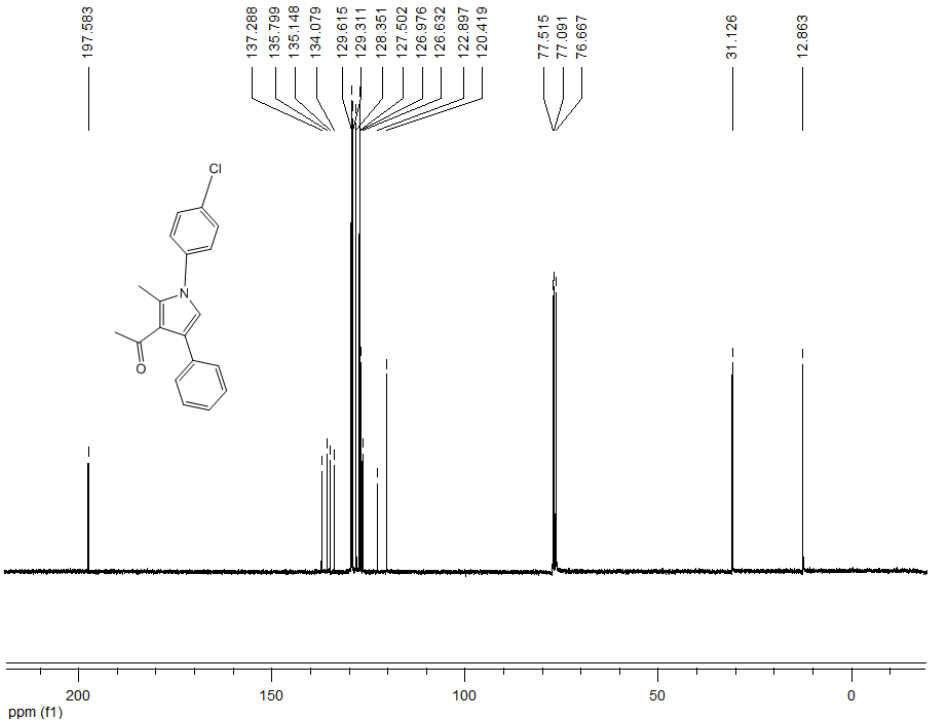


Figure S18: ^{13}C NMR spectrum of 1-(1-(4-chlorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(9)**

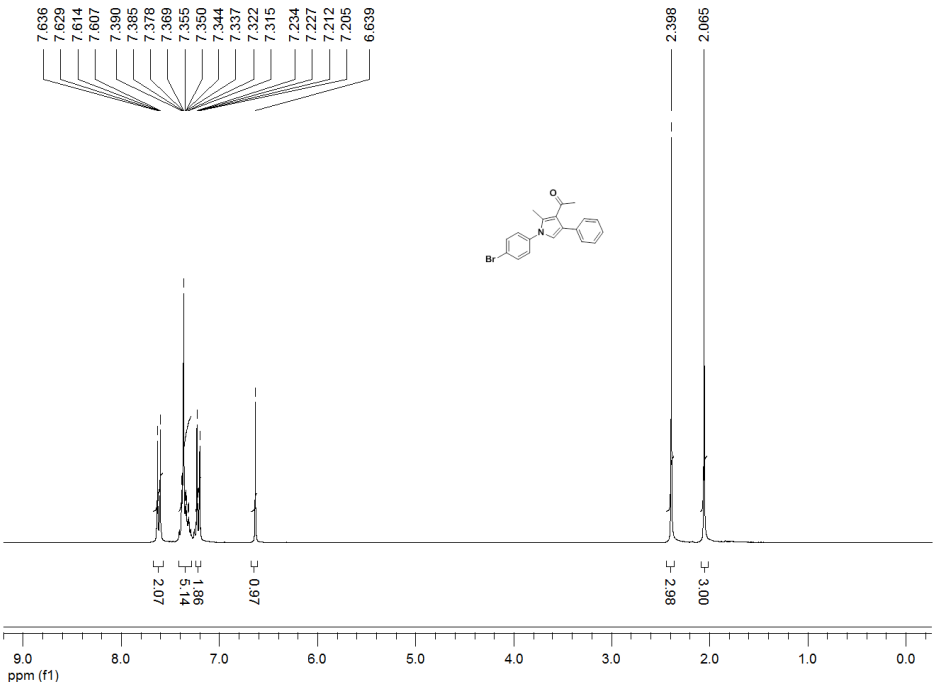


Figure S19: ^{1}H NMR spectrum of 1-(1-(4-bromophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(10)**

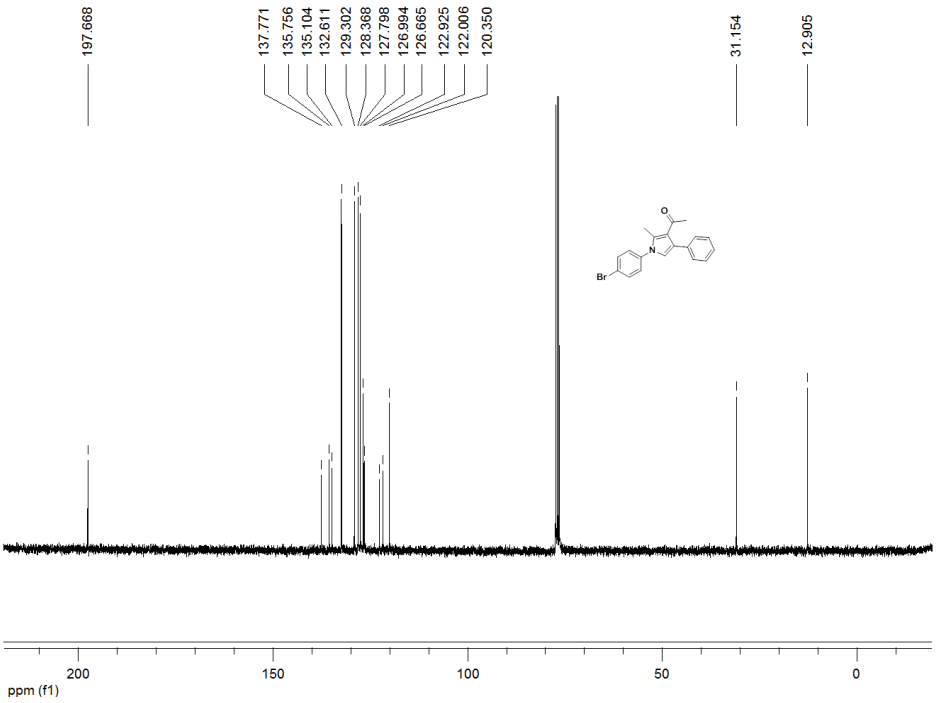


Figure S20: ^{13}C NMR spectrum of 1-(1-(4-bromophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(10)**

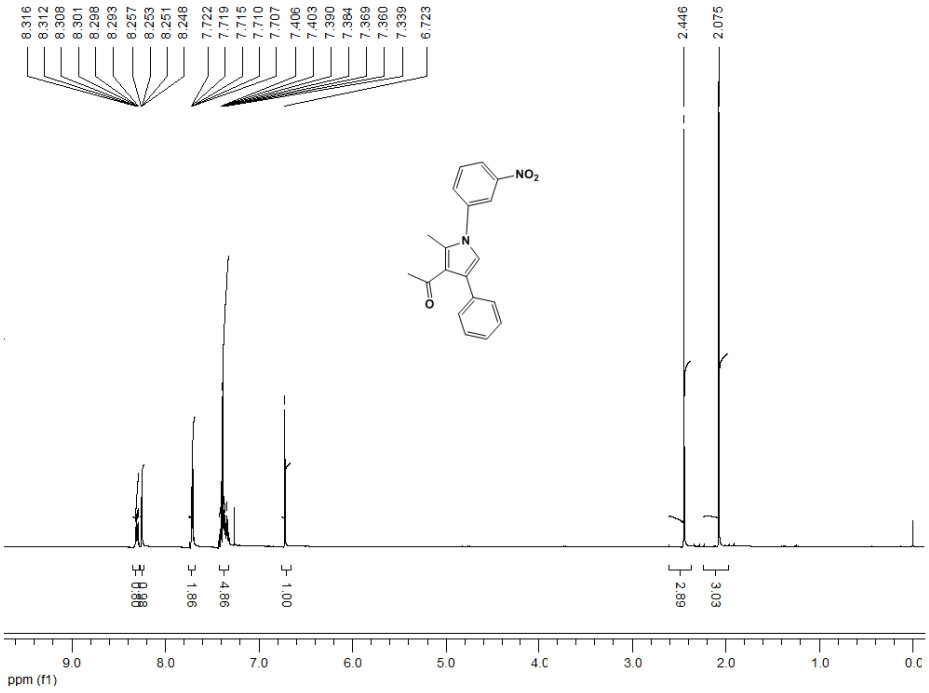


Figure S21: ^{1}H NMR spectrum of 1-(2-methyl-1-(3-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(11)**

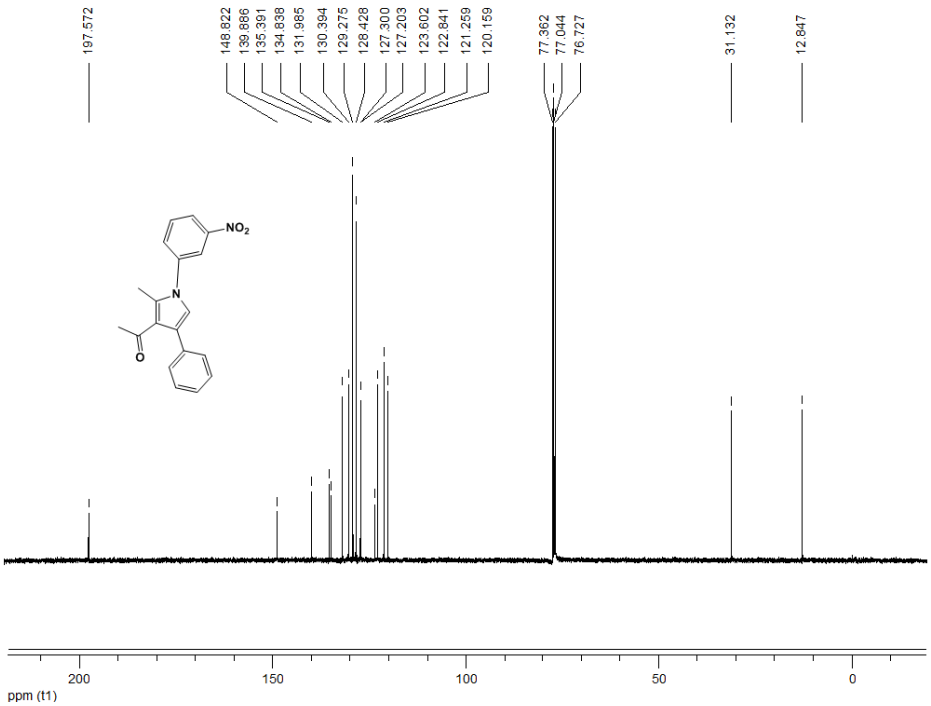


Figure S22: ^{13}C NMR spectrum of 1-(2-methyl-1-(3-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(11)**

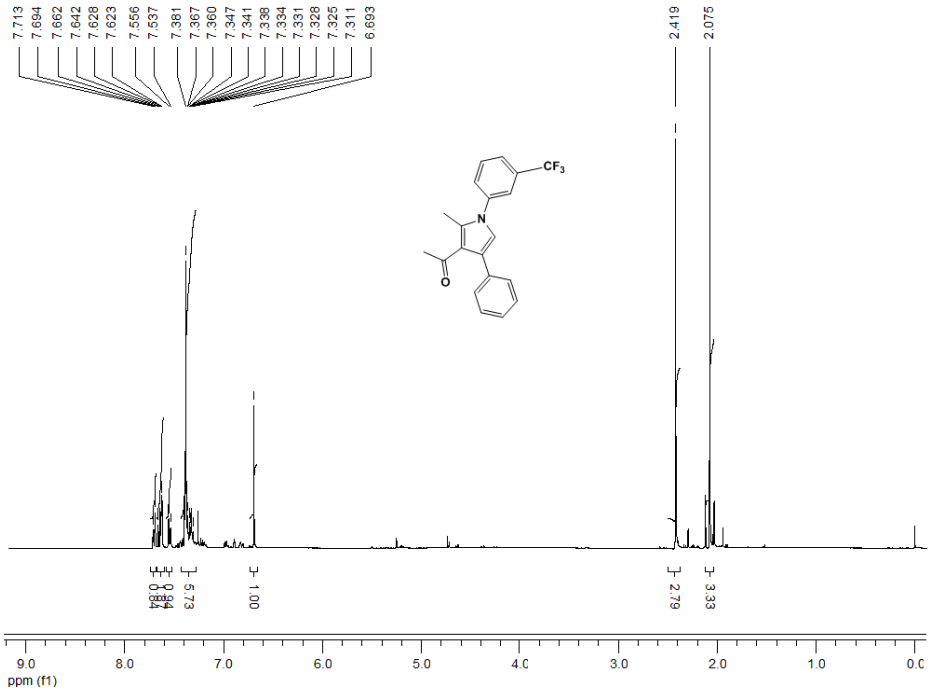


Figure S23: ^{1}H NMR spectrum of 1-(2-methyl-4-phenyl-1-(3-(trifluoromethyl)phenyl)-1*H*-pyrrol-3-yl)ethanone **(12)**

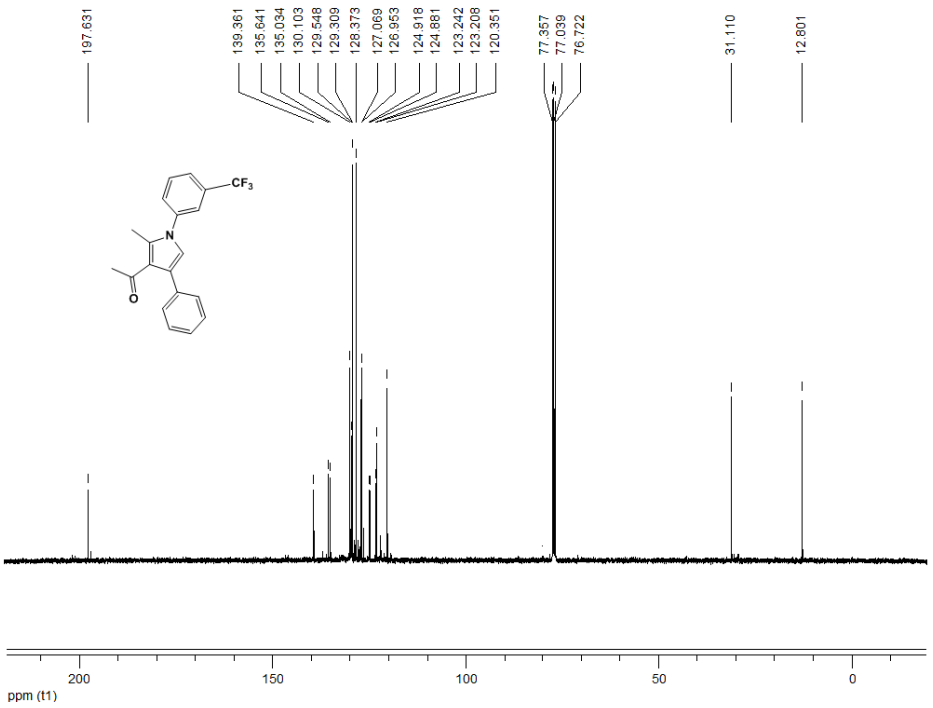


Figure S24: ^{13}C NMR spectrum of 1-(2-methyl-4-phenyl-1-(3-(trifluoromethyl)phenyl)-1*H*-pyrrol-3-yl)ethanone **(12)**

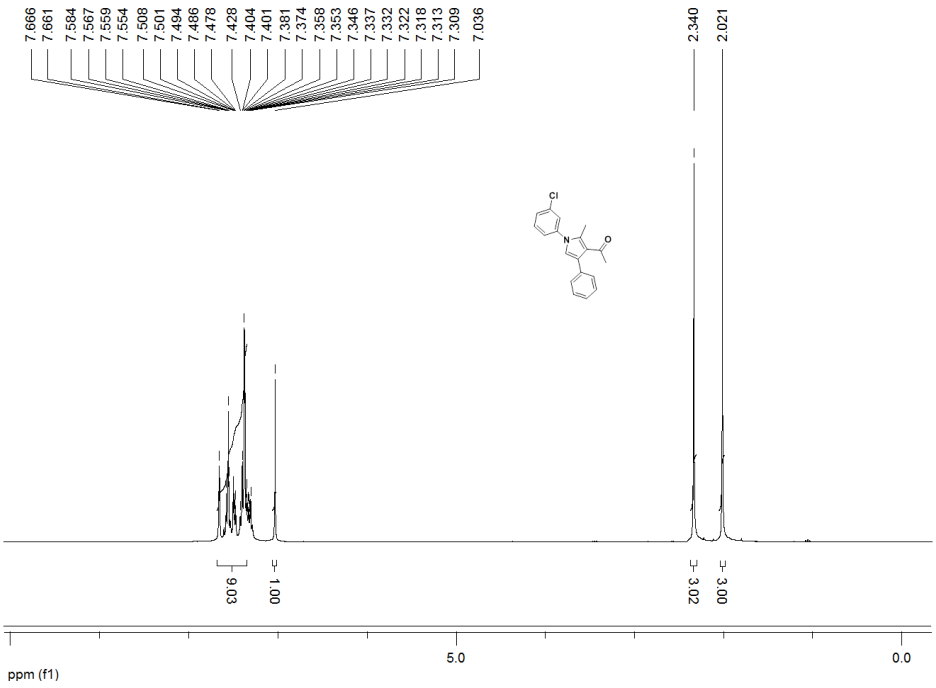


Figure S25: ^{1}H NMR spectrum of 1-(1-(3-chlorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(13)**

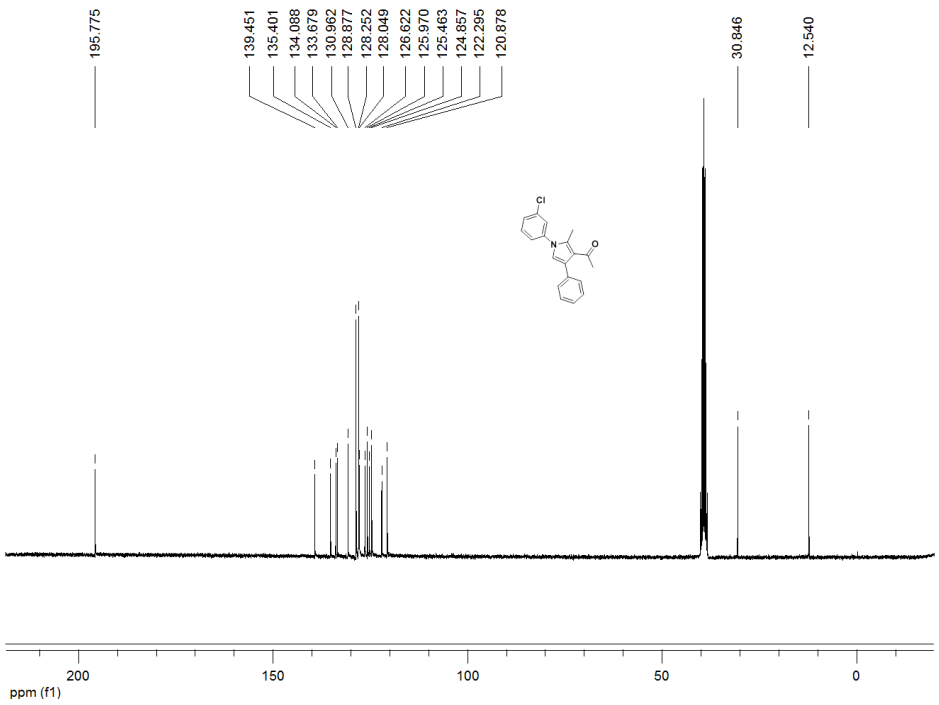


Figure S26: ^{13}C NMR spectrum of 1-(1-(3-chlorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(13)**

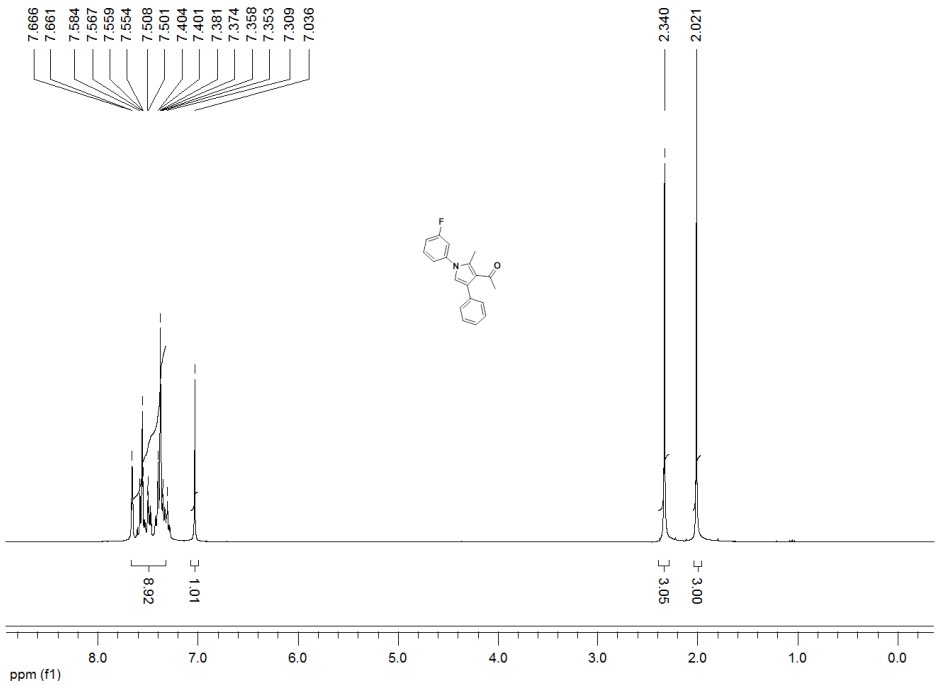


Figure S27: ^{1}H NMR spectrum of 1-(1-(3-fluorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(14)**

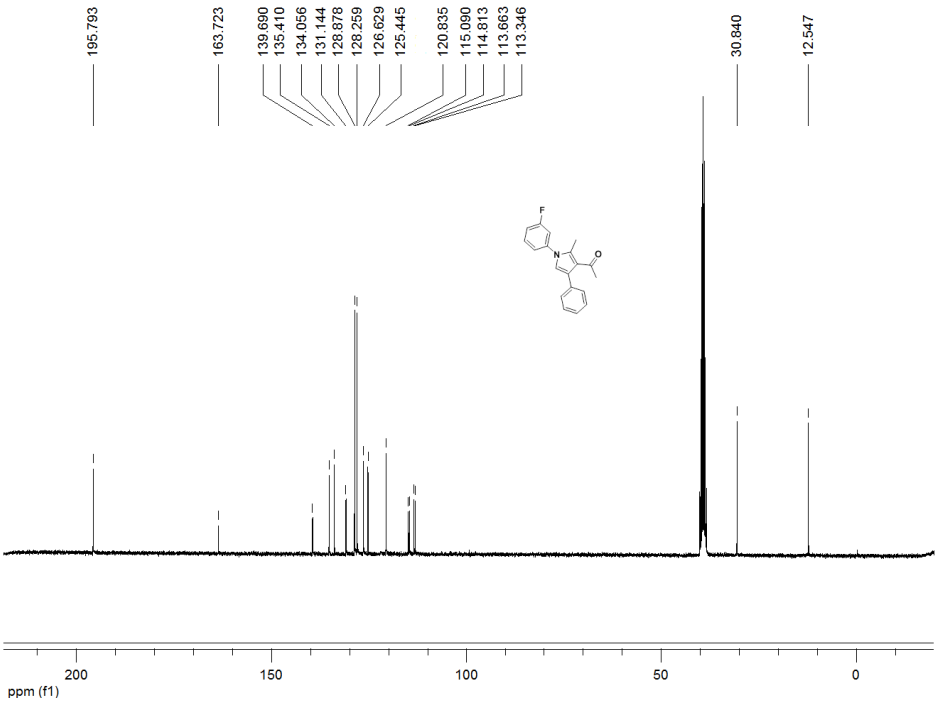


Figure S28: ^{13}C NMR spectrum of 1-(1-(3-fluorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(14)**

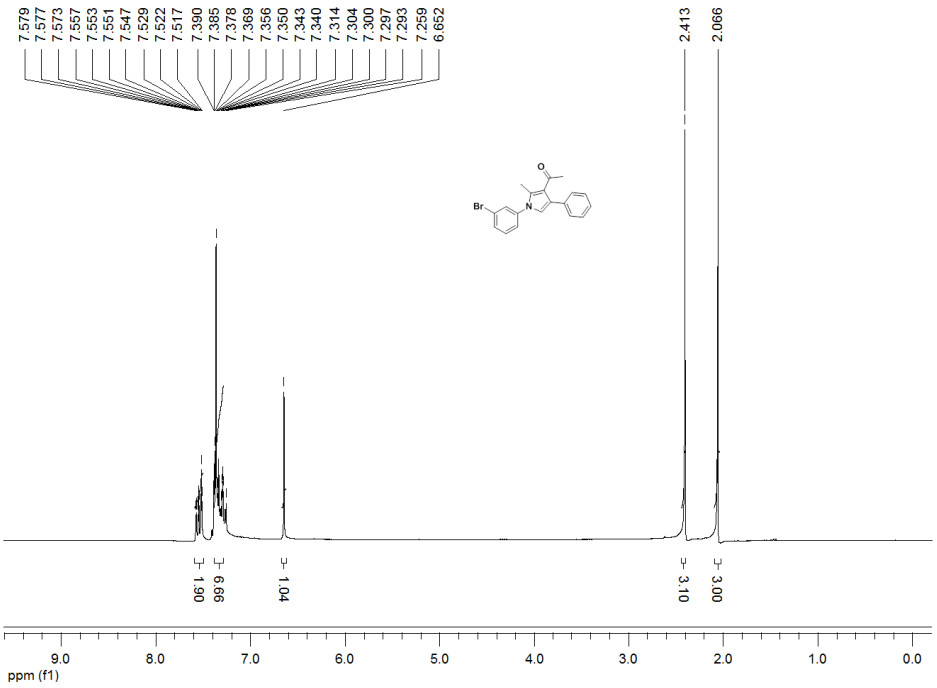


Figure S29: ^{1}H NMR spectrum of 1-(1-(3-bromophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(15)**

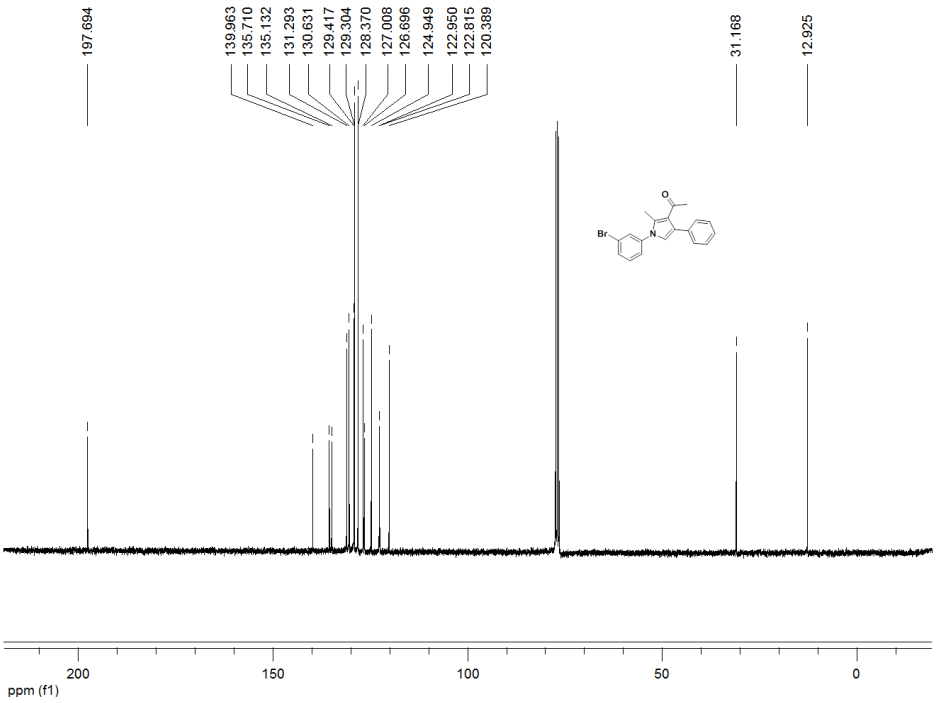


Figure S30: ^{13}C NMR spectrum of 1-(1-(3-bromophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(15)**

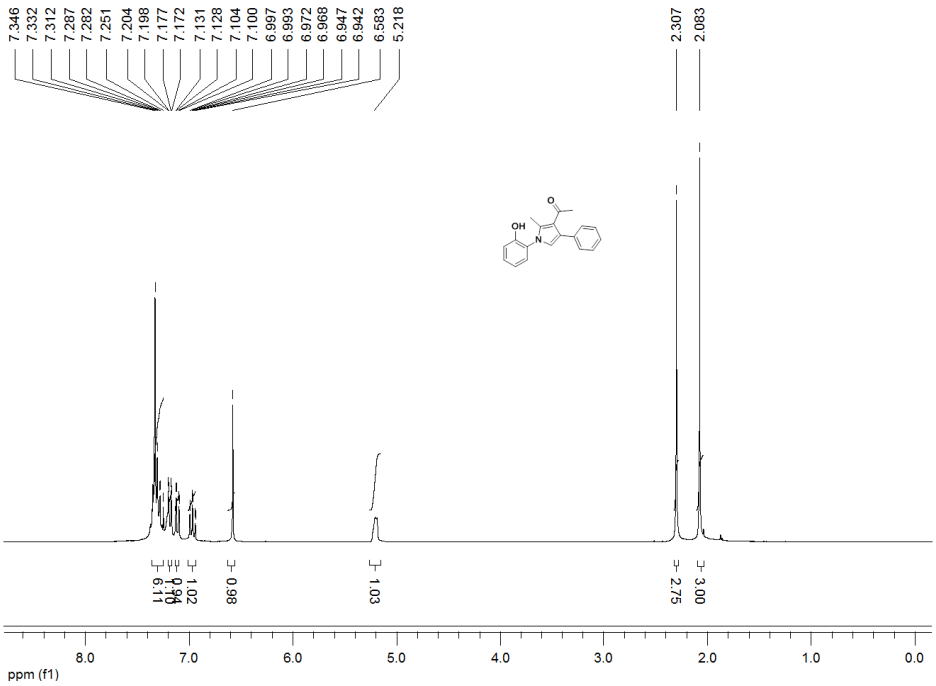


Figure S31: ^{1}HNMR spectrum of 1-(1-(2-hydroxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(16)**

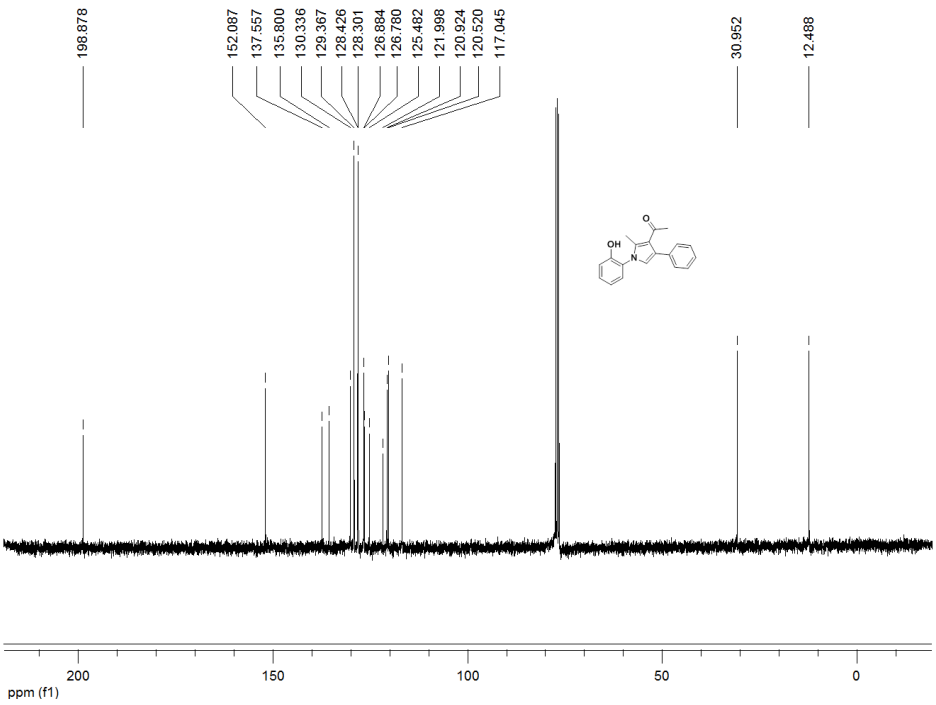


Figure S32: ^{13}C NMR spectrum of 1-(1-(2-hydroxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(16)**

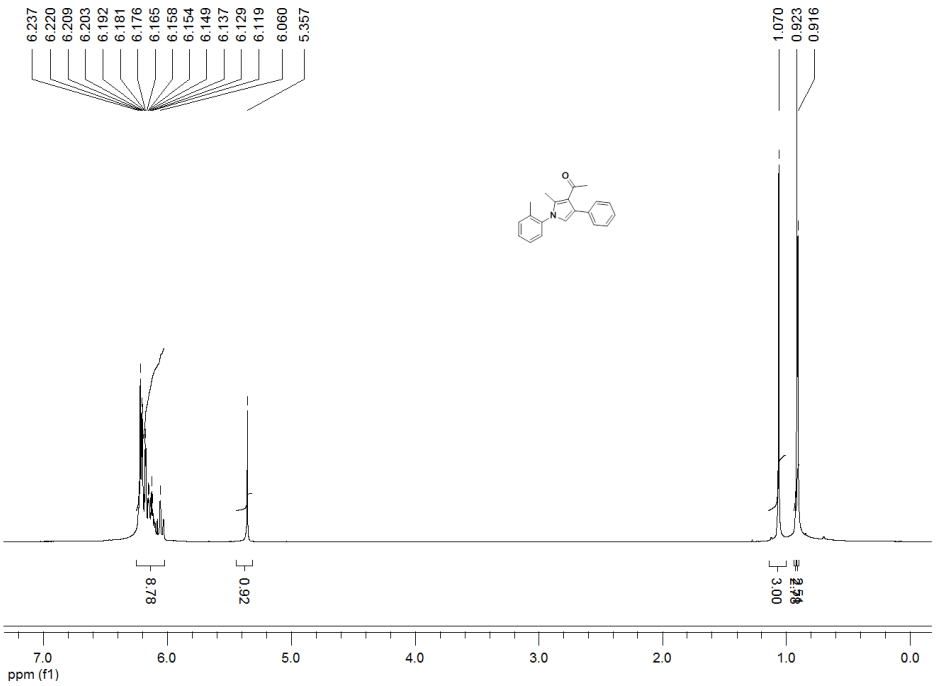


Figure S33: ^{1}H NMR spectrum of 1-(2-methyl-4-phenyl-1-(o-tolyl)-1*H*-pyrrol-3-yl)ethanone **(17)**

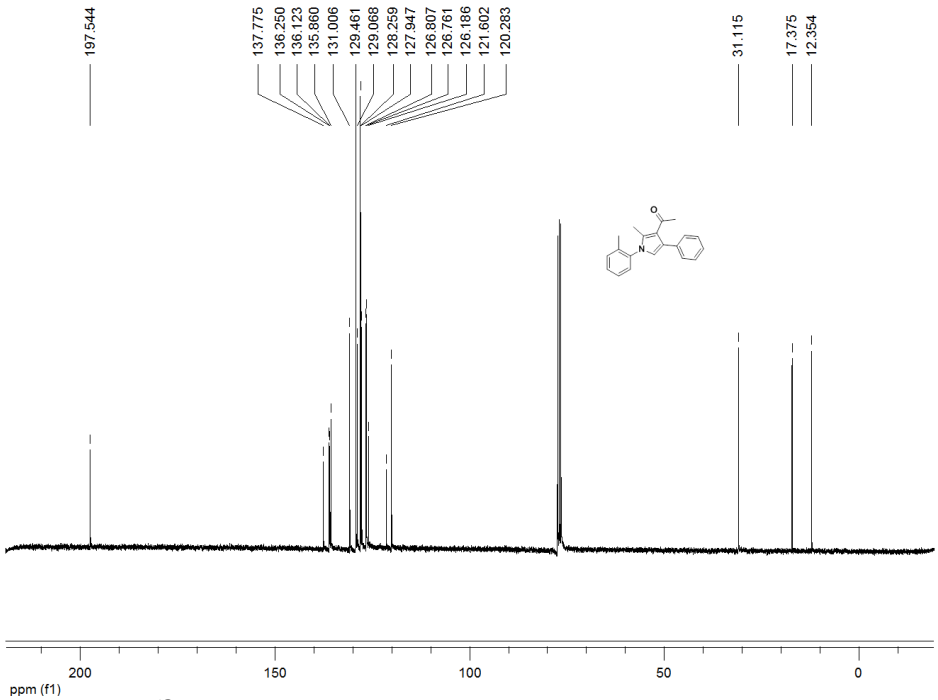


Figure S34: ^{13}C NMR spectrum of 1-(2-methyl-4-phenyl-1-(o-tolyl)-1*H*-pyrrol-3-yl)ethanone **(17)**

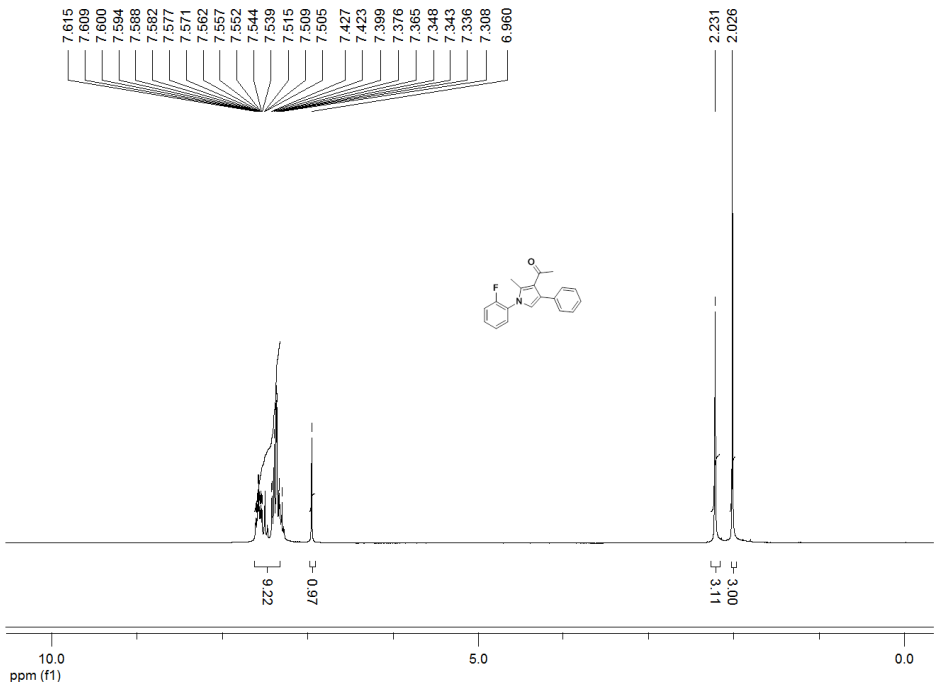


Figure S35: ^{1}H NMR spectrum of 1-(1-(2-fluorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(18)**

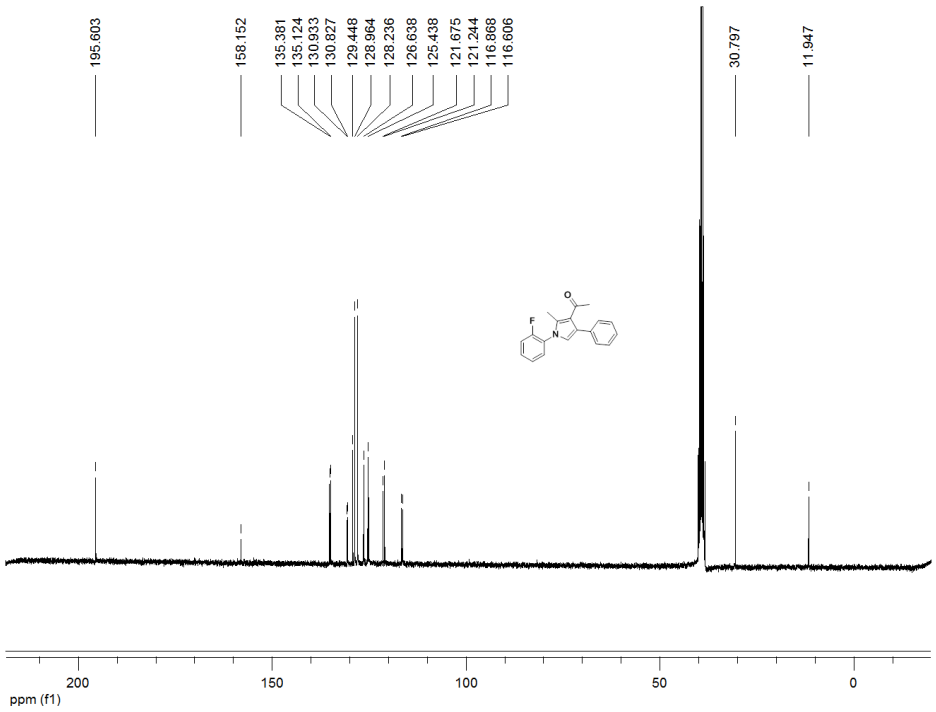


Figure S36: ^{13}C NMR spectrum of 1-(1-(2-fluorophenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(18)**

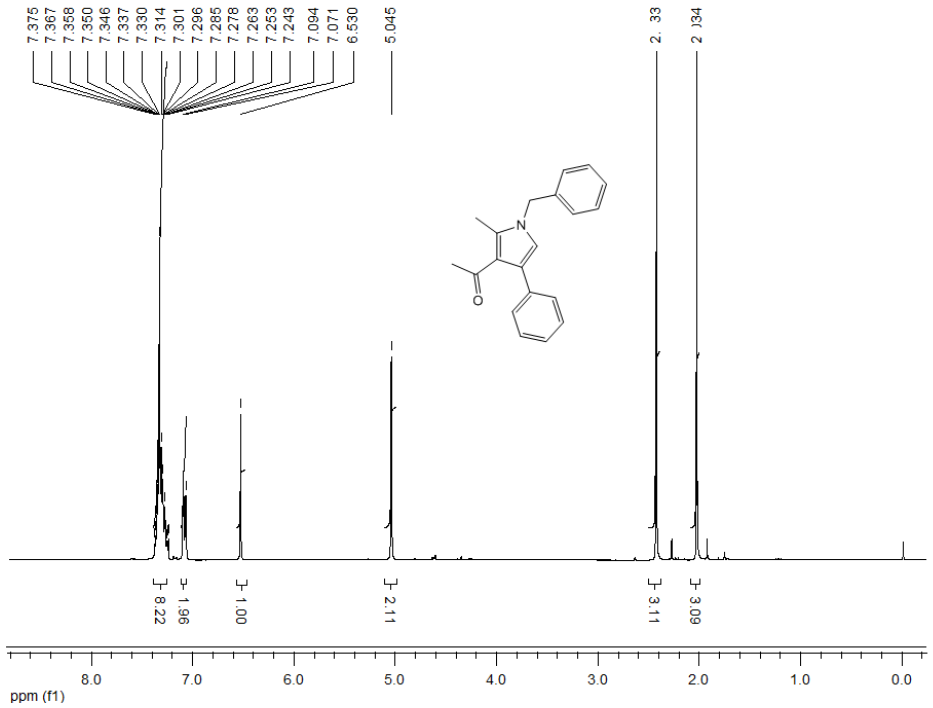


Figure S37: ^{1}H NMR spectrum of 1-(1-benzyl-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(19)**

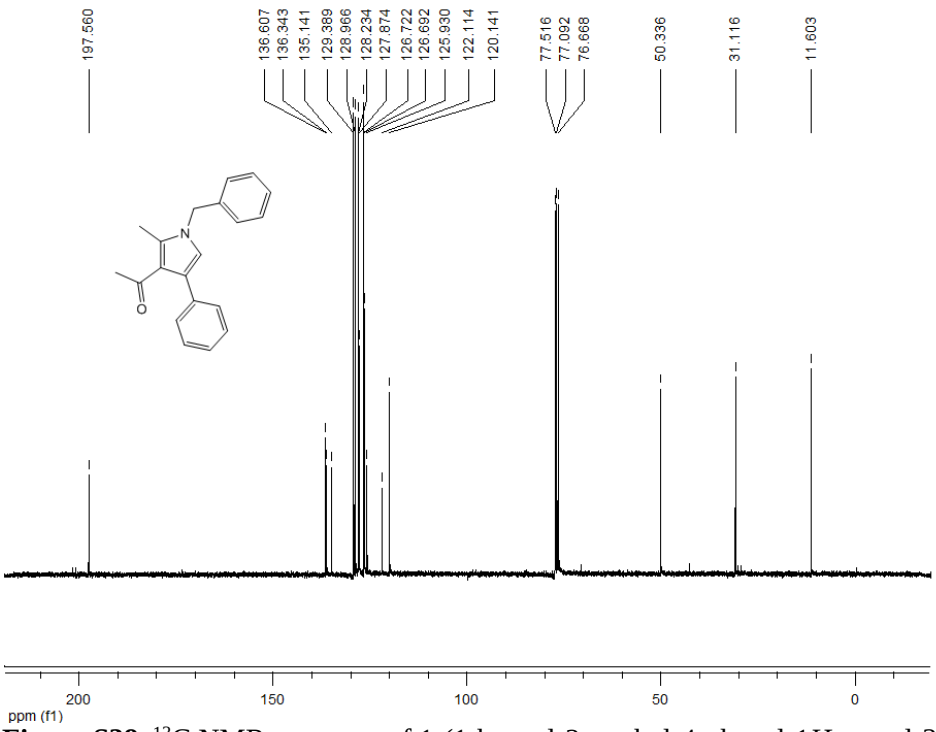


Figure S38: ^{13}C NMR spectrum of 1-(1-benzyl-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(19)**

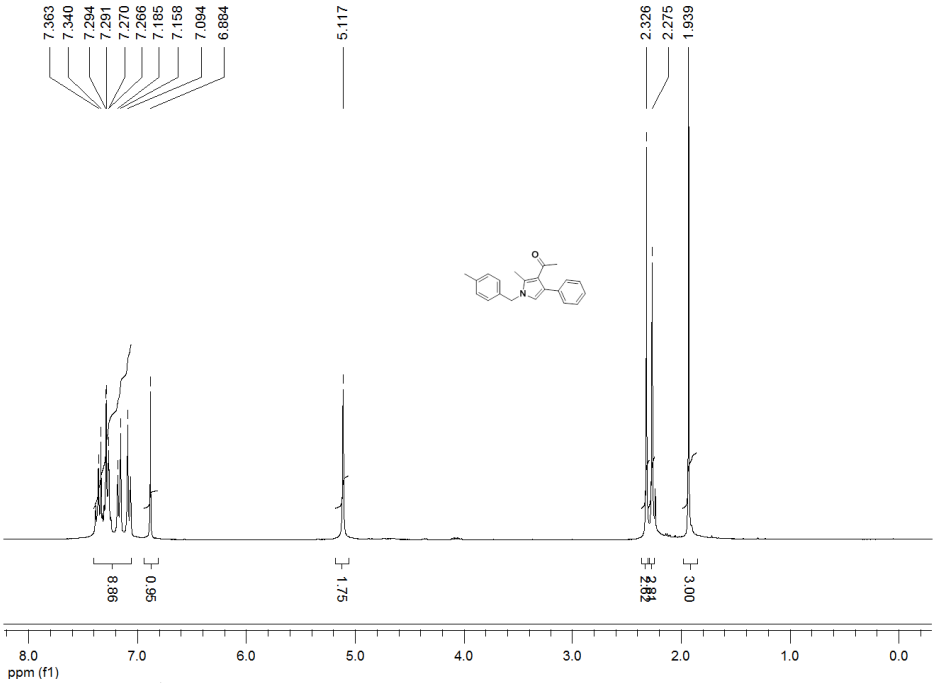


Figure S39: ^{1}H NMR spectrum of 1-(2-methyl-1-(4-methylbenzyl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(20)**

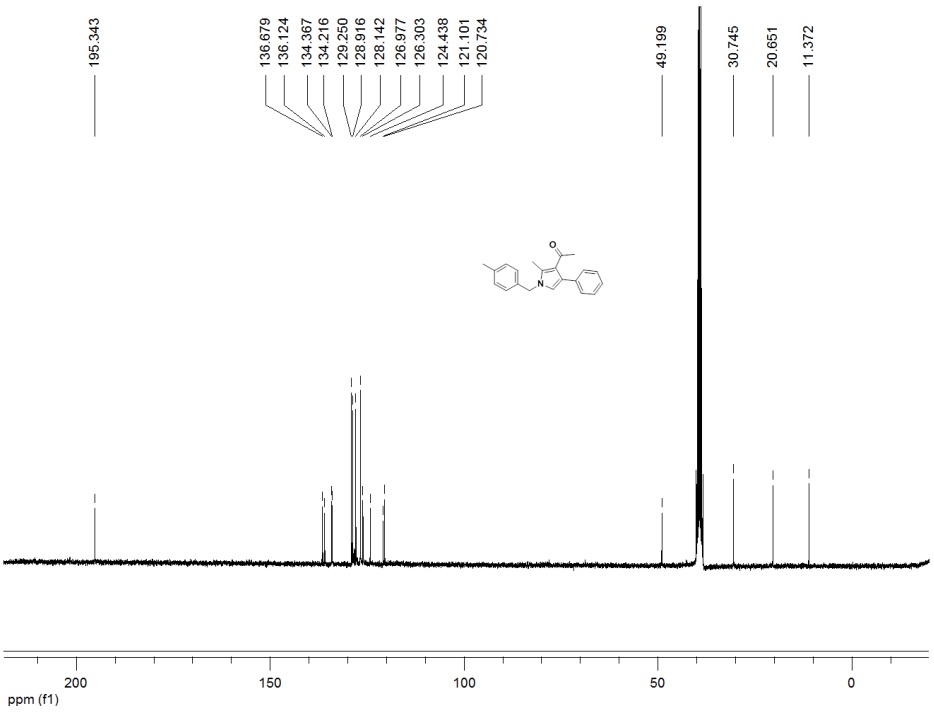


Figure S40: ^{13}C NMR spectrum of 1-(2-methyl-1-(4-methylbenzyl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(20)**

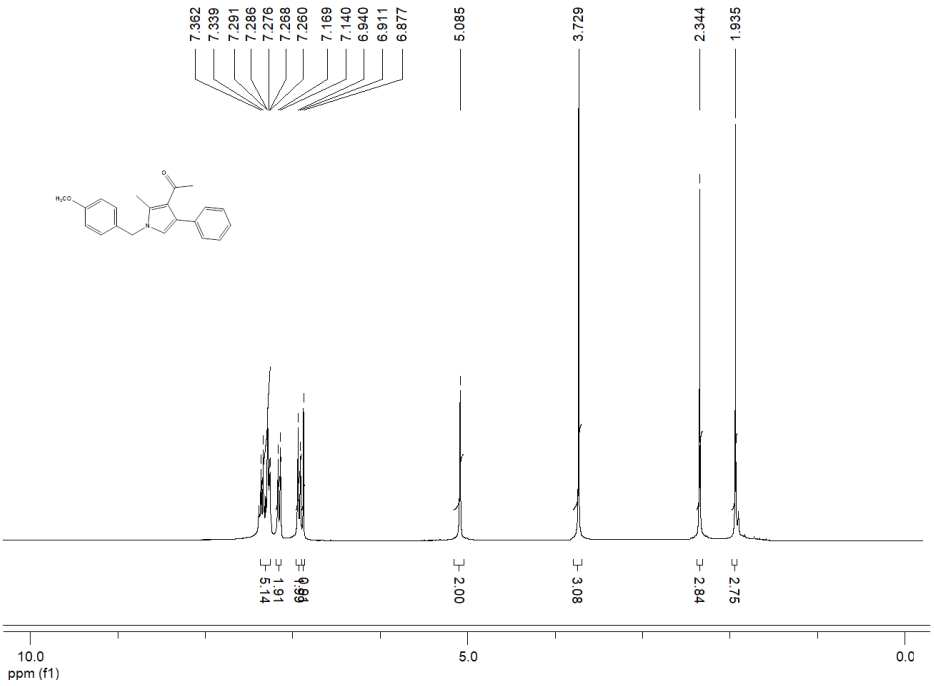


Figure S41: ^{1}H NMR spectrum of 1-(1-(4-methoxybenzyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(21)**

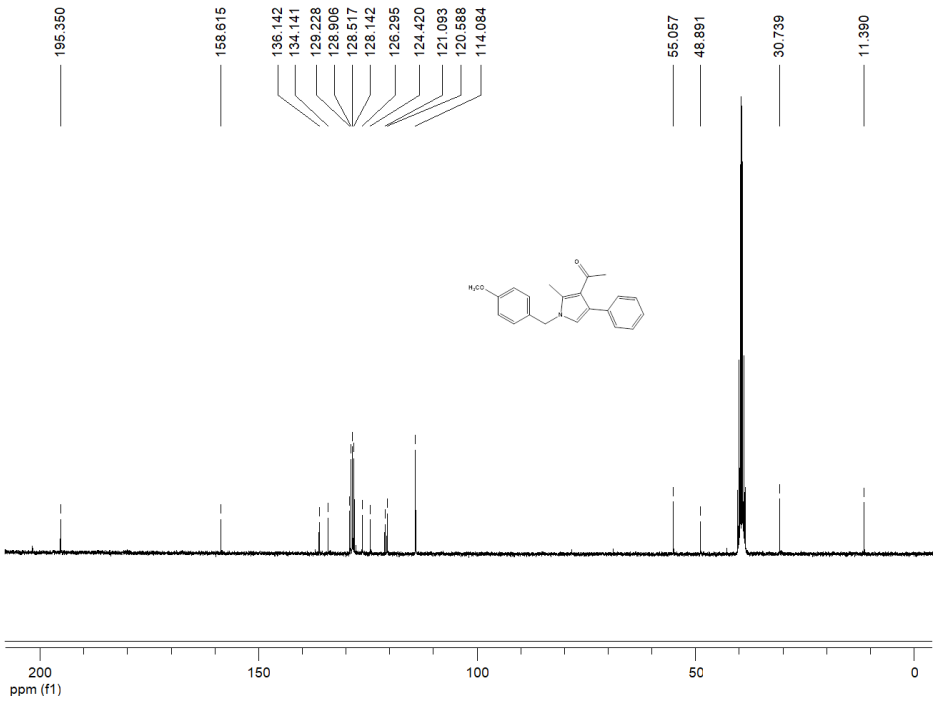


Figure S42: ^{13}C NMR spectrum of 1-(1-(4-methoxybenzyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(21)**

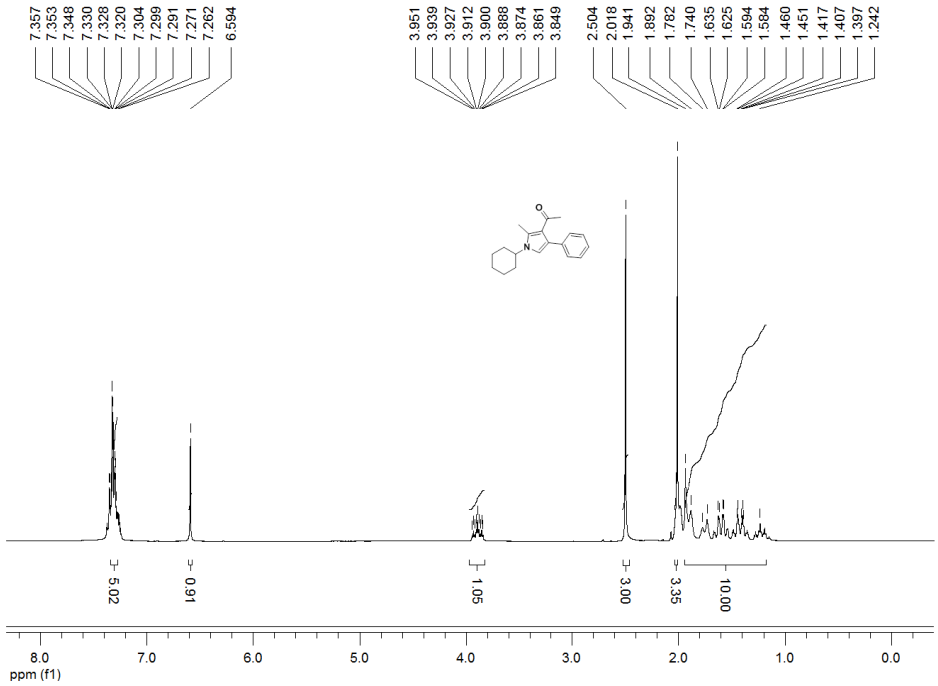


Figure S43: ^{1}H NMR spectrum of 1-(1-cyclohexyl-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(22)**

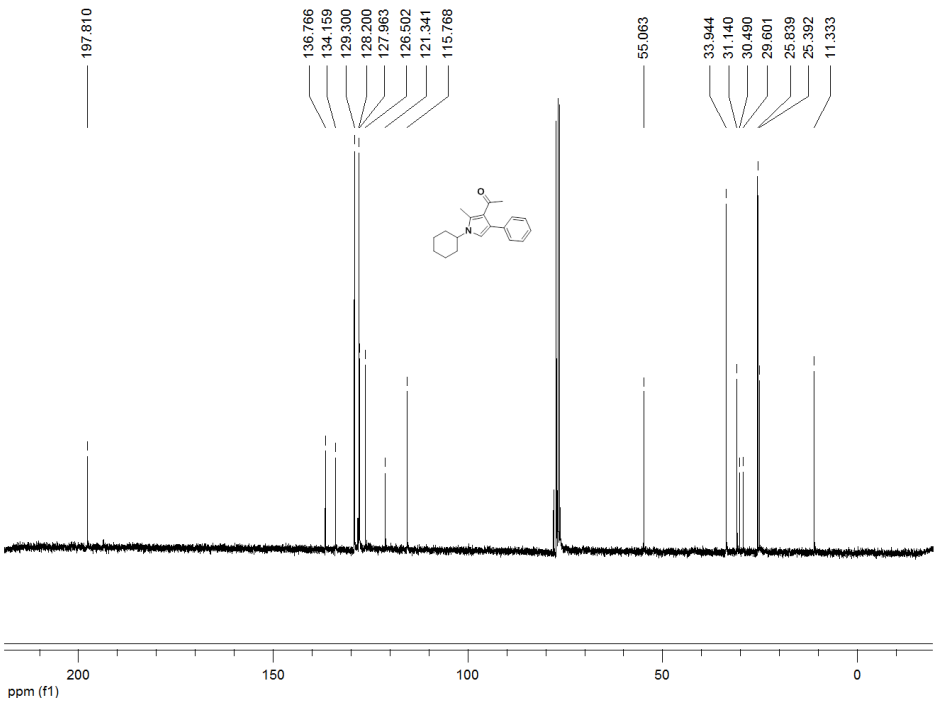


Figure S44: ^{13}C NMR spectrum of 1-(1-cyclohexyl-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(22)**

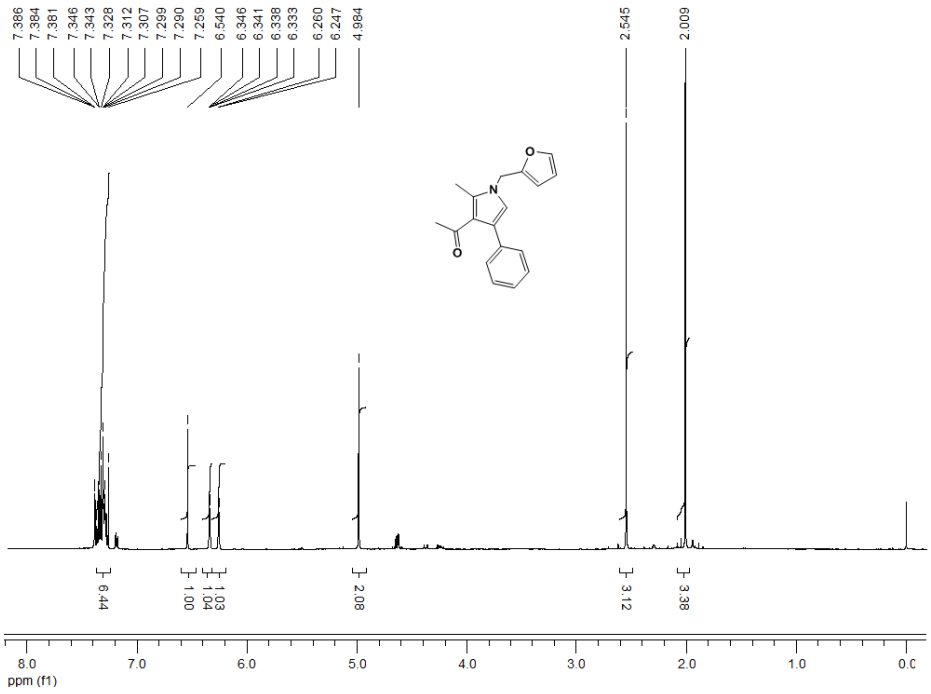


Figure S45: ^{1}H NMR spectrum of 1-(1-(furan-2-ylmethyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(23)**

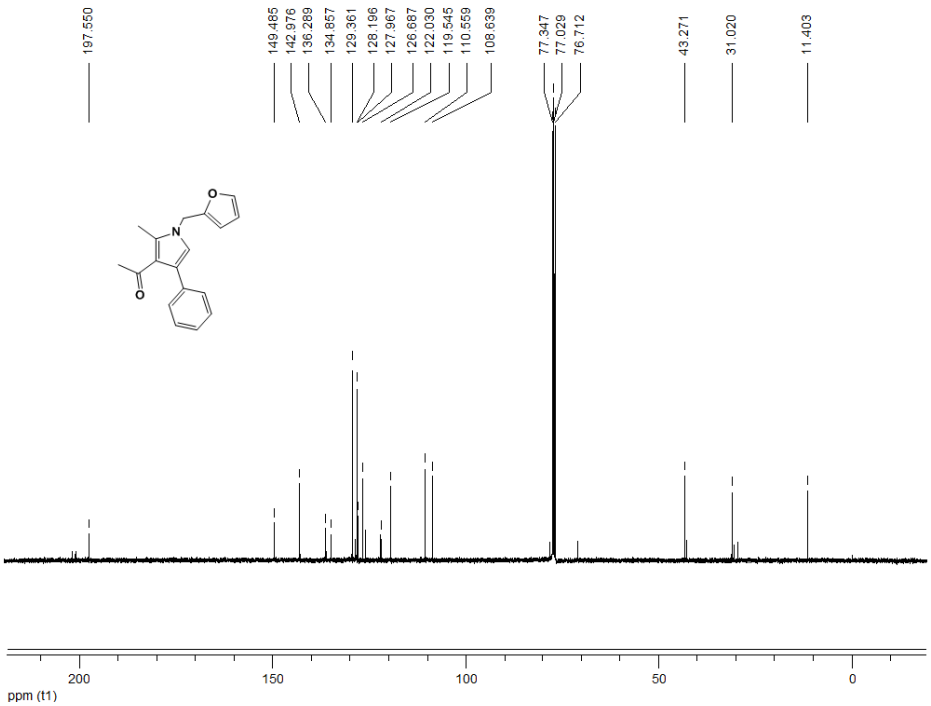


Figure S46: ^{13}C NMR spectrum of 1-(1-(furan-2-ylmethyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(23)**

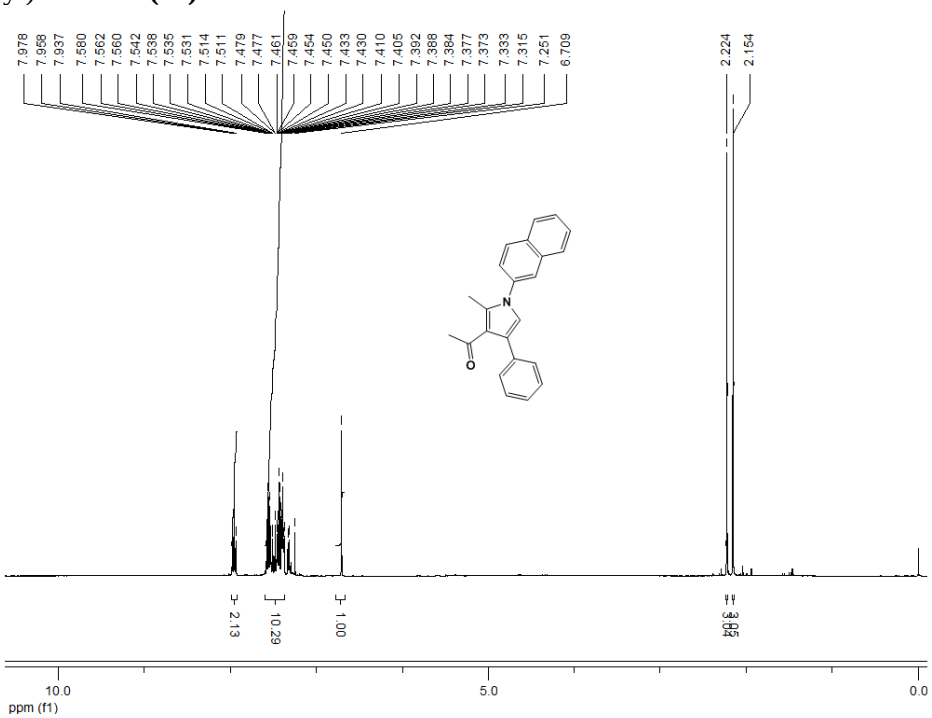


Figure S47: ^{1}H NMR spectrum of 1-(2-methyl-1-(naphthalen-2-yl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(24)**

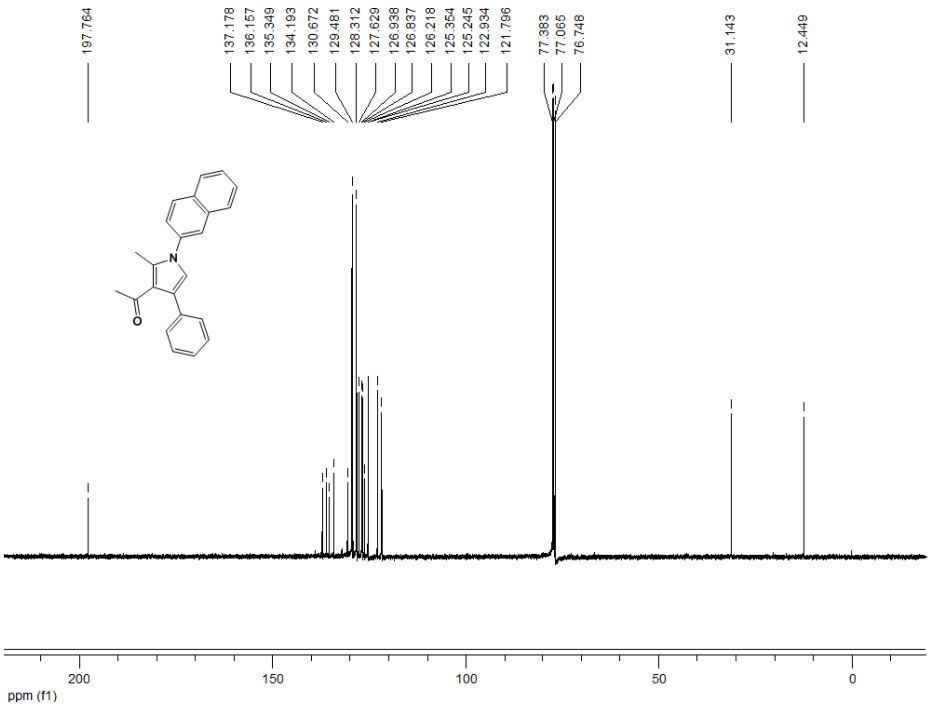


Figure S48: ^{13}C NMR spectrum of 1-(2-methyl-1-(naphthalen-2-yl)-4-phenyl-1*H*-pyrrol-3-yl)ethanone **(24)**

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[1] Li, B. L.; Li, P. H.; Fang, X. N.; Li, C. X.; Sun, J. L.; Mo, L. P.; Zhang, Z. H. One-pot four-component synthesis of highly substituted pyrroles in gluconic acid aqueous solution. *Tetrahedron.* **2013**, 69, 7011-7018.

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[6] Li, B. L.; Zhang, M.; Hu, H. C.; Du, X.; Zhang, Z. H. Nano-CoFe2O4 supported molybdenum as an efficient and magnetically recoverable catalyst for a one-pot, four-component synthesis of functionalized pyrroles. *New J. Chem.* **2014,** 38, 2435-2442.

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