

Supporting Information

β-Cyclodextrin as a recyclable catalyst: Aqueous phase one-pot four-component synthesis of polyfunctionalized pyrroles.

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Contents

General Information.....	2
General procedure for the synthesis of polyfunctionalized pyrroles....	
.....	2
Spectroscopic Data.....	3-17
Copies of ¹H NMR and ¹³C NMR spectra of compounds	18-43

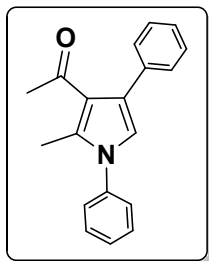
General Information:

All chemical were purchased from Sigma Aldrich with purity not less than 99.9%. Analytical Thin Layer Chromatography (TLC) was carried out by using silica gel 60 F₂₅₄ pre-coated plates. Visualization was accomplished with UV lamp of I₂ stain. All products were characterized by their NMR and Mass spectra. ¹H NMR and ¹³C NMR recorded on 300 or 400 MHz, in CDCl₃ using TMS as the internal standard, chemical shifts were reported in parts per million (ppm, δ) downfield from the tetramethylsilane.

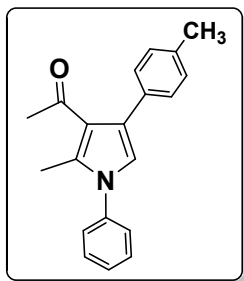
General procedure for the synthesis of polyfunctionalized pyrroles:

β-Cyclodextrin (1.0 mmol, 1.135g) was dissolved in water (15 mL) at 70 °C and to this clear solution, aldehyde (1.0 mmol), nitromethane (1.0 mL) followed by aromatic amine (1.5 mmol) and acetyl acetone (1.0 mmol) after which the reaction mixture was heated at 70-80°C until completion of the reaction as indicated by TLC. The reaction mixture was cooled to the room temperature and β-CD was filtered, the aqueous phase was extracted with ethyl acetate (3×10 mL). The organic layers were washed with water, saturated brine solution and dried over anhydrous NaSO₄. The combined organic layers were evaporated under reduced pressure and the resulting crude product was purified by column chromatography by using ethyl acetate and hexane (1:9) as eluent to give corresponding polyfunctionalized pyrrole

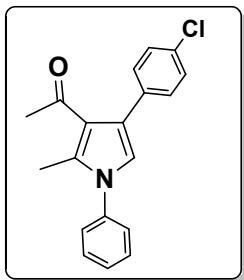
Spectroscopic Data:



1-(2-methyl-1,4-diphenyl-1H-pyrrol-3-yl) ethanone (Table 2, Entry 1): Light brown solid, mp 106-109 °C. IR (KBr) 3060, 2923, 1642, 1495, 1400, 1226 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ=7.30-7.34 (m, 3H), 7.37-7.50 (m, 7H), 6.67 (s, 1H), 2.41 (s, 3H), 2.07(s, 3H) ppm; ¹³C NMR (75MHz, CDCl₃, TMS) δ 12.8, 30.9, 114.5, 120.5, 122.4, 126.1, 126.3, 126.7, 128.0, 128.1, 128.8, 129.2, 135.2, 135.9, 138.6, 197.5 ppm. HRMS: *m/z* calcd for C₁₉H₁₇NONa 298.1207; found 298.1200.

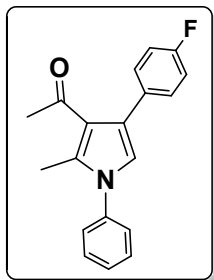


1-(2-methyl-1-phenyl-4-p-tolyl-1H-pyrrol-3-yl) ethanone (Table 2, Entry 2): Brown oil. IR (KBr) 3022, 2924, 1644, 1495, 1410, 1224 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ= 7.41-7.50 (m, 3H), 7.32 (d, *J* = 7.7 Hz, 2H), 7.24-7.26 (m, 2H), 7.18 (d, *J* = 7.7 Hz, 2H), 6.63 (s, 1H), 2.38 (s, 6H), 2.07(s, 3H) ppm; ¹³C NMR (75MHz, CDCl₃, TMS) δ 12.9, 29.7, 31.1, 110.8, 120.6, 122.4, 125.0, 126.2, 128.2, 128.4, 129.3, 130.4, 132.8, 134.5, 135.5, 138.6, 196.9 ppm. HRMS: *m/z* calcd for C₂₀H₂₀NO (M+1) 290.1544; found 290.1548.

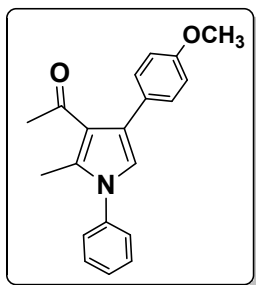


1-(4-(4-chlorophenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (Table 2, Entry 3)
: White solid, mp 119-124°C. IR (KBr) 2922, 2854, 1652, 1499, 1408, 1221 cm⁻¹; ¹H

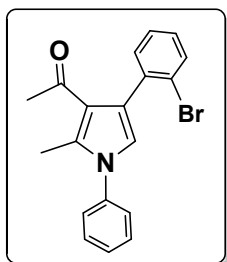
NMR (300MHz, CDCl₃, TMS) δ = 7.42-7.51 (m, 3H), 7.28-7.36 (m, 6H), 6.64 (s, 1H), 2.39 (s, 3H), 2.08 (s, 3H) ppm; ¹³C NMR (75MHz CDCl₃, TMS) δ 12.9, 29.6, 113.2, 120.6, 122.5, 125.0, 126.2, 128.2, 128.4, 129.4, 130.4, 135.5, 197.0 ppm. HRMS: m/z calcd for C₁₉H₁₆ClNNaO 332.0818; found 332.0813.



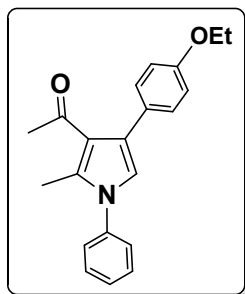
1-(4-(4-fluorophenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (Table 2, Entry 4): Light yellow oil. IR (KBr) 3052, 2922, 1651, 1509, 1408, 1220 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ = 7.42-7.51 (m, 3H), 7.31-7.36 (m, 4H), 7.04-7.12 (m, 2H), 6.64 (s, 1H), 2.40 (s, 3H), 2.07 (s, 3H) ppm; ¹³C NMR (75MHz CDCl₃, TMS) δ 12.8, 29.4, 111.0, 120.4, 122.4, 125.2, 125.9, 128.0, 128.3, 129.2, 130.3, 135.0, 196.6 ppm. ESI-MS: 294 (M+H)⁺.



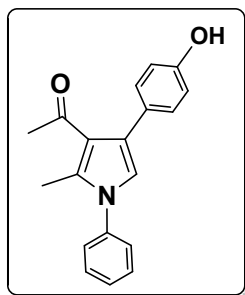
1-(4-(4-methoxyphenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (Table 2, Entry 5): Brown oil. IR (KBr) 2924, 2852, 1649, 1503, 1411, 1232 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ = 7.39-7.49 (m 3H), 7.32 (d, J = 7.1 Hz, 2H), 7.25 (d, J = 8.5 Hz, 2H), 6.88 (d, J = 8.5 Hz, 2H), 6.59 (s, 1H), 3.83 (s, 3H), 2.39 (s, 3H), 2.04 (s, 3H) ppm; ¹³C NMR (75MHz, CDCl₃, TMS) δ 13.0, 31.0, 55.0, 113.6, 120.2, 126.2, 127.9, 128.3, 129.2, 129.7, 130.3, 135.3, 196.6 ppm. HRMS: m/z calcd for C₂₀H₁₉NNaO₂ 328.1313; found 328.1310.



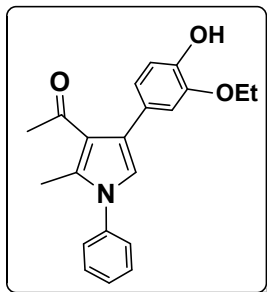
1-(4-(2-bromophenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (Table 2, Entry 6) : Dark brown oil. IR (KBr) 3117, 2922, 1647, 1502, 1404, 1226 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.64 (d, J = 8.3 Hz, 1H), 7.47 (q, J = 7.5 Hz, 3H), 7.35 (t, J = 7.5 Hz, 4H), 7.20 (d, J = 7.5 Hz), 6.63 (s, 1H), 2.46 (s, 3H), 1.98 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 13.1, 30.1, 112.2, 121.0, 124.5, 125.1, 126.1, 127.1, 128.0, 128.7, 129.2, 131.9, 132.6, 135.3, 137.3, 138.4, 196.3 ppm. HRMS: m/z calcd for $\text{C}_{19}\text{H}_{17}\text{BrNO}$ (M+1) 354.0493; found 354.0488.



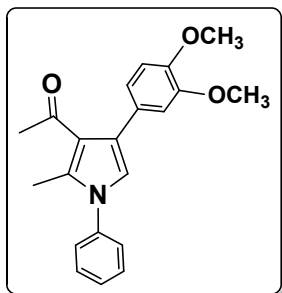
1-(4-(4-ethoxyphenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (Table 2, Entry 7) : Brown oil. IR (KBr) 2926, 2852, 1648, 1502, 1403, 1244 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.50-7.43 (m, 3H), 7.25-7.33 (m, 4H), 6.89 (d, J = 8.5 Hz, 2H), 6.61 (s, 1H), 4.05 (q, J = 6.9 Hz, 2H), 2.40(s, 3H), 2.06 (s, 3H), 1.44 (t, J = 6.9 Hz, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.9, 14.8, 31.1, 63.3, 114.2, 120.3, 125.9, 126.2, 127.9, 129.2, 130.3, 136.5, 197.5 ppm. HRMS: m/z calcd for $\text{C}_{21}\text{H}_{21}\text{NNaO}_2$ 342.1469; found 342.1460.



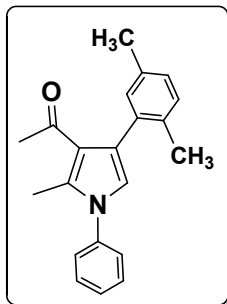
1-(4-(4-hydroxyphenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (Table 2, Entry 8) : Dark brown oil. IR (KBr) 3421, 2925, 1642, 1500, 1400, 1228 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.44-7.51 (m, 3H), 7.31 (d, J = 8.3 Hz, 2H), 7.21 (d, J = 8.3 Hz, 2H), 6.90 (d, J = 8.3 Hz, 2H), 6.62 (s, 1H), 2.41 (s, 3H), 2.10 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 13.0, 30.8, 115.3, 118.9, 120.5, 122.3, 126.1, 128.0, 129.2, 130.4, 135.6, 138.5, 155.4, 198.6 ppm. HRMS: m/z calcd for $\text{C}_{19}\text{H}_{17}\text{NNaO}_2$ 314.1156; found 314.1157.



1-(4-(3-ethoxy-4-hydroxyphenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (Table 2, Entry 9) : Brown oil. IR (KBr) 3420, 2928, 1644, 1502, 1410, 1225 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.42-7.51 (m, 3H), 7.32 (d, J = 7.3 Hz, 2H), 6.94 (d, J = 8.3 Hz, 1H), 6.87 (d, J = 7.3 Hz, 2H), 6.64 (s, 1H), 4.12 (q, J = 6.7 Hz, 2H), 2.40 (s, 3H), 2.11 (s, 3H), 1.45 (t, J = 6.7 Hz, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 13.0, 14.9, 30.9, 64.5, 113.0, 114.2, 120.5, 122.1, 122.5, 126.2, 127.9, 128.1, 129.3, 138.7, 144.9, 145.5, 199.7 ppm. HRMS: m/z calcd for $\text{C}_{21}\text{H}_{21}\text{NNaO}_3$ 358.1419; found 358.1430.

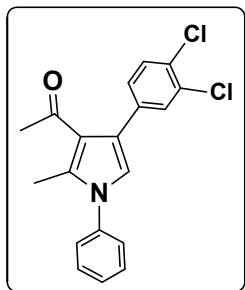


1-(4-(3, 4-dimethoxyphenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl) ethanone (Table 2, Entry 10): Reddish brown oil. IR (KBr) 2924, 2852, 1649, 1503, 1411, 1232 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.44-7.49 (m, 2H), 7.32 (d, J = 8.3 Hz, 2H), 7.26 (s, 1H), 6.88-6.90 (m, 3H), 6.65 (s, 1H), 3.91 (s, 3H), 3.89 (s, 3H), 2.41 (s, 3H), 2.10 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.9, 29.7, 55.8, 111.0, 112.7, 120.4, 121.5, 126.2, 128.0, 128.6, 129.3, 138.7, 148.1, 148.6, 198.5 ppm. ESI-MS: 336 (M+H) $^+$.

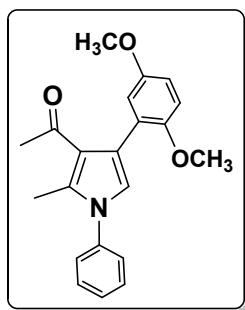


1-(4-(2, 5-dimethylphenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl) ethanone (Table 2, Entry 11): Brown oil. IR (KBr) 2923, 2853, 1653, 1499, 1408, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.41-7.51 (m, 3H), 7.33 (d, J = 8.3 Hz, 2H), 7.07-7.15 (m,

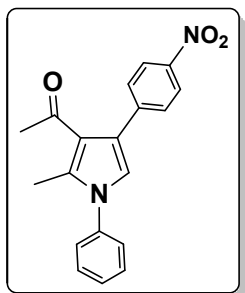
3H), 6.55 (s, 1H), 2.46 (s, 3H), 2.33 (s, 3H), 2.20 (s, 3H), 1.90 (s, 3H) ppm; ^{13}C NMR (75MHz CDCl_3 , TMS) δ 13.2, 19.9, 20.8, 30.1, 110.8, 120.3, 126.1, 127.9, 128.0, 128.9, 129.2, 129.7, 131.3, 133.9, 134.9, 135.7, 138.7, 197.0 ppm. HRMS: m/z calcd for $\text{C}_{21}\text{H}_{21}\text{NNaO}$ 326.1518; found 326.1510.



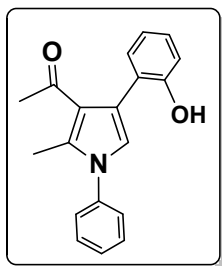
1-(4-(3, 4-dichlorophenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl) ethanone (Table 2, Entry 12): White solid, mp120-125°C. IR (KBr) 2922, 2853, 1652, 1499, 1408, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.42-7.55 (m, 5H), 7.31 (d, J = 6.9 Hz, 2H), 7.20 (d, J = 8.1 Hz, 1H), 6.67 (s, 1H), 2.39 (s, 3H), 2.13 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.8, 29.6, 114.0, 120.9, 122.2, 126.1, 128.3, 128.5, 129.3, 130.0, 130.7, 132.1, 135.7, 136.0, 138.3, 196.7 ppm. ESI-MS: 344 (M+H) $^+$.



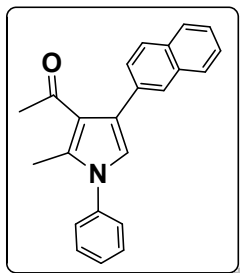
1-(4-(2, 5-dimethoxyphenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl) ethanone (Table 2, Entry 13): Dark brown oil. IR (KBr) 2924, 2852, 1651, 1503, 1411, 1232 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.45-7.49 (m, 2H), 7.40 (d, J = 6.7 Hz, 1H), 7.33 (d, J = 6.7 Hz, 2H), 6.91 (s, 1H), 6.84(s, 2H), 6.67 (s, 1H), 3.79 (s, 3H), 3.75 (s, 3H), 2.41 (s, 3H), 2.07 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.8, 29.6, 55.6, 111.3, 112.6, 116.7, 120.8, 122.9, 126.1, 127.8, 129.1, 134.5, 138.7, 150.9, 153.4, 197.5 ppm. ESI-MS: 336 (M+H) $^+$.



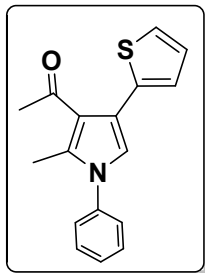
1-(2-methyl-4-(4-nitrophenyl)-1-phenyl-1H-pyrrol-3-yl) ethanone (Table 2, Entry 14): Brown oil. IR (KBr) 2922, 2853, 1649, 1503, 1410, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 8.24(d, J = 8.3 Hz, 2H), 7.49-7.55 (m, 4H), 7.32-7.35 (m, 2H), 7.26 (s, 1H), 6.78 (s, 1H), 2.40 (s, 3H), 2.18 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.8, 31.2, 112.0, 121.6, 122.7, 123.6, 124.1, 126.2, 126.8, 127.8, 128.5, 129.4, 143.9, 145.2, 198.4 ppm. HRMS: m/z calcd for $\text{C}_{19}\text{H}_{17}\text{N}_2\text{O}_3$ (M+1) 321.1239; found 321.1225.



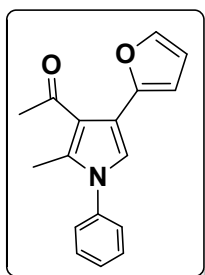
1-(4-(2-hydroxyphenyl)-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (Table 2, Entry 15) : Dark brown oil. IR (KBr) 3441, 2922, 1644, 1501, 1408, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.42-7.50 (m, 3H), 7.30 (d, J = 8.3 Hz, 2H), 7.23 (d, J = 8.3 Hz, 2H), 6.92 (d, J = 8.3 Hz, 2H), 6.60 (s, 1H), 2.41 (s, 3H), 2.08 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.8, 31.2, 115.0, 118.6, 121.0, 122.6, 127.1, 128.0, 129.6, 131.4, 135.8, 139.0, 156.4, 197.6 ppm. HRMS: m/z calcd for $\text{C}_{19}\text{H}_{17}\text{NNaO}_2$ 314.1156; found 314.1157.



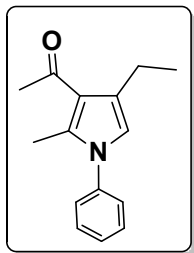
1-(2-methyl-4-(naphthalen-2-yl)-1-phenyl-1H-pyrrol-3-yl) ethanone (Table 2, Entry 16): Light yellow liquid. IR (KBr) 3060, 2923, 1642, 1495, 1400, 1226 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.82-7.87 (m, 5H), 7.43-7.52 (m, 5H), 7.36 (d, J = 6.9 Hz, 2H), 6.77 (s, 1H), 2.43 (s, 3H), 2.09 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.9, 29.6, 110.6, 120.9, 122.6, 125.7, 126.2, 127.3, 127.6, 127.7, 128.0, 128.1, 129.3, 132.2, 133.4, 135.4, 138.6, 197.7 ppm. ESI-MS: 326 (M+H) $^+$.



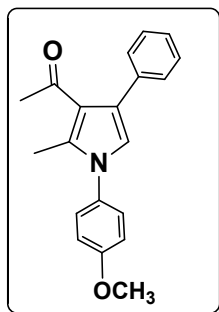
1-(2-methyl-1-phenyl-4-(thiophen-2-yl)-1H-pyrrol-3-yl) ethanone (Table 2, Entry 17): Brown solid, mp 137-142°C. IR (KBr) 2922, 2852, 1636, 1497, 1380, 1232 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ= 7.42-7.51 (m, 3H), 7.25-7.33 (m, 3H), 6.99-7.06 (m, 2H), 6.74 (s, 1H), 2.40 (s, 3H), 2.17 (s, 3H) ppm; ¹³C NMR (75MHz CDCl₃, TMS) δ 13.0, 29.7, 111.2, 121.9, 122.6, 125.0, 126.2, 127.0, 127.2, 128.2, 129.4, 135.6, 196.7 ppm. ESI-MS: 282 (M+H)⁺.



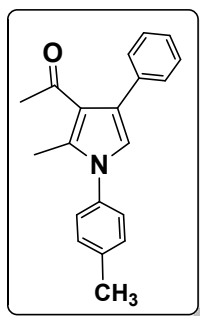
1-(4-(furan-2-yl)-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (Table 2, Entry 18): Brown solid, mp 107-110°C. IR (KBr) 2924, 2850, 1644, 1495, 1444, 1222 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ= 7.54-7.60 (m, 3H), 7.22-7.31 (m, 3H), 6.95-7.04 (m, 2H), 6.68 (s, 1H), 2.40 (s, 3H), 2.10 (s, 3H) ppm; ¹³C NMR (75MHz CDCl₃, TMS) δ 12.8, 29.6, 110.8, 121.7, 122.6, 126.2, 127.2, 128.2, 129.4, 135.6, 141.9, 154.3, 196.7 ppm. ESI-MS: 266 (M+H)⁺.



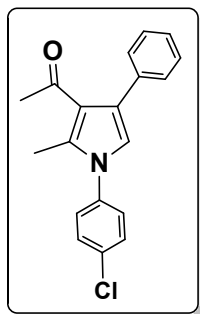
1-(4-ethyl-2-methyl-1-phenyl-1H-pyrrol-3-yl)ethanone (Table 2, Entry 19): Brown oil. IR (KBr) 2922, 2852, 1650, 1501, 1444, 1220 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ= 7.40-7.47 (m, 2H), 7.23-7.26 (m, 2H), 7.08-7.10 (m, 1H), 6.45 (s, 1H), 2.75 (q, *J* = 7.3 Hz, 2H), 2.46 (s, 3H), 2.38 (s, 3H), 0.88 (t, *J* = 7.3 Hz, 3H) ppm; ¹³C NMR (75MHz, CDCl₃, TMS) δ 12.8, 15.0, 25.2, 30.1, 116.0, 120.2, 121.5, 122.6, 126.0, 128.9, 129.4, 135.6, 141.2, 199.7 ppm. ESI-MS: 228 (M+H)⁺.



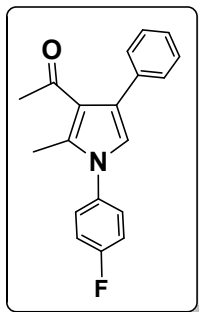
1-(1-(4-methoxyphenyl)-2-methyl-4-phenyl-1H-pyrrol-3-yl)ethanone (Table 3, Entry 1): Light yellow solid, mp 92-95°C. IR (KBr) 2922, 2852, 1651, 1501, 1412, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.36-7.38 (m, 4H), 7.24 (d, J = 8.9 Hz, 3H), 6.98 (d, J = 8.9 Hz, 2H), 6.62 (s, 1H), 3.86 (s, 3H), 2.37 (s, 3H), 2.07 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.7, 31.0, 55.5, 110.0, 114.3, 120.7, 122.0, 125.9, 126.6, 127.3, 128.1, 129.2, 131.5, 135.6, 159.1, 197.6 ppm. HRMS: m/z calcd for $\text{C}_{20}\text{H}_{19}\text{NNaO}_2$ 328.1313; found 328.1310.



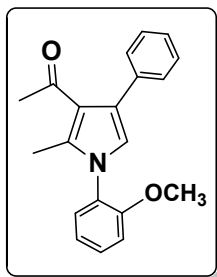
1-(2-methyl-4-phenyl-1-p-tolyl-1H-pyrrol-3-yl) ethanone (Table 3, Entry 2): Brown oil. IR (KBr) 3022, 2924, 1649, 1498, 1408, 1223 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.38-7.45 (m, 3H), 7.32 (d, J = 7.7 Hz, 2H), 7.23-7.25 (m, 2H), 7.20 (d, J = 7.7 Hz, 2H), 6.60 (s, 1H), 2.40 (s, 6H), 2.09 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.8, 29.6, 30.9, 111.8, 120.4, 122.4, 125.2, 126.1, 128.2, 128.4, 129.0, 130.4, 132.5, 134.4, 136.0, 138.6, 157.8, 196.9 ppm. HRMS: m/z calcd for $\text{C}_{20}\text{H}_{20}\text{NO}$ (M+1) 290.1544; found 290.1548.



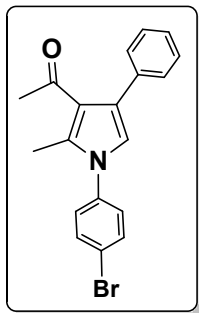
1-(1-(4-chlorophenyl)-2-methyl-4-phenyl-1H-pyrrol-3-yl)ethanone (Table 3, Entry 3)
: White solid, mp 130-132°C. IR (KBr) 2930, 2850, 1651, 1505, 1408, 1224 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ= 7.42-7.48 (m, 3H), 7.26-7.33 (m, 6H), 6.62 (s, 1H), 2.39 (s, 3H), 2.09 (s, 3H) ppm; ¹³C NMR (75MHz CDCl₃, TMS) δ 12.9, 29.6, 114.2, 120.4, 122.6, 125.2, 126.8, 128.0, 128.4, 129.2, 130.4, 135.5, 137.0, 197.0 ppm. HRMS: *m/z* calcd for C₁₉H₁₆ClNNaO 332.0818; found 332.0813.



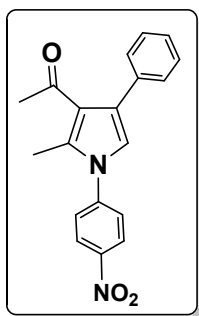
1-(1-(4-fluorophenyl)-2-methyl-4-phenyl-1H-pyrrol-3-yl)ethanone (Table 3, Entry 4)
: Brown solid, mp 79-83°C. IR (KBr) 3051, 2924, 1650, 1509, 1406, 1222 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ= 7.37 (brs, 4H), 7.29-7.33 (m, 3H), 7.18 (t, *J* = 8.6 Hz, 2H), 6.63 (s, 1H), 2.38 (s, 3H), 2.06 (s, 3H) ppm; ¹³C NMR (75MHz, CDCl₃, TMS) δ 12.9, 31.4, 111.6, 120.4, 121.8, 125.2, 126.9, 128.0, 128.6, 129.2, 130.5, 135.0, 153.4, 196.6 ppm. ESI-MS: 294 (M+H)⁺.



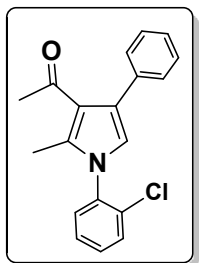
1-(1-(2-methoxyphenyl)-2-methyl-4-phenyl-1H-pyrrol-3-yl)ethanone (Table 3, Entry 5)
: Pale yellow solid, mp 93-96°C. IR (KBr) 2922, 2850, 1649, 1499, 1410, 1226 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ= 7.33-7.37 (m, 4H), 7.20 (d, *J* = 7.7 Hz, 3H), 7.05 (d, *J* = 7.7 Hz, 2H), 6.56 (s, 1H), 3.82 (s, 3H), 2.30 (s, 3H), 2.09 (s, 3H) ppm; ¹³C NMR (75MHz, CDCl₃, TMS) δ 12.9, 31.0, 55.0, 110.9, 114.6, 121.0, 122.5, 125.5, 127.0, 127.3, 128.5, 129.4, 131.2, 135.4, 157.1, 197.6 ppm. HRMS: *m/z* calcd for C₂₀H₁₉NNaO₂ 328.1313; found 328.1310.



1-(1-(4-bromophenyl)-2-methyl-4-phenyl-1H-pyrrol-3-yl)ethanone (Table 3, Entry 6): Red solid, mp 122-125°C. IR (KBr) 3115, 2924, 1649, 1500, 1406, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.60 (d, J = 8.3 Hz, 2H), 7.36 (brs, 3H), 7.17-7.21 (m, 4H), 6.62 (s, 1H), 2.38 (s, 3H), 2.06 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 13.1, 31.1, 111.2, 120.8, 122.6, 124.5, 125.1, 126.1, 127.3, 128.0, 128.5, 129.4, 132.0, 135.3, 137.6, 139.0, 196.3 ppm. HRMS: m/z calcd for $\text{C}_{19}\text{H}_{17}\text{BrNO}$ (M+1) 354.0493; found 354.0488.

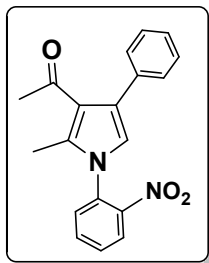


1-(2-methyl-1-(4-nitrophenyl)-4-phenyl-1H-pyrrol-3-yl) ethanone (Table 3, Entry 7): Yellow oil. IR (KBr) 2922, 2853, 1649, 1503, 1410, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 8.40 (d, J = 8.3 Hz, 2H), 7.50-7.62 (m, 4H), 7.45-7.48 (m, 2H), 7.38 (s, 1H), 6.78 (s, 1H), 2.42 (s, 3H), 2.16 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.9, 31.1, 110.0, 116.5, 120.5, 121.6, 122.6, 123.6, 124.5, 126.2, 126.9, 127.5, 129.0, 129.5, 143.9, 146.2, 199.0 ppm. HRMS: m/z calcd for $\text{C}_{19}\text{H}_{17}\text{N}_2\text{O}_3$ (M+1) 321.1239; found 321.1225.

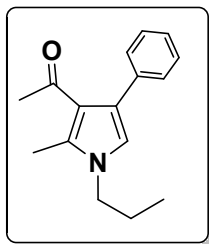


1-(1-(2-chlorophenyl)-2-methyl-4-phenyl-1H-pyrrol-3-yl)ethanone (Table 3, Entry 8): White solid, mp 132-134°C. IR (KBr) 2930, 2851, 1649, 1505, 1402, 1222 cm^{-1} ; ^1H

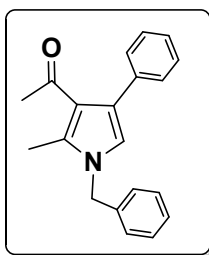
NMR (300MHz, CDCl₃, TMS) δ = 7.53-7.56 (m, 1H), 7.28-7.43 (m, 8H), 6.53 (s, 1H), 2.27 (s, 3H), 2.07 (s, 3H) ppm; ¹³C NMR (75MHz, CDCl₃, TMS) δ 12.8, 29.8, 114.0, 121.0, 122.8, 125.0, 127.0, 128.2, 128.6, 129.0, 131.0, 135.5, 137.2, 157.0, 198.2 ppm. HRMS: *m/z* calcd for C₁₉H₁₆ClNNaO 332.0818; found 332.0813.



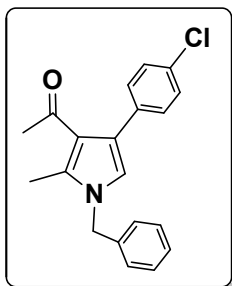
1-(2-methyl-1-(2-nitrophenyl)-4-phenyl-1H-pyrrol-3-yl) ethanone (Table 3, Entry 9): yellow oil. IR (KBr) 2924, 2850, 1651, 1499, 1409, 1224 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ = 8.38 (d, *J* = 8.3 Hz, 2H), 7.54-7.60 (m, 4H), 7.43-7.48 (m, 2H), 7.35 (s, 1H), 6.69 (s, 1H), 2.40 (s, 3H), 2.19 (s, 3H) ppm; ¹³C NMR (75MHz, CDCl₃, TMS) δ 12.8, 31.0, 110.2, 117.0, 120.9, 121.2, 122.5, 124.0, 125.0, 126.2, 127.0, 127.5, 128.7, 129.5, 144.2, 145.8, 197.8 ppm. HRMS: *m/z* calcd for C₁₉H₁₇N₂O₃ (M+1) 321.1239; found 321.1225.



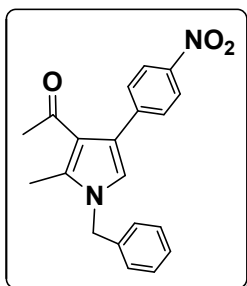
1-(2-methyl-4-phenyl-1-propyl-1H-pyrrol-3-yl)ethanone (Table 3, Entry 10): Brown oil. IR (KBr) 2924, 2850, 1651, 1499, 1409, 1224 cm⁻¹; ¹H NMR (300MHz, CDCl₃, TMS) δ = 7.25-7.33 (m, 5H), 6.44 (s, 1H), 3.80 (t, *J* = 6.7 Hz, 2H), 2.52 (s, 3H), 2.37 (s, 3H), 1.70 (dd, *J* = 6.7 Hz, 2H), 0.96 (t, *J* = 6.7 Hz, 3H) ppm; ¹³C NMR (75MHz, CDCl₃, TMS) δ 12.2, 13.0, 27.5, 31.0, 56.2, 107.1, 122.5, 127.2, 127.5, 128.4, 129.2, 133.2, 137.5, 199.2 ppm. ESI-MS: 242 (M+H)⁺.



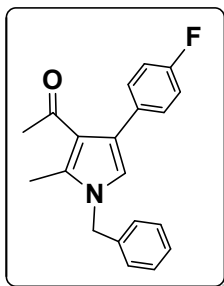
1-(1-Benzyl-2-methyl-4-phenyl-1H-pyrrol-3-yl) ethanone (Table 4, Entry 1): Brown oil. IR (KBr) 3029, 2924, 1651, 1499, 1407, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.44 (d, J = 8.3 Hz, 2H), 7.32-7.38 (m, 5H), 7.22-7.27 (m, 3H), 6.64 (s, 1H), 5.04 (s, 2H), 2.41 (s, 3H), 2.10 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.8, 31.0, 51.0, 110.2, 120.9, 125.2, 125.8, 127.0, 127.2, 127.5, 128.4, 128.8, 129.1, 129.4, 133.0, 136.2, 198.6 ppm. HRMS: m/z calcd for $\text{C}_{20}\text{H}_{19}\text{NNaO}$ 312.1364; found 312.1375.



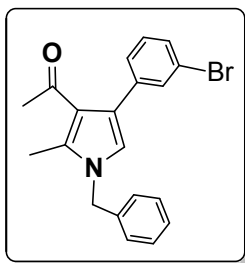
1-(1-Benzyl-4-(4-chlorophenyl)-2-methyl-1H-pyrrol-3-yl) ethanone (Table 4, Entry 2): Yellow oil. IR (KBr) 3030, 2928, 1649, 1501, 1410, 1224 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.28-7.37 (m, 4H), 7.26 (d, J = 8.3 Hz, 2H), 7.20-7.24 (m, 3H), 6.60 (s, 1H), 5.05 (s, 2H), 2.40 (s, 3H), 2.09 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.6, 31.1, 51.1, 120.0, 122.2, 123.8, 126.8, 127.5, 128.4, 128.8, 129.4, 133.0, 134.5, 135.2, 136.2, 197.9 ppm. ESI-MS: 324 (M+H) $^+$.



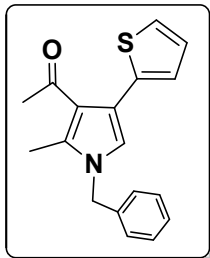
1-(1-Benzyl-2-methyl-4-(4-nitrophenyl)-1H-pyrrol-3-yl) ethanone (Table 4, Entry 3): Red liquid. IR (KBr) 3028, 2926, 1651, 1506, 1414, 1220 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 8.25 (d, J = 8.3 Hz, 2H), 7.46 (d, J = 8.3 Hz, 2H), 7.22-7.38 (m, 3H), 7.09 (d, J = 7.1 Hz, 2H), 6.62 (s, 1H), 5.08 (s, 2H), 2.42 (s, 3H), 2.12 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.0, 31.2, 51.0, 120.9, 122.2, 123.5, 123.7, 126.5, 127.4, 128.2, 129.0, 129.5, 135.2, 136.4, 143.0, 147.1, 198.9 ppm. ESI-MS: 334 (M+H) $^+$.



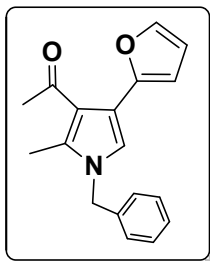
1-(1-Benzyl-4-(4-fluorophenyl)-2-methyl-1H-pyrrol-3-yl) ethanone (Table 4, Entry 4): Yellow oil. IR (KBr) 3030, 2928, 1650, 1498, 1409, 1226 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.25-7.36 (m, 5H), 6.92-7.09 (m, 4H), 6.58 (s, 1H), 5.10 (s, 2H), 2.42 (s, 3H), 2.03 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.2, 30.8, 50.8, 111.9, 120.2, 123.2, 125.7, 126.2, 127.6, 128.5, 129.2, 130.2, 135.0, 136.4, 137.0, 198.9 ppm. ESI-MS: 308 (M+H) $^+$.



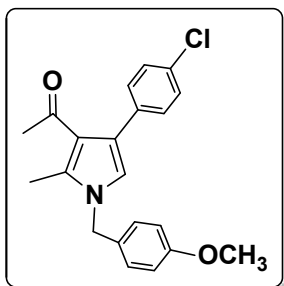
1-(1-Benzyl-4-(3-bromophenyl)-2-methyl-1H-pyrrol-3-yl) ethanone (Table 4, Entry 5): Orange yellow liquid. IR (KBr) 3110, 2924, 1651, 1502, 1406, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.58 (d, J = 8.3 Hz, 2H), 7.40 (brs, 3H), 7.10-7.18 (m, 4H), 6.62 (s, 1H), 5.06(s, 2H), 2.38 (s, 3H), 2.06 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 13.1, 30.8, 51.0, 111.2, 121.0, 122.2, 123.0, 124.6, 125.1, 126.4, 127.0, 128.0, 128.5, 129.2, 132.1, 135.6, 137.6, 139.2, 197.3 ppm. ESI-MS: 368 (M+H) $^+$.



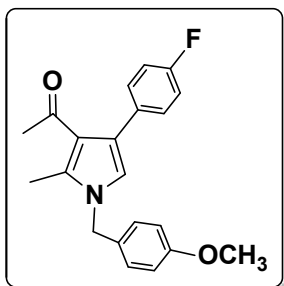
1-(1-Benzyl-2-methyl-4-(thiophen-2-yl)-1H-pyrrol-3-yl) ethanone (Table 4, Entry 6): Brown solid, mp 137-140°C. IR (KBr) 2926, 2854, 1646, 1499, 1382, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.40-7.46 (m, 3H), 7.30-7.37 (m, 3H), 7.04-7.18 (m, 2H), 6.70 (s, 1H), 5.14(s, 2H), 2.40 (s, 3H), 2.14 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 13.0, 30.7, 51.2, 109.8, 111.2, 122.0, 122.6, 125.4, 126.5, 127.0, 127.6, 128.4, 129.0, 136.0, 197.8 ppm. ESI-MS: 318 (M+Na) $^+$.



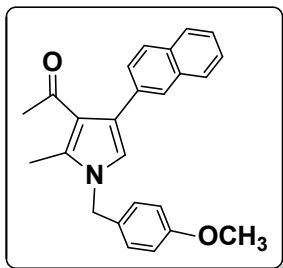
1-(1-Benzyl-4-(furan-2-yl)-2-methyl-1H-pyrrol-3-yl)ethanone (Table 4, Entry 7): Off-white solid, mp 110-114°C. IR (KBr) 3028, 2925, 1650, 1498, 1408, 1224 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.50-7.54 (m, 3H), 7.28-7.32 (m, 3H), 6.98-7.08 (m, 2H), 6.64 (s, 1H), 5.08(s, 2H), 2.42 (s, 3H), 2.10 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.9, 29.8, 51.0, 110.6, 113.0, 121.7, 125.6, 126.2, 127.9, 128.4, 129.4, 135.8, 141.9, 150.3, 197.7 ppm. ESI-MS: 280 (M+H) $^+$.



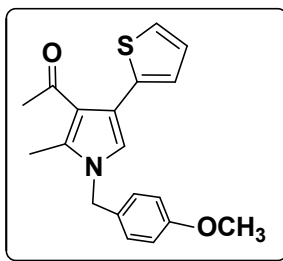
1-(4-(4-Chlorophenyl)-1-(4-methoxybenzyl)-2-methyl-1H-pyrrol-3-yl) ethanone (Table 4, Entry 8): Yellow liquid. IR (KBr) 2928, 2856, 1651, 1501, 1409, 1224 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.20-7.28 (m, 4H), 7.08 (d, J = 8.3 Hz, 2H), 6.82-6.94 (m, 2H), 6.56 (s, 1H), 5.05 (s, 2H), 3.76(s, 3H), 2.41 (s, 3H), 2.09 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.9, 30.8, 50.9, 52.8, 110.7, 114.2, 120.0, 122.6, 123.9, 127.5, 128.2, 128.8, 129.8, 133.0, 134.7, 135.2, 136.6, 156.8, 199.6 ppm. ESI-MS: 354 (M+H) $^+$.



1-(4-(4-Fluorophenyl)-1-(4-methoxybenzyl)-2-methyl-1H-pyrrol-3-yl) ethanone (Table 4, Entry 9): Off-white solid, mp 75-78°C. IR (KBr) 3030, 2926, 1649, 1496, 1410, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.20-7.26 (m, 4H), 7.10 (d, J = 7.1 Hz, 2H), 6.89-6.97 (m, 2H), 6.64 (s, 1H), 5.09 (s, 2H), 3.74 (s, 3H), 2.38 (s, 3H), 2.08 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.2, 30.8, 52.0, 54.2, 111.0, 114.2, 120.4, 123.2, 125.4, 126.2, 128.0, 128.7, 129.8, 130.8, 132.0, 136.4, 137.0, 155.2, 160.4, 199.2 ppm. ESI-MS: 338 (M+H) $^+$.



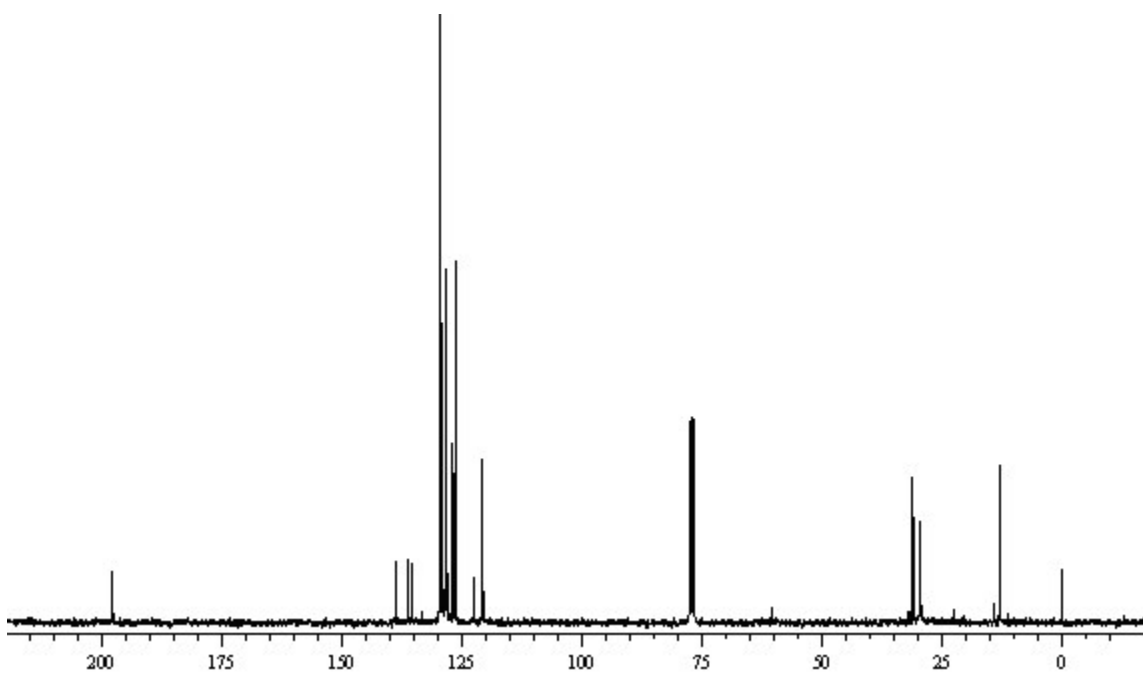
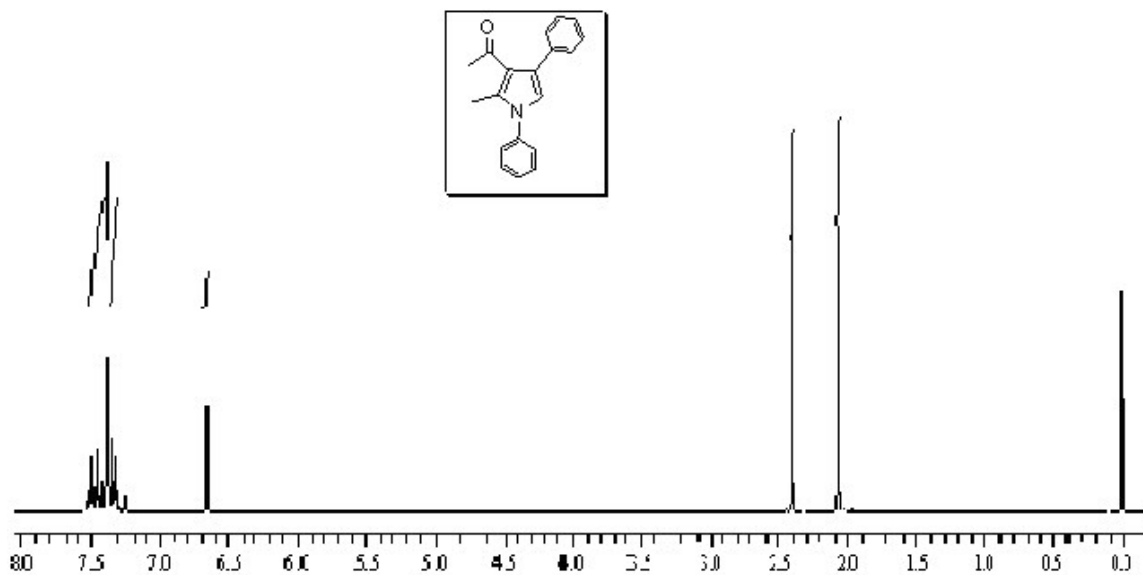
1-(1-(4-Methoxybenzyl)-2-methyl-4-(naphthalen-2-yl)-1H-pyrrol-3-yl) ethanone (Table 4, Entry 10): Yellow orange liquid. IR (KBr) 3030, 2923, 1649, 1499, 1406, 1226 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.80-7.85 (m, 5H), 7.74 (d, J = 8.3 Hz, 2H), 7.46-7.54 (m, 2H), 7.28 (d, J = 8.3 Hz, 2H), 6.70 (s, 1H), 3.80 (s, 3H), 2.43 (s, 3H), 2.10 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 12.9, 29.8, 52.0, 55.4, 108.6, 114.0, 114.2, 123.6, 124.6, 125.7, 126.4, 127.3, 128.0, 128.5, 129.3, 133.8, 134.6, 135.2, 156.9, 197.7 ppm. ESI-MS: 370 (M+H) $^+$.



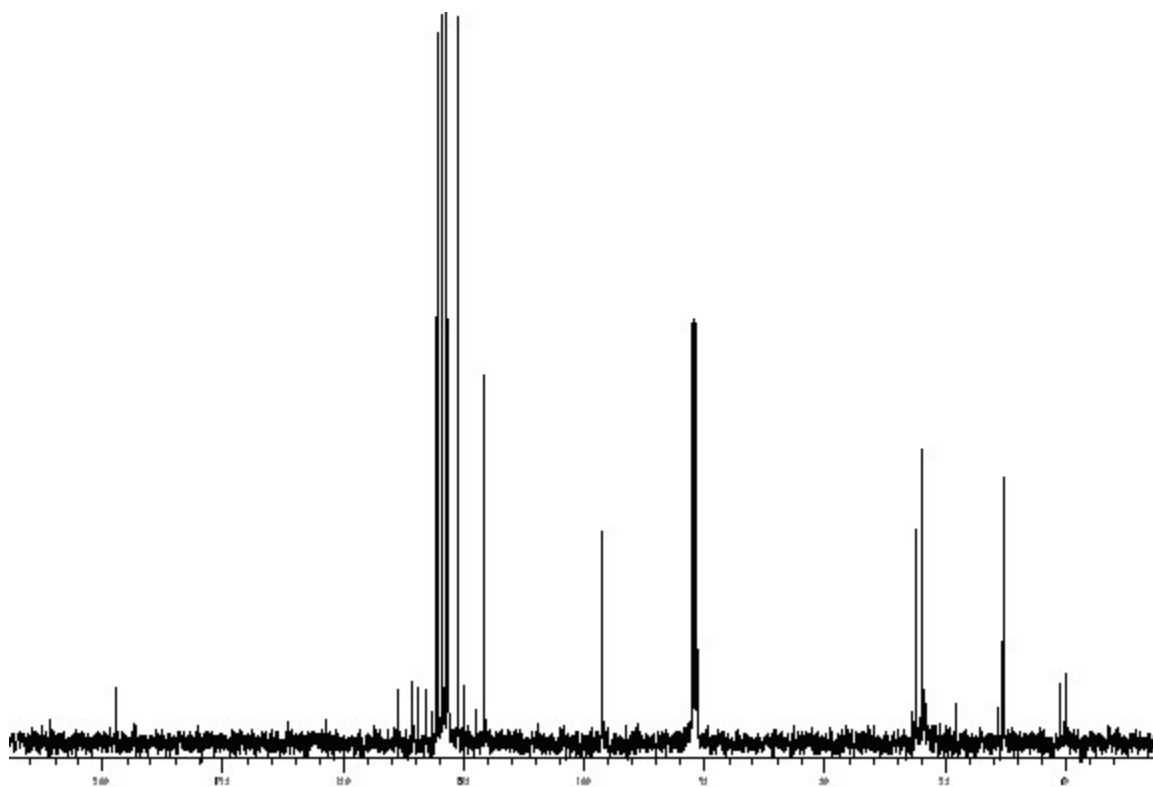
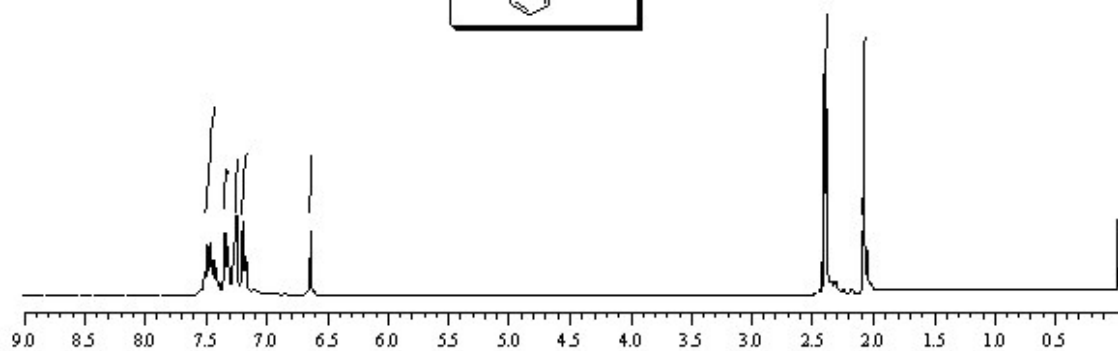
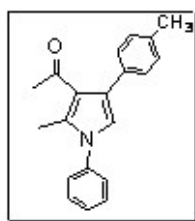
1-(1-(4-Methoxybenzyl)-2-methyl-4-(thiophen-2-yl)-1H-pyrrol-3-yl) ethanone (Table 4, Entry 11): Off-white solid, mp 82-85°C. IR (KBr) 2928, 2850, 1651, 1501, 1396, 1222 cm^{-1} ; ^1H NMR (300MHz, CDCl_3 , TMS) δ = 7.10-7.21 (m, 4H), 6.96-6.98 (m, 1H), 6.90 (d, J = 7.1 Hz, 2H), 6.64 (s, 1H), 5.10 (s, 2H), 2.40 (s, 3H), 2.09 (s, 3H) ppm; ^{13}C NMR (75MHz, CDCl_3 , TMS) δ 13.0, 31.0, 51.2, 56.0, 109.8, 110.9, 117.2, 122.0, 122.6, 125.4, 126.4, 127.2, 127.6, 128.5, 129.2, 135.9, 136.6, 157.8, 197.8 ppm. ESI-MS: 326 (M+H) $^+$.

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

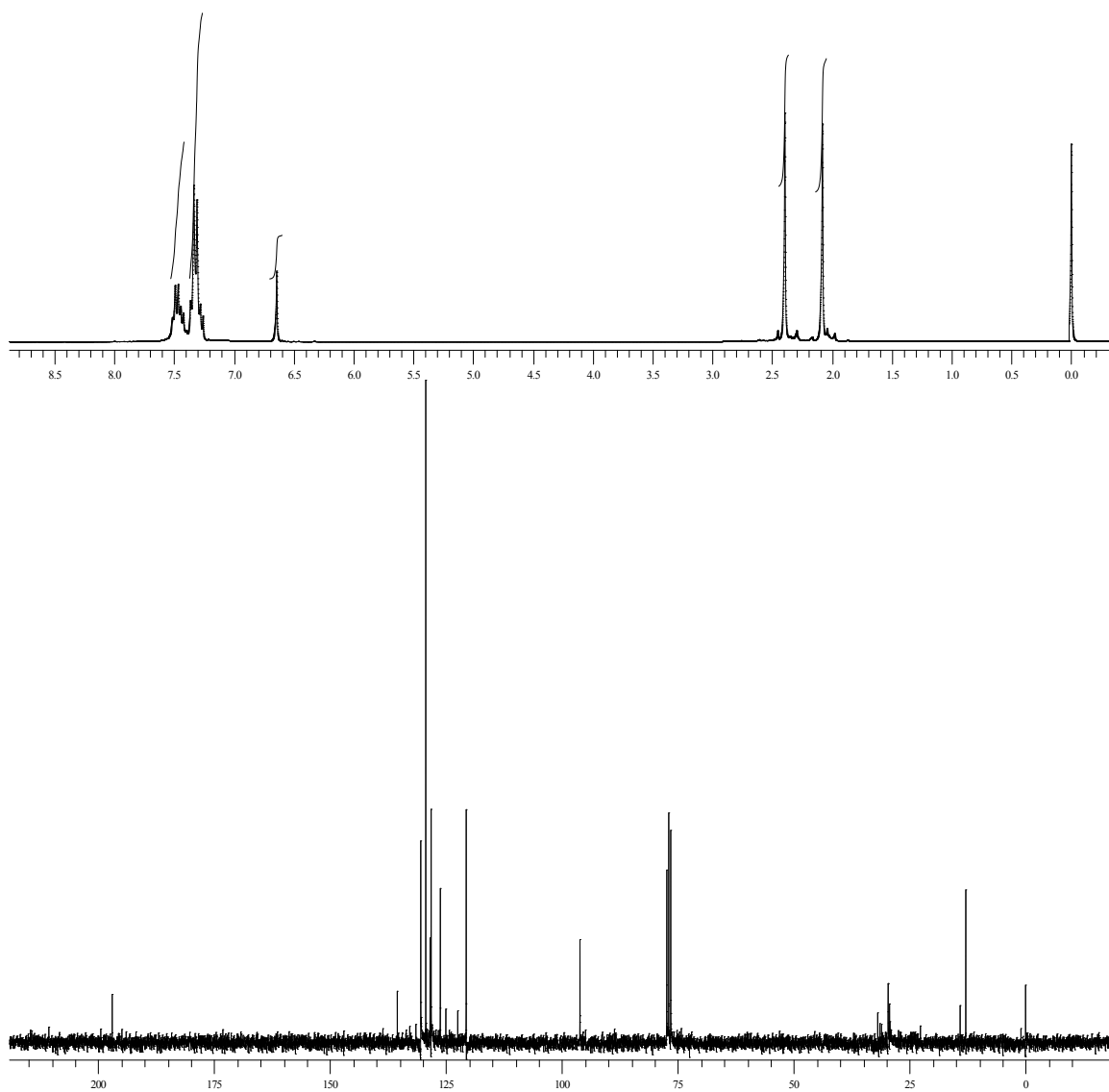
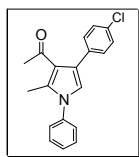
(Table 2, Entry 1)



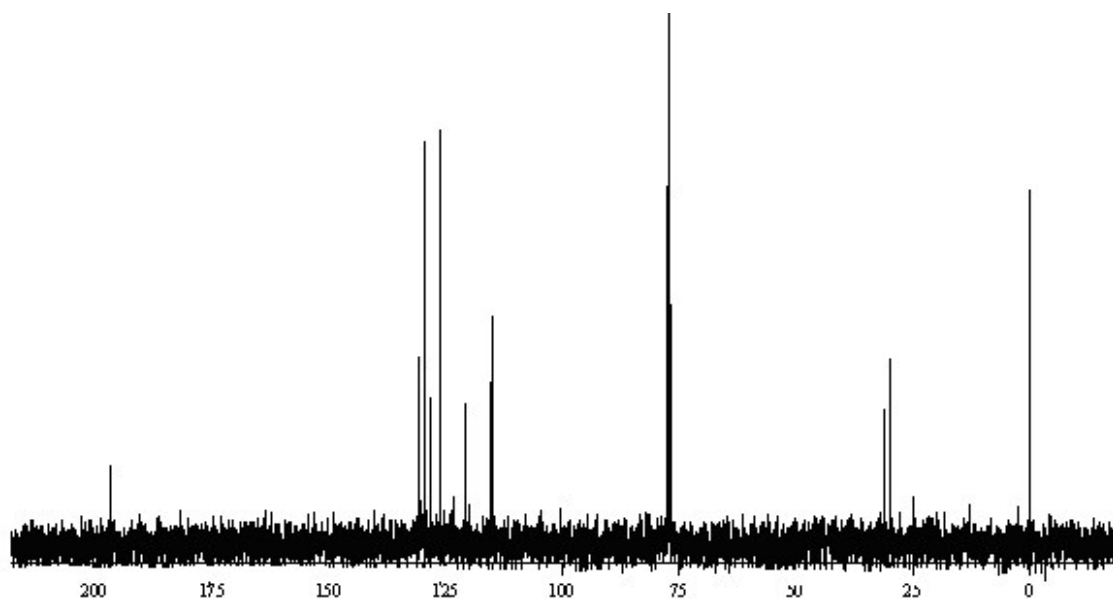
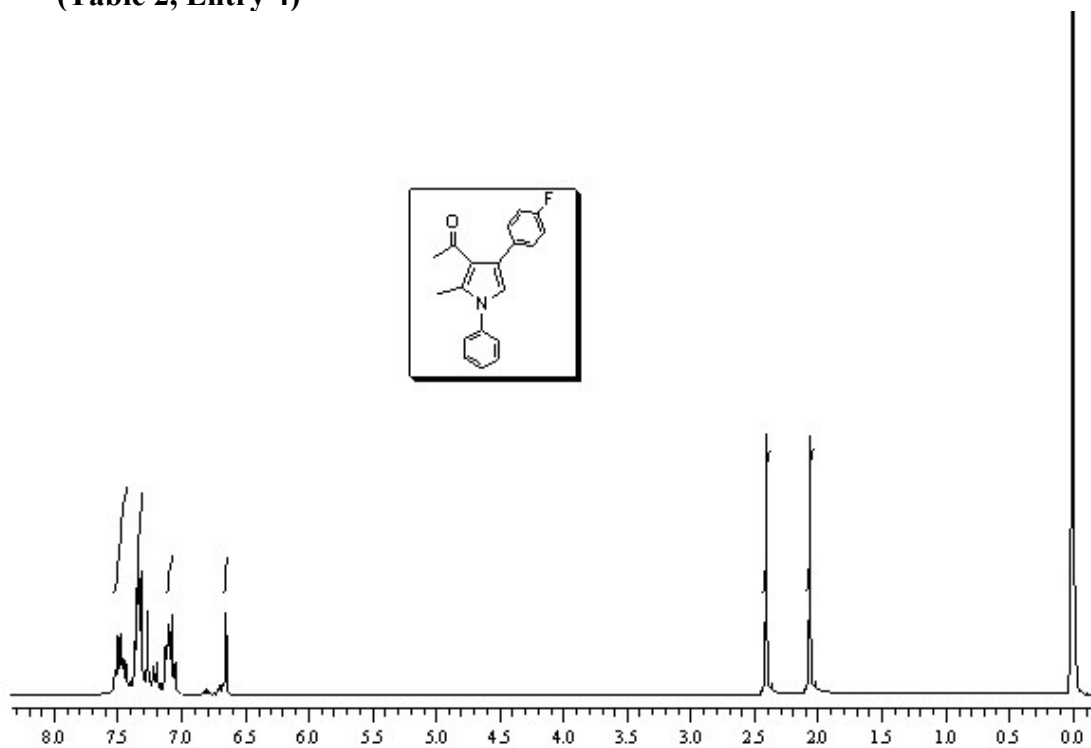
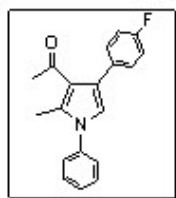
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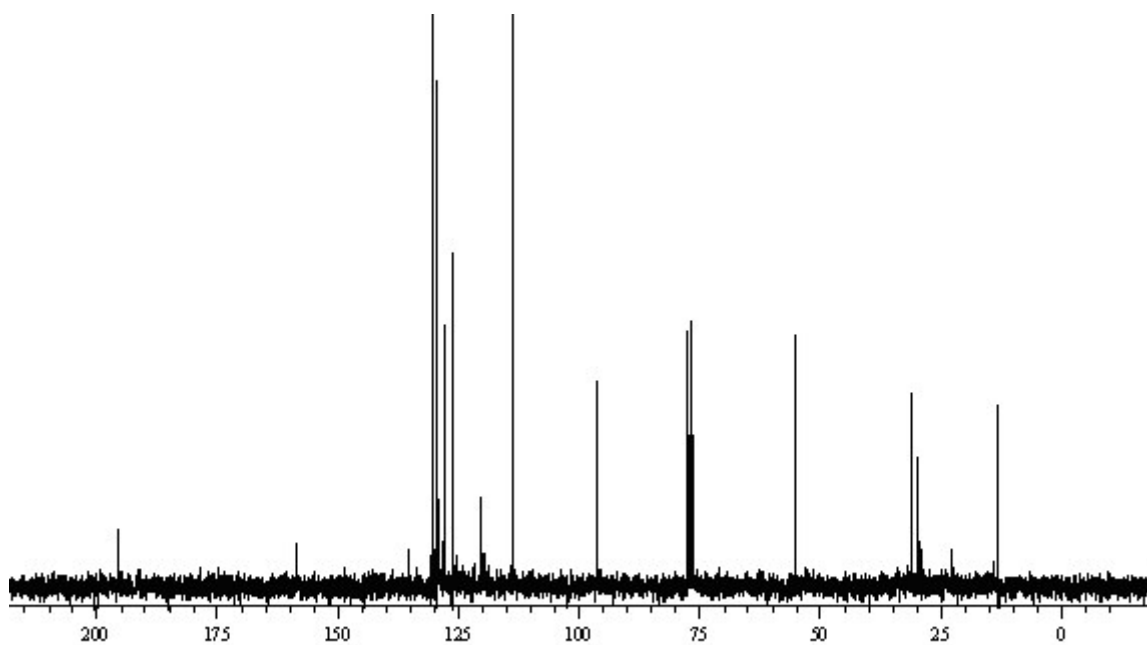
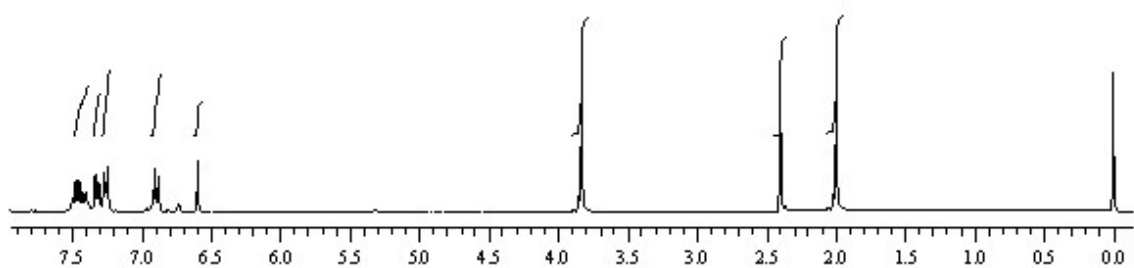
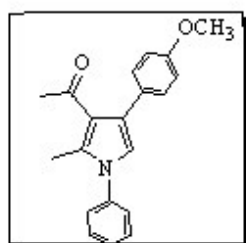
(Table 2, Entry 3)



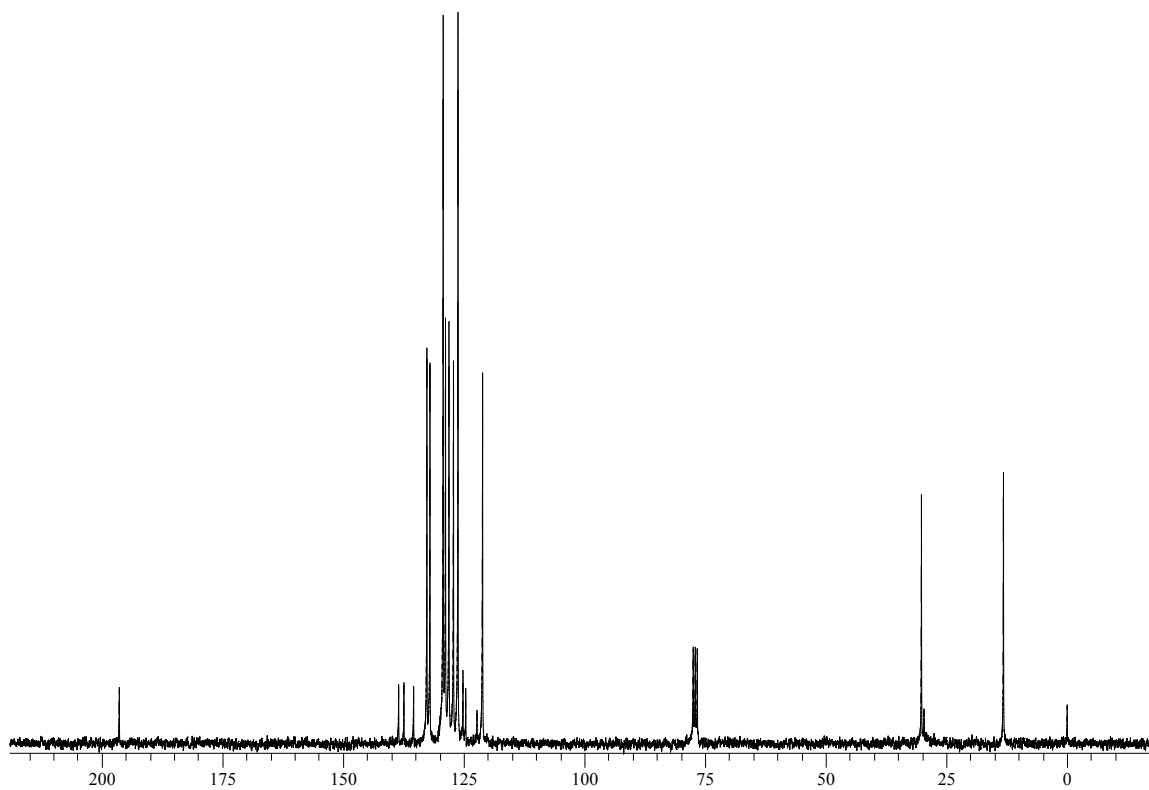
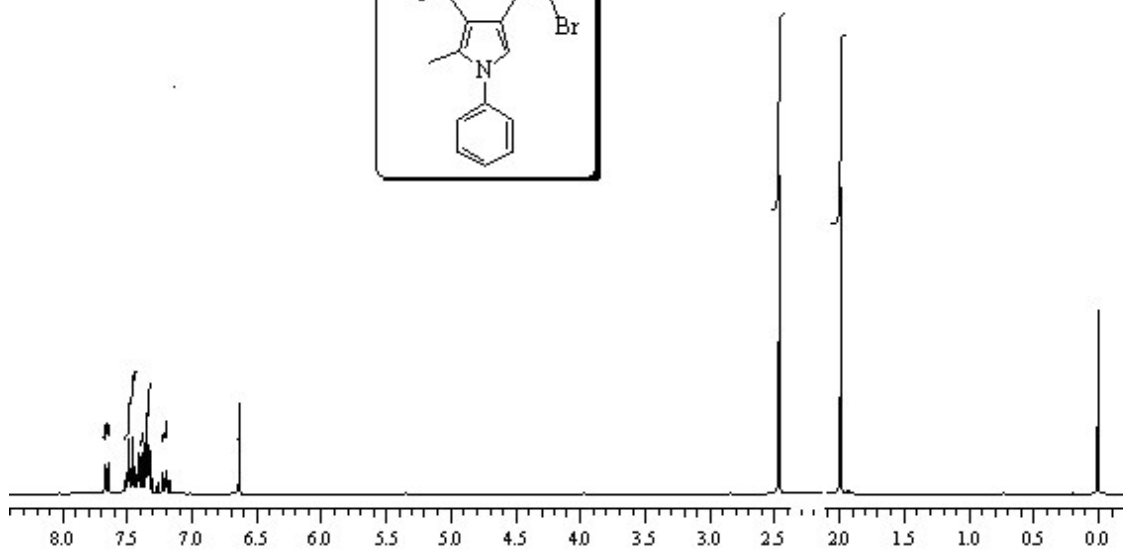
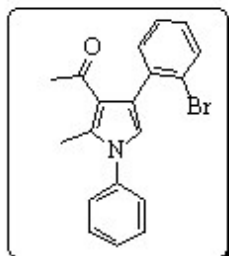
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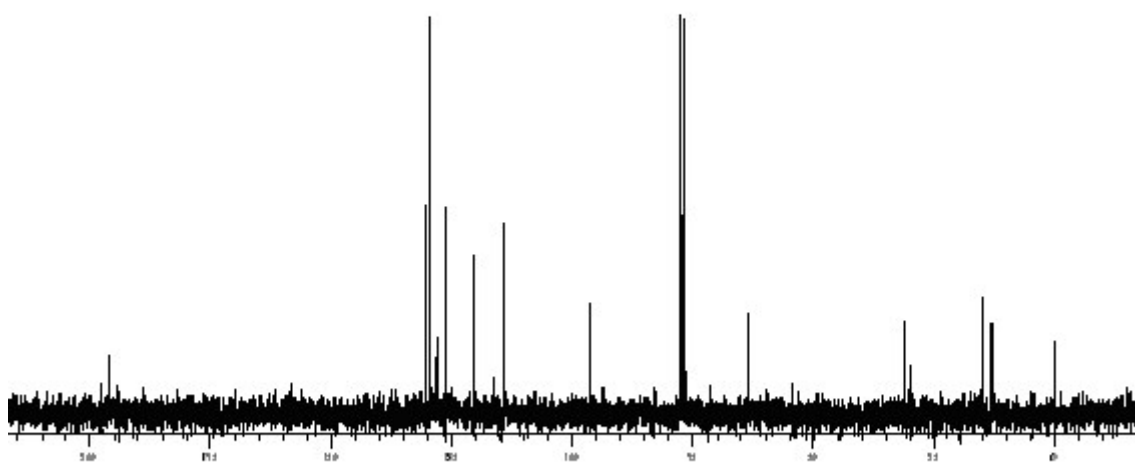
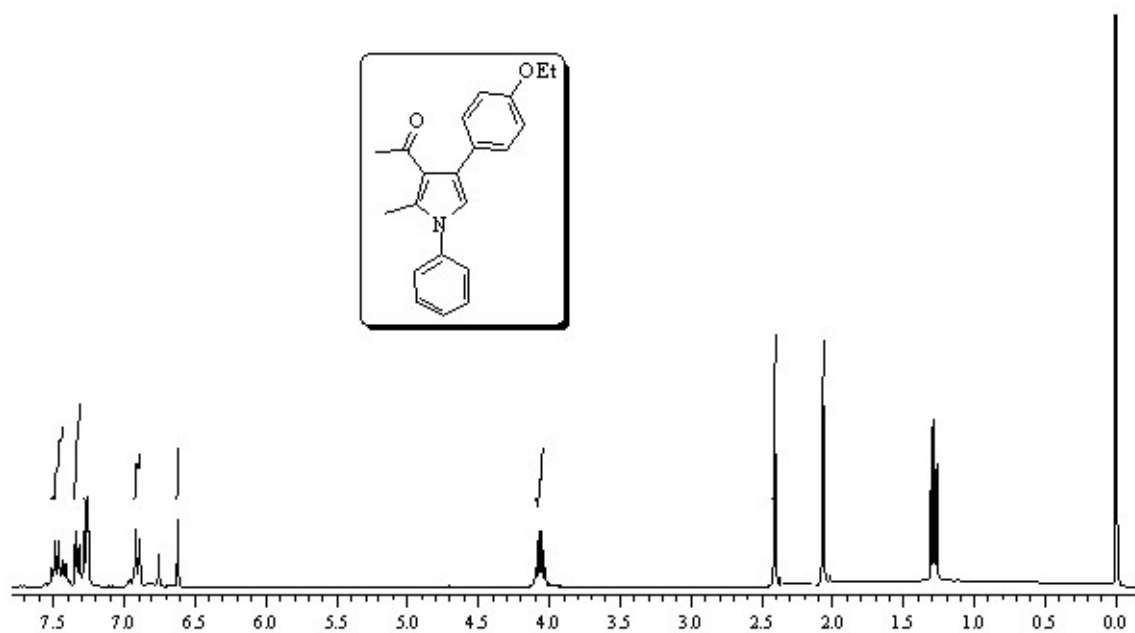
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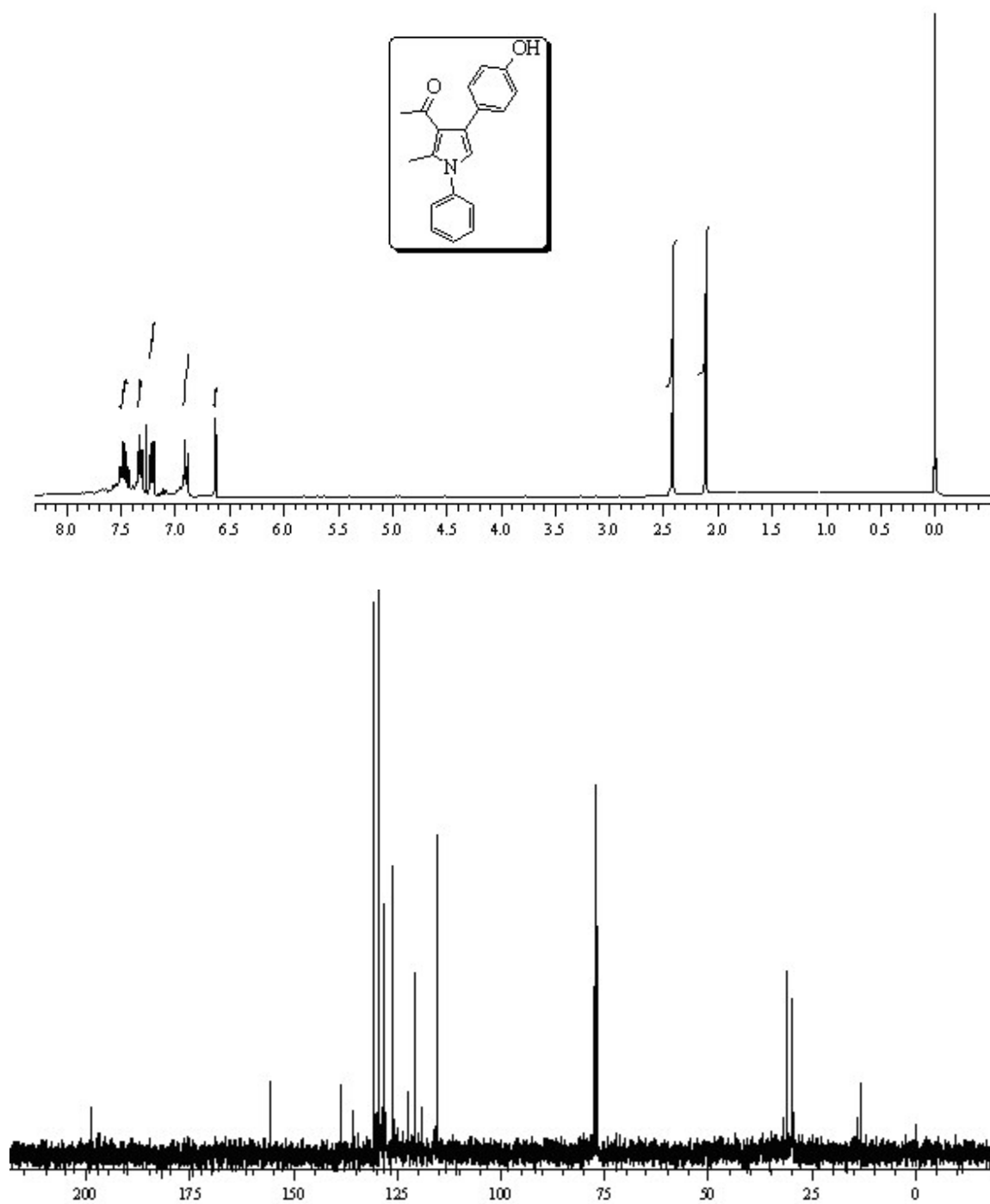
(Table 2, Entry 6)



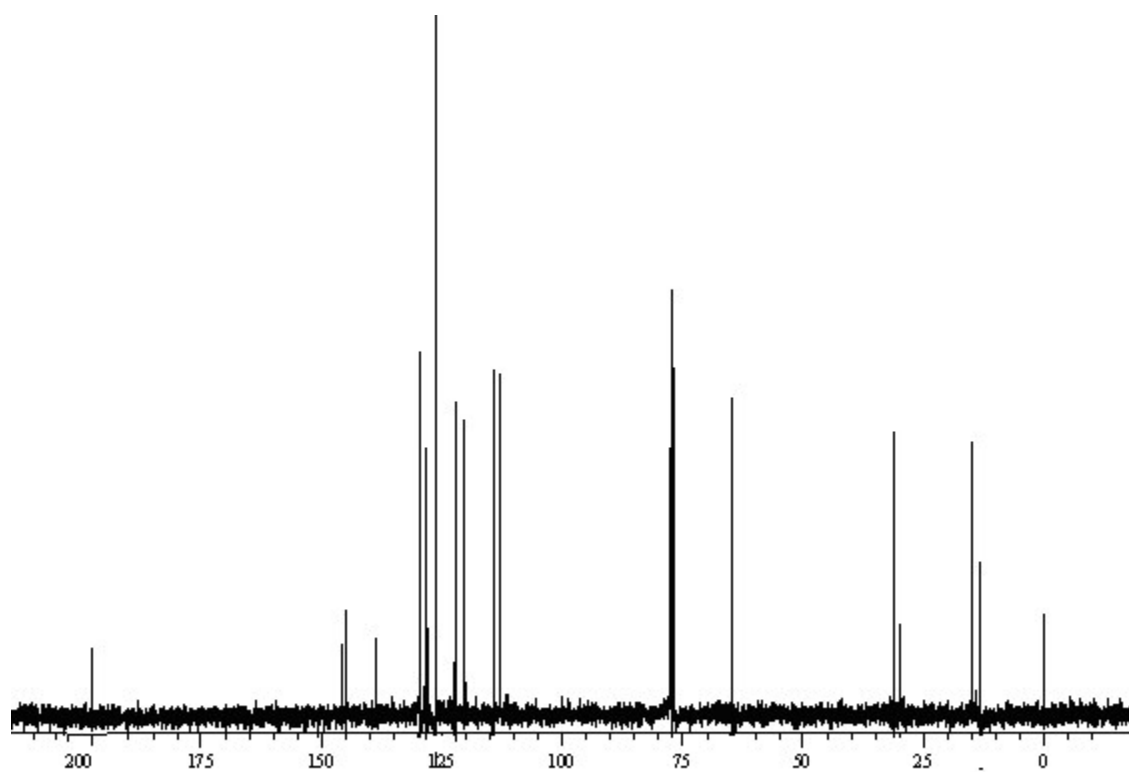
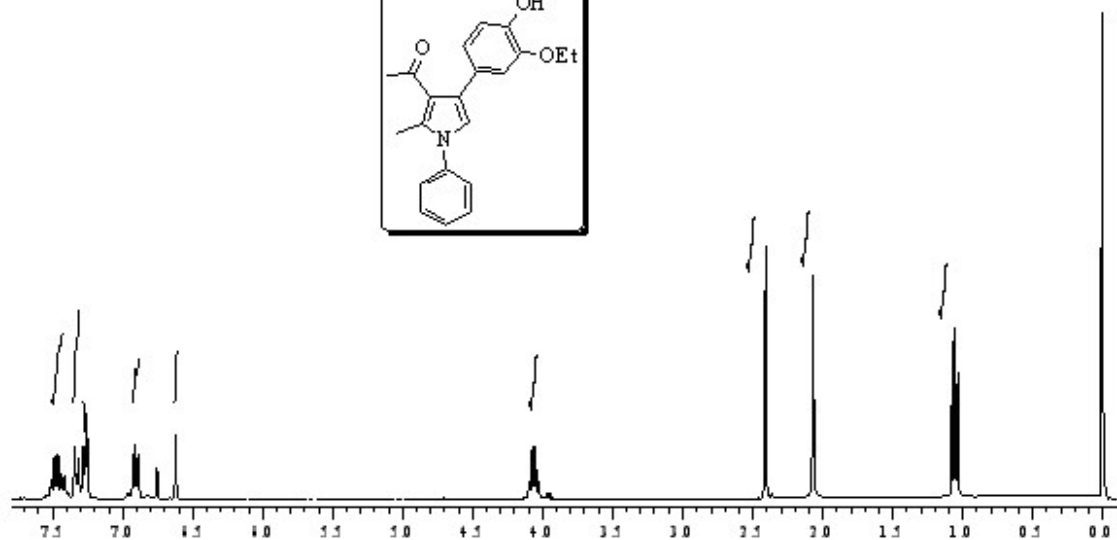
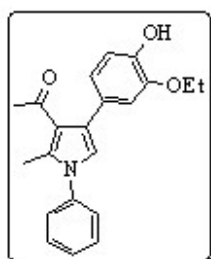
(Table 2, Entry 7)



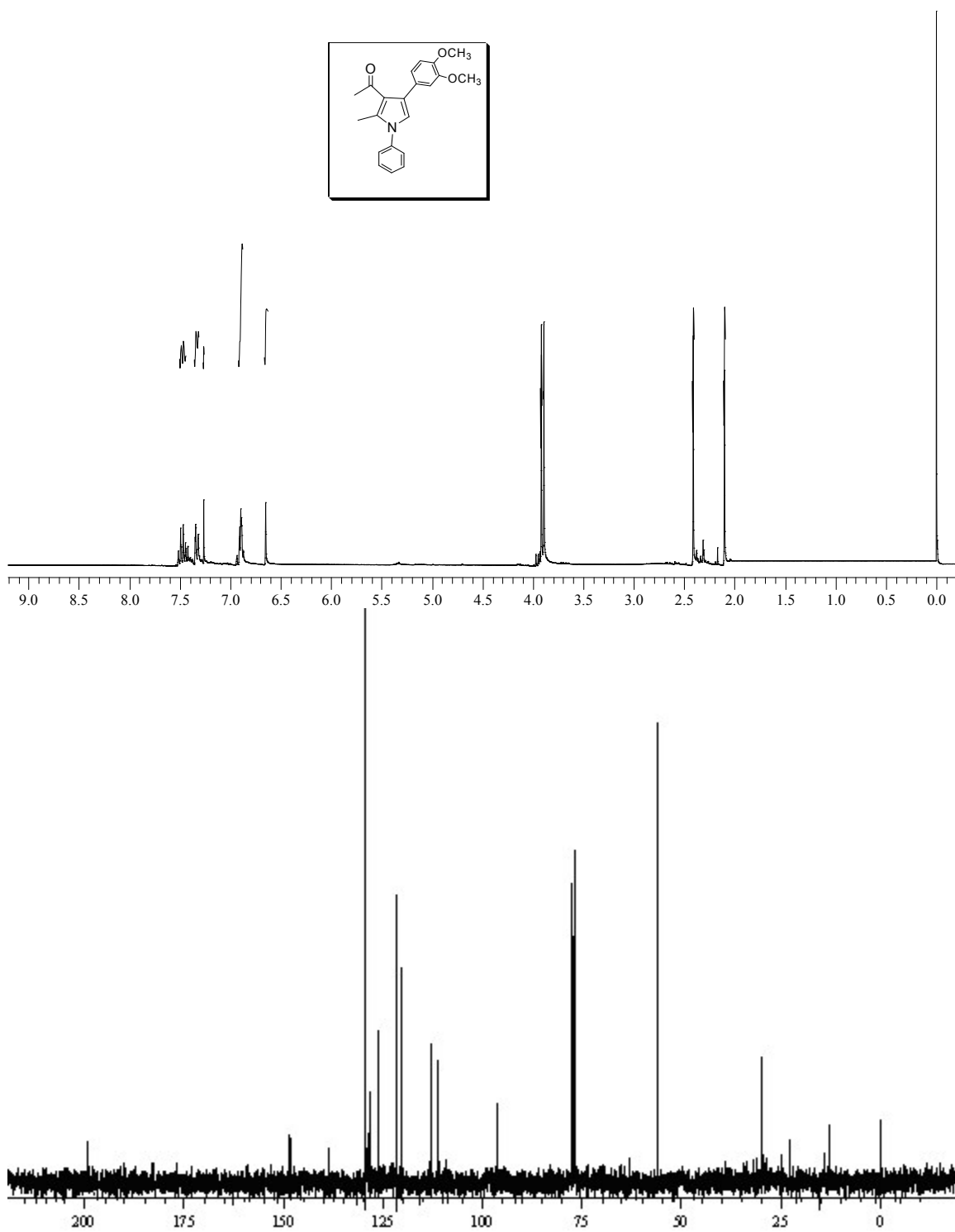
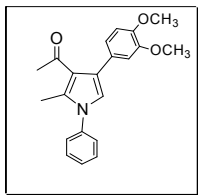
(Table 2, Entry 8)



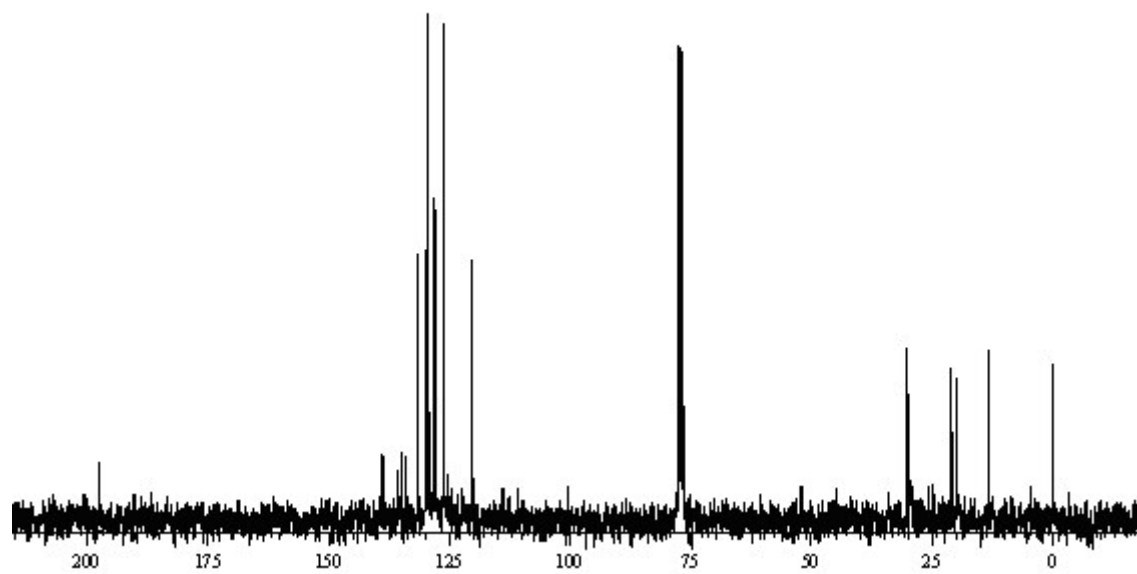
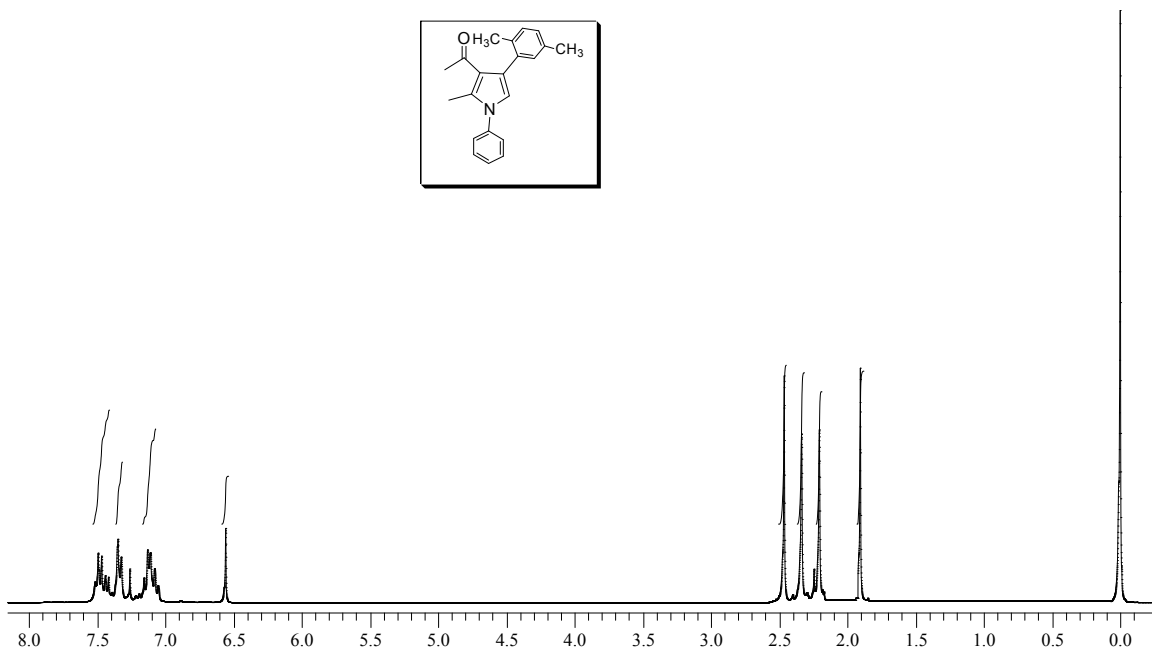
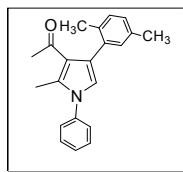
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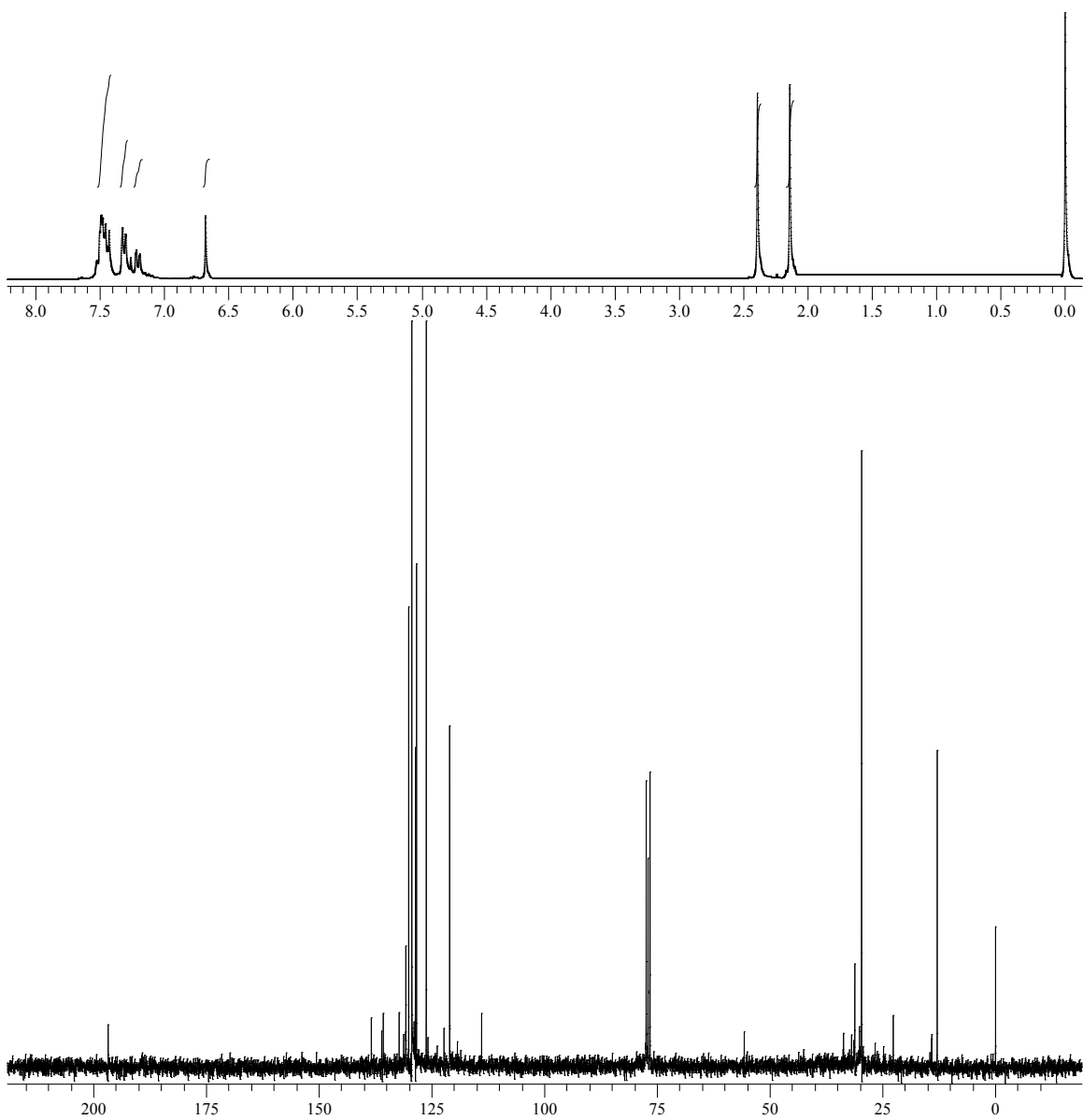
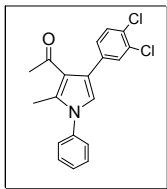
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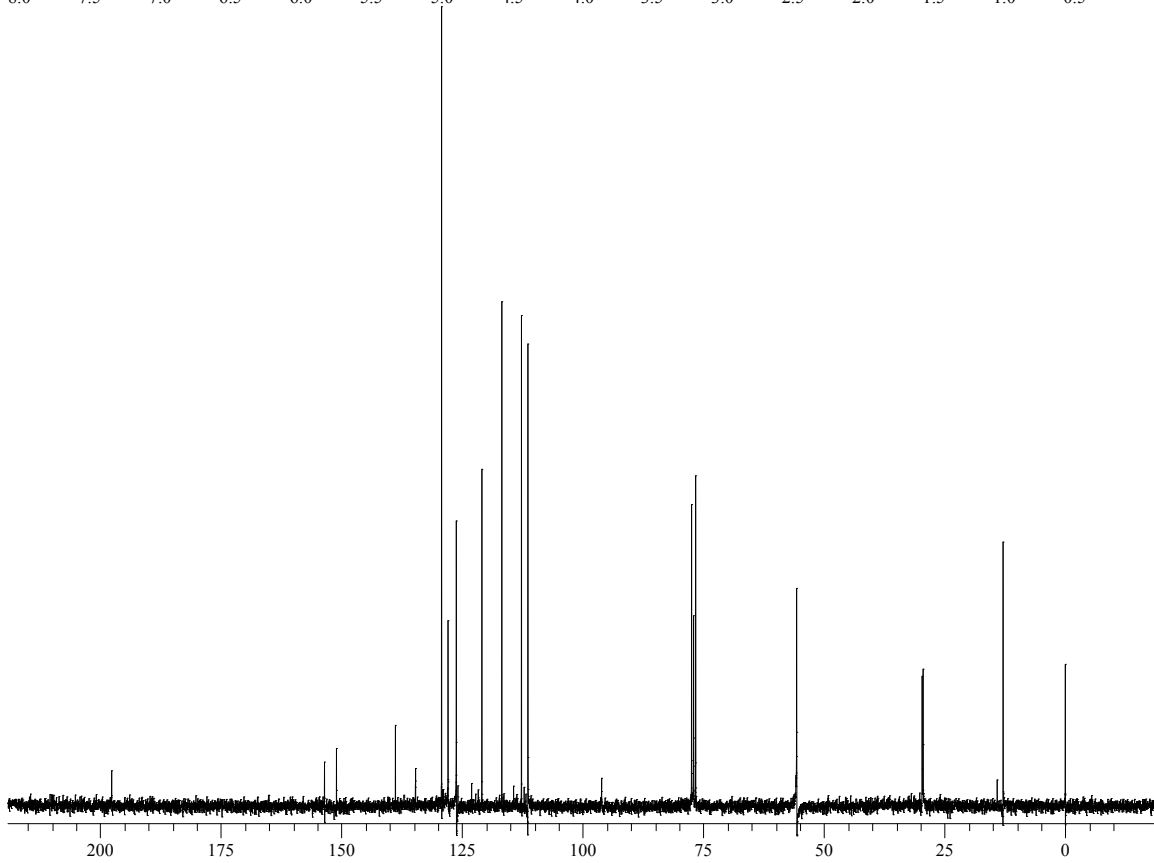
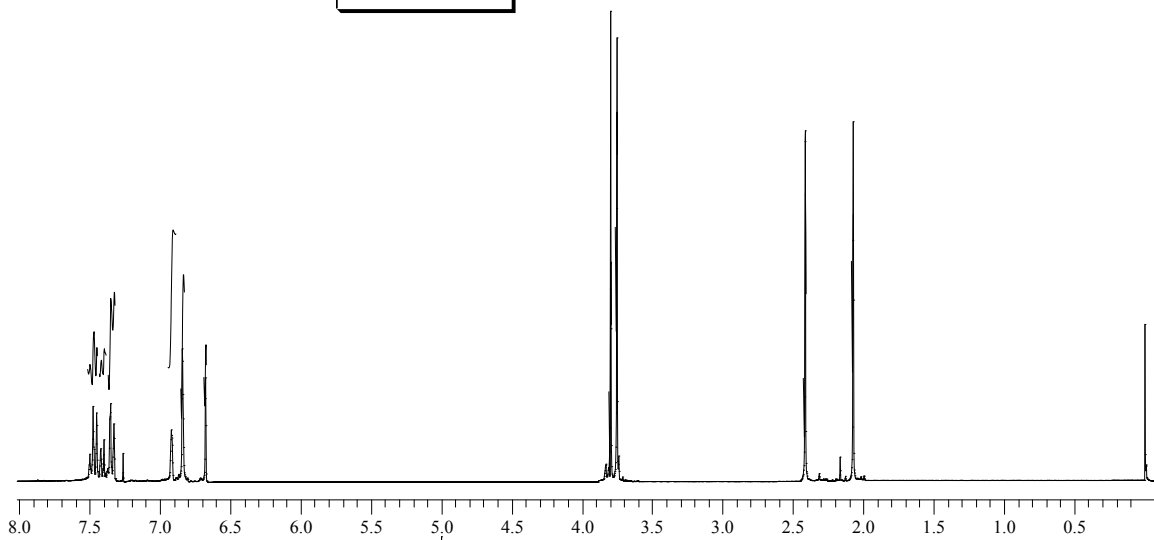
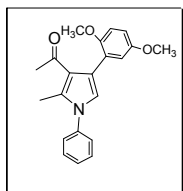
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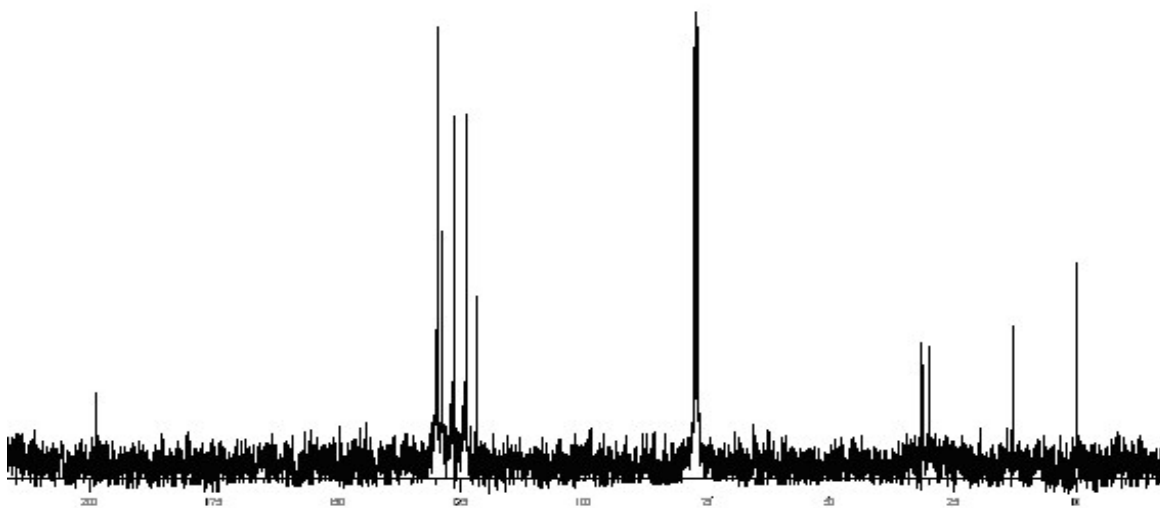
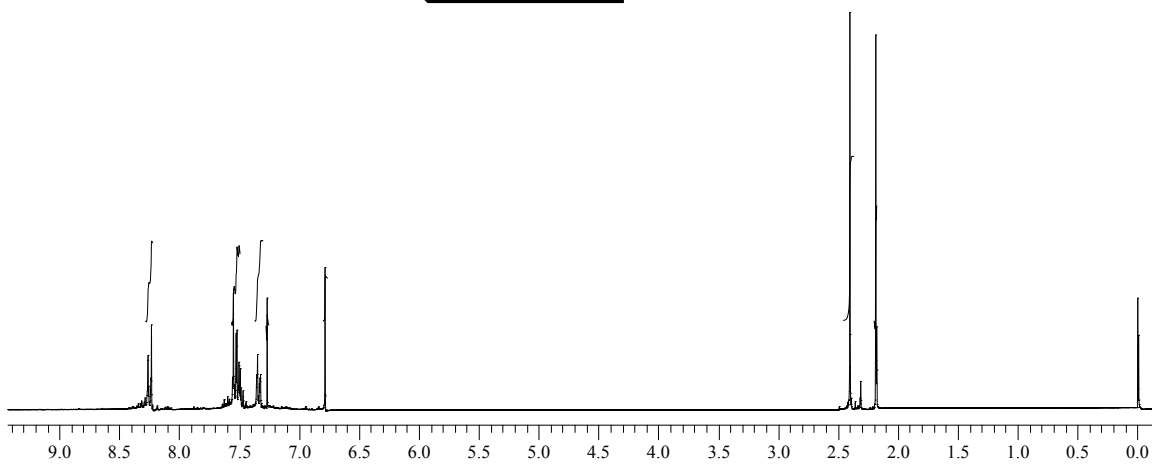
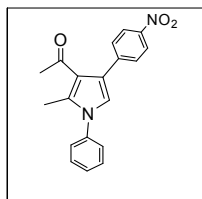
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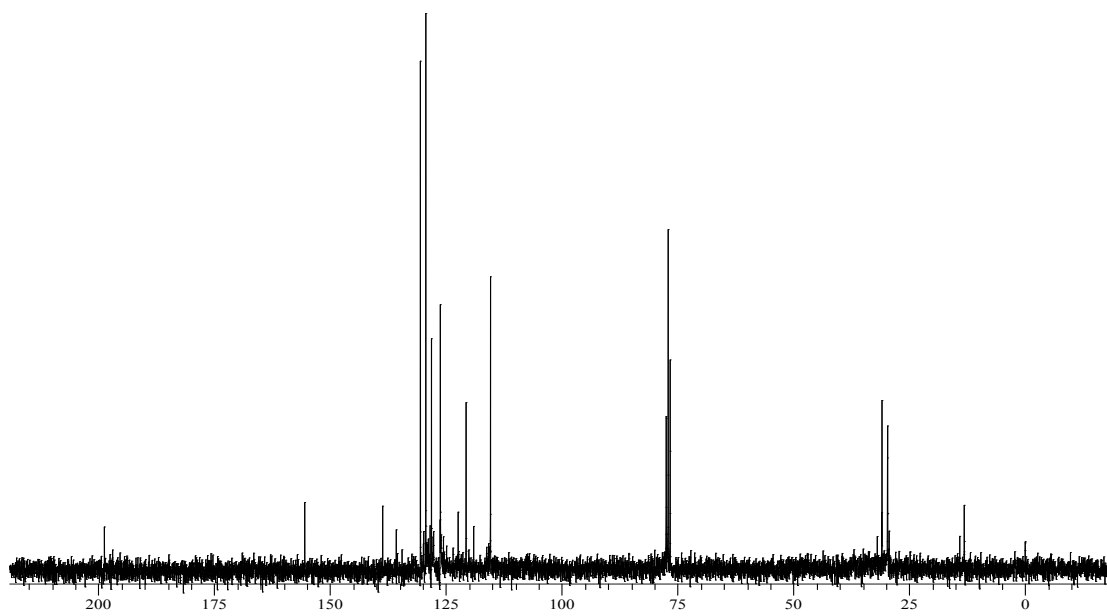
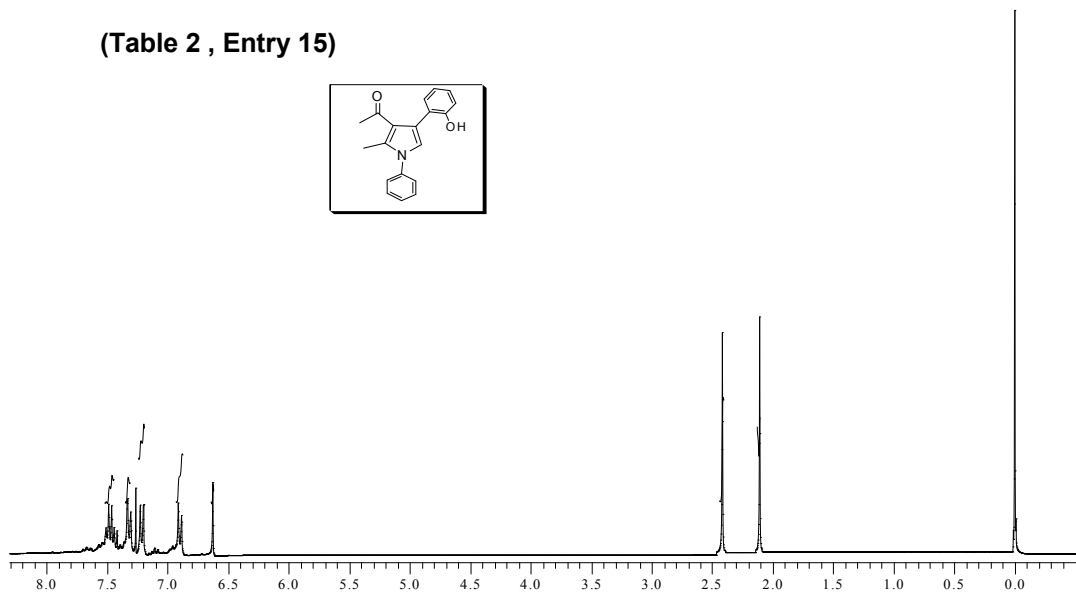
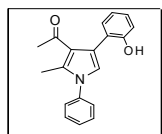
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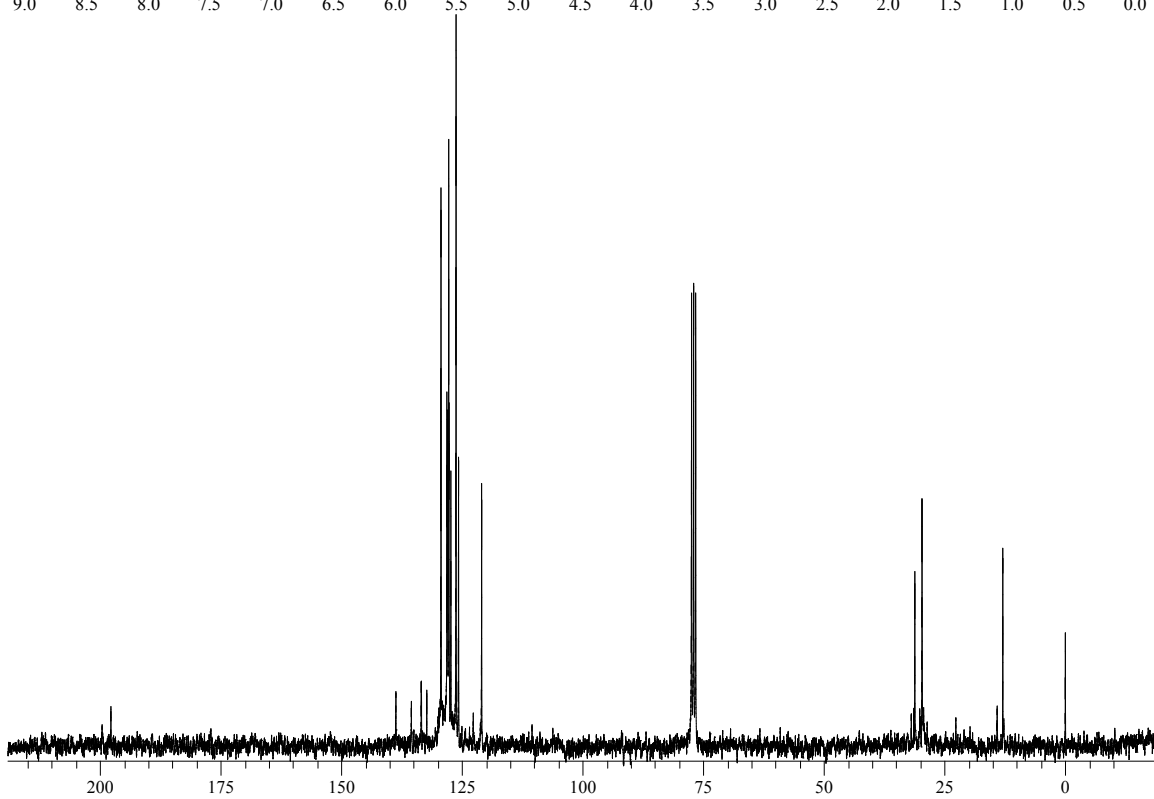
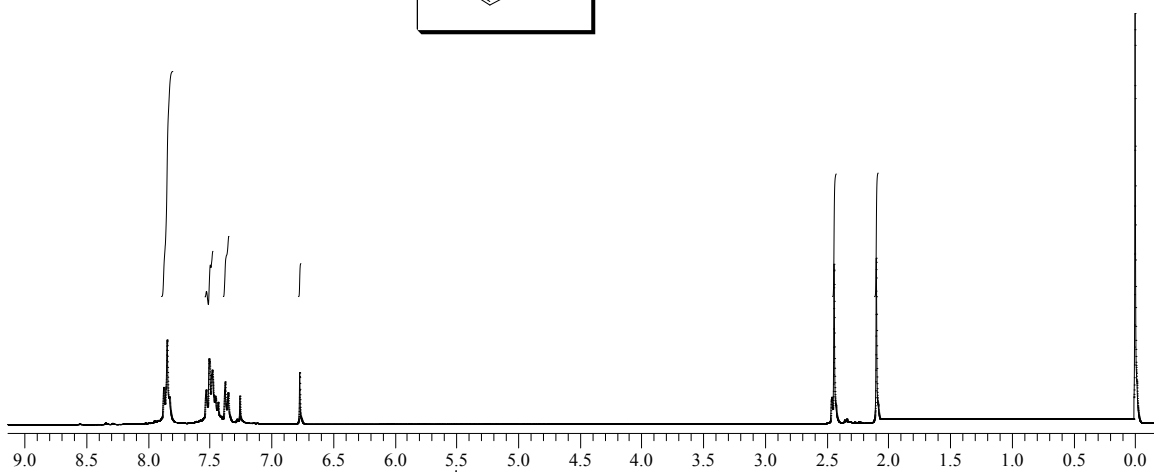
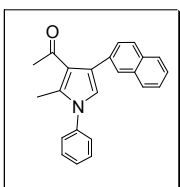
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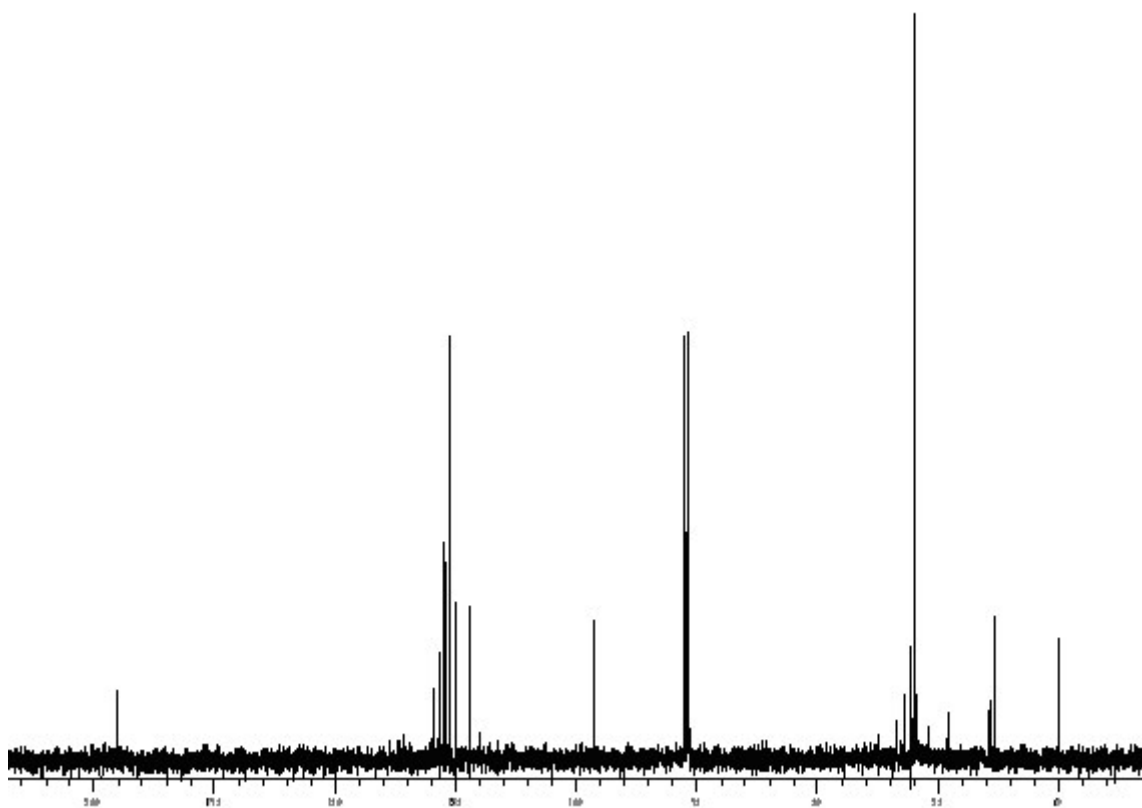
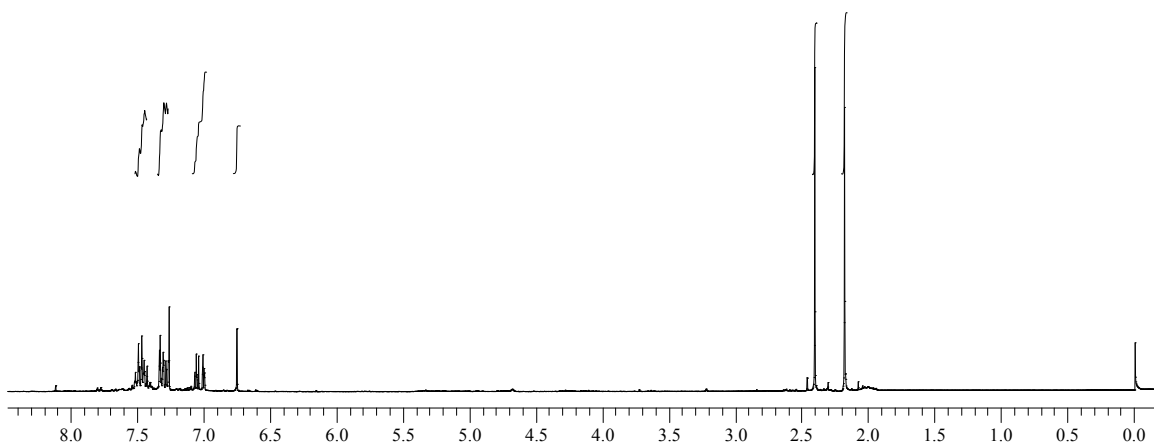
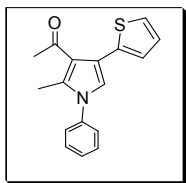
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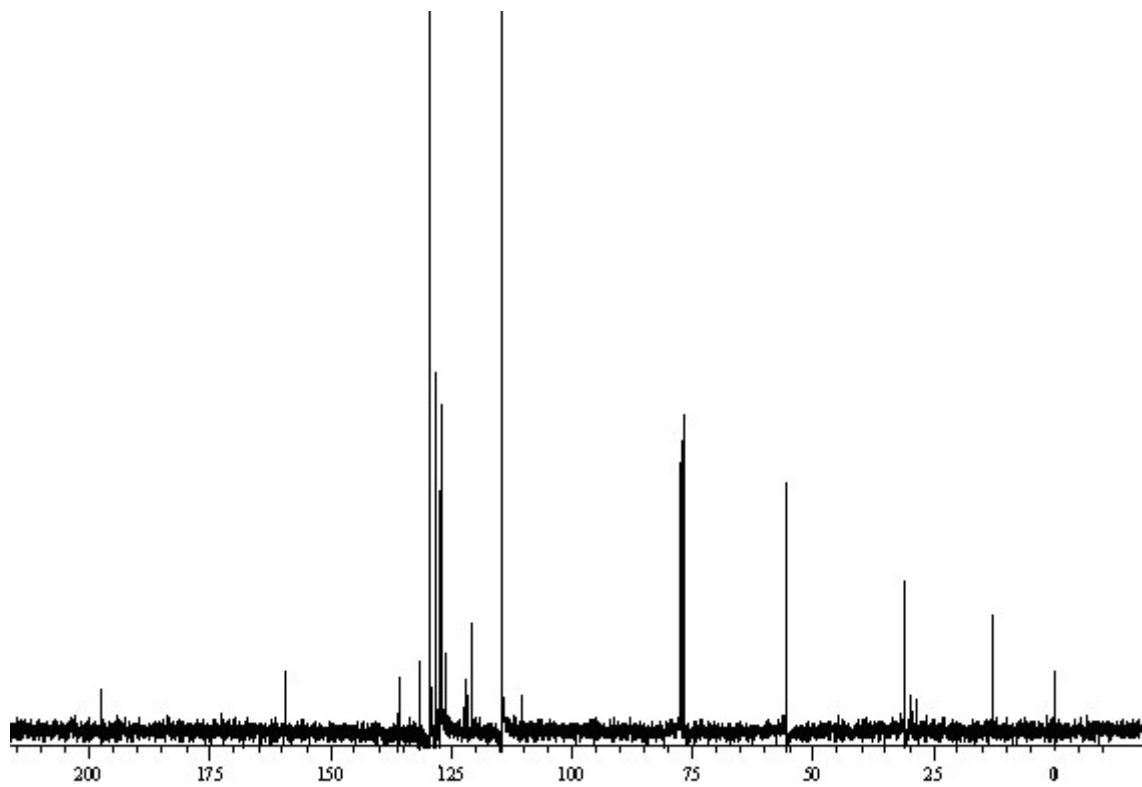
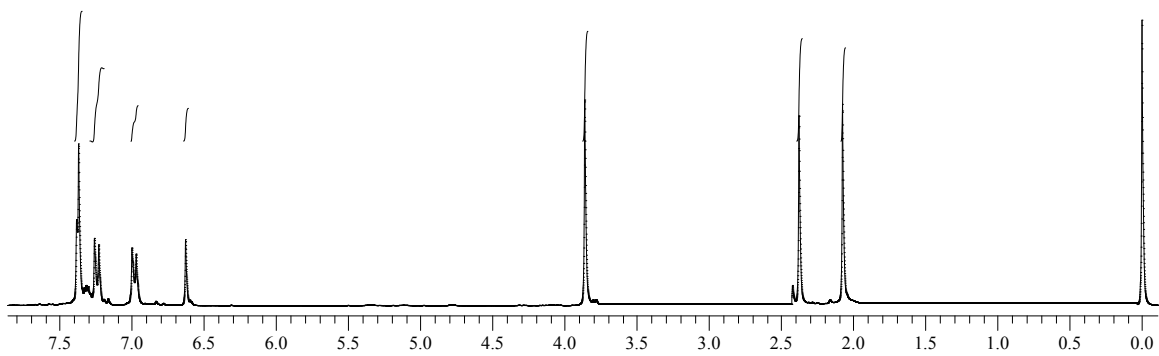
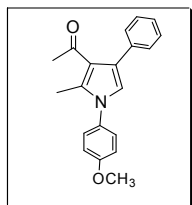
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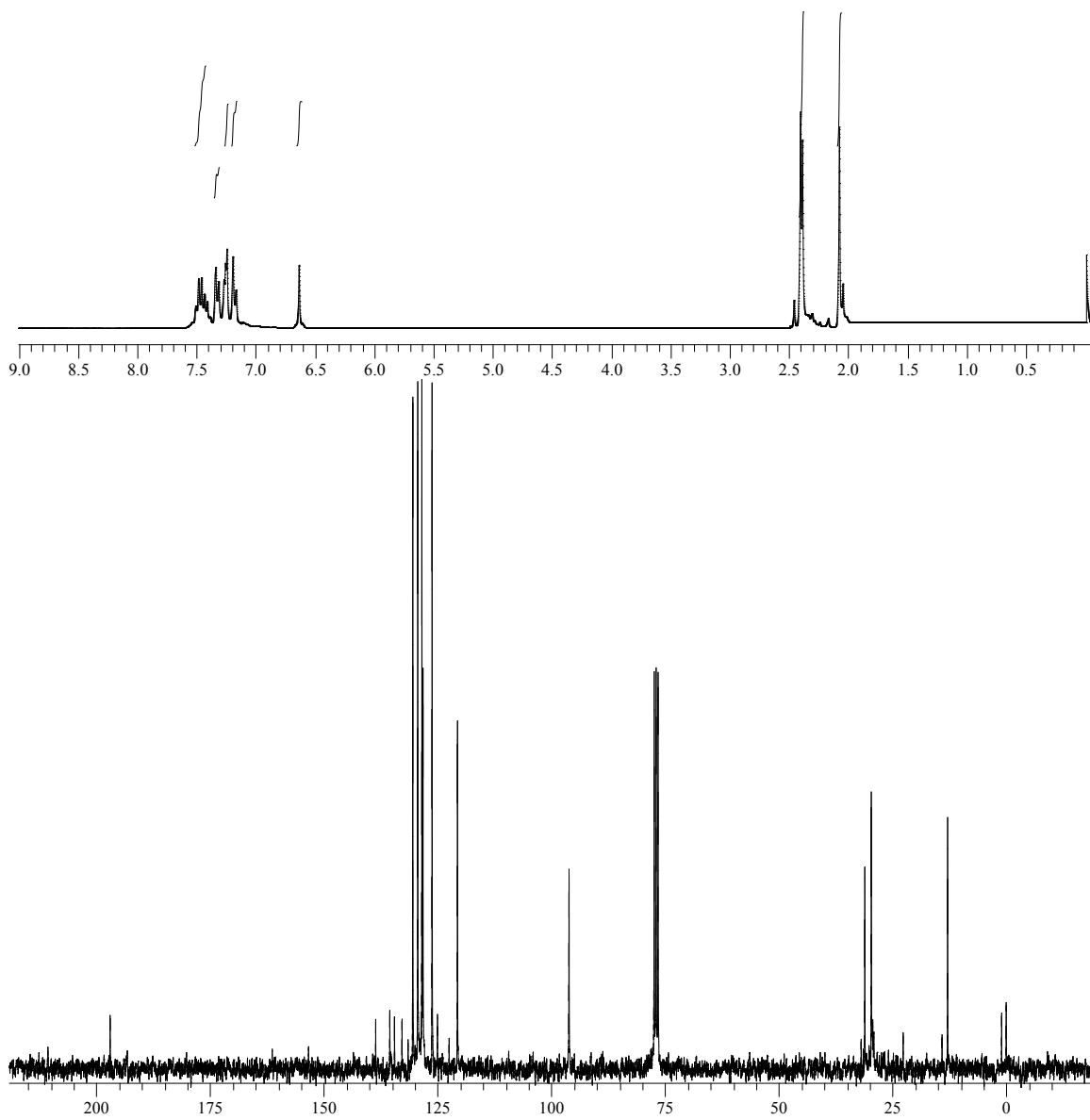
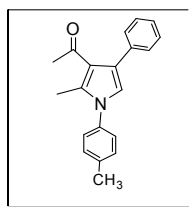
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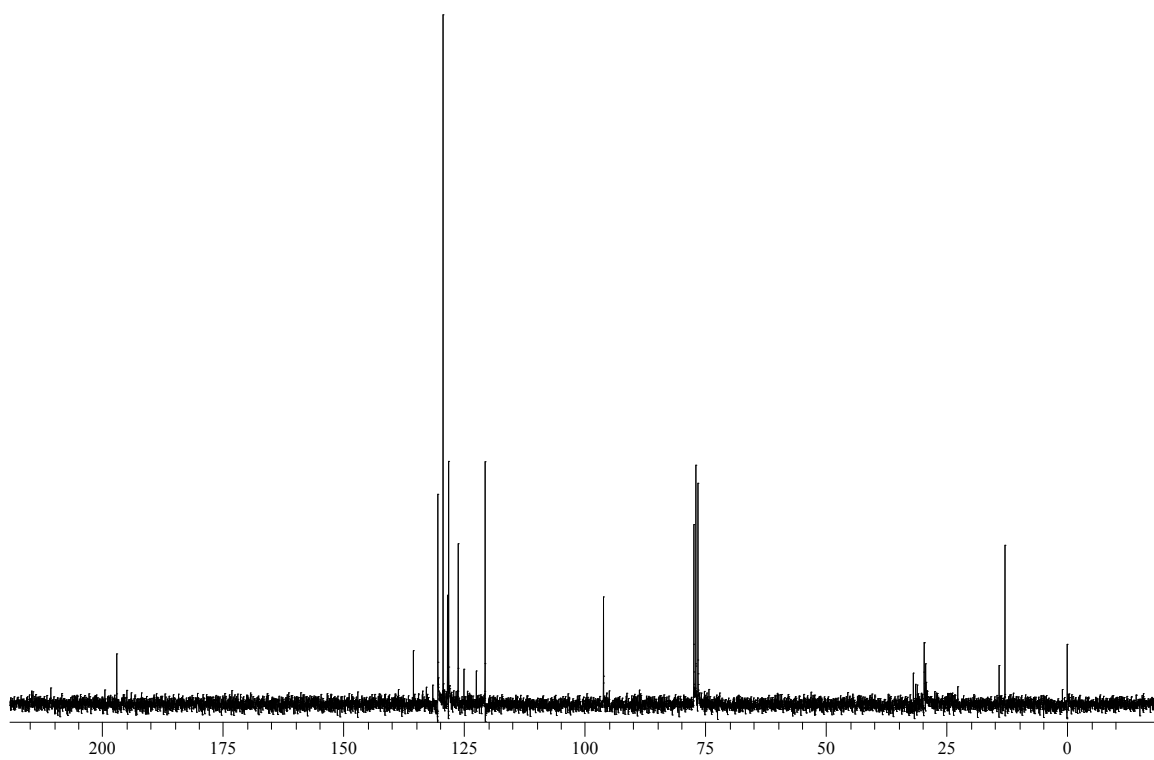
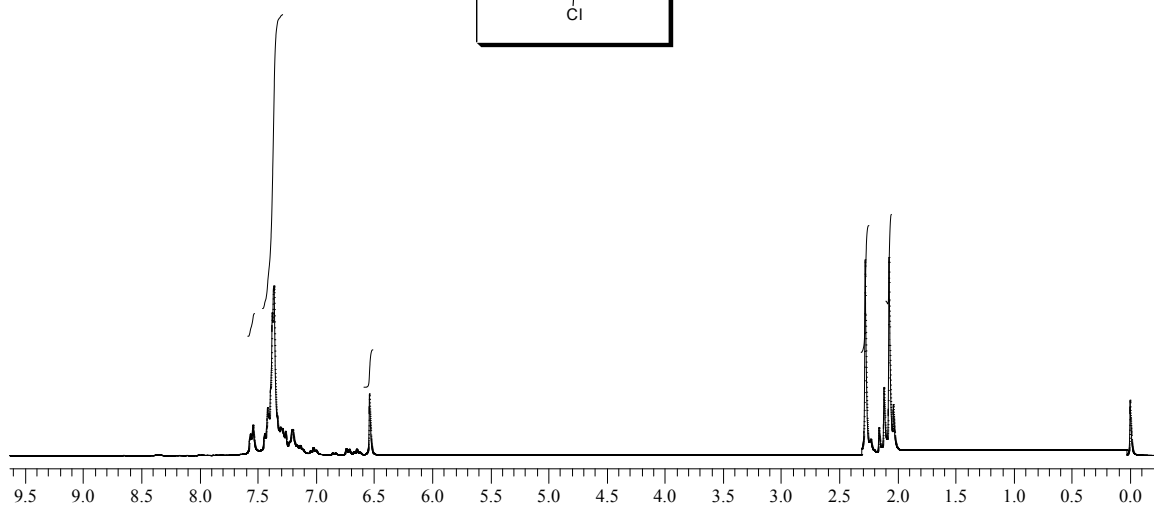
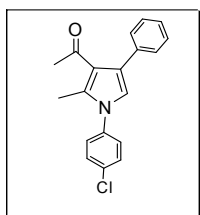
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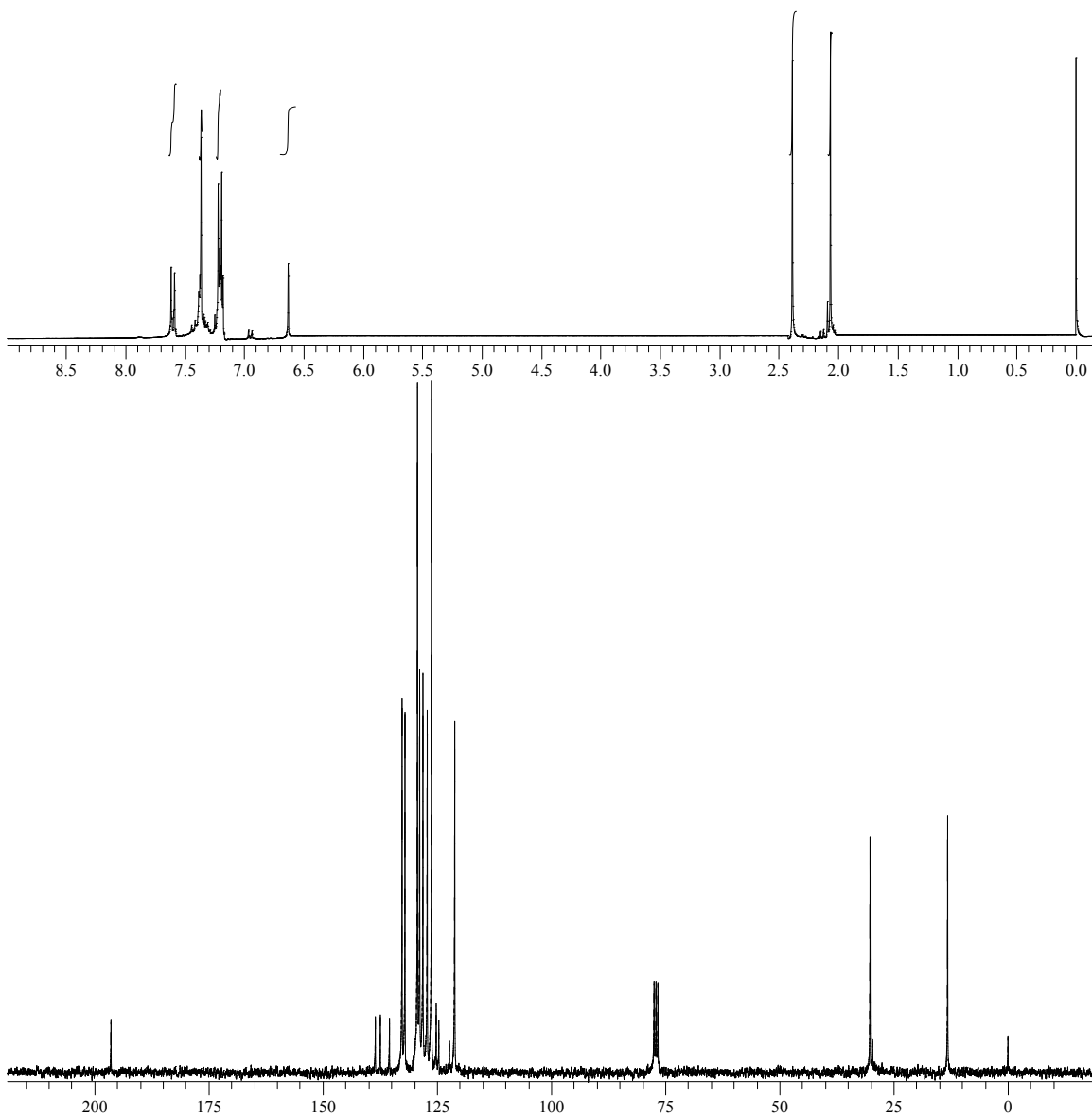
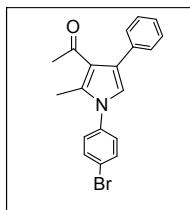
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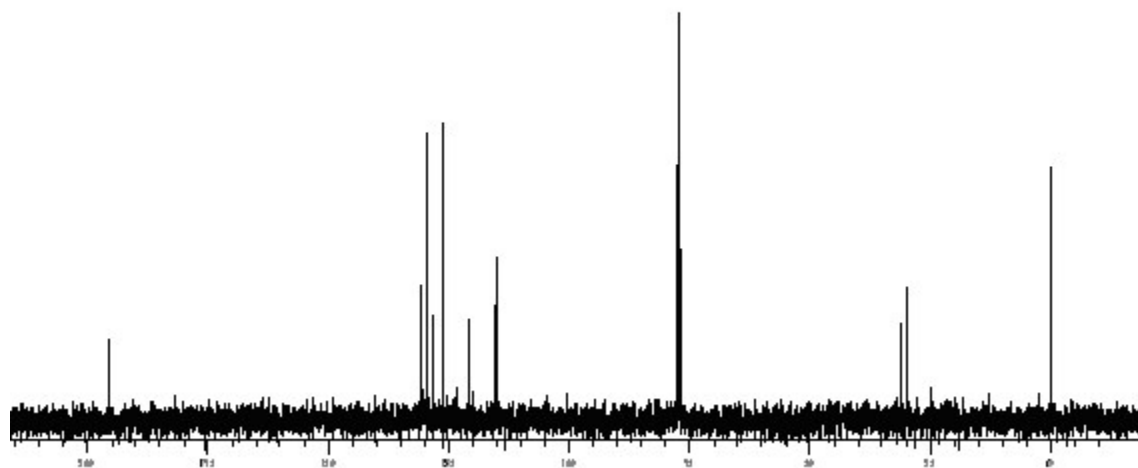
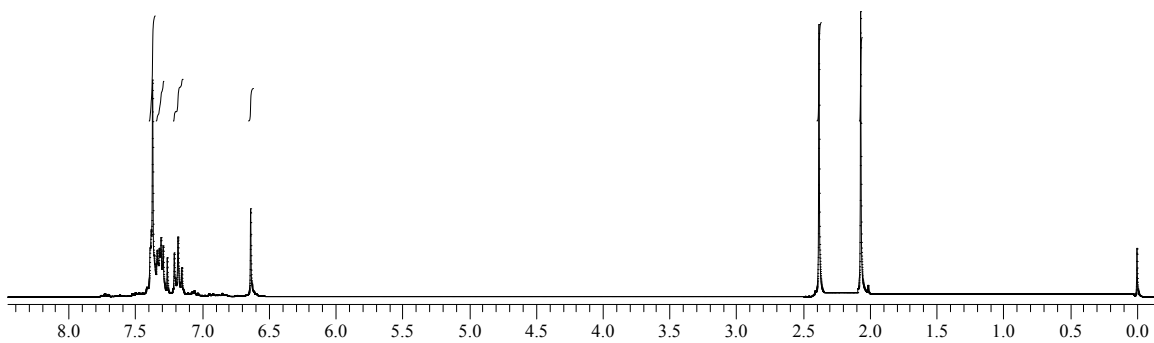
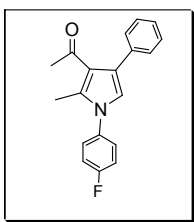
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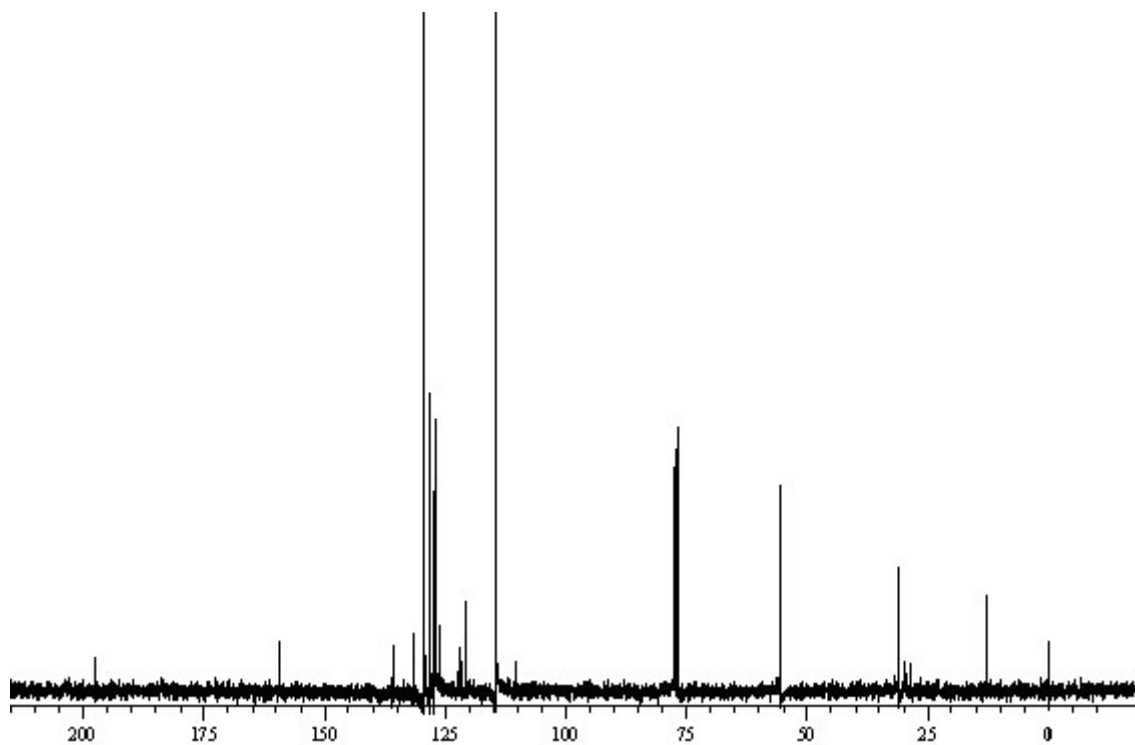
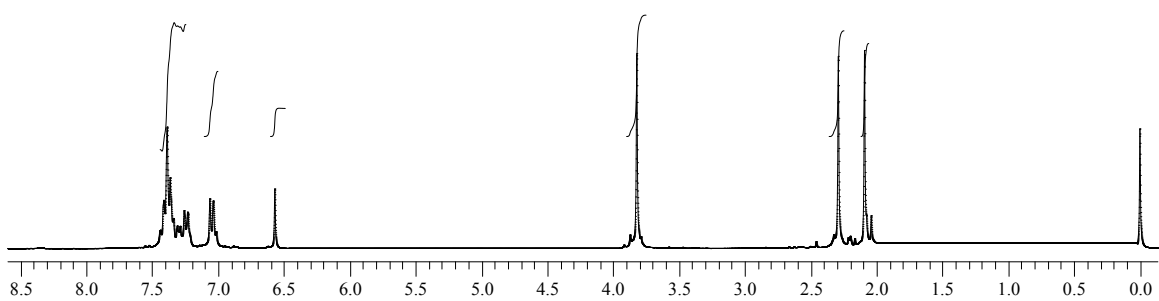
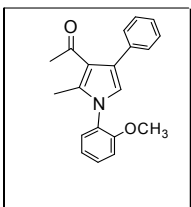
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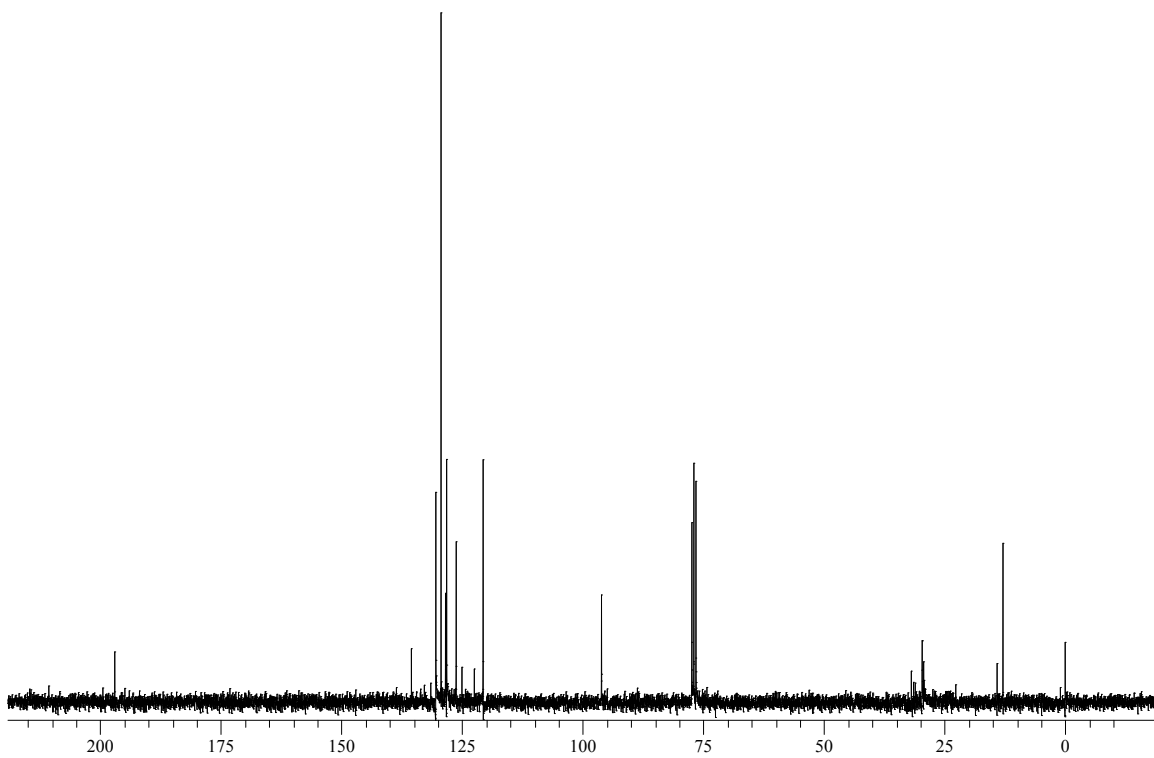
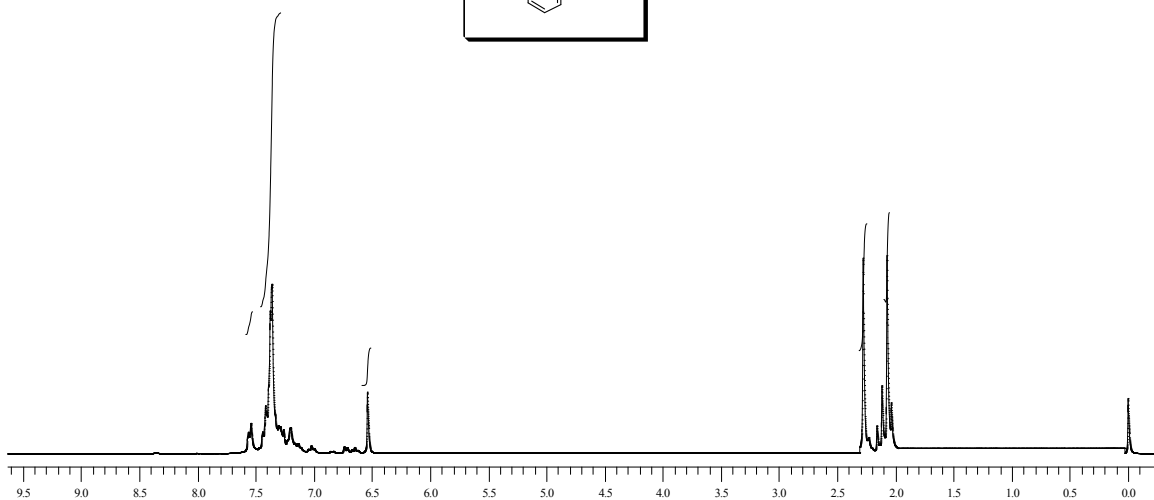
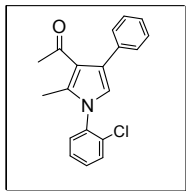
(Table 3, Entry 4)



(Table 3, Entry 5)



(Table 3, Entry 8)



(Table 3, Entry 7)

