Supporting Information

Direct catalytic synthesis of densely substituted 3-formylpyrroles from imines and 1,4-ketoaldehydes

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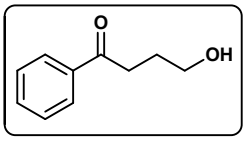
General Experimental Methods:

All reactions under standard conditions were monitored by thin-layer chromatography (TLC) on SiO_2 gel F-254 plates. Unless otherwise noted all reactions have been carried out with distilled and dried solvents. Oven (120 °C) dried glassware were used. All work up and purification were carried out with reagent grade solvents in air. The normal column chromatography was performed on silica gel (100-200 mesh) and Flash column chromatography was performed on silica gel (230-400 meshes) using the mixture of Hexane-EtOAc as eluting solvent. All reagents were of analytical grade and used without further purification. ^{1}H and ^{13}C NMR spectra were recorded on a BRUKER-AV400 (400 MHz and 75 MHz) spectrometer in $CDCl_3$ solution and spectral data were reported in ppm relative to tetramethylsilane (TMS) as internal standard. High resolution mass spectra were recorded using quadrupole electrospray ionization (ESI) technique. Infrared (FT-IR) spectra were recorded on a ABB Bomen MB 3000 FTIR Spectrophotometer system using KBr pellets. Melting points were recorded in open glass capillary tubes on a MPA 120-automated melting point apparatus and are uncorrected.



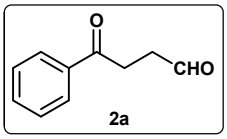
General Experimental procedure for the synthesis of Hydroxy Ketones from Lactones [(1)]:

Synthesis of 4-Hydroxy-1-phenylbutan-1-one:

Bromobenzene (1.81 g, 11.6 mmol, 1.0 equiv.) in dry THF (10.0 mL) was added drop wise with the help of syringe to a stirred solution of crushed magnesium turnings (0.56 g, 23.2 mmol, 2.0 equiv.) in dry THF (10 mL, freshly distilled from sodium/benzophenone) at room temperature for one hour under inert atmosphere. This prepared Grignard reagent solution was cooled at 0 °C and then added drop wise through canula to the stirred solution of butyrolactone (1.0 g, 11.6 mmol, 1 equiv.) in THF (10 mL) at 0 °C over 30 minutes. The combined reaction mixture was stirred at 0 °C for additional 2 h and then quenched by NH_4Cl (15 mL, saturated) and organic

layer was separated. The aqueous layer was again extracted with EtOAc (2 x 10 mL). The combined extracts were washed by brine (15 mL), dried over Na_2SO4, filtered, and concentrated in vacuo. The residue was purified by silica gel (100-200 mesh) column chromatography (Hexane: EtOAc, 20:1 to 5:1) to give the desired keto-alcohol as white semi solid (1.30 g, 68% yield).

White semi solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.89-1.96 (m, 2H), 3.05 (t, *J* = 7.0 Hz, 2H), 3.65 (t, *J* = 6.2 Hz, 2H), 3.98 (bs, 1H), 7.42 (d, *J* = 7.8 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.92 (d, *J* = 7.2 Hz, 2H);



General Experimental procedure for the synthesis of 4-Oxo-4-phenylbutanal (2a):

4-Hydroxy-1-phenylbutan-1-one (0.5 g, 3.0 mmol, 1 equiv.) solution in dichloromethane (2.5 mL) was added to a stirred solution of PCC (0.98 g, 4.6 mmol, 1.5 equiv.) and celite (0.25 g) in dichloromethane (2.5 mL) and stirred for 3 hrs at room temperature. The reaction was monitored by TLC till completion. Filter the reaction mixture over a pad of Na_2SO4 and concentrated in vacuo. The residue was purified by silica gel column chromatography (Hexane: EtOAc = 90:10 to 70:30) to give the desired product **2a** as a yellow oily liquid (0.272 g, 55% yield).

Yellow oily liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.79-2.97 (m, 2H), 3.31 (t, *J* = 6.3Hz, 2H), 7.40-7.48 (m, 2H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 2H), 9.90 (s, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$) δ 30.97, 37.54, 128.00 (2C), 128.60 (2C), 133.27, 136.37, 197.83, 200.70; IR (KBr)/cm$^-$ 2923,1728, 1681, 1211, 979, 694; HRMS (ESI): Calcd for $C_{10}H_{10}O_2$ ($M+H^+$) 163.0759; Found 163.0763.

(1) S.-B. Yang, F.-F. Gan, G.-J. Chen, P.-F. Xu, *SynLett*., 2008, **16**, 2532.

Typical procedure for the synthesis of 2,5-diaryl pyrrole-3-carboxaldehydes (4):

4-Oxo-4-phenylbutanal **2a** (0.9 mmol, 3M solution) was added to a mixture of preformed *N*-PMP aldimine **3c** (0.3 mmol) and L-proline (0.06 mmol) in DMSO (3.0 mL) at room temperature. The reaction mixture was stirred at room temperature until the aldimine was consumed as monitored by TLC. The reaction was quenched with cold water (10 mL) and extracted with ethyl acetate (3 x 5 mL). The combined organic extracts were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. Purification through silica gel column chromatography by eluting the mixture of EtOAc/Hexane to give 2,5-diaryl pyrrole 3-carbxaldehydes **4** with high yields (70%). In almost all the cases, we also obtained about ≤10% of aromatic aldehyde due to cleavage of corresponding imine under these conditions.

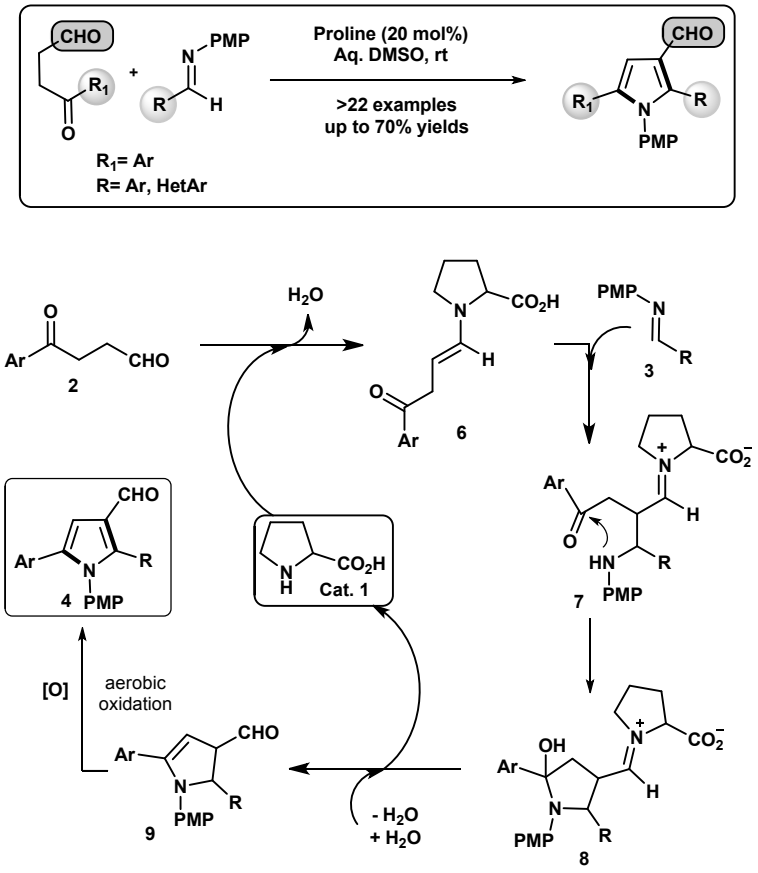
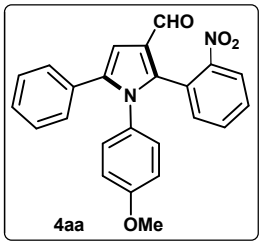


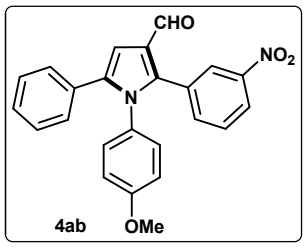
Figure 1: Plausible mechanism of the cascade [4+2] annulation reaction

1-(4-methoxyphenyl)-2-(2-nitrophenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4aa):



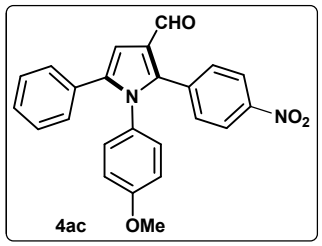
Yellow pasty liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.68 (s, 3H), 6.67 (s, 1H), 6.76 (d, *J* = 8.8 Hz, 2H), 6.92-6.95 (m, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 7.02-7.05 (m, 3H), 7.26-7.30 (m, 2H), 7.68-7.73 (m, 2H), 9.86 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.41, 109.30, 114.61 (2C), 122.32, 125.96, 126.95, 128.03 (2C), 128.11 (2C), 128.31 (2C), 128.54 (2C), 129.35 (2C), 129.60, 131.80, 133.15, 136.14, 142.28, 159.58, 185.93 ; IR (KBr)/cm^{-1} 2932, 1674, 1512, 1250, 1173; HRMS (ESI): Calcd for $C_{24}H_{18}N_2O_4$ ($M+H^+$) 399.1346; Found 399.1348.

1-(4-methoxyphenyl)-2-(3-nitrophenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4ab):



Reddish brown solid (M.P = 154-155 ^{o}C), ^{1}H NMR (400) MHz, $CDCl_3$) δ 3.75 (s, 3H), 6.74 (d, *J* = 8.8 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 6.98 (s, 1H), 7.10-7.12 (m, 2H), 7.20-7.25 (m, 3H) 7.41 (d, *J* = 7.7 Hz, 1H) 7.53-7.57 (m, 1H), 8.05-8.11 (m, 1H), 8.14-8.22 (m, 1H), 9.73 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.33, 107.97, 114.33 (2C), 123.20, 124.39, 125.76, 125.93, 127.54, 128.21(2C), 128.75 (2C), 129.07, 129.56 (2C), 131.17, 131.33, 136.83, 137.63,140.24, 147.65, 159.23, 185.98; IR (KBr)/cm^{-1} 2932, 2854, 1666, 1512, 1342, 1172; HRMS (ESI): Calcd for $C_{24}H_{18}N_2O_4$ ($M+H^+$) 399.1346; Found 399.1342.

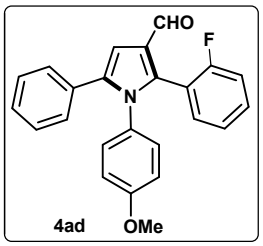
1-(4-methoxyphenyl)-2-(4-nitrophenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4ac);



Yellow solid (M.P = 163-164 ^{o}C), ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.77 (s, 3H), 6.75 (d, *J* = 8.9 Hz, 2H), 6.89 (d, *J* = 8.8 Hz, 2H), 7.09-7.11 (m, 2H), 7.23 (t, *J* = 3.5 Hz, 3H), 7.37 (d, *J* = 8.6 Hz, 2H), 8.15 (d, *J* = 8.7 Hz, 2H), 9.75 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.35,

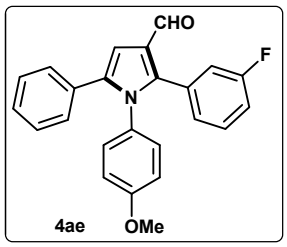
108.33, 114.35 (2C), 123.18 (2C), 124.57, 127.59, 127.97, 128.22 (2C), 128.78 (2C), 129.46 (2C), 131.81 (2C), 133.04, 133.23, 137.91, 140.19, 147.28, 159.25, 186.04; IR (KBr)/cm^{-1} 2924, 2854, 1674, 1596, 1342, 1172; HRMS (ESI): Calcd for $C_{24}H_{18}N_2O_4$ (M+H$^+$) 399.1346; Found 399.1338.

2-(2-fluorophenyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4ad):



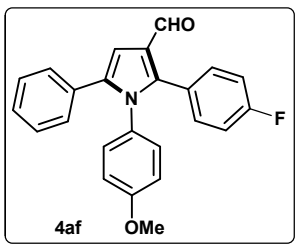
Reddish solid (M.P = 145-146 ^{o}C) ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.73 (s, 3H), 6.69 (d, *J* = 8.3 Hz, 2H), 6.92 (d, *J* = 6.2 Hz, 2H), 6.97 (s, 1H), 7.01 (t, *J* =8.8 Hz, 1H) 7.12 (m, 3H), 7.20 (m, 4H), 7.34 (m, 1H), 9.62 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.26, 107.29, 113.81, 115.66, 115.83, 123.78, 123.81, 124.63, 127.26,128.13 (2C), 128.64 (2C), 129.10, 129.95, 131.16, 131.22, 131.58, 133.30, 137.43, 138.03, 158.90, 161.33, 186.36; IR (KBr)/cm^{-1} 2932, 2854, 1659, 1250, 1180, 1026; HRMS (ESI): Calcd for $C_{24}H_{18}FNO_2$ (M+H$^+$) 372.1400; Found 372.1409.

2-(3-fluorophenyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4ae):



Yellow liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, 3H), 6.73 (d, *J* = 8.9 Hz, 2H), 6.88-6.91 (m, 3H), 6.96 (s, 1H), 6.99-7.05 (m, 2H), 7.09-7.11 (m, 2H), 7.20-7.24 (m, 3H), 7.42 (d, *J* = 7.3 Hz, 1H), 9.71 (s, 1H) ; ^{13}C-NMR (75 MHz, $CDCl_3$) δ 55.34, 107.36, 114.14 (2C), 115.66, 118.22, 124.18, 125.36 (2C), 127.08, 127.34, 128.15, 128.58 (2C), 128.79, 129.50, 129.64, 129.75, 131.55, 137.13, 159.07, 163.30, 186.63; IR (KBr)/cm^{-1} 2908, 1680, 1247, 1174; HRMS (ESI): Calcd for $C_{24}H_{18}FNO_2$ (M+H$^+$) 372.1400; Found 372.1395.

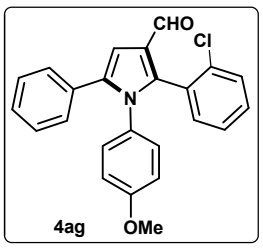
2-(4-fluorophenyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4af):



Yellow liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, 3H), 6.73 (d, *J* = 8.9 Hz, 2H), 6.87 (d, *J* = 8.9 Hz, 2H), 6.95 (s, 1H), 6.99 (t, *J* = 8.7 Hz, 2H), 7.09-7.11 (m, 2H), 7.16-7.22 (m, 5H), 9.68 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.33, 107.21, 114.08 (2C), 115.17, 115.35, 124.02,

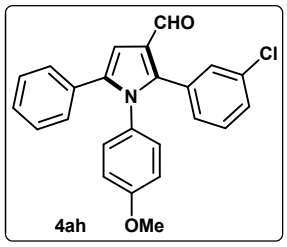
127.28, 128.14 (2C), 128.78 (2C), 129.56 (2C), 129.79, 131.58, 132.90, 132.96, 136.88, 142.96 (2C), 158.93, 176.15, 186.76; IR (KBr)/cm^{-1} 2924, 2854, 1659, 1218, 1157, 1049; HRMS (ESI): Calcd for $C_{24}H_{18}FNO_2$ (MH^+) 372.1400; Found 372.1397.

2-(2-chlorophenyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4ag):



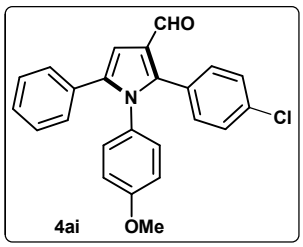
Red oily liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.72 (s, 3H), 6.67 (d, *J* = 9.1 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 6.96 (s, 1H), 7.11-7.14 (m, 2H), 7.19-7.23 (m, 4H), 7.27-7.31 (m, 2H), 7.37 (d, *J* = 8.2 Hz, 1H), 9.53 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.26, 106.98, 113.80 (2C), 124.39, 126.25 (2C), 127.20 (2C), 129.11 (2C), 129.30, 129.51 (2C), 129.96, 135.53 (2C), 131.65, 133.49, 135.57, 136.96, 141.26, 158.89, 186.21; IR (KBr)/cm^{-1} 2924, 2854, 1666, 1250, 1180; HRMS (ESI): Calcd for $C_{24}H_{18}ClNO_2$ ($M+H^+$) 388.1104; Found 388.1106.

2-(3-chlorophenyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4ah):



Brownish red oily liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.75 (s, 3H), 6.72 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.94 (s, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 7.09 (dd, *J* = 7.0 Hz, 5.9 Hz, 2H), 7.17-7.24 (m, 6H), 9.69 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.38, 107.43, 114.18 (2C), 124.28, 127.36, 127.88 (2C), 128.16 (2C), 128.80 (2C), 129.23, 129.31, 129.57 (2C), 131.14, 131.34, 131.56, 134.00, 137.21, 143.03, 159.13 , 186.53; IR (KBr)/cm^{-1} 2932, 1666, 1250, 1165, 1034; HRMS (ESI): Calcd for $C_{24}H_{18}ClNO_2$ ($M+H^+$) 388.1104; Found 388.1094.

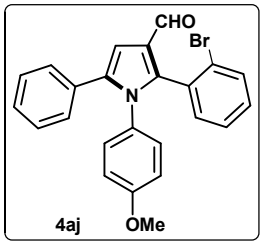
2-(4-chlorophenyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4ai):



Yellow viscous oily liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, 3H), 6.74 (d, *J* = 8.9 Hz, 2H), 6.88 (d, *J* = 8.9 Hz, 2H), 6.96 (s, 1H), 7.08-7.11 (m, 2H), 7.13 (d, *J* = 8.5 Hz, 2H), 7.19-7.24 (m, 3H), 7.27-7.30 (m, 3H) 9.70 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.31, 107.42, 114.14 (2C), 124.08, 127.30, 128.12 (2C), 128.34 (2C), 128.75 (2C), 129.54 (2C), 129.72,

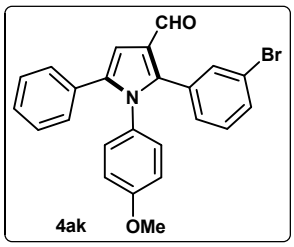
131.53, 132.32 (2C), 134.70, 137.08, 142.68, 152.98, 159.02, 186.55; IR (KBr)/cm^{-1} 2924, 2854, 1659, 1250, 1157, 1088; HRMS (ESI): Calcd for $C_{24}H_{18}ClNO_2$ (M+H$^+$) 388.1104; Found 388.1103.

2-(2-bromophenyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4aj):



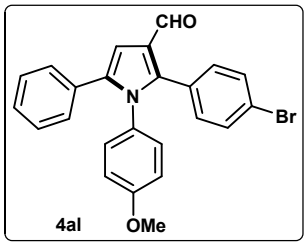
Reddish viscous oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.69 (s, 3H), 6.64 (d, *J* = 9.1 Hz, 2H), 6.93 (m, 3H), 7.07-7.12 (m, 2H), 7.15-7.21 (m, 4H), 7.22-7.25 (m, 2H), 7.53 (d, *J* = 8.0 Hz, 1H), 9.50 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.22, 106.78, 113.74 (2C), 124.12, 125.89, 126.78, 127.15, 128.12 (2C), 128.48, (2C), 129.14 (2C), 129.84, 130.63, 131.32, 131.57, 132.58, 133.48, 136.74, 142.89, 158.82, 186.22; IR (KBr)/cm^{-1} 2924, 2854, 1674, 1242, 1173, 1034; HRMS (ESI): Calcd for $C_{24}H_{18}BrNO_2$ (M+H$^+$) 432.0599; Found 432.0605.

2-(3-bromophenyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4ak):



Slight yellow solid (M.P = 170-171 ^{o}C) ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.73 (s, 3H), 6.75 (d, *J* = 8.8 Hz, 2H), 6.92 (d, *J* = 8.9 Hz, 2H), 7.02 (s, 1H), 7.11-7.17 (m, 5H), 7.20-7.24 (m, 4H), 9.76 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.11, 107.17, 113.99 (2C), 121.76, 124.05, 124.83, 127.18, 127.80, 127.97 (2C), 128.07, 128.14, 128.55 (2C), 129.31, 129.37 (2C), 129.53, 131.28, 133.74 137.01, 158.94, 186.16; IR (KBr)/cm^{-1} 2924, 2854, 1659, 1250, 1157, 1041; HRMS (ESI): Calcd for $C_{24}H_{18}BrNO_2$ (M+H$^+$) 432.0599; Found 432.0602.

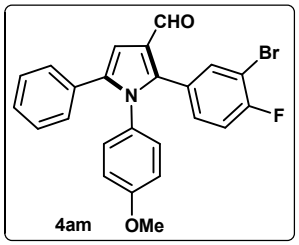
2-(4-bromophenyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4al):



White solid (M.P = 167-168 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.61 (s, 3H), 6.58 (d, *J* = 8.9 Hz, 2H), 6.72 (d, *J* = 8.9 Hz, 2H), 6.80 (s, 1H), 6.91 (d, *J* = 8.4 Hz, 2H), 6.94 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.00-7.08 (m, 3H), 7.27 (d, *J* = 8.3 Hz, 2H), 9.54 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$)

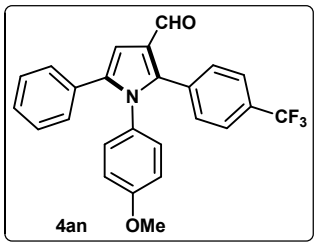
δ 55.31, 107.42, 114.13 (2C), 122.99, 124.00, 125.31, 127.30, 127.83, 128.12 (2C), 128.54, 128.73 (2C), 129.51 (2C), 131.27 (2C), 132.55 (2C), 137.07, 142.65, 158.97, 186.57; IR (KBr)/cm^{-1} 2932, 2847, 1666, 1250, 1168, 1034; HRMS (ESI): Calcd for $C_{24}H_{18}BrNO_2$ (M+H$^+$) 432.0599; Found 432.0595.

2-(3-bromo-4-fluorophenyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3carbaldehyde (4am):



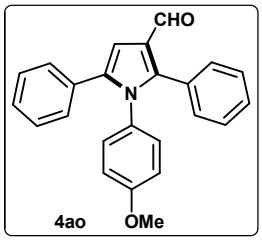
Yellow liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.77 (s, 3H), 6.75 (d, *J* = 8.9 Hz, 2H), 6.89 (d, *J* = 8.9 Hz, 2H), 6.95 (s, 1H), 7.00-7.11 (m, 4H), 7.20-7.23 (m, 3H), 7.46 (dd, 6.5, 2.0 Hz, 1H), 9.70 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.38, 107.42, 108.91, 114.22 (2C), 116.06, 116.24, 124.22, 127.40, 128.17 (2C), 128.73 (2C), 129.52 (2C), 131.36, 131.65, 131.71, 136.08, 137.19, 142.94, 159.11, 176.12, 186.30; IR (KBr)/cm^{-1} 2924, 2854, 1666, 1250, 1157, 1041; HRMS (ESI): Calcd for $C_{24}H_{17}BrFNO_2$ (M+H$^+$) 450.0505; Found 450.0511.

1-(4-methoxyphenyl)-5-phenyl-2-(4-(trifluoromethyl)phenyl)-1*H*-pyrrole carbaldehyde (4an):

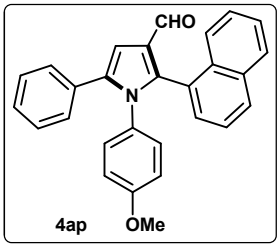


Yellow oily liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.75 (s, 3H), 6.72 (d, *J* = 8.9 Hz, 2H), 6.87 (d, *J* = 8.9 Hz, 2H), 6.97 (s, 1H), 7.04-7.15 (m, 2H), 7.15-7.23 (m, 3H), 7.26 (d, *J* = 6.3 Hz, 2H), 7.54 (d, *J* = 8.1 Hz, 2H), 9.70 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.32, 107.68, 114.20 (2C), 124.32, 124.94, 124.97, 127.41, 127.84 (2C), 128.16 (2C), 128.77(2C), 129.49 (2C), 131.37 (2C), 133.17, 137.38, 141.85, 142.94 (2C), 159.06, 186.41; IR (KBr)/cm^{-1} 2924, 2854, 1674, 1250, 1118; HRMS (ESI): Calcd for $C_{25}H_{18}F_3NO_2$ (M+H$^+$) 422.1368; Found 422.1374.

1-(4-methoxyphenyl)-2,5-diphenyl-1*H*-pyrrole-3-carbaldehyde (4ao):



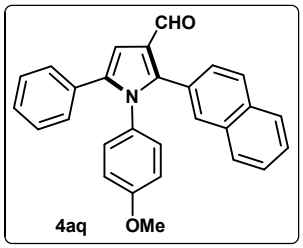
Yellow viscous liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.75 (s, 3H), 6.71 (d, *J* = 8.9 Hz, 2H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.96 (s, 1H), 7.11 (dd, *J* = 7.4 Hz, 5.9 Hz, 2H), 7.18-7.22 (m, 5H), 7.27-7.32 (m, 3H), 9.69 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.32, 107.17, 114.00 (2C), 123.98, 123.37 (2C), 127.20, 127.88, 128.42, 128.59 (2C), 128.80 (2C), 129.45, 129.65 (2C), 130.06, 131.20 (2C), 131.77, 136.81, 158.89, 187.11; IR (KBr)/cm^{-1} 2924, 2854, 1666, 1242, 1165, 1034; HRMS (ESI): Calcd for $C_{24}H_{19}NO_2$ (M+H$^+$) 354.1494; Found 354.1498.



1-(4-methoxyphenyl)-2-(naphthalen-1-yl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4ap):

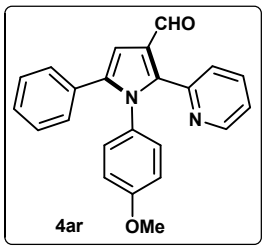
Deep red pasty liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.62 (s, 3H), 6.51 (d, *J* = 8.2 Hz, 2H), 6.82 (d, *J* = 8.2 Hz, 2H), 7.05 (s, 1H), 7.15-7.17 (m, 2H), 7.21-7.24 (m, 3H), 7.38-7.46 (m, 4H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.81-7.85 (m, 2H), 9.39 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.16, 106.86, 113.68 (2C), 124.64, 125.34, 125.80, 126.15, 126.81, 127.16, 127.28, 128.18 (2C), 128.58 (2C), 128.87, 129.53, 130.21, 130.46, 131.82, 133.13, 133.76, 137.01, 143.11, 157.68, 157.87, 158.64, 186.79; IR (KBr)/cm^{-1} 3016, 1658, 1512, 1249, 1172; HRMS (ESI): Calcd for $C_{28}H_{21}NO_2$ (M+H$^+$) 404.1650; Found 404.1654.

1-(4-methoxyphenyl)-2-(naphthalen-2-yl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (4aq):



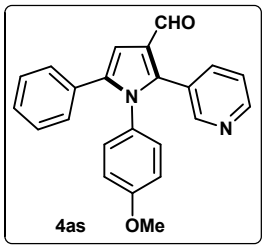
White solid (M.P = 176-177 ^{o}C) ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.72 (s, 3H), 6.68 (d, *J* = 8.9 Hz, 2H), 6.93 (d, *J* = 8.9 Hz, 2H), 7.01 (s, 1H), 7.12 – 7.15 (m, 3H), 7.22-7.24 (m, 3H), 7.52 (dd, *J* = 6.1 Hz, 3.3 Hz, 2H), 7.68 (d, *J* = 8.5 Hz, 1H), 7.81 (dd, *J* = 6.0, 3.4 Hz, 2H), 7.84 (s, 1H), 9.75 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.29, 107.33, 114.07 (2C), 124.25, 126.61, 126.89, 127.24, 127.60, 127.66, 127.81, 127.88, 128.15 (2C), 128.20, 128.81 (2C), 129.60 (2C), 130.06, 131.19, 131.74, 132.60, 132.69, 136.94, 139.28, 158.86, 187.24; IR (KBr)/cm^{-1} 2922, 1668, 1248, 1172; HRMS (ESI): Calcd for $C_{28}H_{21}NO_2$ (M+H$^+$) 404.1650; Found 404.1648.

1-(4-methoxyphenyl)-5-phenyl-2-(pyridin-2-yl)-1*H*-pyrrole-3-carbaldehyde (4ar):



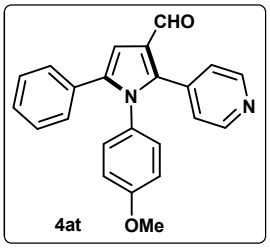
Reddish brown pasty liquid , ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, 3H), 6.73 (d, *J* = 8.9 Hz, 2H), 6.96 (d, *J* = 8.9 Hz, 2H), 6.98 (s, 1H), 7.05 (d, *J* = 7.9 Hz, 1H), 7.08-7.11 (m, 2H), 7.18-7.22 (m, 4H), 7.55 (td, *J* = 7.8, 1.8 Hz, 1H), 8.62 (d, *J* = 4.1, 1H), 9.91 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.33, 107.78, 114.00 (2C), 122.60, 125.10, 126.10, 127.30, 128.11 (2C), 128.89 (2C), 129.51 (2C), 130.19, 131.64, 135.73, 137.23, 141.75, 149.24, 149.53, 158.97, 187.58; IR (KBr)/cm^{-1} 2932, 1659, 1250, 1173; HRMS (ESI): Calcd for $C_{23}H_{18}N_2O_2$ ($M+H^+$) 355.1446; Found 355.1442.

1-(4-methoxyphenyl)-5-phenyl-2-(pyridin-3-yl)-1*H*-pyrrole-3-carbaldehyde (4as):



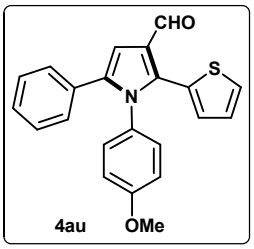
Reddish brown pasty liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, 3H), 6.73 (d, *J* = 8.9 Hz, 2H), 6.90 (d, *J* = 8.9 Hz, 2H), 6.99 (s, 1H), 7.10-7.12 (m, 2H), 7.22 (t, *J* = 3.3 Hz, 4H), 7.49-7.52 (m, 1H), 8.49 (s, 1H), 8.55 (d, *J* = 3.9 Hz, 1H), 9.71 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.33, 107.83, 114.31 (2C), 122.90, 124.69, 126.06, 127.47, 128.18 (2C), 128.77 (2C), 129.35, 129.63 (2C), 131.33, 137.71, 138.39, 139.72, 149.08, 150.93, 159.22, 186.12; IR (KBr)/cm^{-1} 2932, 1666, 1250, 1180, 1026; HRMS (ESI): Calcd for $C_{23}H_{18}N_2O_2$ ($M+H^+$) 355.1446; Found 355.1448.

1-(4-methoxyphenyl)-5-phenyl-2-(pyridin-4-yl)-1*H*-pyrrole-3-carbaldehyde (4at):



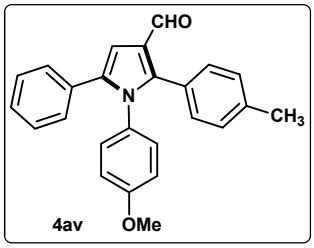
Yellow pasty liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, 3H), 6.74 (d, *J* = 8.9 Hz, 2H), 6.88 (d, *J* = 8.9 Hz, 2H), 6.97 (s, 1H), 7.07-7.09 (m, 4H), 7.21 (m, 3H), 8.55 (bs, 2H), 9.75 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.31, 108.03, 114.25 (2C), 124.41, 125.41, 127.50 (2C), 128.18 (2C), 128.73 (2C), 129.24, 129.38 (2C), 131.08, 137.57, 137.83, 139.88, 149.32 (2C), 159.19, 186.07; IR (KBr)/cm^{-1} 2931, 1674, 1250, 1173, 1026; HRMS (ESI): Calcd for $C_{23}H_{18}N_2O_2$ ($M+H^+$) 355.1446; Found 355.1444.

1-(4-methoxyphenyl)-5-phenyl-2-(thiophen-2-yl)-1*H*-pyrrole-3-carbaldehyde (4au):



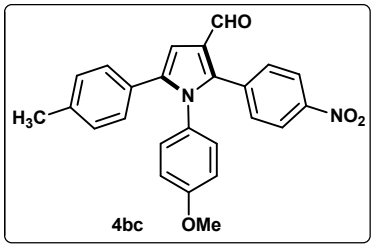
Yellowish orange pasty liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.78 (s, 3H), 6.78 (d, *J* = 8.9 Hz, 2H), 6.96-7.00 (m, 5H),7.11-7.13 (m, 2H), 7.21 (t, *J* = 3.7 Hz, 4H), 9.86 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.36, 89.71, 107.40, 114.08 (2C), 121.88, 126.81, 127.38, 127.88 (2C), 128.15 (2C), 128.73 (2C), 129.87 (2C), 130.81, 131.50, 137.70, 142.99, 159.38, 186.90; IR (KBr)/cm^{-1} 2924, 2854, 1666, 1242, 1173 1034; Found 356.0295. HRMS (ESI): Calcd for $C_{22}H_{17}NO_2S$ ($M+H^+$) 360.1058; Found 360.1064.

1-(4-methoxyphenyl)-5-phenyl-2-(p-tolyl)-1*H*-pyrrole-3-carbaldehyde (4av):



Brown pasty liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.33 (s, 3H), 3.76 (s, 3H), 6.72 (d, *J* = 8.5 Hz, 2H), 6.88 (d, *J* = 8.4 Hz, 2H), 6.95 (s, 1H), 7.08 (m, 5H), 7.20 (m, 2H), 7.35 (t, *J* = 7.3 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 9.69 (s, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$) δ 22.67, 55.34, 107.09, 113.97 (2C), 123.88, 125.34, 126.41, 127.12, 127.86, 128.08, 128.57, 128.75 (2C), 129.62, 130.16, 131.03 (2C), 131.84, 136.69, 138.36, 143.00, 144.79, 158.84, 187.16 ; IR (KBr)/cm^{-1} 2914, 1668, 1248, 1178; HRMS (ESI): Calcd for $C_{25}H_{21}NO_2$ ($M+H^+$) 368.1650; Found 368.1648.

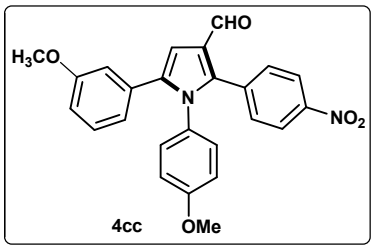
1-(4-methoxyphenyl)-2-(4-nitrophenyl)-5-(p-tolyl)-1*H*-pyrrole-3-carbaldehyde (4bc):



Yellow solid, (M.P = 156-157 ^{o}C) ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.30 (s, 3H), 3.77 (s, 3H), 6.75 (d, *J* = 8.8 Hz, 2H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.95 (s, 1H), 6.98 (d, *J* = 8.1 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 7.36 (d, *J* = 8.6 Hz, 2H), 8.14 (d, *J* = 8.7 Hz, 2H), 9.74 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.15, 55.37, 107.98, 114.34 (2C), 123.19 (2C), 124.55, 128.12, 128.67 (2C), 128.98 (2C), 129.49 (2C), 130.17, 131.82 (2C), 136.26, 137.53, 138.08, 140.08, 147.27, 159.22, 186.14;

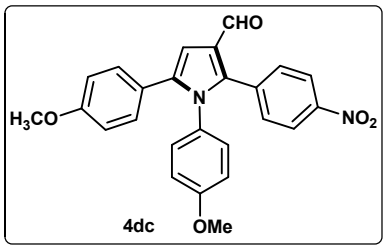
IR (KBr)/cm^{-1} 2936, 2862, 1782, 1234; HRMS (ESI): Calcd for $C_{25}H_{20}N_2O_4$ ($M+H^+$) 413.1501; Found 413.1505.

5-(3-methoxyphenyl)-1-(4-methoxyphenyl)-2-(4-nitrophenyl)-1*H*-pyrrole-3-carbaldehyde (4cc):



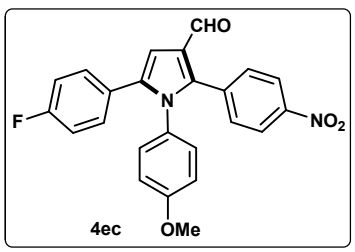
Yellow liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.65 (s, 3H), 3.77 (s, 3H), 6.64-6.69 (m, 2H), 6.75-6.79 (m, 3H), 6.90 (d, *J* = 8.9 Hz, 2H), 7.00 (s, 1H), 7.13 (t, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.8 Hz, 2H), 8.15 (d, *J* = 8.8 Hz, 2H), 9.75 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.09, 55.43, 108.50, 113.70, 114.08, 114.42 (2C), 121.28, 123.21 (2C), 124.63, 129.27, 129.44, 129.50 (2C), 131.86 (2C), 132.40, 136.24, 137.80, 140.29, 147.40, 159.26, 159.39, 186.00; IR (KBr)/cm^{-1} 2962, 2823, 1666, 1519,1342, 1234; HRMS (ESI): Calcd for $C_{25}H_{20}N_2O_5$ (MH^+) 429.1450; Found 429.1454.

1, 5-bis (4-methoxyphenyl)-2-(4-nitrophenyl)-1*H*-pyrrole-3-carbaldehyde (4dc):



Yellow solid (M.P = 145-146 ^{o}C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.77 (s, 6H), 6.75 (dd, *J* = 8.3 Hz, 8.6 Hz, 4H), 6.86 (s, 1H), 6.90 (d, *J* = 8.8 Hz, 2H), 7.01 (d, *J* = 8.7 Hz, 2H), 7.35 (d, *J* = 8.6 Hz, 2H), 8.14 (d, *J* = 8.6 Hz, 2H), 9.74 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.36, 55.37, 107.60, 113.69 (2C), 114.34 (2C), 123.18 (2C), 124.54, 126.78, 129.38 , 129.52 (2C), 130.12 (2C), 131.82 (2C), 136.29, 137.91, 139.88, 147.25, 159.06, 159.21, 186.10; IR (KBr)/cm^{-1} 2924, 2854, 1776, 1250, 1165, 1034; HRMS (ESI): Calcd for $C_{25}H_{20}N_2O_5$ (MH^+) 429.1450; Found 429.1452.

5-(4-fluorophenyl)-1-(4-methoxyphenyl)-2-(4-nitrophenyl)-1*H*-pyrrole-3-carbaldehyde (4ec):



Yellowish oily liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.78 (s, 3H), 6.75 (d, *J* = 8.9 Hz, 2H), 6.86-6.90 (m, 3H), 7.05-7.14 (m, 4H),

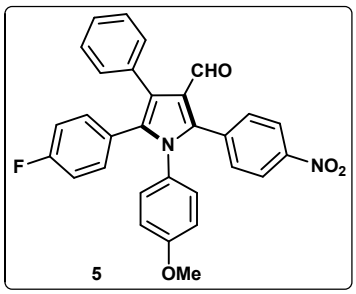
7.36 (d, J = 8.8 Hz, 2H), 8.15 (d, J = 8.8 Hz, 2H), 9.75 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 54.40, 107.34, 113.47 (2C), 114.29, 114.46, 122.25 (2C), 128.09, 128.48 (2C), 128.60, 129.44, 129.51, 129.58, 129.63, 130.51, 131.82 (2C), 135.11, 135.60, 135.94, 158.37, 185.00; IR (KBr)/cm^{-1} 2962, 2885, 1782, 1342, 1172; HRMS (ESI): Calcd for $C_{24}H_{17}FN_2O_4$ (MH^+) 417.1250; Found 417.1257.

Typical procedure for the synthesis of (4-fluorophenyl)-1-(4-methoxyphenyl)-2-(4-nitrophenyl)-4-phenyl-1*H*-pyrrole-3-carbaldehyde (5):

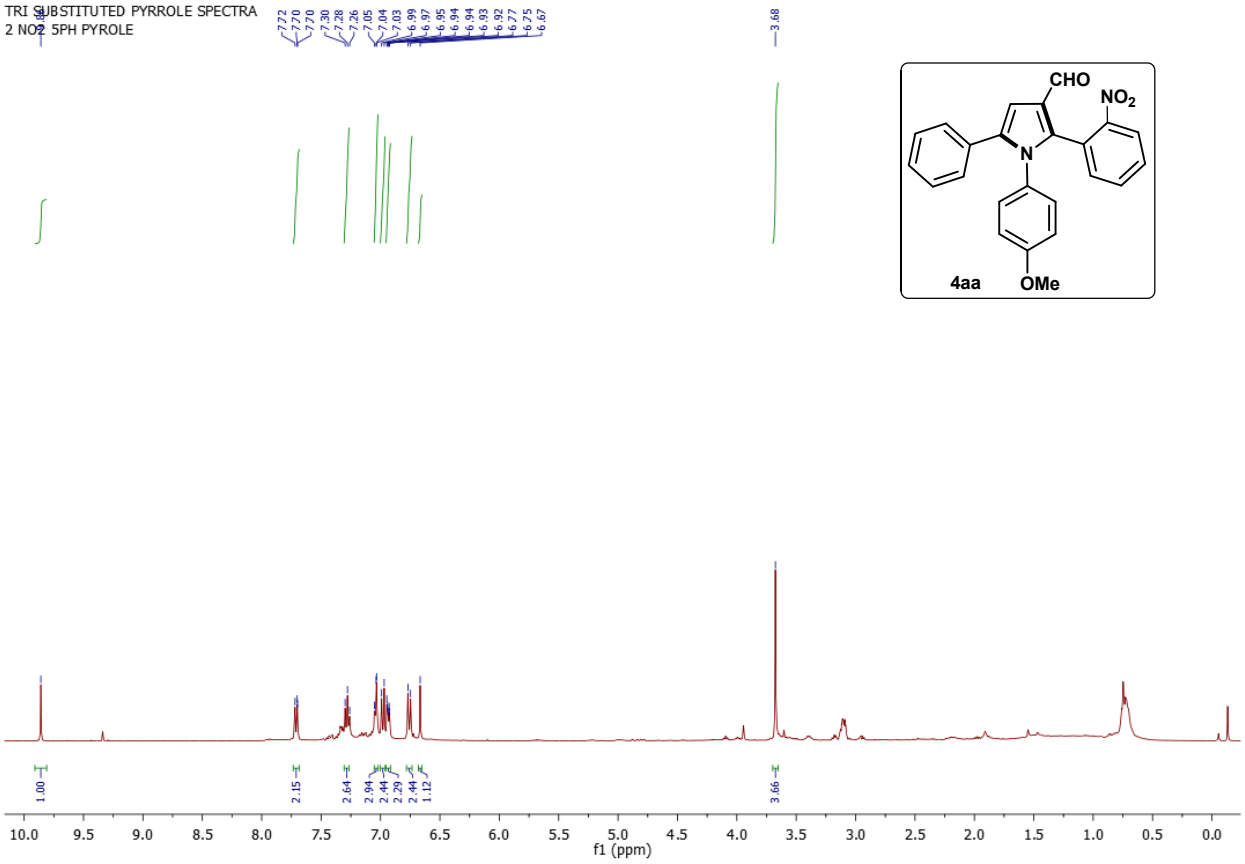
N- Bromosuccinimide (NBS) (22 mg, 0.125 mmol) was added to the stirred solution of pyrrole **4ec** (50 mg, 0.125 mmol) in CH_3CN (4.0 mL) at rt and further heated at 80 ^oC for 4 hrs. The reaction was cooled to room temperature and solvent was evaporated under reduced pressure. The crude material was taken in saturated $NaHCO_3$ solution and extracted with ethyl acetate (2 x 5 mL), the combined organic layer was washed with brine and dried over Na_2SO_4 and concentrated under vacuo. Corresponding intermediate bromo compound (80 mg, 68%,) was obtained as reddish oily liquid after simple chromatographic purification using EtOAc/hexane.

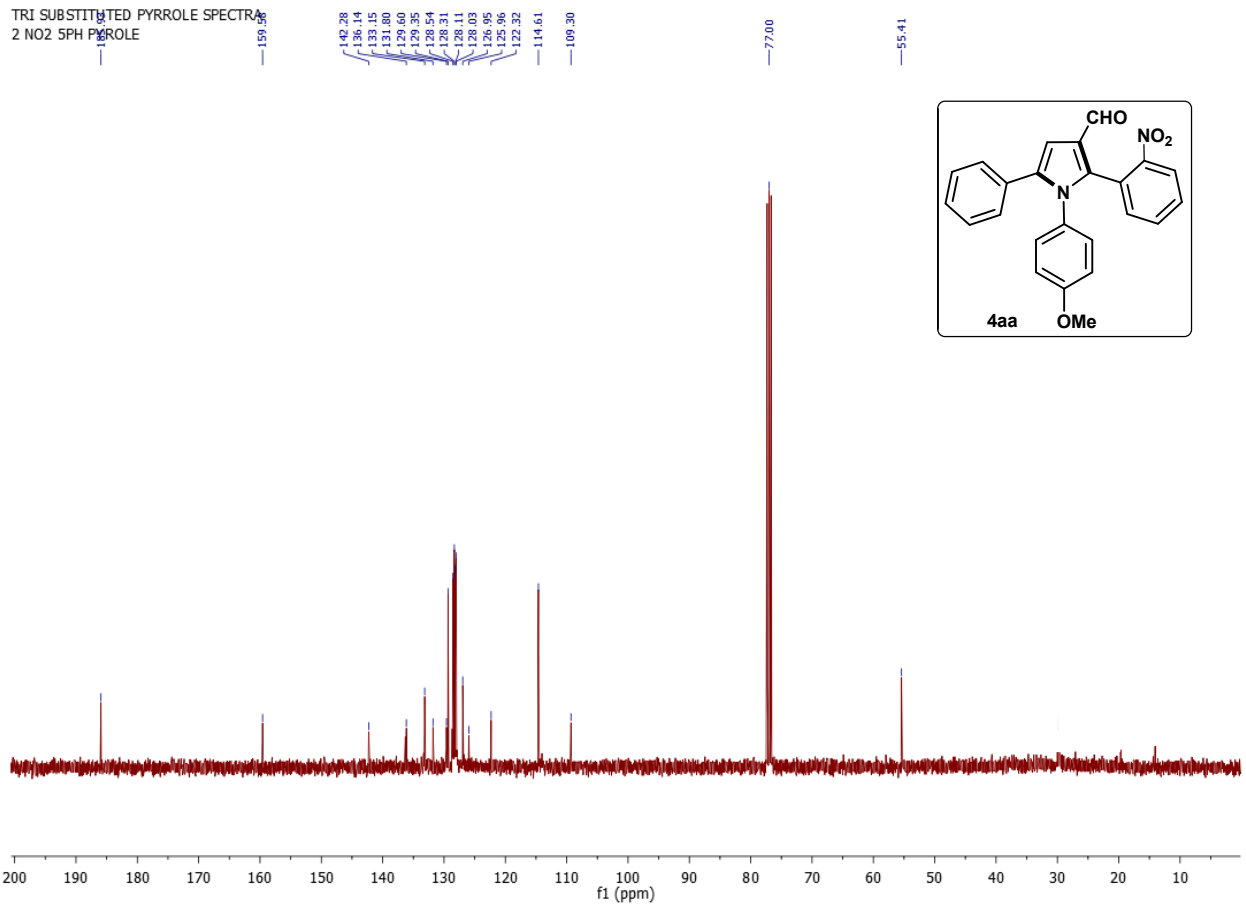
To the stirred solution of crude bromo compound (78 mg, 0.15 mmol) in DMF (3.0 mL) were added $PhB(OH)_2$ (1.5 equiv, 28 mg, 0.23 mmol), Pd (PPh_3)$_4$ (10 mol%, 18 mg, 0.015 mmol) and K_2CO_3 (2M solution, 78 μL, 0.15 mmol) under inert atmosphere. The reaction was then heated to 110 ^oC for 4 hrs. After complete consumption of the intermediate bromo compound on TLC, reaction was cooled and filtered through celite. After standard work up and chromatographic purification using (Hexane : EtOAc = 20:1) gave compound **5** (55 mg, 72%,) as a yellow oily liquid.

(4-fluorophenyl)-1-(4-methoxyphenyl)-2-(4-nitrophenyl)-4-phenyl-1*H*-pyrrole-3-carbaldehyde (5):

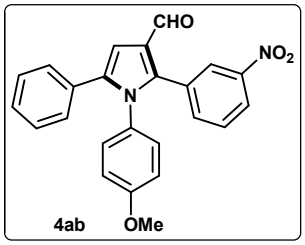


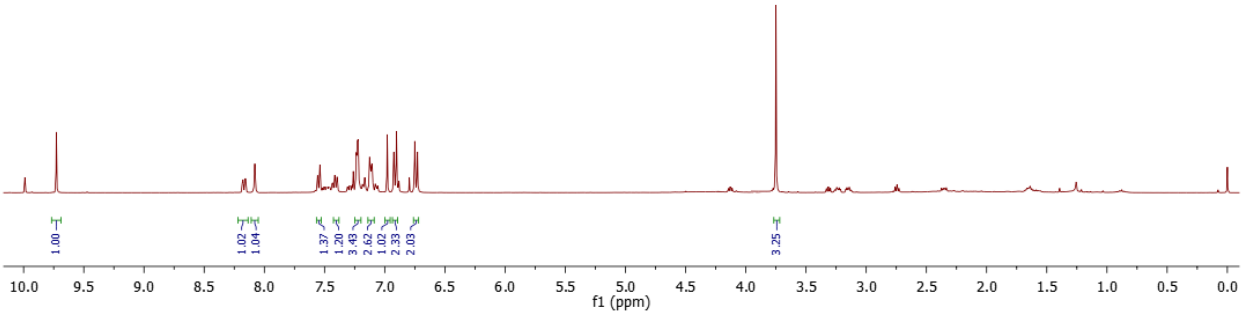
Yellowish pasty liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74 (s, 3H), 6.79 (d, *J* = 8.8 Hz, 2H), 6.79 (t, *J* = 8.7, 3H), 6.84 (d, *J* = 8.8 Hz, 2H), 6.90 (dd, *J* = 8.8 Hz, 5.4 Hz 2H), 7.04 (t, *J* = 8.6 Hz, 1H), 7.29 (m, 2H), 7.36 (dd, *J* = 8.9 Hz, 5.2 Hz, 1H), 7.42 (d, *J* = 8.8 Hz, 2H), 8.13 (d, *J* = 8.8 Hz, 2H) 9.85 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.33, 114.15 (2C), 115.18, 115.69, 122.97 (2C), 125.74, 127.08, 127.19, 127.26, 128.07 (2C), 129.01, 129.65 (2C), 130.86 (2C), 132.06 (2C), 132.60, 132.82, 132.89, 133.58, 136.98, 137.29, 147.22, 159.15, 162.95, 186.91; IR (KBr)/cm^{-1} 2923, 1728, 1512, 1350, 1226; HRMS (ESI): Calcd for $C_{30}H_{21}FN_2O_4$ (MH^+) 493.1563; Found 493.1567.


TRI SUBSTITUTED PYRROLE SPECTRA
2 NO2 5PH PYROLE
7.72
7.70
7.70
7.30
7.28
7.26
7.05
7.04
7.03
6.99
6.97
6.95
6.94
6.94
6.93
6.92
6.77
6.75
6.67
3.68
CHO
NO2
N
4aa
OMe
1.00
2.15
2.64
2.94
2.44
2.29
2.44
1.12
3.66
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

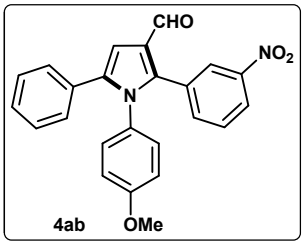

TRI SUBSTITUTED PYRROLE SPECTRA
2 NO2 5PH PYROLE
159.56
142.28
136.14
133.15
131.80
129.60
129.35
128.54
128.31
128.11
128.03
126.95
125.96
122.32
114.61
109.30
77.00
55.41
CHO
NO2
N
4aa
OMe
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

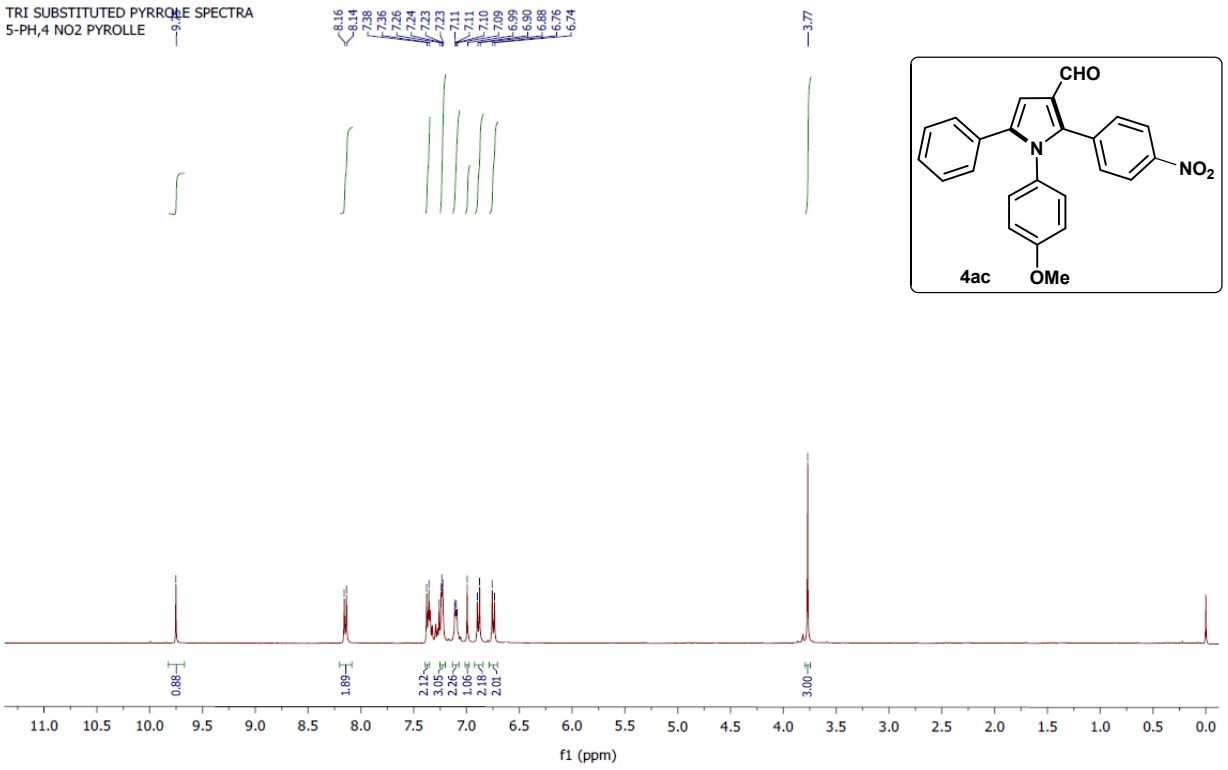
TRI SUBSTITUTED PYRROLE SPECTRA
3-NO2,5Ph-Pyrole

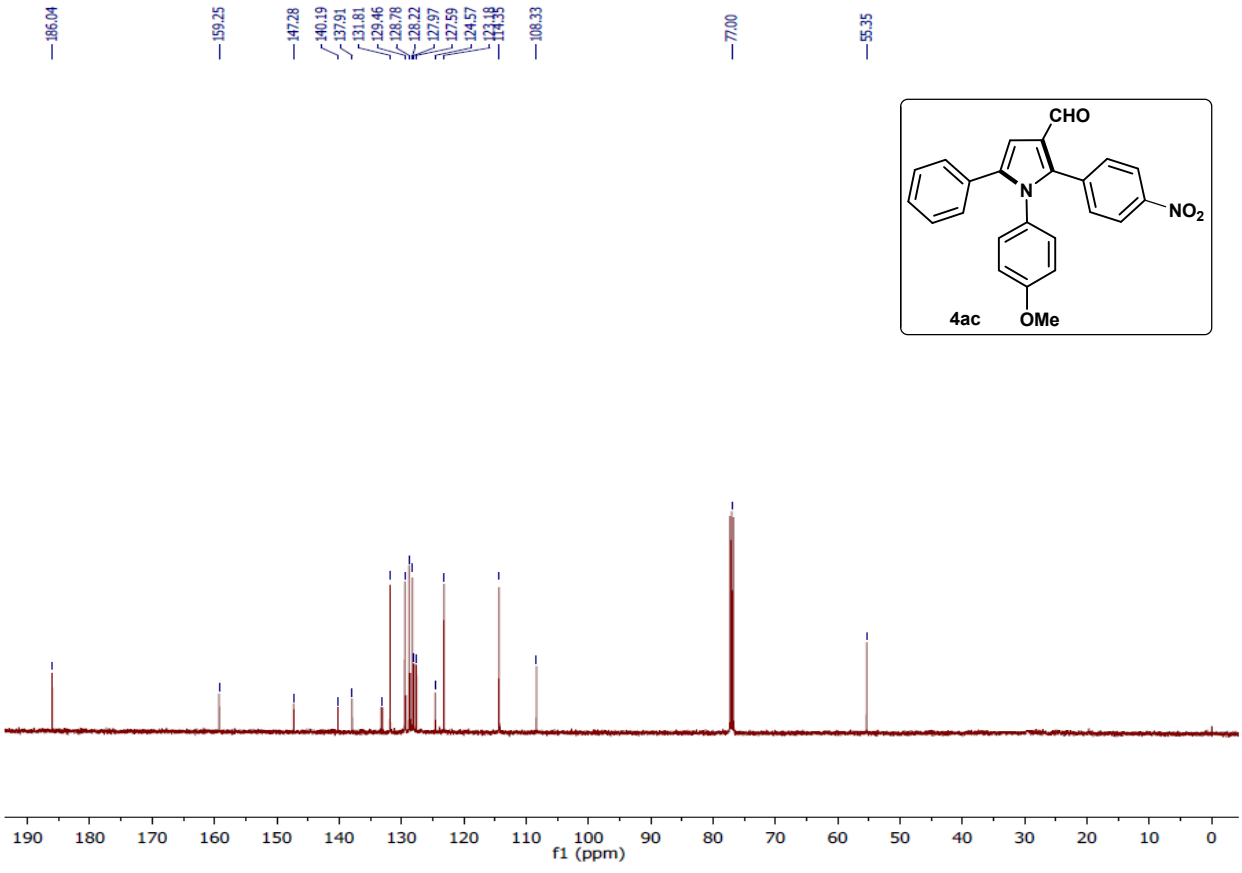


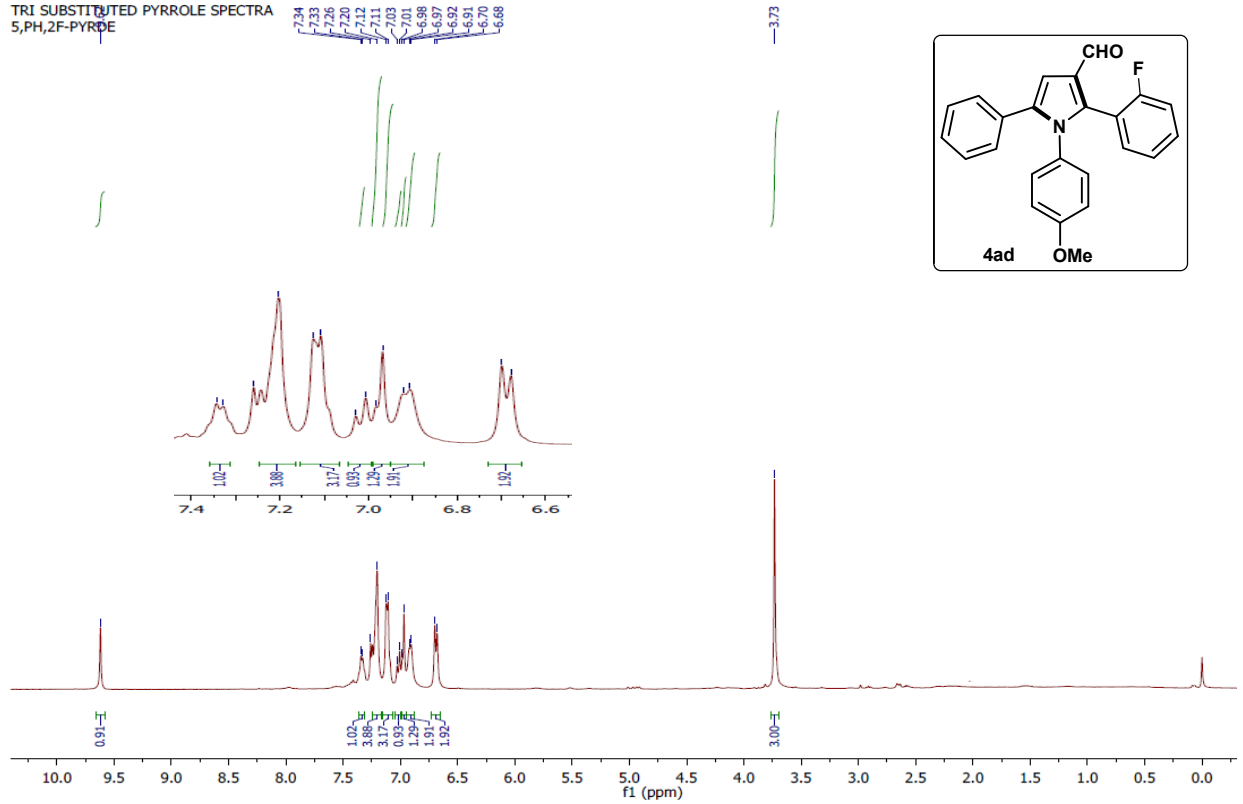


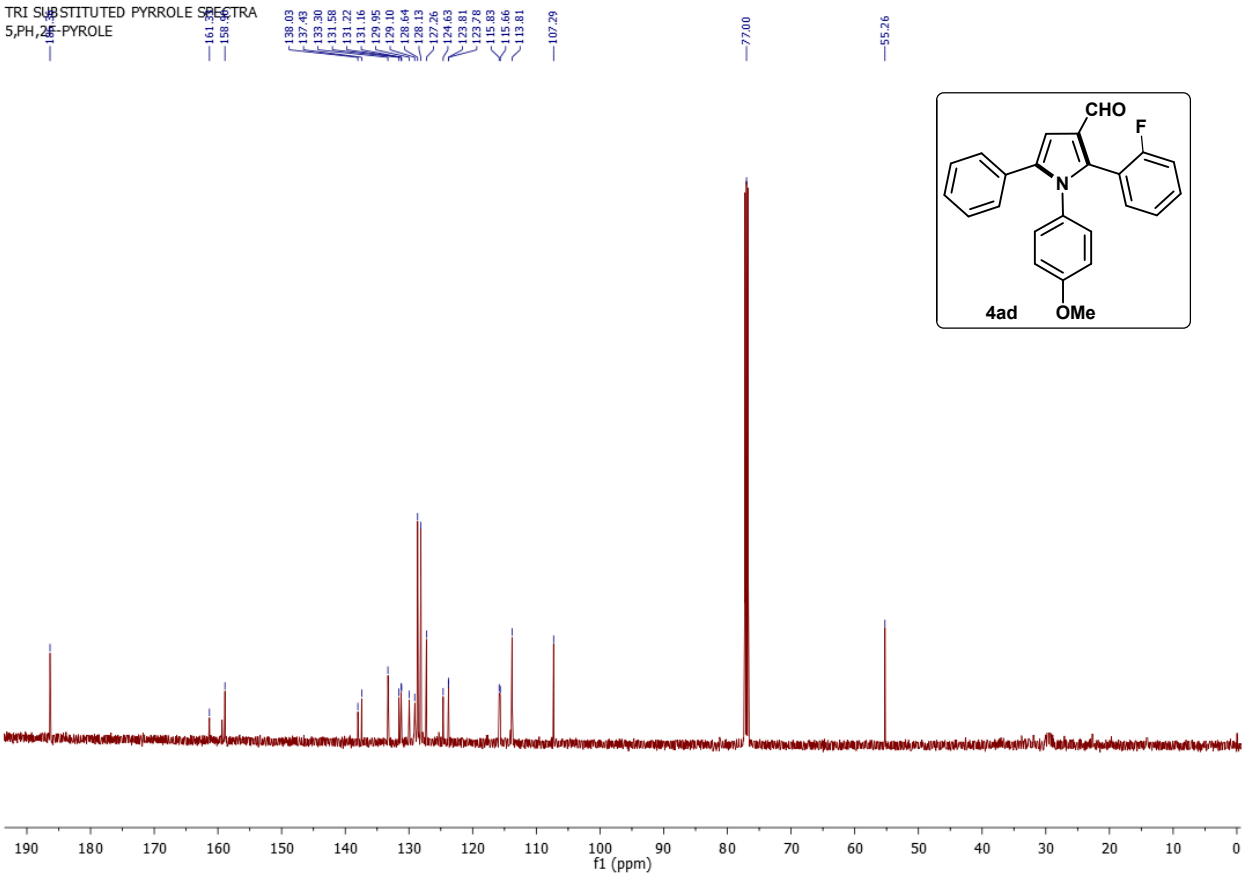
TRI SUBSTITUTED PYRROLE SPECTRA
3-NO2-5Ph-Pyrole

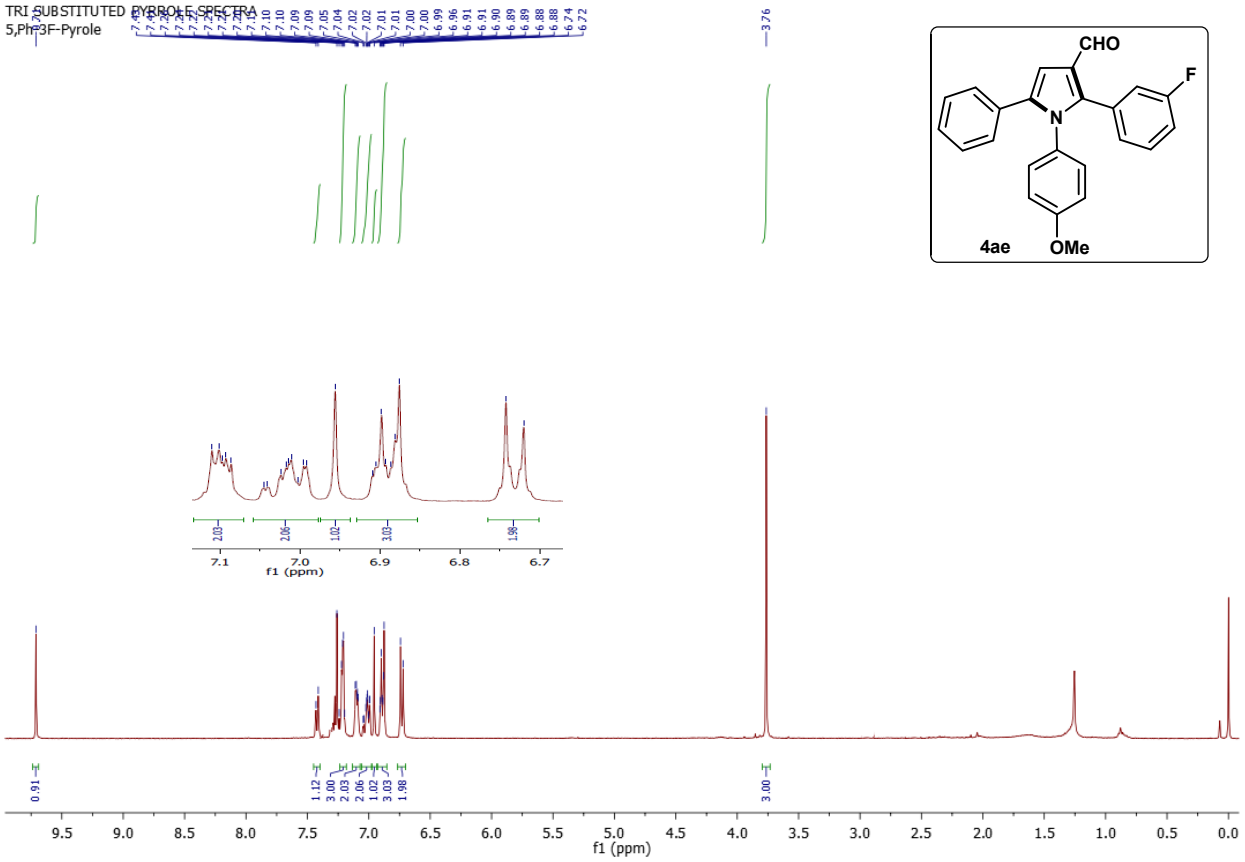


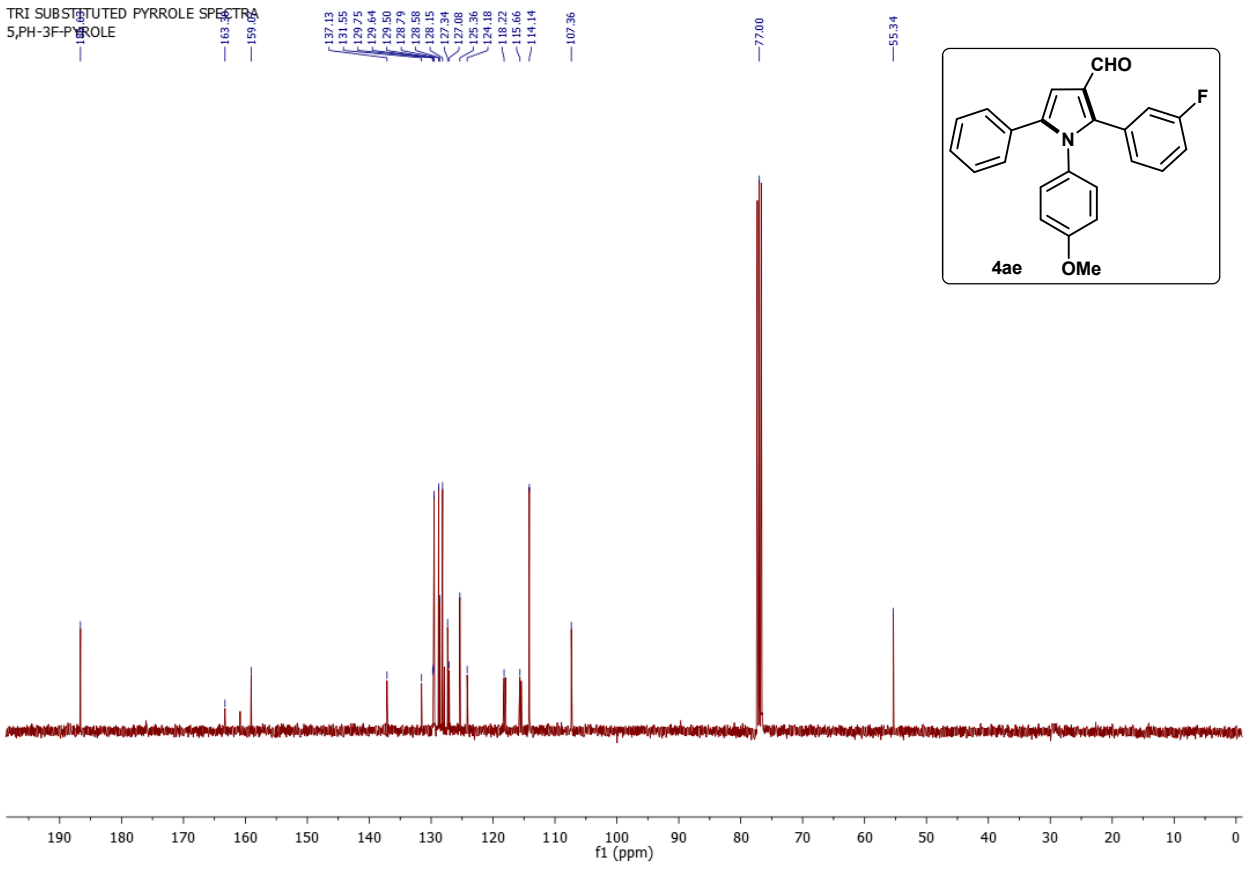

TRI SUBSTITUTED PYRROLE SPECTRA
5-PH,4 NO2 PYROLLE
9.74
8.16
8.14
7.38
7.36
7.26
7.24
7.23
7.23
7.11
7.11
7.10
7.09
6.99
6.90
6.88
6.76
6.74
3.77
CHO
N
NO2
4ac
OMe
0.88
1.89
2.12
3.05
2.26
1.06
2.18
2.01
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

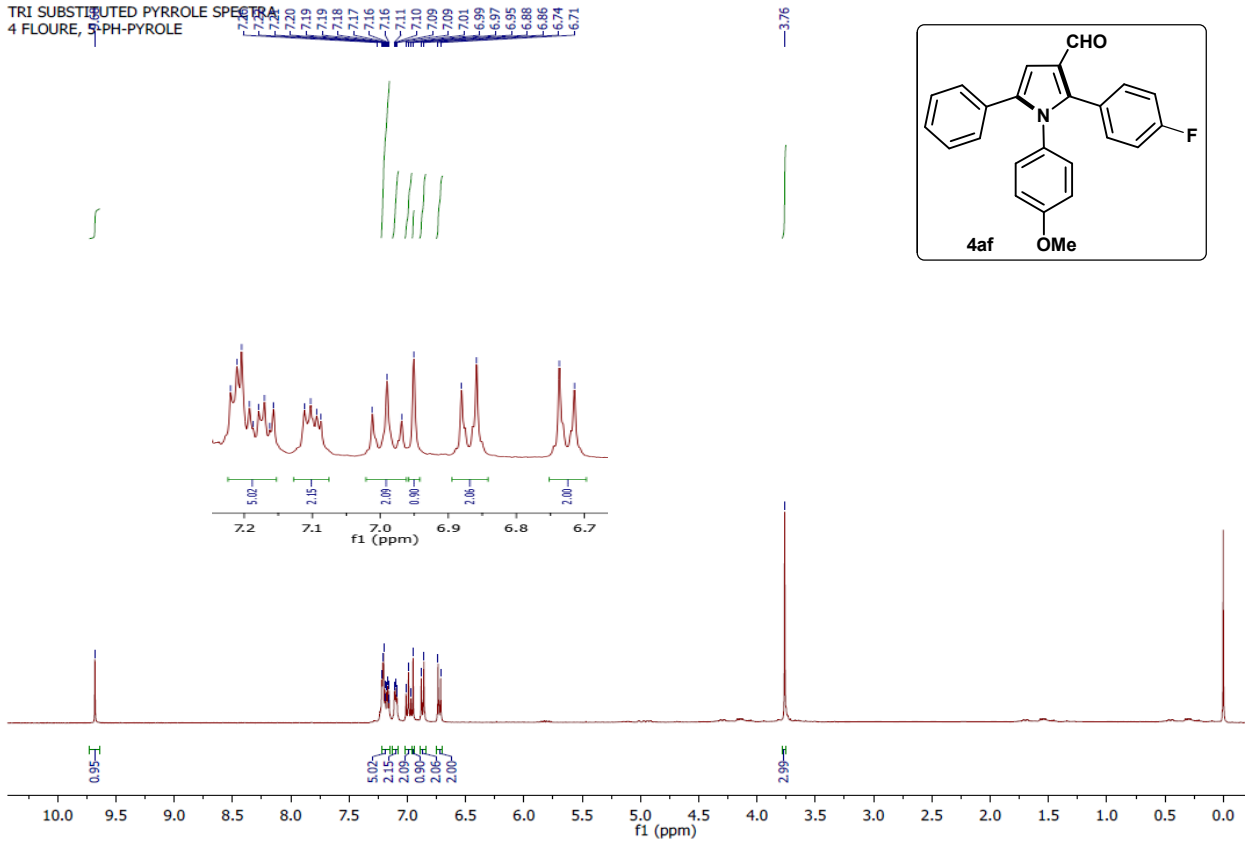

186.04
159.25
147.28
140.19
137.91
131.81
129.46
128.78
128.22
127.97
127.59
124.57
123.18
114.33
108.33
77.00
55.35
CHO
N
NO2
4ac
OMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

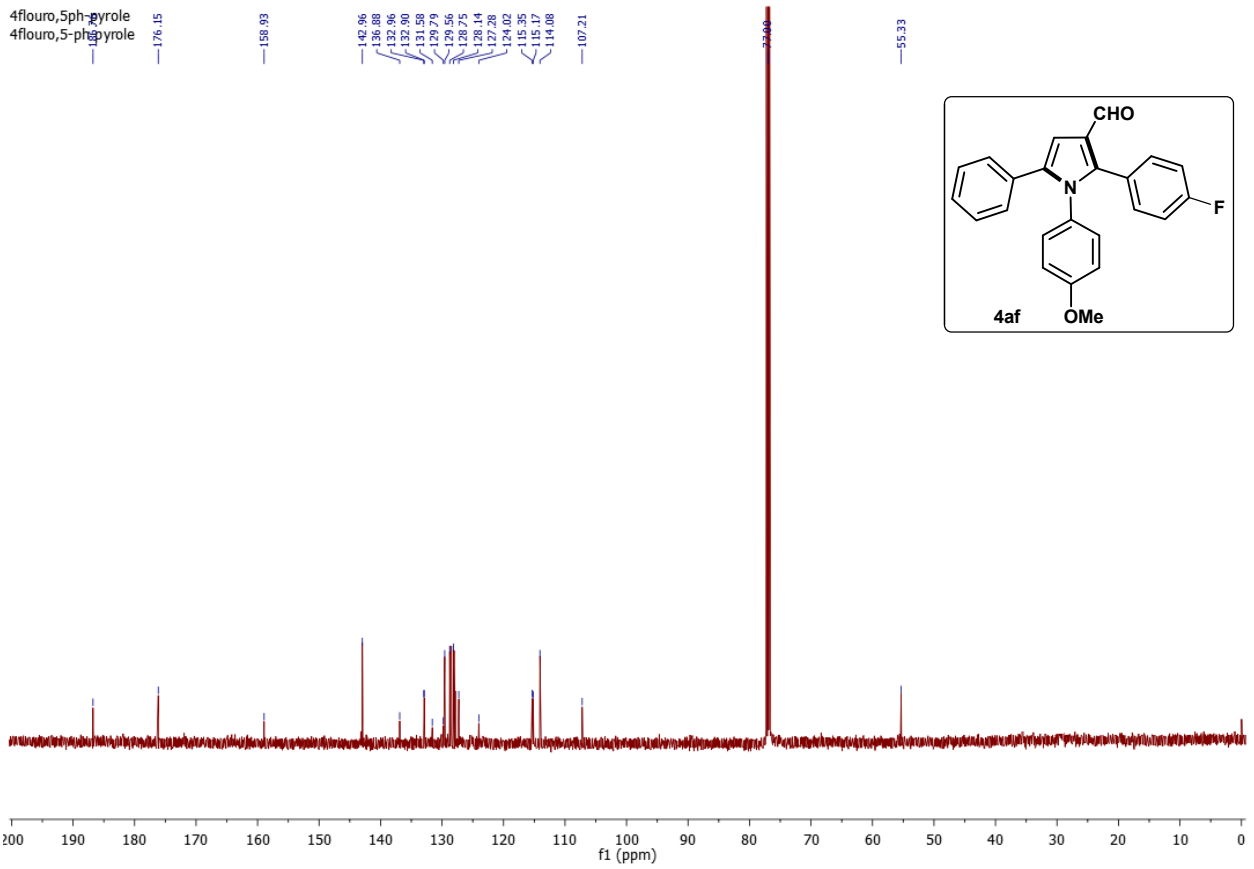

TRI SUBSTITUTED PYRROLE SPECTRA
5,PH,2F-PYRDE
CHO
F
N
4ad
OMe
f1 (ppm)

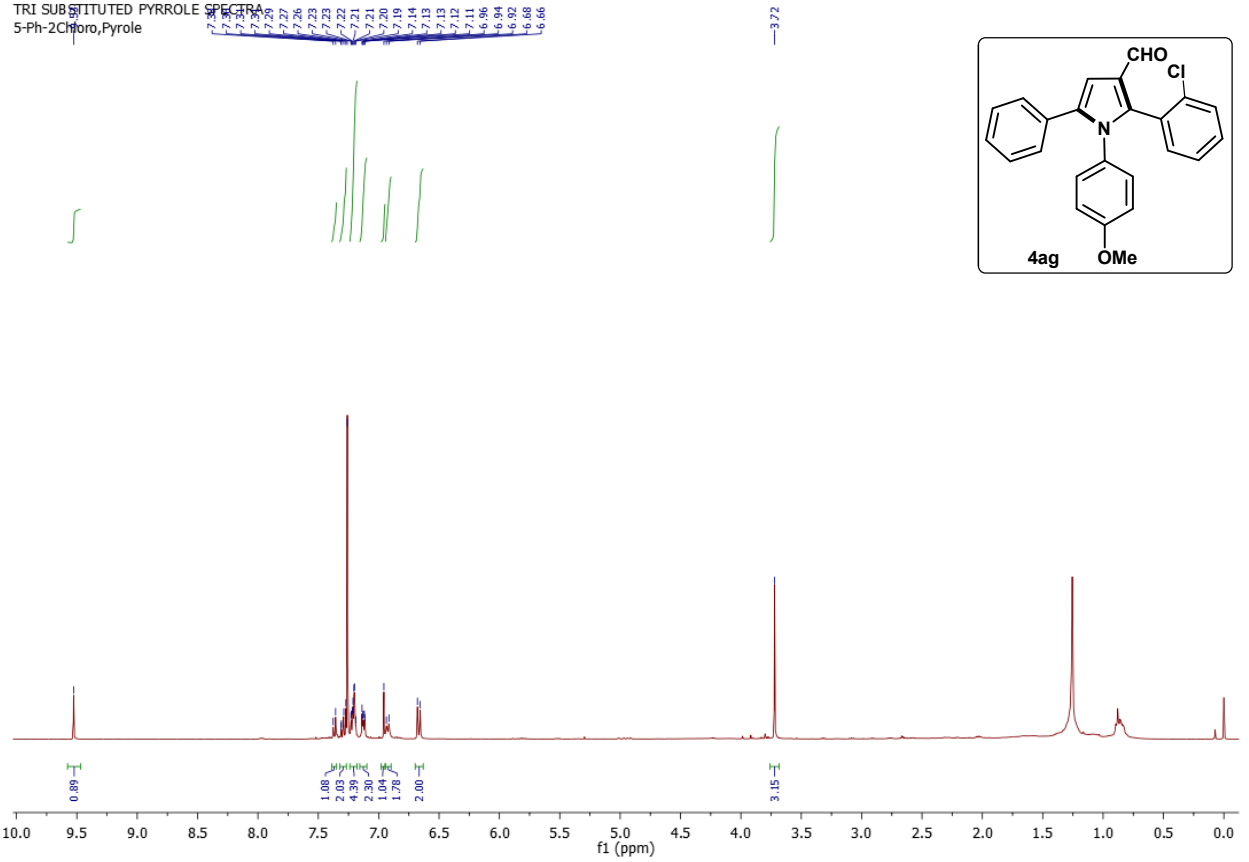

TRI SUBSTITUTED PYRROLE SPECTRA
5,PH,2F-PYROLE
CHO
F
N
4ad
OMe
f1 (ppm)

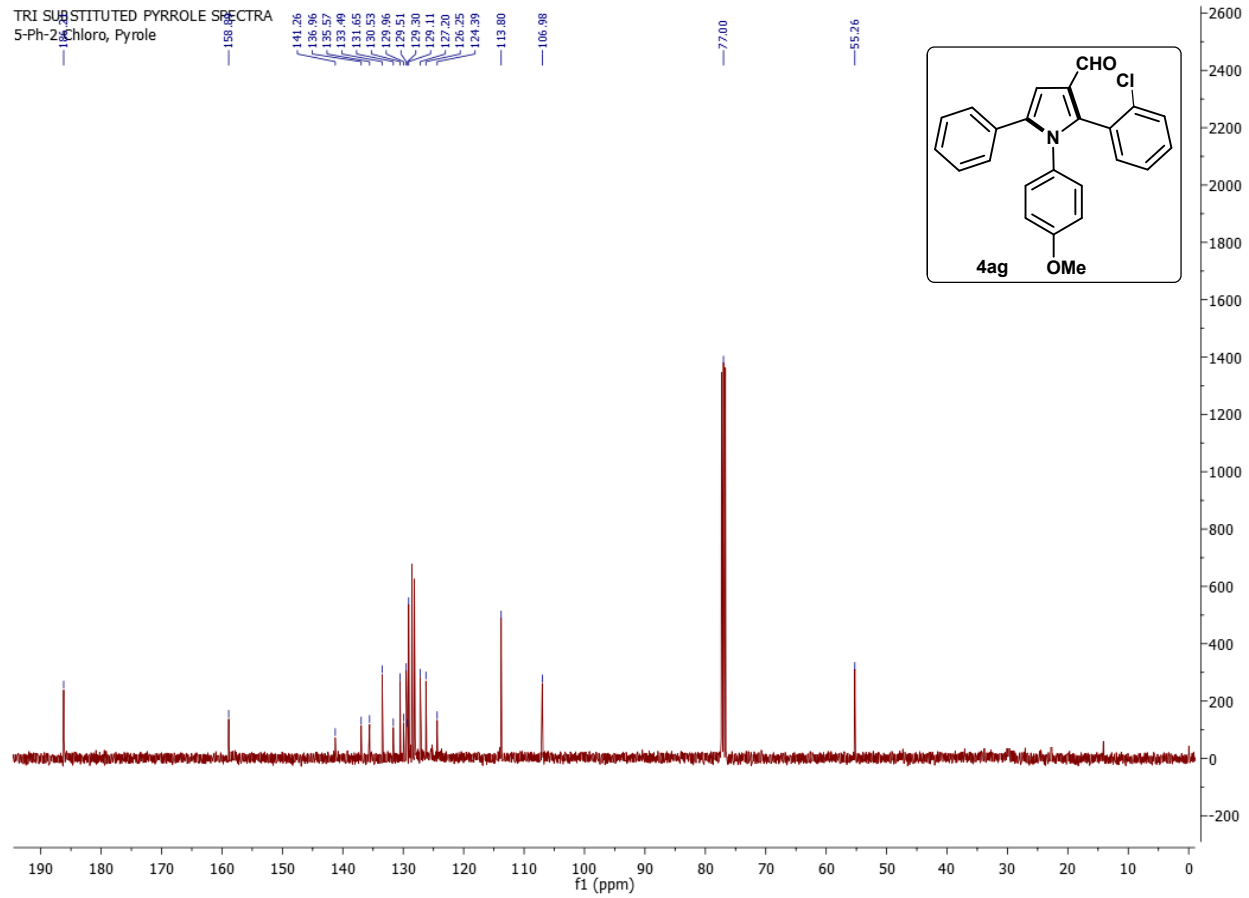

TRI SUBSTITUTED PYRROLE SPECTRA
5,Ph-3F-Pyrole
CHO
F
N
4ae
OMe
f1 (ppm)


TRI SUBSTITUTED PYRROLE SPECTRA
5,PH-3F-PYRROLE
CHO
F
N
4ae
OMe
f1 (ppm)

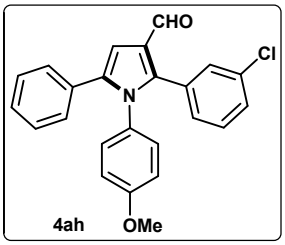

TRI SUBSTITUTED PYRROLE SPECTRA
4 FLOURE, 5-PH-PYROLE
CHO
N
F
4af
OMe
f1 (ppm)

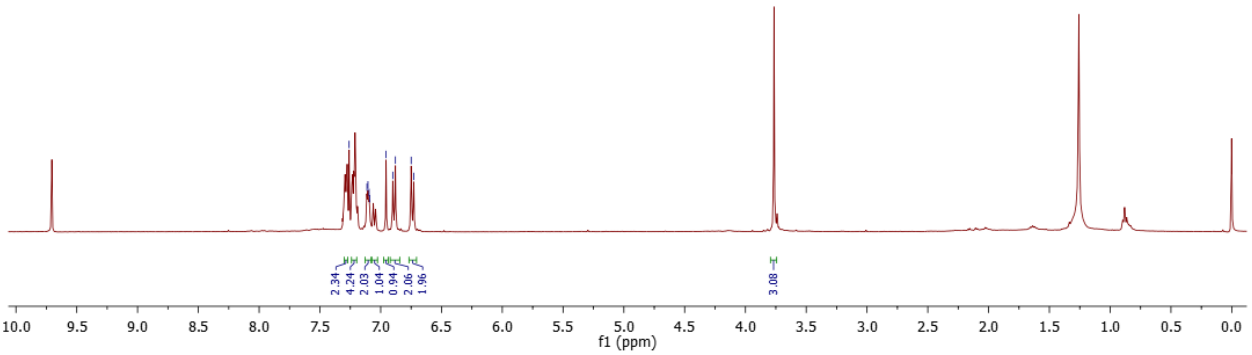

4flouro,5ph-pyrole
4flouro,5-ph-pyrole
CHO
N
F
4af
OMe
f1 (ppm)


TRI SUBSTITUTED PYRROLE SPECTRA
5-Ph-2Chloro,Pyrole
CHO
Cl
N
4ag
OMe
f1 (ppm)

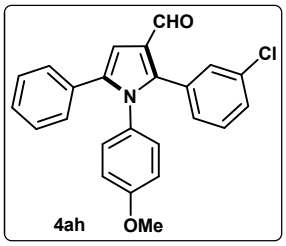

TRI SUBSTITUTED PYRROLE SPECTRA
5-Ph-2Chloro, Pyrole
CHO
Cl
N
4ag
OMe
f1 (ppm)

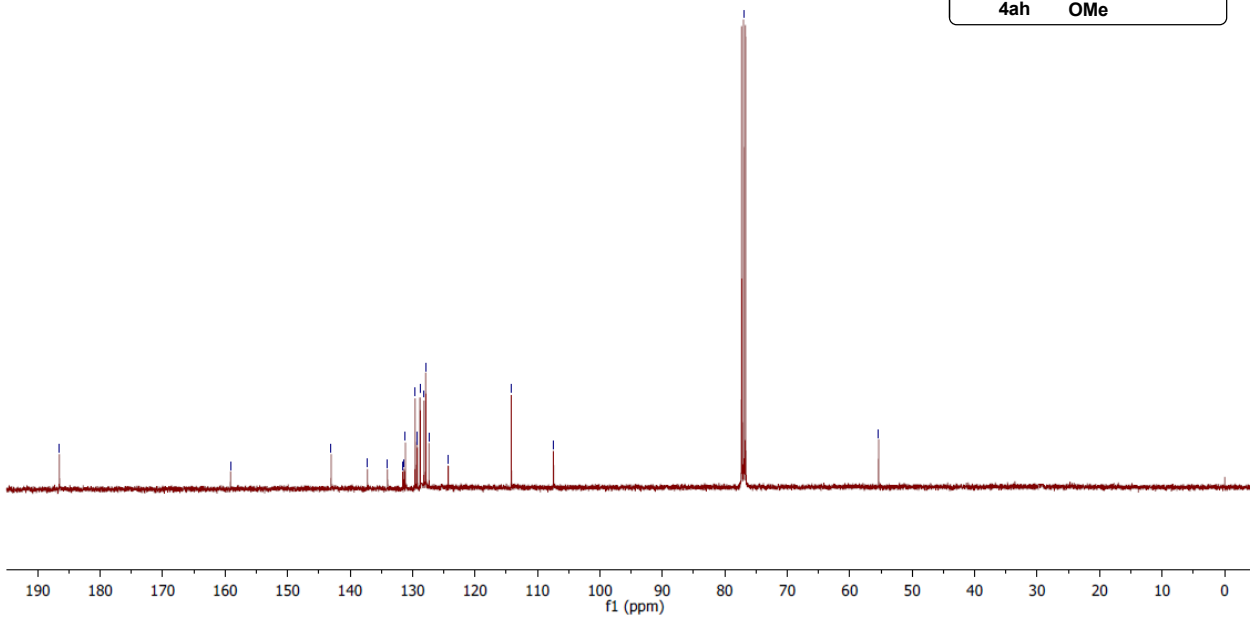
TRI SUBSTITUTED PYRROLE SPECTRA
5-Phenyle-3-3chloroPyrolle



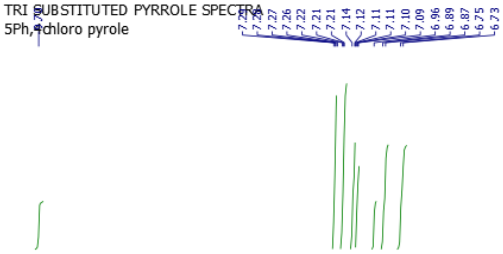


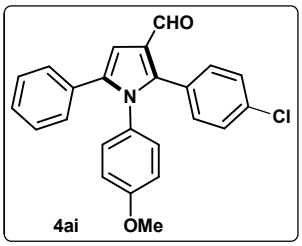
5-Phenyl-3-Chloro-Pyrolle 13C NMR
5Phenyle3-ChloroPyrolle

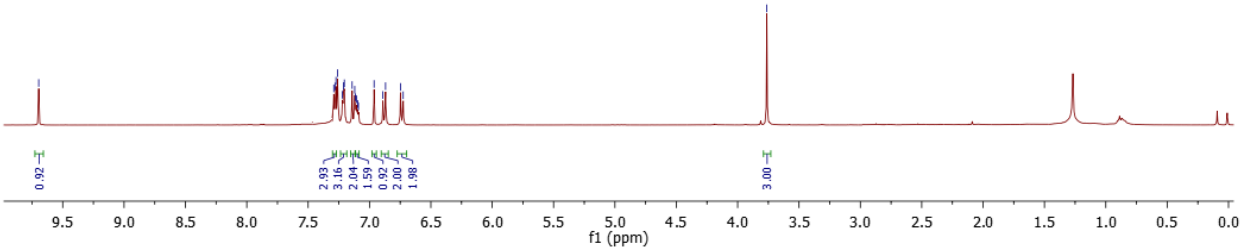




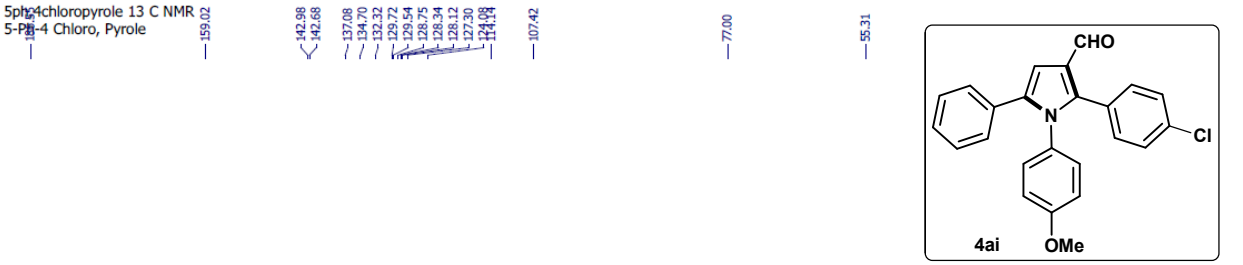
TRI SUBSTITUTED PYRROLE SPECTRA
5Ph, 4chloro pyrole

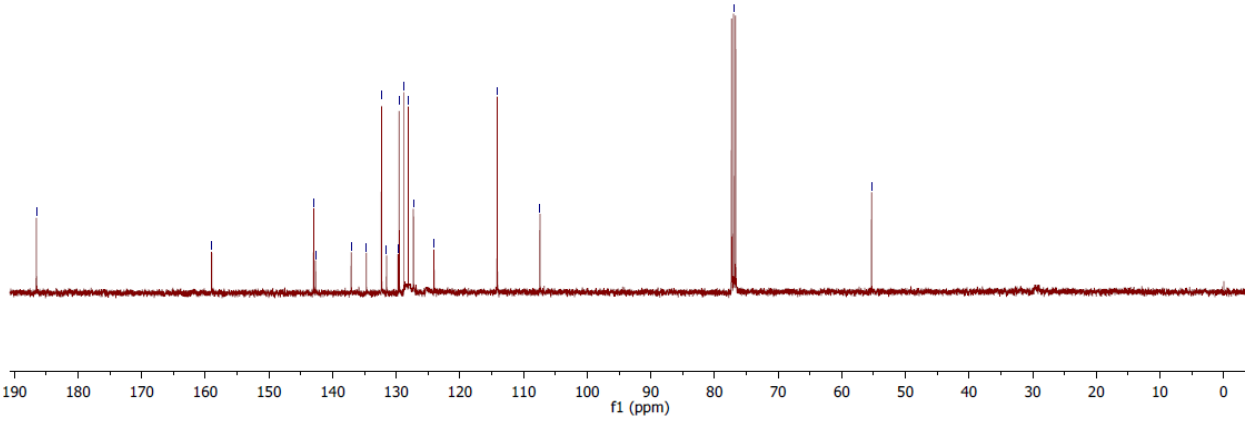


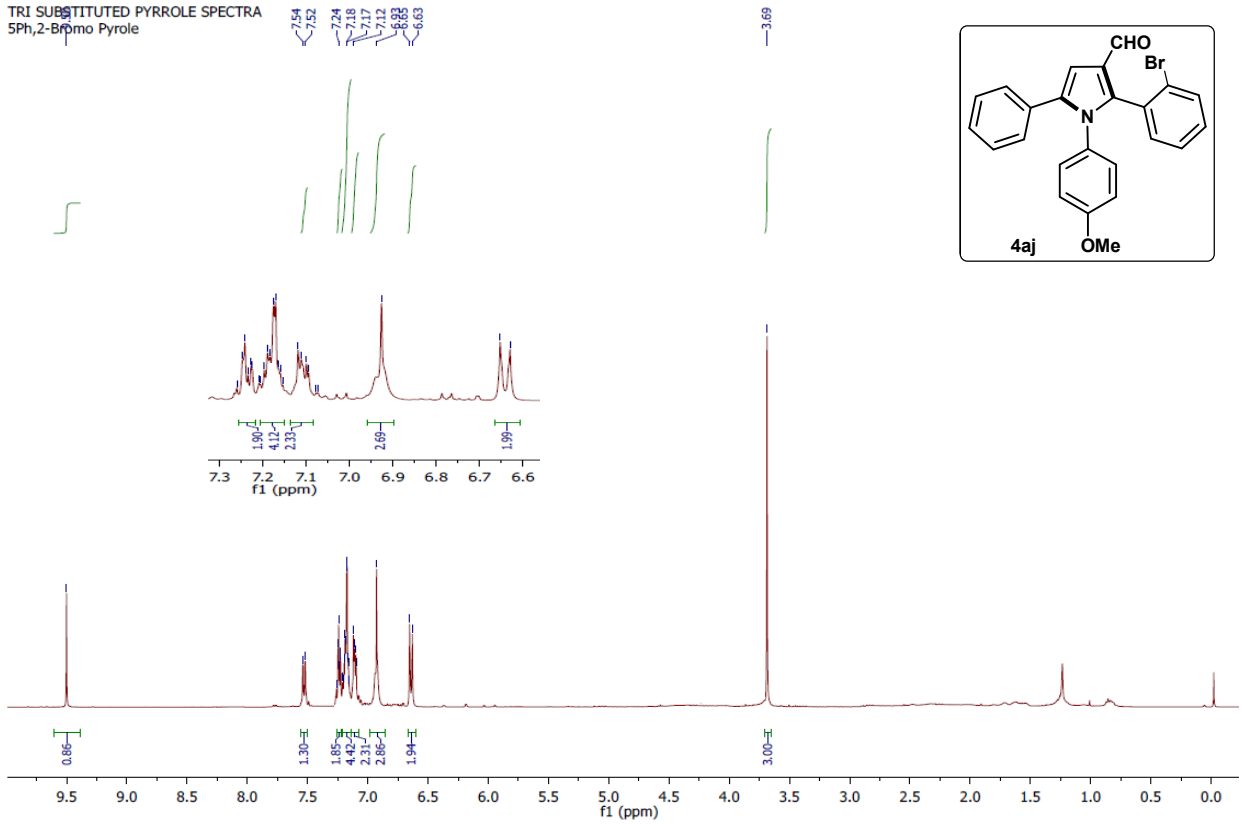


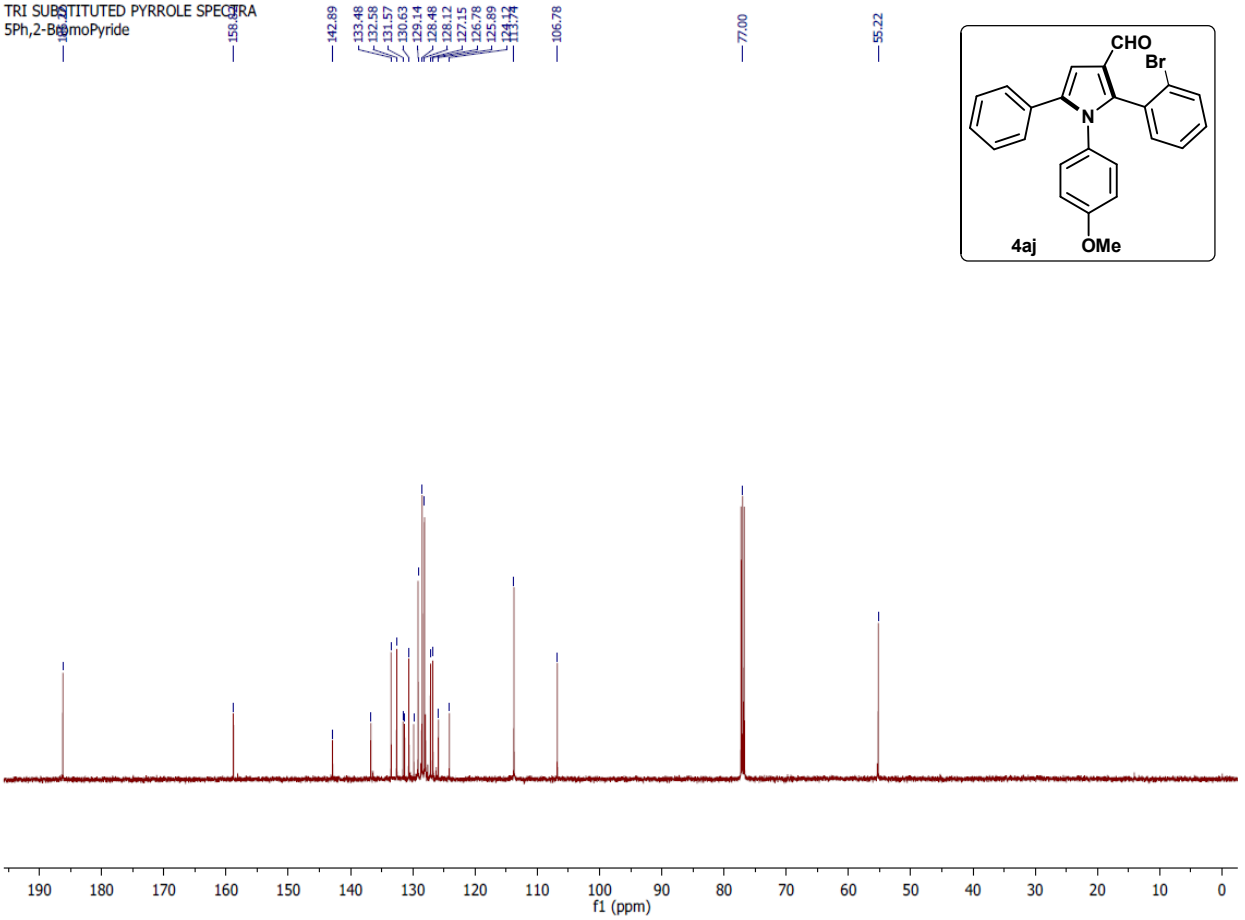


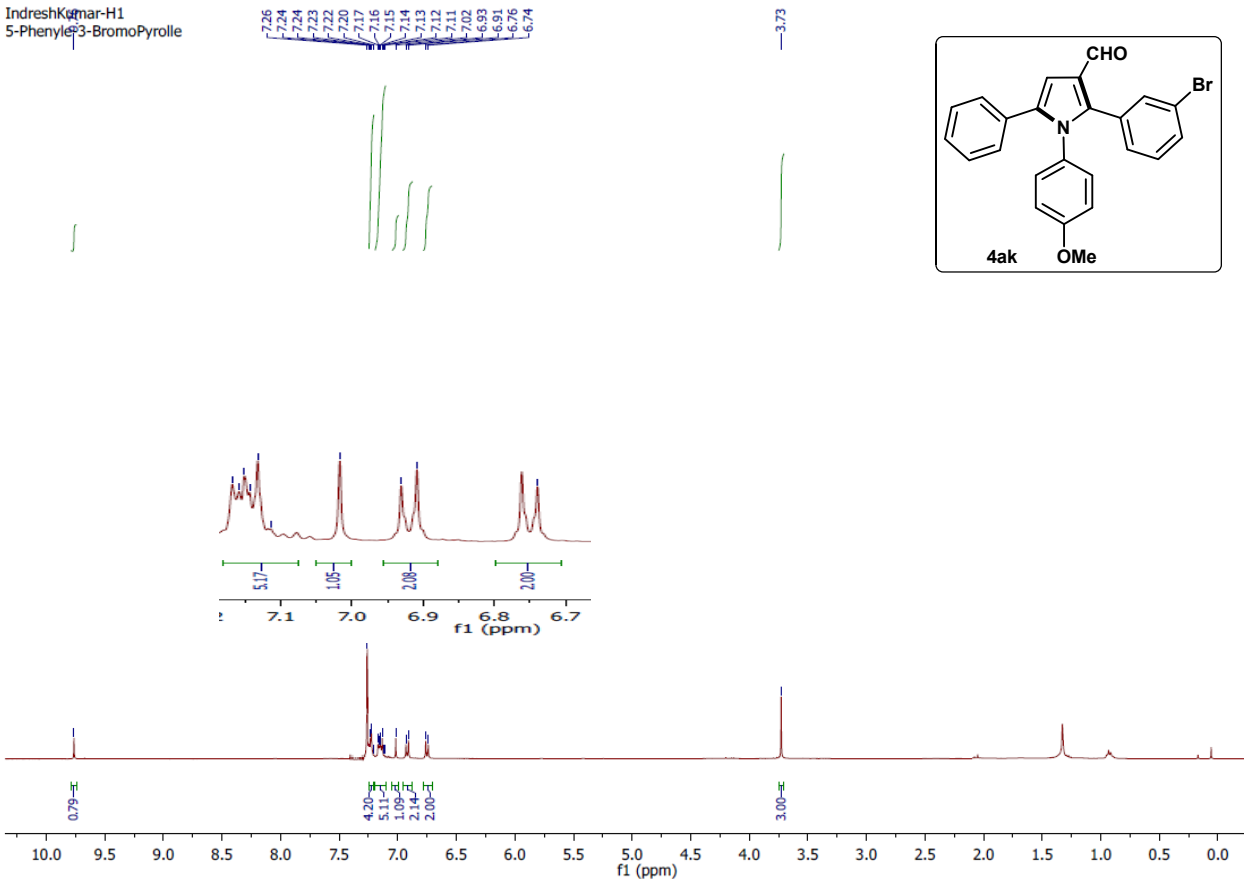
5ph,4chloropyrole 13 C NMR
5-Ph-4 Chloro, Pyrole

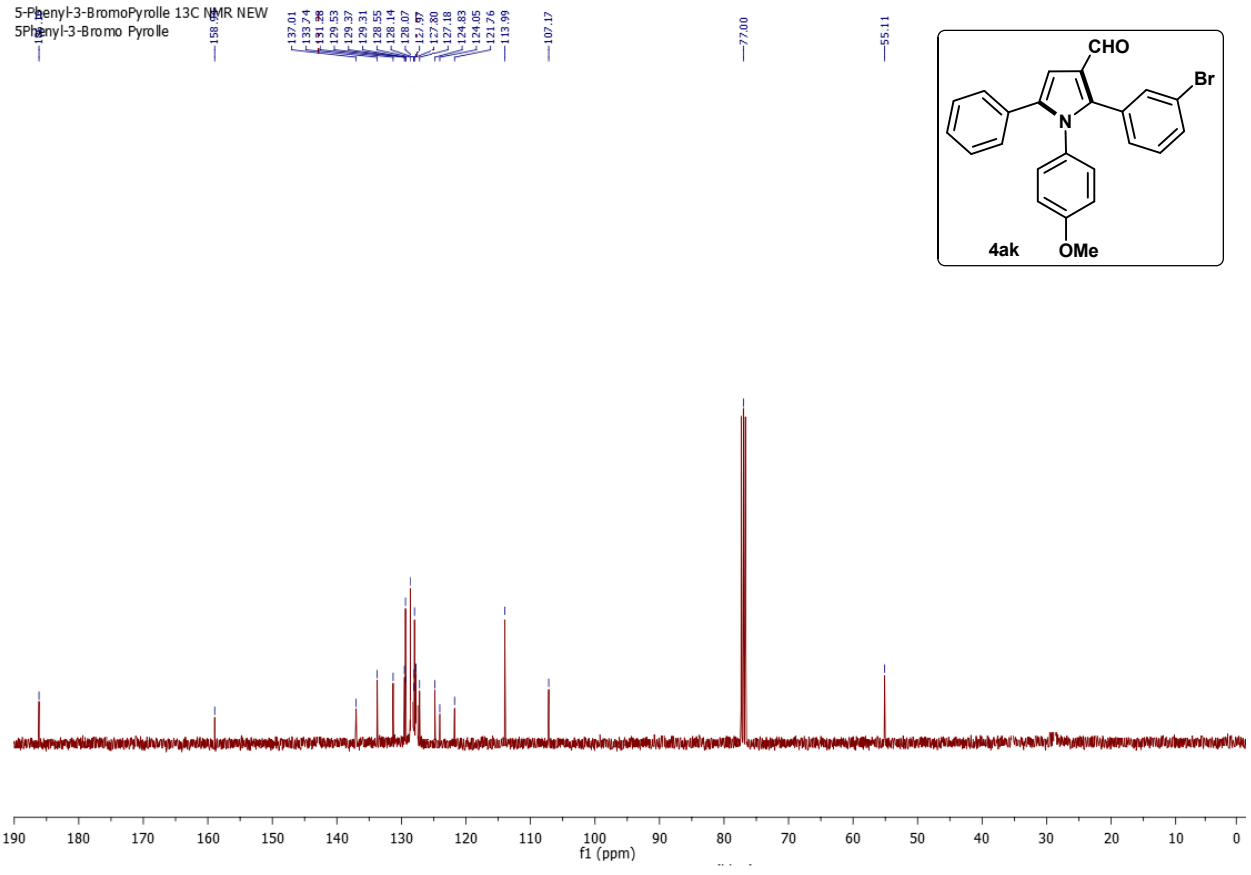


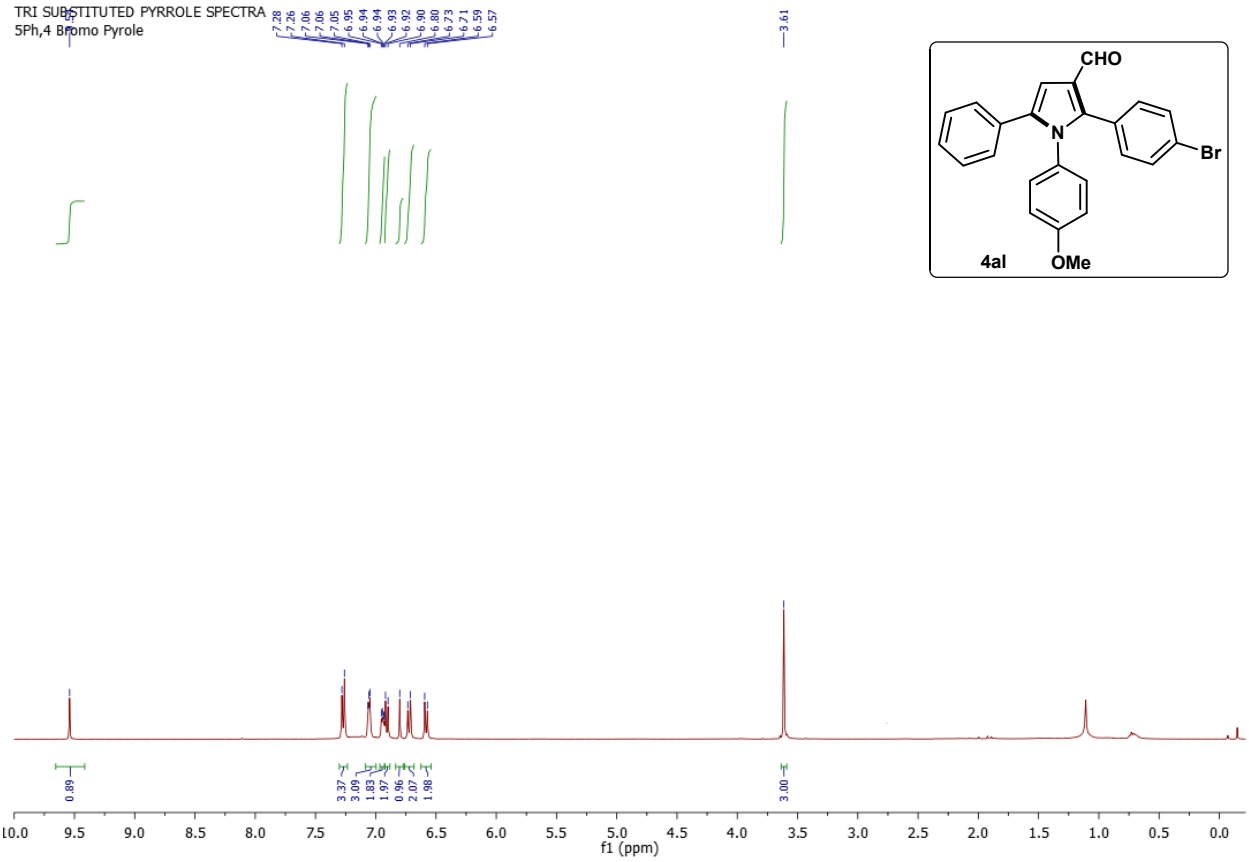


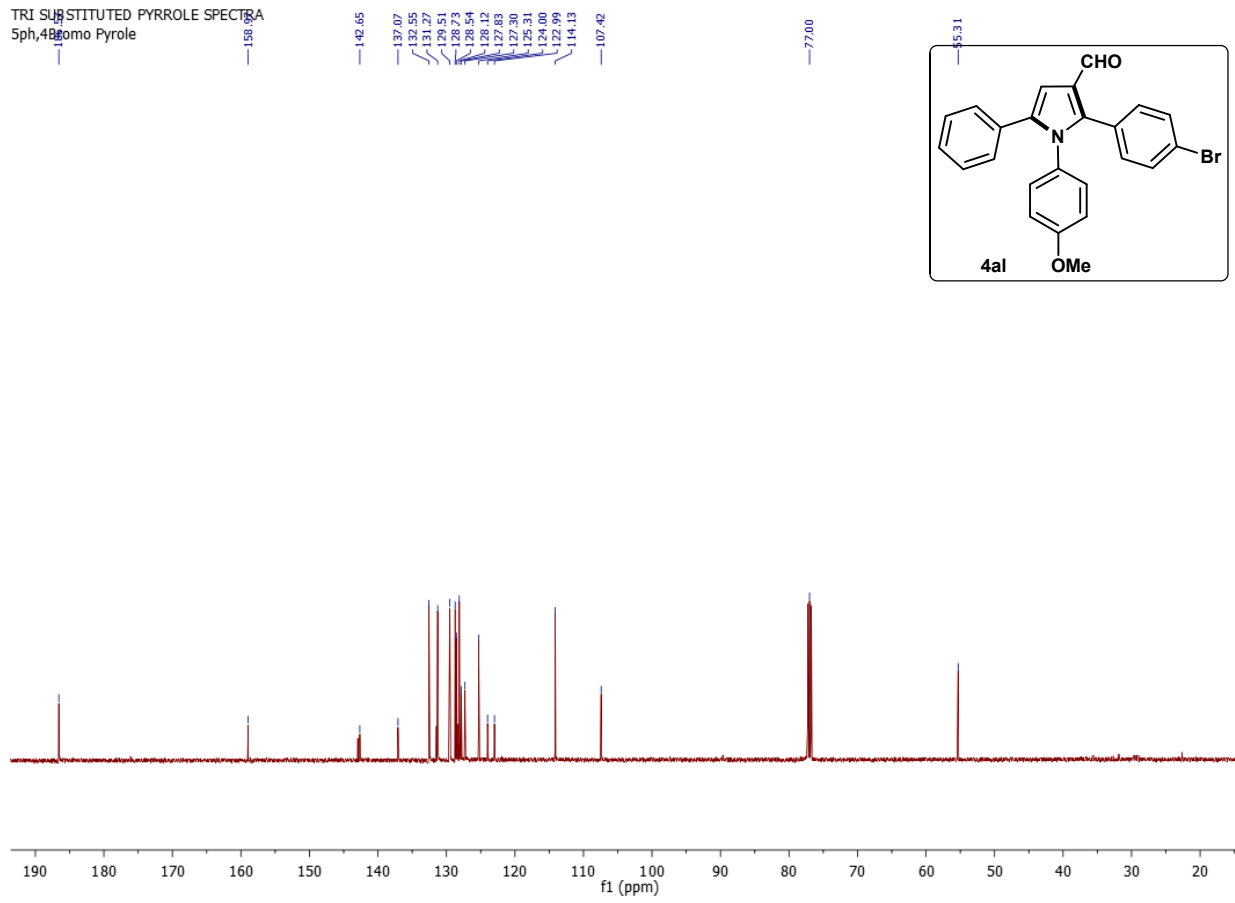

TRI SUBSTITUTED PYRROLE SPECTRA
5Ph,2-Bromo Pyrole
CHO
Br
N
4aj
OMe
f1 (ppm)


TRI SUBSTITUTED PYRROLE SPECTRA
5Ph,2-BromoPyride
CHO
Br
N
4aj
OMe
f1 (ppm)

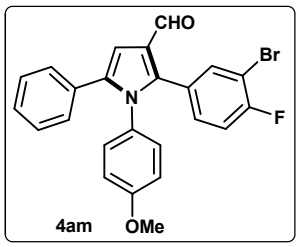

IndreshKumar-H1
5-Phenyle-3-BromoPyrolle
7.26
7.24
7.24
7.23
7.22
7.20
7.17
7.16
7.15
7.14
7.13
7.12
7.11
7.02
6.93
6.91
6.76
6.74
3.73
CHO
Br
N
4ak
OMe
5.17
1.05
2.08
2.00
7.1
7.0
6.9
6.8
6.7
f1 (ppm)
0.79
4.20
5.11
1.09
2.14
2.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


5-Phenyl-3-BromoPyrolle 13C NMR NEW
5Phenyl-3-Bromo Pyrolle
137.01
133.74
131.28
129.53
129.37
129.31
128.55
128.14
128.07
127.80
127.18
124.83
124.05
121.76
113.99
107.17
77.00
55.11
CHO
Br
N
4ak
OMe
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

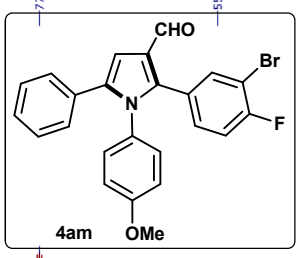

TRI SUBSTITUTED PYRROLE SPECTRA
5Ph,4 Bromo Pyrole
CHO
N
Br
4al
OMe
f1 (ppm)

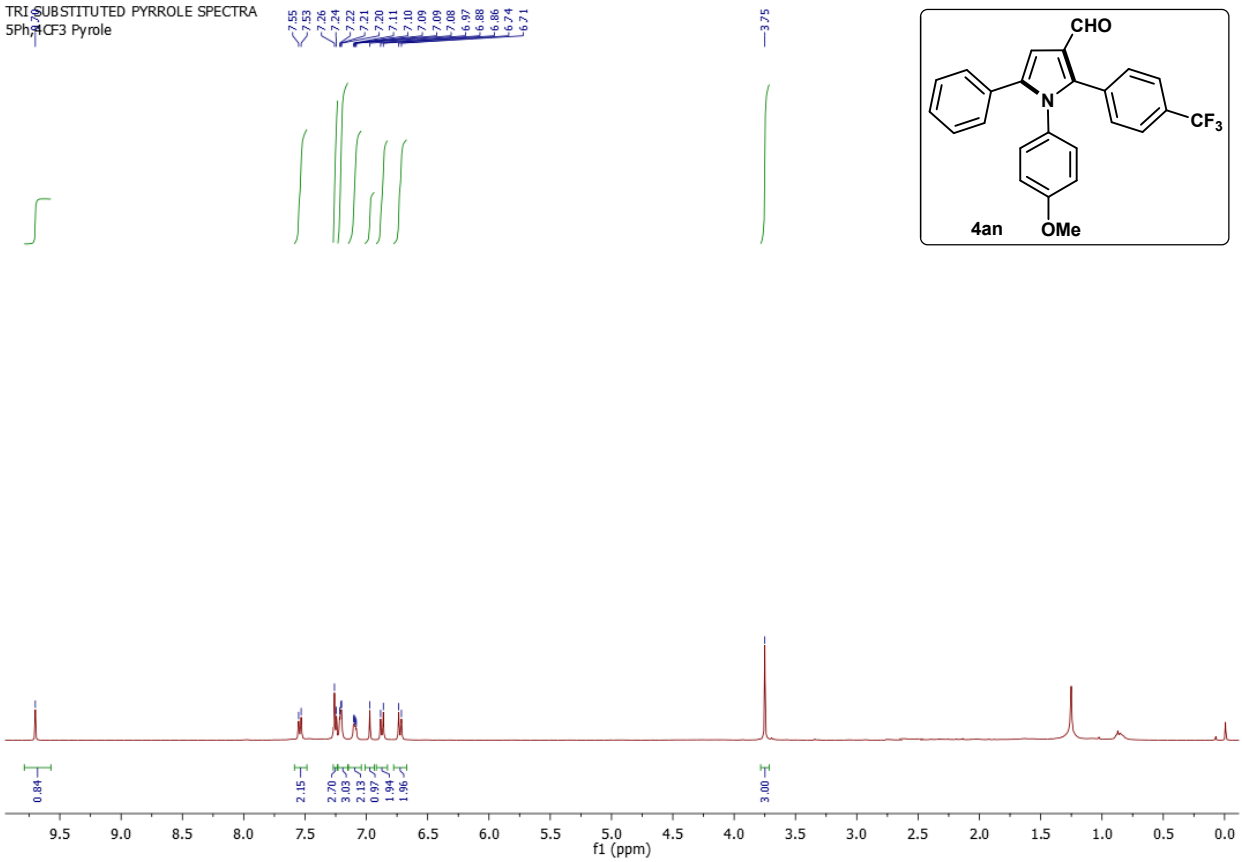

TRI SUBSTITUTED PYRROLE SPECTRA
5ph,4Bromo Pyrole
CHO
N
Br
4al
OMe
f1 (ppm)

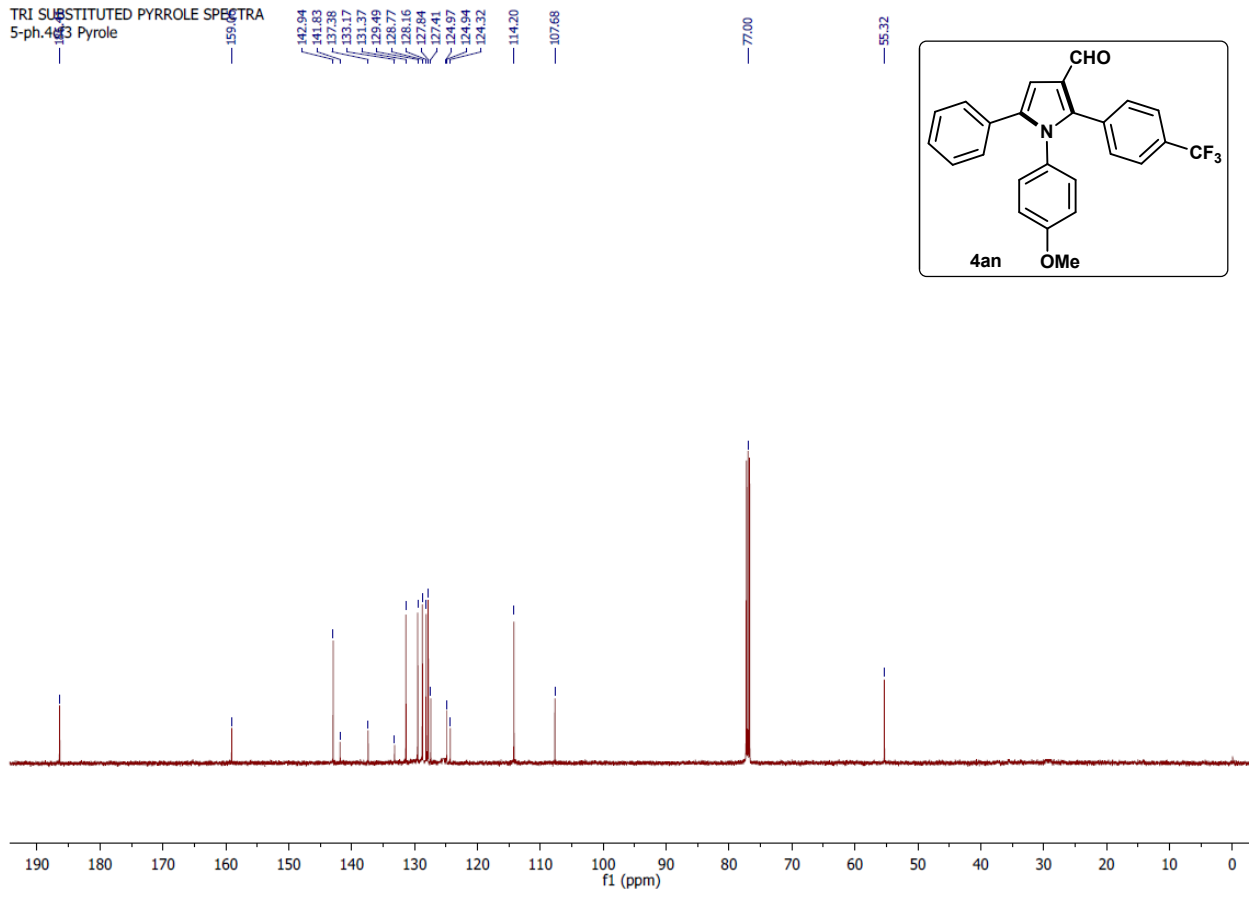
TRI SUBSTITUTED PYRROLE SPECTRA
5PH-3BR-4F-PYRROLE

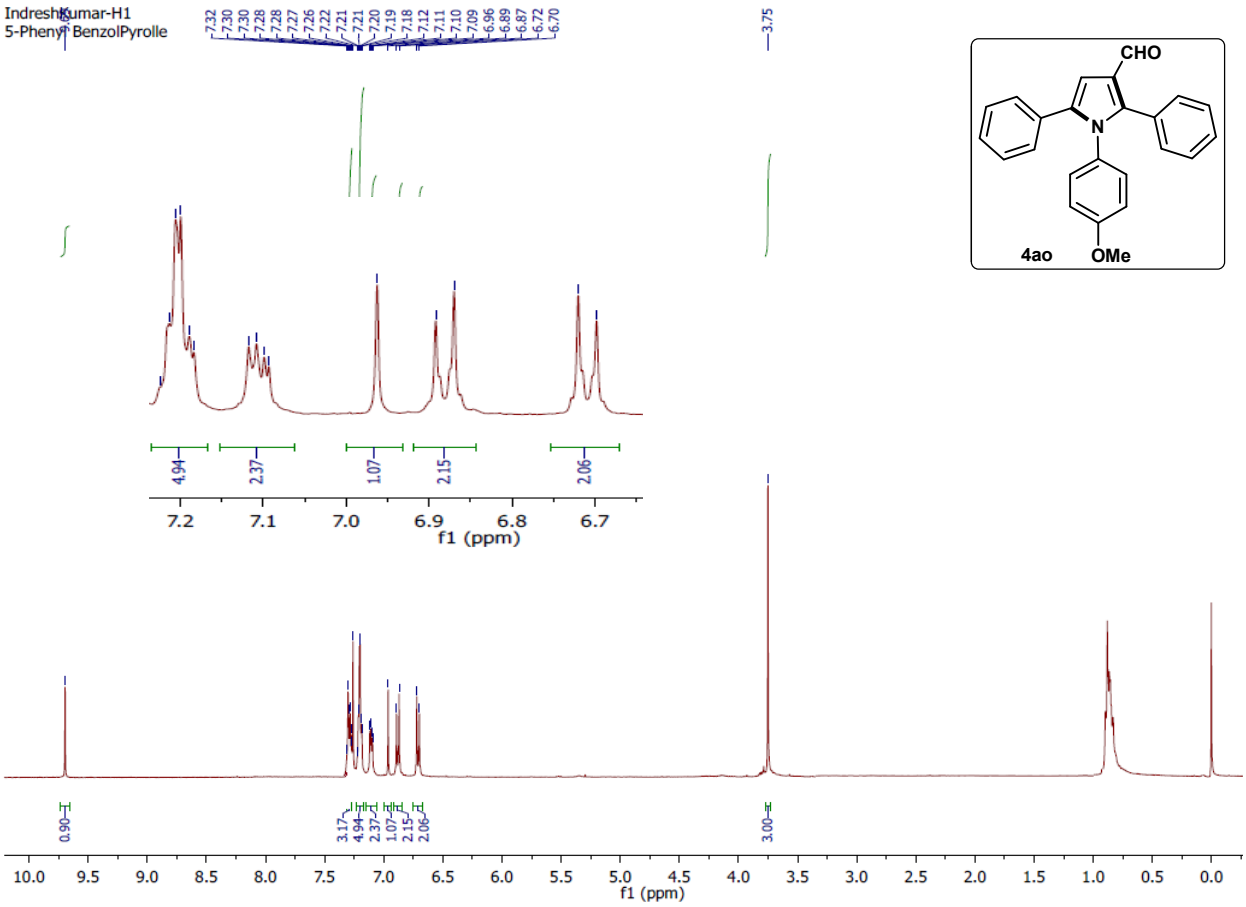


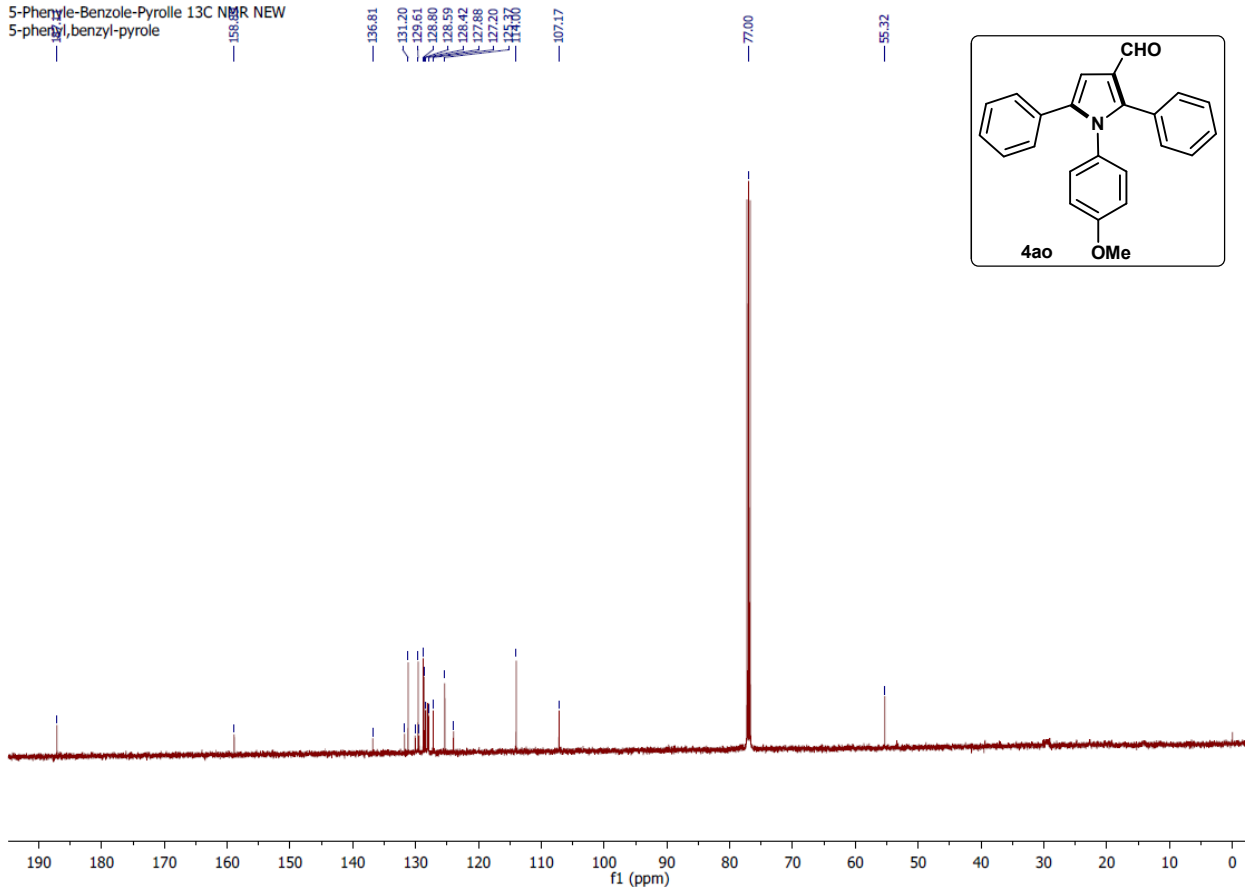
5ph,3br-4f pyrole
5ph-3br-4f-pyrole

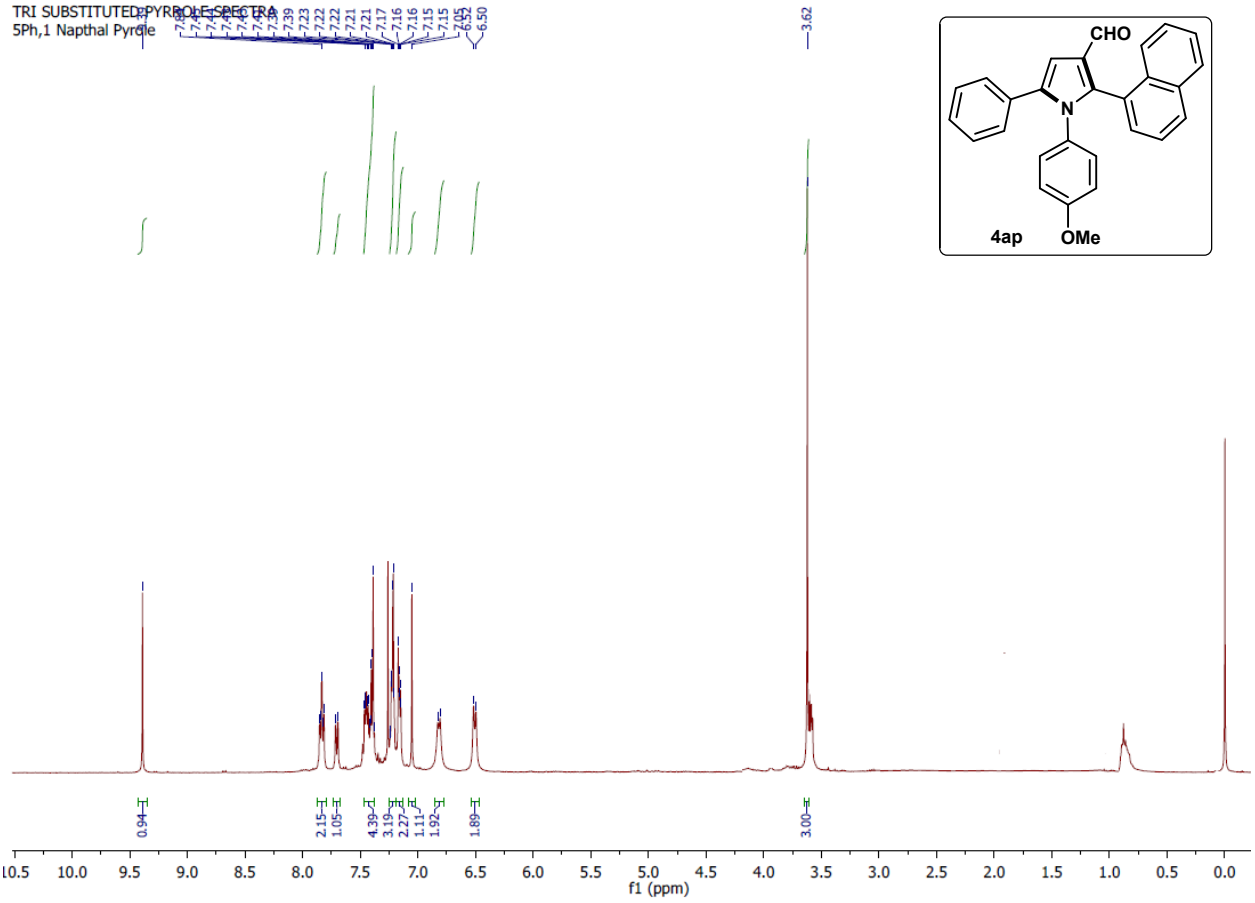


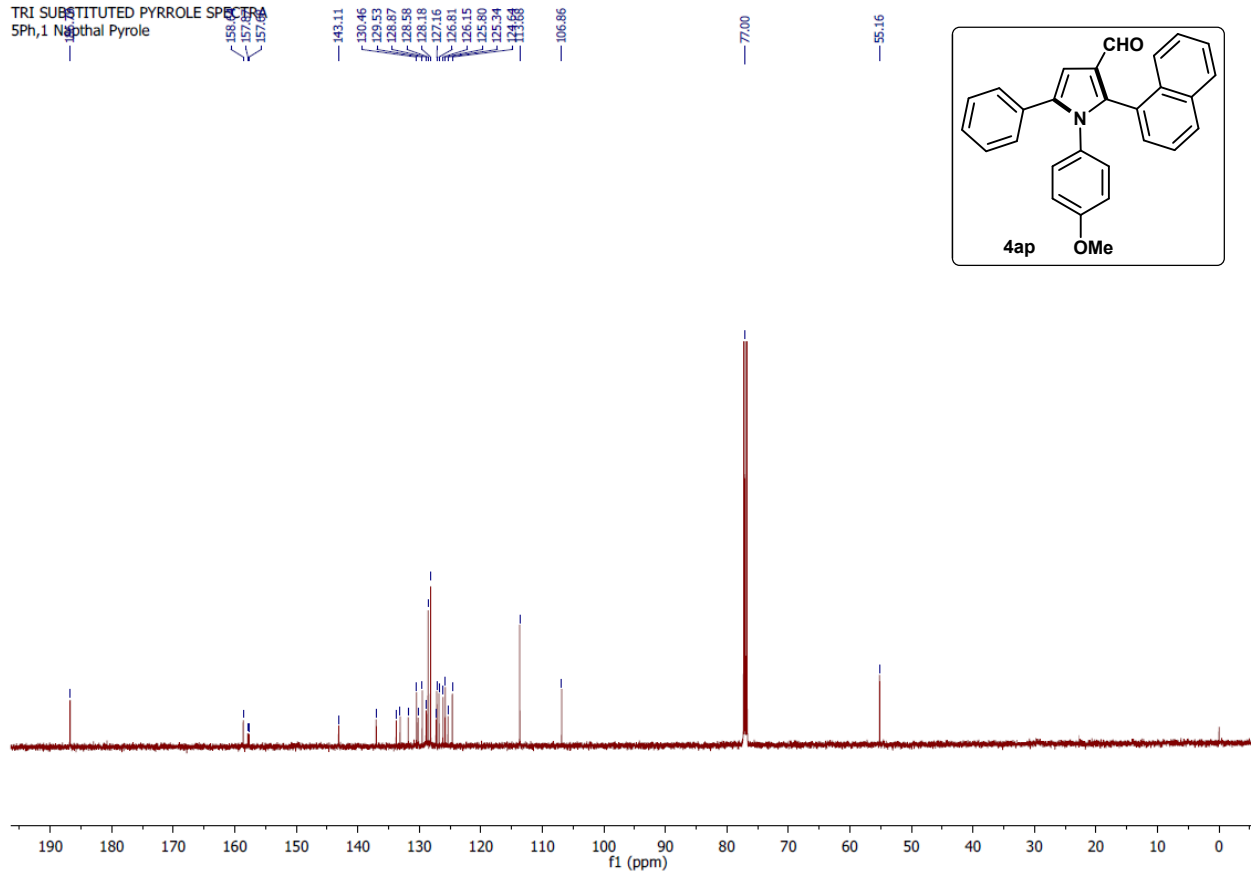

TRI SUBSTITUTED PYRROLE SPECTRA
5Ph,4CF3 Pyrole
7.55
7.53
7.26
7.24
7.22
7.21
7.20
7.11
7.10
7.09
7.09
7.08
6.97
6.88
6.86
6.74
6.71
3.75
CHO
N
CF3
4an
OMe
0.84
2.15
2.70
3.03
2.13
0.97
1.94
1.96
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

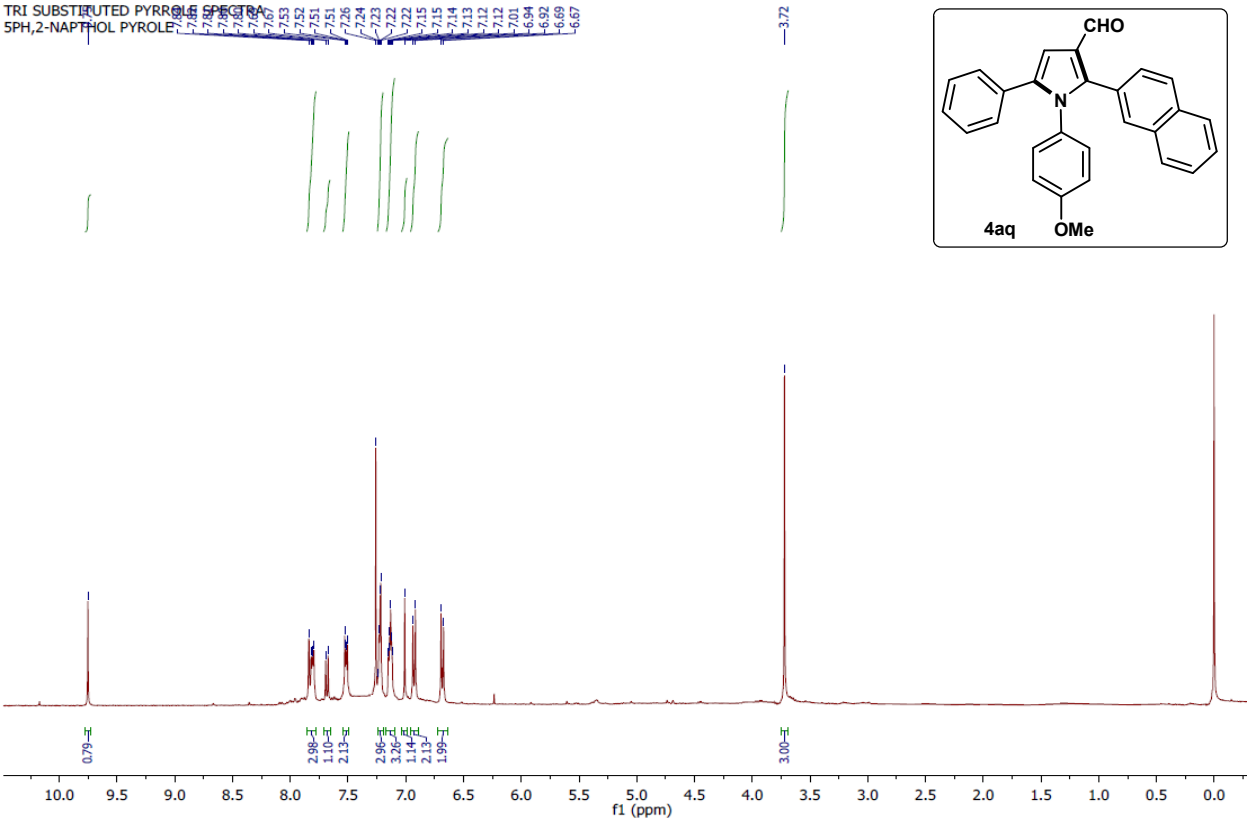

TRI SUBSTITUTED PYRROLE SPECTRA
5-ph,4CF3 Pyrole
159.47
142.94
141.83
137.38
133.17
131.37
129.49
128.77
128.16
127.84
127.41
124.97
124.94
124.32
114.20
107.68
77.00
55.32
CHO
N
CF3
4an
OMe
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

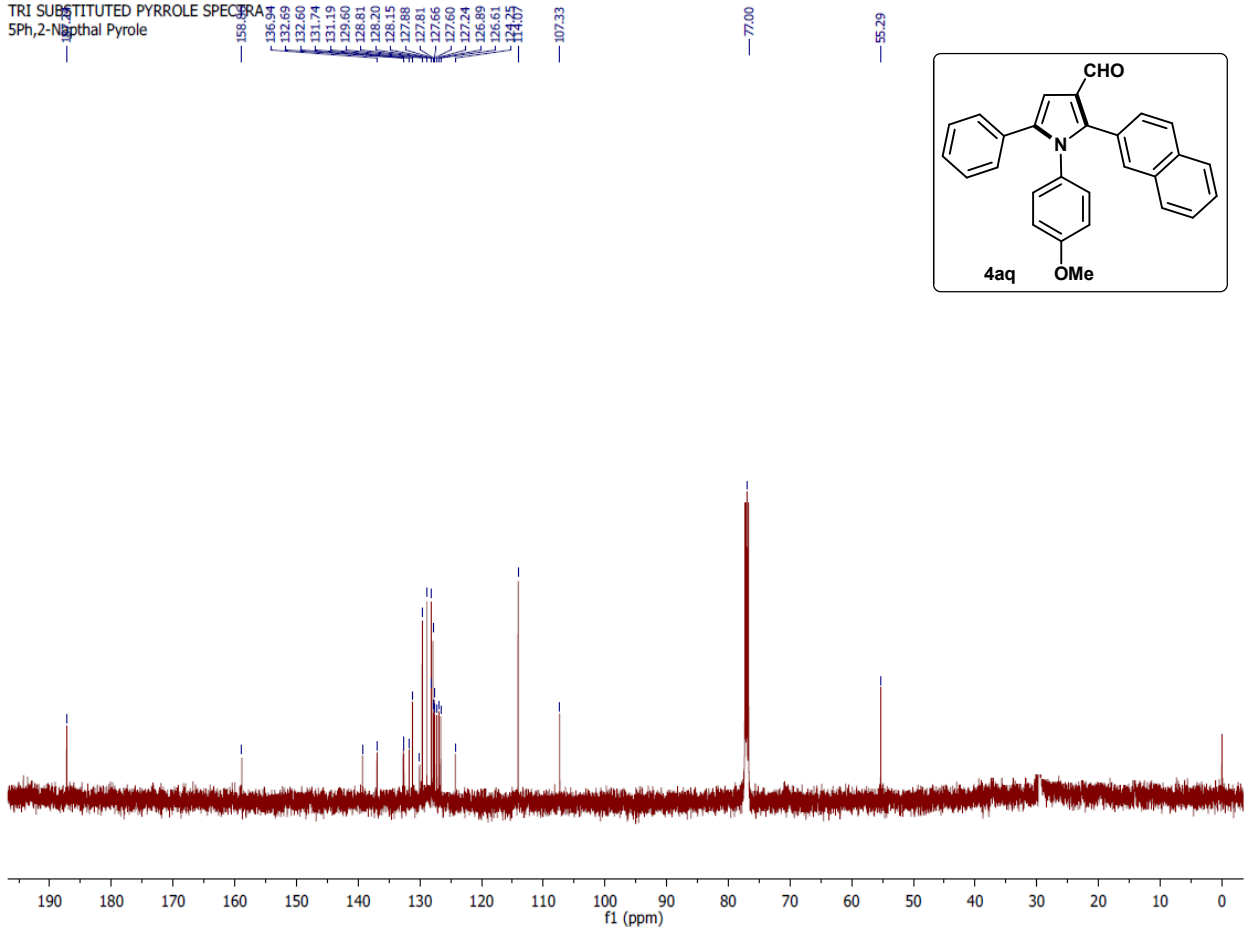

Indresh Kumar-H1
5-Phenyl BenzolPyrolle
CHO
N
4ao
OMe
f1 (ppm)

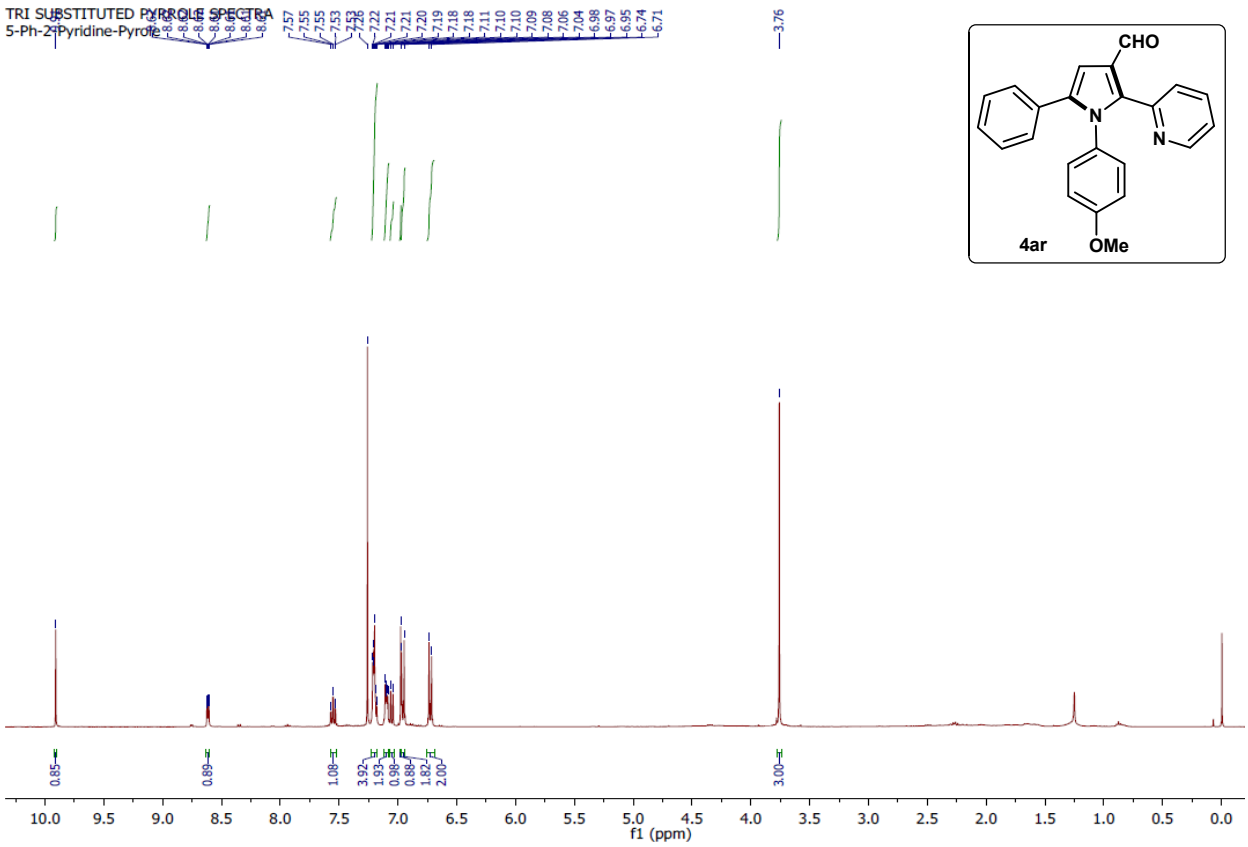

5-Phenyle-Benzole-Pyrolle 13C NMR NEW
5-phenyl,benzyl-pyrole
CHO
N
4ao
OMe
f1 (ppm)

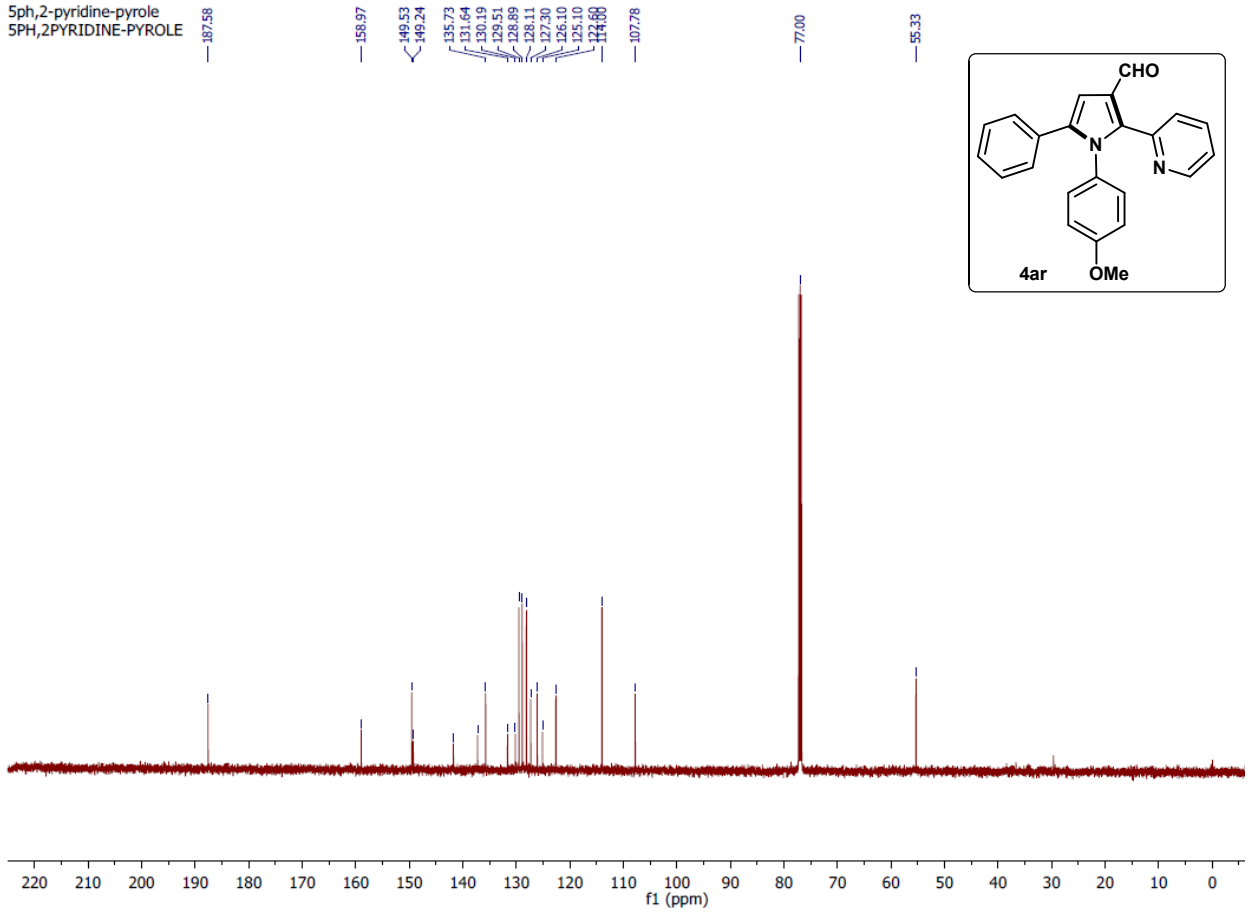

TRI SUBSTITUTED PYRROLE SPECTRA
5Ph,1 Napthal Pyrole
CHO
N
4ap
OMe
f1 (ppm)

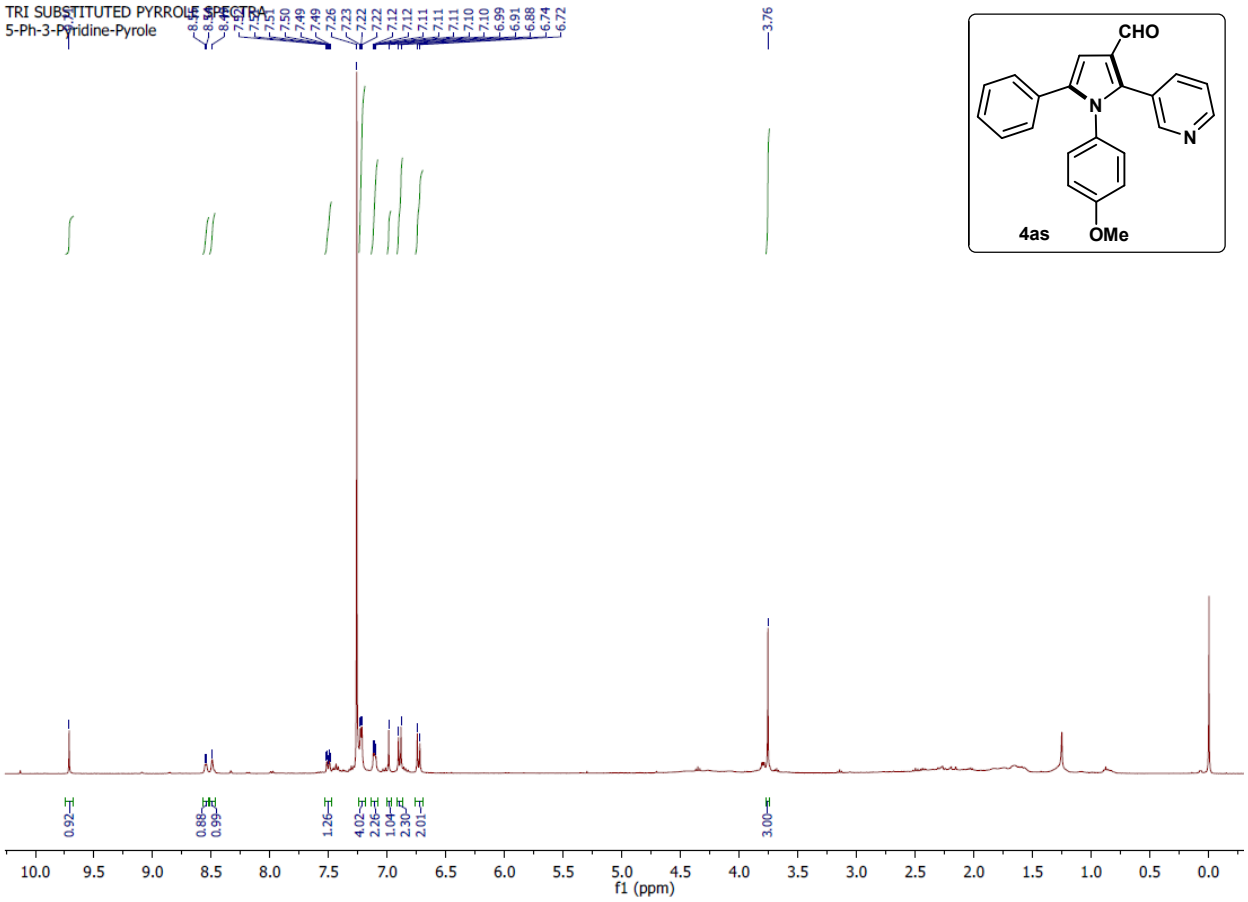

TRI SUBSTITUTED PYRROLE SPECTRA
5Ph,1 Napthal Pyrole
CHO
N
4ap
OMe
f1 (ppm)

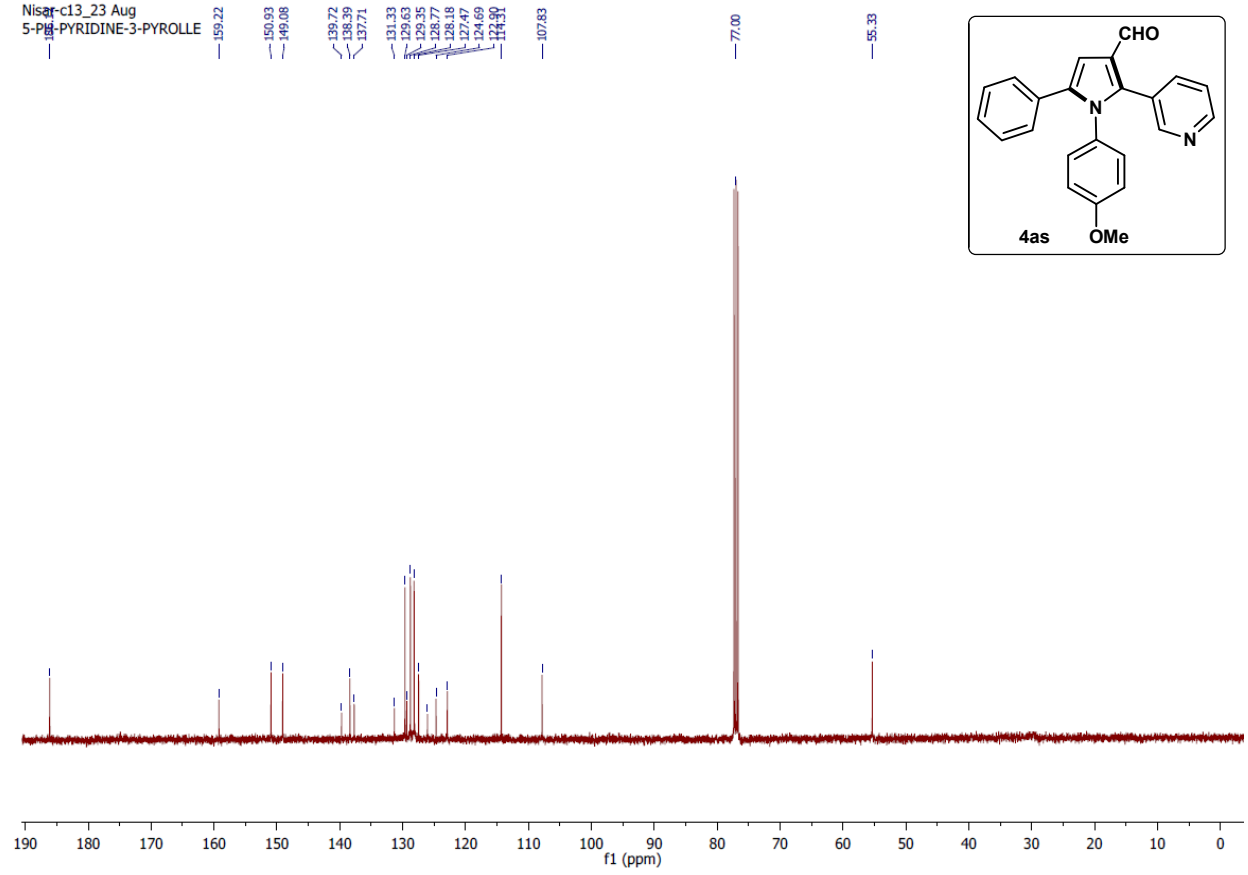

TRI SUBSTITUTED PYRROLE SPECTRA
5PH,2-NAPTHOL PYROLE
CHO
N
4aq
OMe
f1 (ppm)

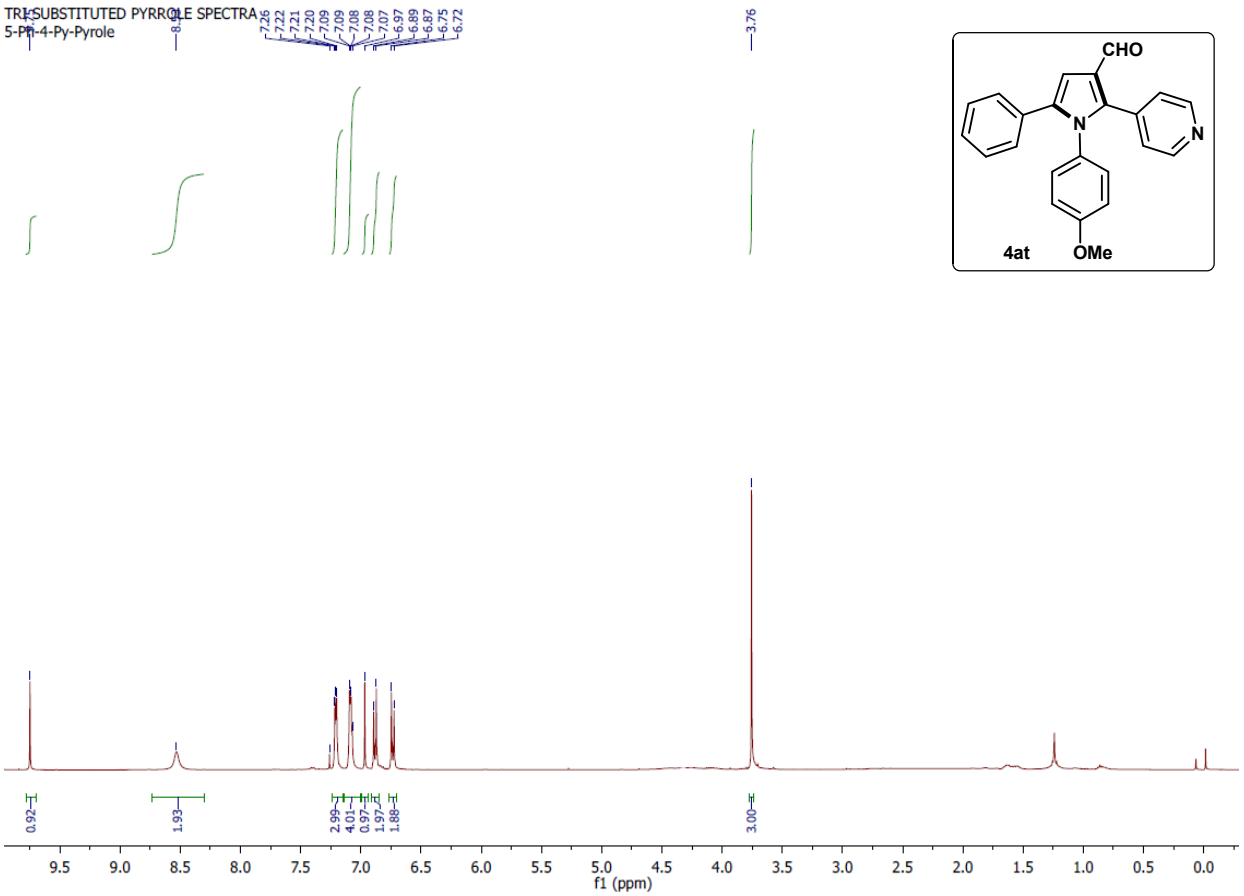

TRI SUBSTITUTED PYRROLE SPECTRA
5Ph,2-Napthal Pyrole
CHO
N
4aq
OMe
f1 (ppm)

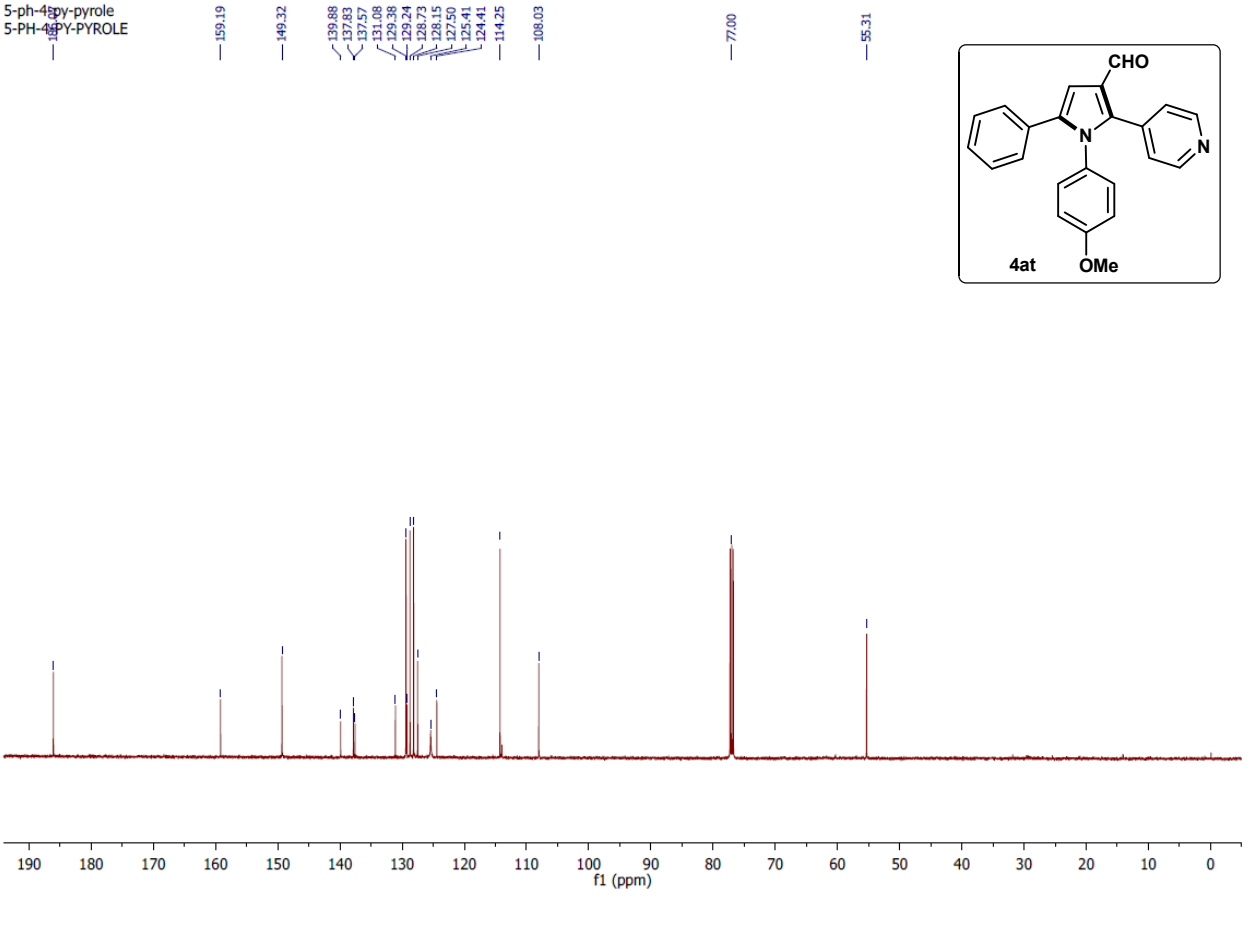

TRI SUBSTITUTED PYRROLE SPECTRA
5-Ph-2-Pyridine-Pyrole
CHO
N
N
4ar
OMe
f1 (ppm)

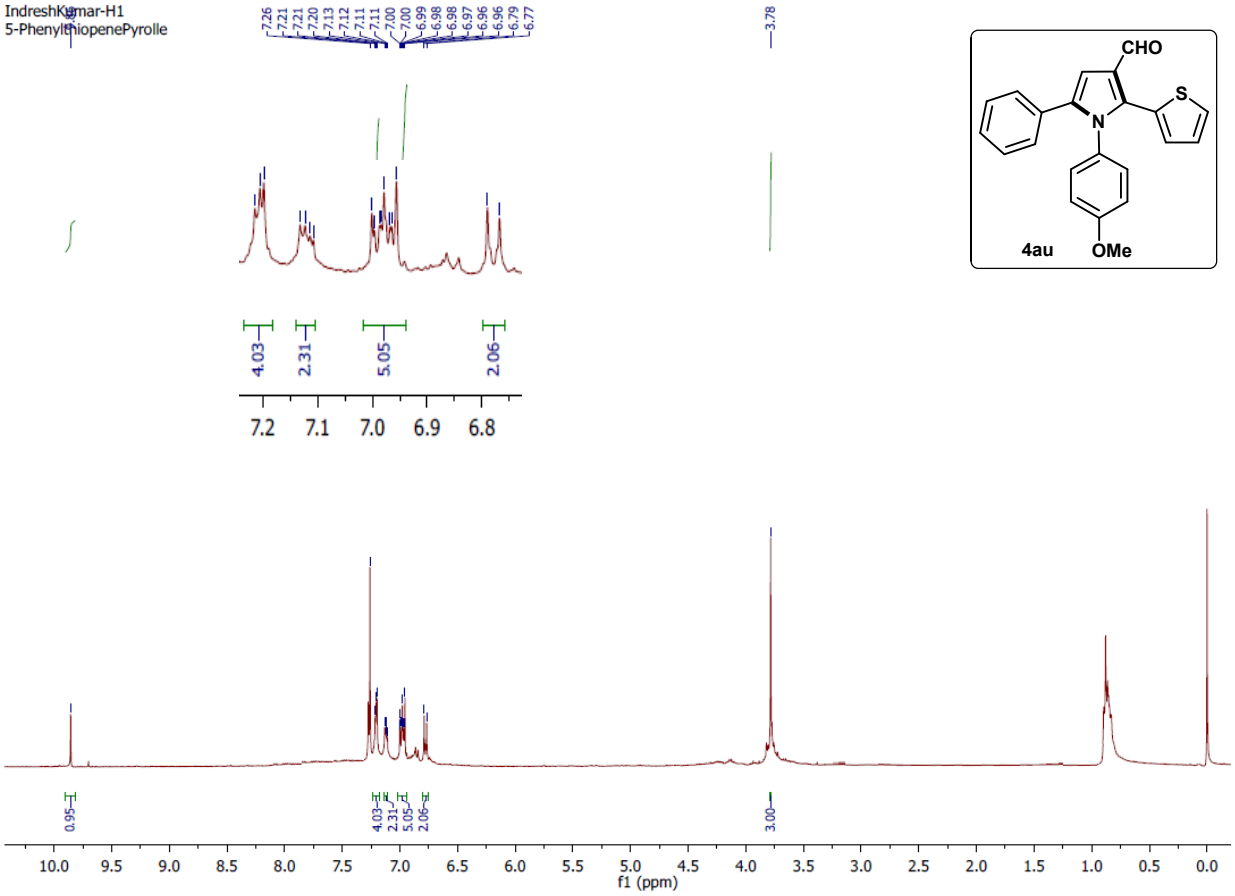

5ph,2-pyridine-pyrole
5PH,2PYRIDINE-PYROLE
CHO
N
N
4ar
OMe
f1 (ppm)

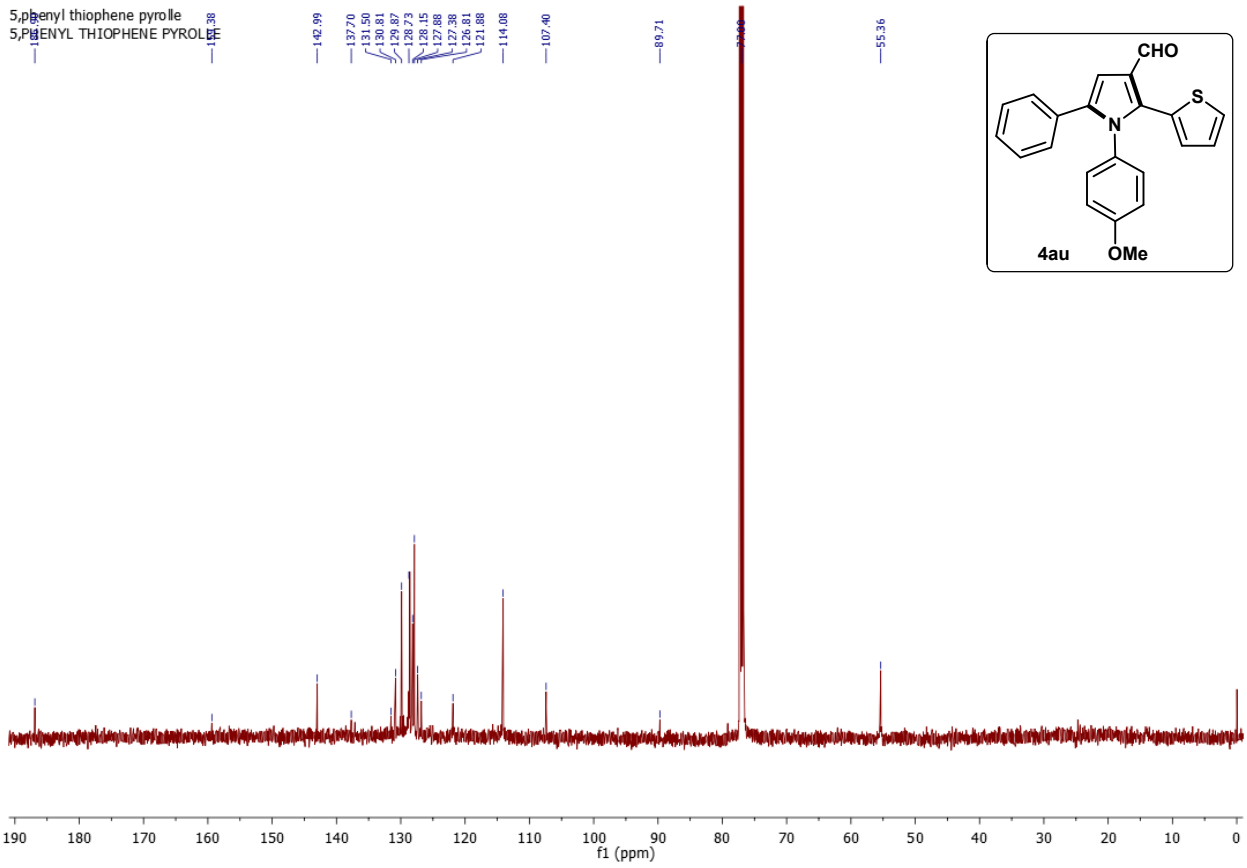

TRI SUBSTITUTED PYRROLE SPECTRA
5-Ph-3-Pyridine-Pyrole
CHO
N
N
4as
OMe
f1 (ppm)

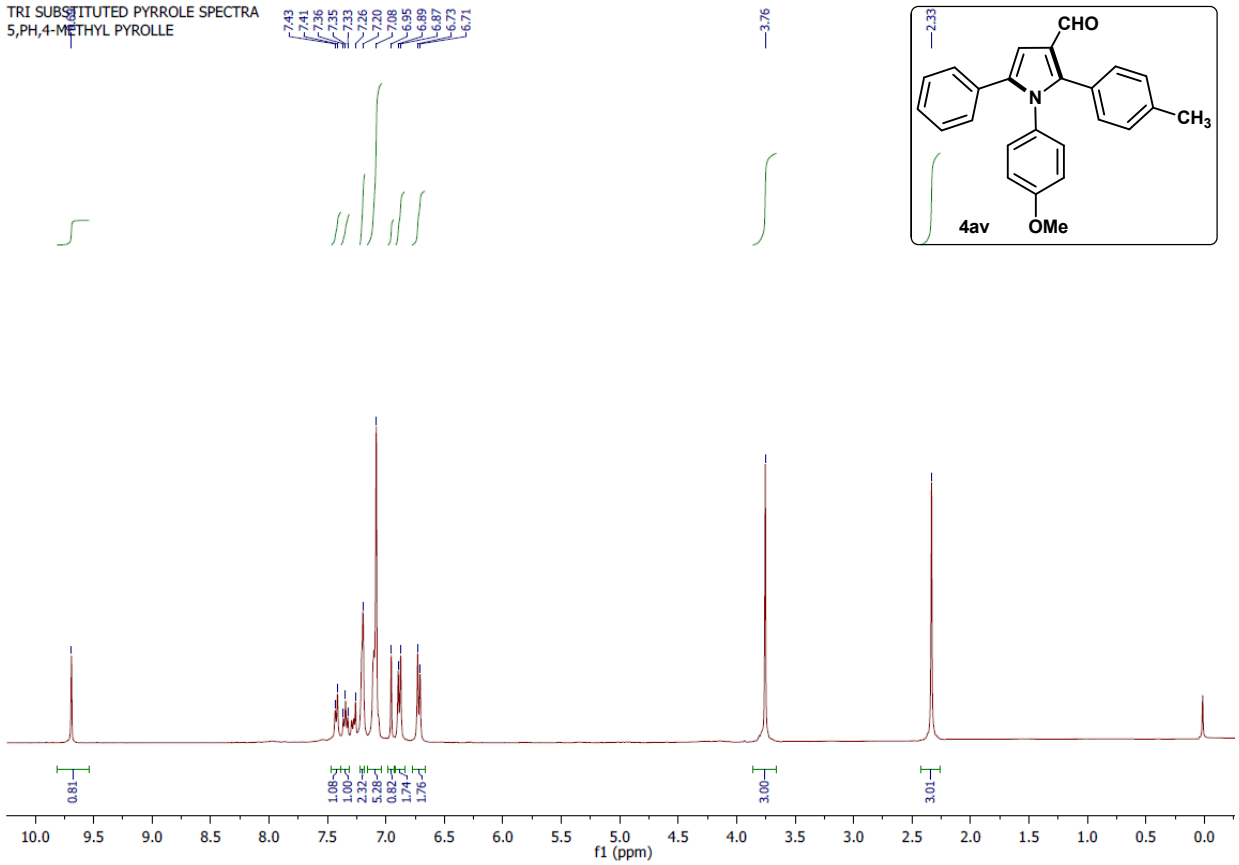

Nisar-c13_23 Aug
5-Ph-PYRIDINE-3-PYROLLE
CHO
N
N
4as
OMe
f1 (ppm)

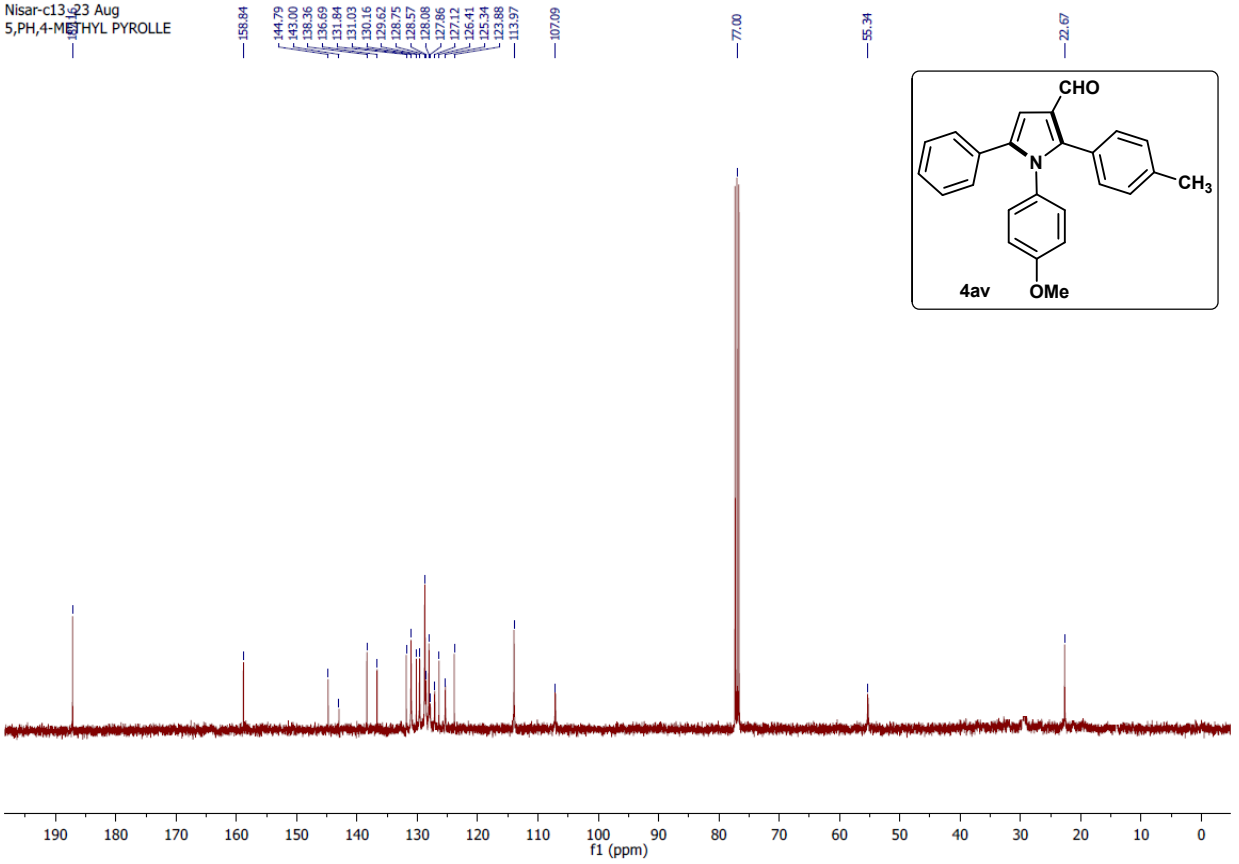

TRI-SUBSTITUTED PYRROLE SPECTRA
5-PH-4-Py-Pyrole
8.52
7.26
7.22
7.21
7.20
7.09
7.09
7.08
7.08
7.07
6.97
6.89
6.87
6.75
6.72
3.76
CHO
N
N
4at
OMe
0.92
1.93
2.99
4.01
0.97
1.97
1.88
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

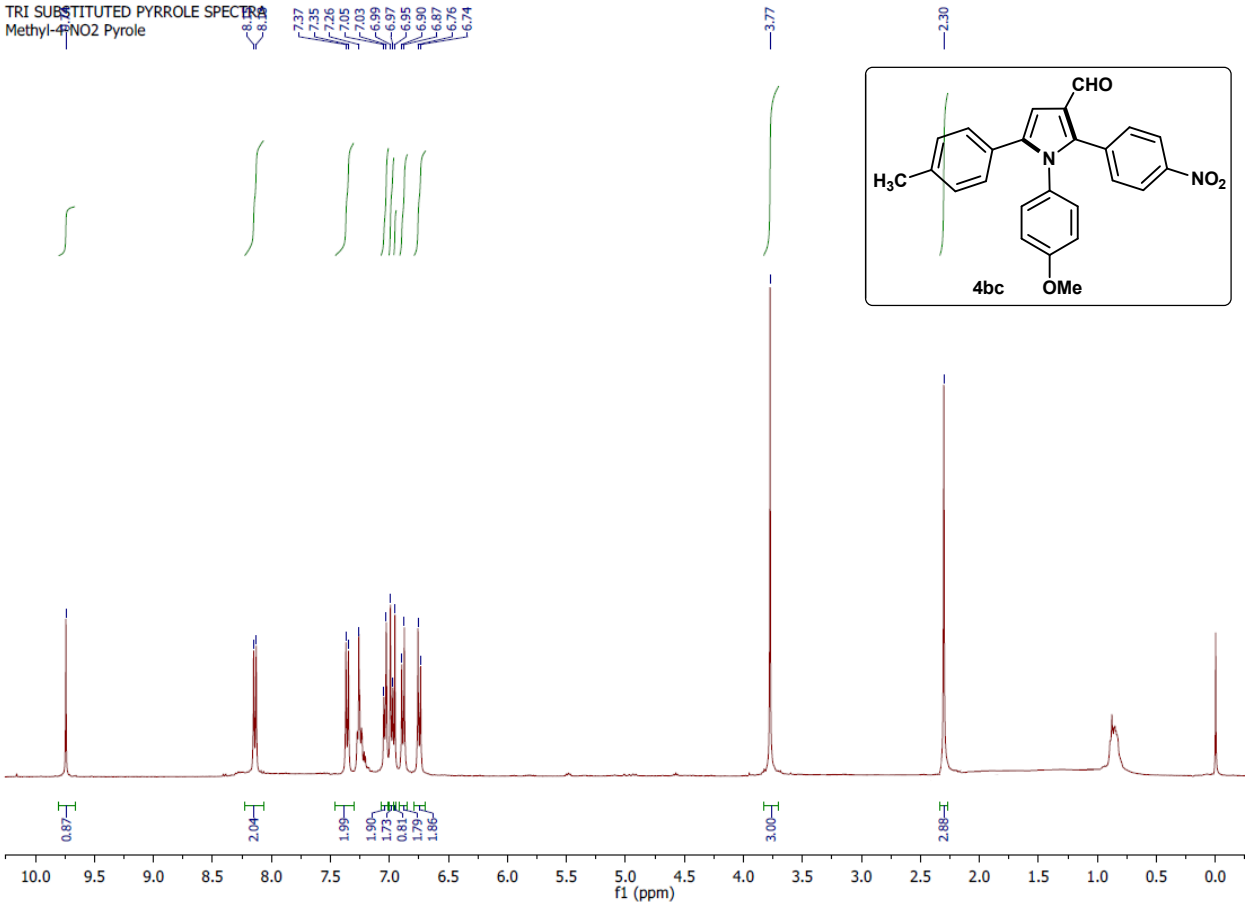

5-ph-4py-pyrole
5-PH-4PY-PYROLE
159.19
149.32
139.88
137.83
137.57
131.08
129.38
129.24
128.73
128.15
127.50
125.41
124.41
114.25
108.03
77.00
55.31
CHO
N
N
4at
OMe
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

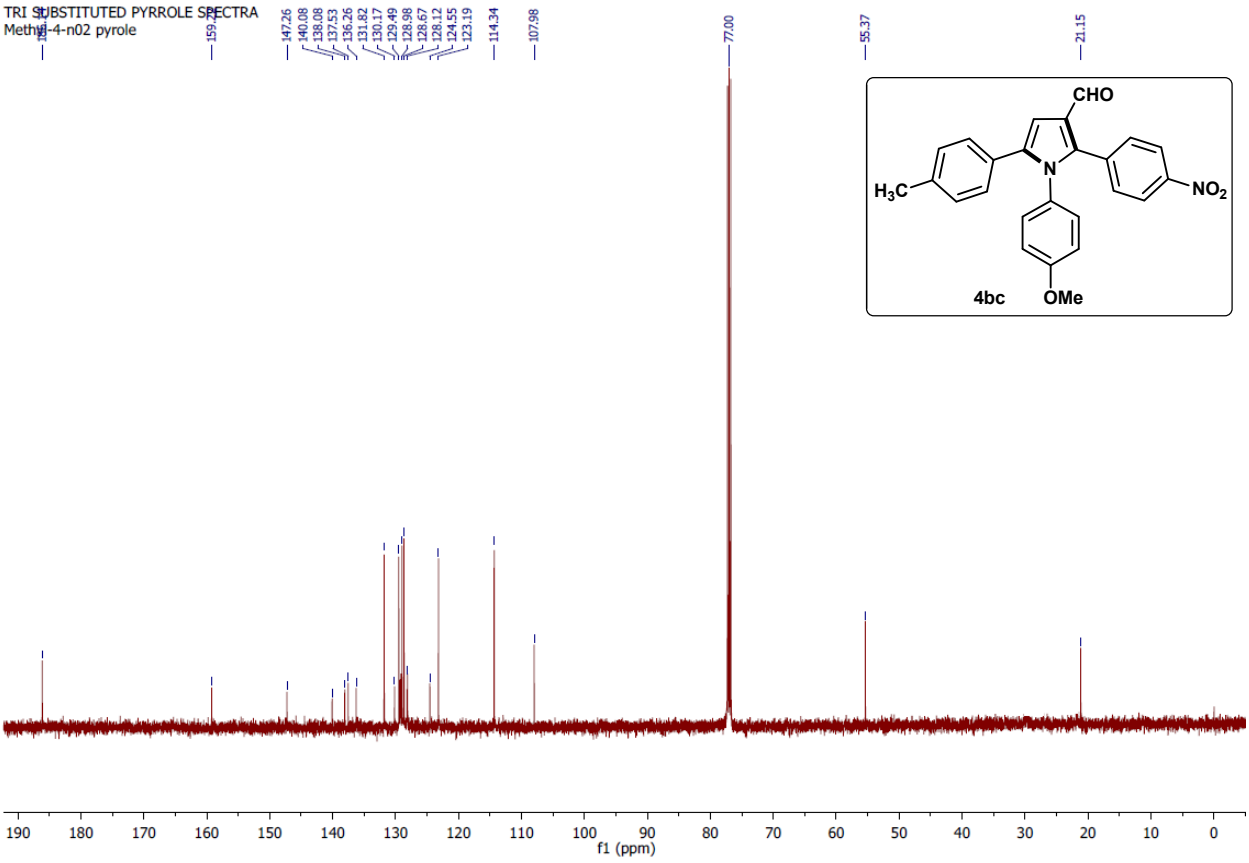

IndreshKumar-H1
5-PhenylThiopenePyrolle
7.26
7.21
7.21
7.20
7.13
7.12
7.11
7.11
7.00
7.00
6.99
6.98
6.98
6.97
6.96
6.96
6.79
6.77
3.78
4.03
2.31
5.05
2.06
7.2
7.1
7.0
6.9
6.8
CHO
S
N
4au
OMe
0.95
4.03
2.31
5.05
2.06
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

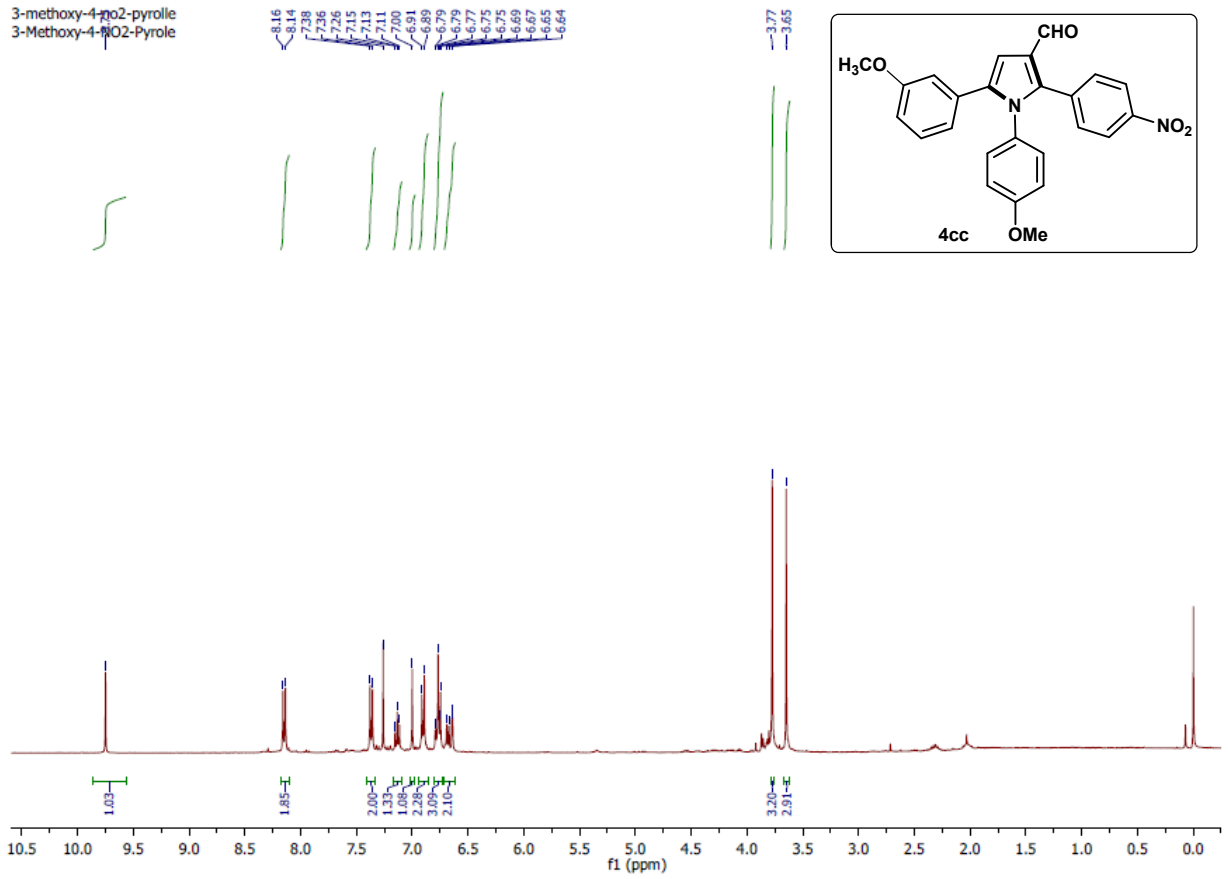

5,phenyl thiophene pyrolle
5,PHENYL THIOPHENE PYROLLE
142.99
137.70
131.50
130.81
129.87
128.73
128.15
127.88
127.38
126.81
121.88
114.08
107.40
89.71
55.36
CHO
S
N
4au
OMe
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

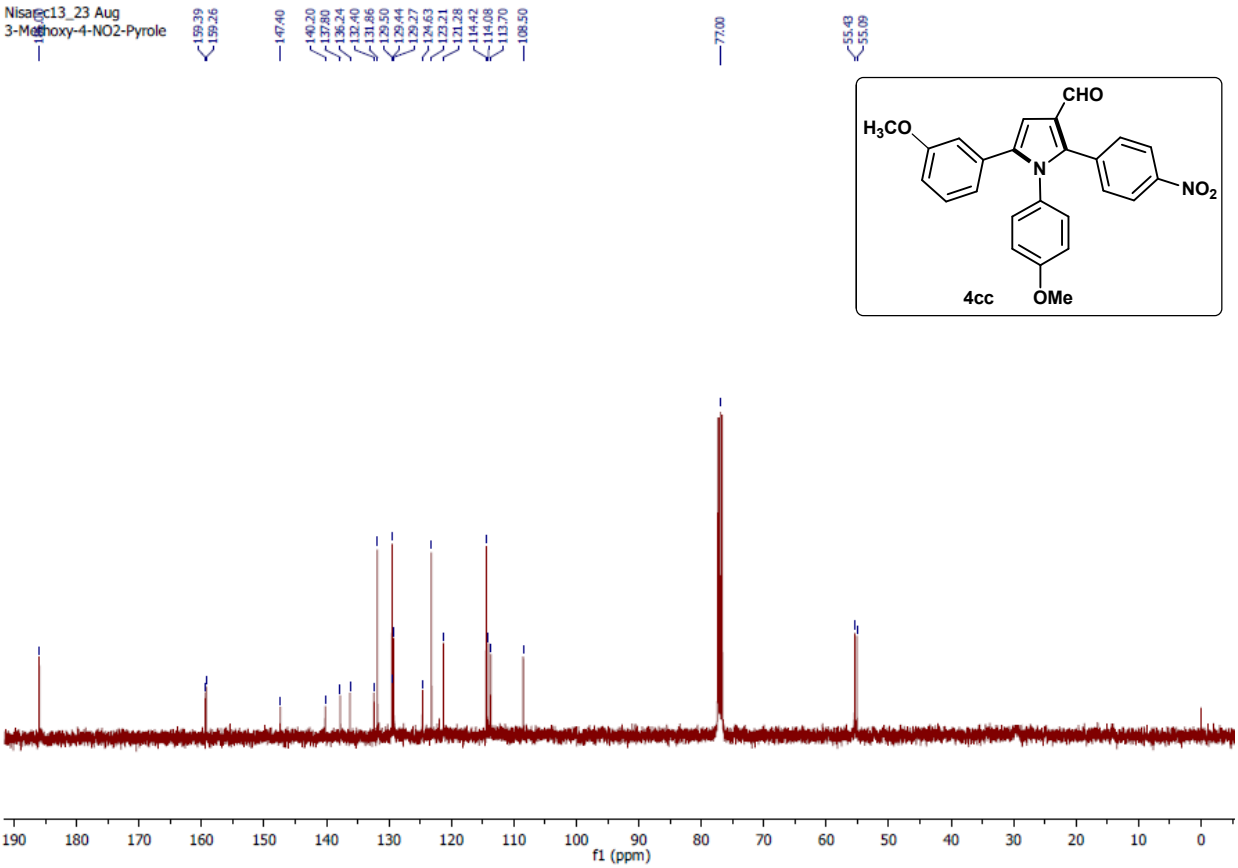

TRI SUBSTITUTED PYRROLE SPECTRA
5,PH,4-METHYL PYROLLE
7.43
7.41
7.36
7.35
7.33
7.26
7.20
7.08
6.95
6.89
6.87
6.73
6.71
3.76
2.33
CHO
N
CH3
4av
OMe
0.81
1.08
1.00
2.32
5.28
0.82
1.74
1.76
3.00
3.01
f1 (ppm)

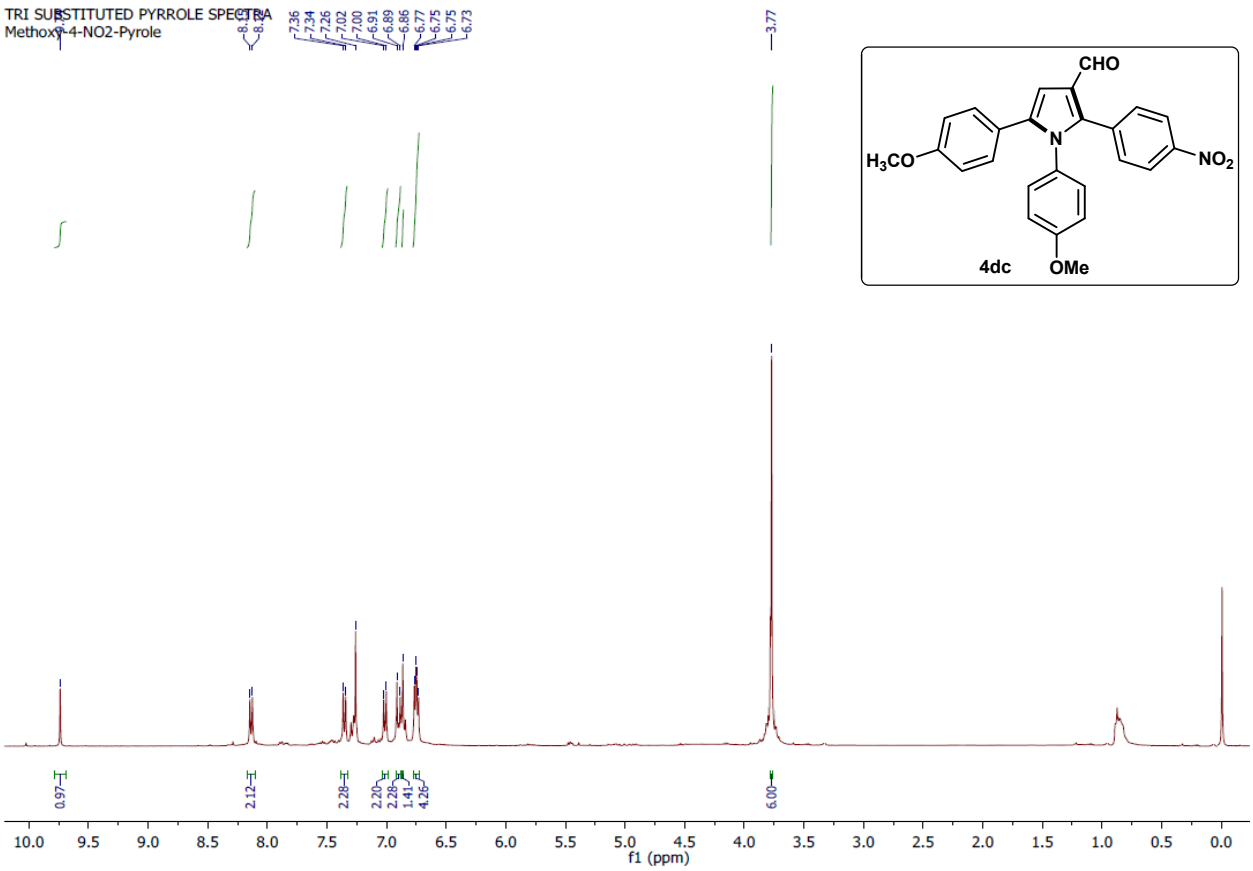

Nisar-c13-23 Aug
5,PH,4-METHYL PYROLLE
158.84
144.79
143.00
138.36
136.69
131.84
131.03
130.16
129.62
128.75
128.57
128.08
127.86
127.12
126.41
125.34
123.88
113.97
107.09
77.00
55.34
22.67
CHO
N
CH3
4av
OMe
f1 (ppm)

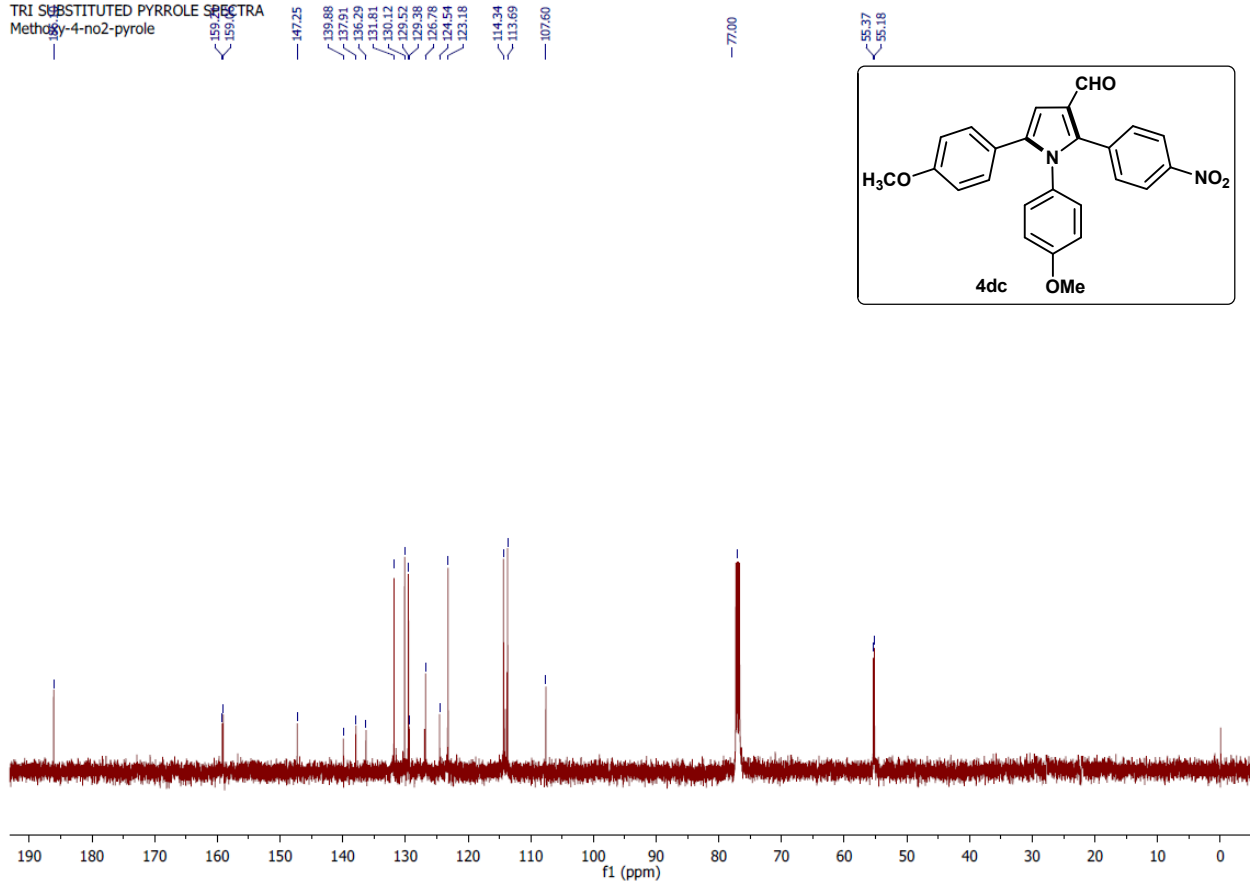

TRI SUBSTITUTED PYRROLE SPECTRA
Methyl-4-NO2 Pyrole
8.13
8.12
7.37
7.35
7.26
7.05
7.03
6.99
6.97
6.95
6.90
6.87
6.76
6.74
3.77
2.30
CHO
N
H3C
NO2
4bc
OMe
0.87
2.04
1.99
1.90
1.73
0.81
1.79
1.86
3.00
2.88
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

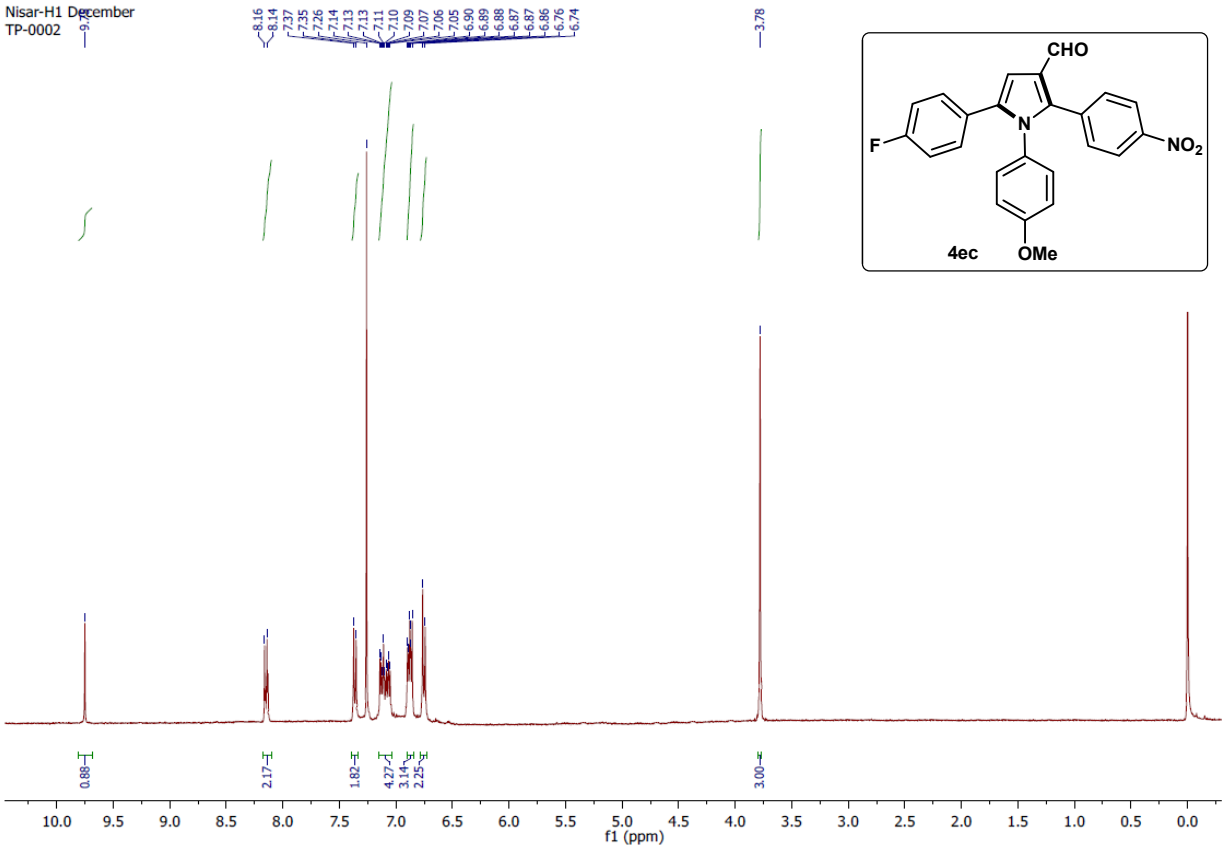

TRI SUBSTITUTED PYRROLE SPECTRA
Methyl-4-n02 pyrole
159.74
147.26
140.08
138.08
137.53
136.26
131.82
130.17
129.49
128.98
128.67
128.12
124.55
123.19
114.34
107.98
77.00
55.37
21.15
CHO
N
H3C
NO2
4bc
OMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

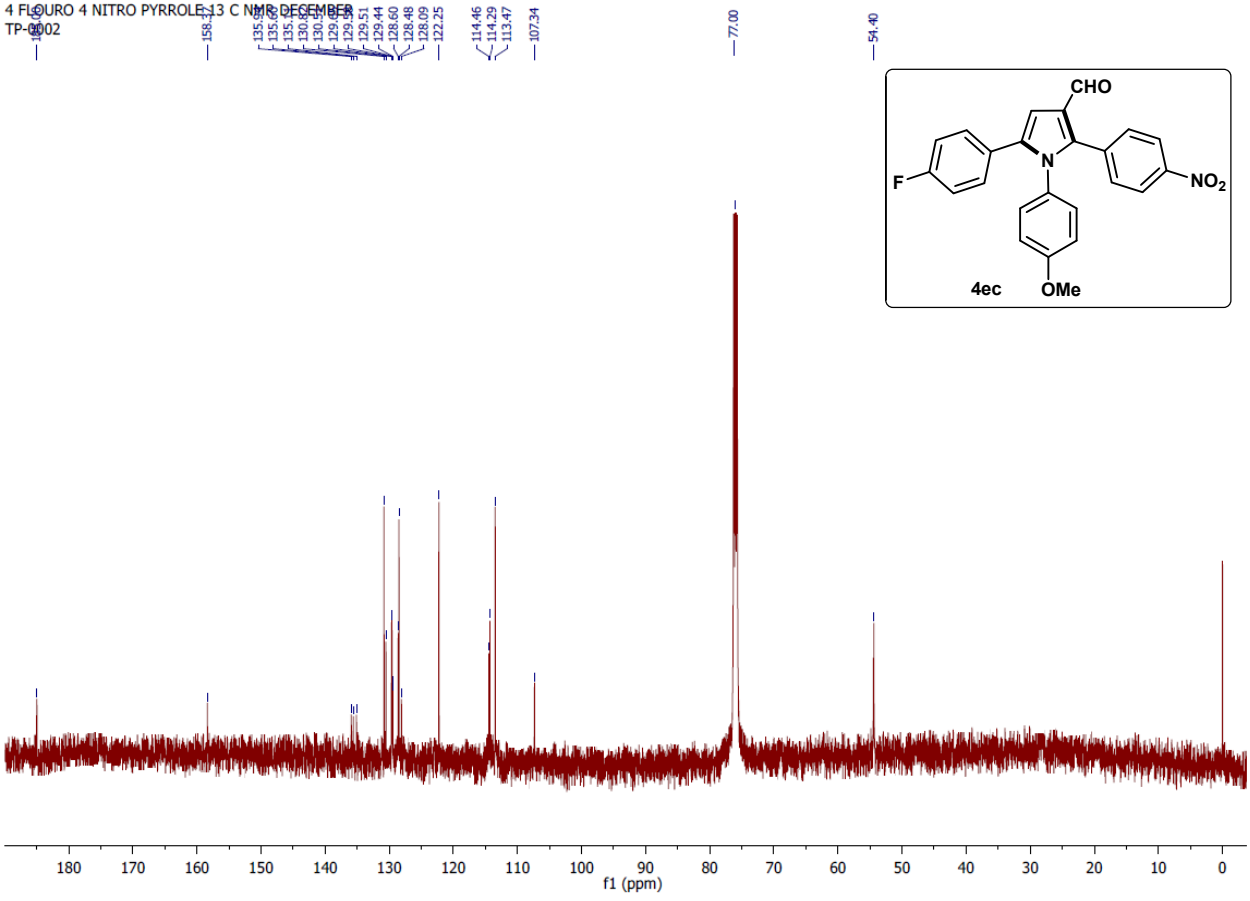

3-methoxy-4-no2-pyrolle
3-Methoxy-4-NO2-Pyrole
8.16
8.14
7.38
7.36
7.26
7.15
7.13
7.11
7.00
6.91
6.89
6.79
6.79
6.77
6.75
6.75
6.69
6.67
6.65
6.64
3.77
3.65
CHO
H3CO
N
NO2
4cc
OMe
1.03
1.85
2.00
1.33
1.08
2.28
3.09
2.10
3.20
2.91
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

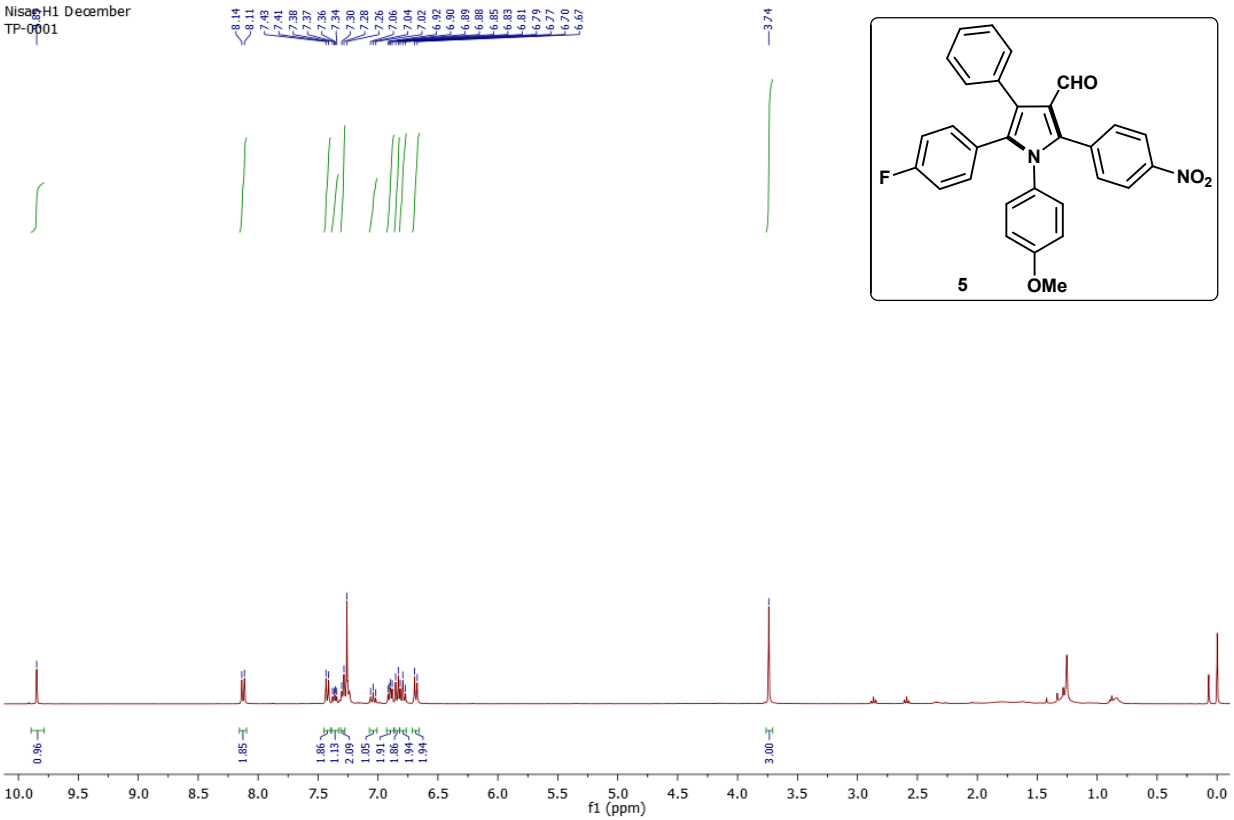

Nisarec13_23 Aug
3-Methoxy-4-NO2-Pyrole
159.39
159.26
147.40
140.20
137.80
136.24
132.40
131.86
129.50
129.44
129.27
124.63
123.21
121.28
114.42
114.08
113.70
108.50
77.00
55.43
55.09
CHO
H3CO
N
NO2
4cc
OMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

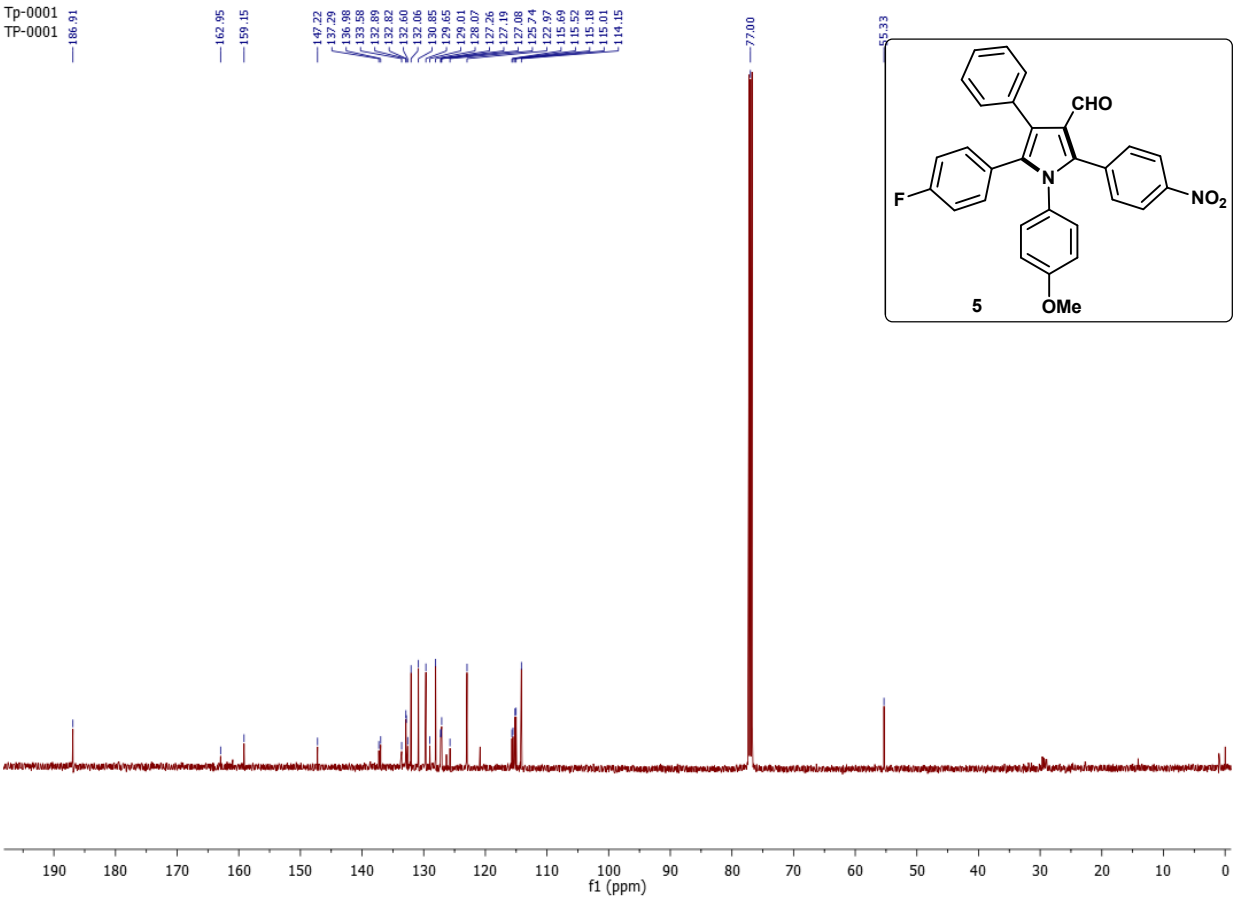

TRI SUBSTITUTED PYRROLE SPECTRA
Methoxy-4-NO2-Pyrole
8.12
8.10
7.36
7.34
7.26
7.02
7.00
6.91
6.89
6.86
6.77
6.75
5.75
6.73
3.77
CHO
N
H3CO
NO2
4dc
OMe
0.97
2.12
2.28
2.20
2.28
1.41
4.26
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


TRI SUBSTITUTED PYRROLE SPECTRA
Methoxy-4-no2-pyrole
159.88
159.44
147.25
139.88
137.91
136.29
131.81
130.12
129.52
129.38
126.78
124.54
123.18
114.34
113.69
107.60
77.00
55.37
55.18
CHO
N
H3CO
NO2
4dc
OMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

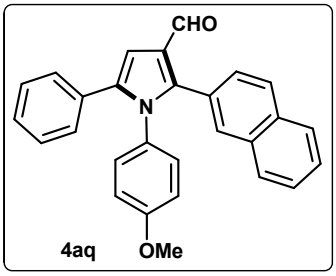

Nisar-H1 December
TP-0002
CHO
F
N
NO2
4ec
OMe
f1 (ppm)


TP-0002
CHO
F
N
NO2
4ec
OMe
f1 (ppm)


Nisar H1 December
TP-0001
CHO
F
NO2
N
5
OMe
f1 (ppm)


Tp-0001
TP-0001
CHO
F
NO2
N
5
OMe
f1 (ppm)

Crystal structure of 1-(4-methoxyphenyl)-2-(naphthalen-2-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (4aq):



[CCDC - 1007133]

The title compound, 1-(4-methoxyphenyl)-2-(naphthalen-2-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde, crystallizes in the monoclinic space group $P2_1/c$ with the following unit-cell parameters: a = 12.6491(8), b = 7.9932(4), c = 21.9541(13) Å, β= 105.450(7), Z = 4. The crystal structure was solved by direct methods using single-crystal X-ray diffraction data and refined by full-matrix least-squares procedures to a final R-value of 0.0489 for 2249 observed reflections.

X-ray intensity data of 7999 reflections (of which 4184 unique) were collected at room temperature on a CCD area-detector diffractometer (*X'calibur system – Oxford diffraction make, U.K.*) equipped with graphite monochromated MoKα radiation (λ=0.71073 Å). The crystal used for data collection was of dimensions 0.30 x 0.20 x 0.20 mm. The intensities were measured by ω scan mode for θ ranges 3.77 to 26.0°. 2249 reflections were treated as observed (I > 2σ(I)). Data were corrected for Lorentz and polarisation factors. The structure was solved by direct methods using SHELXS97.(1) All non-hydrogen atoms of the molecule were located in the best E-map. Full-matrix least-squares refinement was carried out using SHELXL97 [1 All the hydrogen atoms were geometrically fixed and allowed to ride on the corresponding non-hydrogen atoms with C-H= 0.93-0.96 Å, and U_{iso} = 1.5U_{eq} of the attached C atom for methyl H atoms and 1.2 U_{eq} for other H atoms. The final refinement cycles converged to an R = 0.0489 and wR (F^2) = 0.1114 for the observed data. Residual electron densities ranged from -0.172 to 0.158 eÅ^{-3}. Atomic scattering factors were taken from International Tables for X-ray Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4). The crystallographic data are summarized in Table 1. CCDC - 1007133 contains the supplementary crystallographic data for this paper.

Results and discussion

An ORTEP view of the title compound with atomic labeling is shown in Fig.1.[2] The geometry of the molecule was calculated using the WinGX[3] and PARST[4] software's.

References

1. G. M. Sheldrick, *Acta Cryst.*, **2008**, *A64*, 112.
2. L. J. Farrugia, *J. Appl. Cryst.*, **2012**, *45*, 849-854.
3. A. L. Spek, *Acta Cryst.*, **2009**, *D65*, 148–155.
4. M. Naedelli, *J Appl. Cryst.*, **1995**, *28*, 659.

Table 1 Crystal and experimental data

CCDC No	1007133
Crystal description	White block shaped
Crystal size	0.30 x 0.20 x 0.20 mm
Empirical formula	$C_{28}H_{21}N_1O_2$
Formula weight	403.46
Radiation, Wavelength	Mo *K*α, 0.71073 Å
Unit cell dimensions	a = 12.6491(8), b = 7.9932(4), c = 21.9541(13) Å, β= 105.450(7)
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell volume	2139.5(2) $Å^3$

Density (calculated)	1.253 Mgm^{-3}
No. of molecules per unit cell, Z	4
Temperature	273(2) K
Absorption coefficient(μ)	0.078 mm^{-1}
F (000)	848
Scan mode	omega scan
θ range for entire data collection	3.77< θ < 26.00 ^{o}
Reflections collected / unique	7999/4184
Reflections observed (I > 2σ(I))	2249
Structure determination	Direct methods
Refinement	Full-matrix least-squares on F^2
No. of parameters refined	280
Final R	0.0489
wR(F^2)	0.1114
Weight	$1/[\sigma^2(F_o^2)+(0.0277P)^2+0.00P]$
	where $P=[F_o^2+2F_c^2]/3$
Goodness-of-fit	0.918
$(\Delta/\sigma)_{max}$ in the final cycle	0.008
Final residual electron density	-0.172< Δρ <0.158 $eÅ^{-3}$

Measurement	*X'calibur system – Oxford diffraction make, U.K.*
Software for structure solution:	SHELXS97 (Sheldrick, 1997)
Software for refinement:	SHELXL97 (Sheldrick, 1997)
Software for molecular plotting:	ORTEP-3 (Farrugia, 1997) PLATON (Spek, 2003)
Software for geometrical calculation	PLATON (Spek, 2003) PARST (Nardelli, 1995)

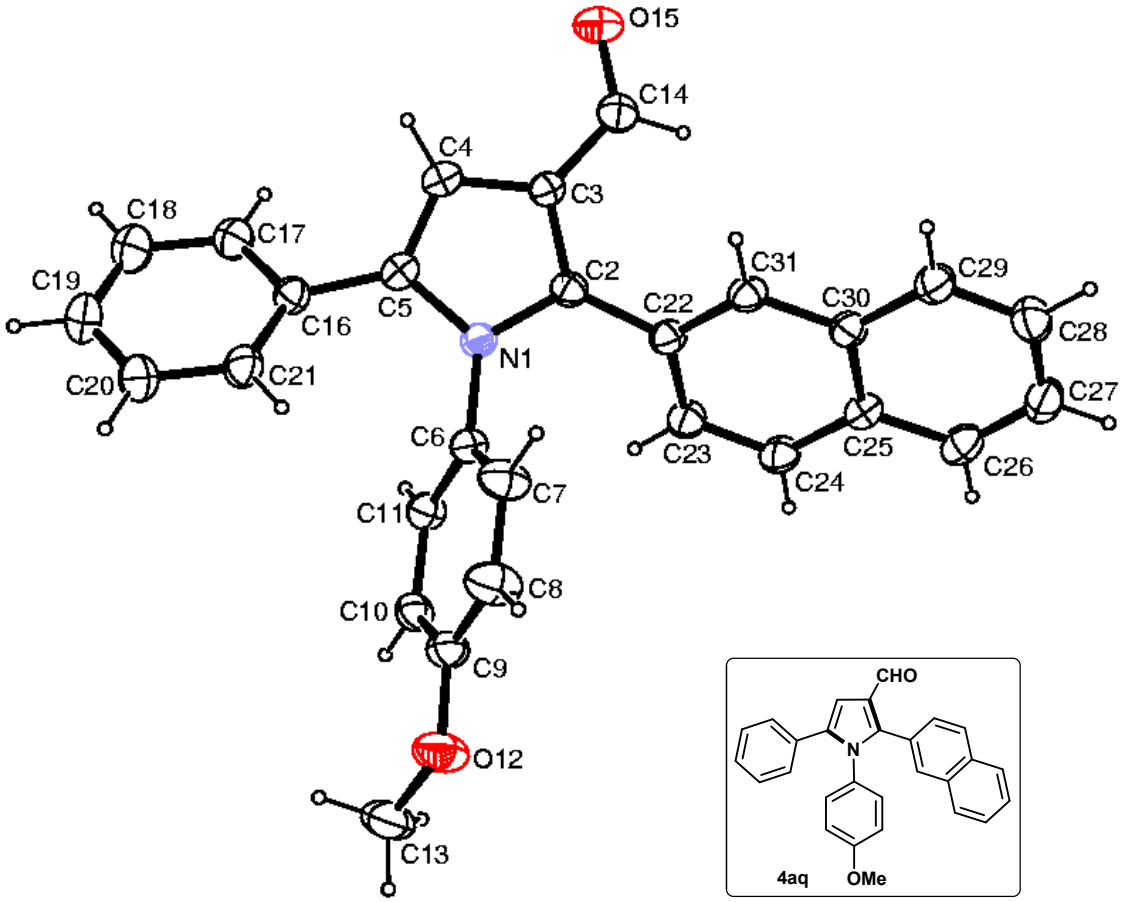


Figure 1 *ORTEP* view of the molecule with displacement ellipsoids drawn at 40%. H atoms are shown as small spheres of arbitrary radii.

CCDC- 1007133 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.