Supporting Information:

Double dehydrogenative coupling of amino alcohols with primary alcohols under Mn(I) catalysis

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1. General Information

All catalytic experiments were carried out using standard Schlenk techniques. All solvents were reagent grade or better. Deuterated solvents were used as received. Manganese salt precursors were used without additional purification. Most of the chemicals used in the catalytic reactions were purified according to standard procedure.[S1] Reactions were monitored using precoated Aluminium supported silica gel 60 F254 TLC (thin layer chromatography) plates (Merck) and are visualized by UV light at 254 nm or under iodine. The final product was purified using column chromatography (230-400 mesh silica gel purchased from Merck). ^{1}H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectra were recorded on the Bruker AVANCE NEO 400 MHz spectrometer. Deuterated chloroform was used as solvents, and Chemical shifts (δ) for ^{1}Hand ^{13}C-NMR spectra are given in ppm relative to tetramethylsilane (TMS) [δ 7.27 for ^{1}H (chloroform-d), δ 77.0 for ^{13}C (chloroform-d)]. Abbreviations used in the NMR follow-up experiments: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; sep, septet; dd, doublet of doublet; m, multiplet. High-resolution mass spectra (HRMS) were obtained from Orbitrap Elite HybridIon Trap-Orbitrap (Thermofischer scientific, Newington, NH, USA) Mass Spectrometer in electrospray ionization mode.

2. Experimental Section

2.1. General procedure for the synthesis of Mn-PNP complex

In a three-necked round-bottom flask (100 mL) under an argon atmosphere, $Mn(CO)_5Br$ (1.0 eq.) was suspended in toluene. Then, the PNP ligand (1.05 eq.) was added at room temperature. The resultant mixture was stirred for 10-15 minutes. After mixing, the reaction mixture was kept at 100°C for 16 h. After the completion of 16 h, the mixture was cooled down to room temperature, and the removal of the solvent under reduced pressure resulted in the formation of a yellow solid. Further washing of this solid with n-octane (3×10 mL) and drying under a high vacuum provide the corresponding manganese complex in 90% yield. The complex was characterized using ^{1}H and ^{31}P NMR spectroscopy, and the data obtained was well correlated with the literature reported once.[S2]

2.2 General procedure for the synthesis of amino alcohol

The compounds 1o, 1d, 1e, 1f, 1g, 1i, 1j, and 1k were synthesized by following the described procedure. The corresponding acetic acid was dissolved in dry THF (40 mL). A solution of $LiAlH_4$ in THF (1M, 60 mL) was added dropwise at 0 ^oC. The resulting mixture was allowed to come to room temperature and then stirred for 2 h. Hydrolyzation of the mixture was done by adding water (2.5 mL) and 5% NaOH (7.5 mL). The suspension was then filtered, and the resulting precipitate was washed with ethyl acetate. After evaporating the organic layer, the resulting residue was recrystallized from ethyl acetate and petroleum ether, and the corresponding amino alcohol was yielded quantitatively.

2.3. General Procedure for the Synthesis of Pyrrole

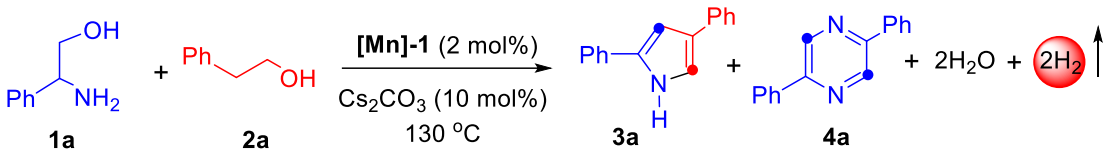
To a 15 mL clean, oven-dried screw cap reaction tube, **[Mn]-1** catalyst (0.01 mmol, 2 mol%), Cs_2CO_3 (0.05 mmol, 10 mol%), **1a** (0.5 mmol, 1 equiv.) and **2a** (0.75 mmol, 1.5 equiv.) were added under a gentle stream of argon. The reaction mixture was kept for stirring (gently) at 130 °C for 8 h. After the completion of 8 h, the crude mixture was cooled down to room temperature, and dichloromethane was used to make it completely dissolve. It was then filtered through a celite filter and again washed with dichloromethane, followed by the solvent was removed under vacuum. Finally, the residue was purified by silica gel column chromatography (230- 400 mesh size) using petroleum ether and ethyl acetate as an eluent system.

2.4. General Procedure for the Synthesis of Pyrazine

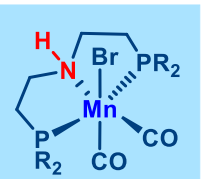
To a 15 mL clean, oven-dried screw cap reaction tube, **[Mn]-1** catalyst (0.01 mmol, 2 mol%), KOH (0.1 mmol, 20 mol%), **1a** (0.5 mmol, 1 equiv.) were added under a gentle stream of argon. The reaction mixture was kept for stirring (gently) at 130 °C for 16 h. After completion of 16 h, the crude mixture was cooled down to room temperature and added dichloromethane to make it completely dissolve then filtered through celite filter and again washed with dichloromethane, followed by the solvent was removed under vacuum and finally, the residue was purified by silica gel column chromatography (230- 400 mesh size) using petroleum-ether and ethyl acetate as an eluent system.

2.5. Reaction Optimization

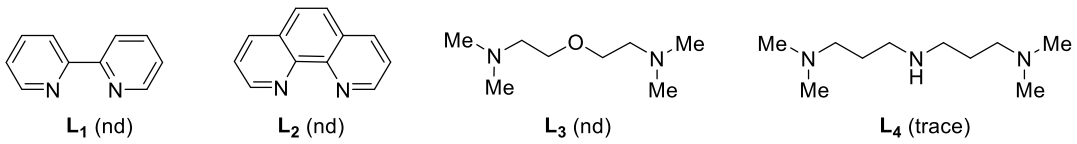
Table S1: Screening of catalyst and ligand.[a]

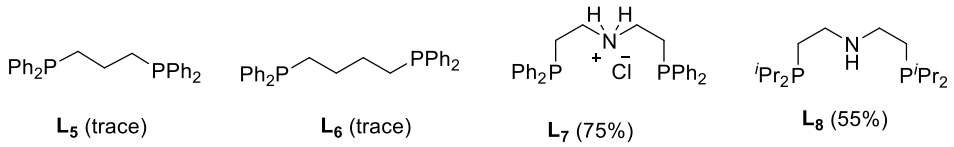


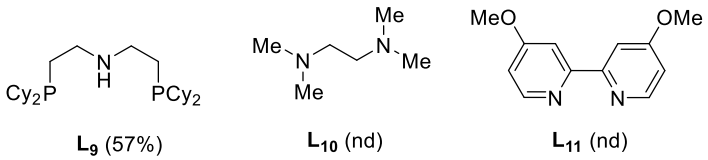
Entry	Deviation from above	**3a** Yield (%)[b]	**4a** Yield (%)[b]
1	No Variation	70	<5
2	**[Mn]-2** as a catalyst	63	<10
3	**[Mn]-3** as a catalyst	60	<10
4	$Mn(CO)_5Br$ / ^{Ph}PNP-Ligand (1:1) (L_7)	57	<15
5	$Mn(CO)_5Br$ / i^{Pr}PNP-Ligand (1:1) (L_8)	46	trace
6	$Mn(CO)_5Br$ / ^{Cy}PNP-Ligand (1:1) (L_9)	43	trace
7	$MnCl_2$ / ^{Ph}PNP-Ligand (1:1) (L_7)	trace	-
8	^{Ph}PNP-Ligand without Mn precursor	NR	NR
9	Mn precursor without ^{Ph}PNP-Ligand (L_7)	NR	NR
10	L1, L2, L3	nd	nd
11	L4, L5, L6	trace	trace



[Mn]-1 R = Ph
[Mn]-2 R = ^{i}Pr
[Mn]-3 R = Cy

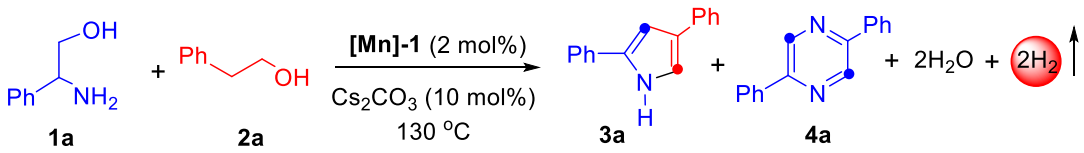




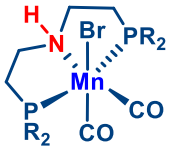


[a]Reaction Conditions: Substrate **1a** (0.5 mmol), **2a** (0.6 mmol), **[Mn]-1** (2 mol%), and Cs_2CO_3 (10 mol%) were heated at 130 °C (silicone oil-bath temperature) for 8 h under an argon atmosphere. [b]Isolated yield.

Table S2: Screening of solvent.[a]



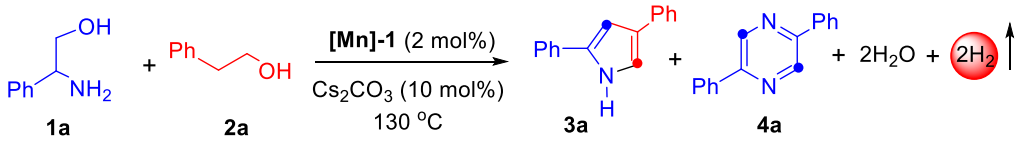
Entry	Deviation from above	**3a** Yield (%)[b]	**4a** Yield (%)[b]
1	No Variation	70	<5
2	n-Octane	46	trace
3	1,4 dioxane	48	trace
4	m-xylene	26	<5
5	THF	30	trace
6	Mesitylene	28	trace
7	Toluene	32	<10



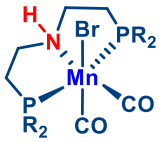
[Mn]-1 R = Ph

[a]Reaction Conditions: Substrate **1a** (0.5 mmol), **2a** (0.6 mmol), **[Mn]-1** (2 mol%) and Cs_2CO_3 (10 mol%) were heated at 130 °C (silicone oil-bath temperature) for 8 h under an argon atmosphere. [b]Isolated yield.

Table S3: Screening of base.[a]



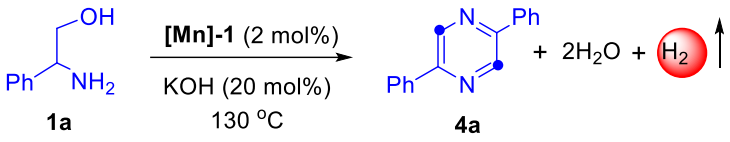
Entry	Deviation from above	**3a** Yield (%)[b]	**4a** Yield (%)[b]
1	No Variation	70	<5
2	KOH	56	30
3	NaOH	51	22
4	KO^{t}Bu	46	21
5	NaO^{t}Bu	43	18
6	K_2CO_3	58	trace
7	[Mn]-1 without base	trace	-
8	Cs_2CO_3 without [Mn]-1	NR	-



[Mn]-1 R = Ph

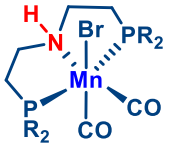
[a]Reaction Conditions: Substrate **1a** (0.5 mmol), **2a** (0.6 mmol), **[Mn]-1** (2 mol%) and Base (10 mol%) were heated at 130 °C (silicone oil-bath temperature) for 8 h under an argon atmosphere. [b]Isolated yield.

Table S4: Optimization for pyrazine.[a]



1a **4a**

Entry	Deviation from above	Base	**4a** Yield (%)[b]
1	No Variation	KOH	80
2	**[Mn]-2** as a catalyst	KOH	75
3	**[Mn]-3** as a catalyst	KOH	72
4	[Mn]-1	NaOH	75
5	[Mn]-1	KO^{t}Bu	72
6	[Mn]-1	NaO^{t}Bu	69
7	[Mn]-1	LiO^{t}Bu	60
8	[Mn]-1	K_2CO_3	25
9	[Mn]-1	Cs_2CO_3	30
10	[Mn]-1	-	30
11	-	KOH	30

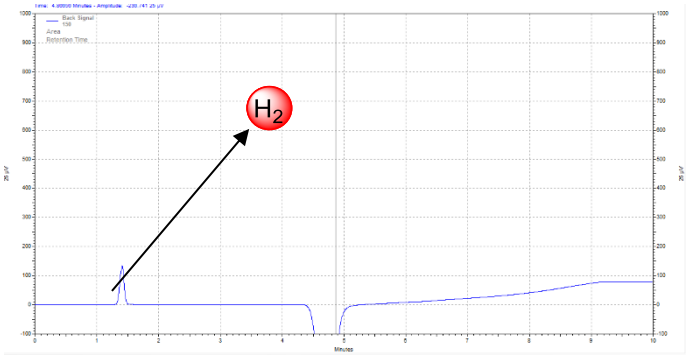


[Mn]-1 R = Ph

[a]Reaction Conditions: Substrate 1 (0.5 mmol), [Mn]-1 (2 mol%), and base (20 mol%) were heated at 130 °C (silicone oil-bath temperature) for 16 h under an argon atmosphere. [b]Isolated yields.

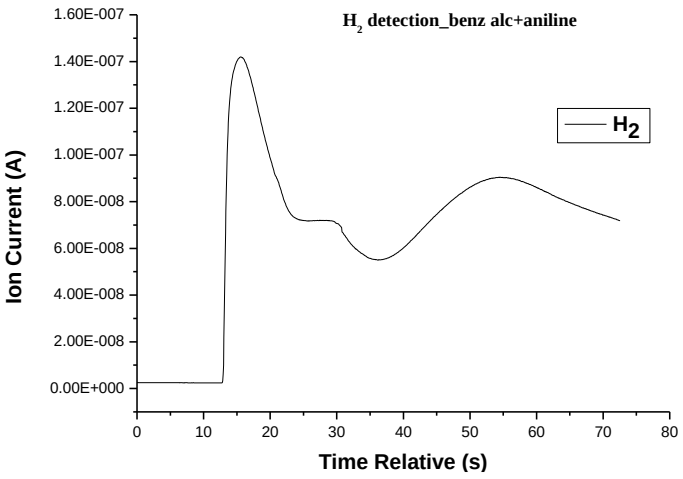
3. H_2 Detection

To a 15 mL clean, oven-dried screw cap with septa reaction tube, **[Mn]-1** catalyst (0.01 mmol, 2 mol%), Cs_2CO_3 (0.05 mmol, 10 mol%), **1a** (0.5 mmol, 1 equiv.) and **2a** (0.75 mmol, 1.5 equiv.) were added under a gentle stream of argon. The reaction mixture was kept for stirring (gently) at 130 °C (oil-bath temperature) for 1 h. After completion of the reaction, the crude mixture was cooled to room temperature, followed by the sample submitted to GC for detection of H_2 gas.



Gas chromatography analysis for the detection of hydrogen gas.

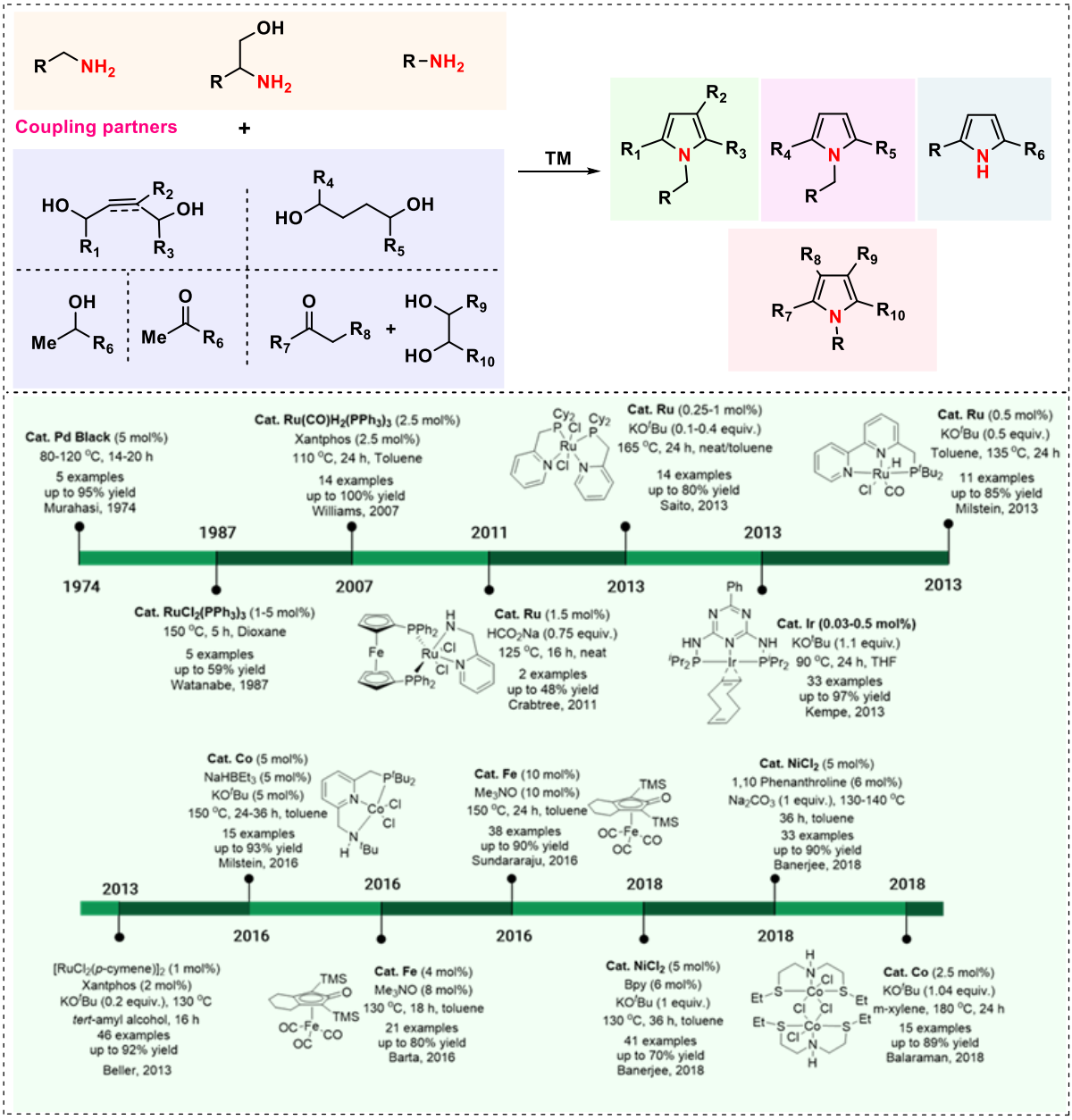
We have determined the formation of hydrogen gas (H_2, m/z = 2) using an online MS with an OmniStarTM Gas Analysis System GSD 320 (Pfeiffer) quadrupole mass spectrometer apparatus.



OmniStar™

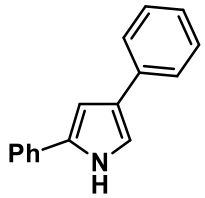
Photograph of OmniStarTM Gas Analysis System GSD 320 (Pfeiffer) quadrupole mass spectrometer apparatus used for the analysis of gases based on following their masses.

4. State-of-the-art: Synthesis of pyrroles *via* ADC approach



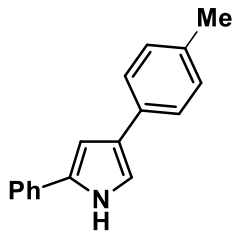
5. Characterization of products

2,4-diphenyl-1H-pyrrole (3a)



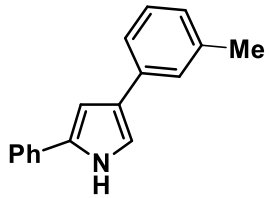
Viscous colourless liquid. Yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.42 (s, 1H), 7.58 – 7.53 (m, 2H), 7.51 – 7.44 (m, 2H), 7.39 – 7.36 (m, 2H), 7.36 – 7.29 (m, 2H), 7.26 – 7.16 (m, 2H), 7.09 (dd, *J* = 2.7, 1.7 Hz, 1H), 6.82 (dd, *J* = 2.8, 1.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 135.55, 133.10, 132.50, 128.99, 128.72, 126.59, 126.52, 125.79, 125.21, 123.89, 115.66, 103.97. HRMS (ESI): m/z Calcd for $C_{16}H_{14}N$ $[M+H]^+$: 220.1121; Found: 220.1126. Ref: M. Adib, N. Ayashi, F. Heidari and P. Mirzaei, *Synlett*, 2016, **27**, 1738–1742.

2-phenyl-4-(p-tolyl)-1H-pyrrole (3b)



Viscous yellowish liquid. Yield: 74%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.44 (s, 1H), 7.56 – 7.46 (m, 2H), 7.43 – 7.33 (m, 4H), 7.27 – 7.21 (m, 2H), 7.12 (d, *J* = 1.3 Hz, 1H), 7.02 (d, *J* = 7.5 Hz, 1H), 6.82 (d, *J* = 1.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 138.17, 135.44, 133.00, 132.55, 128.96, 128.59, 126.46, 126.00, 123.85, 122.33, 115.57, 104.07, 21.58. HRMS (ESI): m/z Calcd for $C_{17}H_{16}N$ $[M+H]^+$: 234.1277; Found: 234.1276. Ref: M. Adib, N. Ayashi, F. Heidari and P. Mirzaei, *Synlett*, 2016, **27**, 1738–1742.

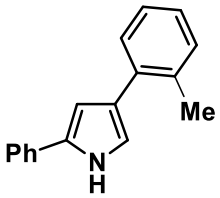
2-phenyl-4-(*m*-tolyl)-1H-pyrrole (3c)



Viscous yellowish liquid. Yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.37 (s, 1H), 7.50 – 7.45 (m, 3H), 7.45 (d, *J* = 1.9 Hz, 1H), 7.36 (dd, *J* = 8.5, 7.0 Hz, 2H), 7.24 – 7.19 (m, 1H), 7.16

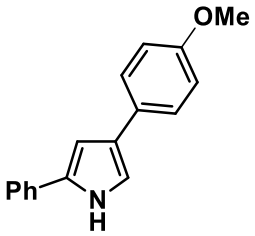
(d, *J* = 7.9 Hz, 2H), 7.06 – 7.05 (m, 1H), 6.80 – 6.79(m, 1H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 135.34, 132.96, 132.67, 132.56, 129.40, 129.40, 128.97, 128.97, 126.60, 126.45, 125.14, 123.85, 115.34, 103.95, 21.15. HRMS (ESI): m/z Calcd for $C_{17}H_{16}N$ $[M+H]^+$: 234.1277; Found: 234.1278. Ref: M. Adib, N. Ayashi, F. Heidari and P. Mirzaei, *Synlett*, 2016, **27**, 1738–1742.

2-phenyl-4-(*o*-tolyl)-1H-pyrrole (3d)



Viscous brown liquid. Yield: 73%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.46 (s, 1H), 7.51 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.45 – 7.39 (m, 2H), 7.39 – 7.34 (m, 1H), 7.28 – 7.18 (m, 3H), 7.17 (td, *J* = 7.3, 1.7 Hz, 1H), 6.93 (dd, *J* = 2.7, 1.7 Hz, 1H), 6.69 (dd, *J* = 2.8, 1.7 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 135.54, 135.32, 132.60, 131.92, 130.61, 129.24, 128.97, 126.39, 126.17, 126.12, 125.86, 123.83, 117.73, 107.00, 21.44. HRMS (ESI): m/z Calcd for $C_{17}H_{16}N$ $[M+H]^+$: 234.1277; Found: 234.1276. Ref: X. Zhang, S. Zheng and S. Zhang, *RSC Adv.*, 2017, **7**, 54254–54257.

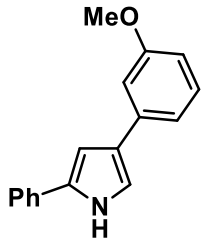
4-(4-methoxyphenyl)-2-phenyl-1H-pyrrole (3e)



Viscous colourless liquid. Yield: 75%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.44 (s, 1H), 7.52 – 7.49 (m, 3H), 7.43 – 7.35 (m, 3H), 7.25 – 7.19 (m, 1H), 7.06 (t, *J* = 2.2 Hz, 1H), 6.94 – 6.89 (m, 2H), 6.76 (dd, *J* = 2.8, 1.7 Hz, 1H), 3.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 157.94, 132.96, 132.59, 128.94, 128.68, 127.20, 126.42, 126.32, 123.85, 114.82, 114.12, 103.89, 55.34. HRMS (ESI): m/z Calcd for $C_{17}H_{15}NO$ $[M+Na]^+$: 272.1051; Found: 272.1072. FTIR: N-H (3317.72 cm^{-1}), C-H stretching (2944.74 cm^{-1}, 2833.43 cm^{-1}), C=C (1694.32 cm^{-1}, 1512 cm^{-1}),

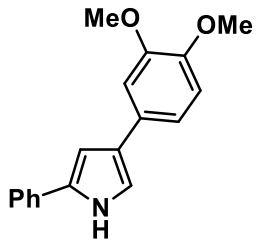
C-O (1252.27 cm^{-1}), C-N (1021.94 cm^{-1}), C-H bending (614.56 cm^{-1}). Ref : M. Adib, N. Ayashi, F. Heidari and P. Mirzaei, *Synlett*, 2016, **27**, 1738–1742.

4-(3-methoxyphenyl)-2-phenyl-1H-pyrrole (3f)



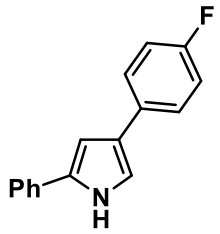
Viscous colourless liquid. Yield: 73%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.47 (s, 1H), 7.54 – 7.49 (m, 2H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.31 – 7.26 (m, 1H), 7.23 (d, *J* = 7.4 Hz, 1H), 7.18 (s, 1H), 7.16 – 7.09 (m, 2H), 6.83 – 6.79 (m, 1H), 6.79 – 6.74 (m, 1H), 3.86 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.96, 136.99, 133.08, 132.47, 129.64, 128.97, 128.97, 126.54, 123.89, 117.88, 115.75, 111.13, 110.96, 104.11, 55.26. HRMS (ESI): m/z Calcd for $C_{17}H_{15}NO$ $[M+H]^+$: 250.1232; Found: 250.1223. FTIR: N-H (3333.05 cm^{-1}), C-H stretching (2942.91 cm^{-1}, 2834.14 cm^{-1}), C=C (1686.54 cm^{-1}, 1605 cm^{-1}), C-O (1287.58 cm^{-1}), C-N (1022.40 cm^{-1}), C-H bending (763.48 cm-1, 692.73 cm^{-1})

4-(3,4-dimethoxyphenyl)-2-phenyl-1H-pyrrole (3g)



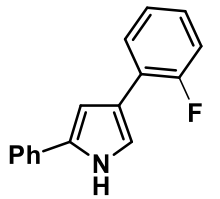
Viscous colourless liquid. Yield: 71%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.46 (s, 1H), 7.55 – 7.48 (m, 2H), 7.38 (m, 2H), 7.25 – 7.19 (m, 1H), 7.15 – 7.04 (m, 3H), 6.89 (d, *J* = 8.2 Hz, 1H), 6.76 (dd, *J* = 2.8, 1.7 Hz, 1H), 3.94 (s, 3H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 149.13, 147.45, 133.02, 132.53, 128.96, 128.83, 126.60, 126.48, 123.86, 117.50, 115.01, 111.66, 109.01, 103.98, 56.01, 55.91. HRMS (ESI): m/z Calcd for $C_{18}H_{17}NO_2$ $[M+Na]^+$: 302.1157; Found: 302.1154. FTIR: N-H (3325.50 cm^{-1}), C-H stretching (2943.89 cm^{-1}, 2832.74 cm^{-1}), C=C (1671.32 cm^{-1}), C-O (1251.22 cm^{-1}), C-N (1021.50 cm^{-1}), C-H bending (628.49 cm^{-1})

4-(4-fluorophenyl)-2-phenyl-1H-pyrrole (3h)



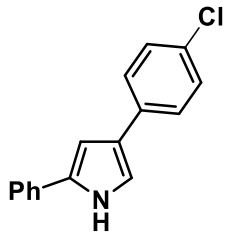
Viscous brown liquid. Yield: 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.44 (s, 1H), 7.52 – 7.49 (m, 4H), 7.40 – 7.36 (m, 2H), 7.28 – 7.21 (m, 1H), 7.09 – 7.00 (m, 3H), 6.76 (dd, *J* = 2.8, 1.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.59, 160.16, 133.22, 132.40, 131.72, 131.69 (F-coupling), 129.04, 129.00, 126.64, 126.62, 126.56, 125.76 (F-coupling), 123.90, 115.57, 115.36, 115.29 (F-coupling), 103.94. ^{19}F NMR (377 MHz, CD_2Cl_2) δ -118.32, -118.33. HRMS (ESI): m/z Calcd for $C_{16}H_{13}FN$ $[M+H]^+$: 238.1027; Found: 238.1026. FTIR: N-H (3326.24 cm^{-1}), C-H stretching (2944.13, 2832.39 cm^{-1}), C=C (1449.14 cm^{-1}), C-N (1114.22 cm^{-1}), C-H bending (634.64 cm^{-1}). Ref: M. Adib, N. Ayashi, F. Heidari and P. Mirzaei, *Synlett*, 2016, **27**, 1738–1742.

4-(2-fluorophenyl)-2-phenyl-1H-pyrrole (3i)



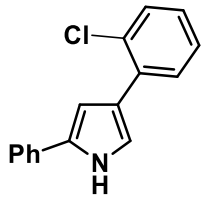
Viscous yellowish liquid. Yield: 71%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.48 (s, 1H), 7.65 – 7.57 (m, 1H), 7.52 – 7.46 (m, 2H), 7.37 (dd, *J* = 8.5, 7.0 Hz, 2H), 7.29 – 7.28 (m, 1H), 7.26 – 7.18 (m, 1H), 7.18 – 7.03 (m, 3H), 6.90 – 6.88 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.95, 158.50, 132.56, 132.36, 129.00, 127.77, 127.72 (F-Coupling), 126.73, 126.64, 126.61 (F-Coupling), 124.23, 124.20 (F-Coupling), 123.95, 123.20, 123.06, 119.89, 119.87 (F-Coupling), 118.76, 118.66 (F-Coupling), 116.10, 115.88, 104.82, 104.80, ^{19}F NMR (377 MHz, Chloroform-*d*) δ -115.07. HRMS (ESI): m/z Calcd for $C_{16}H_{13}FN$ $[M+H]^+$: 238.1027; Found: 238.1023. FTIR: N-H (3326.24 cm^{-1}), C-H stretching (2944.13, 2832.39 cm^{-1}), C=C (1449.14 cm^{-1}), C-N (1114.22 cm^{-1}), C-H bending (634.64 cm^{-1}).

4-(4-chlorophenyl)-2-phenyl-1H-pyrrole (3j)



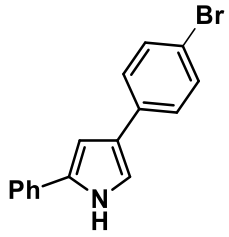
Viscous colourless liquid. Yield: 80%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.47 (s, 1H), 7.51 - 7.46 (m, 4H), 7.41 – 7.37 (m, 2H), 7.34 – 7.29 (m, 2H), 7.27 – 7.21 (m, 1H), 7.11 (s, 1H), 6.78 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 134.06, 133.36, 132.30, 131.23, 129.02, 128.77, 126.70, 126.36, 125.51, 123.92, 115.64, 103.84. HRMS (ESI): m/z Calcd for $C_{16}H_{13}NCl$ $[M+H]^+$: 254.0731; Found: 254.0733. Ref : M. Adib, N. Ayashi, F. Heidari and P. Mirzaei, *Synlett*, 2016, **27**, 1738–1742.

4-(2-chlorophenyl)-2-phenyl-1H-pyrrole (3k)



Viscous colourless liquid. Yield: 78%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 (s, 1H), 7.54 – 7.52 (m, 1H), 7.48 (dd, *J* = 7.5, 2.0 Hz, 2H), 7.44 – 7.34 (m, 3H), 7.30 – 7.20 (m, 2H), 7.15 (d, *J* = 7.7 Hz, 1H), 7.10 – 7.08 (m, 1H), 6.78 (q, *J* = 2.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 137.44, 134.55, 133.38, 132.24, 129.91, 129.03, 126.73, 125.64, 125.31, 125.16, 123.92, 123.21, 116.00, 103.87. HRMS (ESI): m/z Calcd for $C_{16}H_{13}NCl$ $[M+H]^+$: 254.0731; Found: 254.0731.

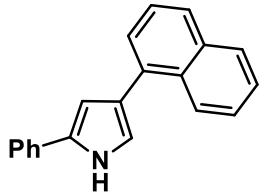
4-(4-bromophenyl)-2-phenyl-1H-pyrrole (3l)



Viscous yellowish liquid. Yield: 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.49 (s, 1H), 7.53 – 7.49 (m, 2H), 7.49 – 7.41 (m, 4H), 7.41 – 7.38 (m, 1H), 7.28 – 7.21 (m, 2H), 7.13 (dd, *J* = 2.7, 1.7 Hz, 1H), 6.78 (dd, *J* = 2.8, 1.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 134.51, 133.39, 132.29, 131.69, 129.01, 126.73, 126.71, 125.52, 123.93, 119.21, 115.64, 103.81. HRMS (ESI): m/z Calcd for $C_{16}H_{13}NBr$ $[M+H]^+$: 298.0226; Found: 254.0231.

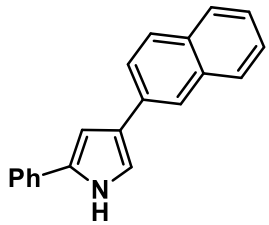
(Ref : M. Adib, N. Ayashi, F. Heidari and P. Mirzaei, *Synlett*, 2016, **27**, 1738–1742)

4-(naphthalen-1-yl)-2-phenyl-1H-pyrrole (3m)



Viscous colourless liquid. Yield: 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.53 (s, 1H), 8.43 – 8.34 (m, 1H), 7.91 – 7.85 (m, 1H), 7.79 – 7.77 (m, 1H), 7.55 – 7.52 (m, 3H), 7.51 – 7.44 (m, 3H), 7.41 – 7.37 (m, *J* = 7.8 Hz, 2H), 7.27 – 7.21 (m, 1H), 7.05 (dd, *J* = 2.6, 1.6 Hz, 1H), 6.82 (dd, *J* = 2.9, 1.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 134.39, 134.03, 132.57, 132.29, 131.96, 129.03, 128.33, 126.75, 126.50, 126.28, 125.81, 125.65, 125.62, 125.17, 123.90, 123.90, 118.24, 107.92. HRMS (ESI): m/z Calcd for $C_{20}H_{15}N$ $[M+H]^+$: 270.1283; Found: 270.1275. FTIR: N-H (3326.75 cm^{-1}), C-H stretching (3005.61 cm^{-1}), C=C (1685.81 cm^{-1}, 1449.50 cm^{-1}), C-N (1017.22 cm^{-1}), C-H bending (760.20 cm^{-1}, 694.46 cm^{-1}).

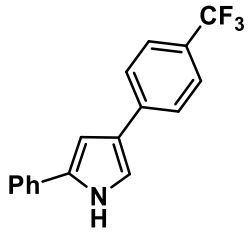
4-(naphthalen-2-yl)-2-phenyl-1H-pyrrole (3n)



Viscous colourless liquid. Yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.52 (s, 1H), 8.00 (d, *J* = 1.7 Hz, 1H), 7.84 – 7.80 (m, 3H), 7.73 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.59 – 7.52 (m, 2H), 7.47 (dd, *J* = 6.8, 1.3 Hz, 1H), 7.44 – 7.37 (m, 3H), 7.29 – 7.26 (m, 1H), 7.26 – 7.24 (m, 1H), 6.97 (dd, *J* = 2.7, 1.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 134.00, 133.35, 132.93, 132.47, 132.08, 129.00, 129.00, 128.19, 127.70, 127.67, 126.60, 126.10, 124.99, 124.51, 123.93, 122.70, 116.01, 104.12. HRMS (ESI): m/z Calcd for $C_{20}H_{15}N$ $[M+H]^+$: 270.1283; Found:

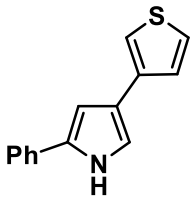
270.1277. FTIR: N-H (3326.70 cm^{-1}), C-H stretching (2944.60, 2832.76 cm^{-1}), C=C (1687.09 cm^{-1}, 1449.60 cm-1), C-N (1021.10 cm^{-1}), C-H bending (776.86 cm^{-1}, 641.74 cm^{-1}).

2-phenyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrrole (3o)



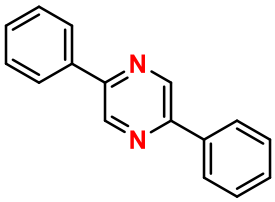
Viscous brown liquid. Yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.55 (s, 1H), 7.67 – 7.63 (m, 2H), 7.62 – 7.57 (m, 2H), 7.54 – 7.49 (m, 2H), 7.44 – 7.36 (m, 2H), 7.29 – 7.25 (m, 1H), 7.21 (dd, *J* = 2.8, 1.7 Hz, 1H), 6.84 (dd, *J* = 2.8, 1.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 139.10, 133.63, 132.16, 129.05, 127.69, 127.37 (F couplings), 126.85, 125.86, 125.70, 125.66, 125.63, 125.59 (CF_3 group, F couplings), 125.29, 125.05 (F couplings), 123.98, 123.16, 116.37, 103.96. ^{19}F NMR (377 MHz, CD_2Cl_2) δ -62.48. HRMS (ESI): m/z Calcd for $C_{17}H_{12}F_3N$ $[M+NH_4]^+$: 305.1266; Found: 305.1258.

2-phenyl-4-(thiophen-3-yl)-1H-pyrrole (3p)



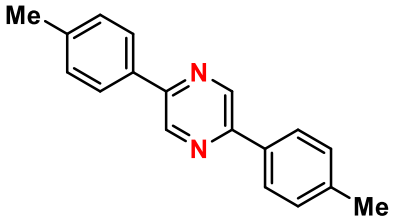
Viscous brown liquid. Yield: 69%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.40 (s, 1H), 7.54 – 7.47 (m, 2H), 7.39 (dd, *J* = 8.5, 7.1 Hz, 2H), 7.33 (dd, *J* = 5.0, 2.9 Hz, 1H), 7.28 (dd, *J* = 5.0, 1.4 Hz, 1H), 7.26 (d, *J* = 2.4 Hz, 1H), 7.25 – 7.20 (m, 1H), 7.06 (dd, *J* = 2.8, 1.6 Hz, 1H), 6.74 (dd, *J* = 2.8, 1.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 136.78, 132.86, 132.45, 128.97, 126.53, 126.08, 125.59, 123.89, 122.15, 117.13, 115.58, 104.39. HRMS (ESI): m/z Calcd for $C_{14}H_{11}NS$ $[M+H]^+$: 226.0690; Found: 226.0685. FTIR: N-H (3337.84 cm^{-1}), C-H stretching (2950.0 cm^{-1}), C=C (1687.19 cm^{-1}), C-N (1022.16 cm^{-1}), C-H bending (764.98 cm^{-1}, 692.15 cm^{-1}).

2,5-diphenylpyrazine (4a)



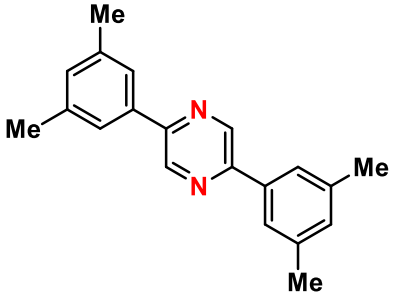
White solid. Yield: 80%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.98 (s, 2H), 8.20 – 8.13 (m, 4H), 7.57 – 7.54 (m, 2H), 7.54 – 7.47 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 151.61, 139.92, 136.54, 129.93, 129.02, 127.05. HRMS (ESI): m/z Calcd for $C_{16}H_{13}N_2$ $[M+H]^+$: 233.1079; Found: 233.1072. Ref: M. Nitta and T. Kobayashi, *Chem. Lett.*, 1983, **12**, 1715–1718.

2,5-di-*p*-tolylpyrazine (4b)



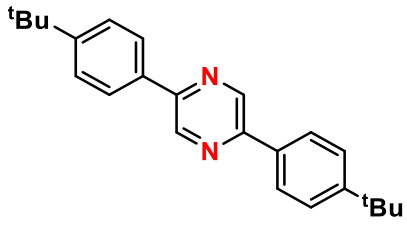
Yellow solid. Yield: 72%. ^{1}H NMR (400 MHz, $CDCl_3$-*d*) δ = 8.91 (s, 2H), 8.09 – 8.02 (m, 4H), 7.37 – 7.29 (m, 4H), 2.44 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 151.52, 140.03, 139.34, 133.85, 129.72, 126.91, 21.40. HRMS (ESI): m/z Calcd for $C_{18}H_{17}N_2$ $[M+H]^+$: 261.1393; Found: 261.1386. Ref: P. Vitale, L. Cicco, F. Messa, F. M. Perna, A. Salomone and V. Capriati, *Eur. J. Org. Chem.*, 2019, **2019**, 5557–5562.

2,5-bis(3,5-dimethylphenyl)pyrazine (4c)



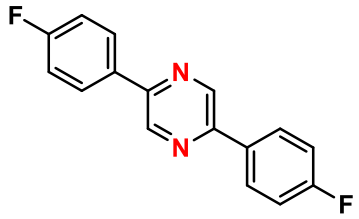
Yellowish-brown solid. Yield: 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.55 (s, 2H), 7.33 (d, *J* = 7.5 Hz, 2H), 7.07 (s, 3H), 7.05 (s, 2H), 2.37 (s, 6H), 2.31 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 154.35, 142.22, 139.02, 136.25, 134.21, 131.86, 130.04, 126.87, 21.20, 20.57 HRMS (ESI): m/z Calcd for $C_{20}H_{21}N_2$ $[M+H]^+$: 289.1705; Found: 289.1698.

2,5-bis(4-(tert-butyl)phenyl)pyrazine (4d)



Yellow solid. Yield: 67%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.92 (s, 2H), 8.13 – 8.04 (m, 4H), 7.60 – 7.52 (m, 4H), 1.39 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 153.18, 151.57, 139.45, 133.87, 126.78, 125.97, 34.83, 31.28. HRMS (ESI): m/z Calcd for $C_{24}H_{29}N_2$ $[M+H]^+$: 345.2325; Found: 345.2337. Ref: Z. Chen, D. Ye, G. Xu, M. Ye and L. Liu, *Org. Biomol. Chem.*, 2013, **11**, 6699–6702.

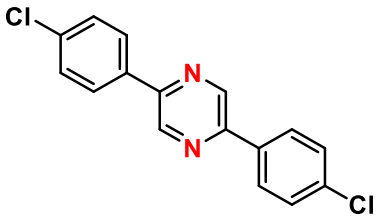
2,5-bis(4-fluorophenyl)pyrazine (4e)



Yellow solid. Yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.93 (s, 2H), 8.14 (dd, J = 8.9, 5.3 Hz, 4H), 7.26 -7.21 (m, 4H). ^{13}C NMR (101 MHz, CDCl3) δ = 165.43, 162.94, 150.86, 138.99, 132.43 (F-coupling), 129.03 - 128.95 (F-coupling), 116.26 -116.05 (F-coupling), ^{19}F NMR (377 MHz, $CDCl_3$) δ -110.64. HRMS (ESI): m/z Calcd for $C_{16}H_{11}N_2F_2$ $[M+H]^+$: 269.0890; Found: 269.0893. FTIR: N-H (3337.84 cm^{-1}), C-H stretching (2923.72.0 cm^{-1}), C=C (1602.21 cm-1, 1511.47 cm^{-1}), C-N (1228.33 cm^{-1}, 1436.53 cm^{-1}), C-H bending (1157.84 cm^{-1}, 827.66

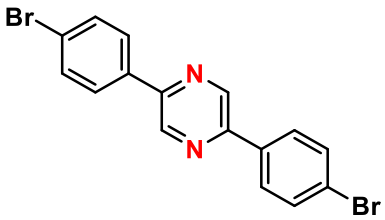
cm^{-1}). Ref: P. Vitale, L. Cicco, F. Messa, F. M. Perna, A. Salomone and V. Capriati, *European J. Org. Chem.*, 2019, **2019**, 5557–5562).

2,5-bis(4-chlorophenyl)pyrazine (4f)



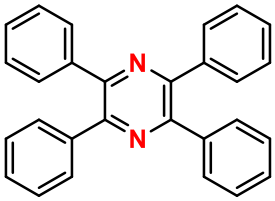
Yellow solid. Yield: 60%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.04 (s, 2H), 8.05 – 7.98 (m, 4H), 7.54 – 7.47 (m, 4H). ^{13}C NMR (101 MHz, CDCl3) δ = 149.78, 141.00, 136.20, 134.57, 129.37, 128.04. HRMS (ESI): m/z Calcd for $C_{16}H_{11}N_2Cl_2$ $[M+H]^+$: 301.0299; Found: 301.0304. Ref: P. Vitale, L. Cicco, F. Messa, F. M. Perna, A. Salomone and V. Capriati, *Euro. J. Org. Chem.*, 2019, **2019**, 5557–5562.

2,5-bis(4-bromophenyl)pyrazine (4g)



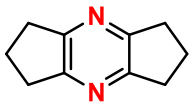
White solid. Yield: 60%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.96 (s, 2H), 8.06 – 7.97 (m, 4H), 7.68 (dd, *J* = 6.3, 4.3 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 150.62, 139.92, 135.18, 132.28, 128.54, 124.74. HRMS (ESI): m/z Calcd for $C_{16}H_{11}N_2Br_2$ $[M+H]^+$: 388.9289; Found: 388.9301.

2,3,5,6-tetraphenylpyrazine (4h)



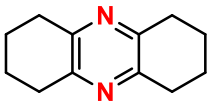
Yellow solid. Yield: 63%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (m, 8H), 7.25 (m, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 148.46, 138.50, 129.92, 128.64, 128.27. HRMS (ESI): m/z Calcd for $C_{28}H_{21}N_2$ $[M+H]^+$: 385.1705; Found: 385.1703. Ref: L. O. Khafizova, M. G. Shaibakova and U. M. Dzhemilev, *ChemistrySelect*, 2018, **3**, 11451–11453.

1,2,3,5,6,7-hexahydrodicyclopenta[b,e]pyrazine (4i)



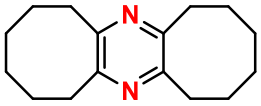
White solid. Yield: 59%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.00 (t, *J* = 7.6 Hz, 4H), 2.20 (t, *J* = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.09, 31.60, 21.40. HRMS (ESI): m/z Calcd for $C_{10}H_{13}N_2$ $[M+H]^+$: 161.1079; Found: 161.1074.

1,2,3,4,6,7,8,9-octahydrophenazine (4j)



White solid. Yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.92 – 2.84 (m, 4H), 1.90 (td, *J* = 4.1, 2.2 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 149.35, 31.64, 22.82. HRMS (ESI): m/z Calcd for $C_{12}H_{17}N_2$ $[M+H]^+$: 189.1386; Found: 189.1377

1,2,3,4,5,6,8,9,10,11,12,13-dodecahydrodicycloocta[b,e]pyrazine (4k)



White solid. Yield: 61%.^{1}H NMR (400 MHz, Chloroform-*d*) δ 2.96 – 2.82 (m, 8H), 1.73 (dt, *J* = 3.7, 1.6 Hz, 8H), 1.40 – 1.27 (m, 8H). HRMS (ESI): m/z Calcd for $C_{14}H_{26}N_2Na$ $[M+H]^+$: 245.1994 ; Found: 245.2005.

6. References

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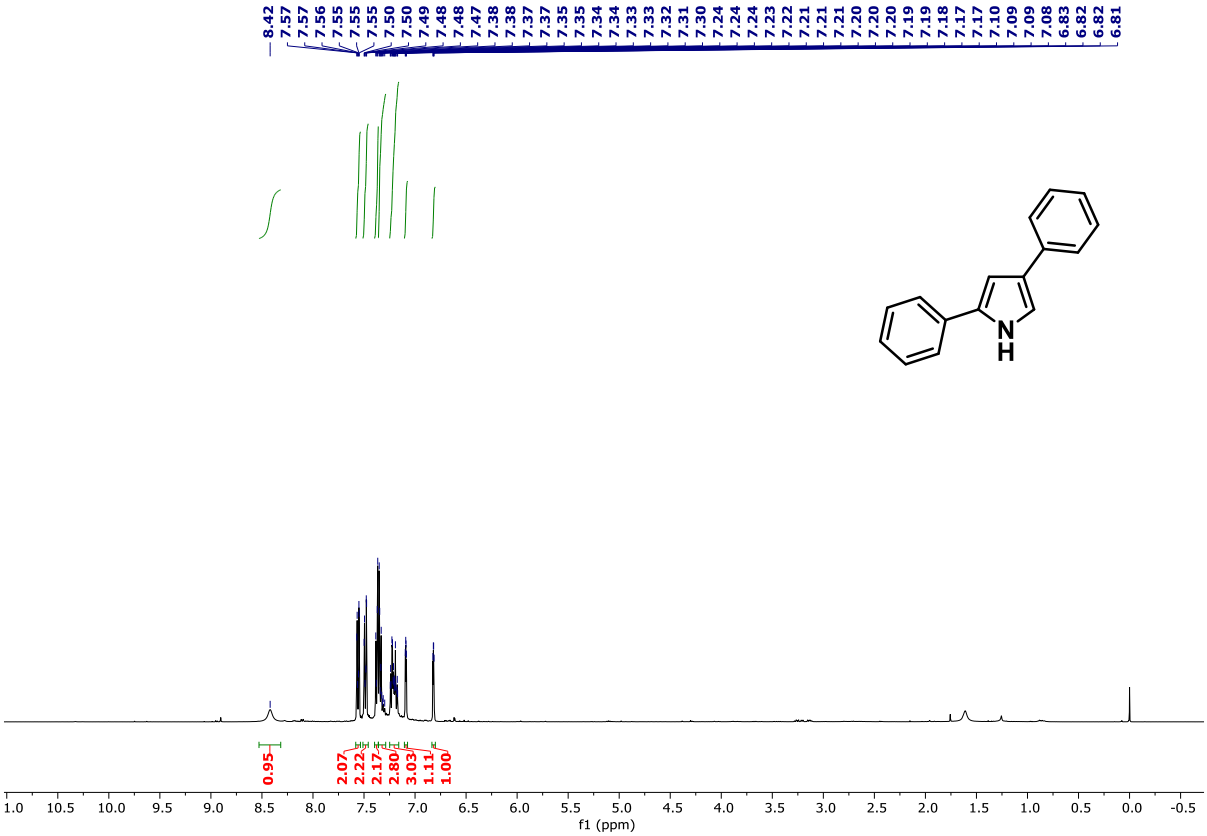
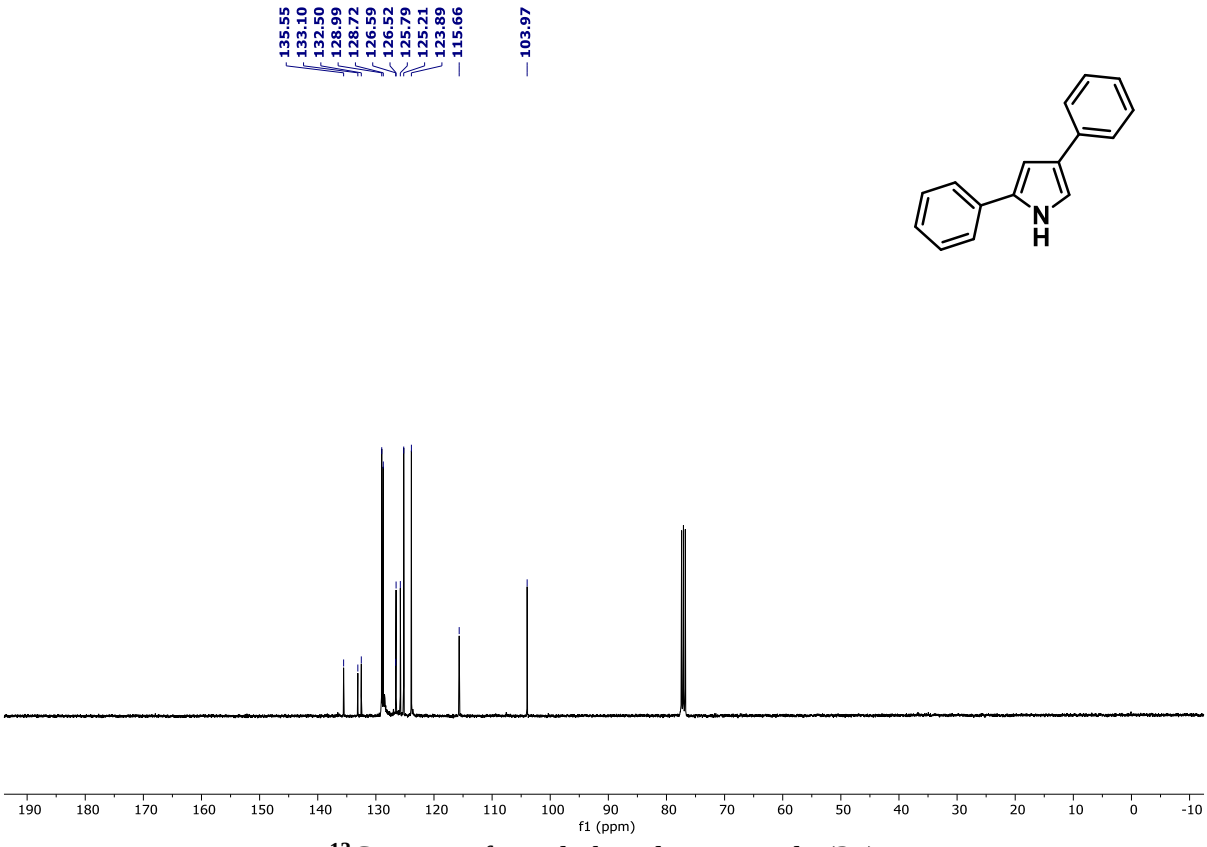
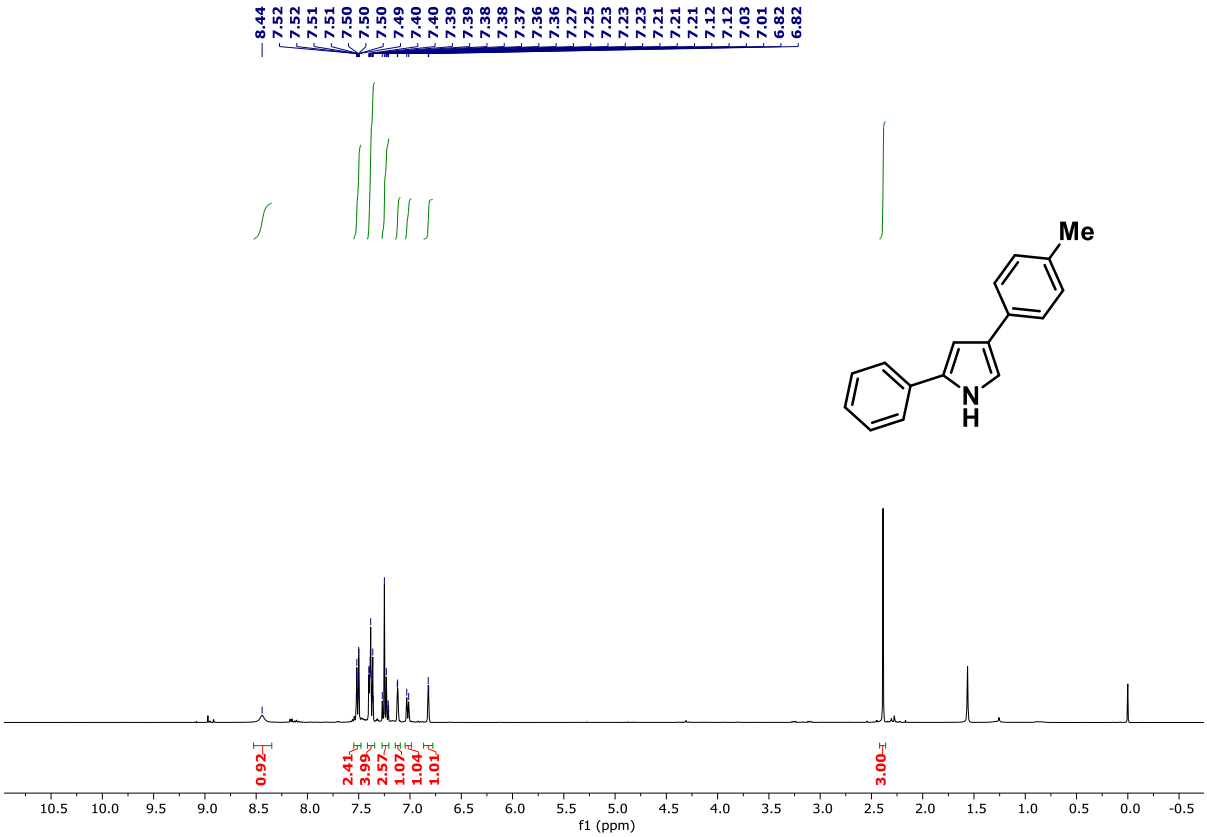
7. Copy of Spectra



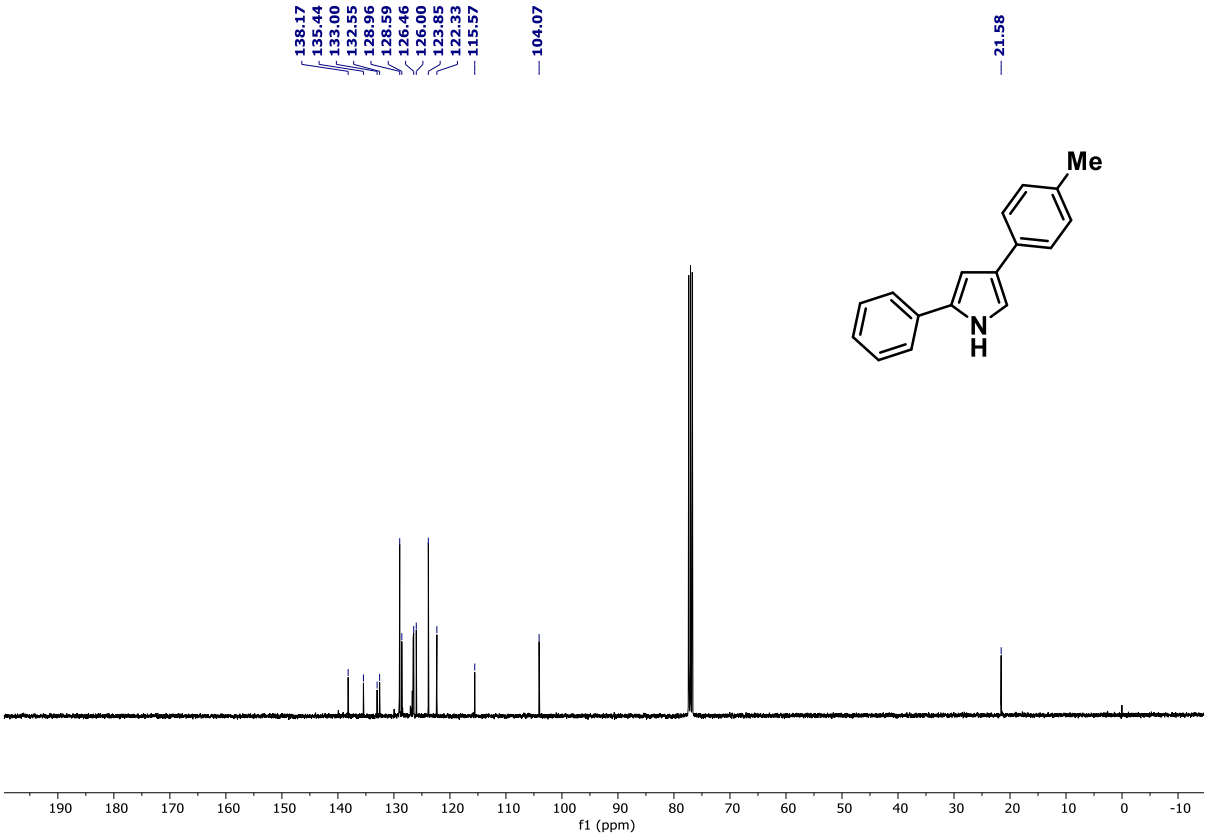
^{1}H NMR of 2,4-diphenyl-1H-pyrrole (**3a**)



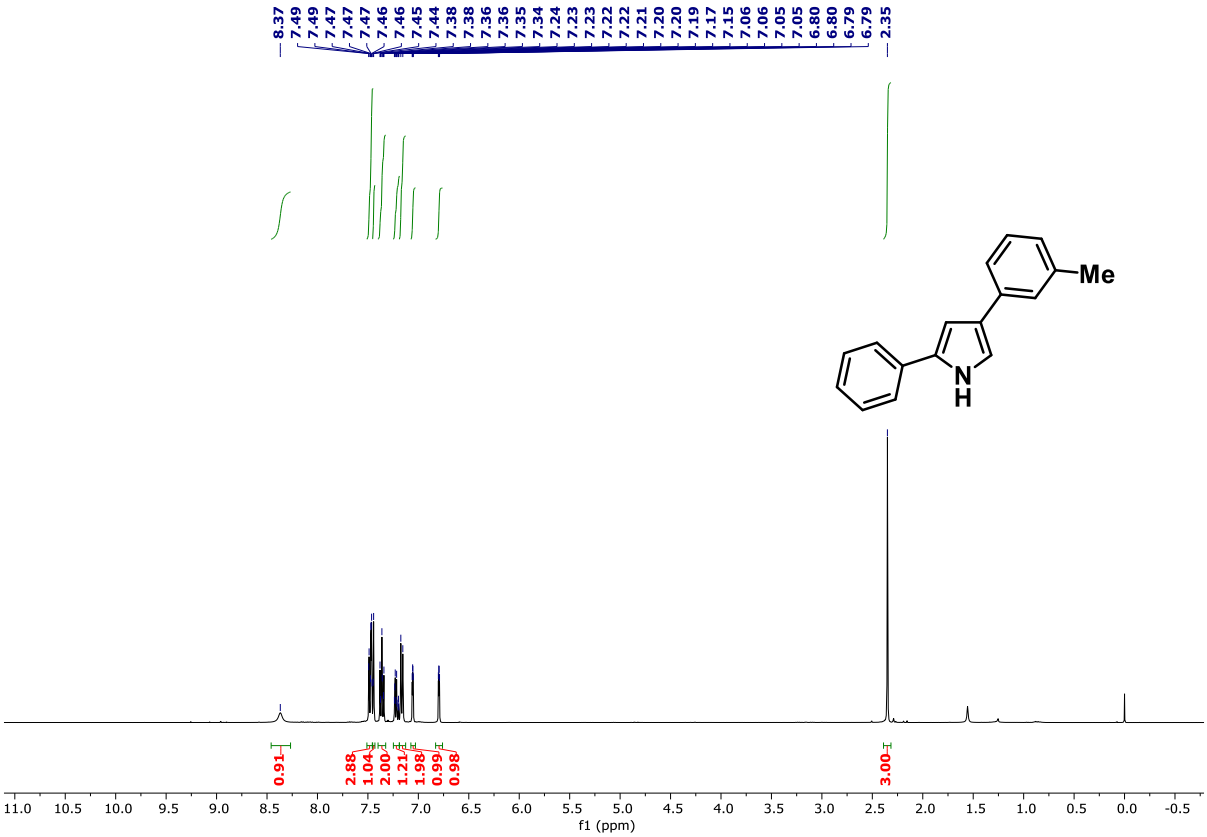
^{13}C NMR of 2,4-diphenyl-1H-pyrrole (**3a**)



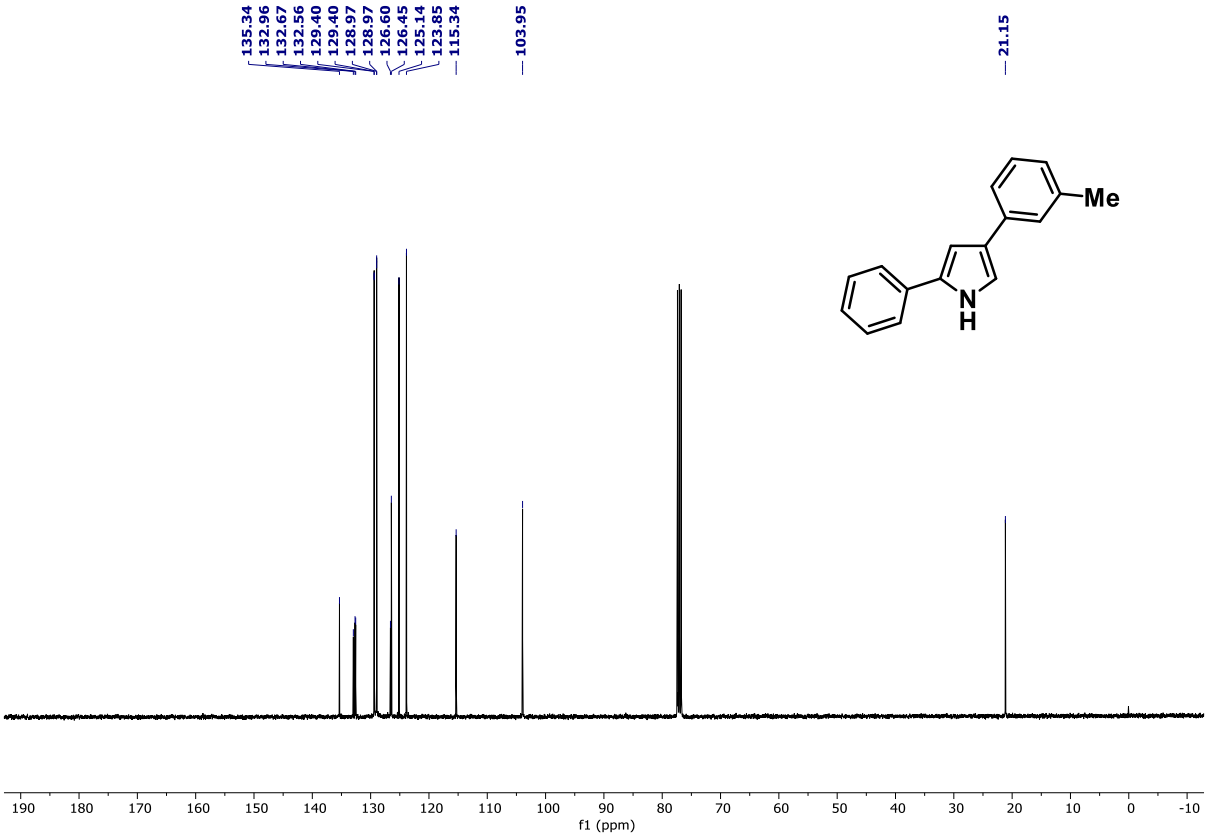
^{1}H NMR of 2-phenyl-4-(*p*-tolyl)-1H-pyrrole (**3b**)



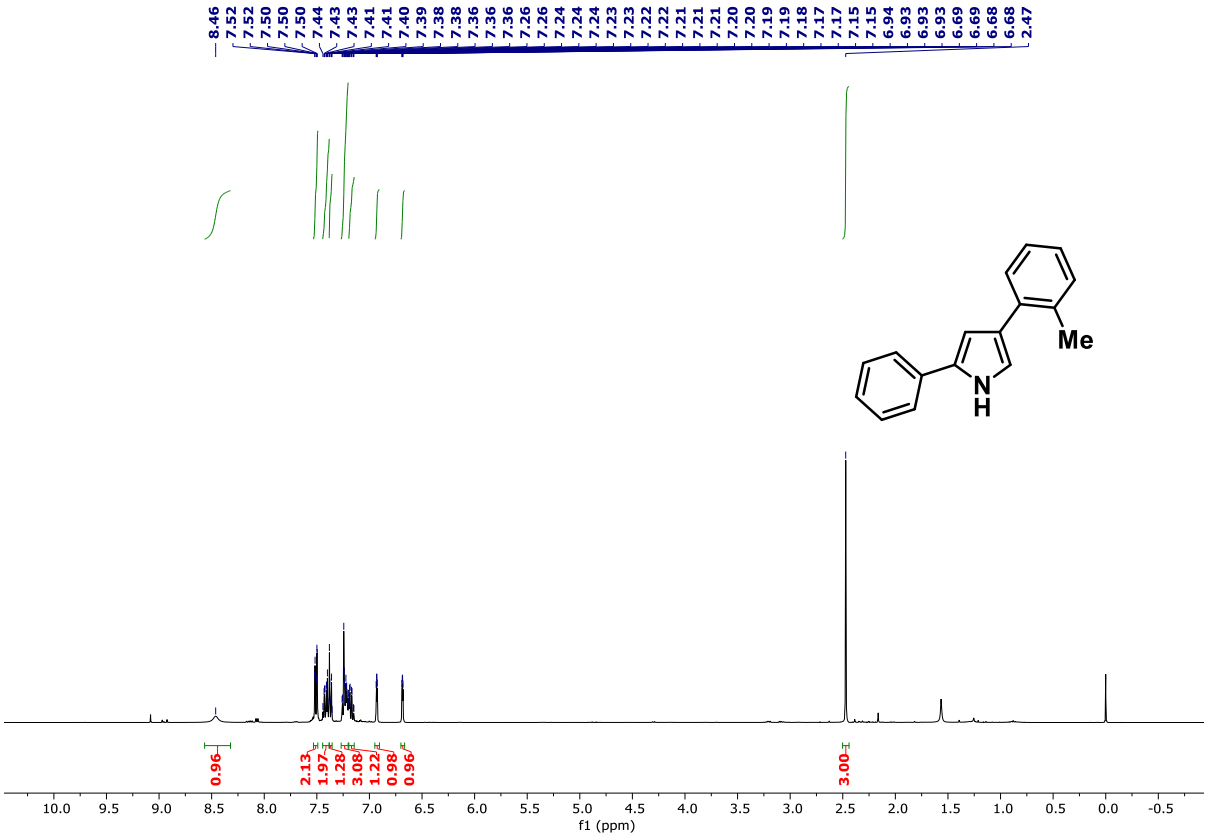
^{13}C NMR of 2-phenyl-4-(*p*-tolyl)-1H-pyrrole (**3b**)



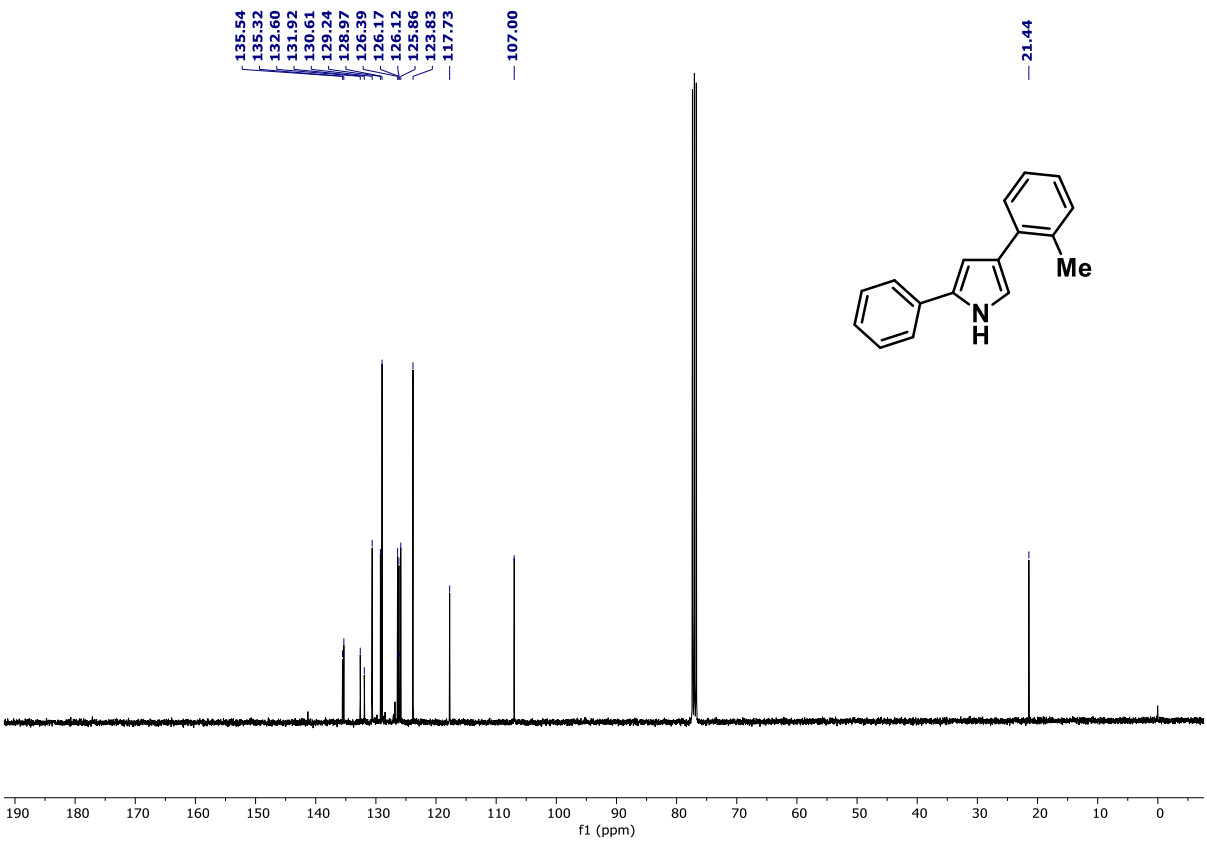
^{1}H NMR of 2-phenyl-4-(*m*-tolyl)-1H-pyrrole (**3c**)



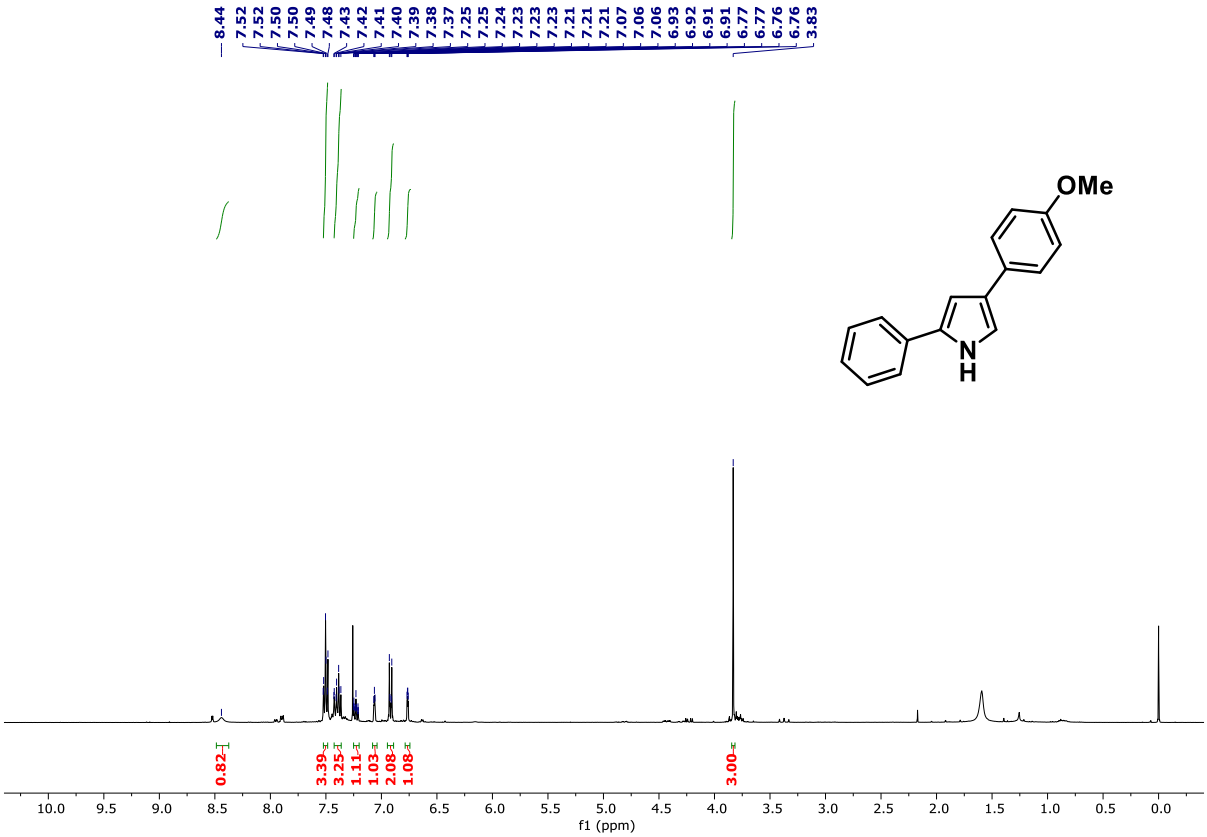
^{13}C NMR of 2-phenyl-4-(*m*-tolyl)-1H-pyrrole (**3c**)



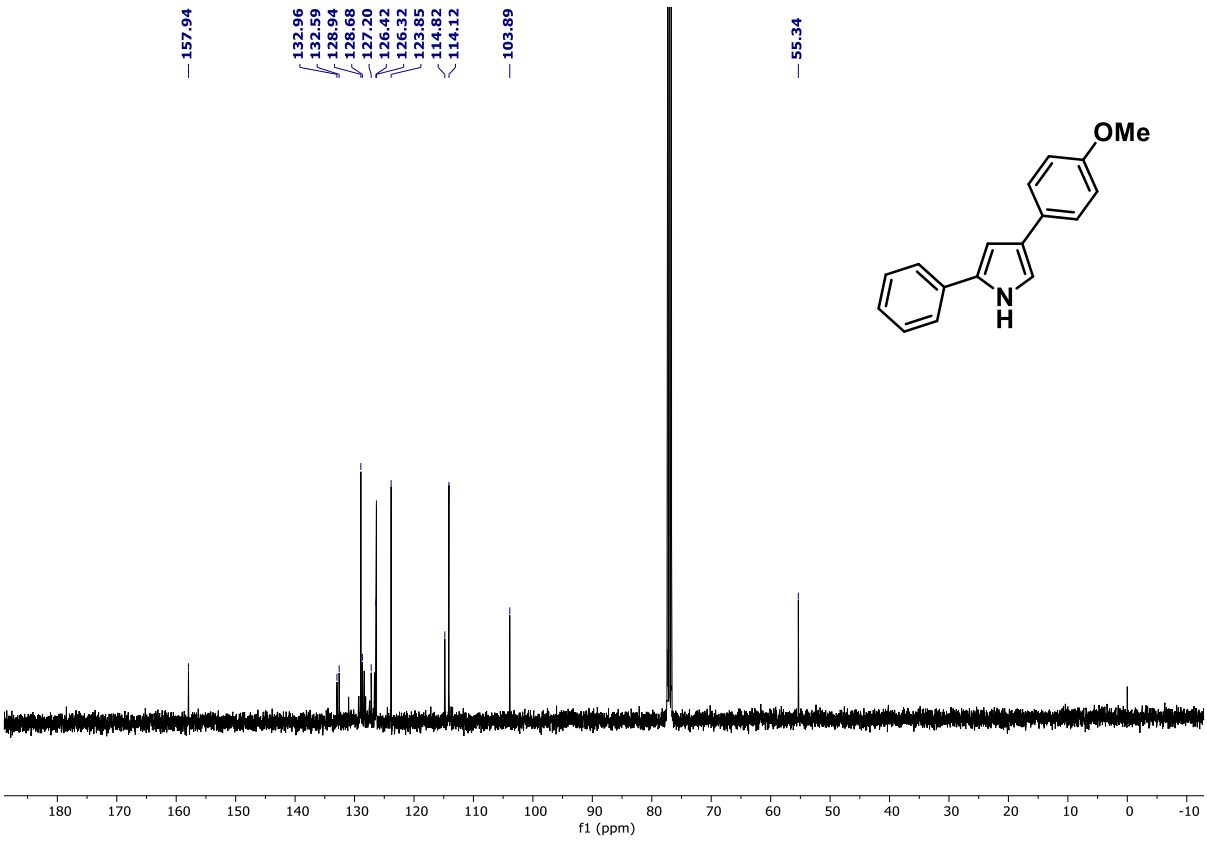
^{1}H NMR of 2-phenyl-4-(*o*-tolyl)-1H-pyrrole (**3d**)



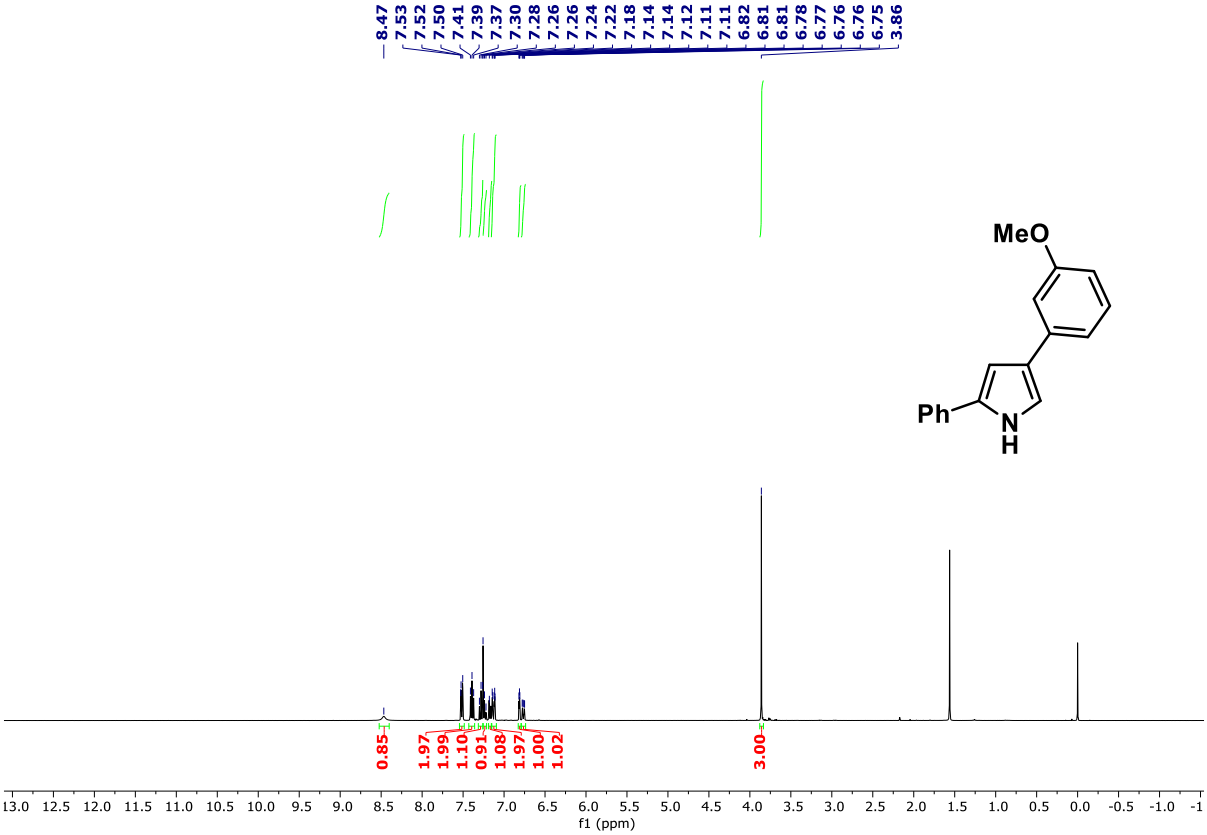
^{13}C NMR of 2-phenyl-4-(*o*-tolyl)-1H-pyrrole (**3d**)



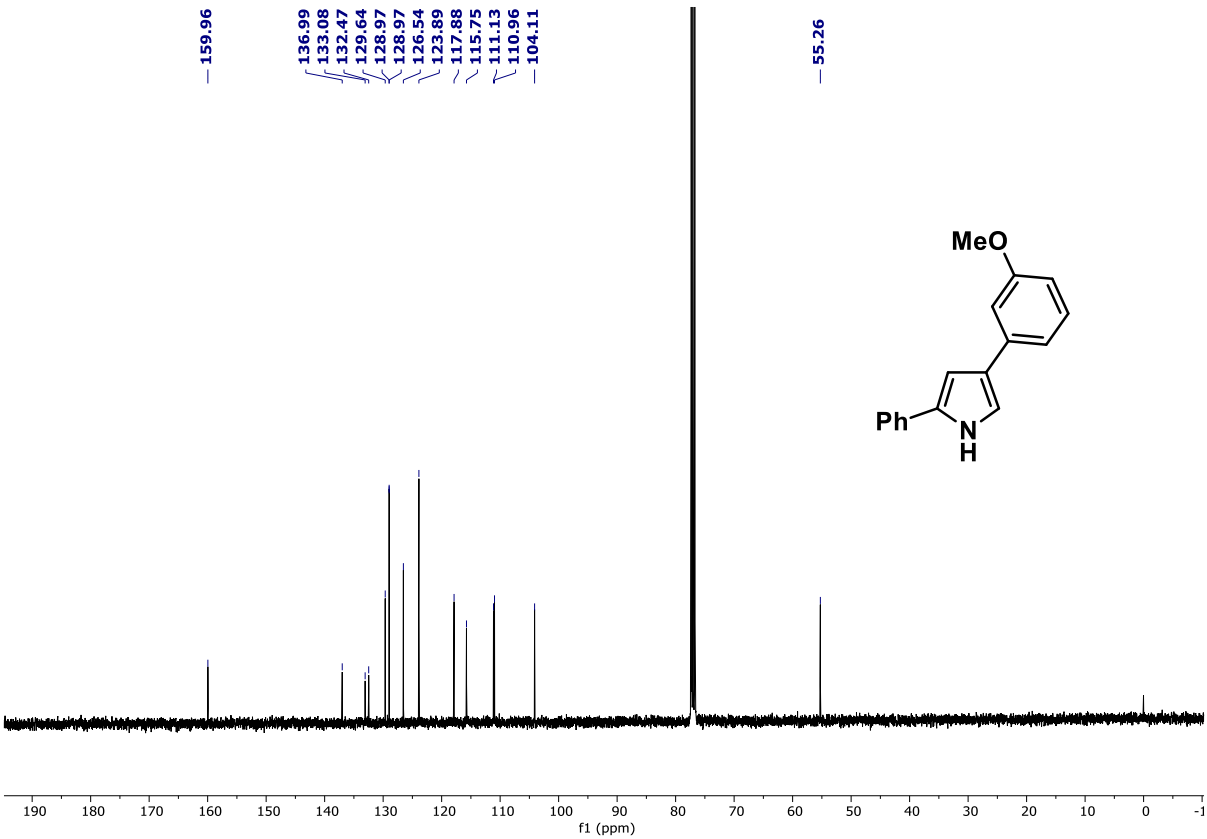
^{1}H NMR of 4-(4-methoxyphenyl)-2-phenyl-1H-pyrrole (**3e**)



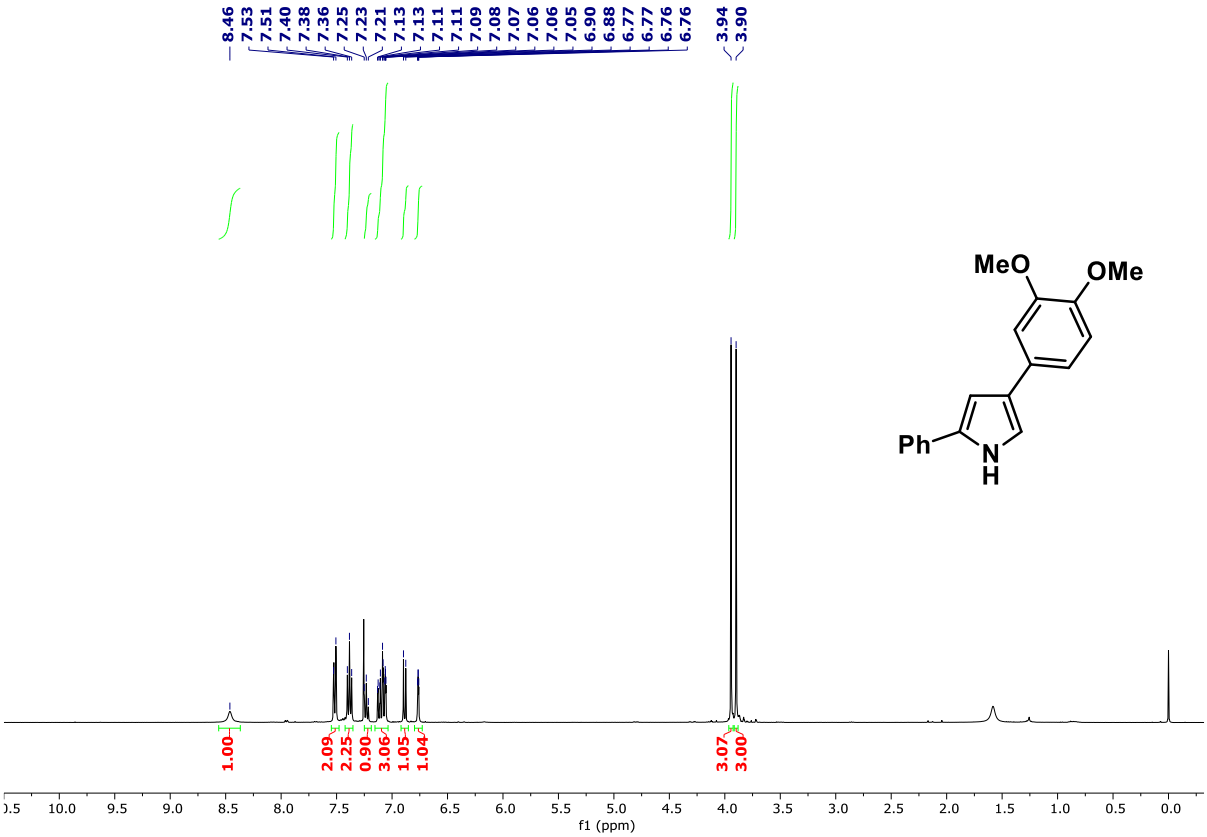
^{13}C NMR of 4-(4-methoxyphenyl)-2-phenyl-1H-pyrrole (**3e**)



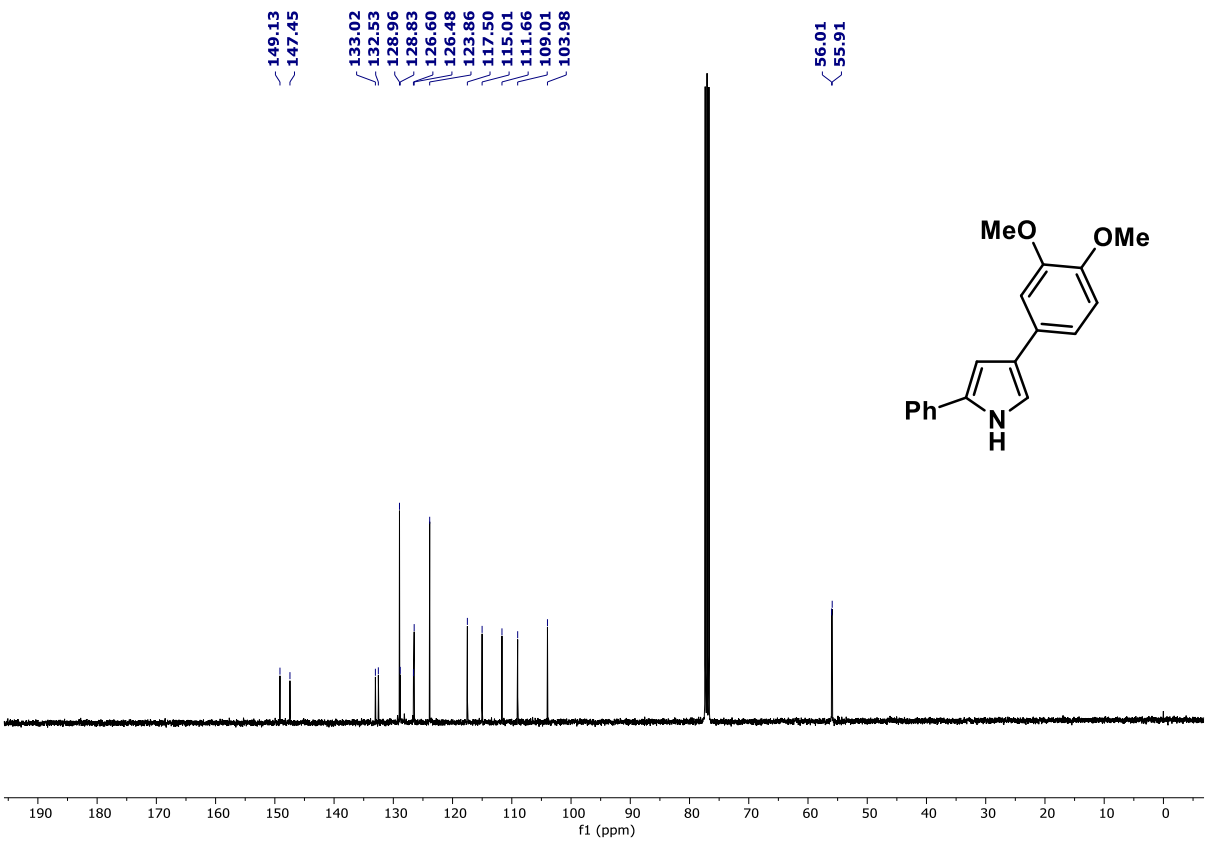
^{1}H NMR of 4-(3-methoxyphenyl)-2-phenyl-1H-pyrrole (**3f**)



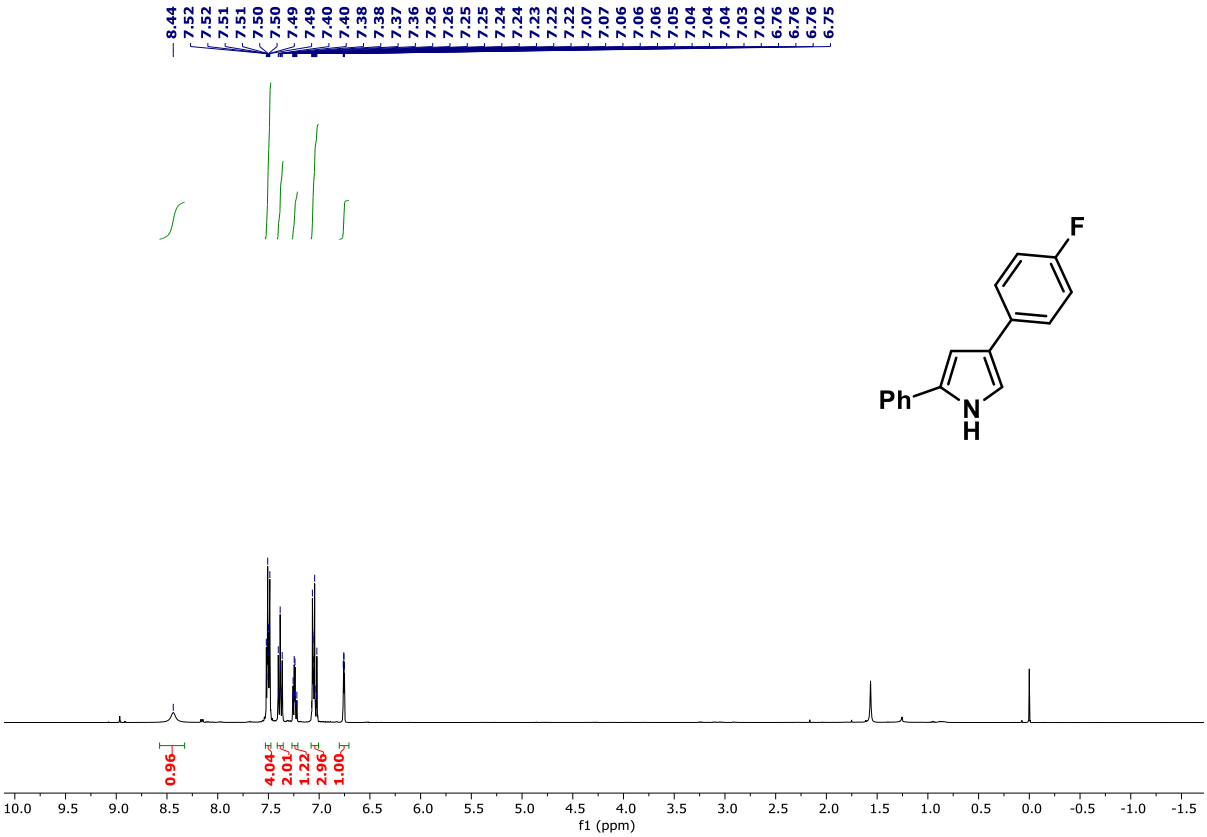
^{13}C NMR of 4-(3-methoxyphenyl)-2-phenyl-1H-pyrrole (**3f**)



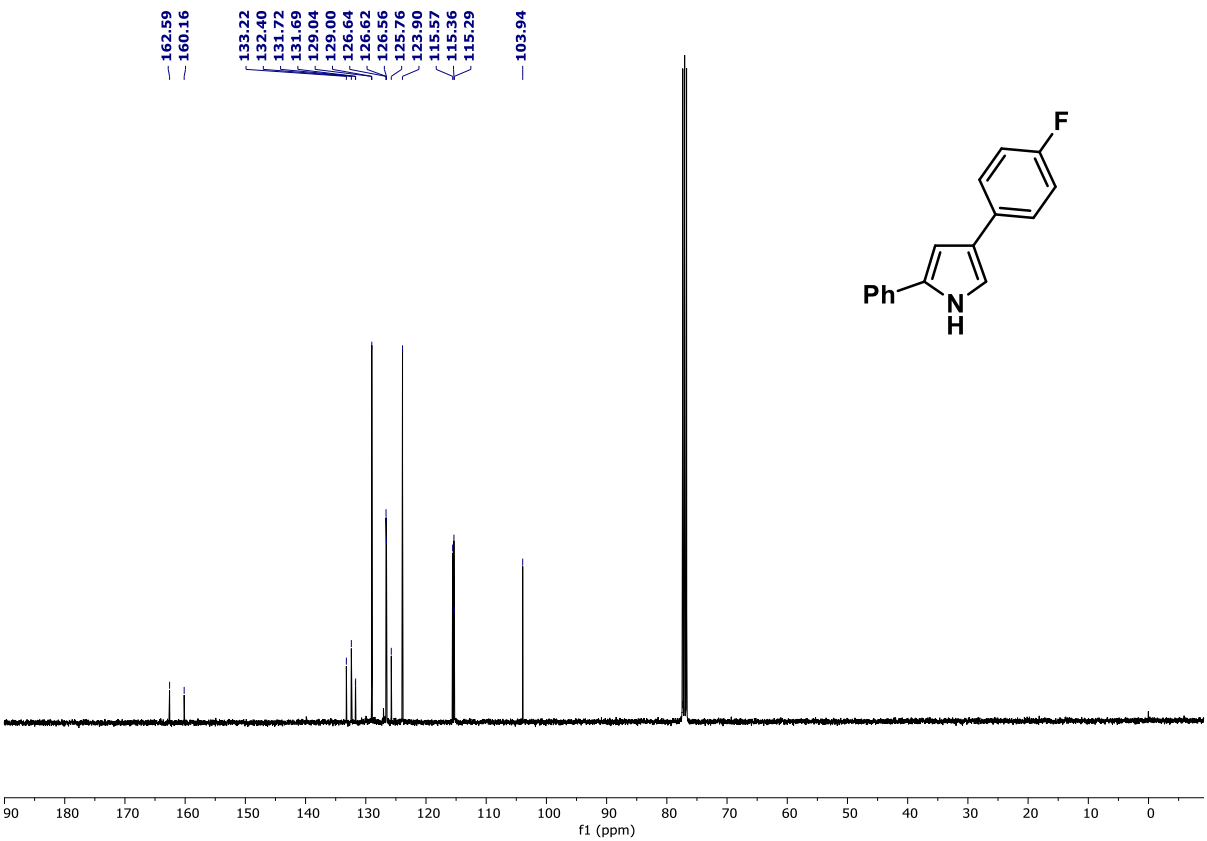
^{1}H NMR of 4-(3,4-dimethoxyphenyl)-2-phenyl-1H-pyrrole (**3g**)



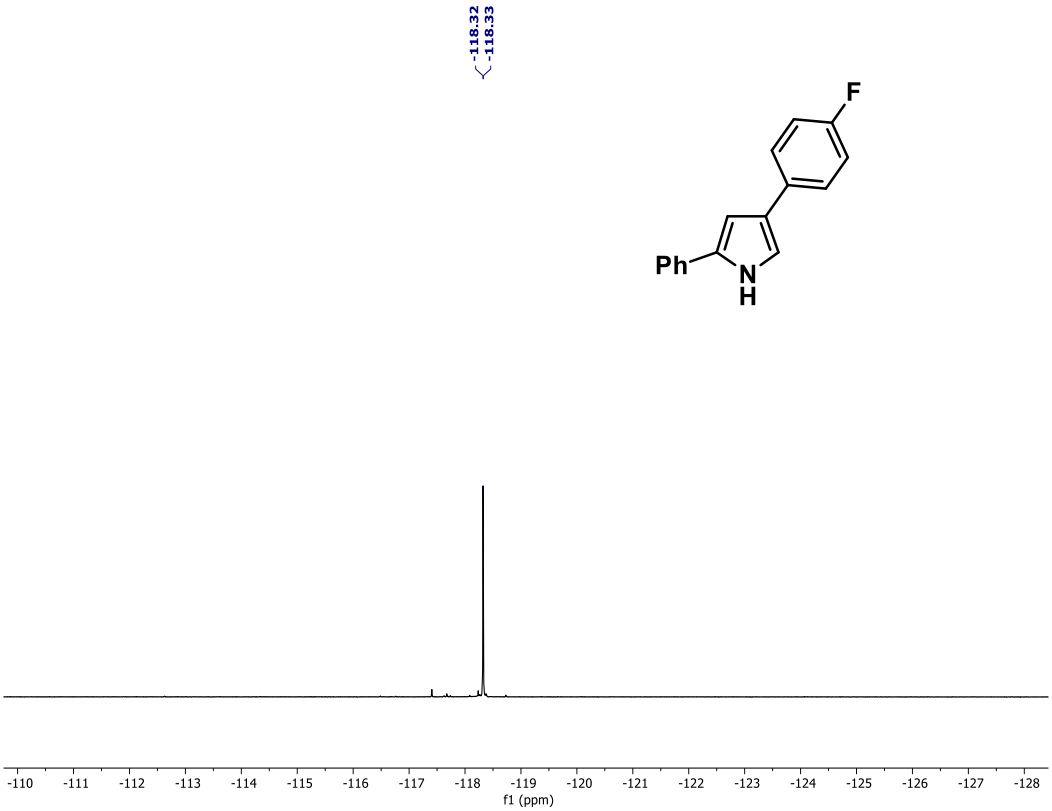
^{13}C NMR of 4-(3,4-dimethoxyphenyl)-2-phenyl-1H-pyrrole (**3g**)



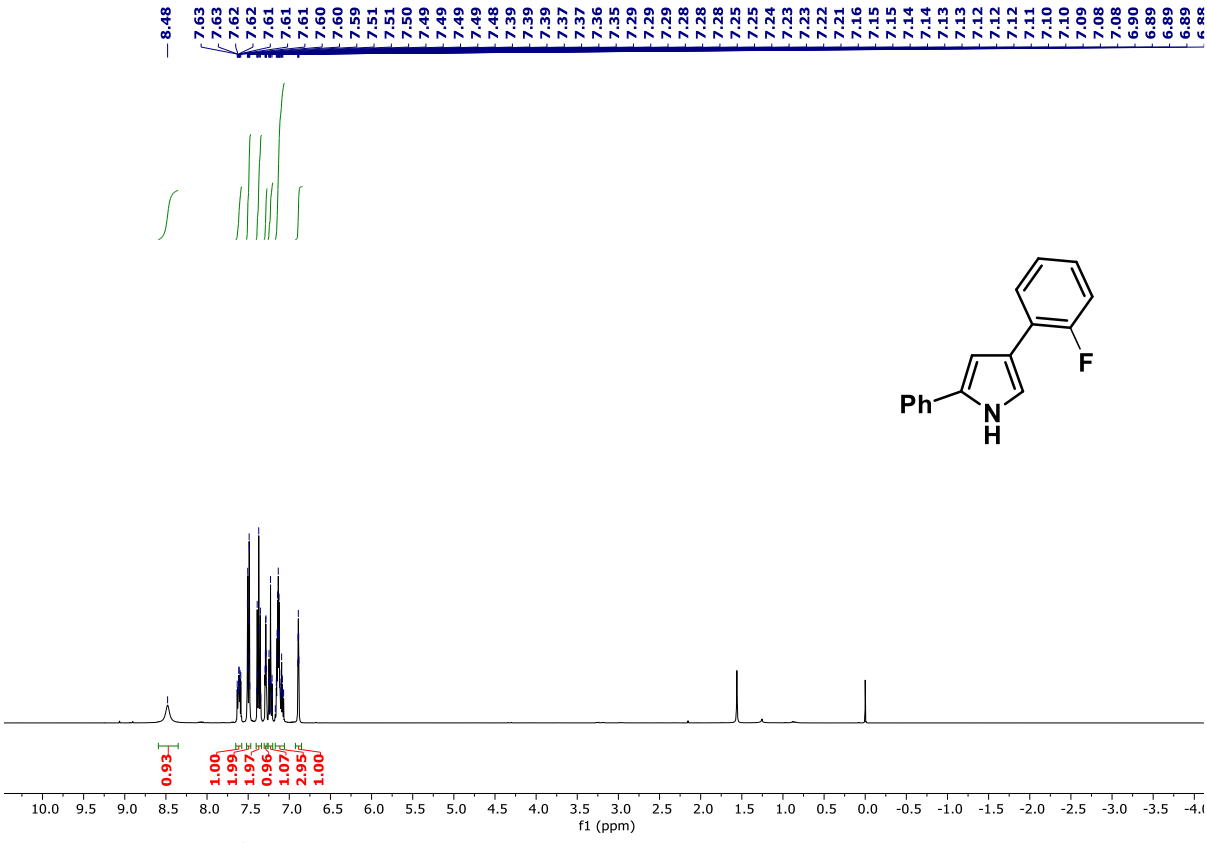
^{1}H NMR of 4-(4-fluorophenyl)-2-phenyl-1H-pyrrole (**3h**)



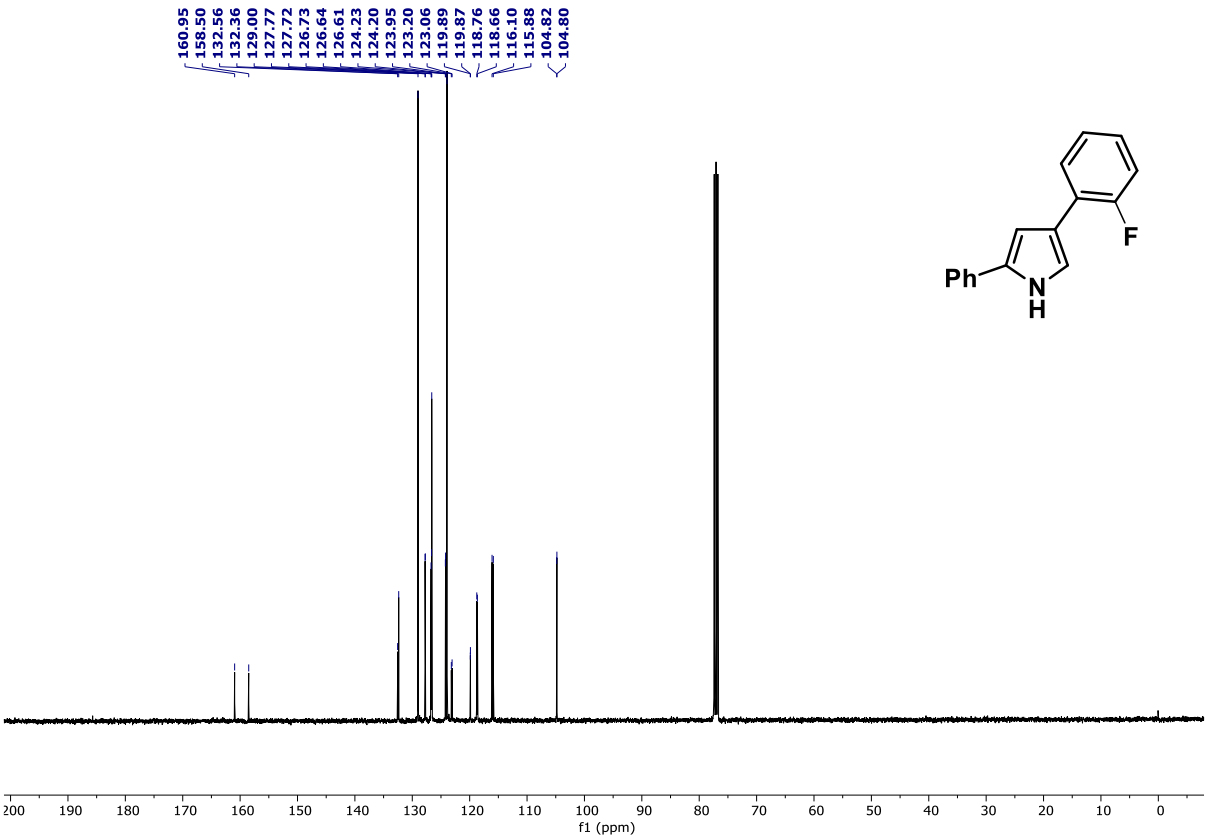
^{13}C NMR of 4-(4-fluorophenyl)-2-phenyl-1H-pyrrole (**3h**)



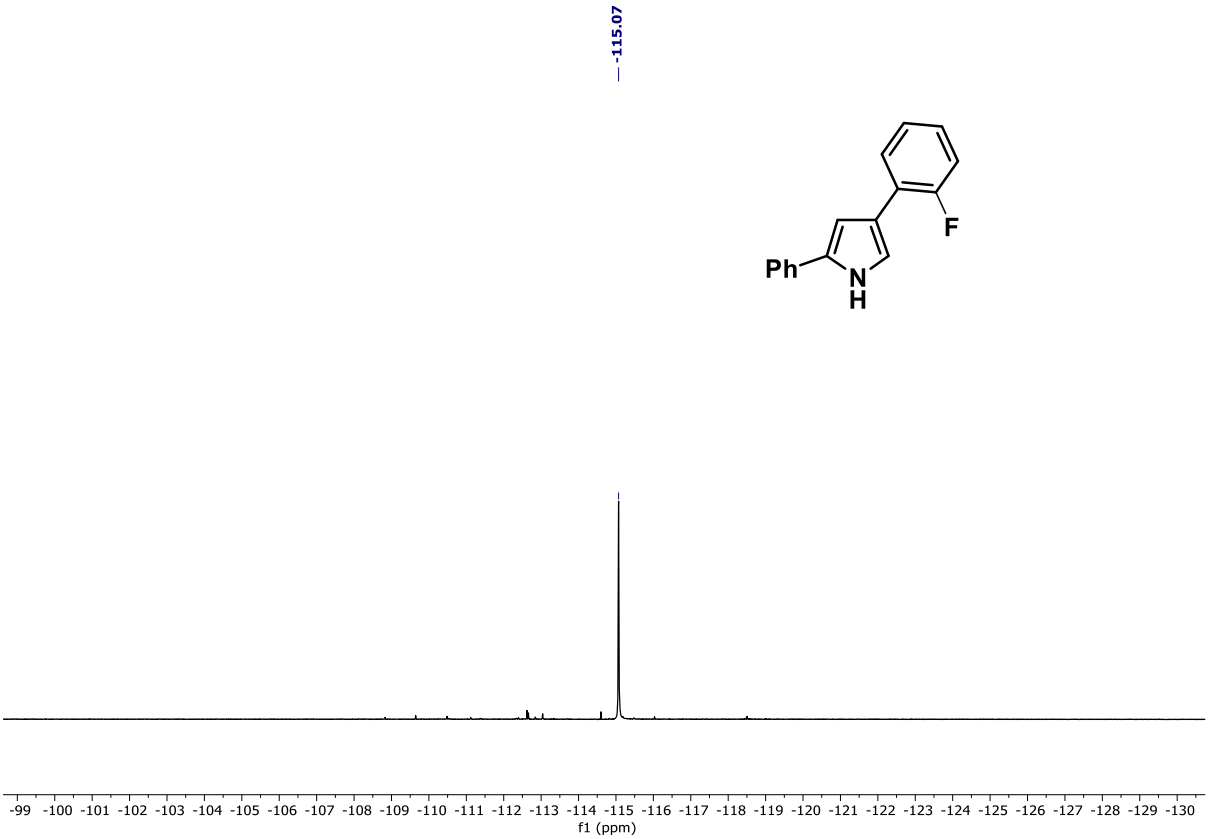
^{19}F NMR of 4-(4-fluorophenyl)-2-phenyl-1H-pyrrole (**3h**)



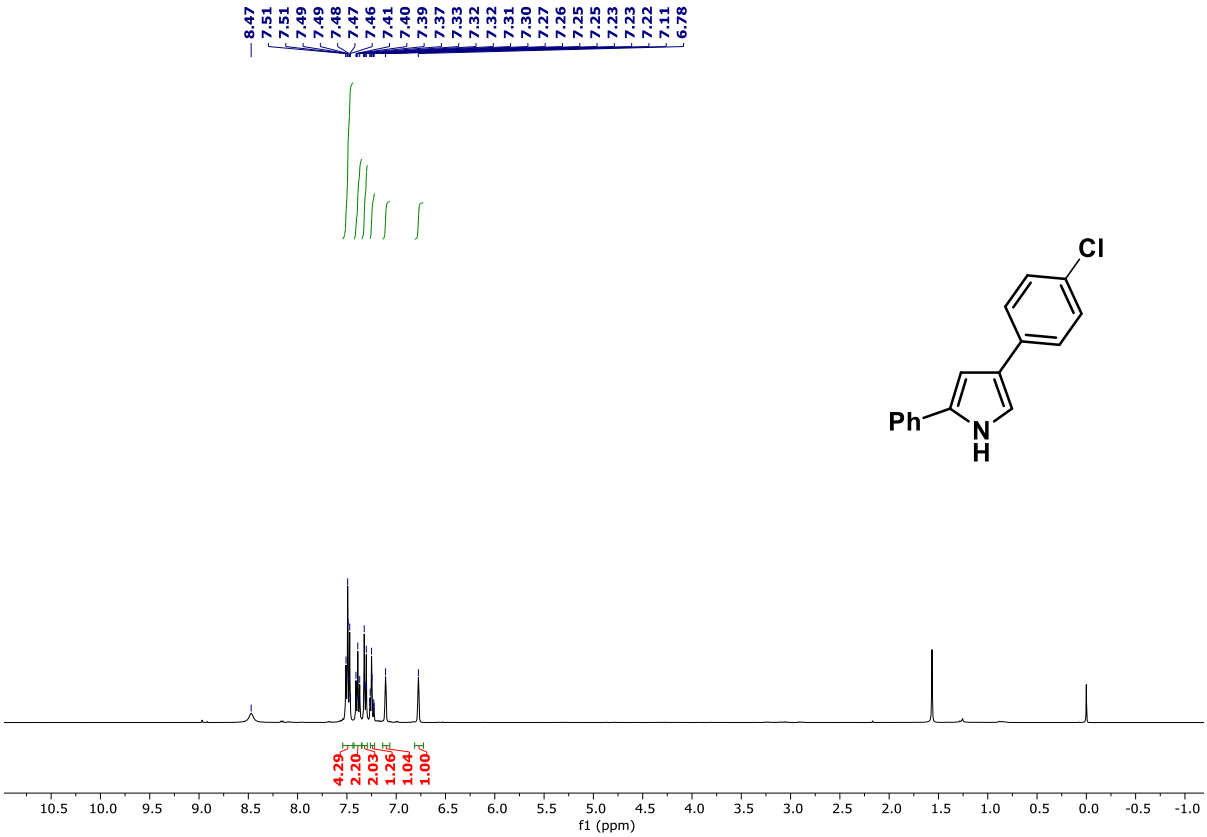
^{1}H NMR of 4-(2-fluorophenyl)-2-phenyl-1H-pyrrole (**3i**)



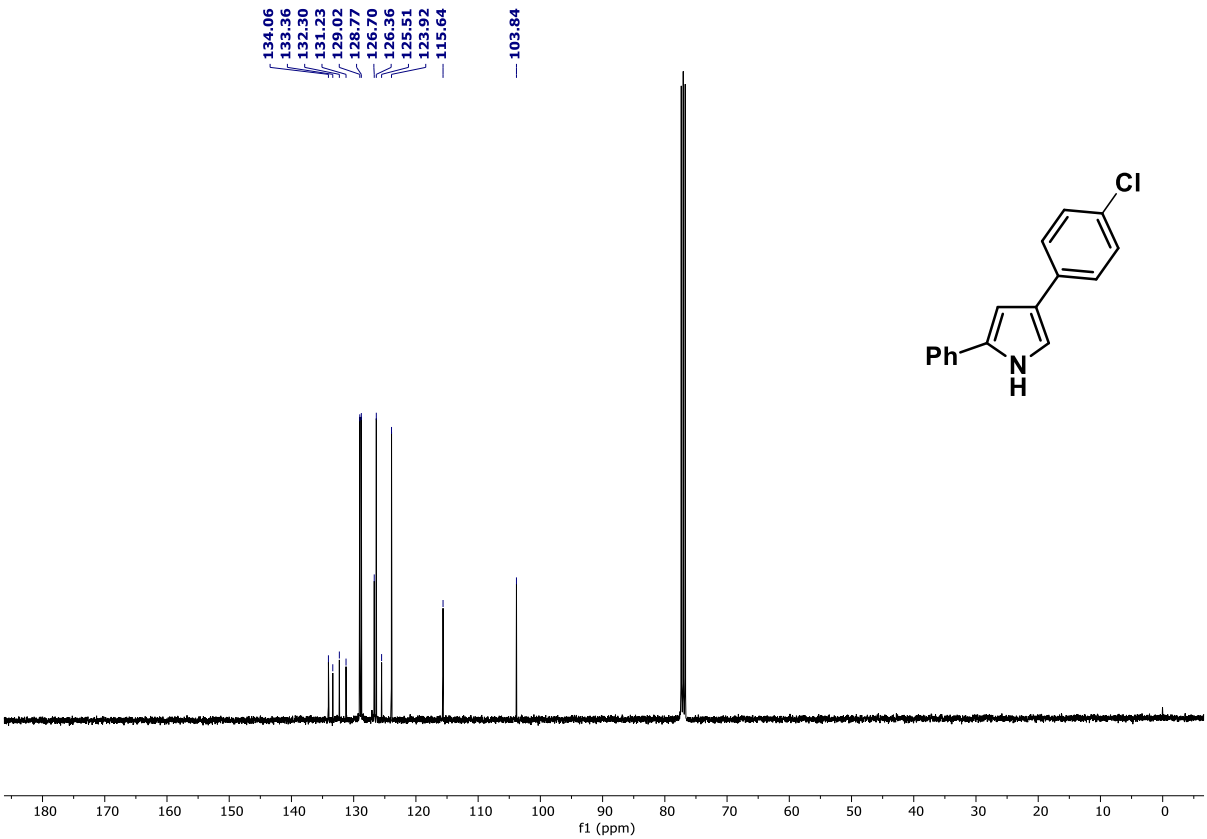
^{13}C NMR of 4-(2-fluorophenyl)-2-phenyl-1H-pyrrole (**3i**)



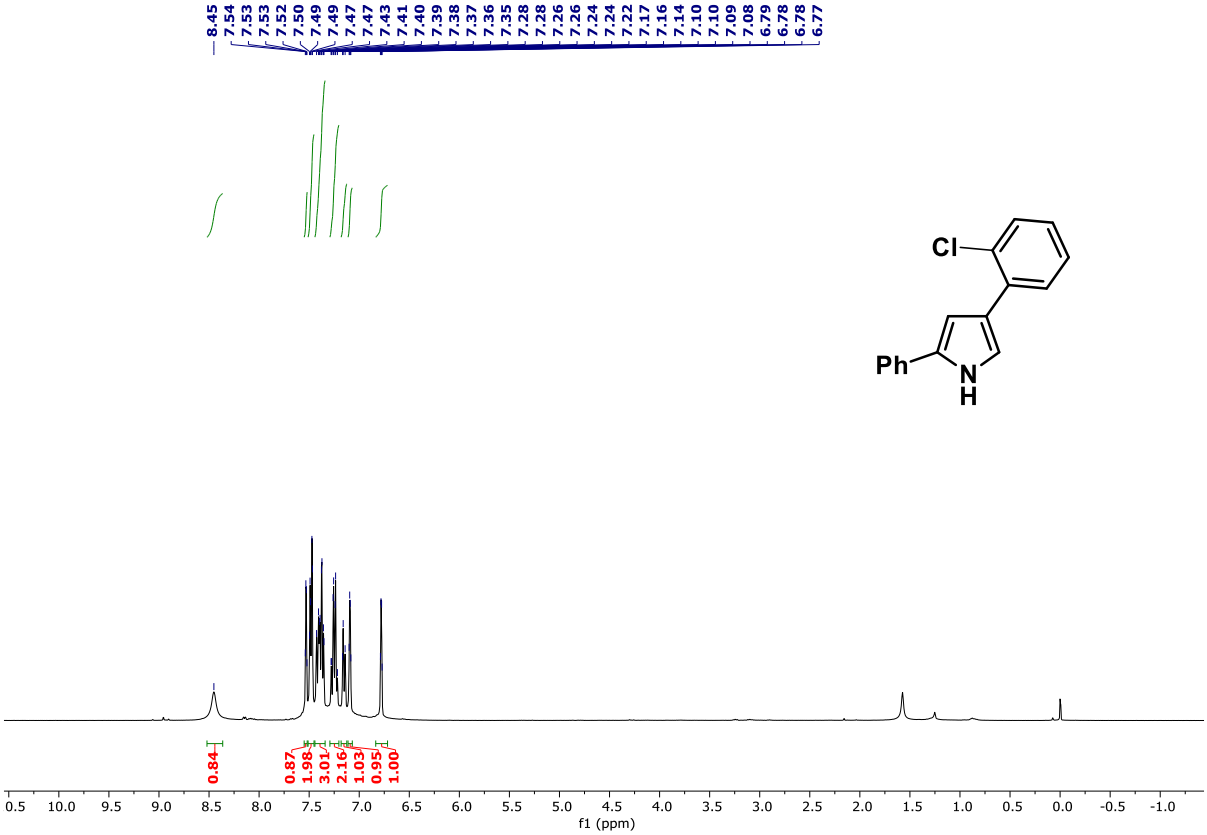
^{19}F NMR of 4-(2-fluorophenyl)-2-phenyl-1H-pyrrole (**3i**)



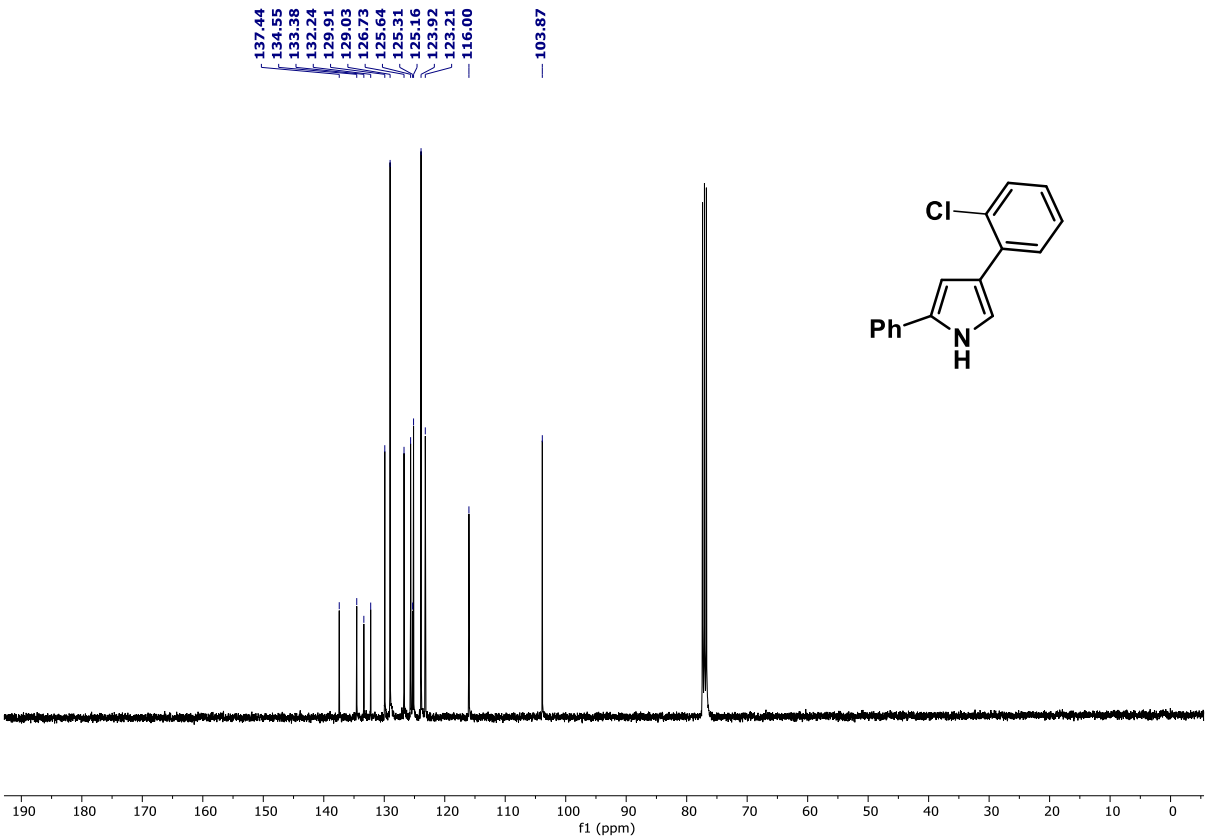
^{1}H NMR of 4-(4-chlorophenyl)-2-phenyl-1H-pyrrole (**3j**)



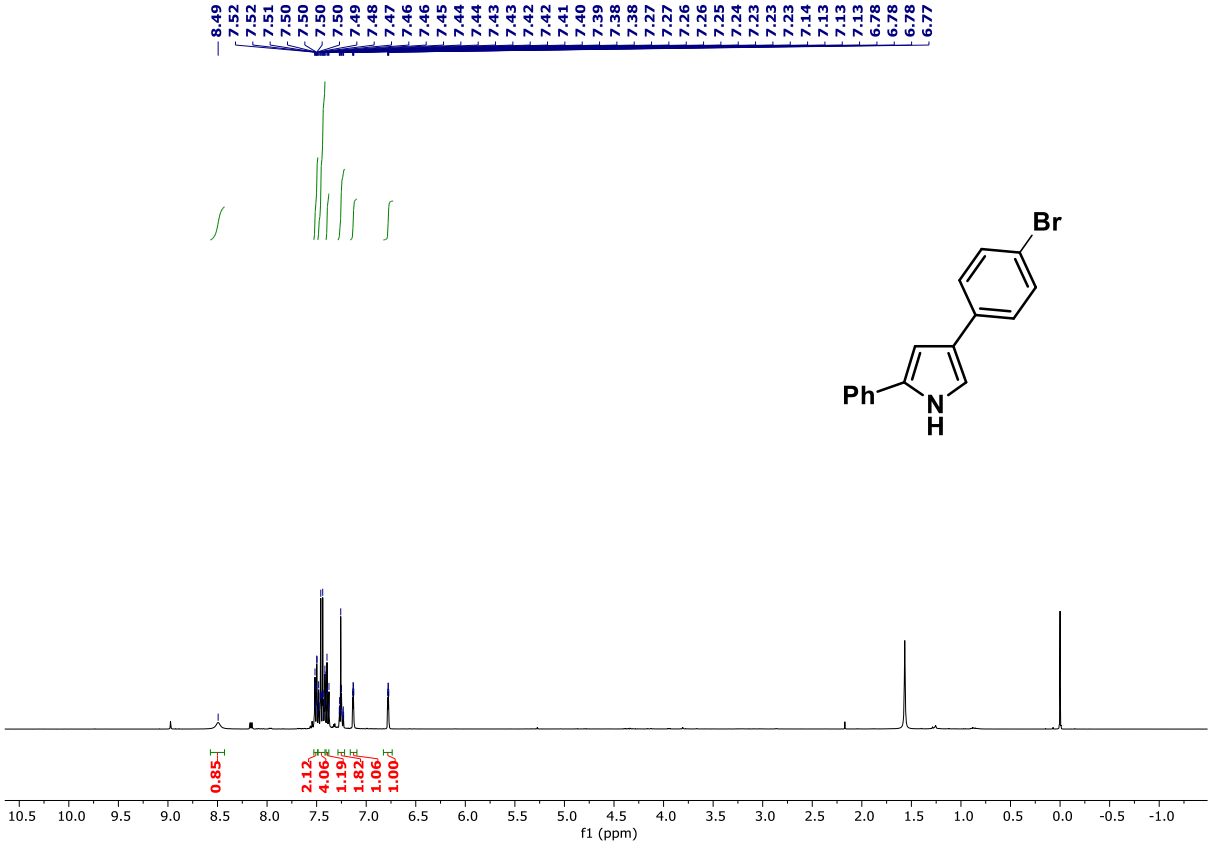
^{13}C NMR of 4-(4-chlorophenyl)-2-phenyl-1H-pyrrole (**3j**)



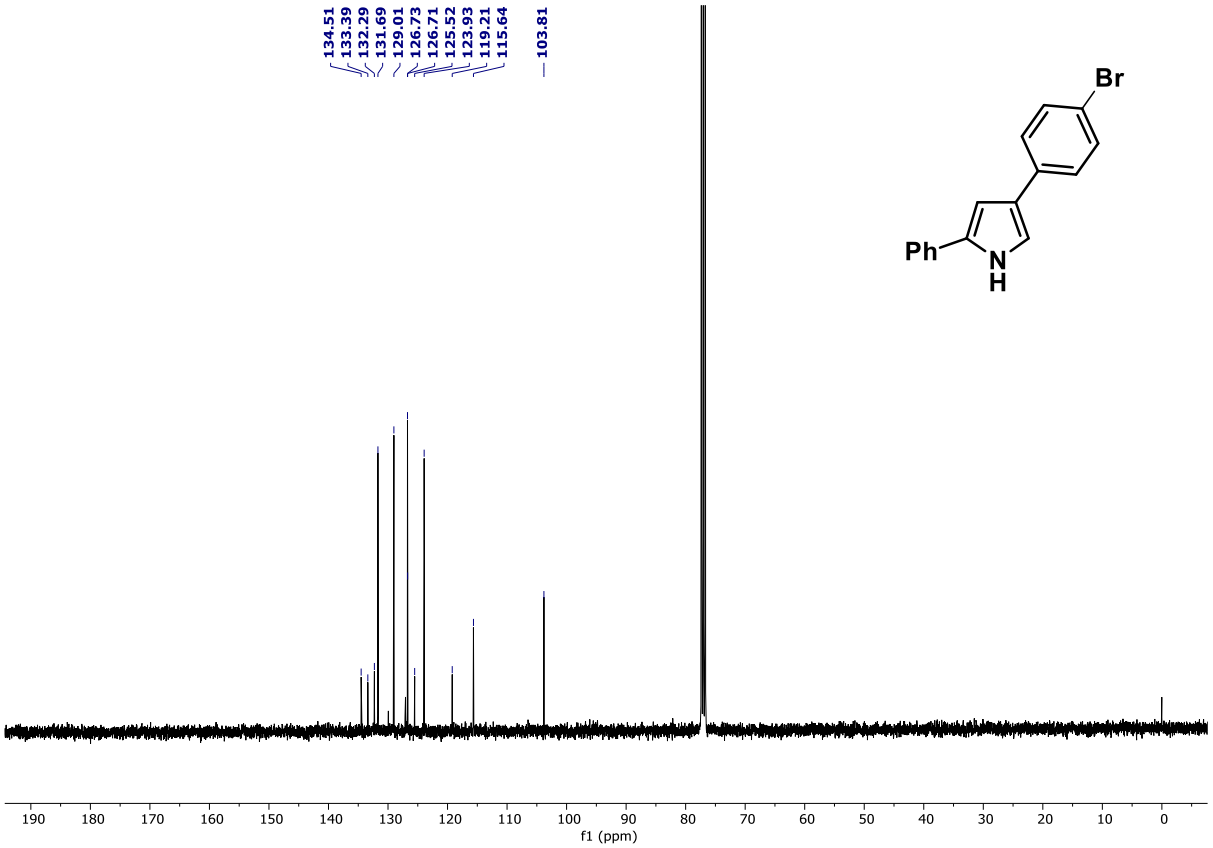
^{1}H NMR of 4-(2-chlorophenyl)-2-phenyl-1H-pyrrole (**3k**)



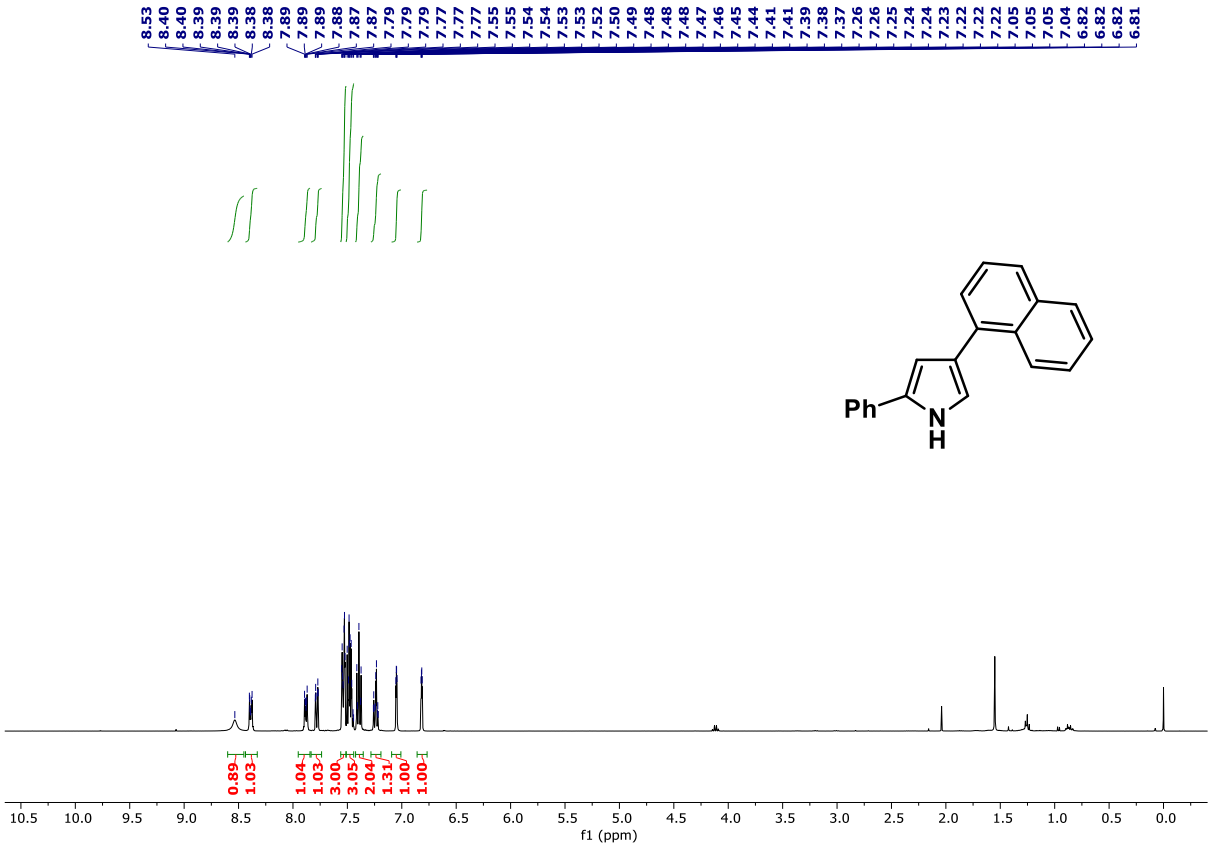
^{13}C NMR of 4-(2-chlorophenyl)-2-phenyl-1H-pyrrole (**3k**)



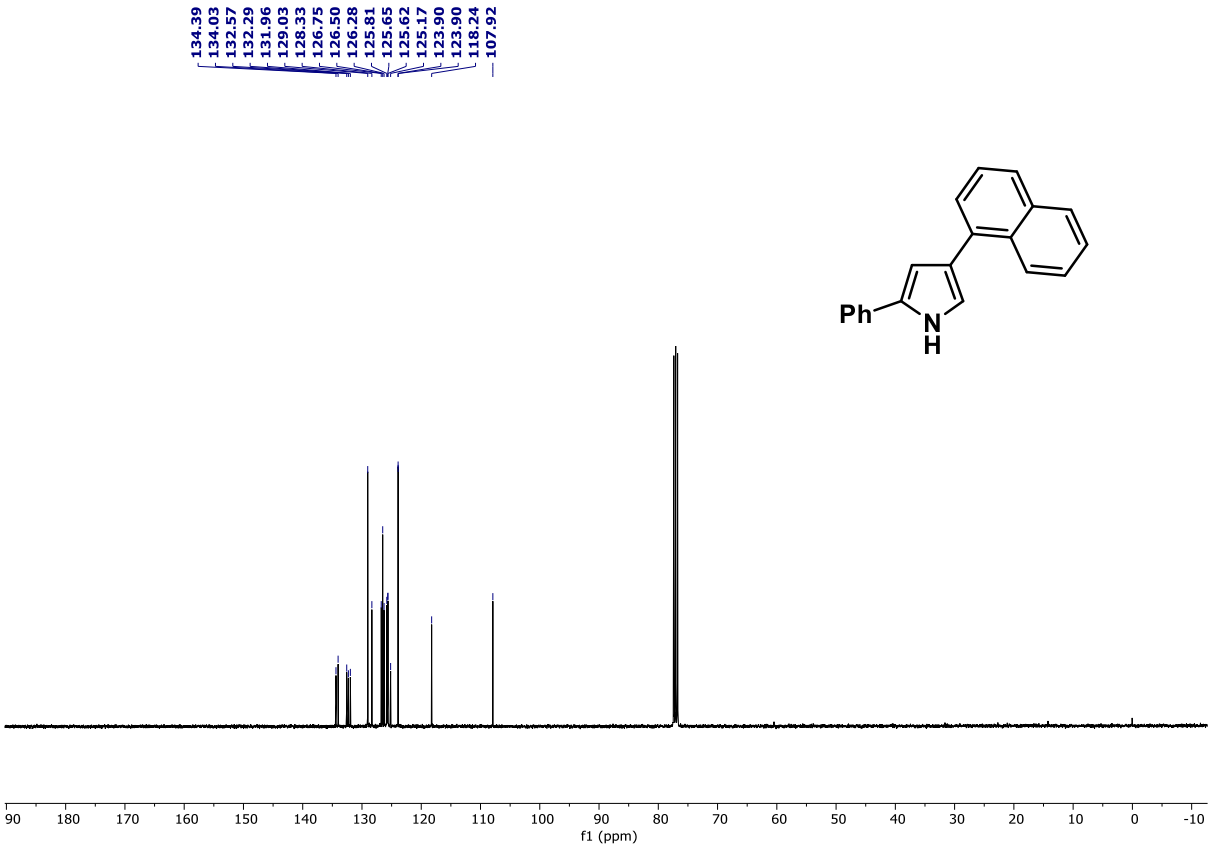
^{1}H NMR of 4-(4-bromophenyl)-2-phenyl-1H-pyrrole (**3l**)



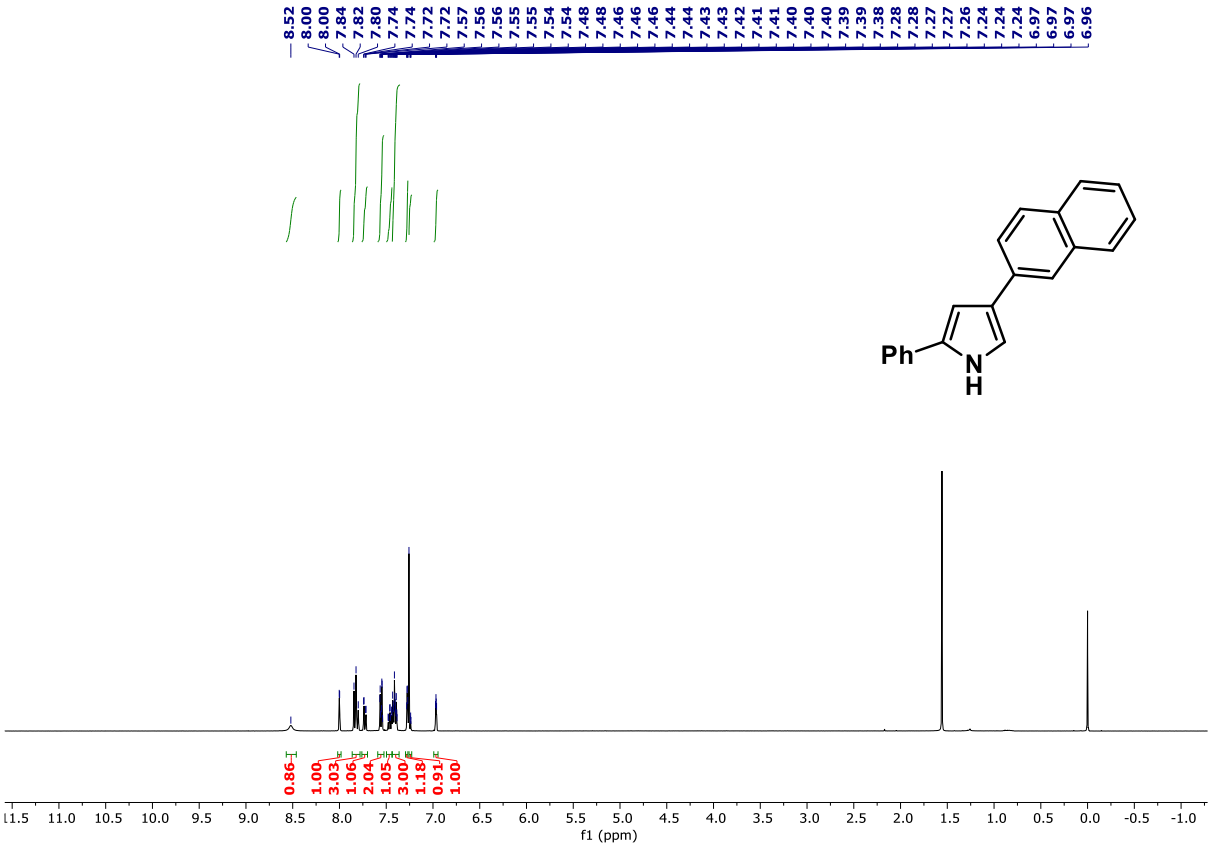
^{13}C NMR of 4-(4-bromophenyl)-2-phenyl-1H-pyrrole (**3l**)



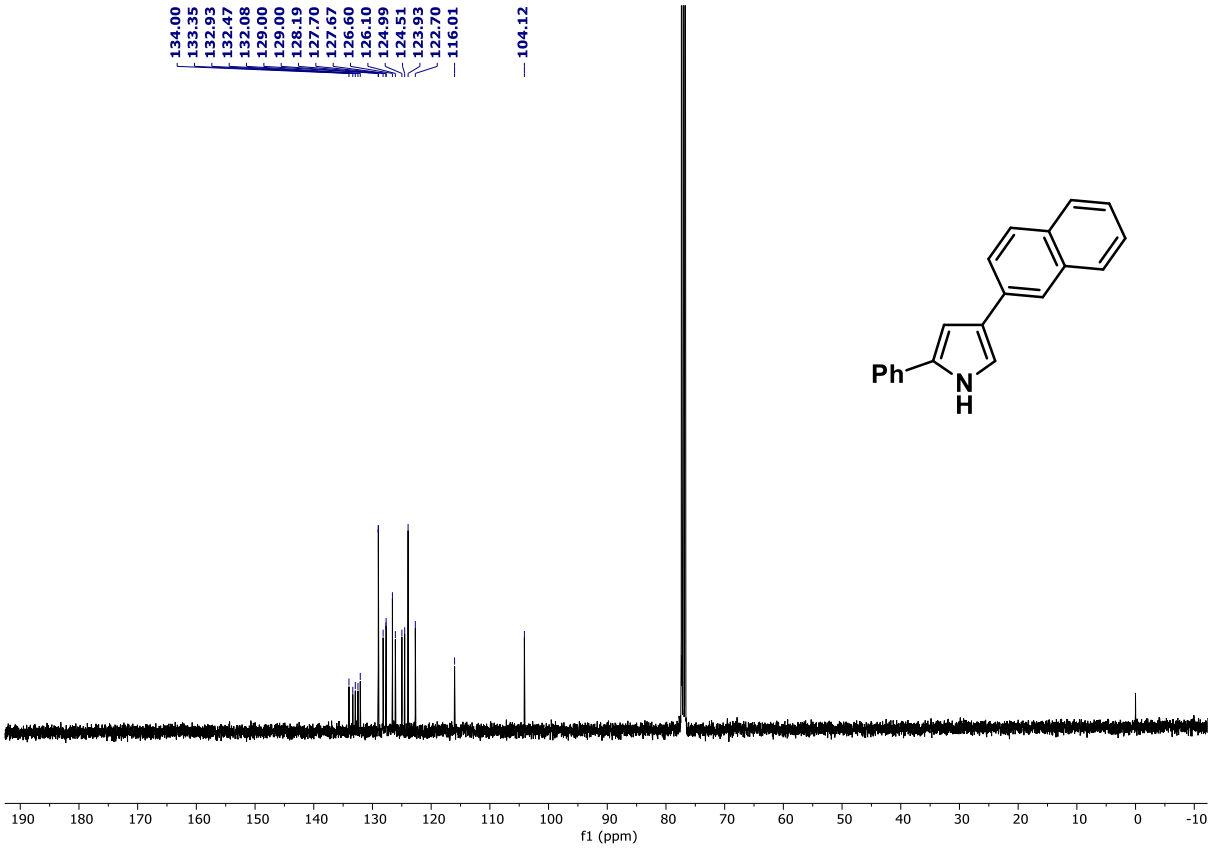
^{1}H NMR of 4-(naphthalen-1-yl)-2-phenyl-1H-pyrrole (**3m**)



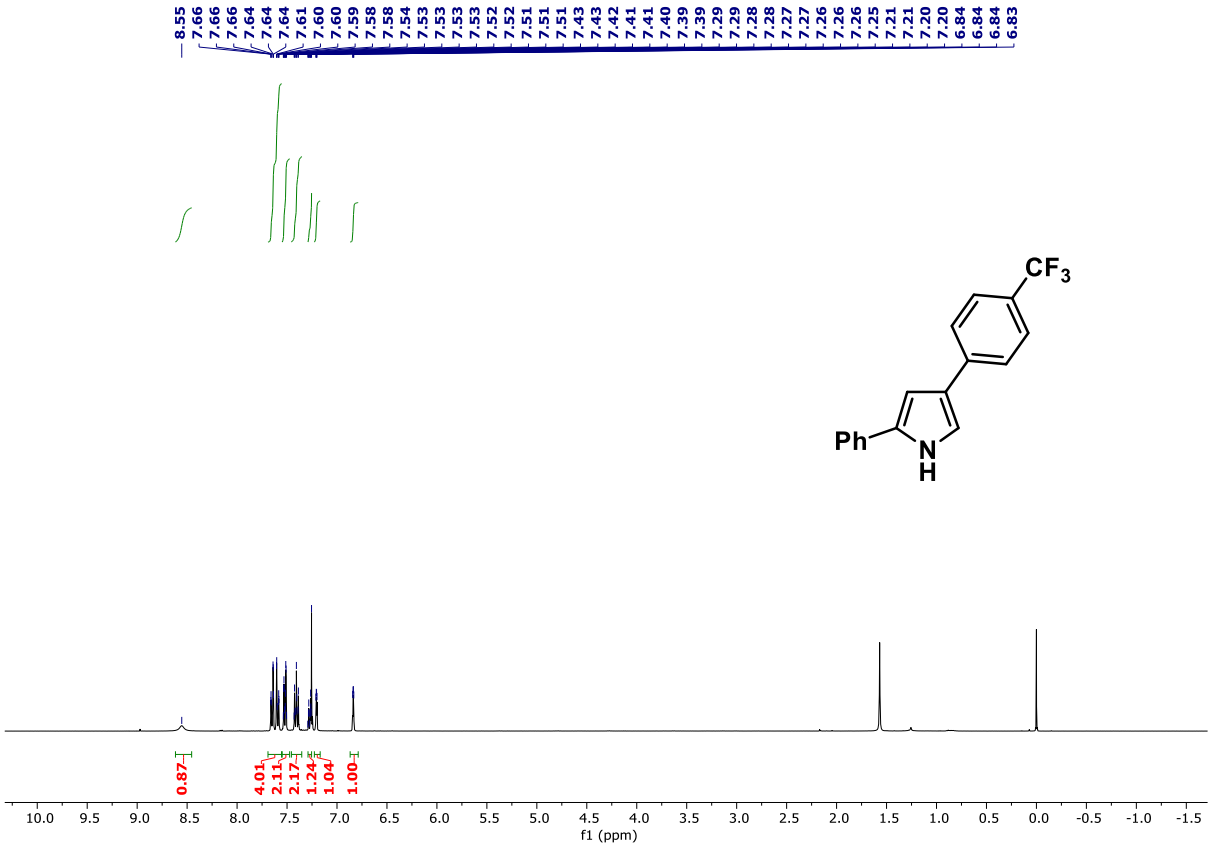
^{13}C NMR of 4-(naphthalen-1-yl)-2-phenyl-1H-pyrrole (**3m**)



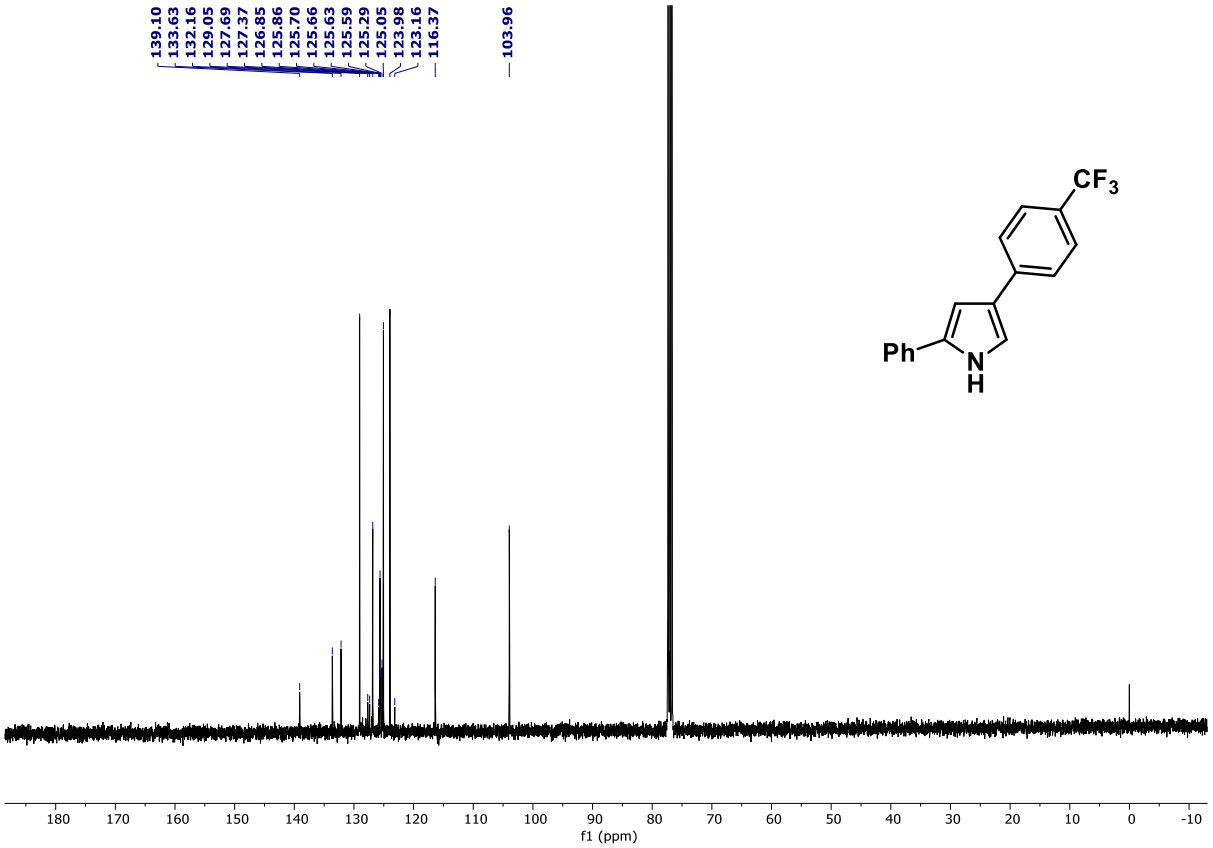
^{1}H NMR of 4-(naphthalen-2-yl)-2-phenyl-1H-pyrrole (**3n**)



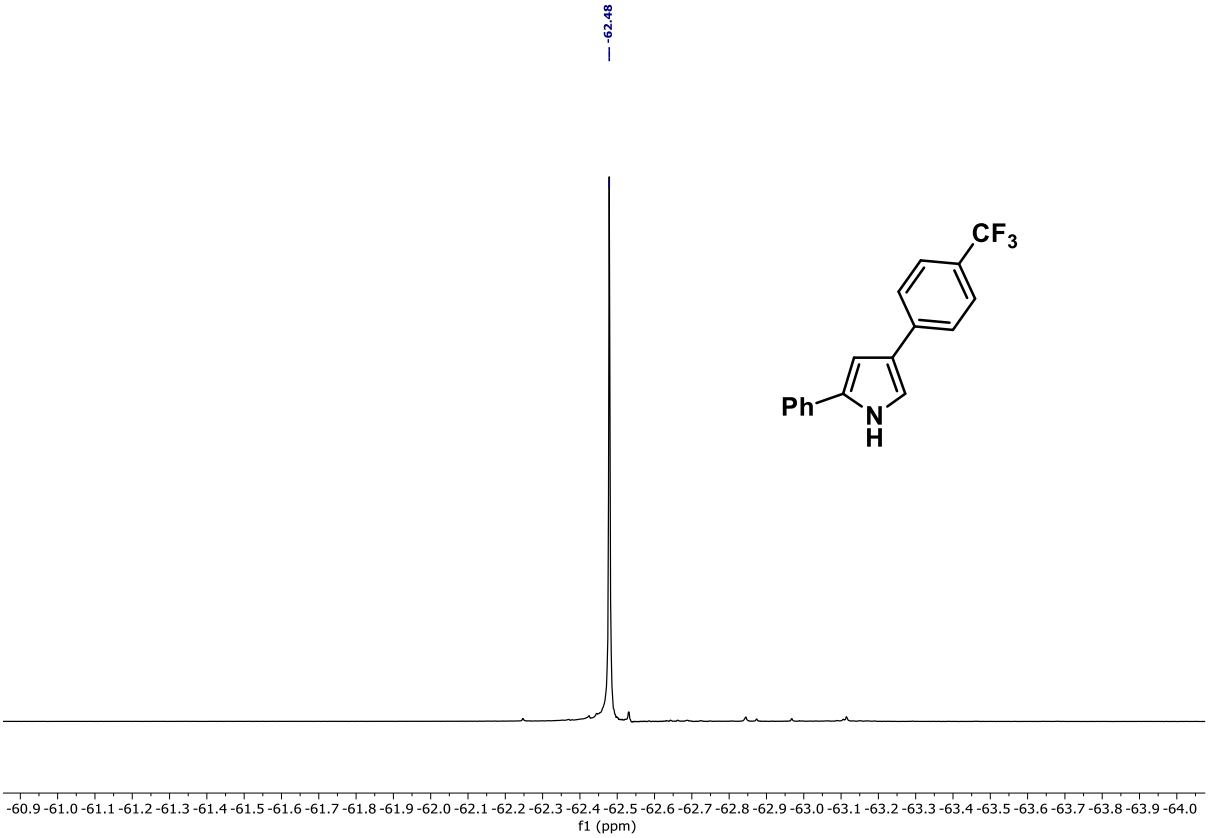
^{13}C NMR of 4-(naphthalen-2-yl)-2-phenyl-1H-pyrrole (**3n**)



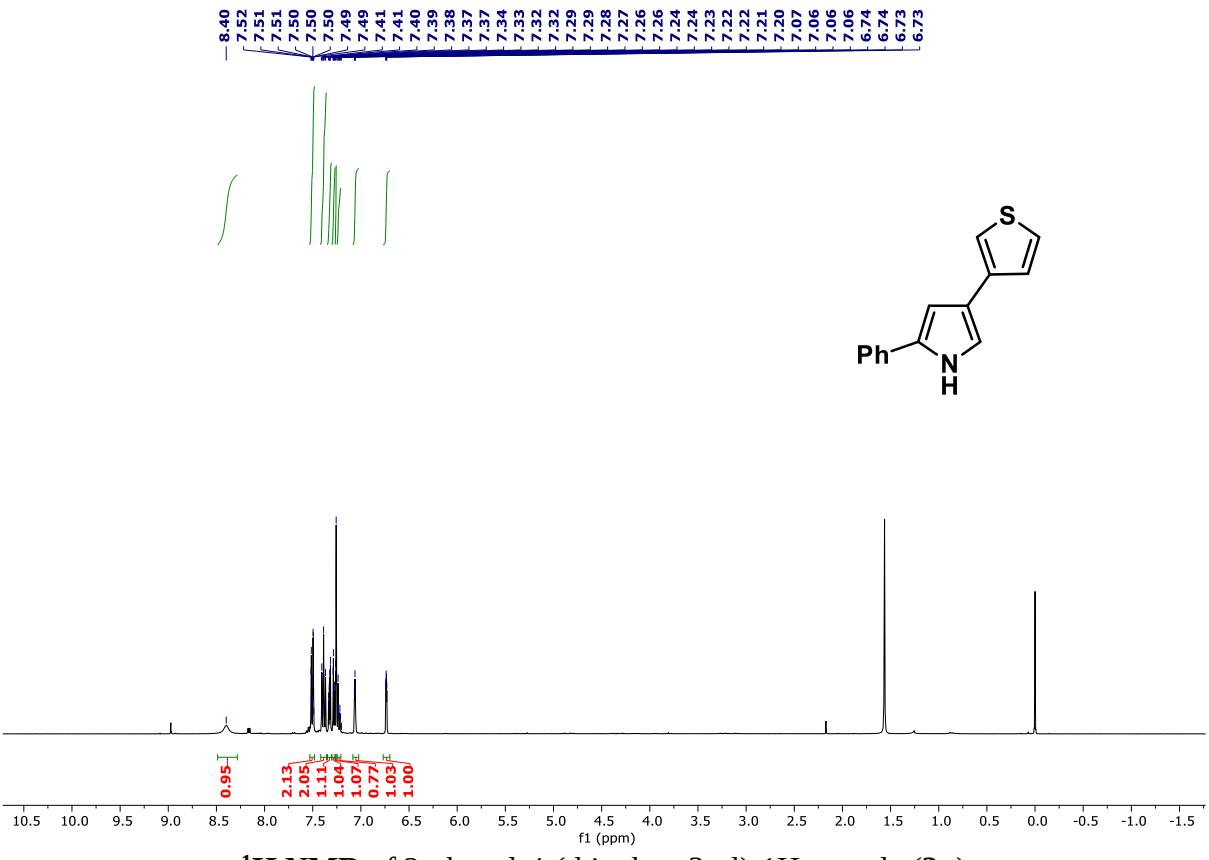
^{1}H NMR of 2-phenyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrrole (**3o**)



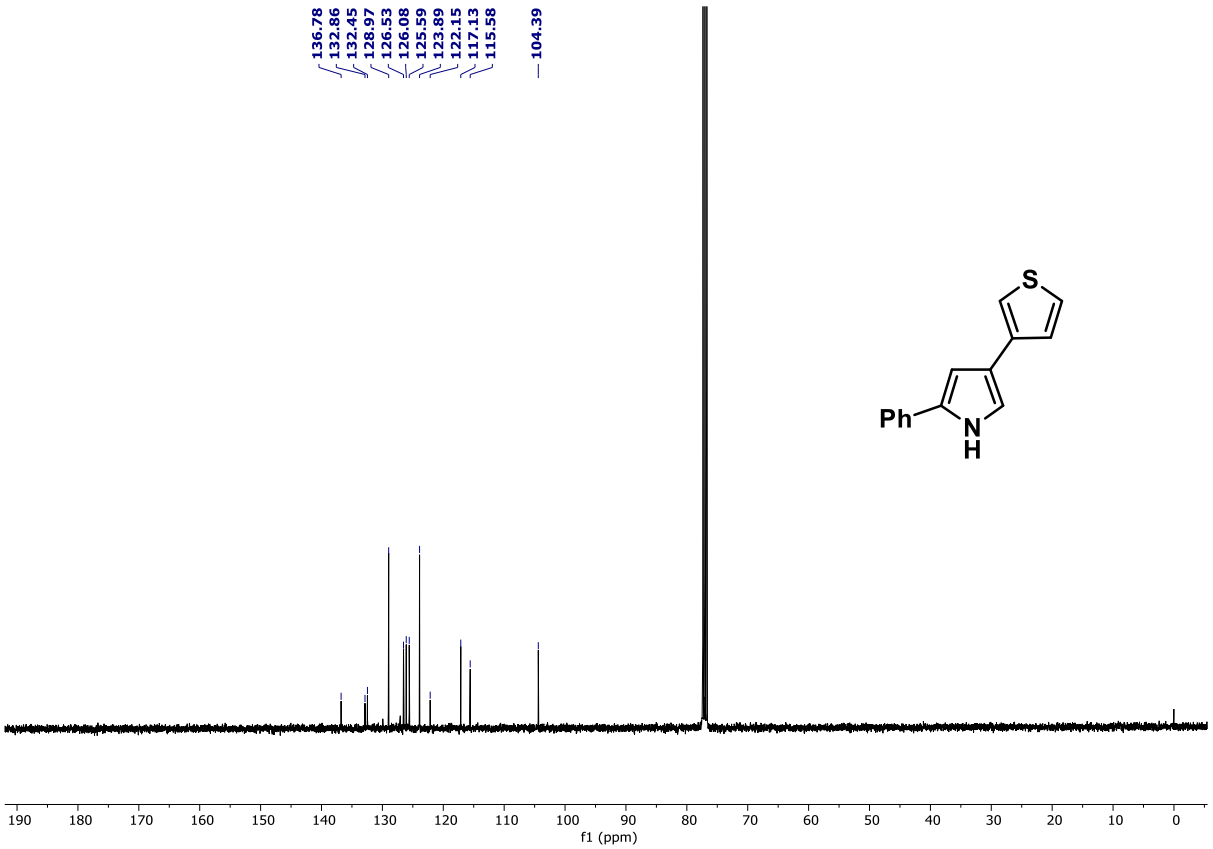
^{13}C NMR of 2-phenyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrrole (**3o**)



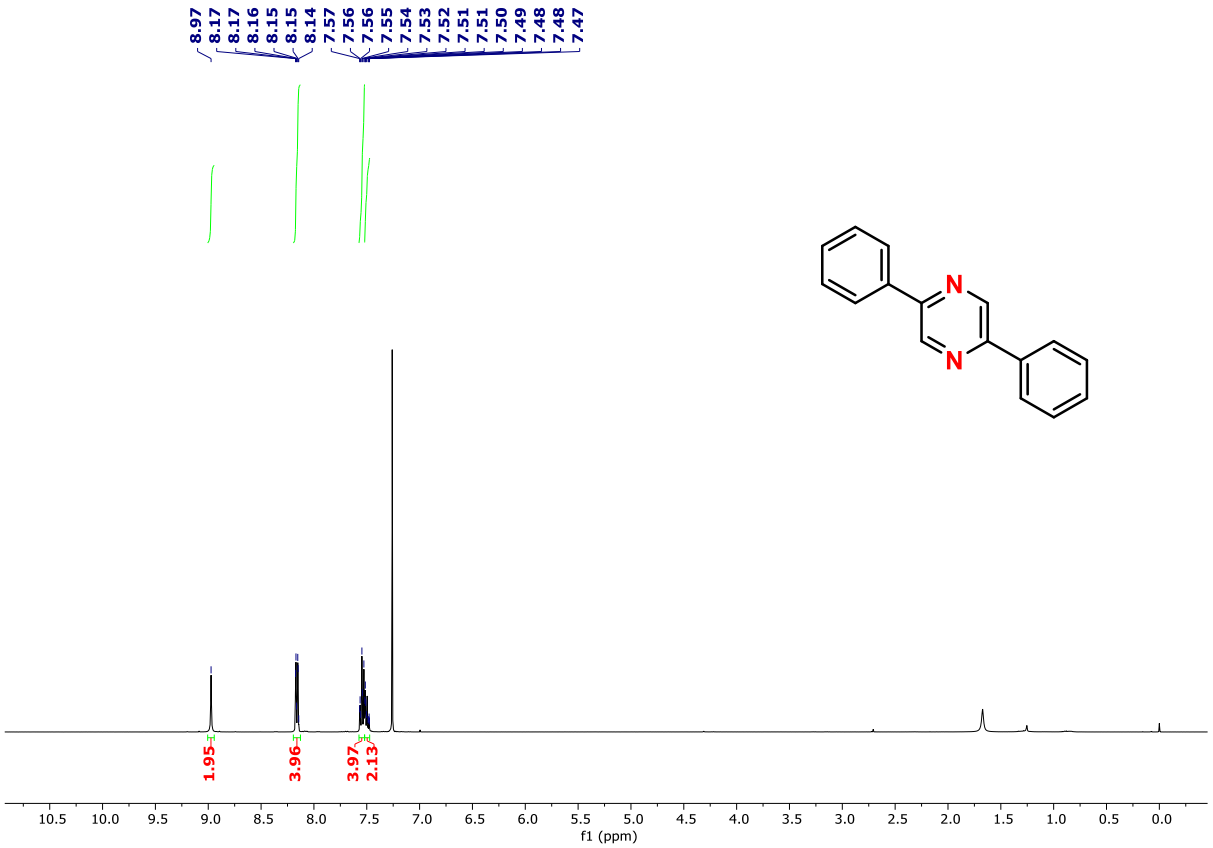
^{19}F NMR of 2-phenyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrrole (**3o**)



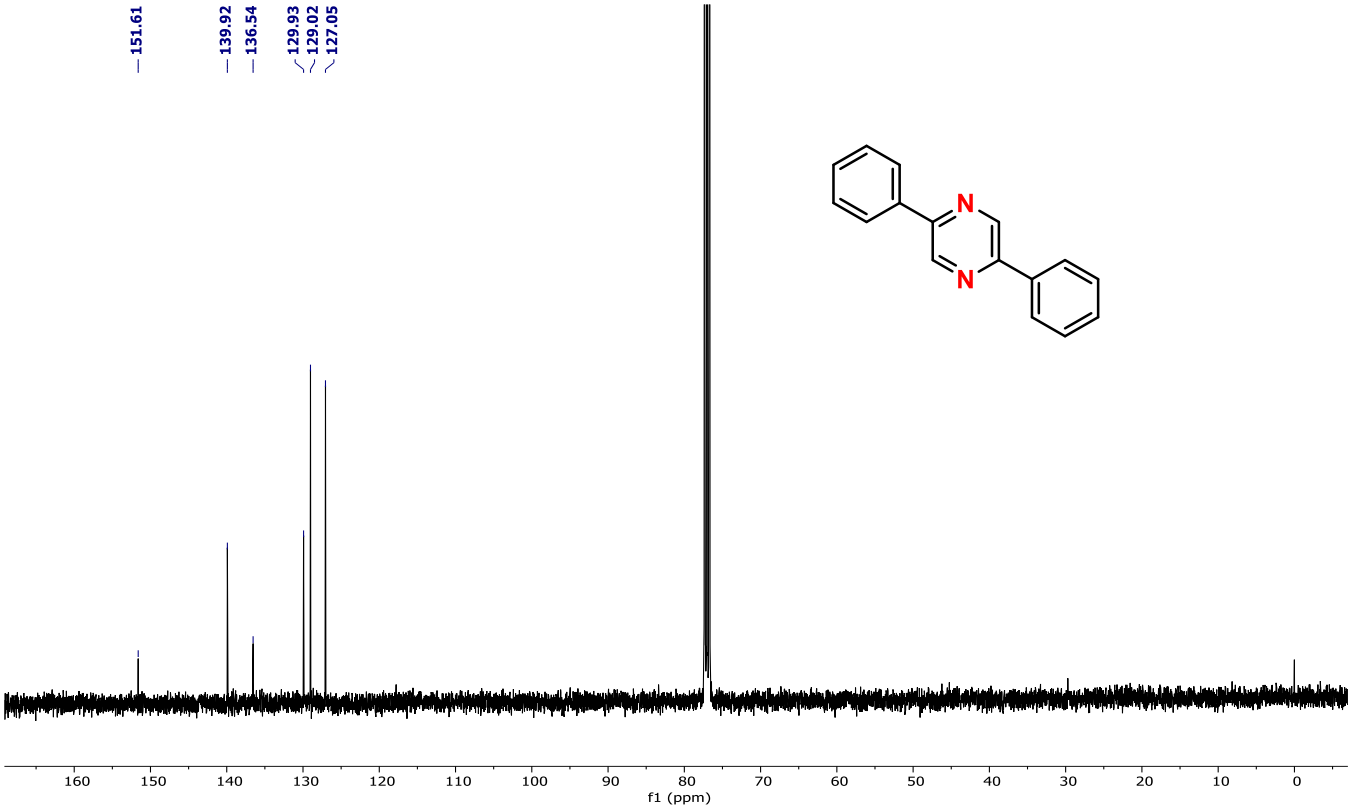
^{1}H NMR of 2-phenyl-4-(thiophen-3-yl)-1H-pyrrole (**3p**)



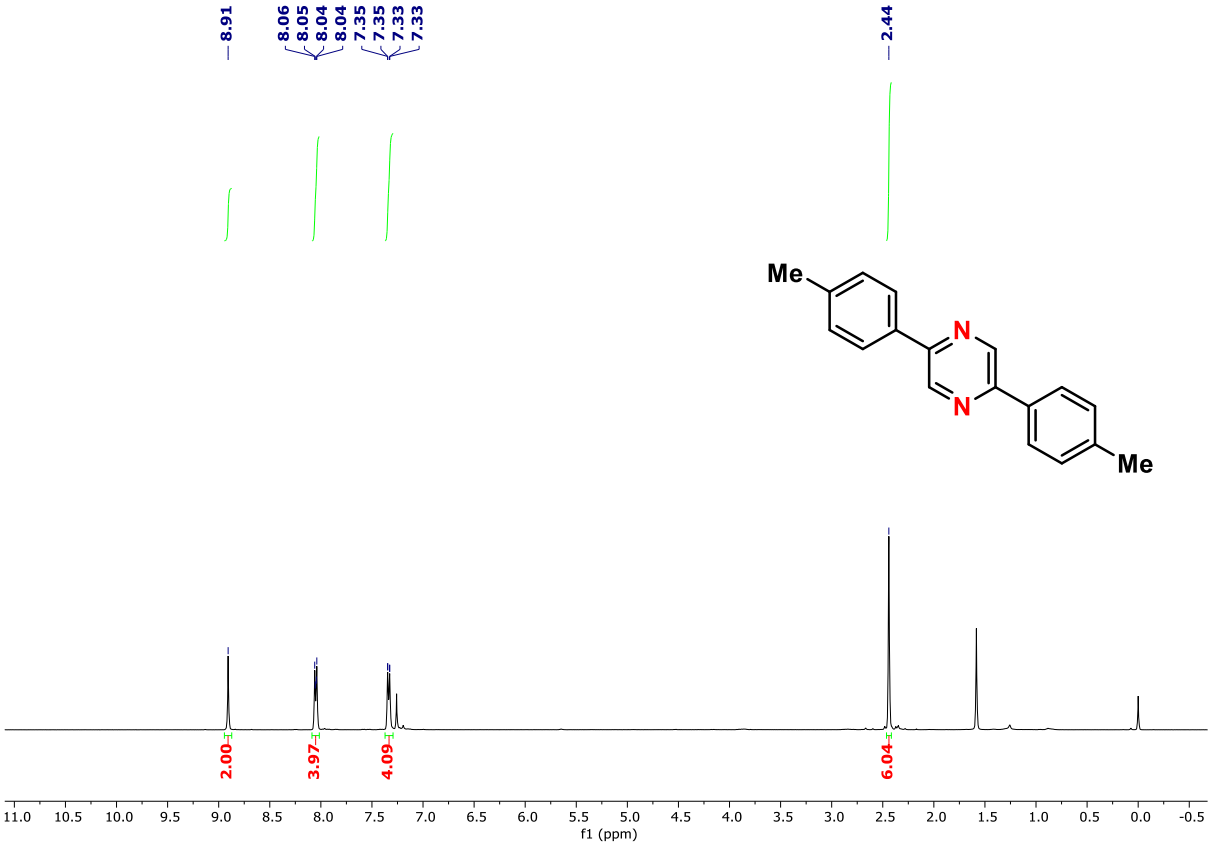
^{13}C NMR of 2-phenyl-4-(thiophen-3-yl)-1H-pyrrole (**3p**)



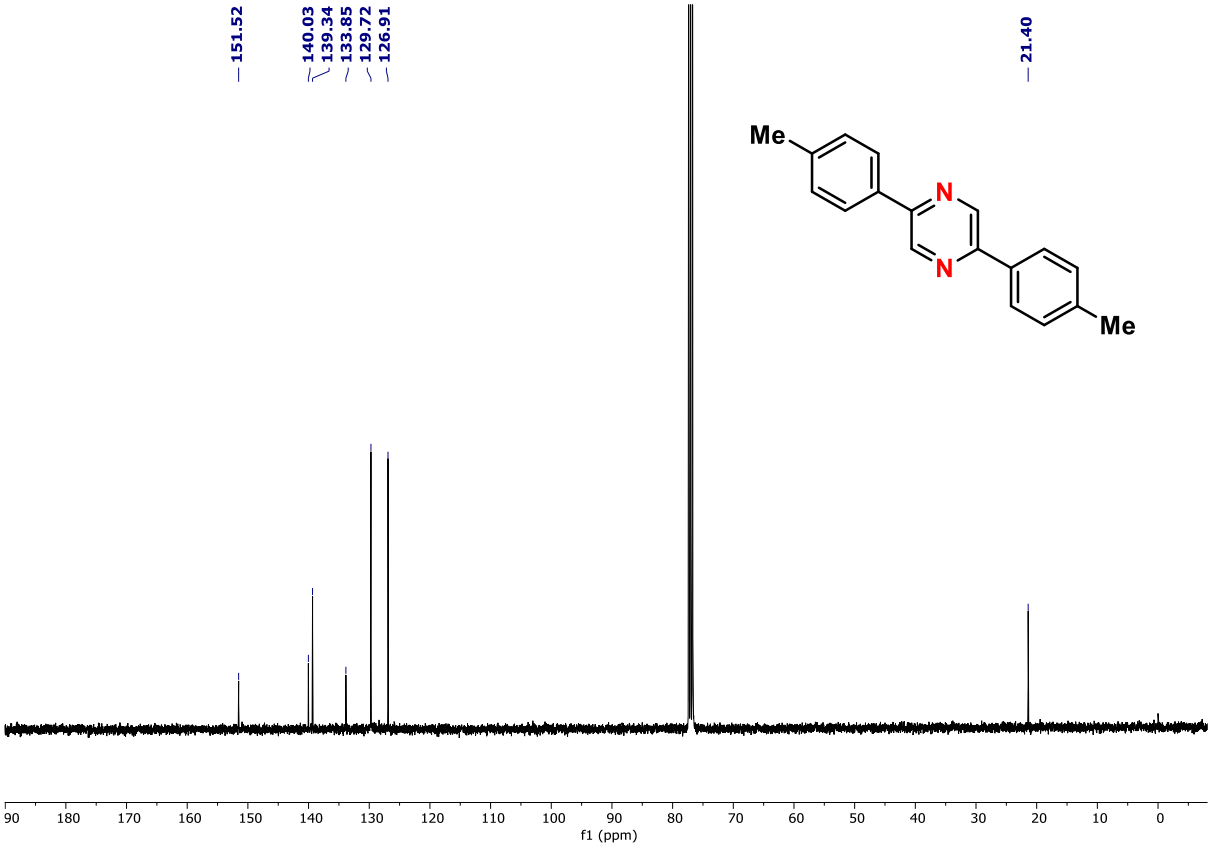
^{1}H NMR of 2,5-diphenylpyrazine (**4a**)



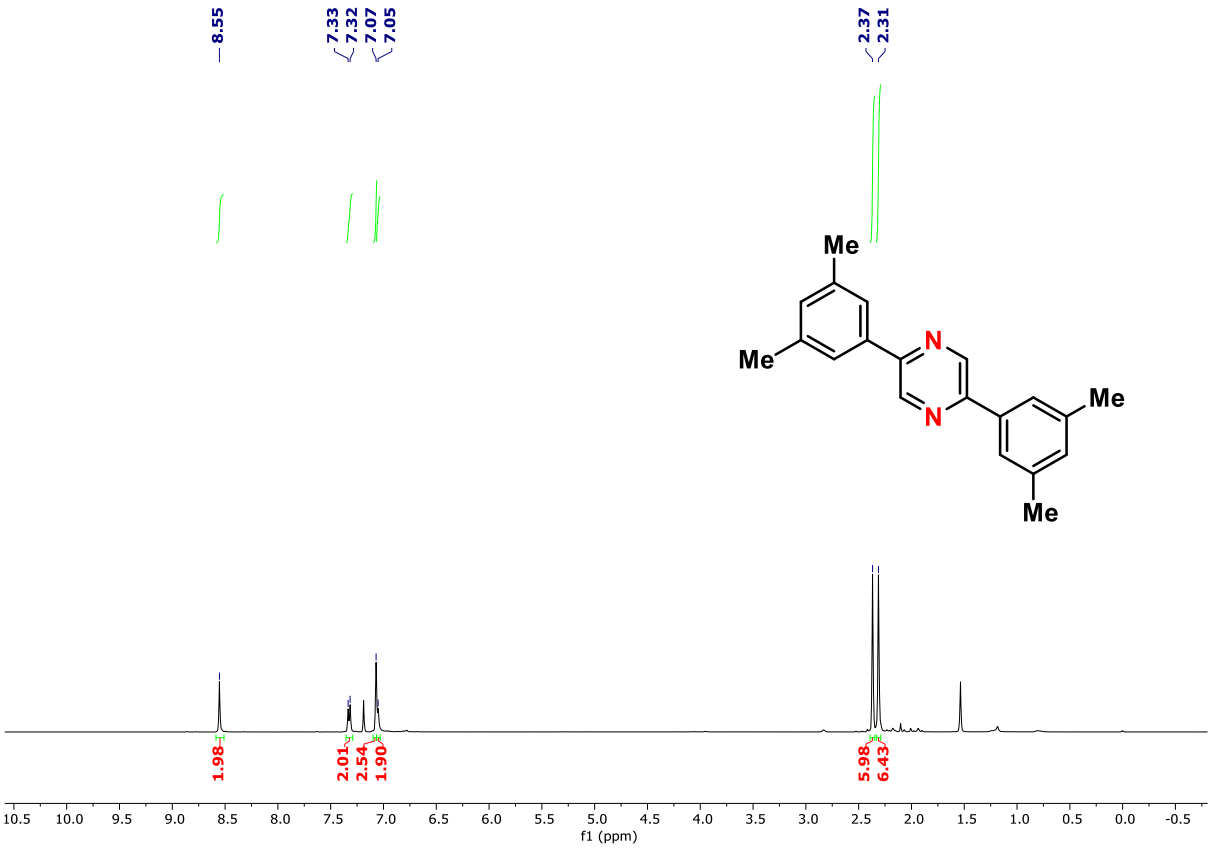
^{13}C NMR of 2,5-diphenylpyrazine (**4a**)



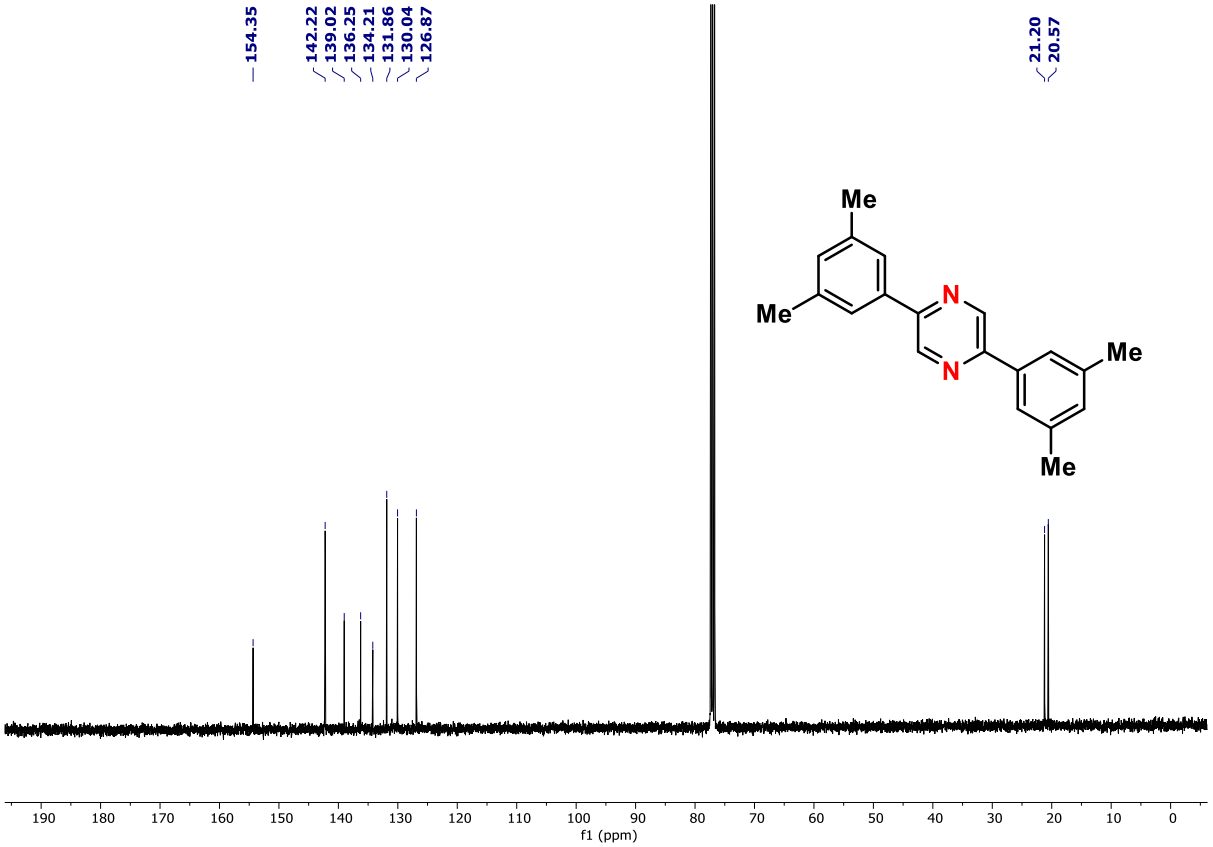
^{1}H NMR of 2,5-di-p-tolylpyrazine (**4b**)



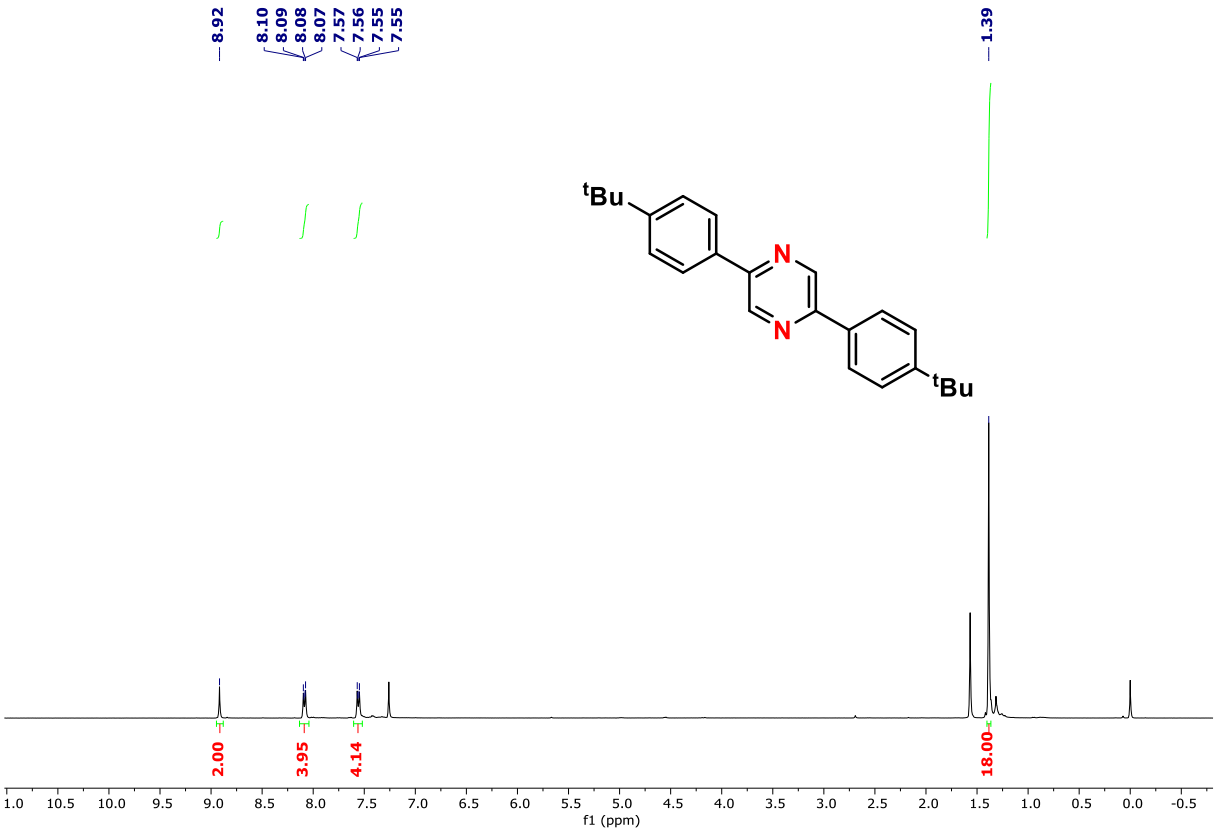
^{13}C NMR of 2,5-di-p-tolylpyrazine (**4b**)



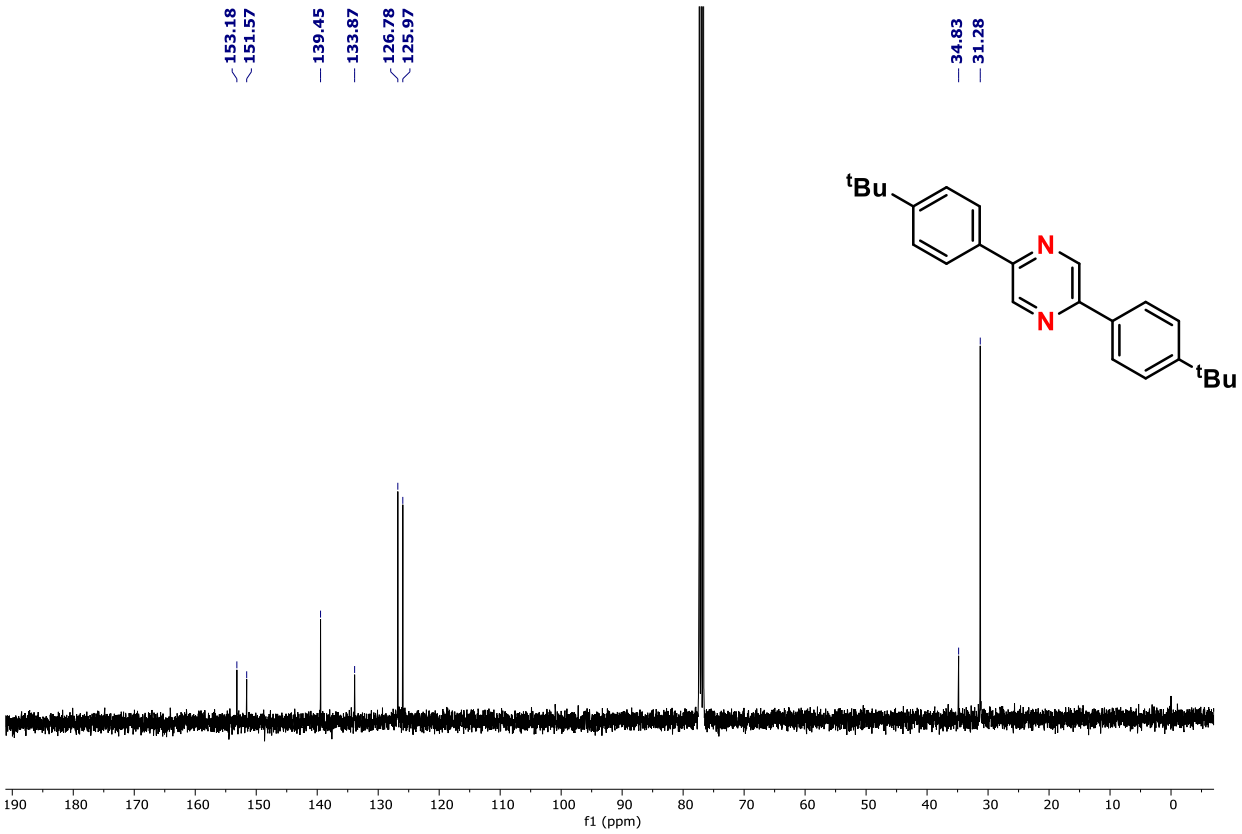
^{1}H NMR of 2,5-bis(3,5-dimethylphenyl)pyrazine (**4c**)



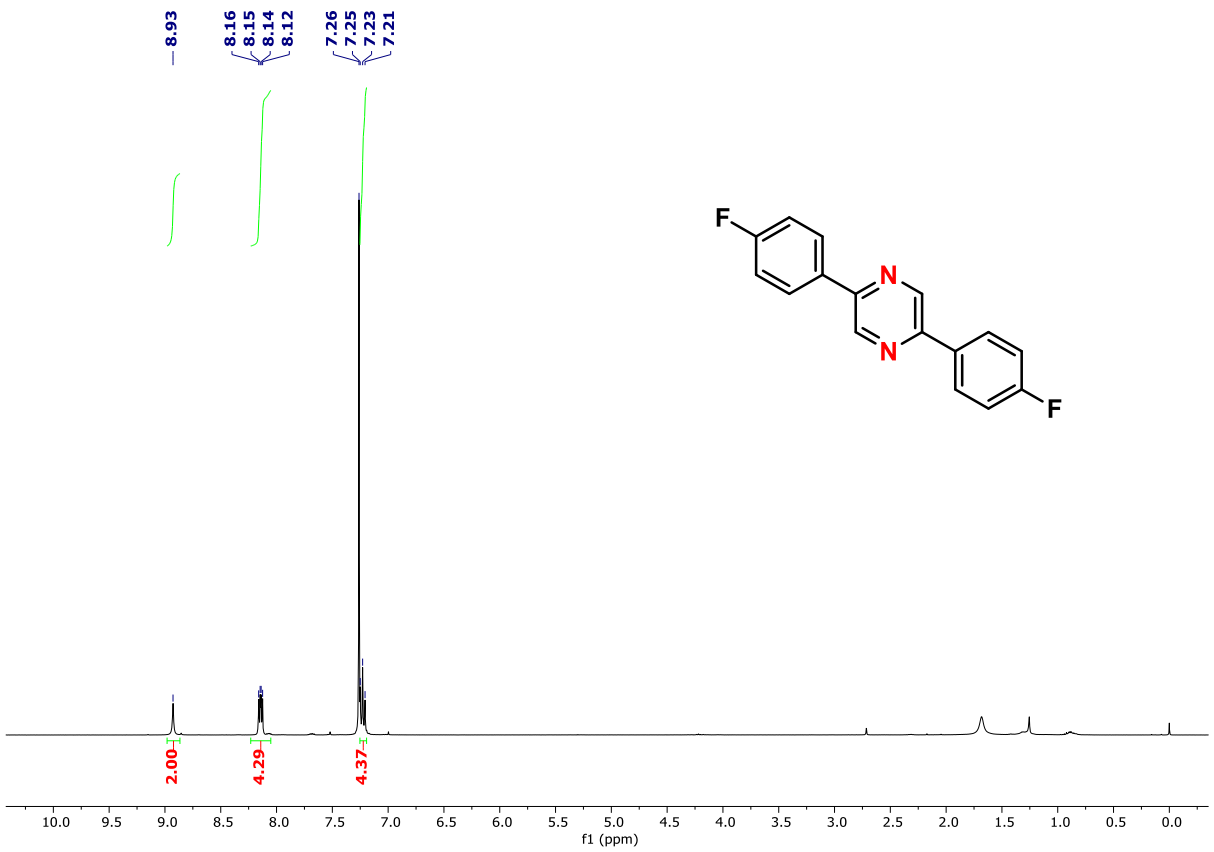
^{13}C NMR of 2,5-bis(3,5-dimethylphenyl)pyrazine (**4c**)



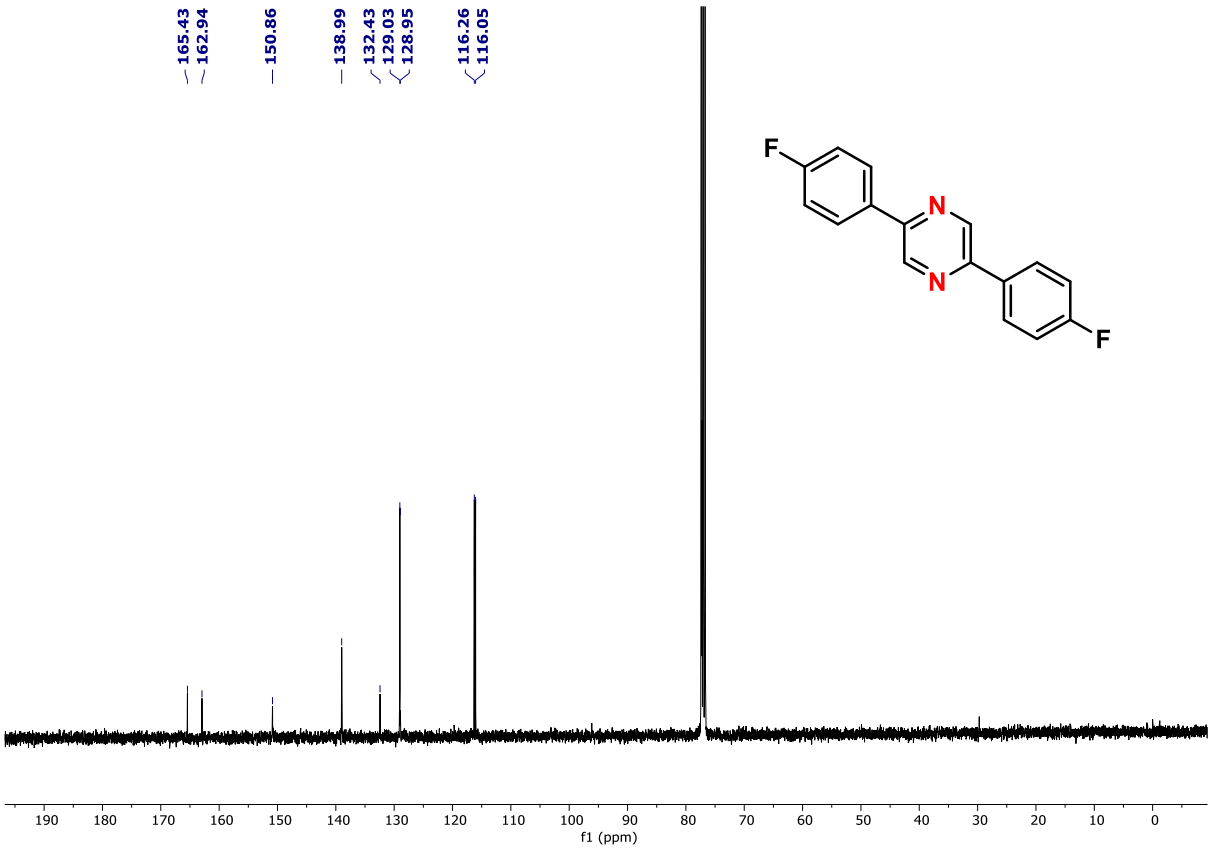
^{1}H NMR of 2,5-bis(4-(tert-butyl)phenyl)pyrazine (**4d**)



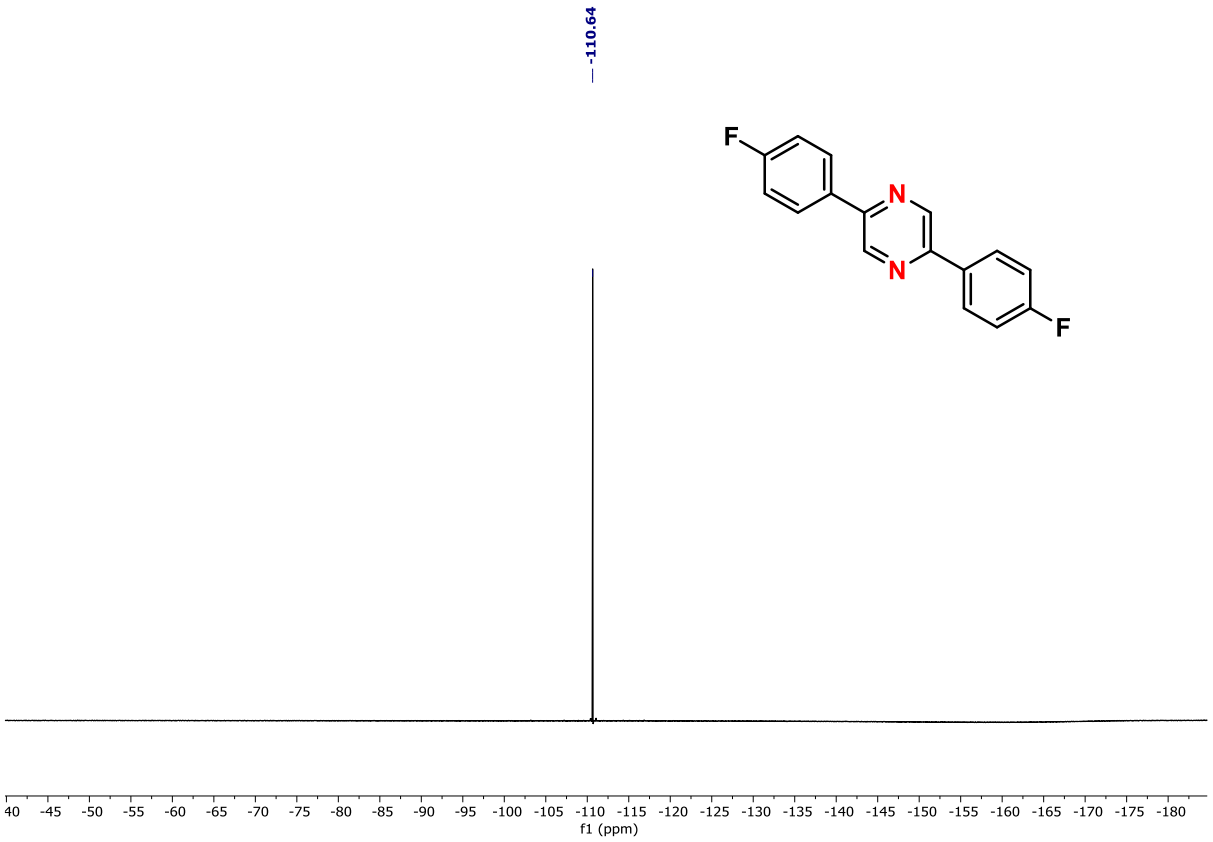
^{13}C NMR of 2,5-bis(4-(tert-butyl)phenyl)pyrazine (**4d**)



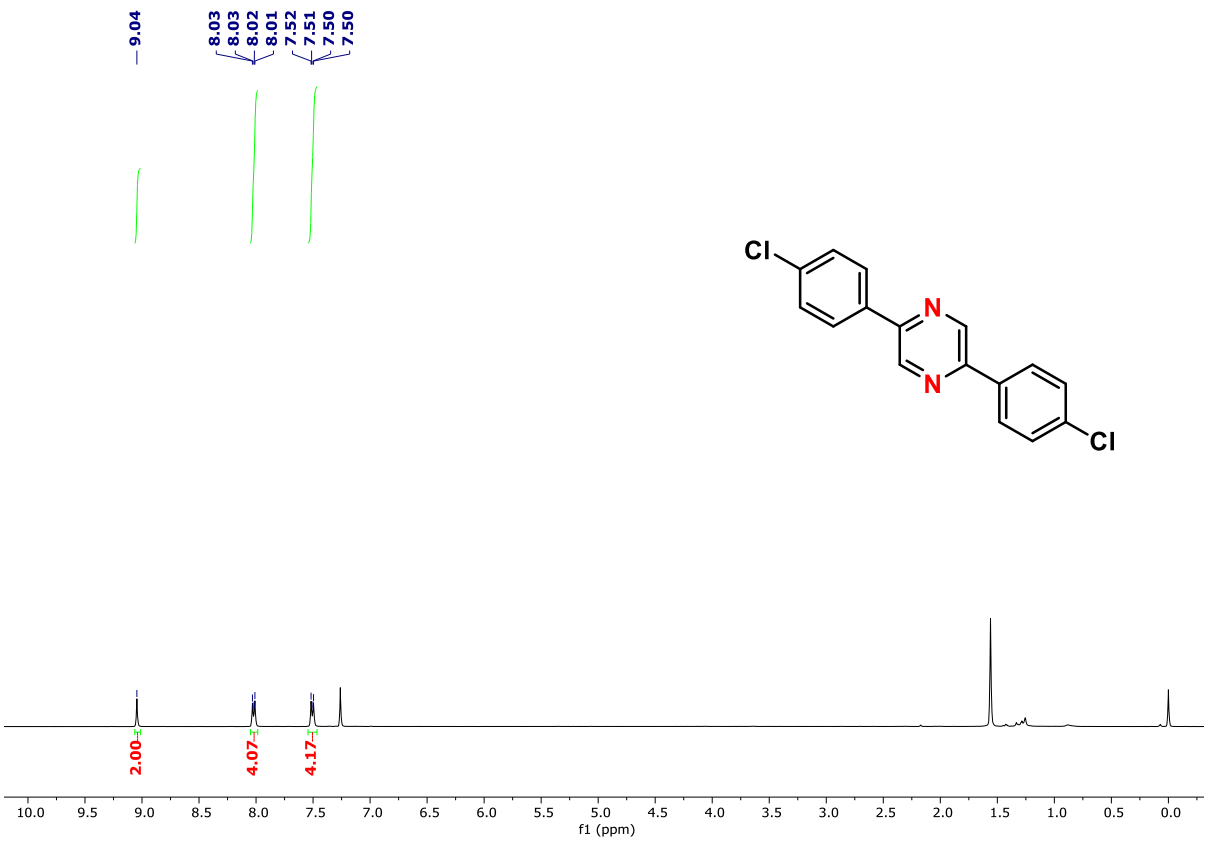
^{1}H NMR of 2,5-bis(4-fluorophenyl)pyrazine (**4e**)



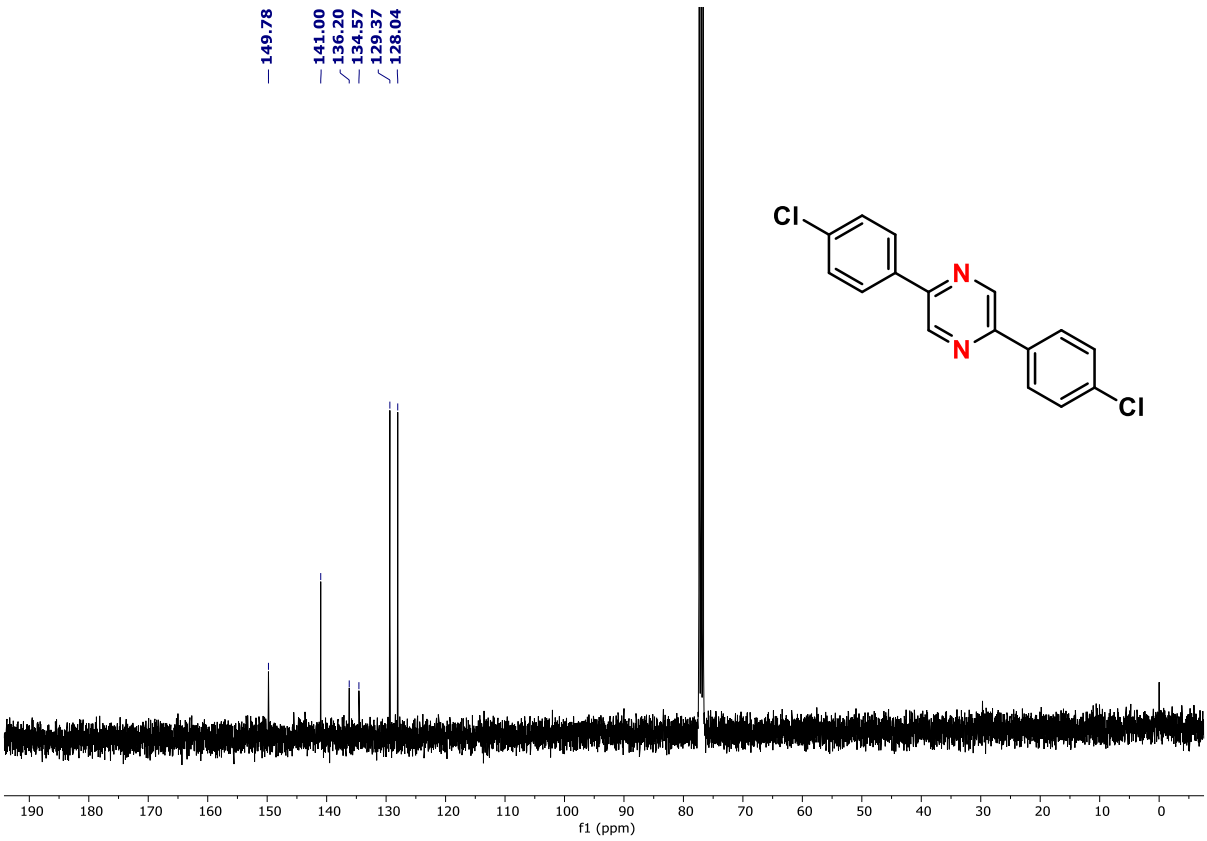
^{13}C NMR of 2,5-bis(4-fluorophenyl)pyrazine (**4e**)



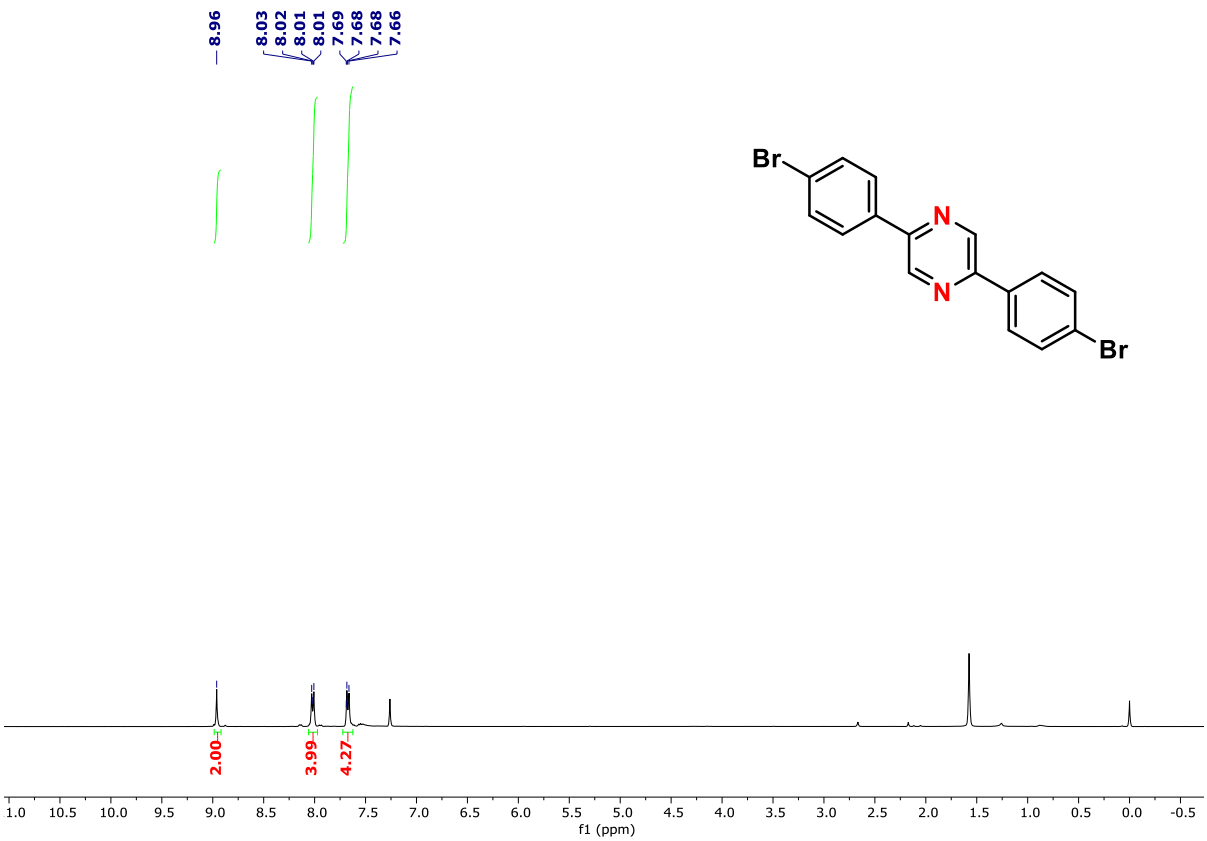
^{19}F NMR of 2,5-bis(4-fluorophenyl)pyrazine (**4e**)



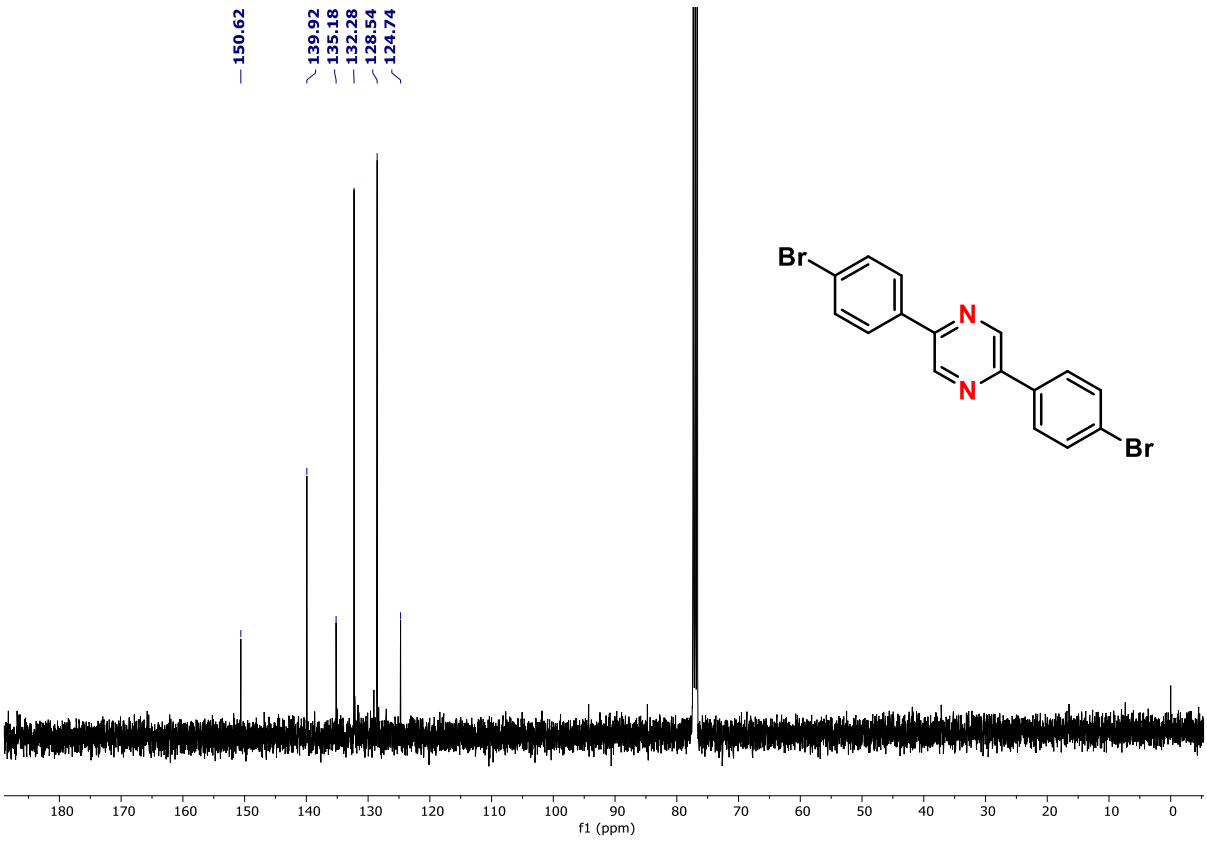
^{1}H NMR of 2,5-bis(4-chlorophenyl)pyrazine (**4f**)



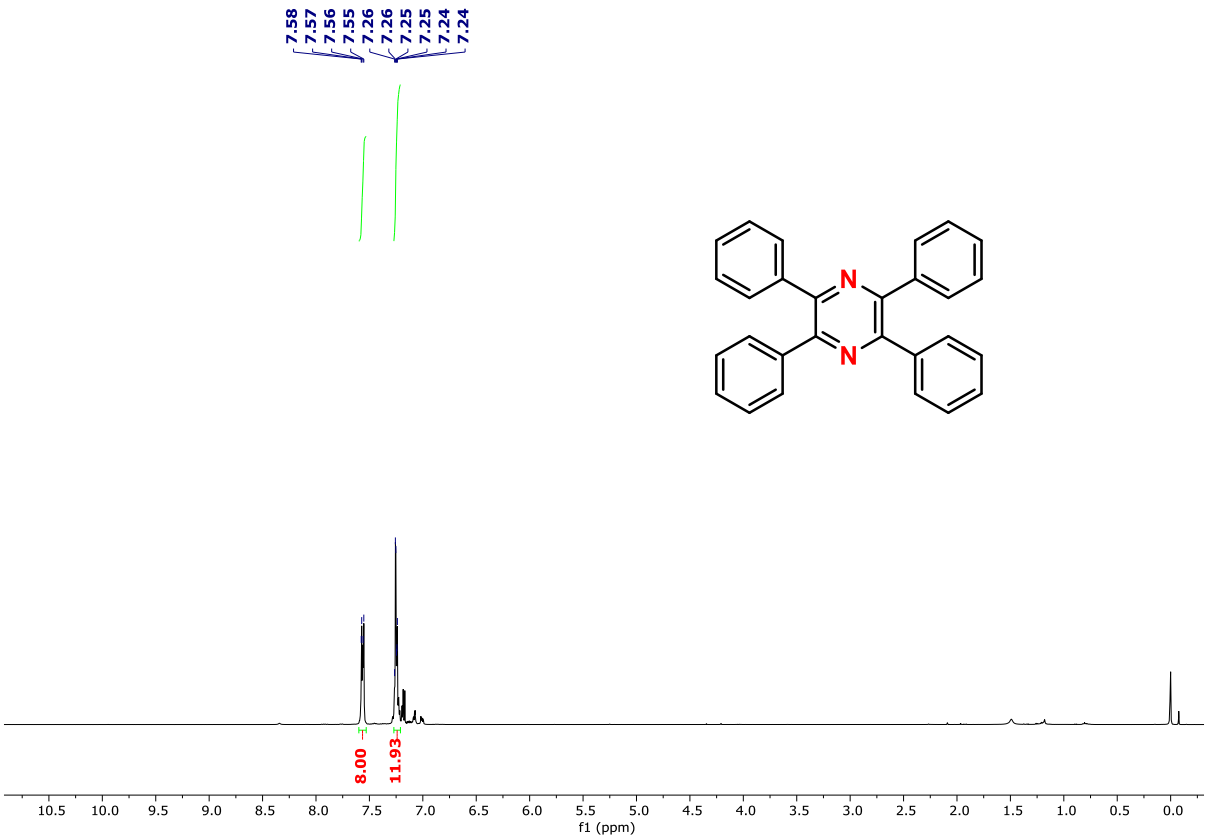
^{13}C NMR of 2,5-bis(4-chlorophenyl)pyrazine (**4f**)



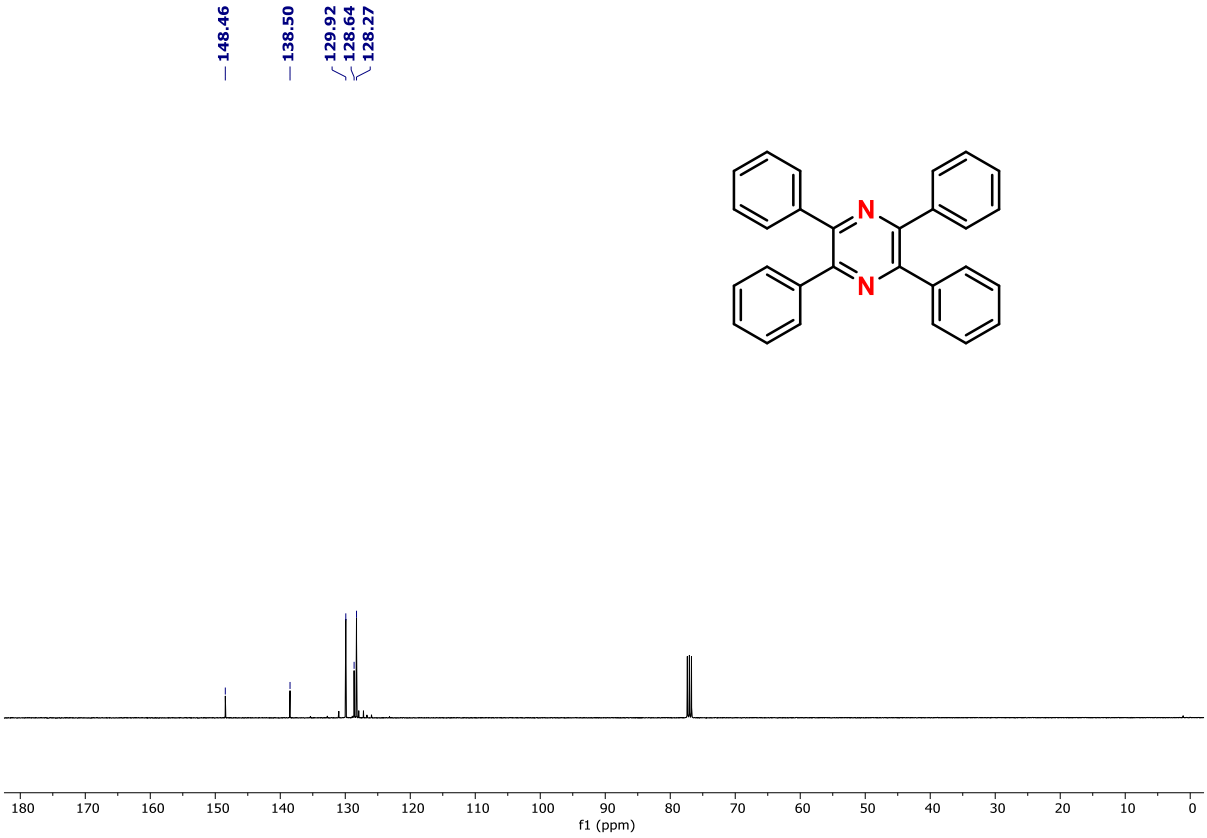
^{1}H NMR of 2,5-bis(4-bromophenyl)pyrazine (**4**g)



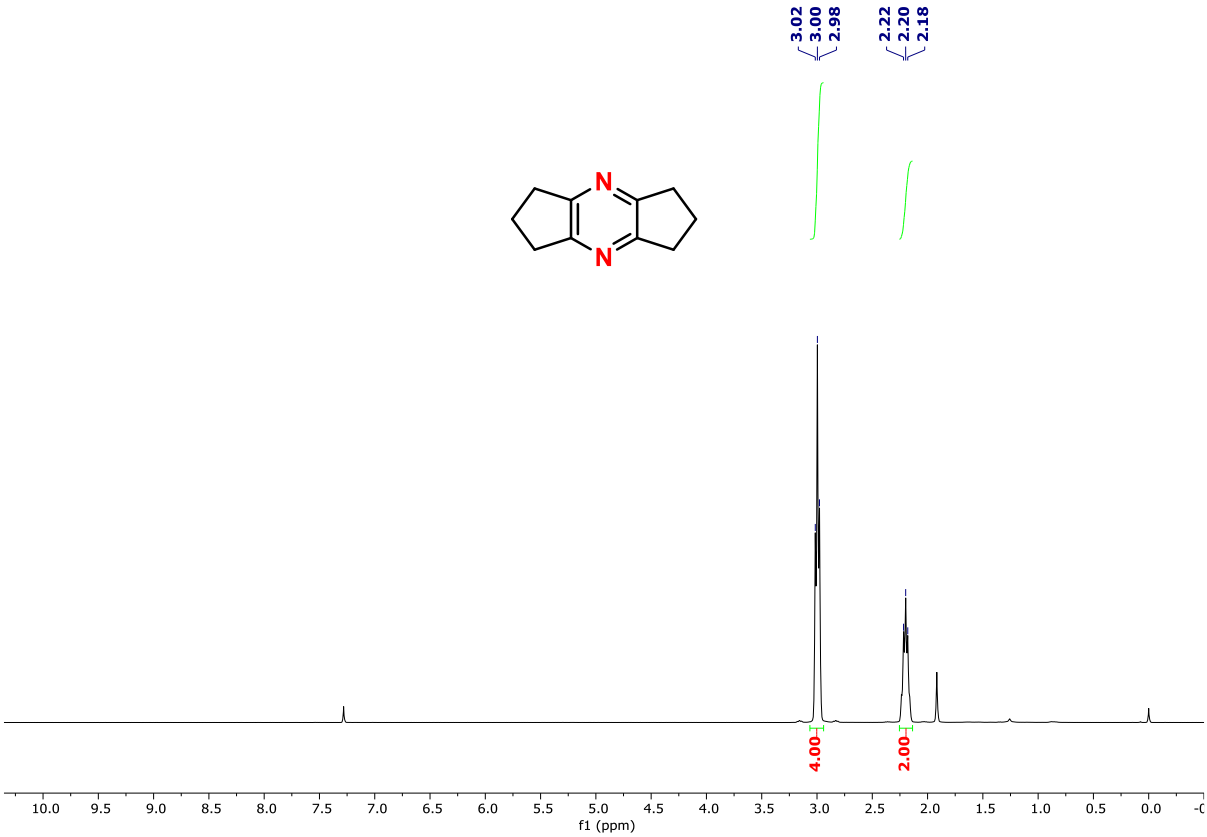
^{13}C NMR of 2,5-bis(4-bromophenyl)pyrazine (**4g**)



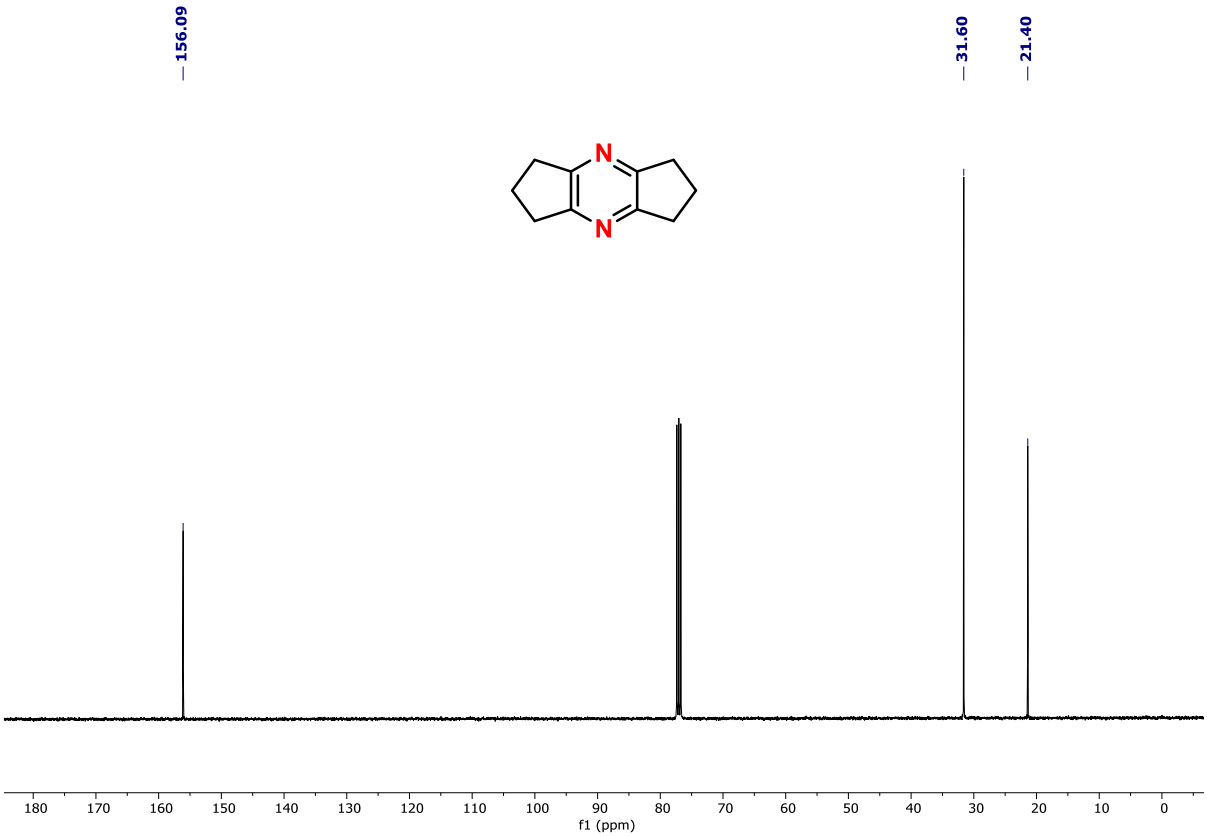
^{1}H NMR of 2,3,5,6-tetraphenylpyrazine (**4h**)



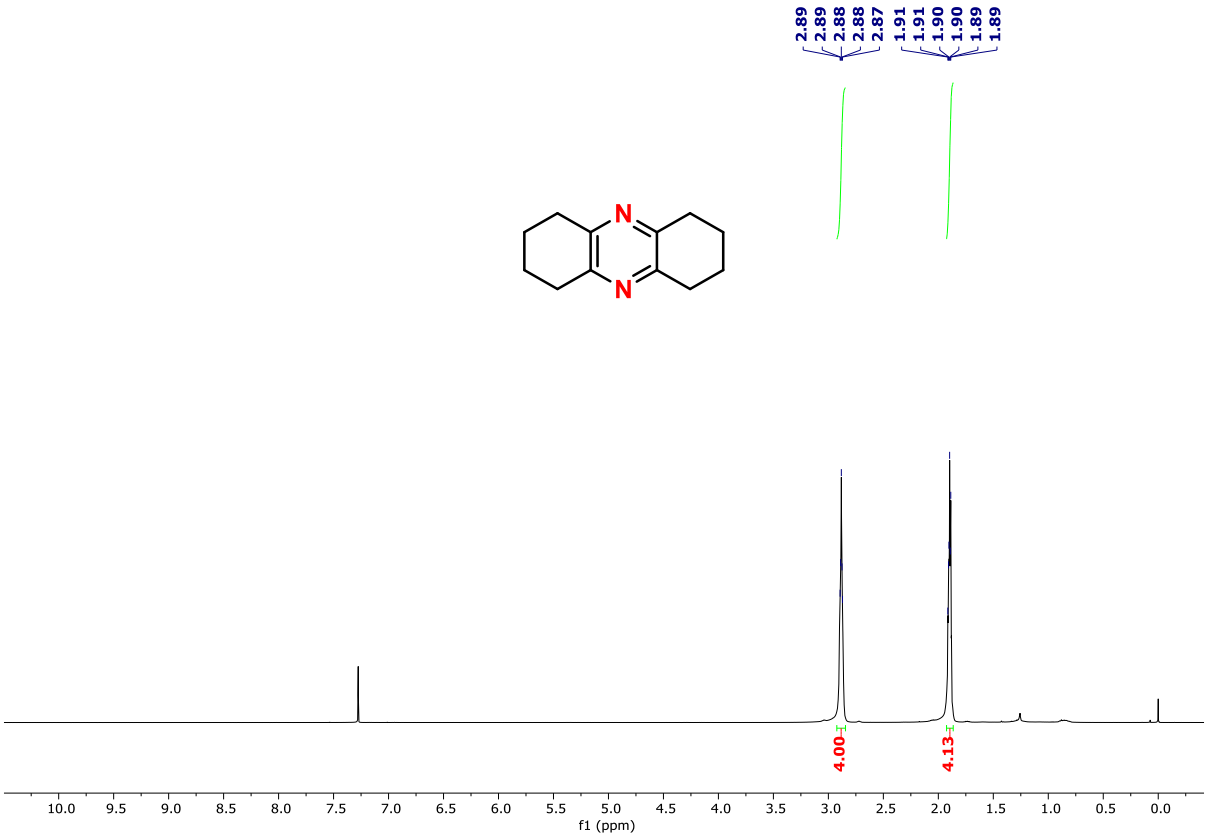
^{13}C NMR of 2,3,5,6-tetraphenylpyrazine (**4h**)



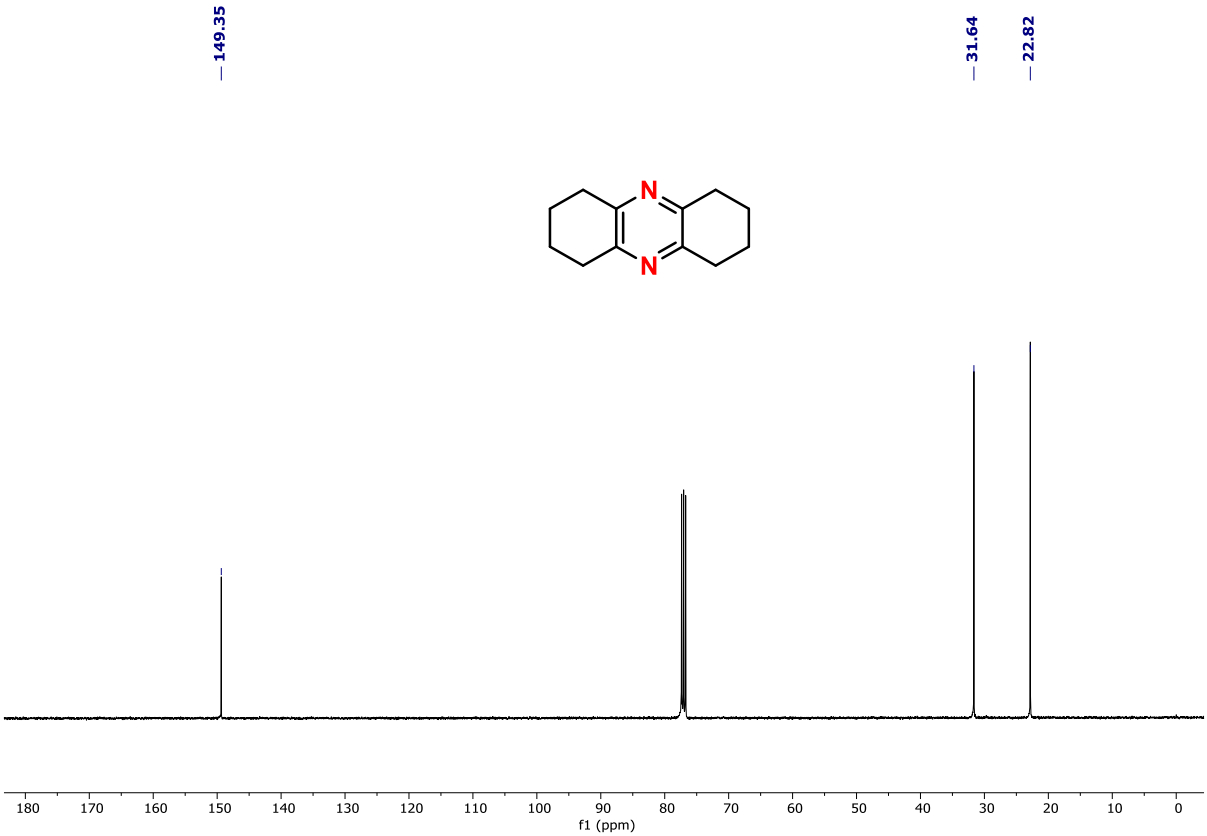
^{1}H NMR of 1,2,3,5,6,7-hexahydrodicyclopenta[b,e]pyrazine (**4i**)



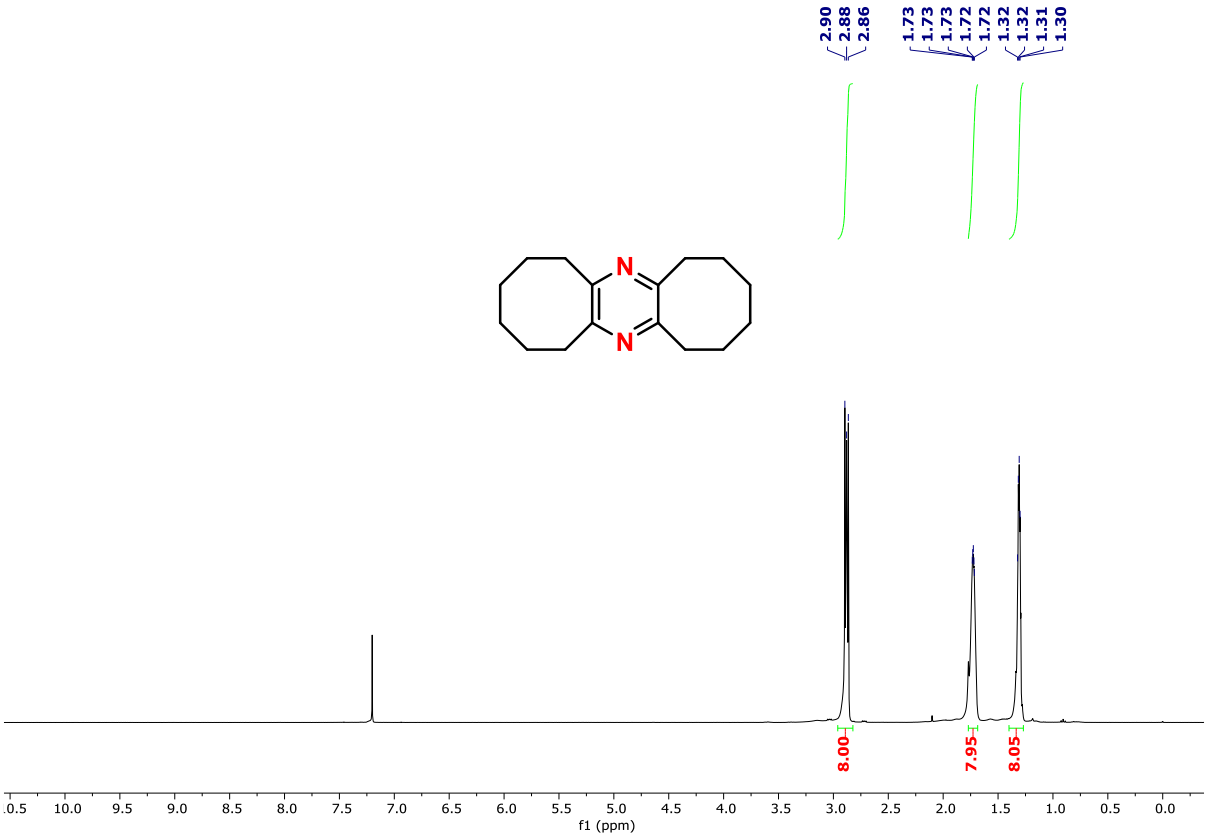
^{13}C NMR of 1,2,3,5,6,7-hexahydrodicyclopenta[b,e]pyrazine (**4i**)



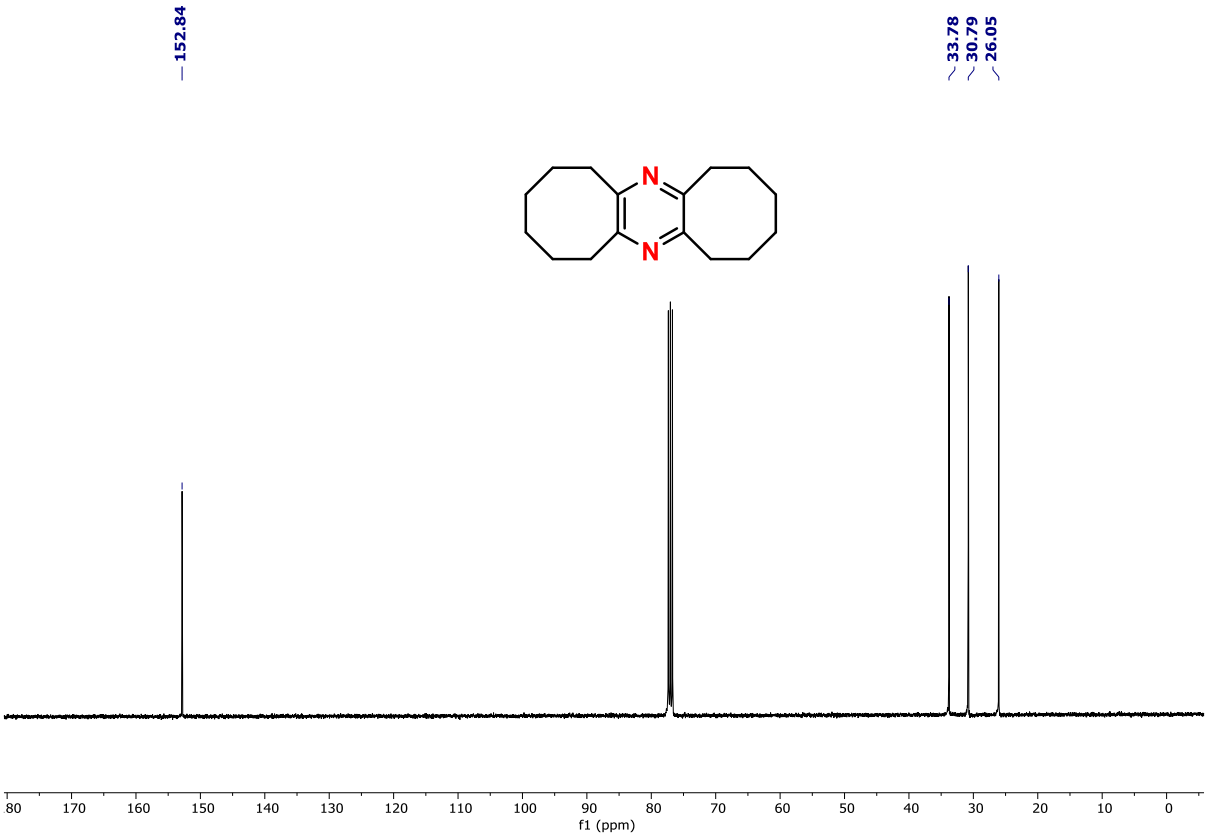
^{1}H NMR of 1,2,3,4,6,7,8,9-octahydrophenazine (**4j**)



^{13}C NMR of 1,2,3,4,6,7,8,9-octahydrophenazine (**4j**)

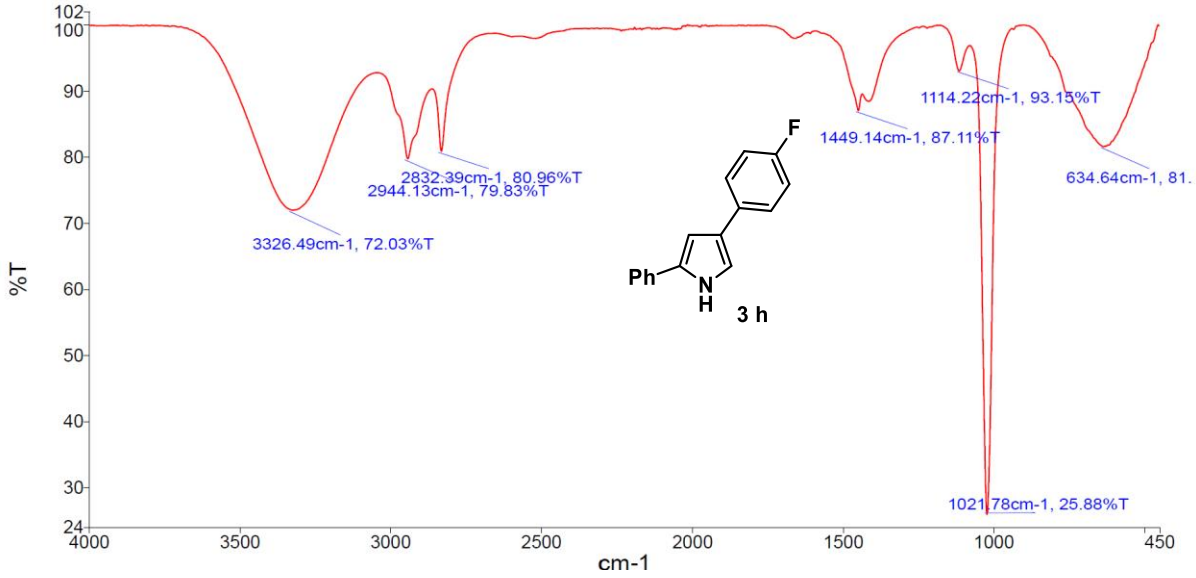


^{1}H NMR of 1,2,3,4,5,6,8,9,10,11,12,13-dodecahydrodicycloocta[b,e]pyrazine (**4k**)



^{13}C NMR of 1,2,3,4,5,6,8,9,10,11,12,13-dodecahydrodicycloocta[b,e]pyrazine (**4k**)

FTIR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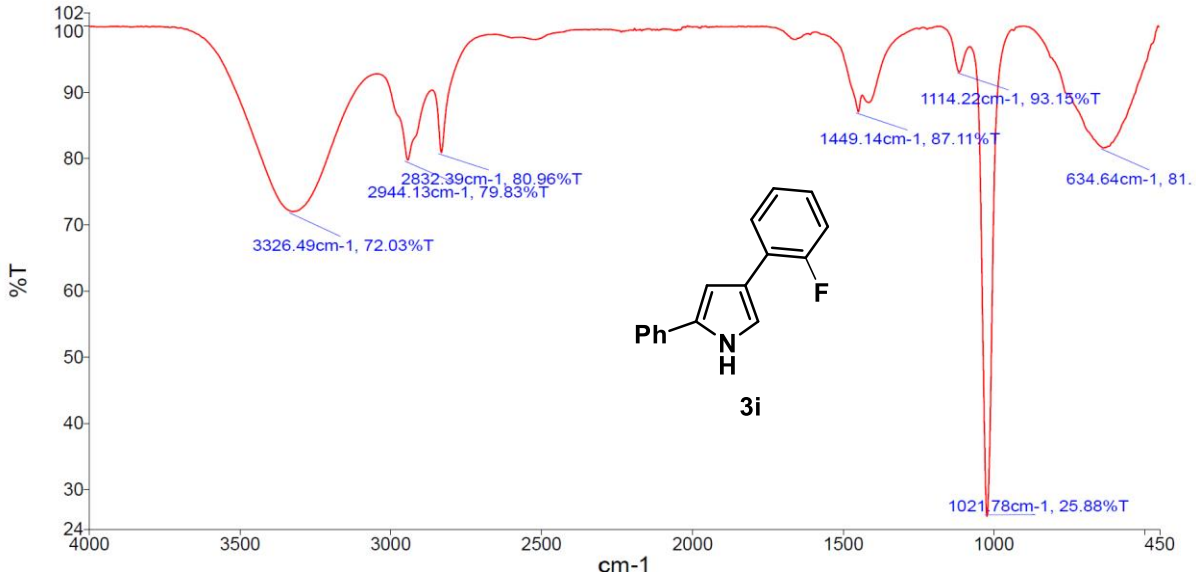
2832.39cm-1, 80.96%T
2944.13cm-1, 79.83%T
1449.14cm-1, 87.11%T
1114.22cm-1, 93.15%T
634.64cm-1, 81.
1021.78cm-1, 25.88%T
F
Ph
N
H
3 h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cm-1
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2832.39cm-1, 80.96%T
2944.13cm-1, 79.83%T
1449.14cm-1, 87.11%T
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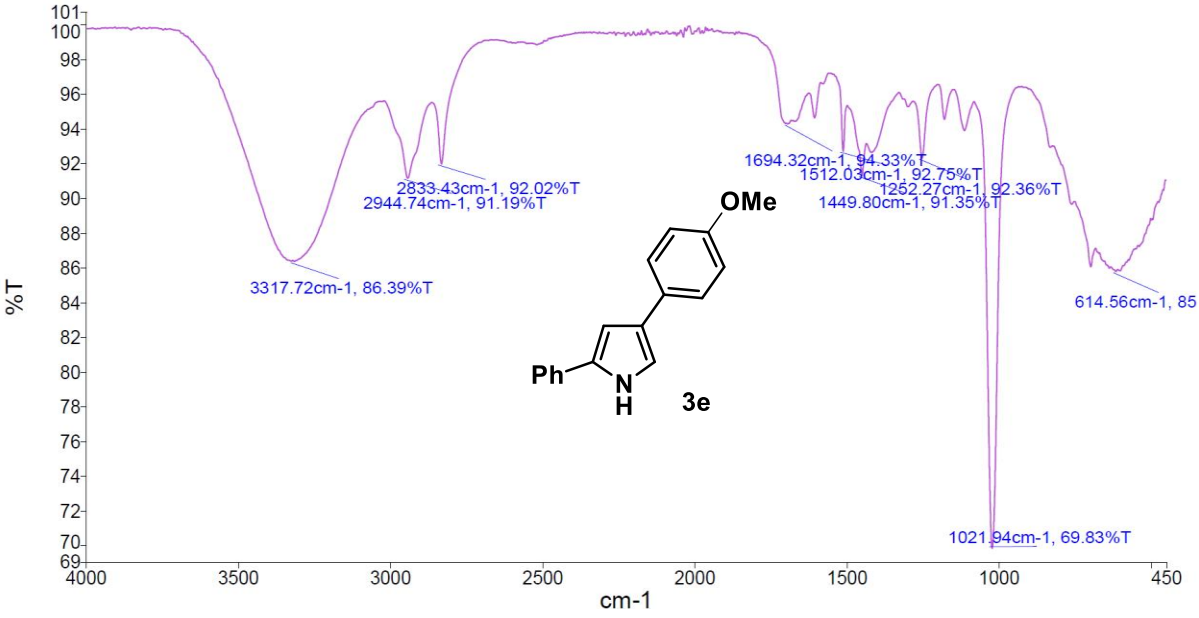
634.64cm-1, 81.
1021.78cm-1, 25.88%T
F
Ph
N
H
3i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1694.32cm-1, 94.33%T
1512.03cm-1, 92.75%T
1252.27cm-1, 92.36%T
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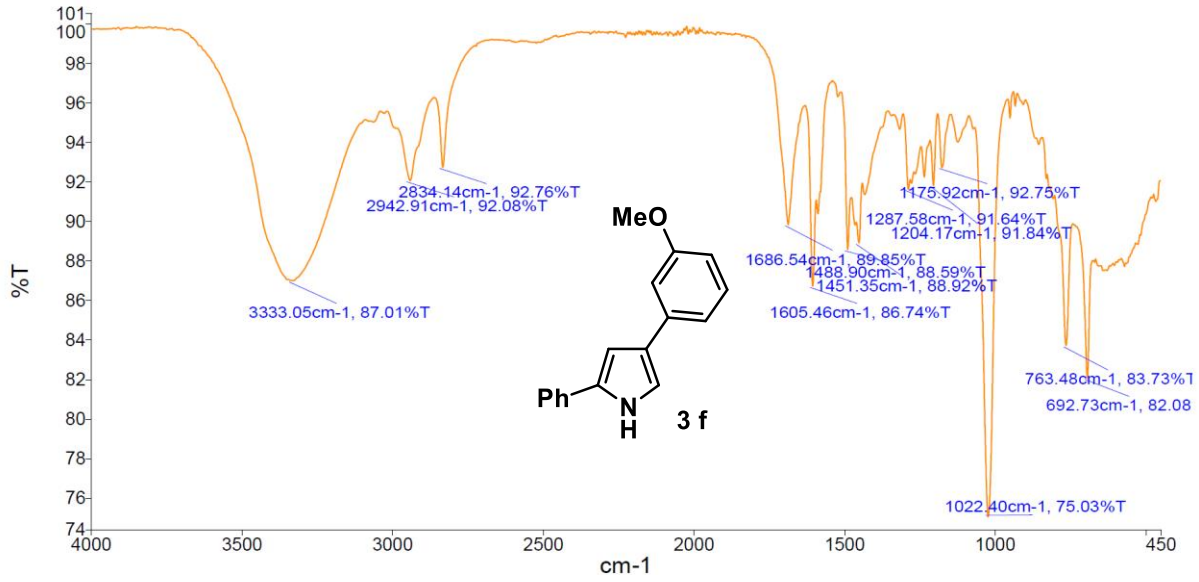
OMe
Ph
N
H
3e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1488.90cm-1, 88.59%T
1451.35cm-1, 88.92%T
1605.46cm-1, 86.74%T
1175.92cm-1, 92.75%T
1287.58cm-1, 91.64%T
1204.17cm-1, 91.84%T
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692.73cm-1, 82.08
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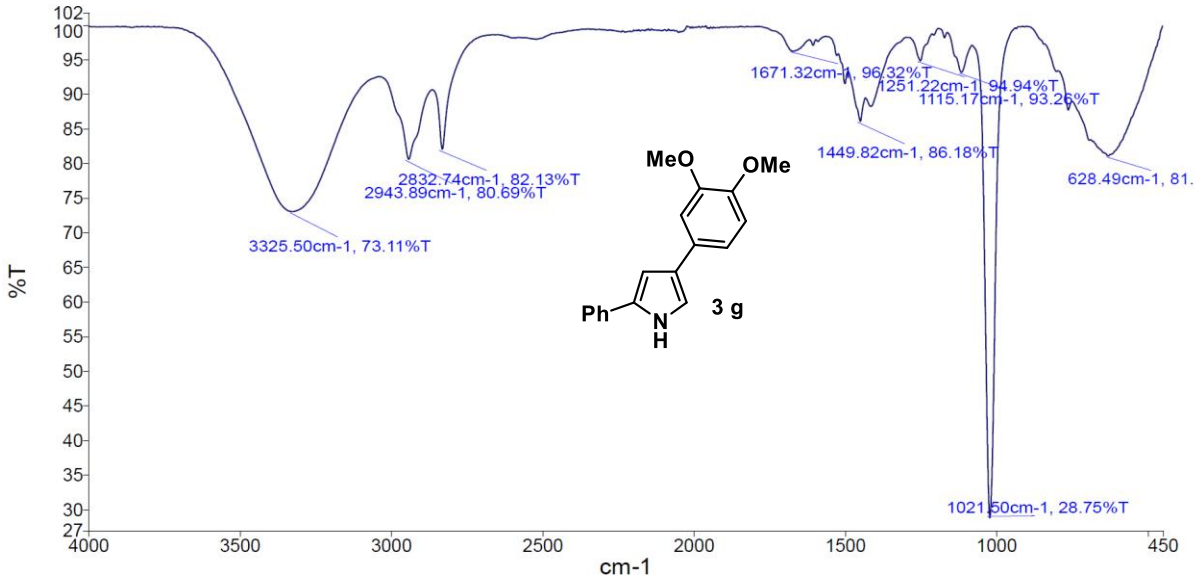
MeO
Ph
N
H
3 f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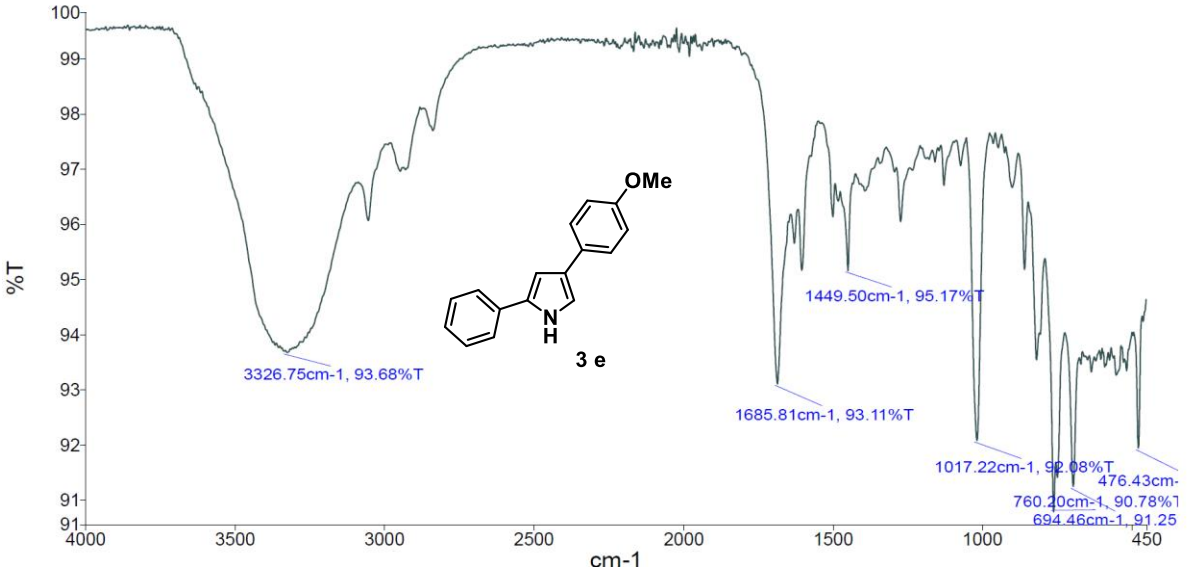
MeO
OMe
Ph
N
H
3 g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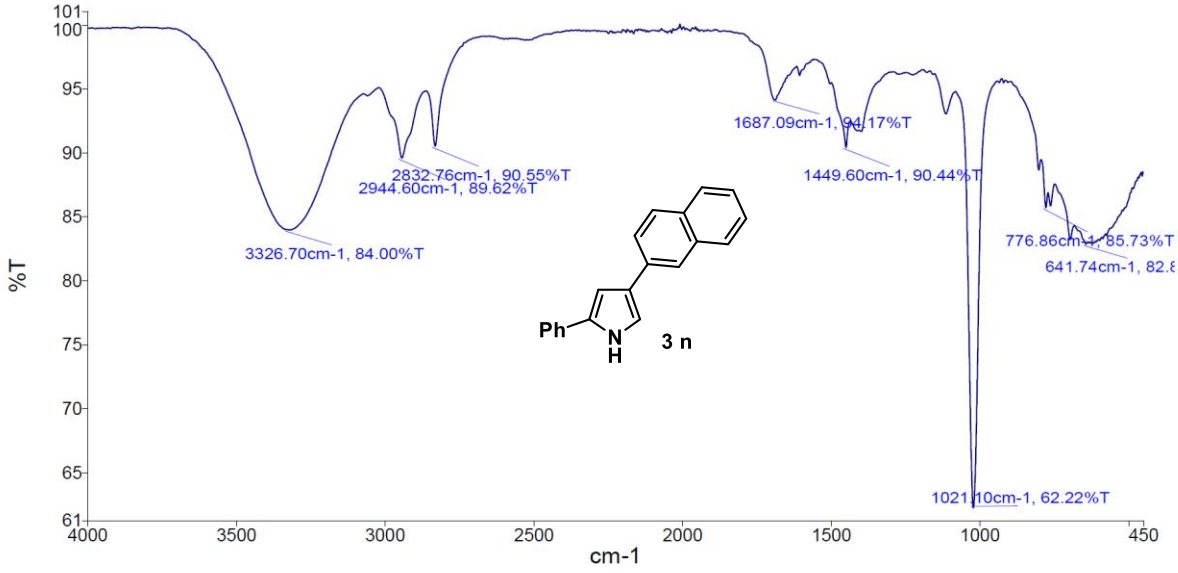
694.46cm-1, 91.25
OMe
N
H
3 e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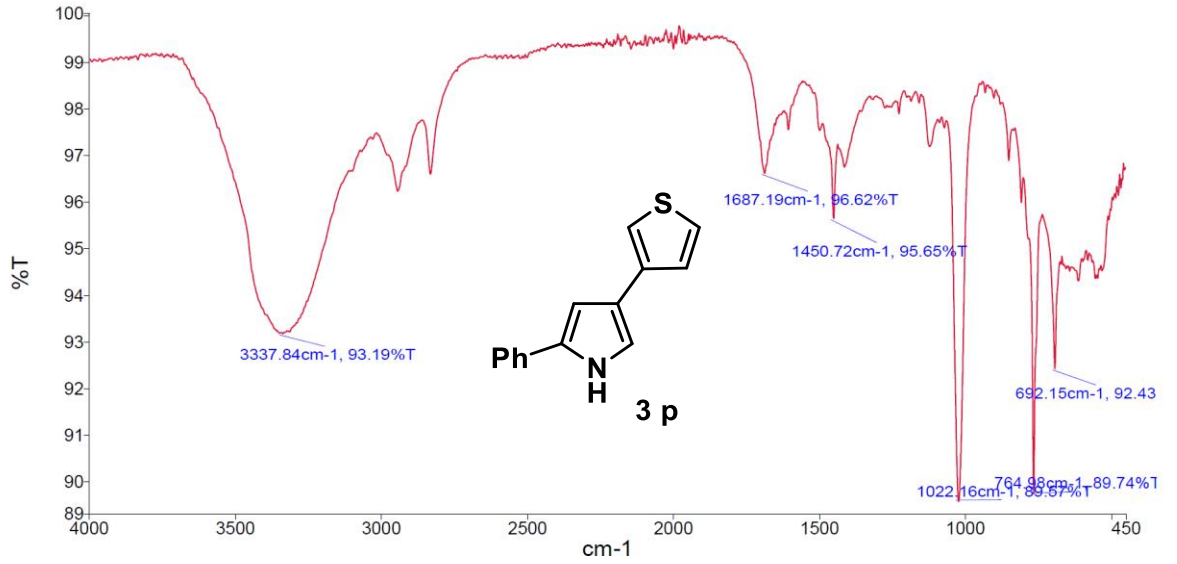
Ph
N
H
3 n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S
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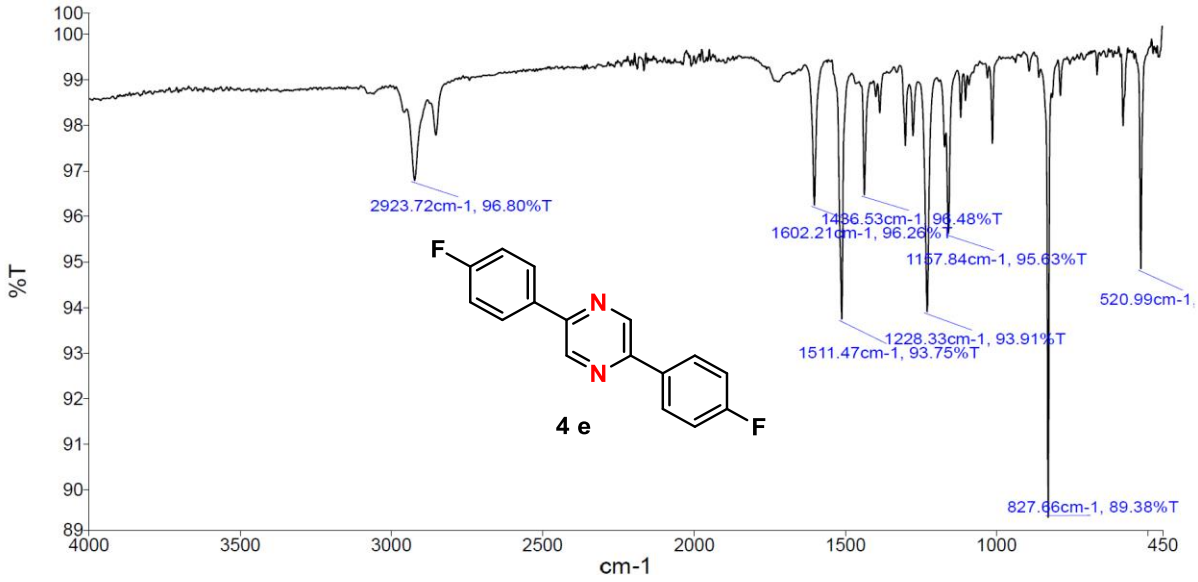
3 p


100
100
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98
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96
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94
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92
91
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89
%T
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3500
3000
2500
2000
1500
1000
450
cm-1
2923.72cm-1, 96.80%T
1602.21cm-1, 96.26%T
1511.47cm-1, 93.75%T
1228.33cm-1, 93.91%T
827.66cm-1, 89.38%T
520.99cm-1,
F
N
N
F
4 e