Supporting Information

Synthesis and antiproliferative activities of 2,3,5-trisubstituted 1*H*-pyrroles *via* formal [3+2] cycloaddition of 1-arylpropynes and nitriles

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Contents

General Information

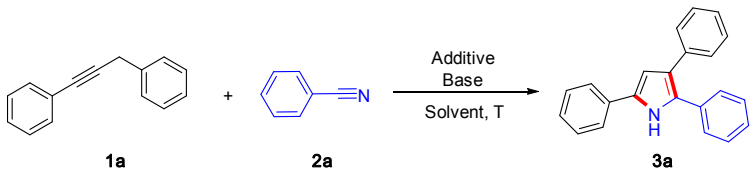
Melting points were determined with a WRX-4 Melting-point instrument. ^{1}H and ^{13}C NMR spectra were recorded using Bruker DRX-400 spectrometer or Bruker DRX-600 spectrometer using $CDCl_3$ or DMSO-d_6 as solvent. The peaks were internally referenced to $SiMe_3$ (0.00 ppm) or residual solvent signals (7.26 and 77.0 ppm for Chloroform-*d*, and 2.50 and 39.5 ppm for DMSO-d_6). The data of HRMS was carried out on a high-resolution mass spectrometer (LCMSIT-TOF). TLC was performed by using commercially prepared 100- 400 mesh silica gel plates and visualization was effected at 254 nm. Unless otherwise noted, all reagents and solvents were obtained from commercial suppliers and used without further purification.

Experimental procedures, bioassay and spectroscopic data

1. Experimental procedures

1) Condition optimization

Table S1. Optimization of the reaction conditions[a]



1a 2a 3a

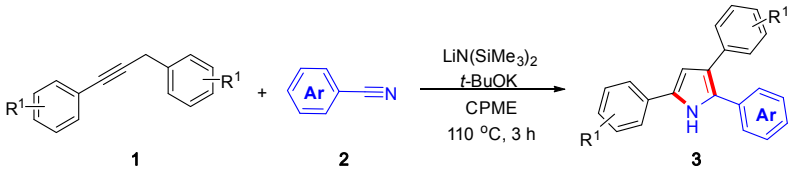
Entry[a]	Base	Additive	Solvent	T/°C	Time/h	Yield of **3a** (%)[b]
1	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	110	**1**	55
2	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	110	**2**	57
3	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	110	**3**	**82**
4	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	110	**4**	73
5	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	110	**5**	57
6	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	110	**6**	56
7	**$NaN(SiMe_3)_2$**	*t*-BuOK	CPME	110	3	64
8	**$KN(SiMe_3)_2$**	*t*-BuOK	CPME	110	3	68
9	$LiN(SiMe_3)_2$	***t*-BuOLi**	CPME	110	3	trace
10	$LiN(SiMe_3)_2$	**t-BuONa**	CPME	110	3	80
11	$LiN(SiMe_3)_2$	**Cs_2CO_3**	CPME	110	3	51
12	$KN(SiMe_3)_2$	**-**	CPME	110	3	65
13	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	**120**	3	80
14	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	**60**	3	57
15	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	**70**	3	65
16	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	**80**	3	70
17	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	**90**	3	74

18	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	**100**	3	77
19	$LiN(SiMe_3)_2$	*t*-BuOK	**THF**	110	3	63
20	$LiN(SiMe_3)_2$	*t*-BuOK	**1,4-dioxane**	110	3	69
21	$LiN(SiMe_3)_2$	*t*-BuOK	**toluene**	110	3	50
22	$LiN(SiMe_3)_2$	*t*-BuOK	**benzene**	110	3	60
23	$LiN(SiMe_3)_2$	*t*-BuOK	**DMF**	110	3	36
24[c]	$LiN(SiMe_3)_2$	*t*-BuOK	CPME	110	3	**87 (82)**[d]

[a]All reactions were performed with **1** (0.2 mmol), **2** (2 equiv), base (2 equiv), additive (1.5 equiv), solvent (1 mL) under N_2 . [b]Yield was determined by ^{1}H-NMR with CH_2Br_2 as internal standard. [c]Solvent (0.5 mL). [d]Isolated yield. CPME = cyclopentyl methyl ether.

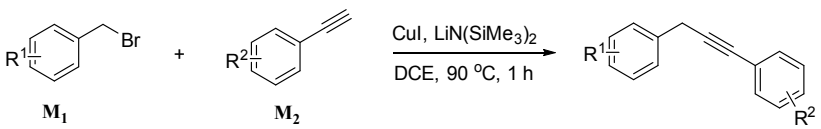
2) General experimental procedure

A. General procedure for the synthesis of 2,3,5-triphenyl-1*H*-pyrrole



A mixture of **1** (0.2 mmol), **2** (2.0 equiv), $Li(SiMe_3)_2$ (2.0 equiv), and *t*-BuOK (1.5 equiv) dissolved in 0.5 mL dry CPME was added to an oven-dried Schlenk tube equipped with a magnetic stirring bar and stirred at 110 °C under N_2 for 3 h (***Cautious:*** the rising pressure produced by CPME). After finished, the reaction mixture was cooled to room temperature and quenched by 10 mL of water. The product was extracted with ethyl acetate (10 mL × 3). The organic phase was dried over Na_2SO_4 and concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography using petroleum ether/ethyl acetate/(100:1) as eluent to afford the corresponding product.

B. General procedure for the preparation of compound 1[1]



An oven-dried Schlenk tube equipped with a magnetic stirring bar was added successively $\mathbf{M_1}$ (2 mmol), $\mathbf{M_2}$ (3 mol), CuI (5 mol %), $Li(SiMe_3)_2$ (1.2 equiv), and DCE (4 mL) under N_2. The mixture was stirred at 90 °C for 1 h and monitored by TLC. Upon completion, the reaction mixture was diluted with water (15 mL) and extracted with ethyl acetate (15 mL × 3). The combined organic layers were washed with water and brine, dried over Na_2SO_4, and filtered. The solvent was removed under vacuum. The residue was purified by chromatography on silica gel (petroleum

ether/ethyl acetate 200:1~100:1 v/v).

2. Biological assays

1) Cell lines and culture conditions

The cytotoxic activity of the synthesized compounds against MDA-MB-231 (human breast cancer cell line), SGC-7901 (human gastric cancer cell line), HCT-116 (human colon cancer cells) was investigated. The cells were cultured in RPMI-1640 (Hyclon) or high glucose DMEM (Hyclon) medium with 10% heat-inactivated fetal bovine serum (Hyclon) 1% penicillin–streptomycin (Hyclon), and incubated at standard culture conditions (37 ℃, 5% CO_2 in air) (Thermo Fisher Scientific, Wisconsin, USA). The culture medium was refreshed every 2 days. The cells were subcultured twice each week, seeding at a density of about 1×10^5 cells/mL. Before the analysis of the compounds, cells were washed with PBS and fresh medium was added. For fifinal analysis, exponentially growing cells were collected and resuspended in fresh culture medium with 10% FBS. Cells were maintained in a humidified incubator with 5% CO_2 at 37 ℃.

2) MTT assay

Cytotoxic activity was determined by the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay as described. 5-fluorouracil (**5-Fu**) was selected as a positive control. Cell suspensions were prepared at a concentration of 1×10^5μg/mL, added to 96-well plates at 100μL per well, and incubated at 37 °C in a 5% CO_2 incubator for 24 h. Different concentrations of subjects were added to the 96-well plates of cultured tumor cells, and incubation was continued for 48h and observed under an inverted microscope. The culture medium was discarded, and 100 μL of 0. 05% MTT application solution was added to each well and incubated for 4 h. The culture medium was discarded, 100 μL of DMSO was added to each well and shaken for 10 min to dissolve the methylzan crystals, and the absorbance (OD) of the cells was measured at 490 nm.

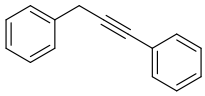
The concentration and growth inhibition curves were obtained by plotting the growth inhibition rates at different doses and plotted using GraphPad Prism 9.0 software to calculate the semi-inhibitory concentration IC_{50} of the target compounds on three tumor cells and one normal cell.

compound	IC50(uM)		
	MDA-MB-231	SGC-7901	HCT116
3e	227.6(±93.0)	119.9(±2.7)	201.3(±3.4)
3m	47.9(±1.2)	50.8(±0.9)	91.75(±1.9)
3n	43.3(±0.6)	141.5(±1.9)	174.3(±3.9)
3r	3.5(±0.2)	8.3(±0.3)	10.7(±0.4)
3x	41.1(±0.8)	66.0(±0.8)	98.05(±1.4)
5-Fu	4.7(±0.4)	10.7(±0.3)	12.9(±0.3)

(±) Standard deviation; n = 3. NA: not active up to significant concentrations.

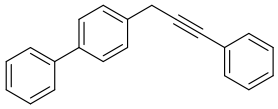
3. Spectroscopic data

prop-1-yne-1,3-diyldibenzene (1a):



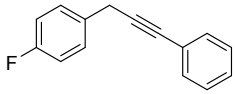
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.46 – 7.43 (m, 2H), 7.40 (d, J = 7.0 Hz, 2H), 7.32 (t, J = 7.7 Hz, 2H), 7.27 (m, J = 5.1, 2.1 Hz, 3H), 7.23 (t, J = 7.4 Hz, 1H), 3.81 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 136.7, 131.6, 128.5, 128.2, 127.9, 127.8, 126.6, 123.6, 87.5, 82.6, 25.7. The spectroscopic data are in agreement with literature data.[1]

1-4-(3-phenylprop-2-yn-1-yl)-1,1'-biphenyl (1b):



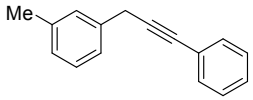
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm7.56 (dd, J = 11.3, 7.7 Hz, 4H), 7.46 (d, J = 7.8 Hz, 4H), 7.40 (t, J = 7.7 Hz, 2H), 7.29 (m, J = 25.3, 6.3 Hz, 4H), 3.84 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 140.8, 139.6, 135.8, 131.6, 128.7, 128.3, 128.2, 127.8, 127.3, 127.1, 127.0, 123.6, 87.4, 82.7, 25.4. The spectroscopic data are in agreement with literature data.[2]

2-fluoro-4-(3-phenylprop-2-yn-1-yl)benzene (1c):



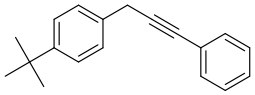
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.44 (dd, J = 6.7, 3.0 Hz, 2H), 7.35 (dd, J = 8.5, 5.5 Hz, 2H), 7.28 (dd, J = 5.0, 2.1 Hz, 3H), 7.01 (t, J = 8.7 Hz, 2H), 3.78 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 161.7 (d, J = 243.0 Hz), 132.4 (d, J = 3.0 Hz), 131.6, 129.4 (d, J = 7.8 Hz), 128.2, 127.9, 123.5, 115.3 (d, J = 21.3 Hz), 87.3, 82.8, 25.0. The spectroscopic data are in agreement with literature data.[2]

1-methyl-3-(3-phenylprop-2-yn-1-yl)benzene (1d):



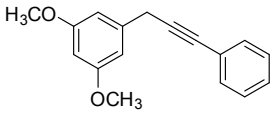
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.44 (dd, J = 7.5, 2.3 Hz, 2H), 7.30 – 7.26 (m, 3H), 7.21 (d, J = 6.5 Hz, 3H), 7.05 (d, J = 7.5 Hz, 1H), 3.78 (s, 2H), 2.35 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ ppm 138.2, 136.6, 131.6, 128.7, 128.4, 128.2, 127.7, 127.3, 125.0, 123.7, 87.7, 82.5, 25.61, 21.38. The spectroscopic data are in agreement with literature data.[1]

1-(tert-butyl)-4-(3-phenylprop-2-yn-1-yl)benzene (1e)



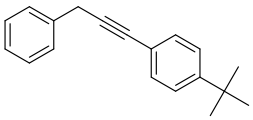
Yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ ppm 7.47 – 7.42 (m, 2H), 7.35 (d, J = 1.7 Hz, 4H), 7.26 (dd, J = 5.1, 2.0 Hz, 3H), 3.78 (s, 2H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 149.5, 133.7, 131.6, 128.2, 127.7, 127.6, 125.4, 123.8, 87.8, 82.4, 34.4, 31.4, 25.2. The spectroscopic data are in agreement with literature data.[1]

1,3-dimethoxy-5-(3-phenylprop-2-yn-1-yl)benzene (1f):



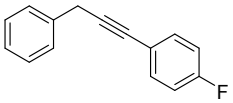
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.44 (d, J = 5.3 Hz, 2H), 7.29 (d, J = 5.2 Hz, 3H), 6.58 (s, 2H), 6.36 (s, 1H), 3.79 (s, 6H), 3.77 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 160.9, 139.1, 131.6, 128.2, 127.8, 123.6, 106.1, 98.6, 87.2, 82.7, 55.3, 25.9. The spectroscopic data are in agreement with literature data.[3]

1-(tert-butyl)-4-(3-phenylprop-1-yn-1-yl)benzene (1g):



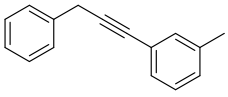
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.43 – 7.37 (m, 4H), 7.34 – 7.30 (m, 4H), 7.23 (t, J = 8.2 Hz, 1H), 3.82 (s, 2H), 1.30 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 151.0, 136.9, 131.3, 128.5, 127.9, 126.5, 125.2, 120.6, 86.7, 82.7, 34.7, 31.2, 25.7. The spectroscopic data are in agreement with literature data.[2]

1-fluoro-4-(3-phenylprop-1-yn-1-yl)benzene (1h):



Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.36 – 7.28 (m, 4H), 7.25 (t, J = 7.7 Hz, 2H), 7.16 (t, J = 7.4 Hz, 1H), 6.89 (t, J = 8.7 Hz, 2H), 3.72 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 162.2 (d, J = 247.1 Hz), 136.6, 133.4 (d, J = 8.4 Hz), 128.5, 127.9, 126.7, 119.7 (d, J = 3.4 Hz), 115.4 (d, J = 21.8 Hz), 87.2, 81.5, 25.6. The spectroscopic data are in agreement with literature data.[1]

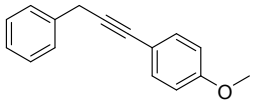
1-methyl-3-(3-phenylprop-1-yn-1-yl)benzene (1i):



Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.41 (d, J = 6.7 Hz, 2H), 7.34 (t, J = 7.8 Hz, 2H), 7.28 – 7.23 (m, 3H), 7.18 (t, J = 7.6 Hz, 1H), 7.10 (d, J = 7.6 Hz, 1H), 3.83 (s, 2H), 2.32 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 137.9, 136.8,

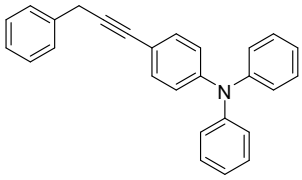
132.2, 128.7, 128.7, 128.5, 128.1, 127.9, 126.6, 123.4, 87.1, 82.8, 25.7, 21.2. The spectroscopic data are in agreement with literature data.[1]

1-methoxy-4-(3-phenylprop-1-yn-1-yl)benzene(1j):



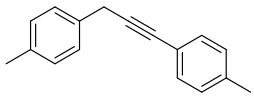
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.33 (d, J = 7.1 Hz, 2H), 7.31 – 7.29 (m, 2H), 7.24 (t, J = 7.7 Hz, 2H), 7.15 (t, J = 7.3 Hz, 1H), 6.74 – 6.73 (m, 2H), 3.73 (s, 2H), 3.69 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 159.2, 137.0, 132.9, 128.5, 127.9, 126.5, 115.8, 113.8, 85.9, 82.4, 55.2, 25.7. The spectroscopic data are in agreement with literature data.[1]

N,N-diphenyl-4-(3-phenylprop-1-yn-1-yl)aniline(1k):



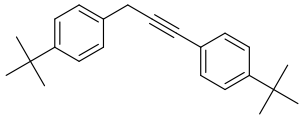
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.29 (d, J = 7.1 Hz, 2H), 7.21 – 7.17 (m, 4H), 7.13 – 7.10 (m, 5H), 6.97 (d, J = 7.3 Hz, 4H), 6.90 (t, J = 7.4 Hz, 2H), 6.85 (d, J = 8.7 Hz, 2H), 3.69 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 147.4, 147.2, 136.9, 132.5, 129.3, 128.4, 127.9, 126.5, 124.6, 123.2, 122.6, 116.8, 86.5, 82.6, 25.74. HRMS (ESI): calculated $[M+H]^+$ for $C_{27}H_{22}N$: 360.1747, found :360.1743

2-4,4'-(prop-1-yne-1,3-diyl)bis(methylbenzene) (1l):



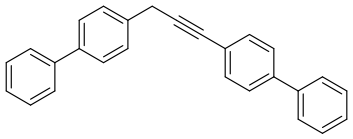
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.25 (d, J = 8.1 Hz, 2H), 7.21 (d, J = 7.8 Hz, 2H), 7.05 (d, J = 7.8 Hz, 2H), 7.00 (d, J = 7.8 Hz, 2H), 3.69 (s, 2H), 2.25 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 137.7, 136.1, 133.8, 131.5, 129.2, 128.9, 127.8, 120.6, 87.0, 82.4, 25.3, 21.4, 21.0. The spectroscopic data are in agreement with literature data.[4]

4,4'-(prop-1-yne-1,3-diyl)bis(tert-butylbenzene) (1m):



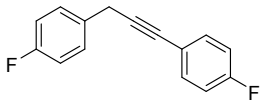
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.38 (d, J = 8.4 Hz, 2H), 7.35 (s, 4H), 7.31 (d, J = 8.4 Hz, 2H), 3.79 (s, 2H), 1.32 (s, 9H), 1.30 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 150.9, 149.5, 133.9, 131.3, 127.6, 125.4, 125.2, 120.7, 87.0, 82.5, 34.7, 34.4, 31.4, 31.2, 25.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{29}$: 305.2264, found :305.2259

4,4''-(prop-1-yne-1,3-diyl)di-1,1'-biphenyl (1n):



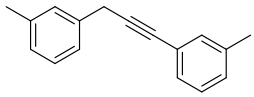
Yellow solid. M.p.: 98.3-100.2 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.60 – 7.57 (m, 6H), 7.55 – 7.52 (m, 4H), 7.50 (d, J = 7.9 Hz, 2H), 7.43 (t, J = 7.6 Hz, 4H), 7.34 (m, J = 7.4, 3.5 Hz, 2H), 3.90 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 140.9, 140.6, 140.5, 139.7, 135.9, 132.1, 128.9, 128.8, 128.4, 127.6, 127.4, 127.2, 127.1, 127.0, 127.0, 122.6, 88.2, 82.6, 25.6. HRMS (ESI): calculated $[M+H]^+$ for $C_{27}H_{21}$: 345.1638, found :345.1633

4,4'-(prop-1-yne-1,3-diyl)bis(fluorobenzene) (1o):



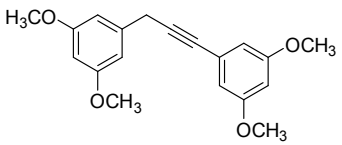
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.32 (dd, J = 8.7, 5.5 Hz, 2H), 7.26 (dd, J = 8.4, 5.5 Hz, 2H), 6.91 (m, J = 20.2, 8.7 Hz, 4H), 3.68 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 162.2 (d, J = 247.4 Hz), 161.7 (d, J = 243.1 Hz), 133.4 (d, J = 8.1 Hz), 132.2 (d, J = 3.3 Hz), 129.3 (d, J = 8.0 Hz), 119.5 (d, J = 3.5 Hz), 115.5 (d, J = 22.2 Hz), 115.3 (d, J = 21.6 Hz), 86.9, 81.7, 24.9. HRMS (ESI): calculated $[M-H]^-$ for $C_{15}H_9F_2$: 227.0678, found :227.0675

3,3'-(prop-1-yne-1,3-diyl)bis(methylbenzene) (1p):



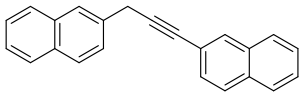
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.28 (s, 1H), 7.25 (d, J = 7.7 Hz, 1H), 7.22 (d, J = 6.6 Hz, 3H), 7.18 (t, J = 7.6 Hz, 1H), 7.10 (d, J = 7.7 Hz, 1H), 7.06 (d, J = 6.5 Hz, 1H), 3.79 (s, 2H), 2.36 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 138.2, 137.8, 136.7, 132.2, 128.7, 128.7, 128.6, 128.4, 128.1, 127.3, 125.0, 123.5, 87.3, 82.6, 25.6, 21.4, 21.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{17}H_{17}$: 221.1325, found :221.1323

5,5'-(prop-1-yne-1,3-diyl)bis(1,3-dimethoxybenzene) (1q):



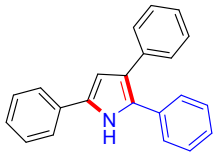
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 6.60 (d, J = 2.3 Hz, 2H), 6.57 (d, J = 2.3 Hz, 2H), 6.42 (s, 1H), 6.36 (s, 1H), 3.79 (s, 6H), 3.77 (s, 6H), 3.76 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 160.9, 160.4, 138.9, 124.9, 109.4, 106.1, 101.3, 98.6, 86.9, 82.6,55.3, 55.3, 25.9. HRMS (ESI): calculated $[M+H]^+$ for $C_{19}H_{21}O_4$: 313.1434, found :313.1429

2,2'-(prop-1-yne-1,3-diyl)dinaphthalene (1r):



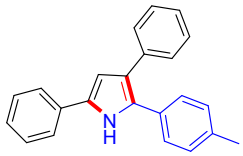
Yellow solid. M.p.: 107.2-110.5 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 7.98 (s, 1H), 7.89 (s, 1H), 7.82 (d, J = 8.5 Hz, 3H), 7.79 – 7.74 (m, 3H), 7.52 (d, J = 5.4 Hz, 2H), 7.45 (s, 4H), 4.02 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 134.2, 133.5, 133.0, 132.6, 132.4, 131.3, 128.7, 128.2, 127.9, 127.7, 127.6, 127.6, 126.5, 126.4, 126.4, 126.3, 126.1, 125.4, 120.9, 87.8, 83.2, 26.1. HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{17}$: 293.1325, found :293.1320

2,3,5-triphenyl-1*H*-pyrrole (3a):



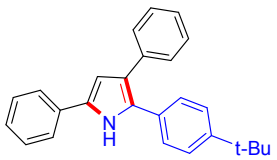
Yellow solid. M.p.: 126.6-128.4 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.35 (s, 1H), 7.47 (d, J = 8.1 Hz, 2H), 7.34 – 7.30 (m, 6H), 7.25 – 7.12 (m, 7H), 6.63 (d, J = 2.9 Hz, 1H); ^{13}C NMR (150MHz, $CDCl_3$) δ ppm 136.5, 133.2, 132.4, 132.4, 129.5, 129.1, 128.9, 128.6, 128.5, 127.6, 127.1, 126.7, 126.1, 124.0, 123.9, 108.7. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{18}N$: 296.1434, found :296.1431. The spectroscopic data are in agreement with literature data.[5]

3,5-diphenyl-2-(p-tolyl)-1*H*-pyrrole (3b):



Yellow solid. M.p.: 69.8-73.3 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.27 (s, 1H), 7.43 (d, J = 7.5 Hz, 2H), 7.34 – 7.25 (m, 4H), 7.23 – 7.15 (m, 4H), 7.15 – 7.08 (m, 2H), 7.04 (d, J = 7.8 Hz, 2H), 6.60 (s, 1H), 2.26 (s, 3H); ^{13}C NMR (150 MHz, Chloroform-*d*) δ ppm 136.8, 136.5, 132.3, 131.9, 130.2, 129.4, 128.9, 128.3, 128.3, 127.4, 126.4, 125.8, 123.7, 123.4, 108.4, 21.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{20}N$: 310.1590, found :310.1586. The spectroscopic data are in agreement with literature data.[5]

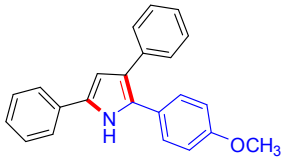
2-(4-(tert-butyl)phenyl)-3,5-diphenyl-1*H*-pyrrole (3c):



Yellow solid. M.p.: 121.6-127.3 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.38 (s, 1H), 7.53 (d, J = 7.4 Hz, 2H), 7.44 – 7.36 (m, 4H), 7.33 (s, 4H), 7.29 (t, J = 7.6 Hz,

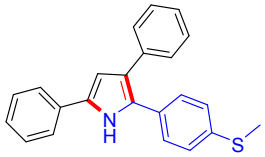
2H), 7.25 – 7.18 (m, 2H), 6.69 (d, J = 2.8 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (150 MHz, Chloroform-*d*) δ ppm 150.0, 136.6, 132.3, 131.9, 130.2, 129.4, 129.0, 128.4, 128.3, 127.1, 126.4, 125.7, 125.7, 123.7, 123.5, 108.5, 34.6, 31.3. HRMS (ESI): calculated $[M+H]^+$ for $C_{26}H_{26}N$: 352.2060, found :352.2056. The spectroscopic data are in agreement with literature data.[5]

1-(4-methoxyphenyl)-3,5-diphenyl-1*H*-pyrrole (3d):



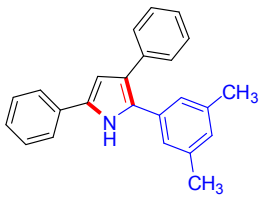
Yellow solid. M.p.: 95.2-98.4 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.25 (s, 1H), 7.43 (d, J = 7.5 Hz, 2H), 7.31 – 7.26 (m, 4H), 7.23 – 7.17 (m, 4H), 7.14 – 7.08 (m, 2H), 6.77 (d, J = 8.7 Hz, 2H), 6.60 (d, J = 2.7 Hz, 1H), 3.70 (s, 3H); ^{13}C NMR (150 MHz, Chloroform-*d*) δ ppm 158.7, 136.4, 132.3, 131.7, 129.3, 128.9, 128.3, 128.2, 126.3, 125.7, 125.7, 123.7, 123.0, 114.1, 108.2, 55.2; HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{20}NO$:326.1539 , found :326.1535. The spectroscopic data are in agreement with literature data.[5]

2-(4-(methylthio)phenyl)-3,5-diphenyl-1*H*-pyrrole (3e):



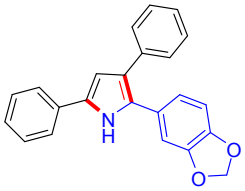
Yellow solid. M.p.: 165.0-169.3 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.40 (s, 1H), 7.55 – 7.52 (m, 2H), 7.40 – 7.37 (m, 4H), 7.31 – 7.27 (m, 4H), 7.22 (m, J = 7.4, 5.6 Hz, 2H), 7.18 (d, J = 8.4 Hz, 2H), 6.68 (d, J = 2.8 Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 137.1, 136.3, 132.2, 132.1, 129.8, 128.9, 128.8, 128.4, 128.3, 127.8, 126.6, 126.5, 126.0, 123.8, 123.8, 108.6, 15.6. HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{20}N_1S$:342.1311 , found :342.1308.

2-(3,5-dimethylphenyl)-3,5-diphenyl-1*H*-pyrrole (3f):



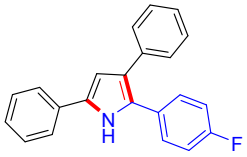
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.36 (s, 1H), 7.52 (d, J = 7.6 Hz, 2H), 7.40 (d, J = 7.4 Hz, 2H), 7.37 (t, J = 7.7 Hz, 2H), 7.27 (t, J = 7.6 Hz, 2H), 7.22 – 7.16 (m, 2H), 7.01 (s, 2H), 6.89 (s, 1H), 6.68 (d, J = 2.8 Hz, 1H), 2.25 (s, 6H); ^{13}C NMR (150 MHz, Chloroform-*d*) δ ppm 138.2, 136.4, 133.0, 132.3, 131.9, 129.6, 128.9, 128.7, 128.3, 128.2, 126.4, 125.8, 125.3, 123.7, 123.5, 108.4, 21.3. HRMS (ESI): calculated $[M+H]^+$ for $C_{24}H_{22}N$: 324.1747, found :324.1744.

2-(benzo[*d*][1,3]dioxol-5-yl)-3,5-diphenyl-1*H*-pyrrole (3g):



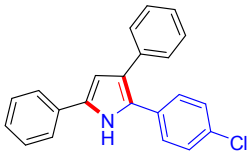
Yellow solid. M.p.: 108.6-113.6 ºC. ^{1}H NMR (600 MHz, Chloroform-d) δ ppm 8.26 (s, 1H), 7.45 (d, J = 7.7 Hz, 2H), 7.33 – 7.27 (m, 4H), 7.21 (t, J = 7.7 Hz, 2H), 7.16 – 7.10 (m, 2H), 6.80 (d, J = 8.0 Hz, 1H), 6.76 (s, 1H), 6.70 (d, J = 8.0 Hz, 1H), 6.59 (d, J = 2.9 Hz, 1H), 5.87 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 148.0, 146.9, 136.4, 132.4, 131.9, 129.3, 129.1, 128.5, 128.5, 127.3, 126.6, 126.0, 123.9, 123.4, 121.4, 108.8, 108.5, 108.4, 101.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{18}NO_2$: 340.1332, found :340.1330.

2-(4-fluorophenyl)-3,5-diphenyl-1*H*-pyrrole (3h):



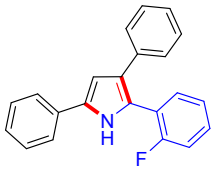
Yellow solid. M.p.: 105.9-107.9 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.34 (s, 1H), 7.52 (d, *J* = 6.8 Hz, 2H), 7.39 – 7.32 (m, 6H), 7.28 (t, *J* = 7.7 Hz, 2H), 7.24 – 7.19 (m, 2H), 7.00 (t, *J* = 8.6 Hz, 2H), 6.67 (d, *J* = 2.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 161.9 (d, *J* = 245.4 Hz), 136.1, 132.2 (d, *J* = 19.0 Hz), 129.3 (d, *J* = 8.1 Hz), 129.2 (d, *J* = 3.2 Hz), 129.0, 128.4, 128.3, 126.6, 126.0, 123.8, 123.8, 115.7 (d, *J* = 21.3 Hz), 108.4. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{17}FN$: 314.1340, found :314.1335. The spectroscopic data are in agreement with literature data.[5]

1-(4-chlorophenyl)-3,5-diphenyl-1*H*-pyrrole (3i):



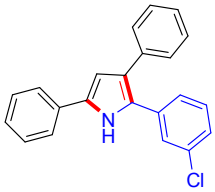
Yellow solid. M.p.: 94.4-100.3 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.34 (s, 1H), 7.51 (d, *J* = 7.3 Hz, 2H), 7.39 – 7.33 (m, 4H), 7.30 – 7.19 (m, 8H), 6.65 (d, *J* = 2.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 136.1, 132.7, 132.7, 132.1, 131.6, 129.1, 129.0, 128.7, 128.5, 128.5, 128.1, 126.8, 126., 1324.4, 124.0, 108.9. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{17}ClN$: 330.1044, found: 330.1040. The spectroscopic data are in agreement with literature data.[5]

2-(2-fluorophenyl)-3,5-diphenyl-1*H*-pyrrole (3j):



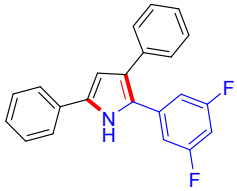
Yellow solid. M.p.: 75.1-80.4 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.80 (s, 1H), 7.54 (d, J = 7.3 Hz, 2H), 7.39 (t, J = 7.7 Hz, 4H), 7.33 – 7.17 (m, 6H), 7.17 – 7.10 (m, 1H), 6.98 (t, J = 7.5 Hz, 1H), 6.69 (d, J = 2.9 Hz, 1H); ^{13}C NMR (150 MHz, Chloroform-*d*) δ ppm 159.4 (d, J = 244.1 Hz), 136.5, 132.6, 132.1, 130.7 (d, J = 3.4 Hz), 129.0, 128.4, 128.4, 128.3, 126.7, 126.2, 125.8, 124.2 (d, J = 3.2 Hz), 123.9, 122.7, 120.4 (d, J = 12.6 Hz), 116.1 (d, J = 22.4 Hz), 108.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{17}FN$: 314.1340, found: 314.1336.

2-(3-chlorophenyl)-3,5-diphenyl-1*H*-pyrrole (3k):



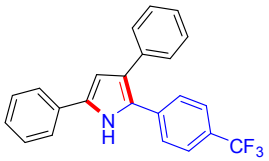
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.37 (s, 1H), 7.52 (d, J = 7.2 Hz, 2H), 7.37 (m, J = 15.8, 8.2 Hz, 5H), 7.29 (t, J = 8.4, 6.8 Hz, 2H), 7.25 – 7.16 (m, 5H), 6.66 (d, J = 2.9 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm136.0, 134.9, 134.6, 132.9, 132.1, 130.0, 129.1, 128.6, 127.8, 127.1, 126.9, 126.9, 126.4, 125.9, 124.9, 124.0, 109.0. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{17}ClN$: 330.1044, found: 330.1041.

2-(3,5-difluorophenyl)-3,5-diphenyl-1*H*-pyrrole (3l):



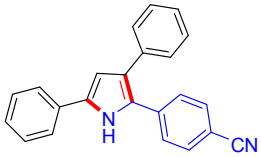
Yellow solid. M.p.: 106.4-112.4 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.34 (s, 1H), 7.48 (d, J = 8.4 Hz, 2H), 7.34 (t, J = 7.8 Hz, 2H), 7.30 (d, J = 6.8 Hz, 2H), 7.26 (t, J = 7.7 Hz, 2H), 6.80 (d, J = 6.6 Hz, 2H), 6.64 – 6.54 (m, 2H); ^{13}C NMR (150 MHz, Chloroform-*d*) δ ppm 164.0 (d, J = 13.5 Hz), 162.4 (d, J = 13.3 Hz), 135.9, 135.6, 132.5 (d, J = 219.2 Hz), 129.0, 128.6, 126.8 (d, J = 60.6 Hz), 126.7, 125.6, 124.0, 109.7 (d, J = 25.9 Hz), 109.7 (d, J = 15.0 Hz), 109.2, 102.0 (d, J = 50.6 Hz), 101.8. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{16}F_2N$: 332.1245, found: 332.1241.

3,5-diphenyl-2-(4-(trifluoromethyl)phenyl)-1*H*-pyrrole (3m):



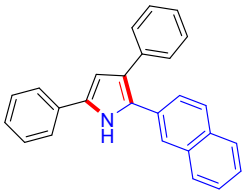
Yellow solid. M.p.: 79.4-83.6 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.37 (s, 1H), 7.45 (t, J = 6.9 Hz, 4H), 7.37 (d, J = 8.1 Hz, 2H), 7.32 (t, J = 7.7 Hz, 2H), 7.28 (d, J = 7.2 Hz, 2H), 7.23 (t, J = 7.5 Hz, 2H), 7.19 – 7.12 (m, 2H), 6.59 (d, J = 2.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 136.4, 135.9, 133.3, 131.8, 129.0, 128.5, 128.5, 127.5, 127.1, 126.9, 126.4, 125.6 (q, J = 3.8 Hz), 125.5, 124.2 (q, J = 270.4 Hz), 124.0, 109.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{17}F_3N$: 364.1308, found: 364.1304. The spectroscopic data are in agreement with literature data.[6]

4-(3,5-diphenyl-1*H*-pyrrol-2-yl)benzonitrile (3n):



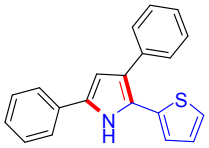
Yellow solid. M.p.: 168.6-170.0 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*)δ ppm 8.66 (s, 1H), 7.57 (d, J = 8.5 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 7.45 – 7.39 (m, 4H), 7.37 – 7.31 (m, 4H), 7.27 (m, J = 7.3 Hz, 2H), 6.66 (d, J = 2.7 Hz, 1H); ^{13}C NMR (150MHz, $CDCl_3$) δ ppm 137.3, 135.7, 134.1, 132.4, 131.6, 129.0, 128.6, 127.1, 127.0, 126.8, 126.5, 124.1, 119.1, 109.7, 109.3. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{17}N_2$: 321.1386, found: 321.1383.

2-(naphthalen-2-yl)-3,5-diphenyl-1*H*-pyrrole (3o):



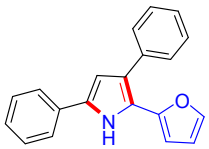
Yellow solid. M.p.: 122.8-127.5 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.44 (s, 1H), 7.82 (s, 1H), 7.74 (m, J = 15.5, 8.2 Hz, 2H), 7.68 (d, J = 8.5 Hz, 1H), 7.52 (d, J = 6.8 Hz, 2H), 7.47 – 7.33 (m, 7H), 7.27 – 7.15 (m, 4H), 6.71 (d, J = 2.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 136.4, 133.7, 132.7, 132.5, 132.3, 130.80, 129.4, 129.1, 128.6, 128.5, 128.3, 127.9, 127.6, 126.7, 126.5, 126.4, 126.2, 126.0, 125.4, 124.4, 124.0, 108.9. HRMS (ESI): calculated $[M+H]^+$ for $C_{26}H_{20}N$: 346.1590, found: 346.1586.

3,5-diphenyl-2-(thiophen-2-yl)-1*H*-pyrrole (3p):



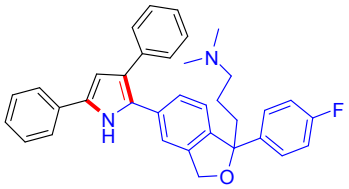
Yellow solid. M.p.: 93.8-99.0 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.37 (s, 1H), 7.52 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 8.4 Hz, 2H), 7.38 (t, J = 7.8 Hz, 2H), 7.32 (t, J = 7.9 Hz, 2H), 7.26 – 7.22 (m, 2H), 7.20 (d, J = 5.0 Hz, 1H), 7.03 – 7.00 (m, 1H), 6.98 (dd, J = 5.0, 3.5 Hz, 1H), 6.66 (d, J = 2.7 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 135.8, 134.8, 132.3, 131.9, 129.0, 128.6, 128.3, 127.4, 126.7, 126.3, 124.9, 124.8, 124.5, 123.8, 123.0, 108.5. HRMS (ESI): calculated $[M+H]^+$ for $C_{20}H_{16}NS$: 302.0998, found: 302.0995.

2-(furan-2-yl)-3,5-diphenyl-1*H*-pyrrole (3q):



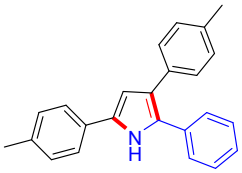
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.78 (s, 1H), 7.54 (d, J = 7.3 Hz, 4H), 7.41 – 7.36 (m, 5H), 7.29 (t, J = 7.4 Hz, 1H), 7.23 (t, J = 7.4 Hz, 1H), 6.60 (d, J = 3.0 Hz, 1H), 6.35 (dd, J = 3.4, 1.8 Hz, 1H), 6.28 (d, J = 3.4 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 147.3, 140.3, 136.1, 132.0, 131.9, 128.9, 128.7, 128.3, 126.6, 126.6, 124.1, 123.8, 120.6, 111.6, 108.7, 104.3. HRMS (ESI): calculated $[M+H]^+$ for $C_{20}H_{16}NO$: 286.1226, found: 286.1223.

3-(5-(3,5-diphenyl-1*H*-pyrrol-2-yl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-1-yl)-N,N-dimethylpropan-1-amine (3r):



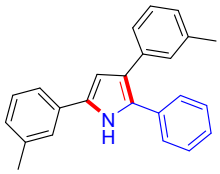
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.56 (s, 1H), 7.56 – 7.51 (m, 2H), 7.49 – 7.42 (m, 2H), 7.40 – 7.34 (m, 4H), 7.30 – 7.24 (m, 3H), 7.24 – 7.17 (m, 4H), 6.98 (t, J = 8.7 Hz, 2H), 6.67 (d, J = 2.8 Hz, 1H), 5.30 – 4.96 (m, 2H), 2.23 (t, J = 7.3 Hz, 2H), 2.20 – 2.07 (m, 2H), 2.12 (s, 6H), 1.53 – 1.34 (m, 2H); ^{13}C NMR (150 MHz, Chloroform-*d*) δ ppm 161.8 (d, J = 243.7 Hz), 142.9, 140.9 (d, J = 3.1 Hz), 139.6, 136.2, 132.8, 132.3, 132.1, 128.9, 128.9, 128.3, 127.0, 126.8, 126.7, 126.5, 125.9, 123.9, 123.8, 122.0, 120.0, 115.0 (d, J = 21.1 Hz), 108.6, 90.8, 71.7, 59.5, 45.2, 39.4, 22.1. HRMS (ESI): calculated $[M+H]^+$ for $C_{35}H_{34}FN_2O$: 517.2650, found: 517.2646.

2-phenyl-3,5-di-p-tolyl-1*H*-pyrrole (3s):



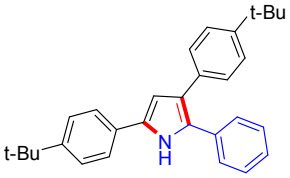
Yellow solid. M.p.: 132.4-134.3 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.18 (s, 1H), 7.28 (m, J = 14.8, 7.7 Hz, 4H), 7.19 – 7.16 (m, 4H), 7.11 (t, J = 7.4 Hz, 1H), 7.06 (d, J = 7.8 Hz, 2H), 6.98 (d, J = 7.7 Hz, 2H), 6.51 (d, J = 2.8 Hz, 1H), 2.23 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 136.1, 135.4, 133.4, 133.2, 132.3, 129.6, 129.4, 129.0, 128.6, 128.2, 127.3, 126.7, 123.7, 123.6, 108.1, 21.1. HRMS (ESI): calculated $[M+H]^+$ for $C_{24}H_{22}N$: 324.1747, found: 324.1744.

2-phenyl-3,5-di-m-tolyl-1*H*-pyrrole (3t):



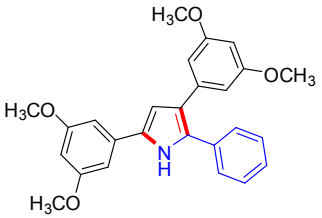
Yellow oil.^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.36 (s, 1H), 7.39 (d, J = 6.9 Hz, 2H), 7.36 – 7.30 (m, 3H), 7.30 – 7.20 (m, 4H), 7.16 (t, J = 5.8 Hz, 2H), 7.03 (m, J = 14.4, 6.8 Hz, 2H), 6.67 (d, J = 2.8 Hz, 1H), 2.39 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 138.5, 137.8, 136.3, 133.1, 132.3, 132.2, 129.1, 129.1, 128.8, 128.6, 128.1, 127.2, 127.3, 126.8, 126.7, 125.5, 124.5, 123.8, 120.9, 108.2, 21.5, 21.4. HRMS (ESI): calculated $[M+H]^+$ for $C_{24}H_{22}N$: 324.1747, found: 324.1745.

3,5-bis(4-(tert-butyl)phenyl)-2-phenyl-1*H*-pyrrole (3u):



Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.32 (s, 1H), 7.45 (d, J = 8.3 Hz, 2H), 7.42 – 7.39 (m, 4H), 7.33 – 7.28 (m, 6H), 7.24 – 7.20 (m, 1H), 6.63 (d, J = 2.8 Hz, 1H), 1.34 (s, 9H), 1.32 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 149.4, 148.6, 133.4, 133.4, 132.2, 129.5, 128.7, 128.6, 127.9, 127.4, 126.7, 125.8, 125.2, 123.6, 123.5, 108.3, 34.5, 34.4, 31.4, 31.3. HRMS (ESI): calculated $[M+H]^+$ for $C_{30}H_{34}N$: 408.2686, found: 408.2684.

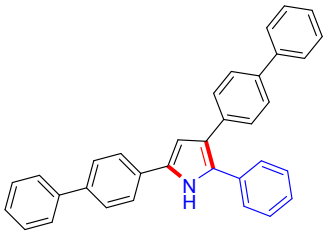
3,5-bis(3,5-dimethoxyphenyl)-2-phenyl-1*H*-pyrrole (3v):



Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.44 (s, 1H), 7.42 (d, J = 6.7 Hz, 2H), 7.33 (t, J = 7.7 Hz, 2H), 7.27 – 7.24 (m, 1H), 6.68 (t, J = 2.6 Hz, 3H), 6.55 (d, J = 2.3 Hz, 2H), 6.37 (s, 1H), 6.34 (s, 1H), 3.83 (s, 6H), 3.68 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 161.3, 160.6, 138.2, 134.1, 132.9, 132.0, 129.6, 128.6,

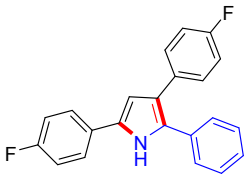
127.7, 127.1, 123.6, 108.7, 106.3, 102.2, 98.6, 98.6, 55.4, 55.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{26}H_{26}NO_4$: 416.1856, found: 416.1853.

3,5-di([1,1'-biphenyl]-4-yl)-2-phenyl-1*H*-pyrrole (3w):



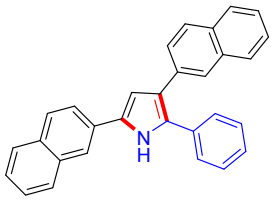
Yellow solid. M.p.: 203.7-209.2 ºC. ^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 11.51 (s, 1H), 7.91 (d, J = 8.1 Hz, 2H), 7.72 (t, J = 8.5 Hz, 4H), 7.68 (d, J = 7.7 Hz, 2H), 7.60 (d, J = 8.1 Hz, 2H), 7.49 – 7.44 (m, 6H), 7.41 – 7.39 (t, 3H), 7.38 – 7.29 (m, 4H), 6.89 (d, J = 2.7 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ ppm 139.8, 139.7, 137.3, 137.1, 135.7, 132.9, 131.7, 131.4, 129.9, 128.9, 128.9, 128.4, 128.3, 127.2, 127.1, 126.8, 126.8, 126.5, 126.3, 124.4, 122.2, 108.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{34}H_{26}N$: 448.2060, found: 448.2056.

3,5-bis(4-fluorophenyl)-2-phenyl-1*H*-pyrrole (3x):



Yellow solid. M.p.: 151.5-155.9 ºC. ^{1}H NMR (600 MHz, Chloroform-d) δ ppm 8.35 (s, 1H), 7.50 (dd, J = 8.5, 5.2 Hz, 2H), 7.36 (d, J = 6.9 Hz, 2H), 7.34 – 7.31 (m, 4H), 7.28 – 7.25 (t, 1H), 7.09 (t, J = 8.6 Hz, 2H), 6.98 (t, J = 8.7 Hz, 2H), 6.58 (d, J = 2.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 161.7 (d, J = 244.6 Hz), 161.5 (d, J = 243.2 Hz), 132.7, 132.2(d, J = 3.0 Hz), 131.4, 129.8(d, J = 7.6 Hz), 129.2, 128.8, 128.5(d, J = 3.2 Hz), 127.4, 127.1, 125.5(d, J = 7.6 Hz), 122.8, 116.0 (d, J = 21.6 Hz), 115.2(d, J = 21.1 Hz), 108.3. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{16}F_2N$: 332.1245, found: 332.1242.

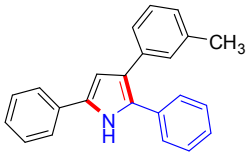
3,5-di(naphthalen-2-yl)-2-phenyl-1*H*-pyrrole (3y):



Yellow solid. M.p.: 139.2-142.0 ºC. ^{1}H NMR (600 MHz, Chloroform-d) δ ppm 8.61 (s, 1H), 7.93 (d, J = 9.9 Hz, 2H), 7.89 – 7.78 (m, 4H), 7.78 – 7.70 (m, 3H), 7.55 – 7.39 (m, 7H), 7.33 (t, J = 7.4 Hz, 2H), 7.27 (t, J = 7.3 Hz, 1H), 6.93 (d, J = 2.8 Hz, 1H); ^{13}C NMR (150 MHz, Chloroform-d) δ ppm 133.9, 133.8, 133.8, 133.0, 132.4, 132.3, 132.0, 130.1, 129.5, 128.8, 128.7, 127.8, 127.8, 127.7, 127.7, 127.6, 127.5,

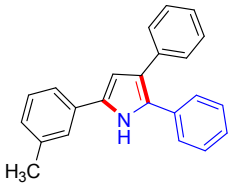
127.5, 127.1, 126.6, 126.4, 125.9, 125.6, 125.3, 124.0, 123.0, 121.1, 109.4. HRMS (ESI): calculated $[M+H]^+$ for $C_{30}H_{22}N$: 396.1747, found: 396.1743.

2,5-diphenyl-3-(m-tolyl)-1*H*-pyrrole (3aa):



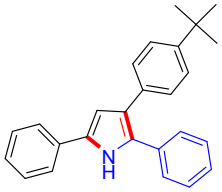
Yellow oil. ^1H NMR (600 MHz, Chloroform-*d*) δ ppm 8.42 (s, 1H), 7.55 (d, J = 8.2 Hz, 2H), 7.43 – 7.37 (m, 4H), 7.32 (t, J = 7.8 Hz, 2H), 7.24 (m, J = 7.6 Hz, 3H), 7.17 (d, J = 5.1 Hz, 2H), 7.03 (d, J = 3.6 Hz, 1H), 6.69 (d, J = 2.8 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 137.8, 136.2, 133.1, 132.2, 132.1, 129.2, 129.1, 128.9, 128.6, 128.2, 127.4, 126.9, 126.7, 126.5, 125.6, 123.9, 123.8, 108.6, 21.4. HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{20}N$: 310.1590, found: 310.1586.

2,3-diphenyl-5-(m-tolyl)-1*H*-pyrrole (3aa'):



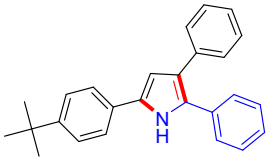
Yellow oil. ^1H NMR (600 MHz, Chloroform-*d*) δ ppm 8.40 (s, 1H), 7.40 (d, J = 8.3 Hz, 4H), 7.36 (d, J = 5.5 Hz, 1H), 7.34 (d, J = 5.6 Hz, 1H), 7.32 (s, 1H), 7.31 – 7.26 (m, 4H), 7.25 (d, J = 4.7 Hz, 1H), 7.21 (t, J = 7.4 Hz, 1H), 7.06 (d, J = 7.5 Hz, 1H), 6.69 (d, J = 2.9 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 138.6, 136.4, 133.1, 132.3, 132.1, 129.1, 128.9, 128.7, 128.4, 128.3, 127.4, 127.4, 126.9, 125.9, 124.5, 123.7, 120.9, 108.5, 21.5. HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{20}N$: 310.1590, found: 310.1585.

3-(4-(tert-butyl)phenyl)-2,5-diphenyl-1*H*-pyrrole (3ba):



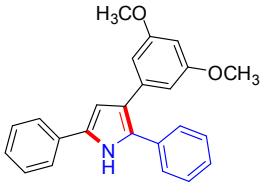
Yellow solid. M.p.: 115.4-119.5 ºC. ^1H NMR (400 MHz, Chloroform-*d*) δ ppm 8.33 (s, 1H), 7.45 (d, J = 8.6 Hz, 2H), 7.41 – 7.36 (m, 5H), 7.34 – 7.23 (m, 5H), 7.23 – 7.15 (m, 2H), 6.64 (d, J = 2.9 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 149.5, 136.4, 133.2, 132.4, 129.4, 128.9, 128.7, 128.4, 128.3, 127.4, 126.8, 125.8, 123.7, 123.6, 108.2, 34.5, 31.3. HRMS (ESI): calculated $[M+H]^+$ for $C_{26}H_{26}N$: 352.2060, found: 352.2056.

5-(4-(tert-butyl)phenyl)-2,3-diphenyl-1*H*-pyrrole (3ba'):



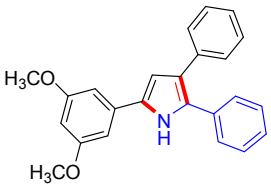
Yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ ppm 8.37 (s, 1H), 7.53 (d, J = 7.7 Hz, 2H), 7.44 – 7.36 (m, 4H), 7.35 – 7.29 (m, 6H), 7.27 – 7.21 (m, 2H), 6.69 (d, J = 2.8 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 148.7, 133.3, 132.3, 132.1, 129.1, 128.9, 128.7, 127.9, 127.5, 126.9, 126.4, 125.2, 123.7, 123.7, 108.6, 34.4, 31.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{26}H_{26}N$: 352.2060, found: 352.2057.

3-(3,5-dimethoxyphenyl)-2,5-diphenyl-1*H*-pyrrole (3ca):



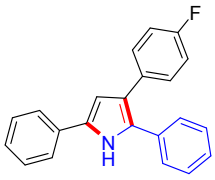
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.44 (s, 1H), 7.54 (d, J = 7.7 Hz, 2H), 7.43 (d, J = 8.4 Hz, 2H), 7.39 (t, J = 7.8 Hz, 2H), 7.33 (t, J = 7.7 Hz, 2H), 7.26 – 7.22 (m, 2H), 6.70 (d, J = 2.8 Hz, 1H), 6.56 (d, J = 2.3 Hz, 2H), 6.34 (t, J = 2.3 Hz, 1H), 3.68 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 160.6, 138.2, 132.9, 132.1, 129.6, 129.0, 128.6, 127.7, 127.1, 126.5, 123.8, 123.7, 108.3, 106.3, 98.6, 55.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{24}H_{22}NO_2$: 356.1645, found: 356.1642.

5-(3,5-dimethoxyphenyl)-2,3-diphenyl-1*H*-pyrrole (3ca'):



Yellow solid. M.p.: 121.3-124.1 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.41 (s, 1H), 7.39 (d, J = 8.1 Hz, 4H), 7.32 (t, J = 7.6 Hz, 2H), 7.28 (t, J = 7.7 Hz, 2H), 7.25 (d, J = 5.6 Hz, 1H), 7.21 (t, J = 7.3 Hz, 1H), 6.69 (dd, J = 5.2, 2.4 Hz, 3H), 6.37 (s, 1H), 3.84 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 161.3, 136.3, 134.1, 133.0, 132.1, 129.3, 128.7, 128.4, 128.3, 127.5, 127.0, 125.9, 123.7, 108.9, 102.3, 98.5, 55.4. HRMS (ESI): calculated $[M+H]^+$ for $C_{24}H_{22}NO_2$: 356.1645, found: 356.1640.

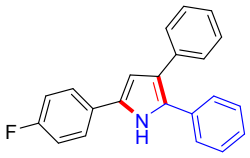
3-(4-fluorophenyl)-2,5-diphenyl-1*H*-pyrrole (3da):



Yellow solid. M.p.: 138.0-143.1 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ ppm 8.27 (s, 1H), 7.45 – 7.41 (m, 2H), 7.34 – 7.29 (m, 4H), 7.28 – 7.17 (m, 6H), 7.14 (t, J = 7.4 Hz, 1H),

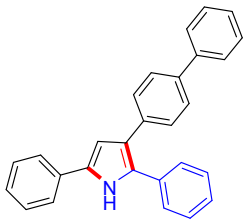
7.02 (t, J = 8.7 Hz, 2H), 6.55 (d, J = 2.9 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 161.7 (d, J = 244.8 Hz), 136.2, 133.0, 131.4, 129.3, 128.7, 128.6 (d, J = 3.1 Hz), 128.4, 128.3, 127.5, 127.0, 126.0, 125.5 (d, J = 8.0 Hz), 123.8, 116.0 (d, J = 21.7 Hz), 108.5. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{17}FN$: 314.1340, found: 314.1335. The spectroscopic data are in agreement with literature data.[5]

5-(4-fluorophenyl)-2,3-diphenyl-1*H*-pyrrole (3da'):



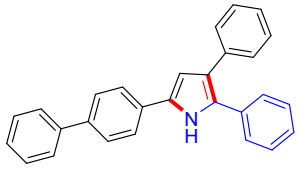
Yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ ppm 8.34 (s, 1H), 7.47 (d, J = 7.1 Hz, 2H), 7.37 – 7.28 (m, 4H), 7.28 – 7.23 (m, 4H), 7.22 – 7.09 (m, 2H), 6.91 (t, J = 8.7 Hz, 2H), 6.58 (d, J = 2.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 161.2 (d, J = 243.2 Hz), 132.9, 132.4 (d, J = 3.3 Hz), 132.2(d, J = 24.4 Hz), 129.9, 129.8, 129.2, 129.0, 128.8, 127.4, 127.1, 126.6, 123.8, 122.8, 115.2 (d, J = 21.1 Hz), 108.5. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{17}FN$: 314.1340, found: 314.1336.

3-([1,1'-biphenyl]-4-yl)-2,5-diphenyl-1*H*-pyrrole (3ea):



Yellow solid. M.p.: 91.3-96.3 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ ppm 8.30 (s, 1H), 7.52 (d, J = 7.1 Hz, 2H), 7.46 – 7.42 (m, 4H), 7.39 – 7.29 (m, 8H), 7.27 (d, J = 6.3 Hz, 1H), 7.25 – 7.22 (m, 2H), 7.19 – 7.16 (t, 1H), 7.13 (t, J = 11.0 Hz, 1H), 6.64 (d, J = 2.8 Hz, 1H); ^{13}C NMR (100 MHz, CDCl3) δ ppm140.9, 138.5, 135.4, 133.1, 132.3, 132.1, 129.5, 129.0, 128.7, 128.6, 127.6, 127.0, 127.0, 127.0, 126.8, 126.5, 123.8, 123.3, 108.4. HRMS (ESI): calculated $[M+H]^+$ for $C_{28}H_{22}N$: 372.1747, found: 372.1745.

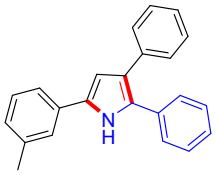
5-([1,1'-biphenyl]-4-yl)-2,3-diphenyl-1*H*-pyrrole (3ea'):



Yellow solid. M.p.: 151.3-156.8 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 11.47 (s, 1H), 7.90 (d, J = 8.3 Hz, 2H), 7.73 – 7.68 (t, 4H), 7.45 (m, J = 13.8, 7.3 Hz, 4H), 7.37 – 7.25 (m, 8H), 7.18 (t, J = 7.0 Hz, 1H), 6.83 (d, J = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ ppm 139.7, 137.3, 136.6, 132.9, 131.6, 131.4, 129.7, 128.9, 128.3, 128.1,

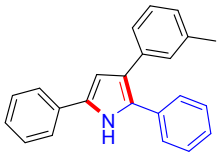
128.0, 127.2, 126.8, 126.7, 126.3, 125.6, 124.4, 122.8, 108.4. HRMS (ESI): calculated $[M+H]^+$ for $C_{28}H_{22}N$: 372.1747, found: 372.1743.

2,3-diphenyl-5-(m-tolyl)-1*H*-pyrrole (3ab):



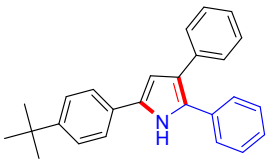
Yellow oil. ^1H NMR (600 MHz, Chloroform-*d*) δ ppm 8.38 (s, 1H), 7.39 (d, J = 7.6 Hz, 4H), 7.36 – 7.18 (m, 9H), 7.05 (d, J = 7.5 Hz, 1H), 6.68 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 138.5, 136.4, 133.1, 132.3, 132.1, 129.1, 128.8, 128.7, 128.4, 128.3, 127.4, 127.3, 126.9, 125.9, 124.5, 123.7, 120.9, 108.5, 21.5. HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{20}N$: 310.1590, found: 310.1586.

2,5-diphenyl-3-(m-tolyl)-1*H*-pyrrole (3ab'):



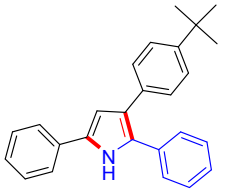
Yellow oil. ^1H NMR (600 MHz, Chloroform-*d*) δ ppm 8.39 (s, 1H), 7.54 (d, J = 6.9 Hz, 2H), 7.41 – 7.37 (m, 4H), 7.31 (t, J = 7.7 Hz, 2H), 7.24 (m, J = 7.8 Hz, 3H), 7.18 – 7.15 (m, 2H), 7.03 (d, J = 3.4 Hz, 1H), 6.69 (d, J = 2.9 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 137.8, 136.2, 133.1, 132.2, 132.1, 129.2, 129.1, 128.9, 128.6, 128.2, 127.4, 126.9, 126.7, 126.5, 125.6, 123.9, 123.8, 108.7, 21.4. HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{20}N$: 310.1590, found: 310.1587.

5-(4-(tert-butyl)phenyl)-2,3-diphenyl-1*H*-pyrrole (3ac):



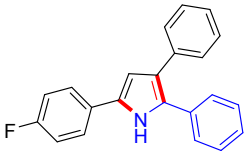
Yellow oil. ^1H NMR (400 MHz, Chloroform-*d*) δ ppm 8.36 (s, 1H), 7.52 (dd, J = 8.3, 1.3 Hz, 2H), 7.43 – 7.35 (m, 4H), 7.34 – 7.28 (m, 6H), 7.26 – 7.20 (m, 2H), 6.68 (d, J = 2.9 Hz, 1H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 148.7, 133.3, 133.2, 132.2, 132.0, 129.1, 128.9, 128.6, 127.9, 127.5, 126.8, 126.4, 125.2, 123.7, 123.7, 108.6, 34.4, 31.2. HRMS (ESI): calculated $[M+H]^+$ for $C_{26}H_{26}N$: 352.2060, found: 352.2057.

3-(4-(tert-butyl)phenyl)-2,5-diphenyl-1*H*-pyrrole (3ac'):



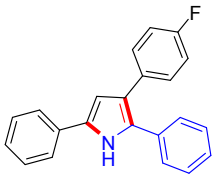
Yellow solid. M.p.: 115.8-118.7 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ ppm 8.37 (s, 1H), 7.47 (d, J = 8.5 Hz, 2H), 7.43 – 7.38 (m, 5H), 7.30 (m, J = 12.9, 7.4 Hz, 5H), 7.24 – 7.17 (m, 2H), 6.65 (d, J = 2.8 Hz, 1H), 1.34 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 149.6, 136.4, 133.2, 132.4, 129.5, 128.9, 128.7, 128.4, 128.3, 127.4, 126.8, 125.9, 123.7, 123.6, 108.2, 34.5, 31.3. HRMS (ESI): calculated $[M+H]^+$ for $C_{26}H_{26}N$:352.2060, found: 352.2058.

5-(4-fluorophenyl)-2,3-diphenyl-1*H*-pyrrole (3ad):



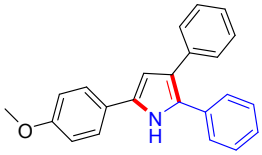
Yellow oil. ^{1}H NMR (400 MHz, Chloroform-d) δ ppm 8.33 (s, 1H), 7.49 (dd, J = 8.8, 5.2 Hz, 2H), 7.38 (d, J = 8.4 Hz, 4H), 7.35 – 7.23 (m, 6H), 7.21 (t, J = 7.3 Hz, 1H), 7.09 (t, J = 8.7 Hz, 2H), 6.62 (d, J = 2.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.7 (d, J = 244.5 Hz), 136.2, 133.0, 131.4, 129.3, 128.7, 128.6 (d, J = 3.2 Hz), 128.4, 128.3, 127.5, 127.0, 126.0, 125.5 (d, J = 7.8 Hz), 123.8, 115.9 (d, J = 21.6 Hz), 108.4. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{17}FN$: 314.1340, found: 314.1336.

3-(4-fluorophenyl)-2,5-diphenyl-1*H*-pyrrole (3ad'):



Yellow solid. M.p.: 138.7-142.4 ºC. ^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.42 (s, 1H), 7.54 (d, J = 7.0 Hz, 2H), 7.40 (d, J = 7.5 Hz, 1H), 7.37 (t, J = 12.5 Hz, 2H), 7.35 – 7.31 (m, 4H), 7.25 (m, J = 7.4 Hz, 3H), 6.98 (t, J = 8.7 Hz, 2H), 6.65 (d, J = 2.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 161.5 (d, J = 243.2 Hz), 160.7, 132.9, 132.3 (d, J = 3.2 Hz), 132.3, 132.1, 129.9 (d, J = 7.6 Hz), 129.2, 129.0, 128.8, 127.4, 127.0, 126.6, 123.8, 122.8, 115.2 (d, J = 21.1 Hz), 108.4. HRMS (ESI): calculated $[M+H]^+$ for $C_{22}H_{17}FN$: 314.1340, found: 314.1336.

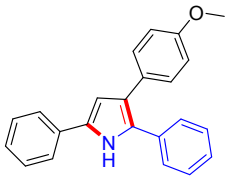
5-(4-methoxyphenyl)-2,3-diphenyl-1*H*-pyrrole(3ae):



Yellow oil.^{1}H NMR (600 MHz, Chloroform-*d*) δ ppm 8.39 (s, 1H), 7.53 (d, J = 6.8

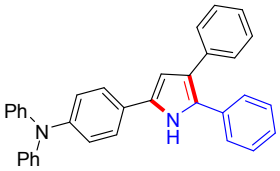
Hz, 2H), 7.38 (t, J = 7.7 Hz, 4H), 7.32 – 7.29 (m, 4H), 7.23 (m, J = 7.4 Hz, 2H), 6.84 (d, J = 8.7 Hz, 2H), 6.64 (d, J = 2.8 Hz, 1H), 3.79 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ ppm 158.0, 133.1, 132.2, 132.1, 129.5, 128.9, 128.8, 128.7, 127.3, 126.8, 126.4, 123.7, 123.5, 113.8, 108.5, 55.2; HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{20}NO$: 326.1539, found: 326.1534

3-(4-methoxyphenyl)-2,5-diphenyl-1*H*-pyrrole(3ae')：



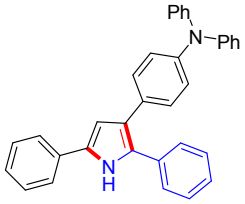
Yellow solid. M.p.: 71.4-75.7 ºC. ^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 11.26 (s, 1H), 7.72 (d, J = 8.7 Hz, 2H), 7.40 (d, J = 7.0 Hz, 2H), 7.33 (t, J = 7.6 Hz, 2H), 7.26 (m, J = 14.6, 7.0 Hz, 5H), 7.16 (t, J = 7.0 Hz, 1H), 6.96 (d, J = 8.7 Hz, 2H), 6.62 (d, J = 2.7 Hz, 1H), 3.78 (s, 3H); ^{13}C NMR (150 MHz, DMSO) δ ppm 157.7, 136.8, 133.1, 132.1, 128.5, 128.2, 128.0, 127.9, 126.4, 125.5, 125.3, 125.2, 122.5, 114.1, 106.9, 55.1; HRMS (ESI): calculated $[M+H]^+$ for $C_{23}H_{20}NO$: 326.1539, found: 326.1535

4-(4,5-diphenyl-1*H*-pyrrol-2-yl)-N,N-diphenylaniline(3af):



Yellow solid. M.p.: 90.3-94.5 ºC.^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 11.31 (s, 1H), 7.72 (d, J = 8.6 Hz, 2H), 7.39 (d, J = 6.8 Hz, 2H), 7.34 – 7.28 (m, 7H), 7.27 – 7.23 (m, 4H), 7.16 (t, J = 6.7 Hz, 1H), 7.03 (t, J = 7.4 Hz, 6H), 7.00 (d, J = 8.6 Hz, 2H), 6.66 (d, J = 2.7 Hz, 1H); ^{13}C NMR (150 MHz, DMSO) δ ppm 147.2, 145.1, 136.6, 132.9, 131.8, 129.5, 129.0, 128.2, 128.0, 127.9, 127.2, 126.5, 125.5, 125.1, 123.9, 123.6, 122.8, 122.6, 107.5; HRMS (ESI): calculated $[M+H]^+$ for $C_{34}H_{27}N_2$: 463.2169, found: 463.2162

4-(2,5-diphenyl-1*H*-pyrrol-3-yl)-N,N-diphenylaniline(3af'):



Yellow solid. M.p.: 78.5-81.6 ºC.^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 11.35 (s, 1H), 7.78 (d, J = 7.8 Hz, 2H), 7.45 (d, J = 7.2 Hz, 2H), 7.36 (m, J = 9.0, 8.5 Hz, 4H), 7.28 (t, J = 7.2 Hz, 4H), 7.25 (d, J = 7.3 Hz, 1H), 7.22 (d, J = 8.3 Hz, 2H), 7.18 (d, 1H), 7.00 (d, J = 7.1 Hz, 6H), 6.90 (d, J = 8.1 Hz, 2H), 6.74 (d, J = 2.7 Hz, 1H); ^{13}C NMR (150 MHz, DMSO) δ ppm 147.2, 144.8, 133.0, 132.3, 131.9, 131.4, 129.4, 129.2,

128.8, 128.6, 128.3, 128.0, 126.6, 125.8, 123.9, 123.7, 123.5, 122.7, 122.2, 107.9; HRMS (ESI): calculated $[M+H]^+$ for $C_{34}H_{27}N_2$: 463.2169, found: 463.2162

References

[1] Zhang, H.; Sun, N.; Hu, B.; Shen, Z.; Hu. X.; Jin, L. Copper-catalyzed direct couplings of terminal alkynes with primary and secondary benzyl bromides. *Org. Chem. Front*. **2019**, *6*, 1983–1988.

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[3] Biradar, D.; Gau, H. Simple and efficient nickel-catalyzed cross-coupling reaction of alkynylalanes with benzylic and aryl bromides. *Chem. Commun*. **2011**, 47, 10467–10469

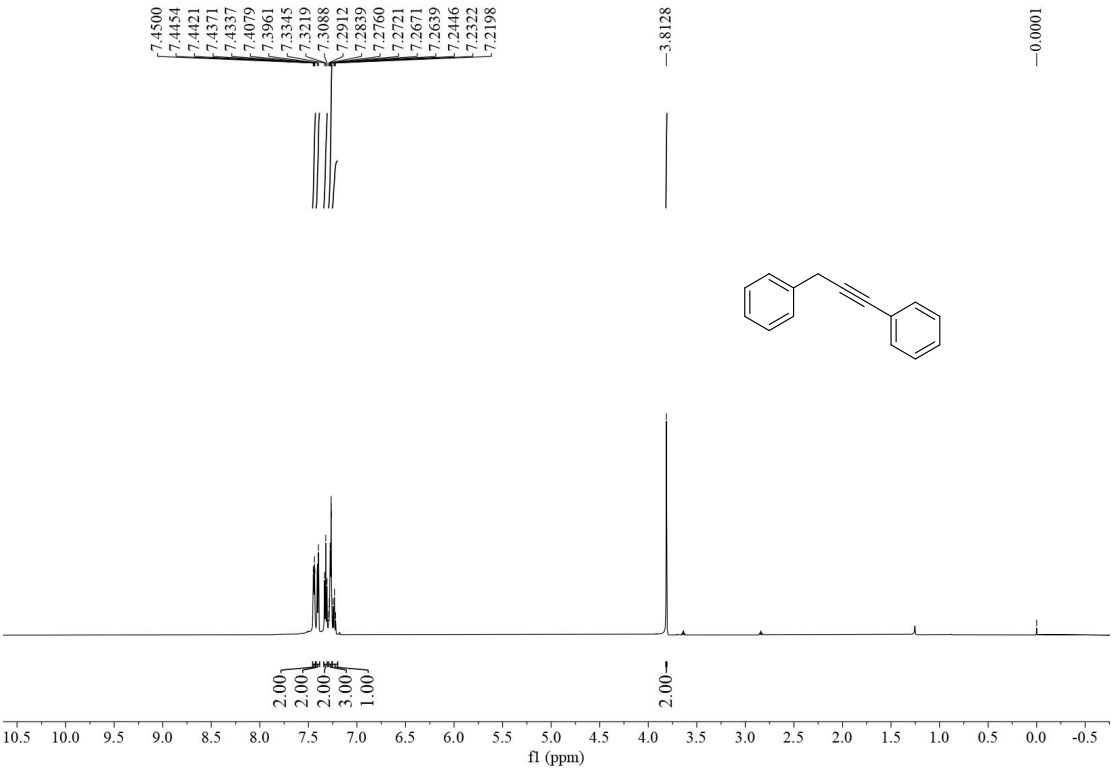
[4] Han, J.; San, H.; Guo, A.;Wang, L.; Tang, X. Boryl Radical-mediated C−H activation of inactivated alkanes for the synthesis of internal alkynes. *Adv. Synth. Catal*. **2021**, 363, 2366–2370.

[5] Zhao, M.; Ren Z.; Yang, D.; Guan, Z. Iron-catalyzed radical cycloaddition of 2 H-azirines and enamides for the synthesis of pyrroles. *Org. Lett*. **2018**, 205, 1287–1290.

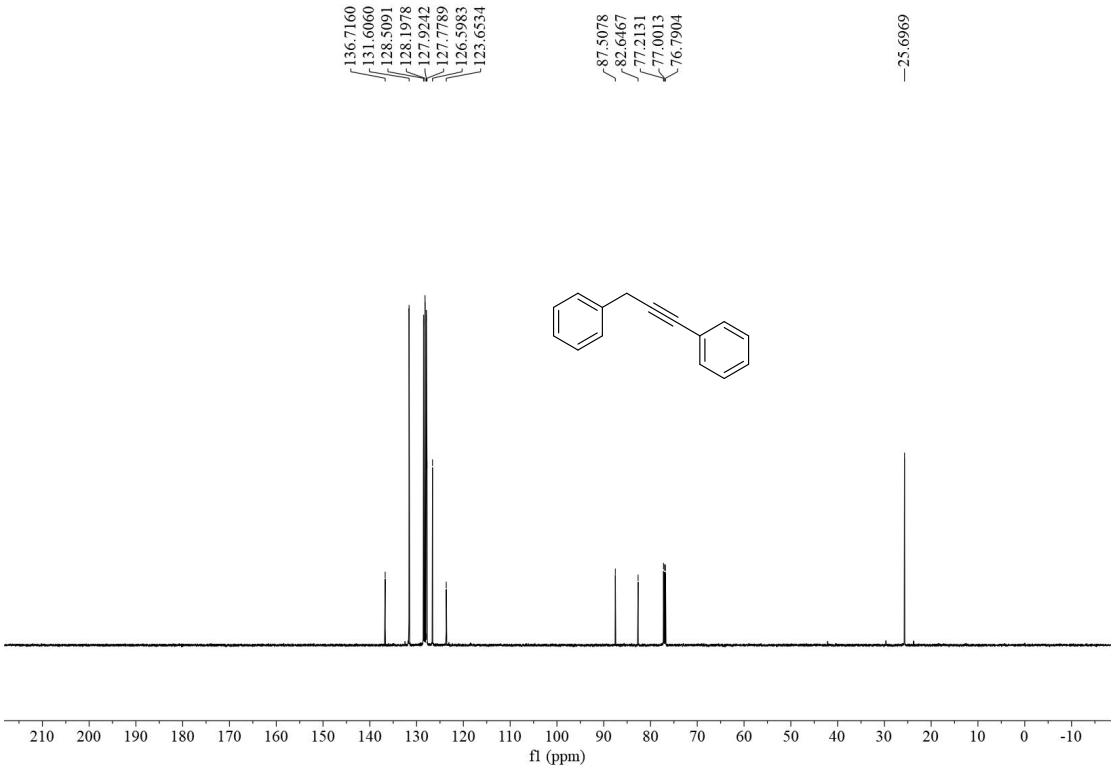
[6] Shen. J.; Cheng, G.; Cui, X. “One pot” regiospecific synthesis of polysubstituted pyrroles from benzylamines and ynones under metal free conditions. *Chem. Commun.* **2013**, 49, 10641–10643.

NMR Spectra for the compounds

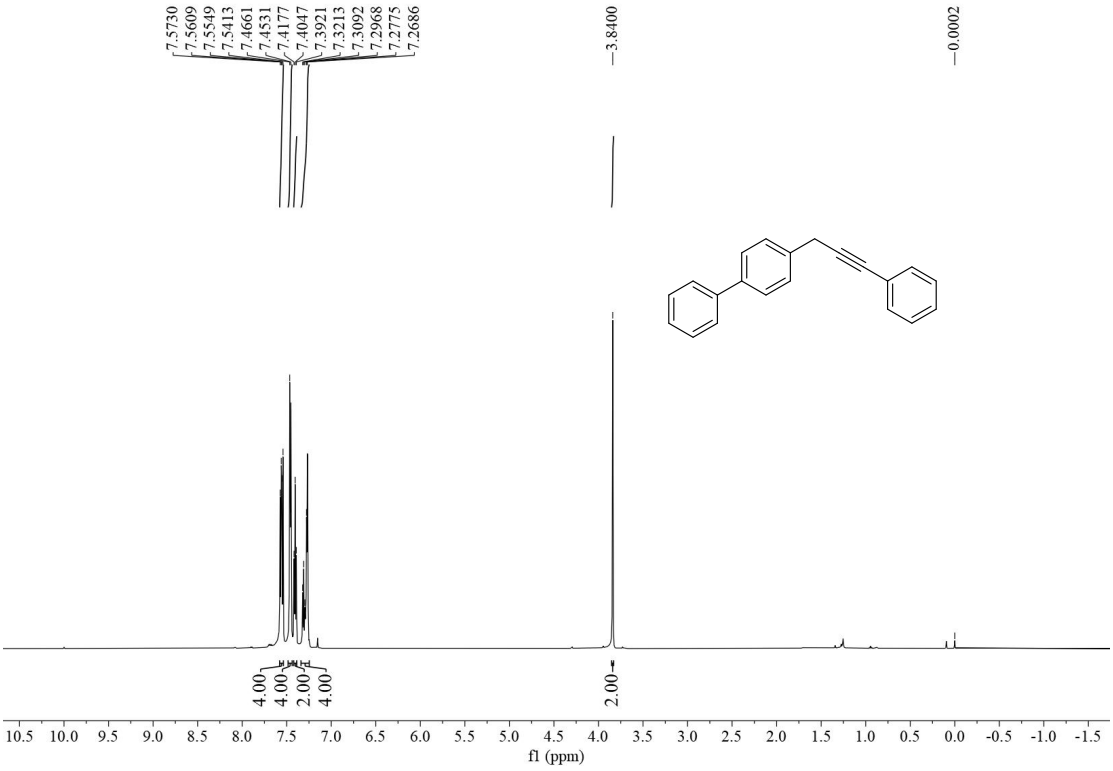
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1a



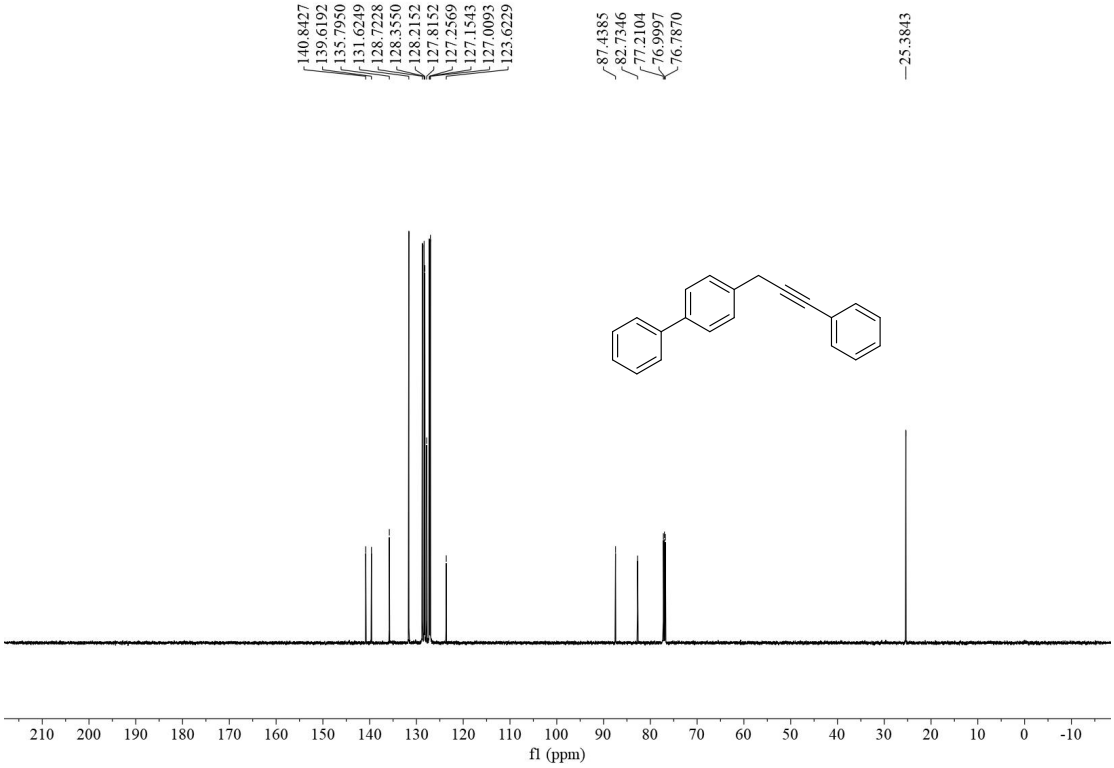
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1a



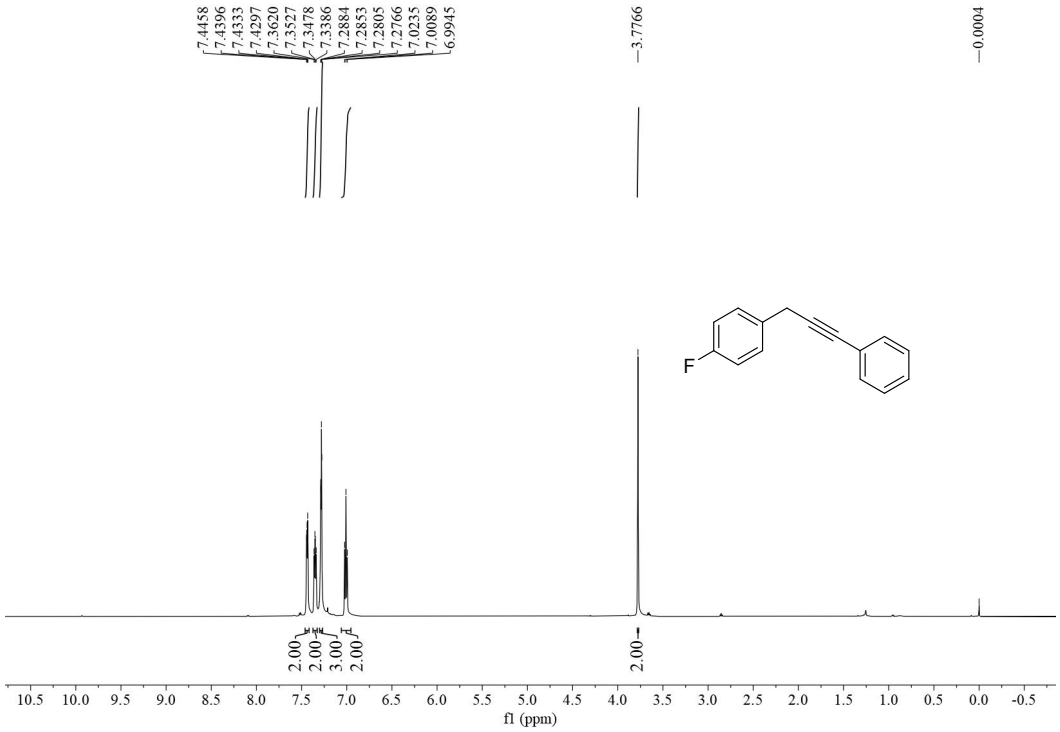
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1b



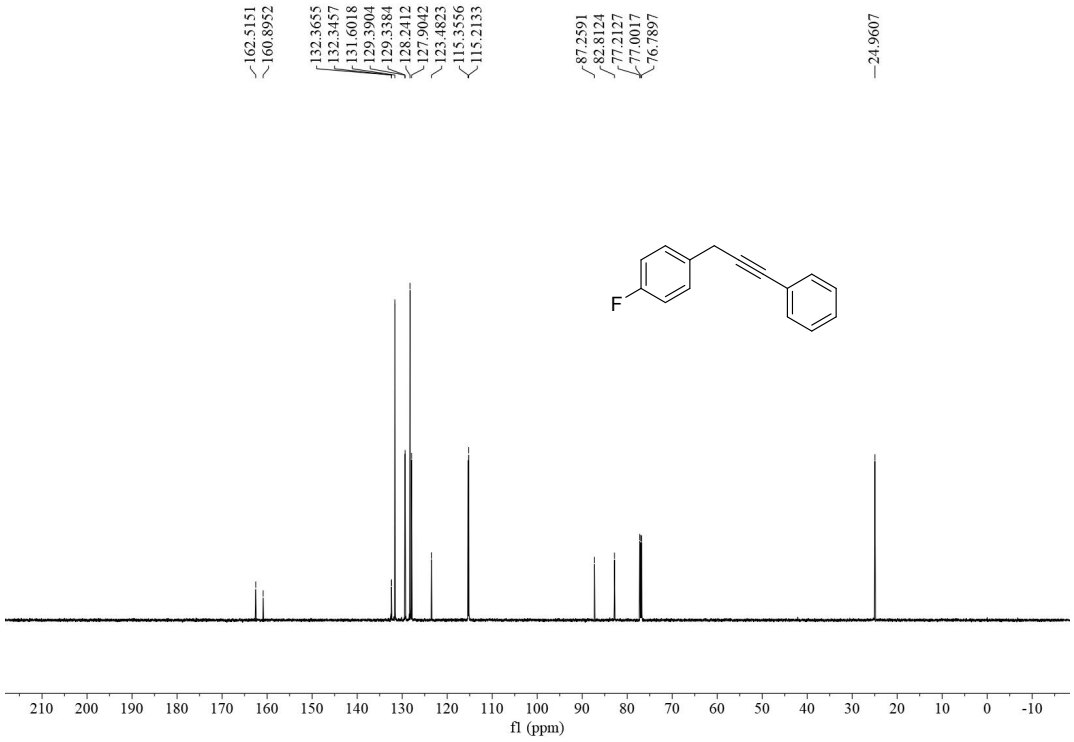
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1b



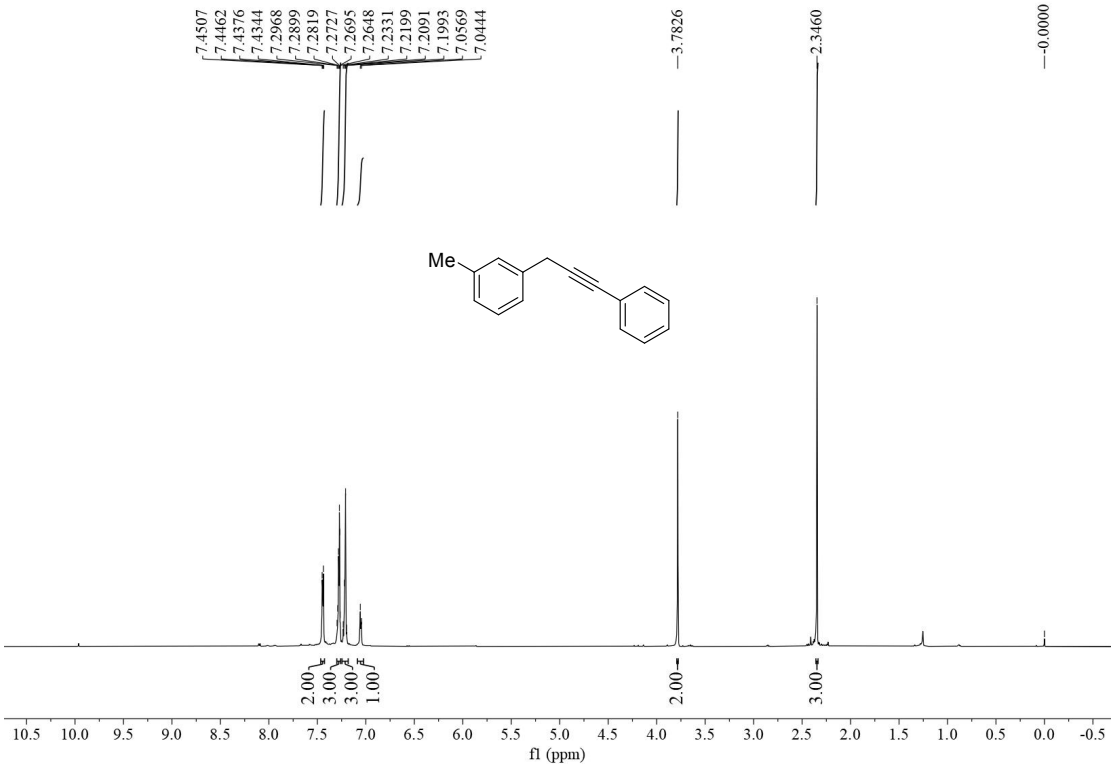
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1c



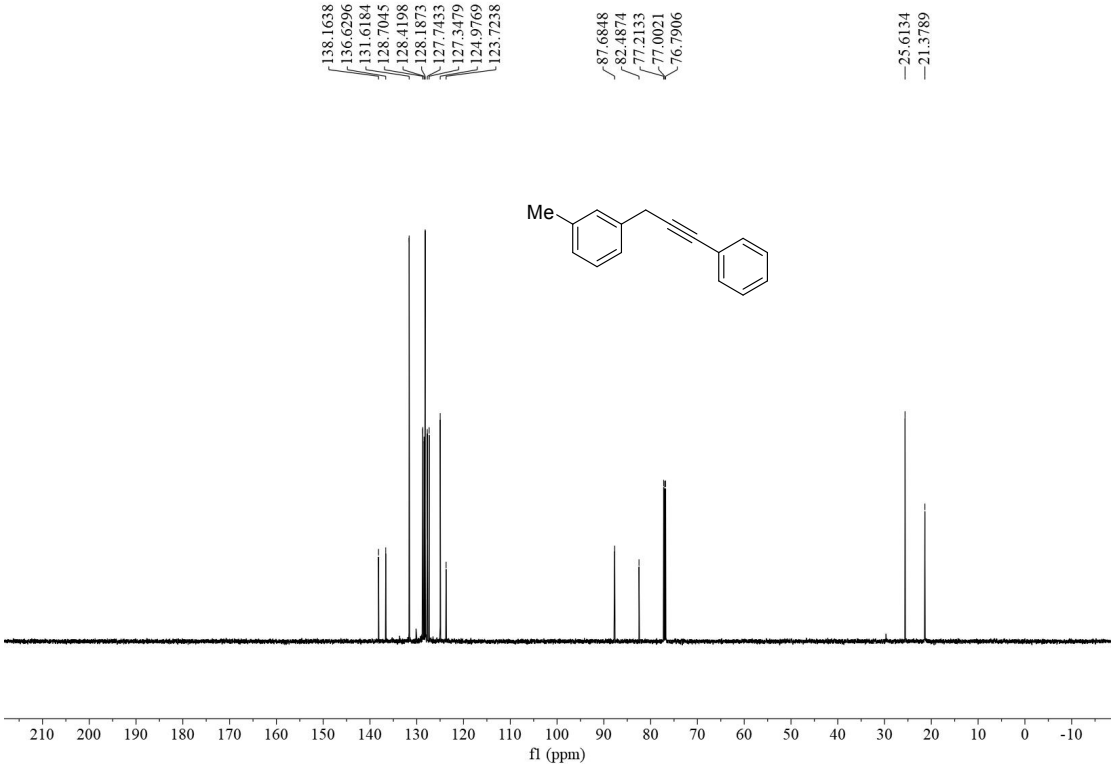
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1c



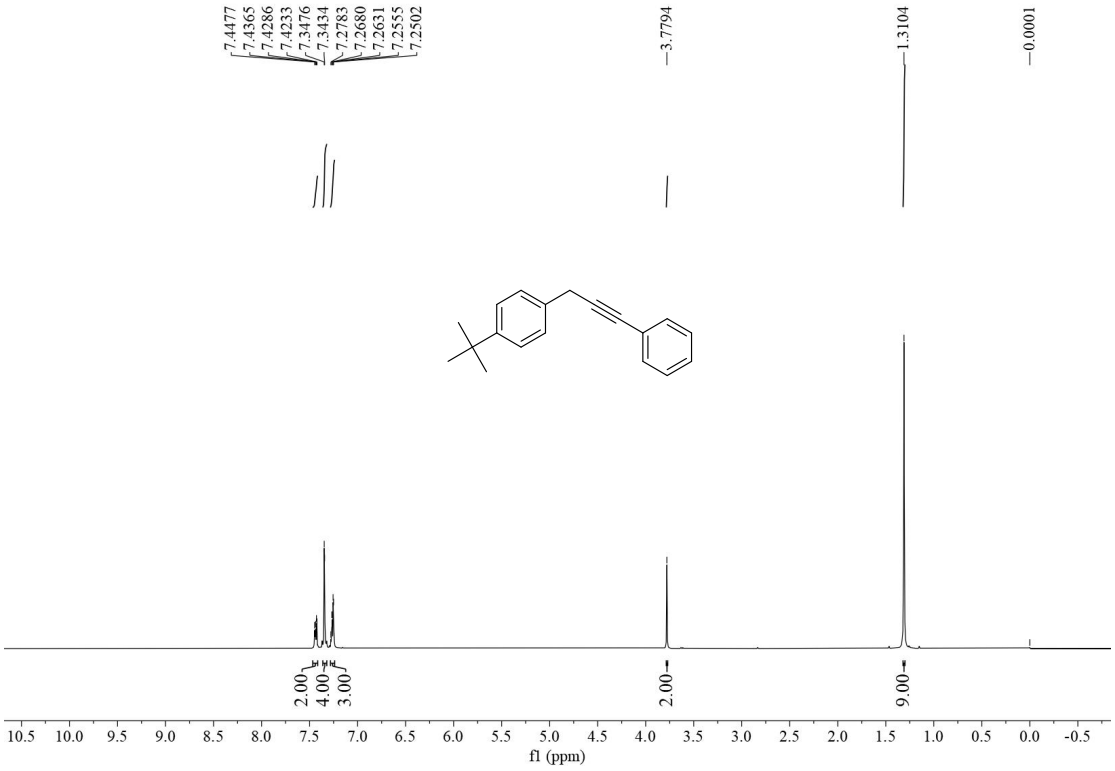
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1d



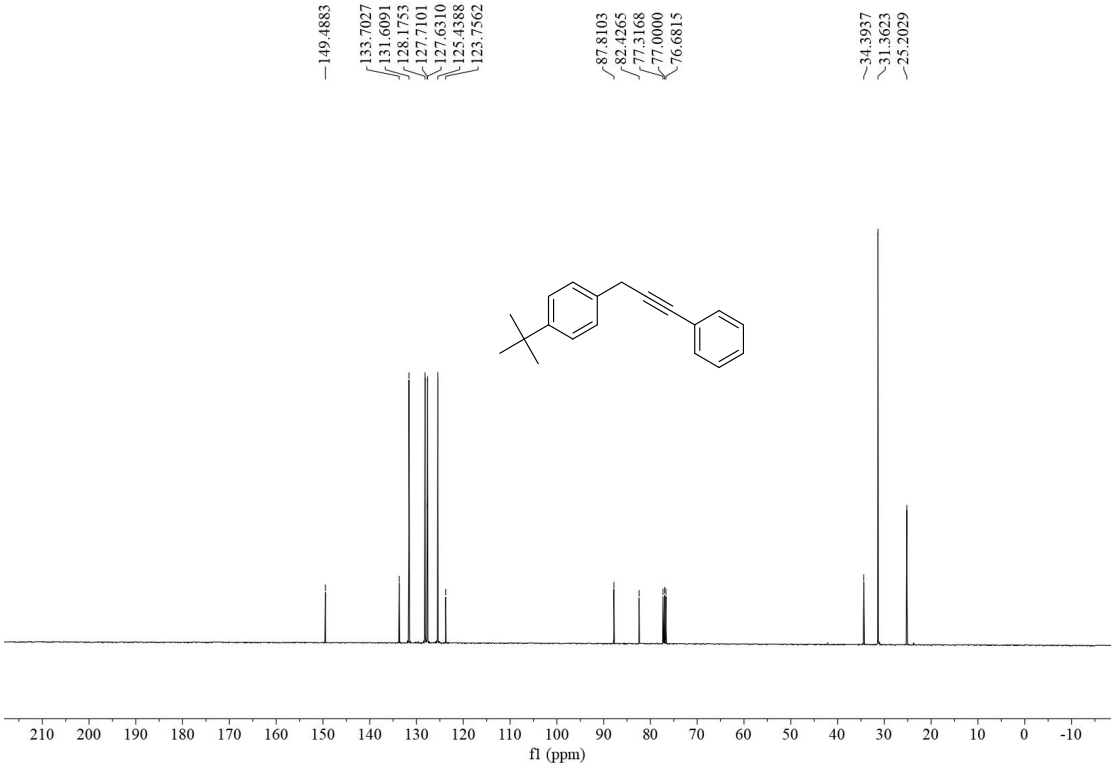
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1d



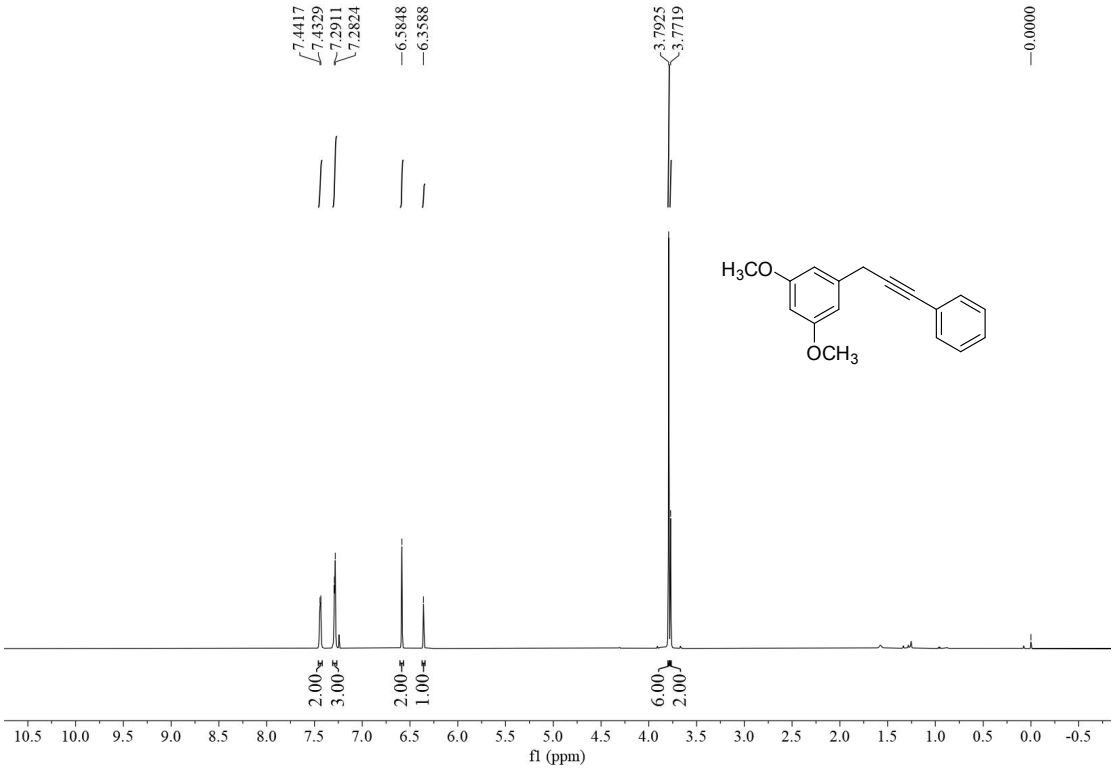
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 1e



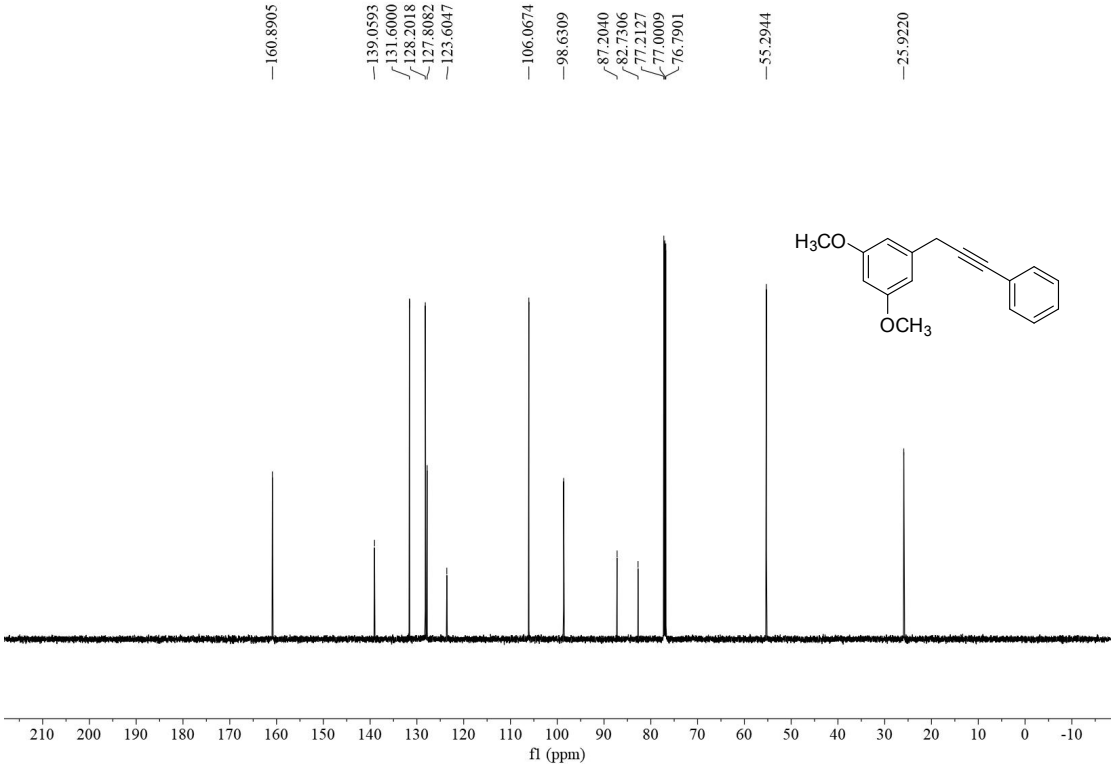
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 1e



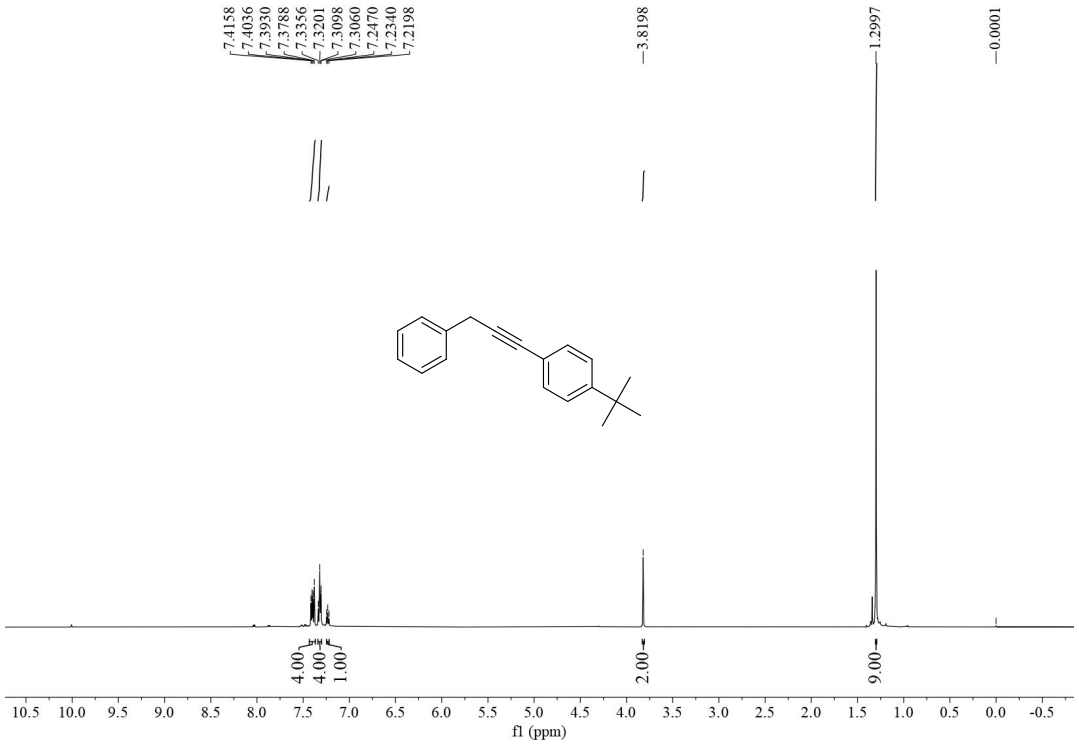
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1f



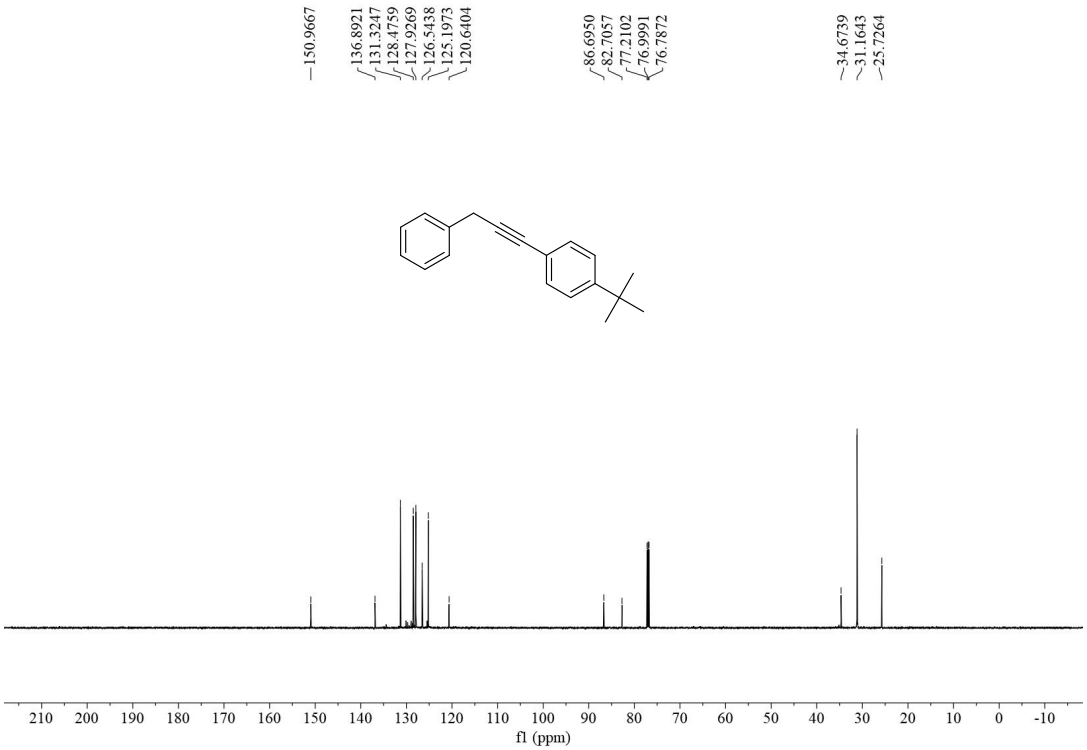
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1f



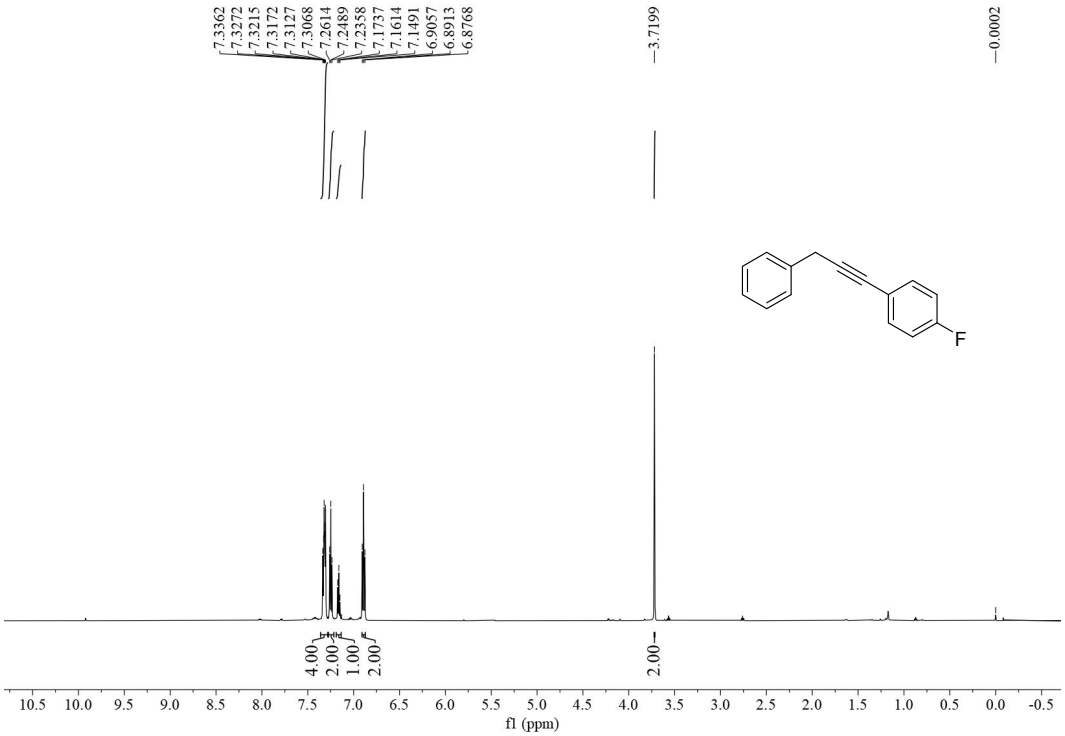
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1g



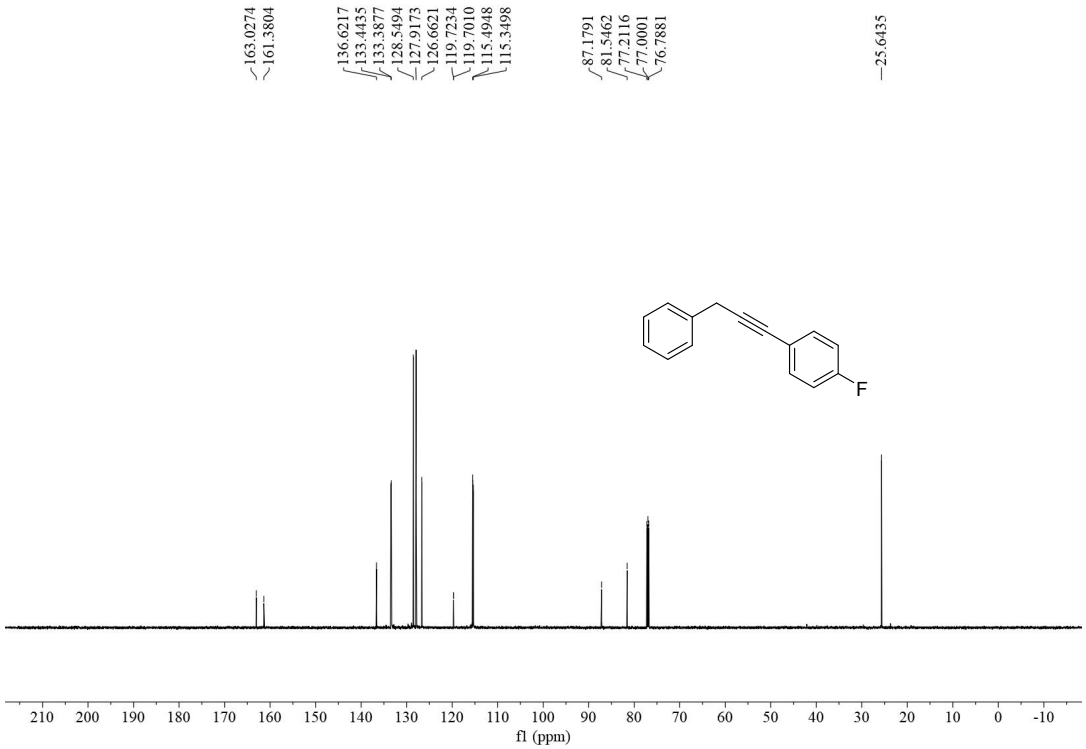
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1g



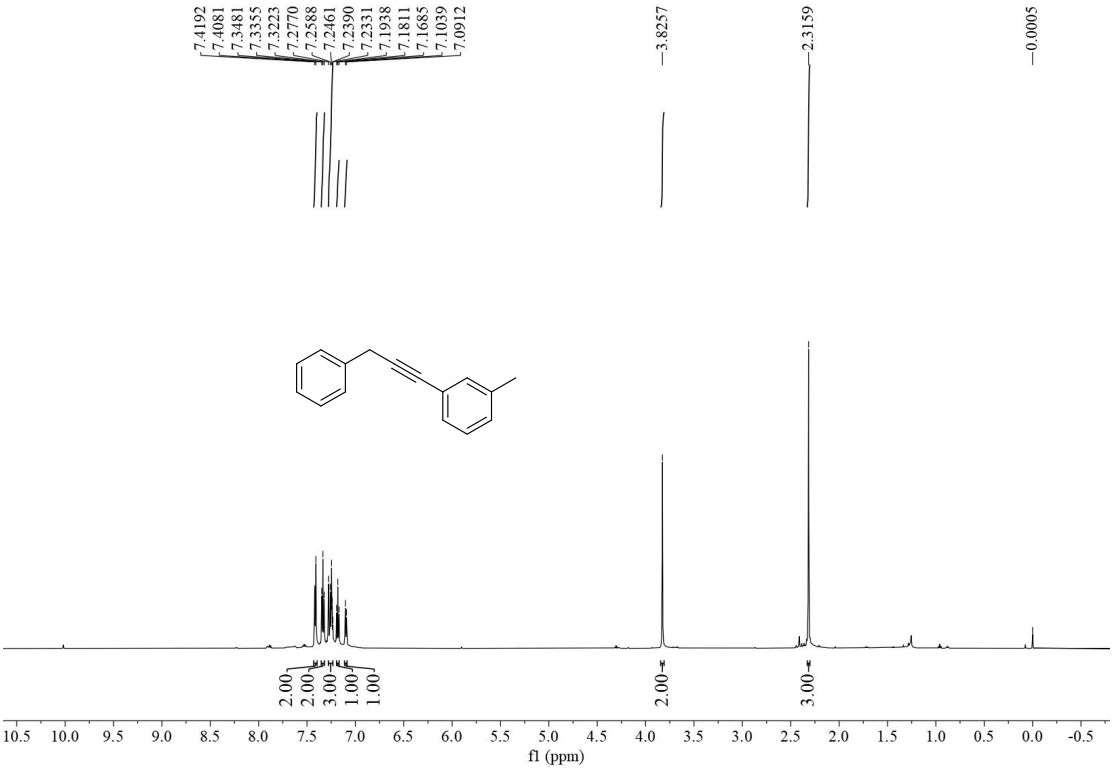
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1h



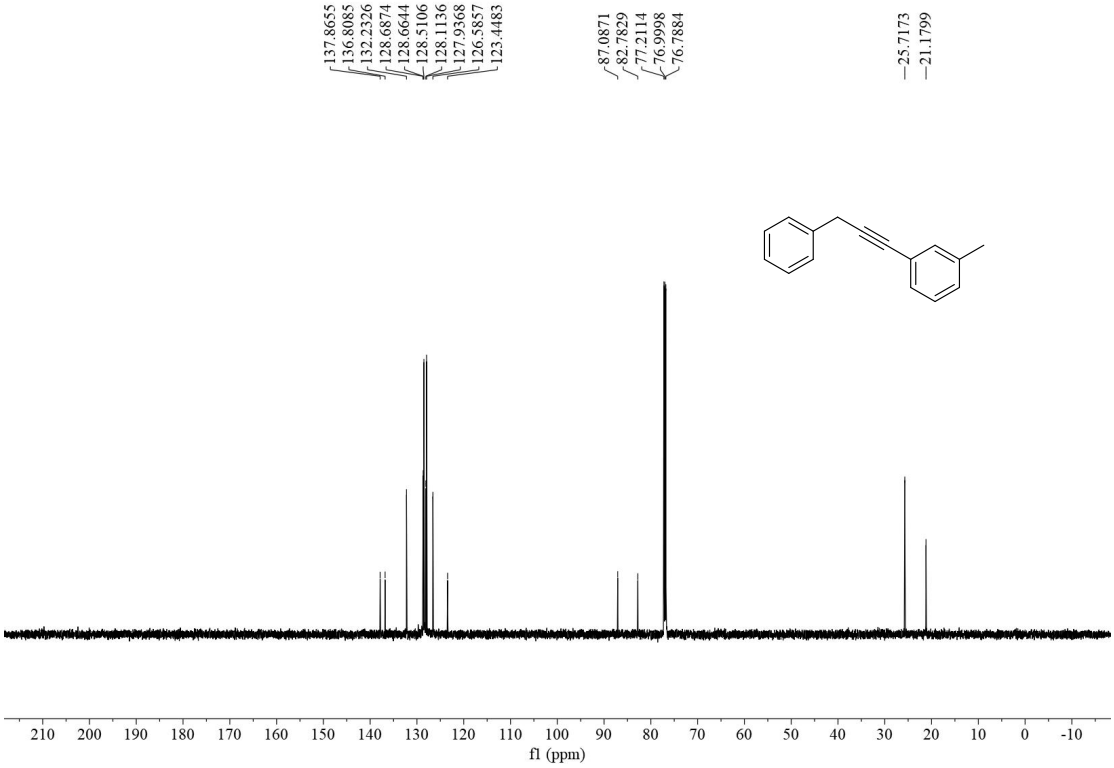
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1h



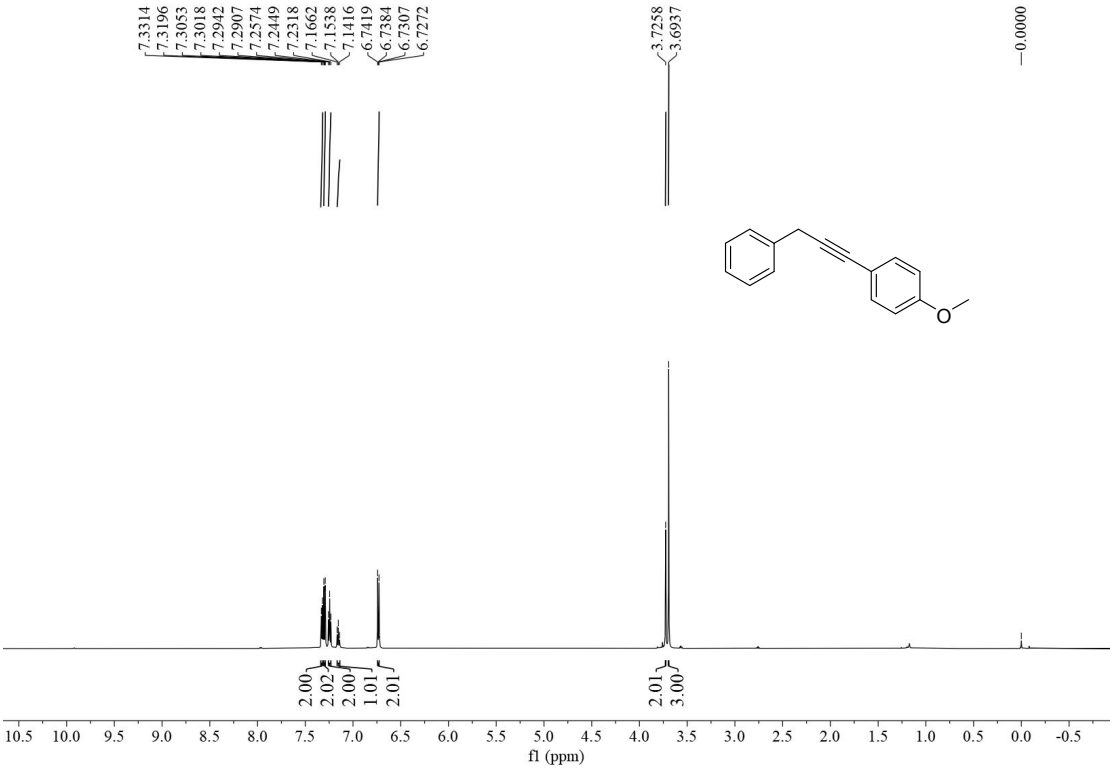
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1i



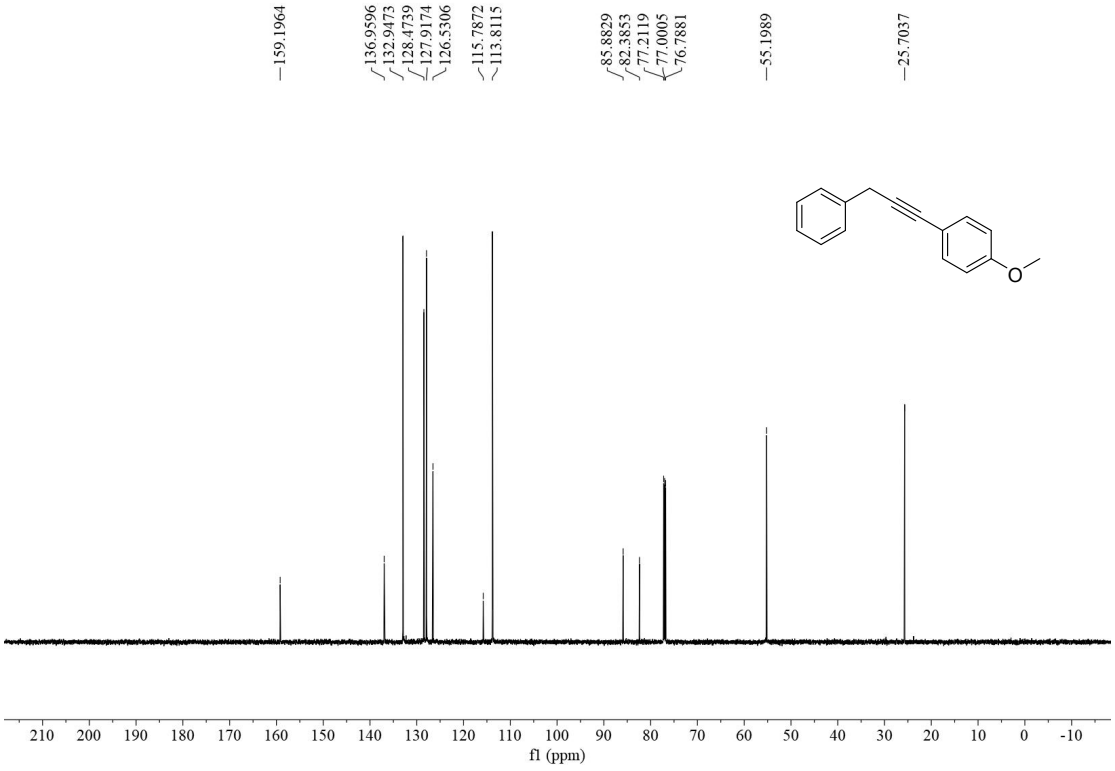
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1i



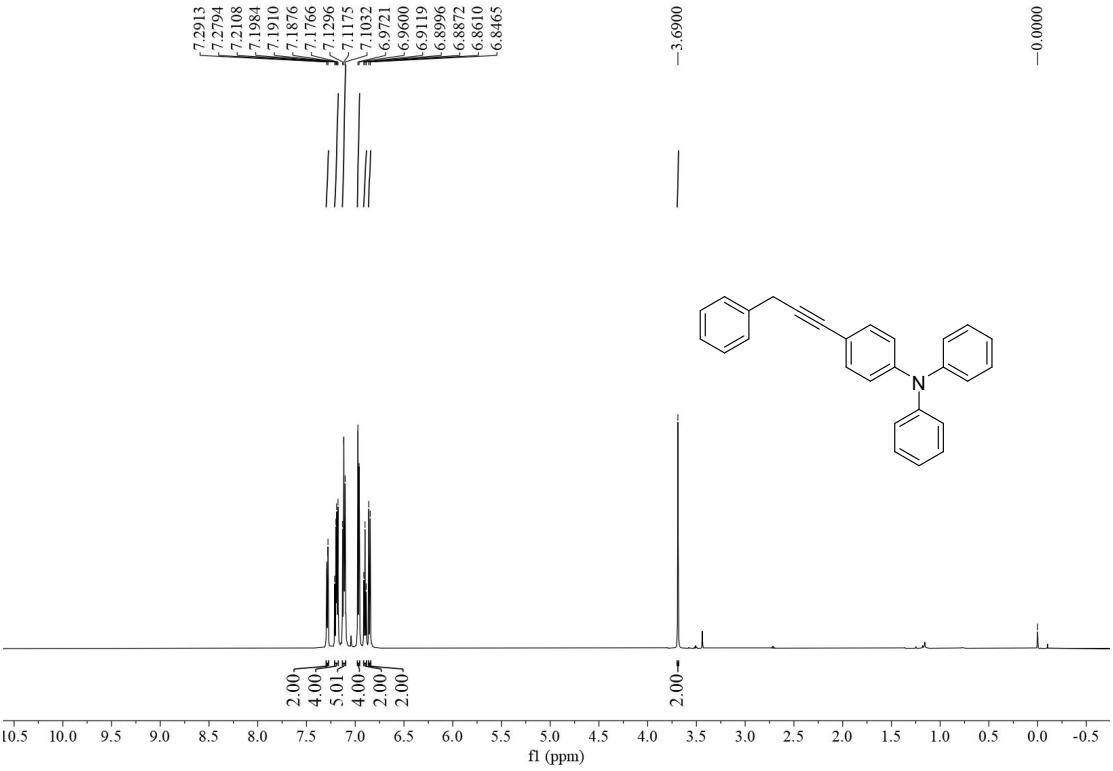
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1j



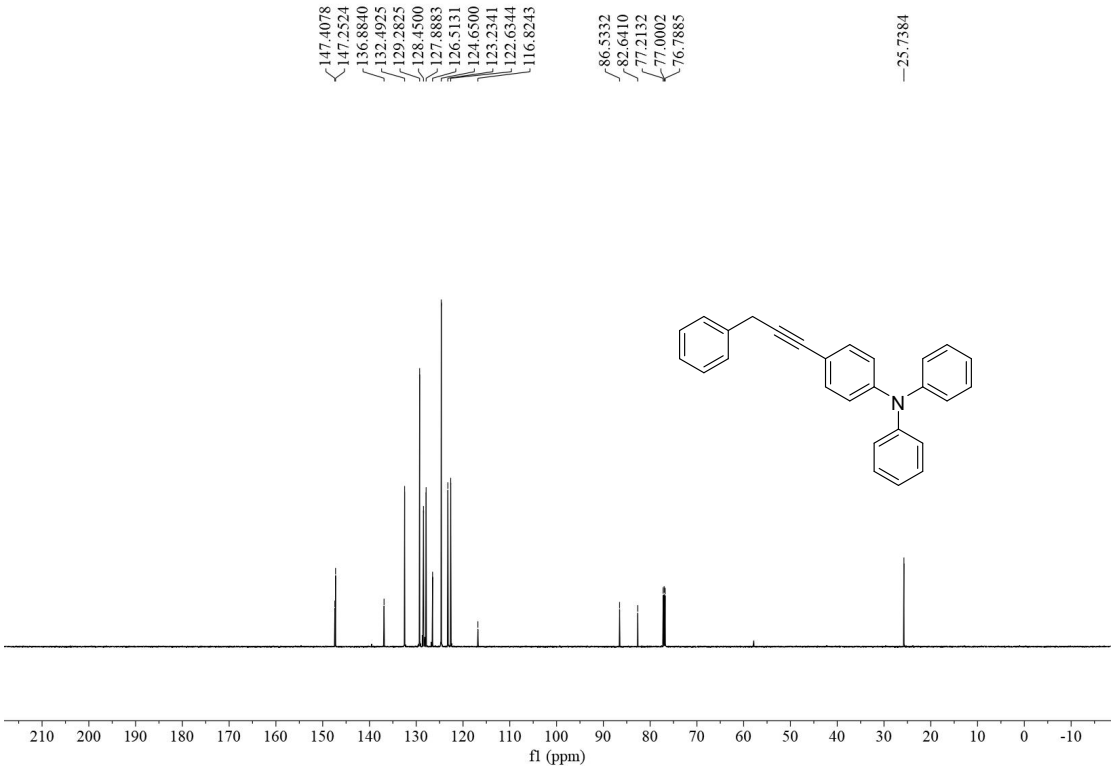
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1j



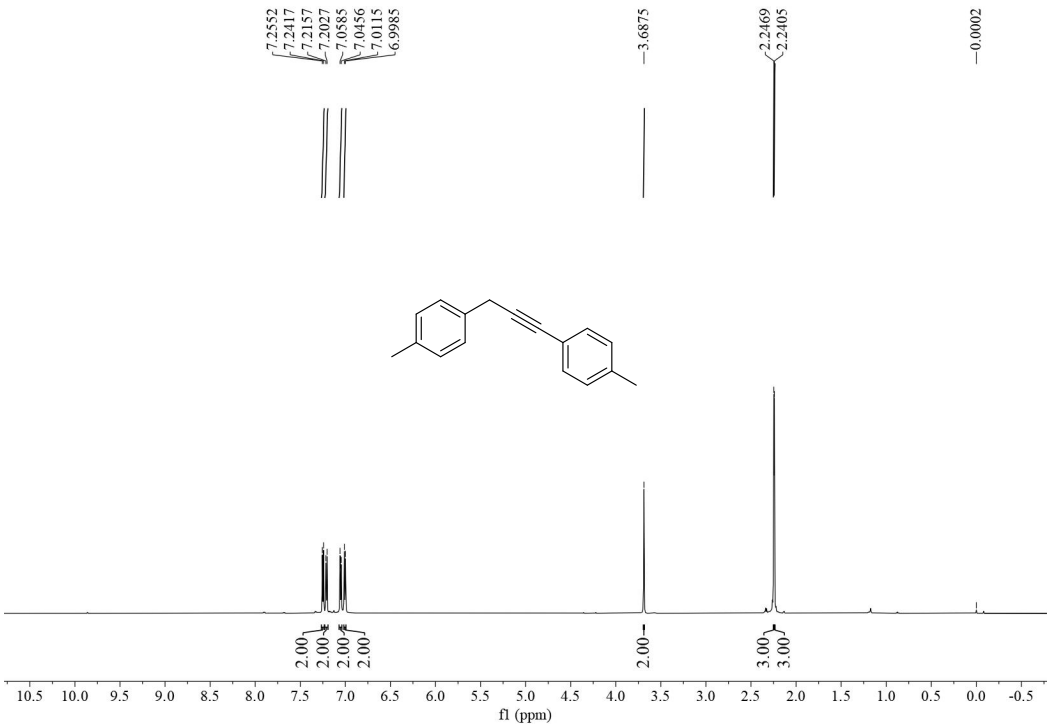
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1k



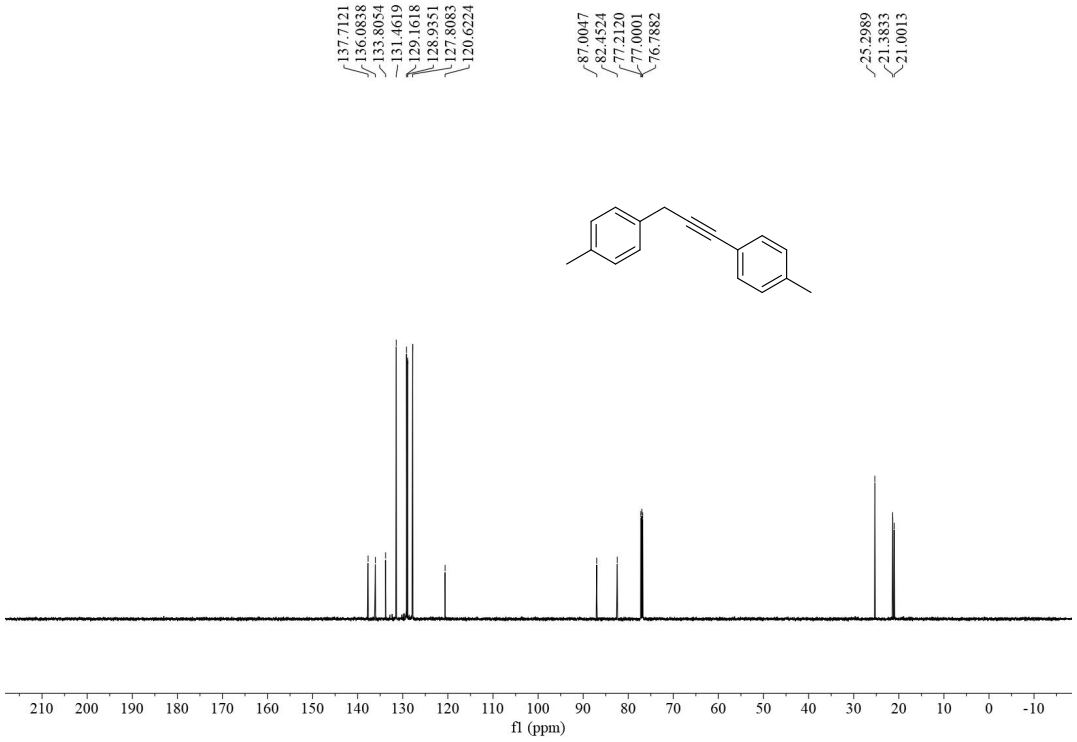
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1k



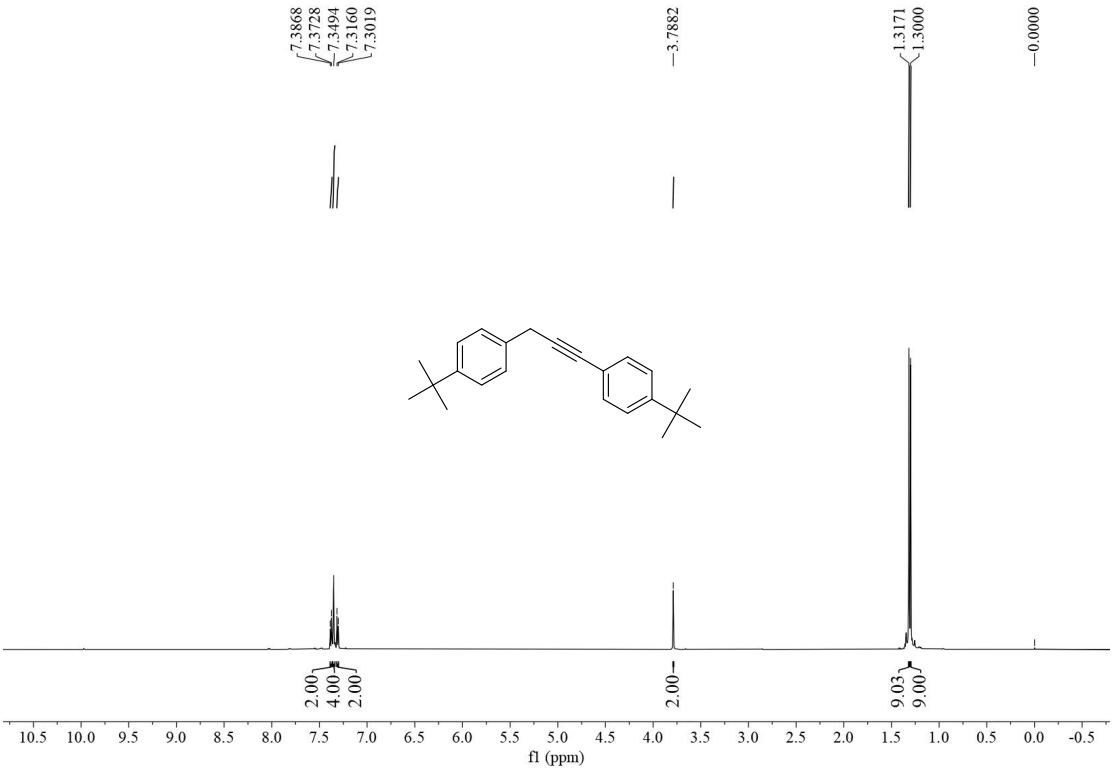
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1l



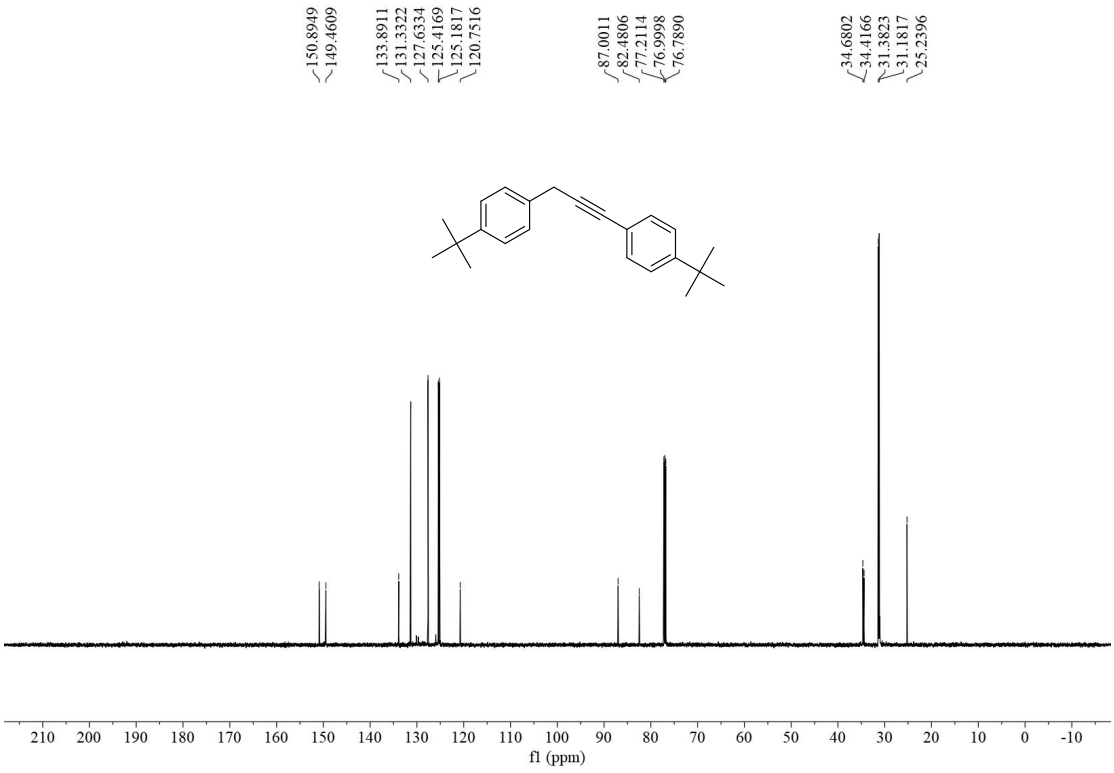
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1l



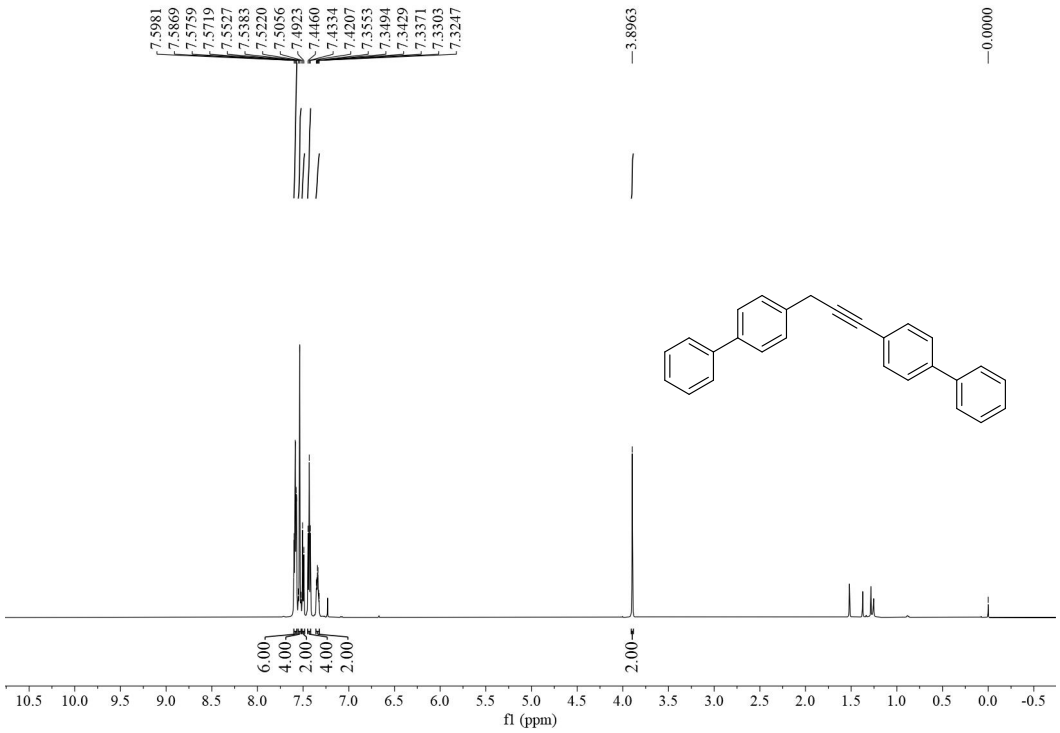
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1m



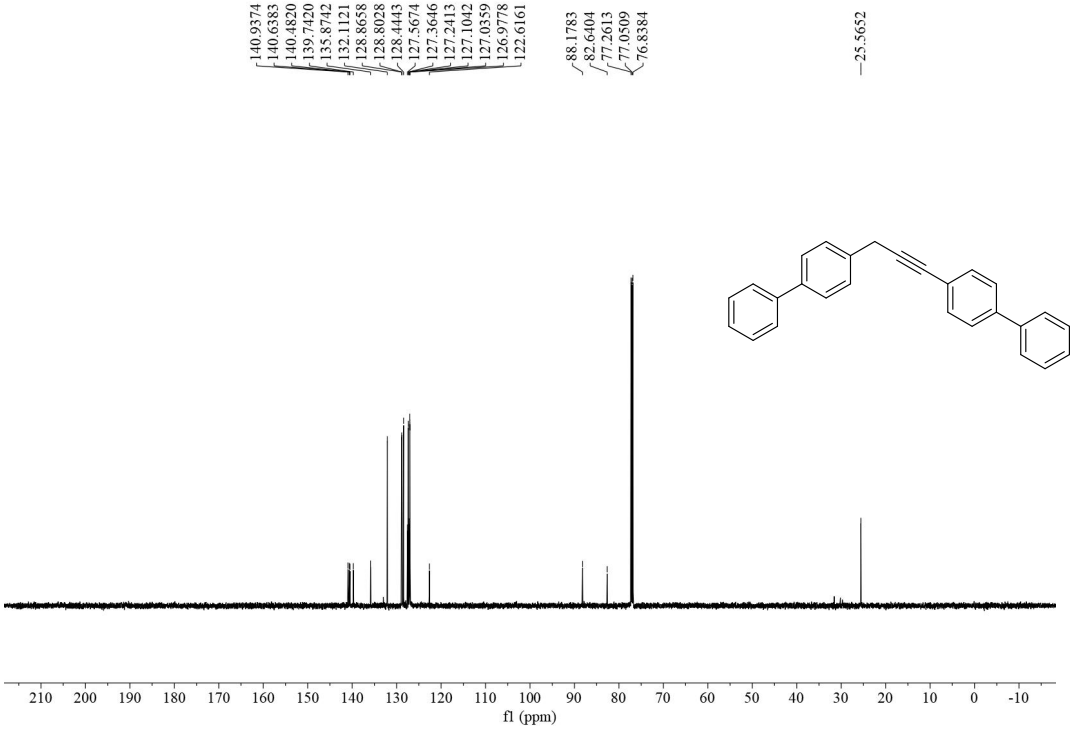
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1m



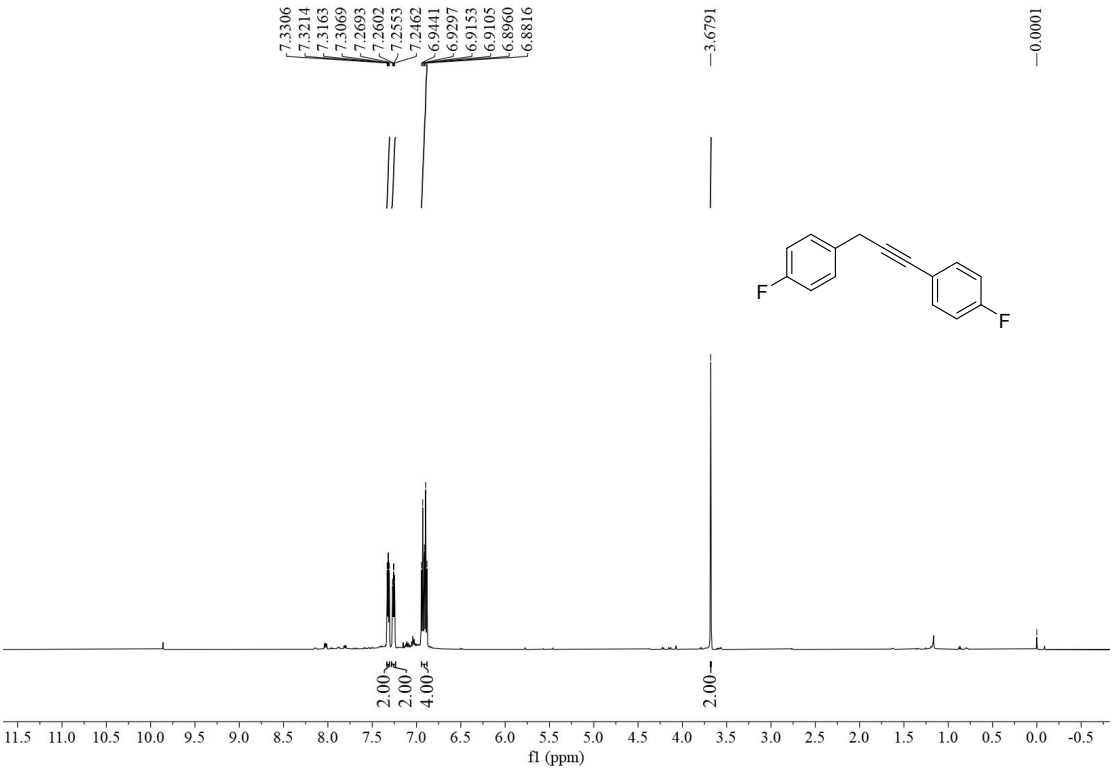
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1n



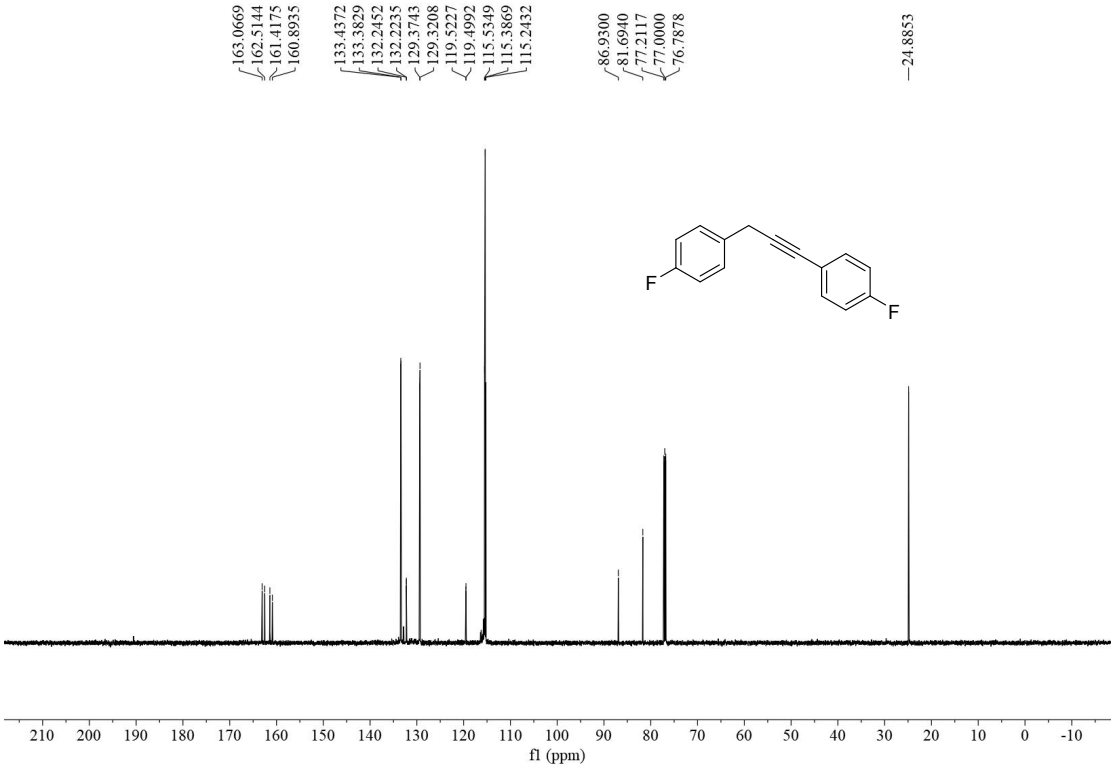
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1n



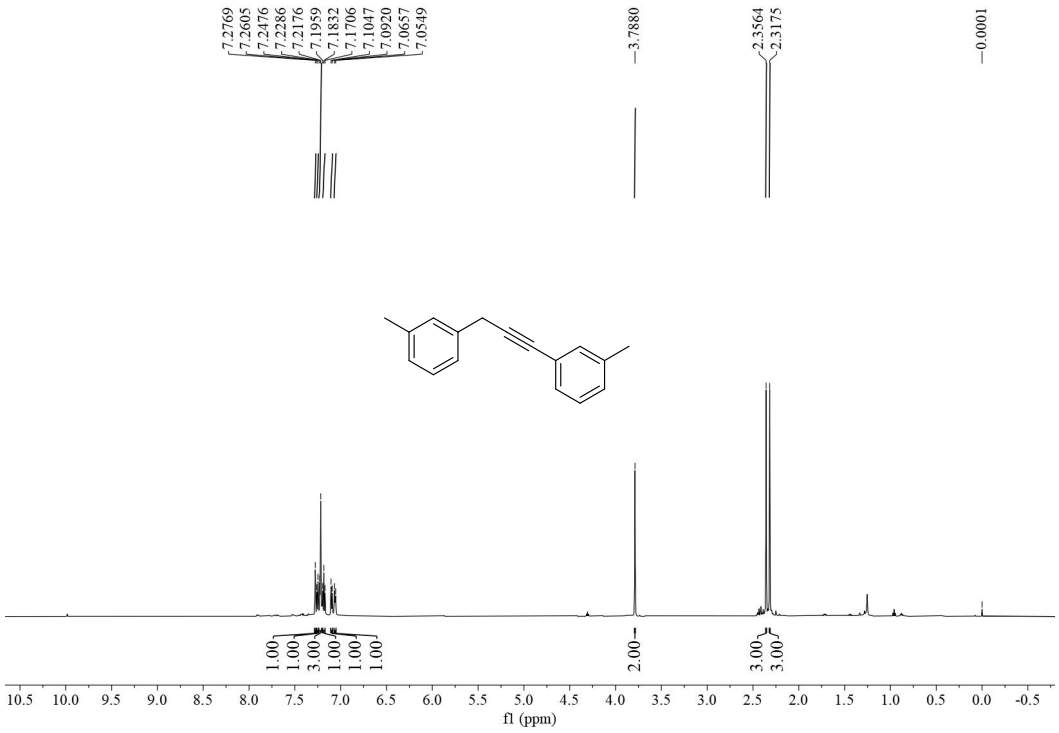
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1o



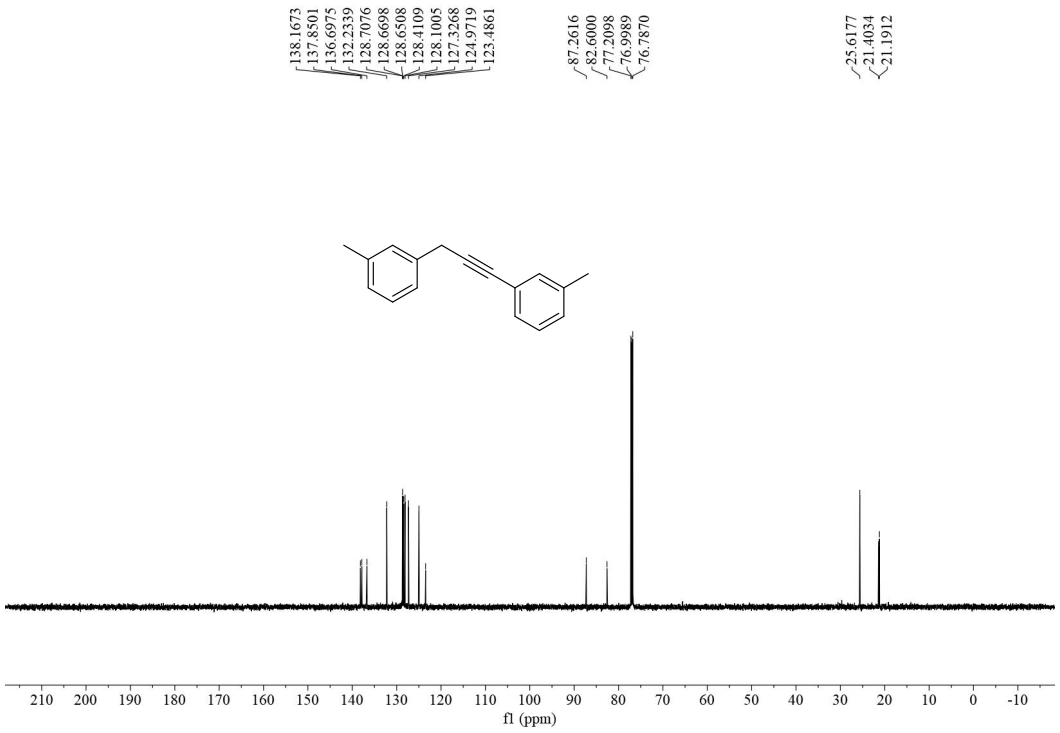
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1o



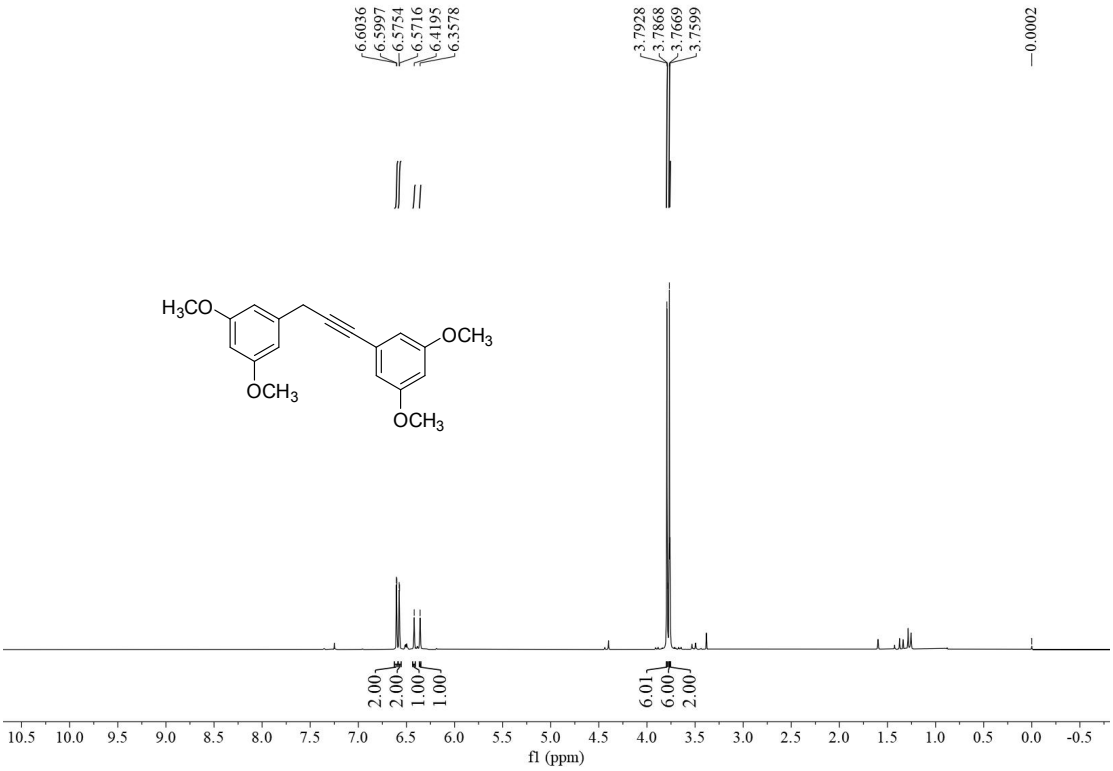
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1p



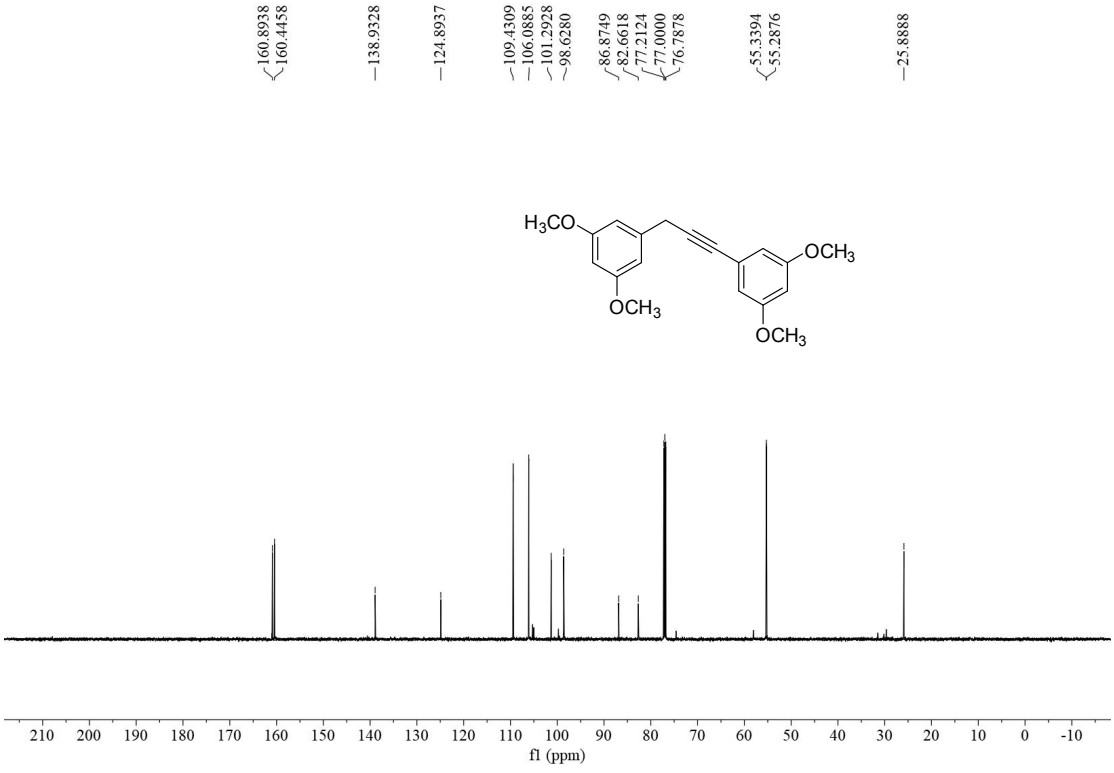
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1p



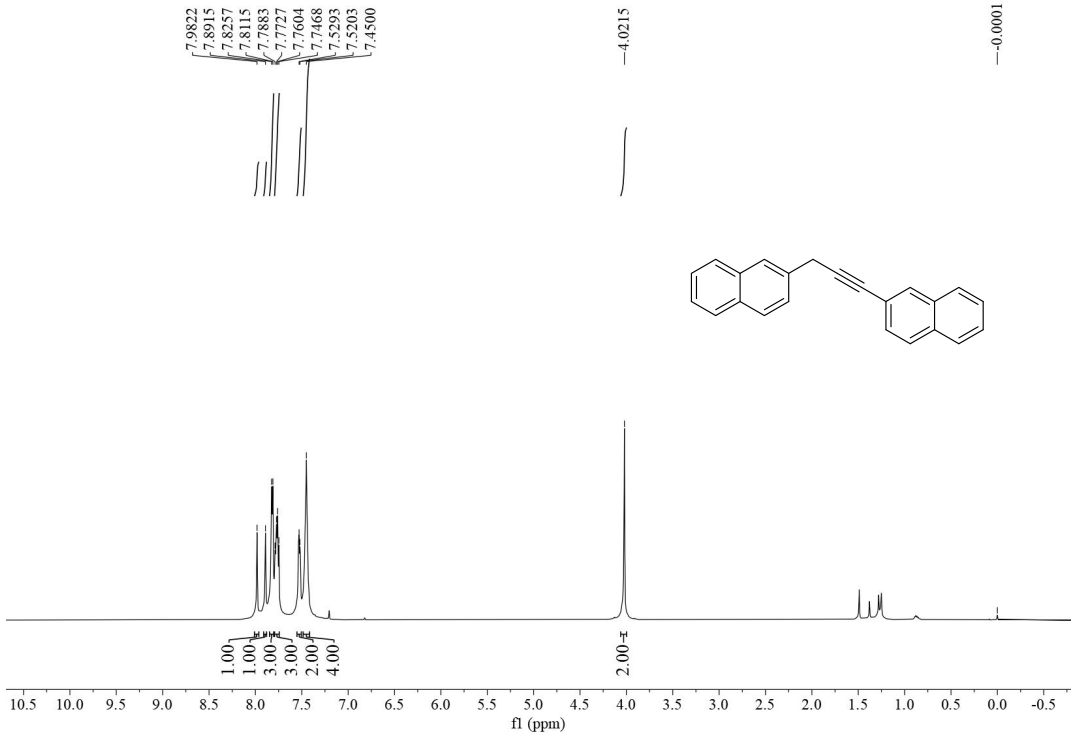
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1q



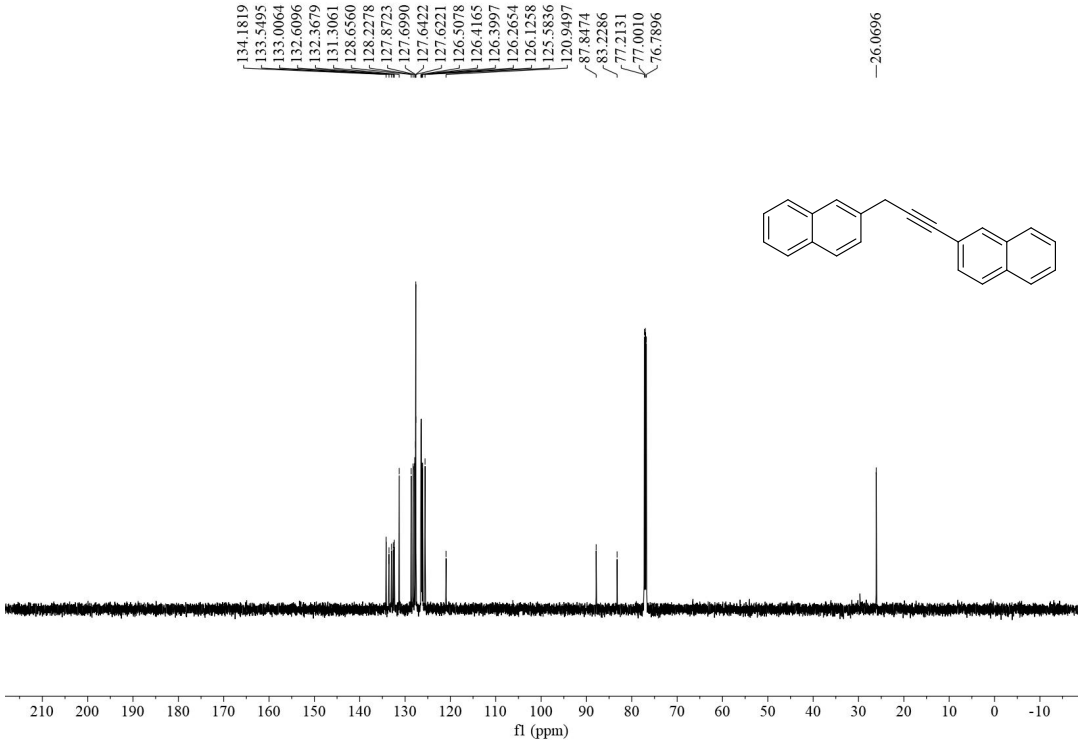
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1q



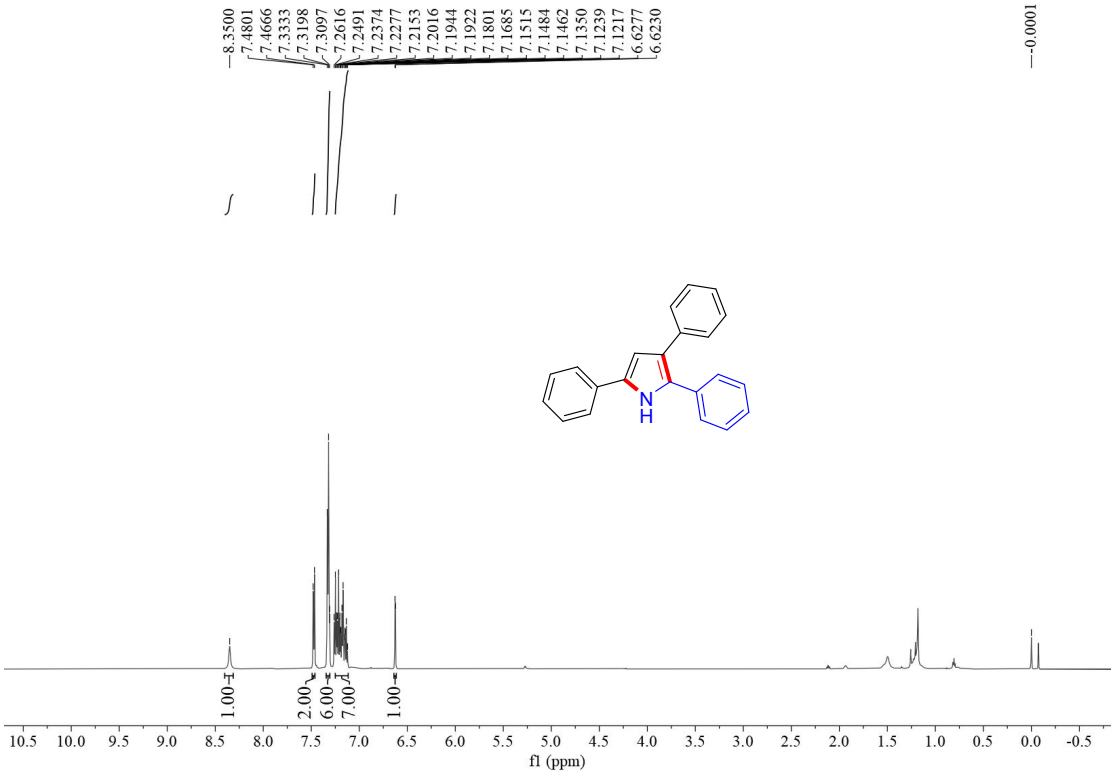
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 1r



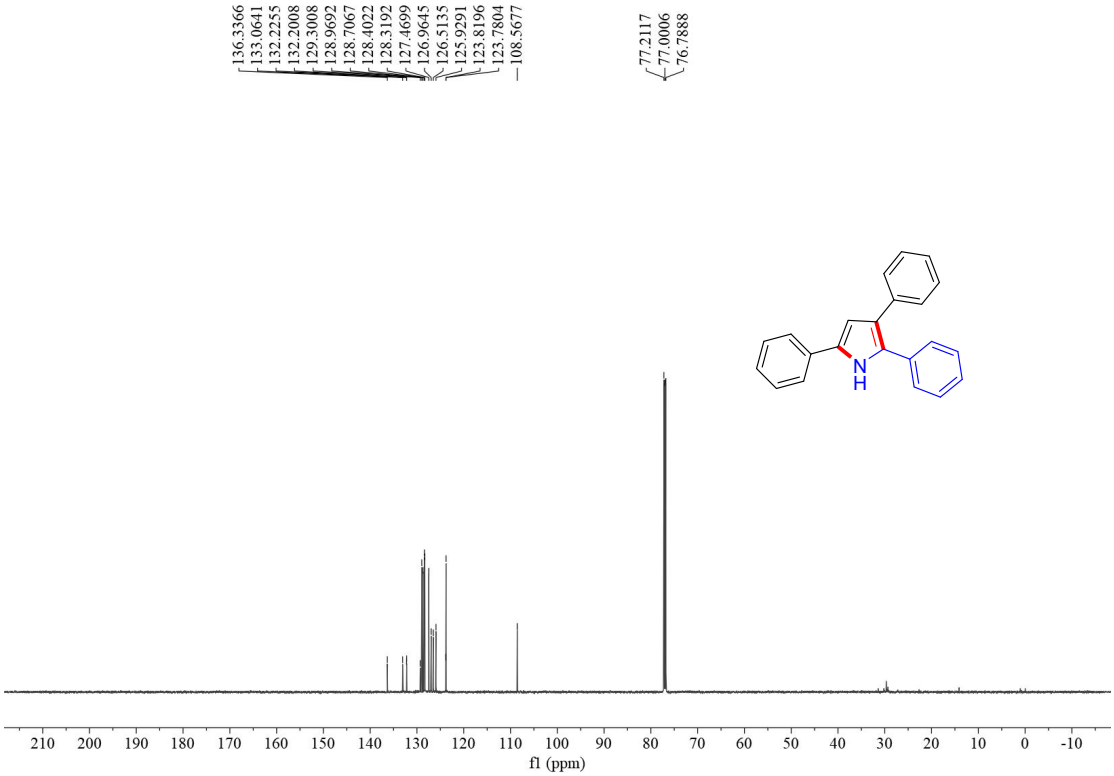
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 1r



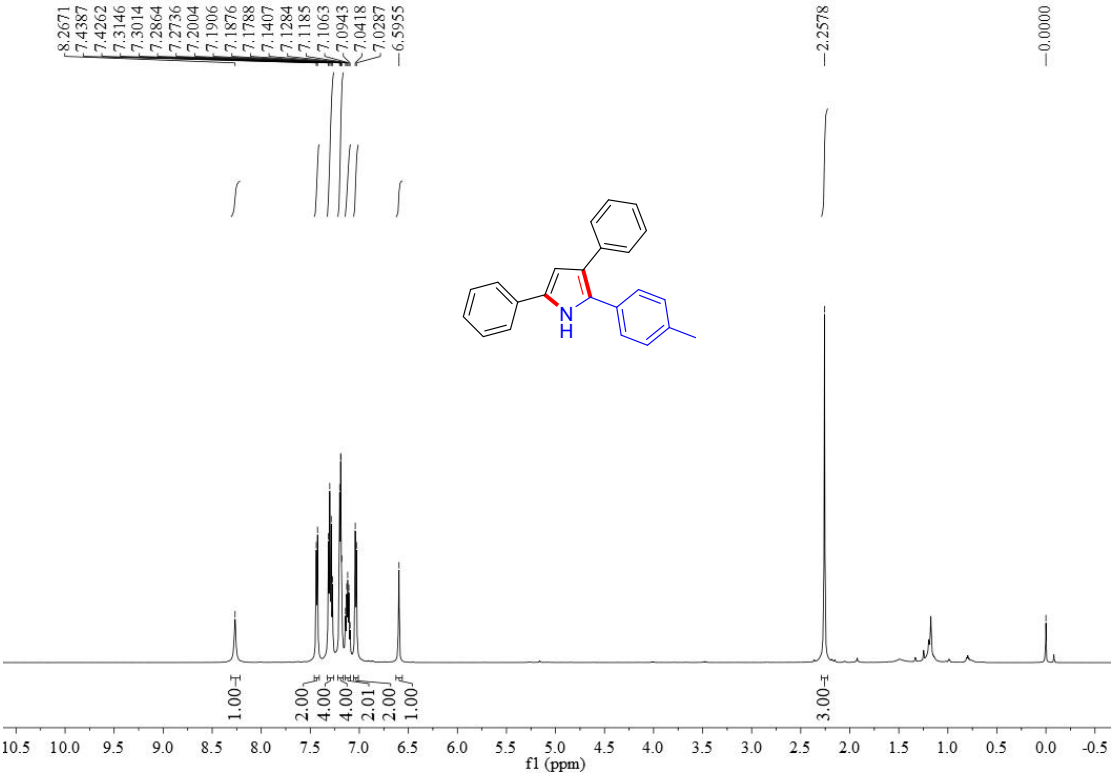
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3a



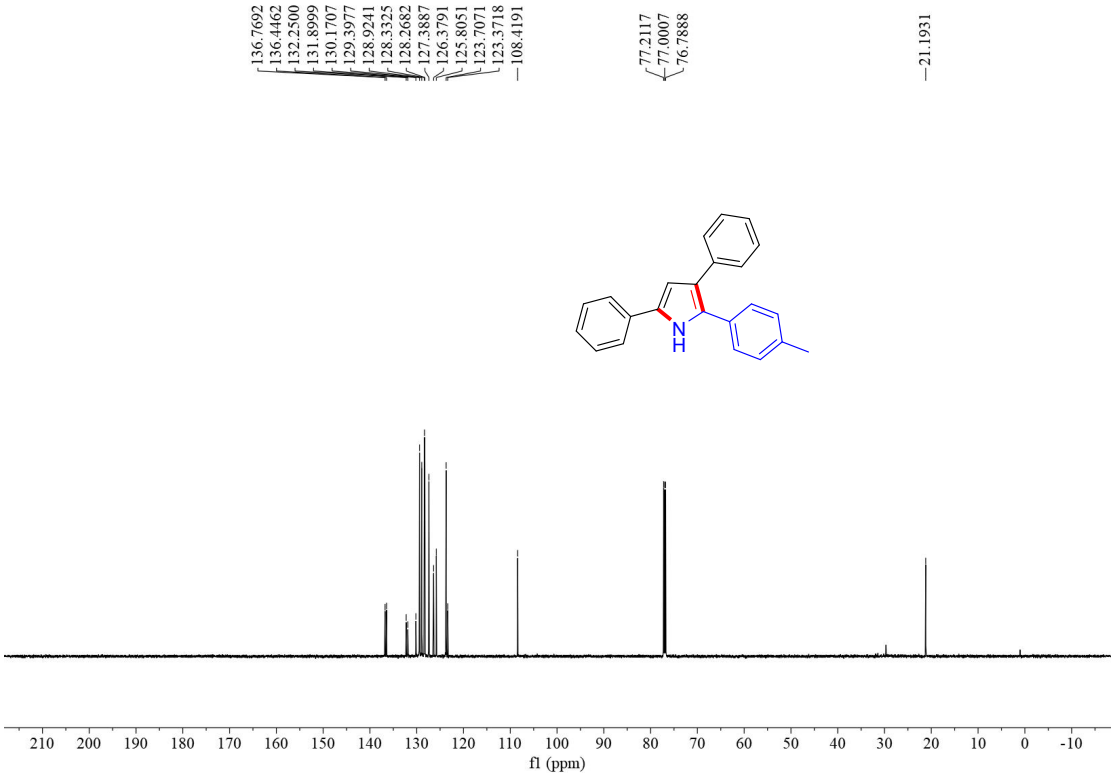
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3a



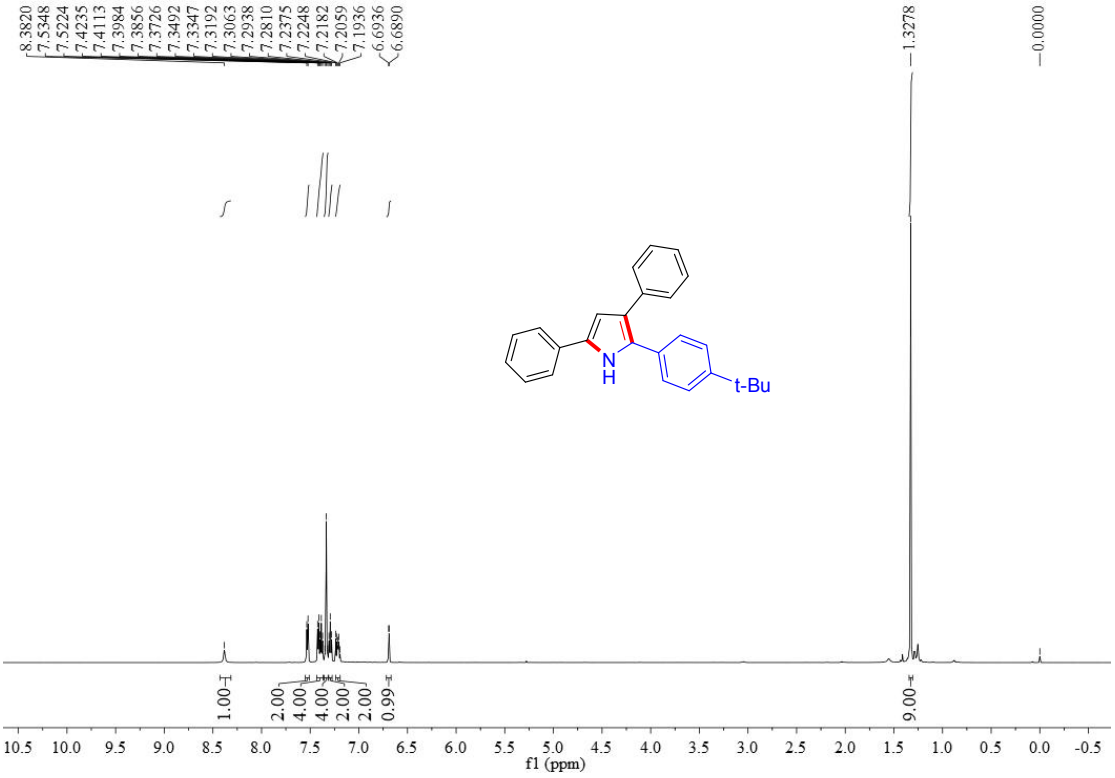
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3b



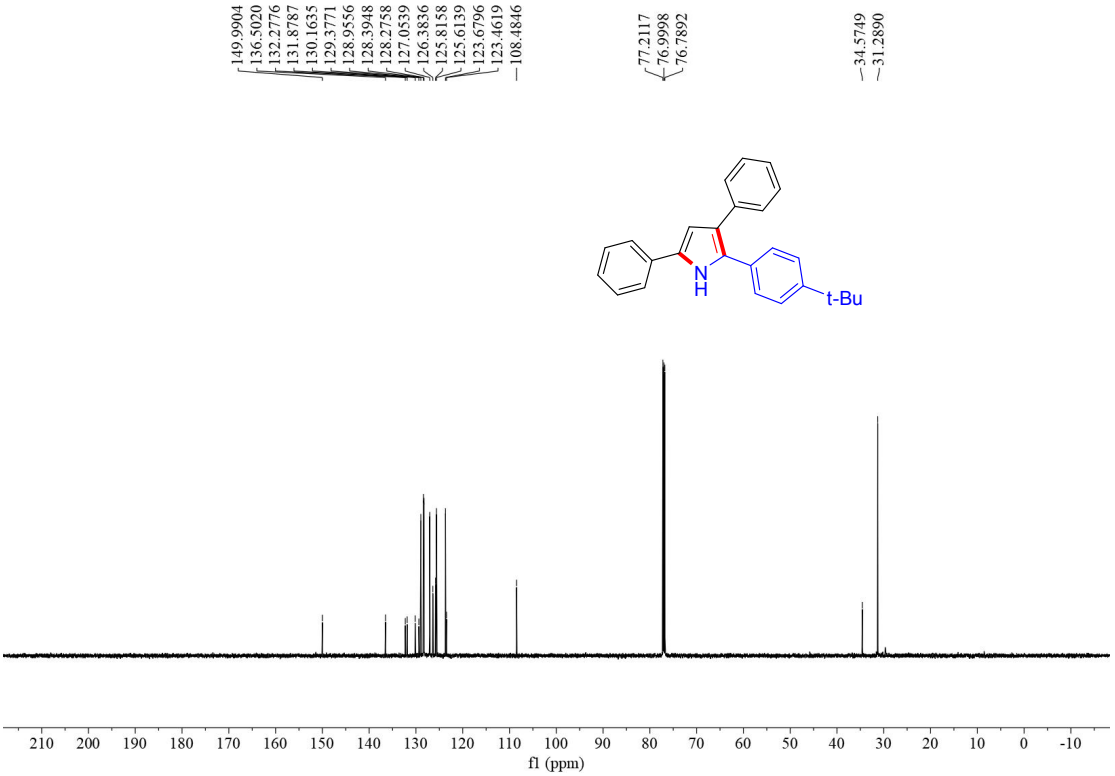
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3b



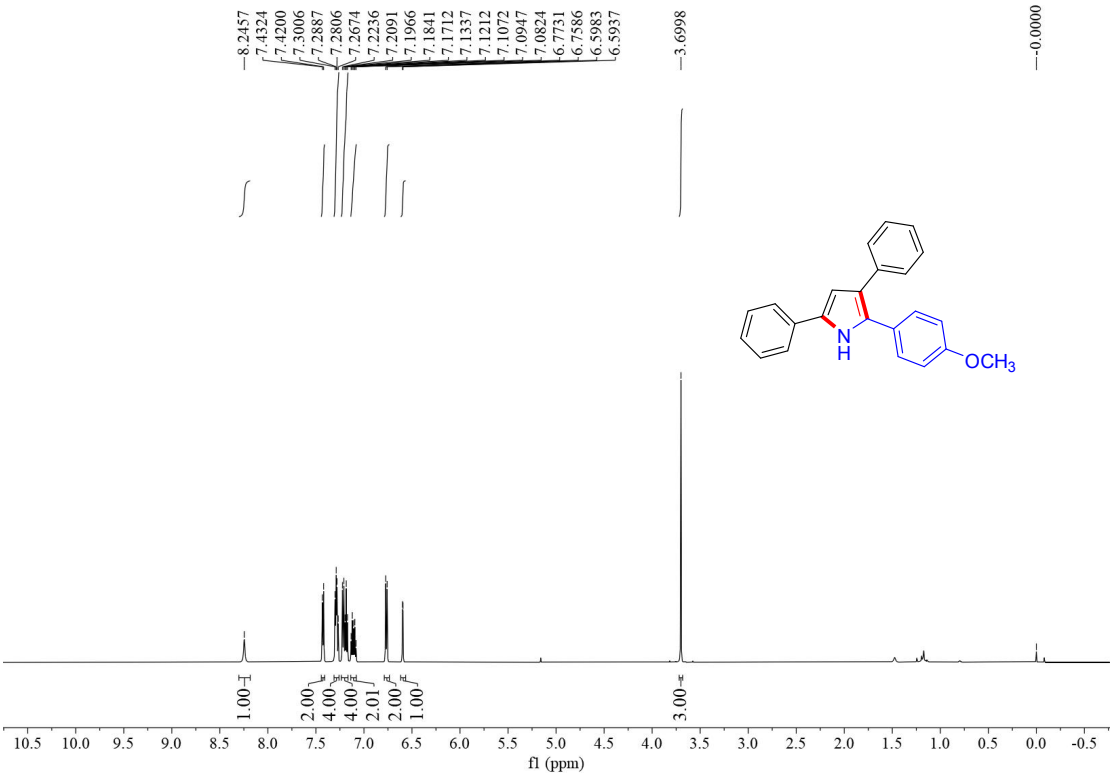
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3c



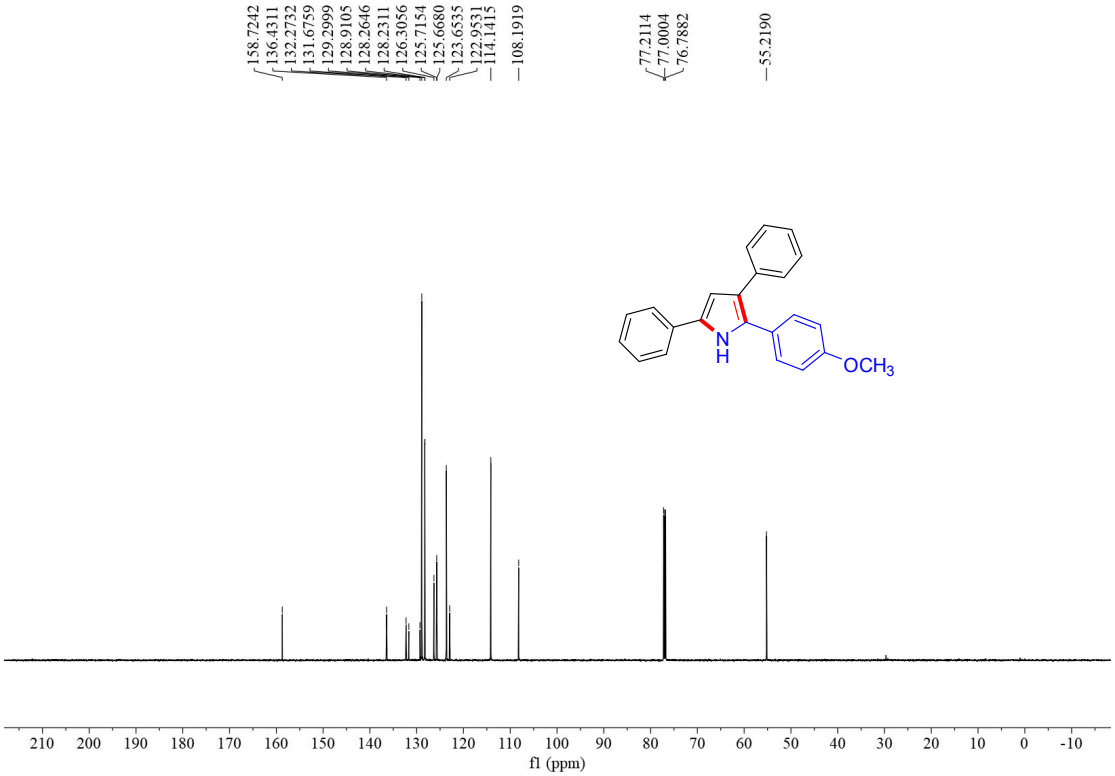
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3c



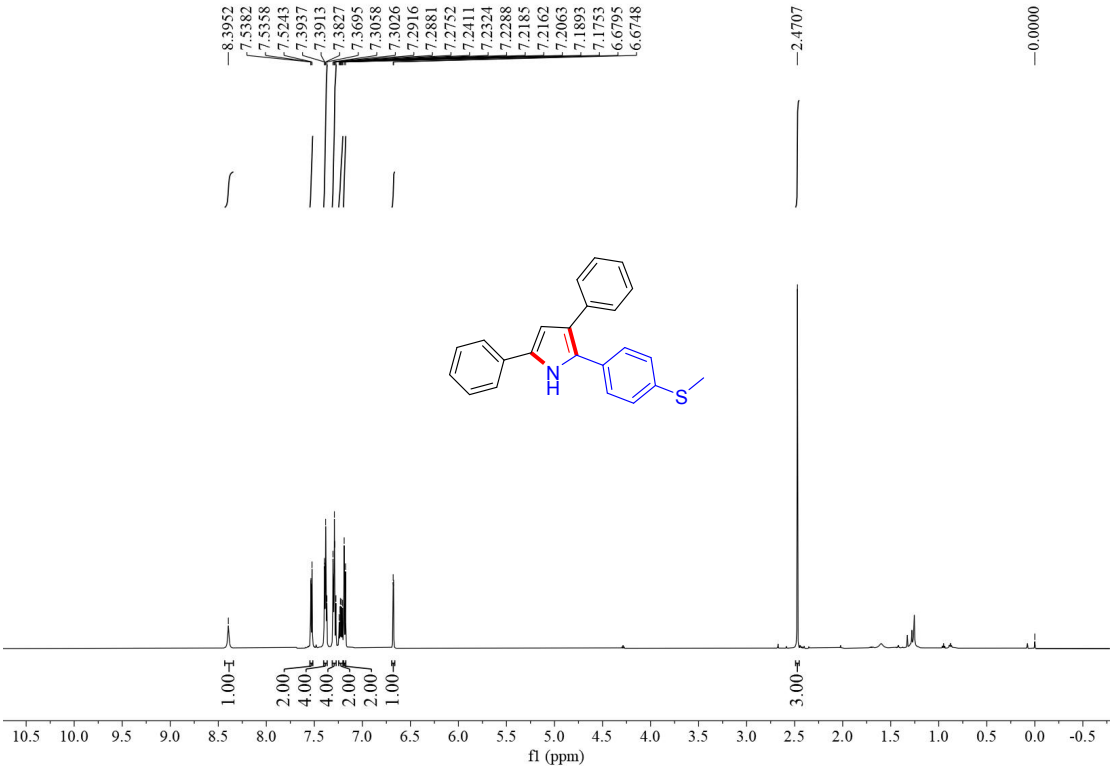
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3d



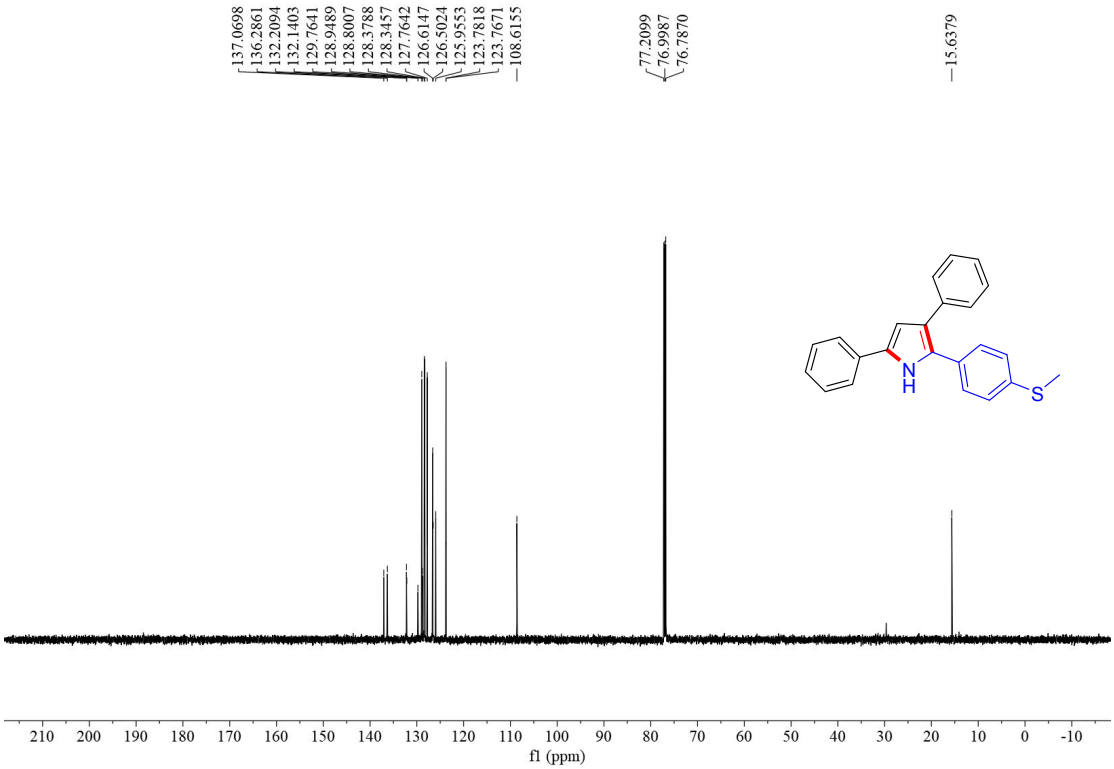
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3d



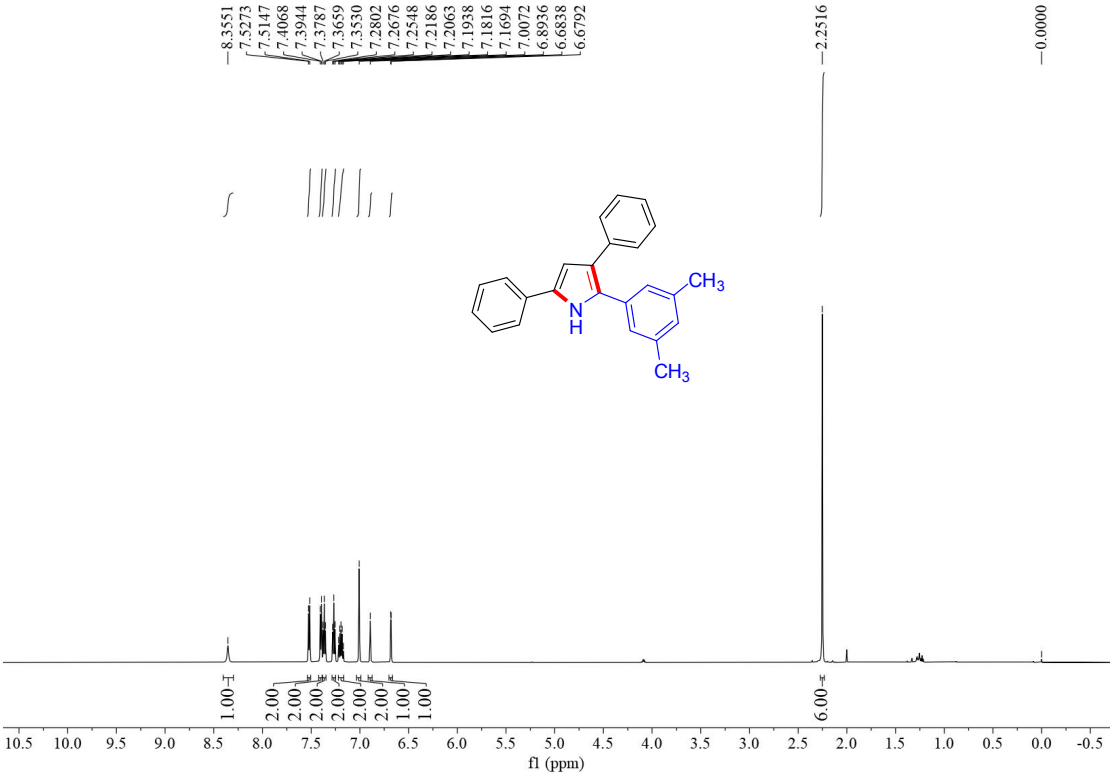
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3e



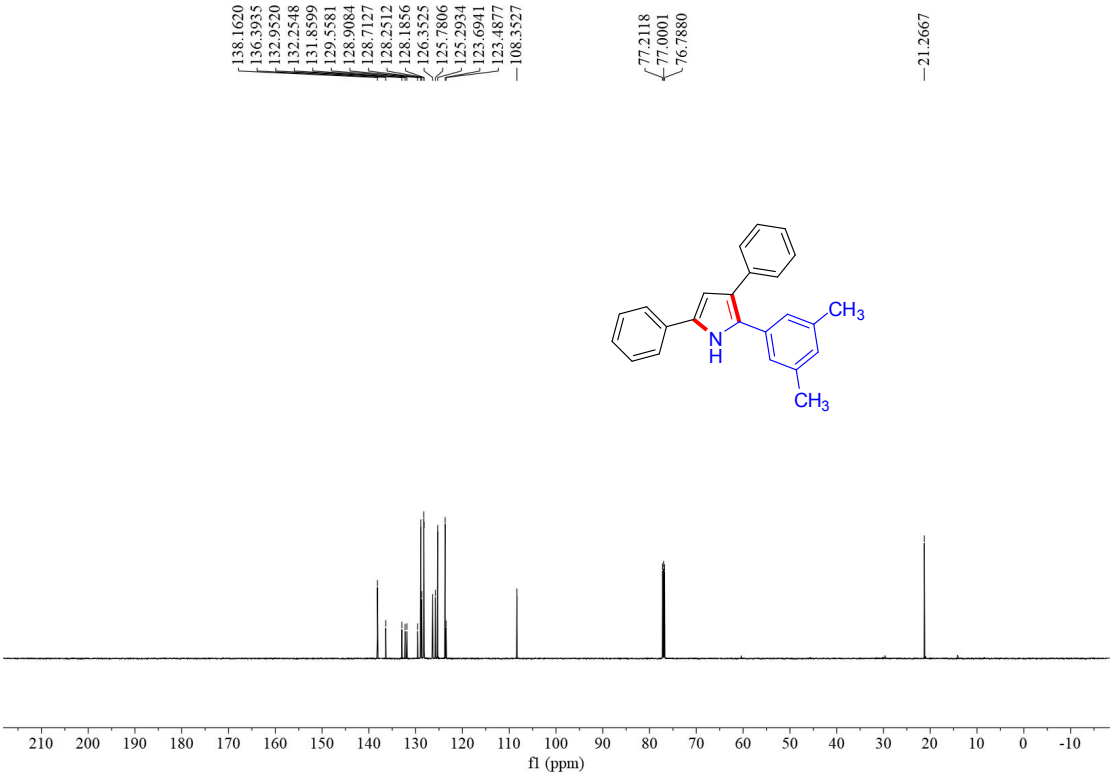
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3e



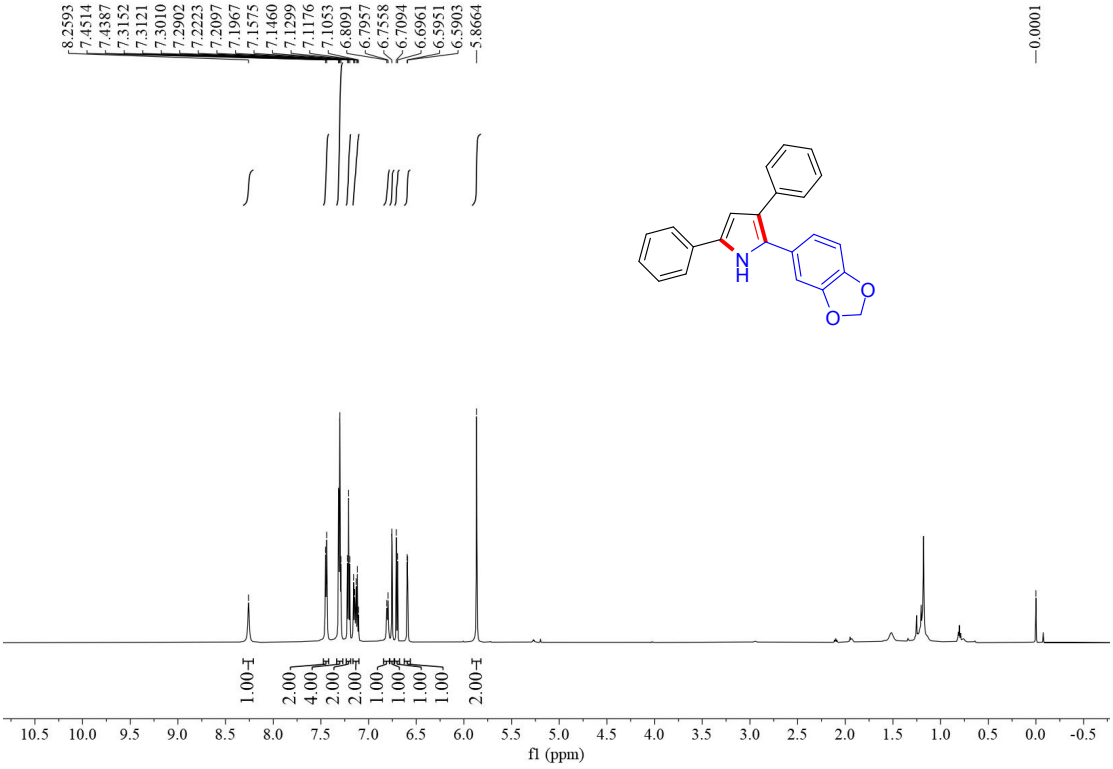
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3f



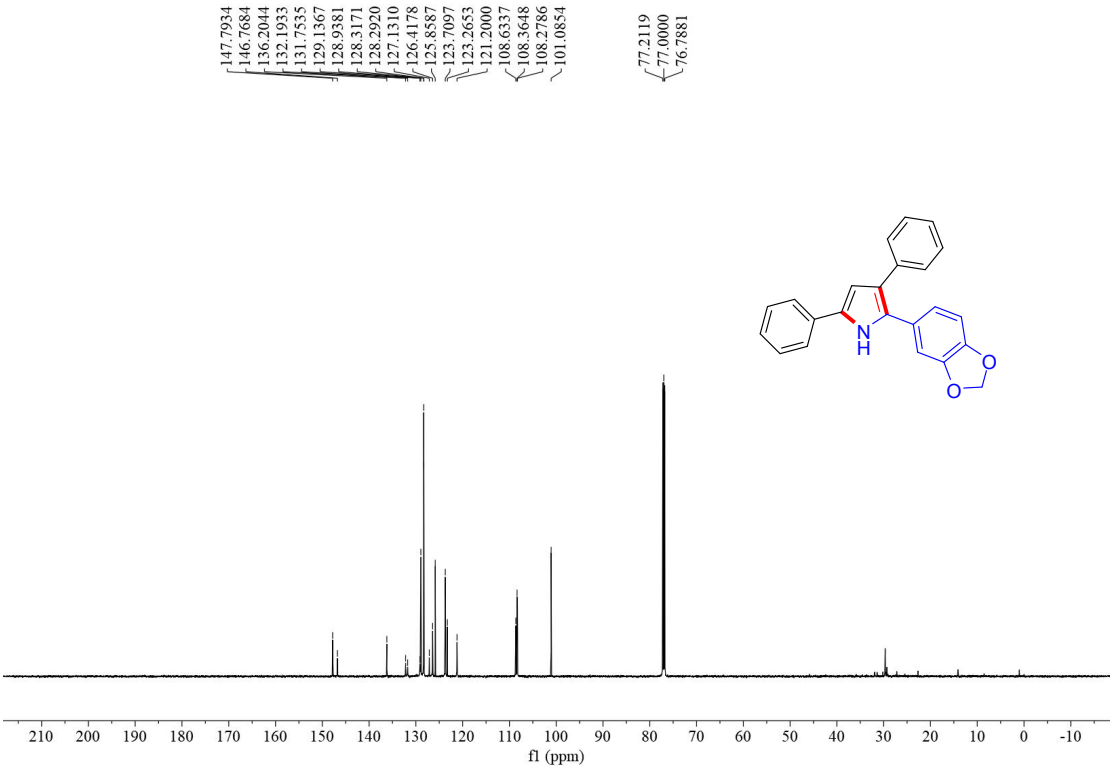
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3f



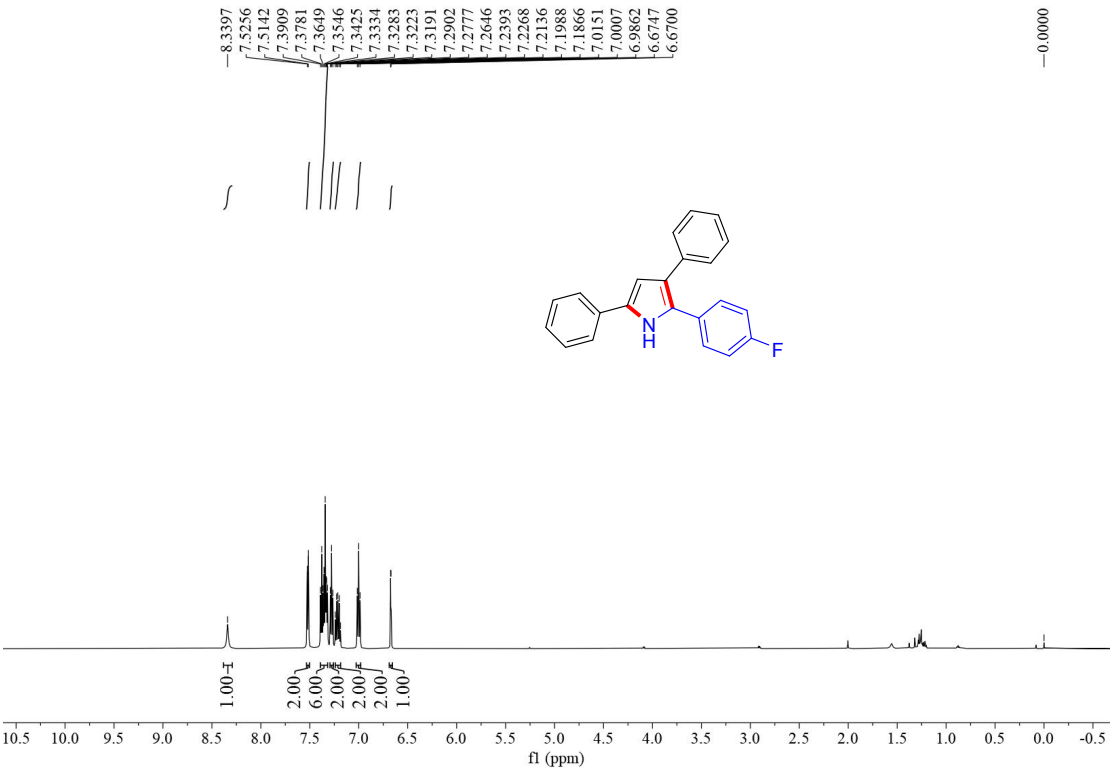
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3g



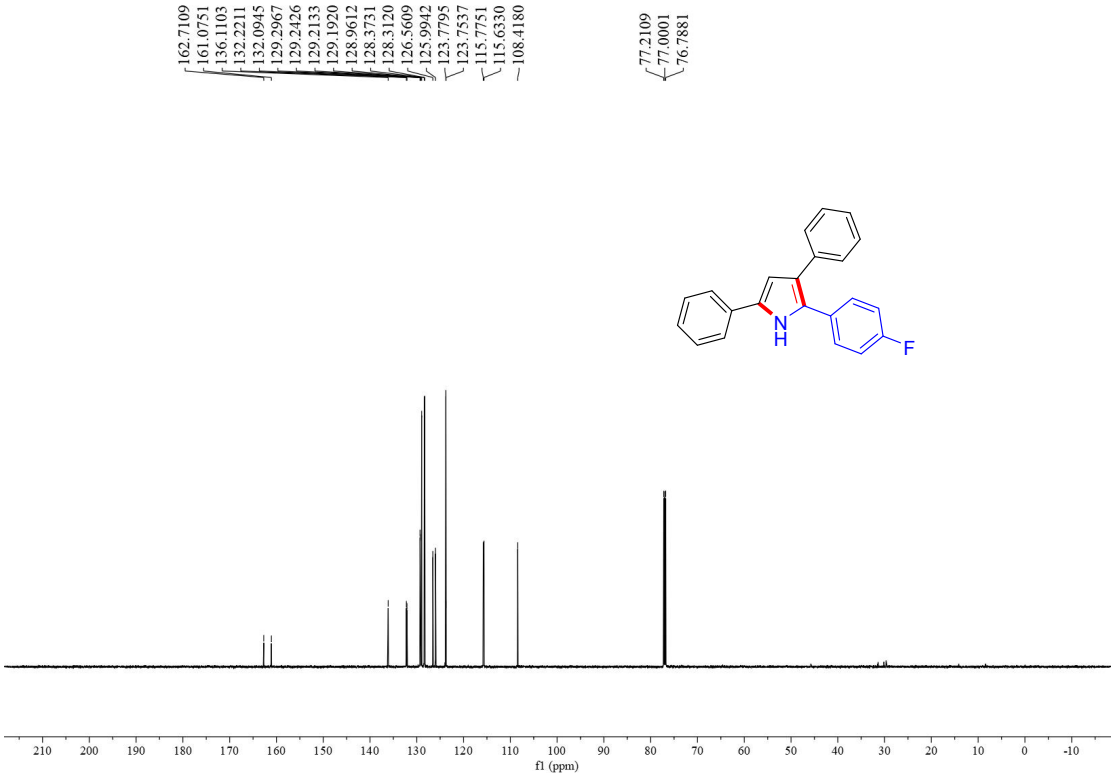
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3g



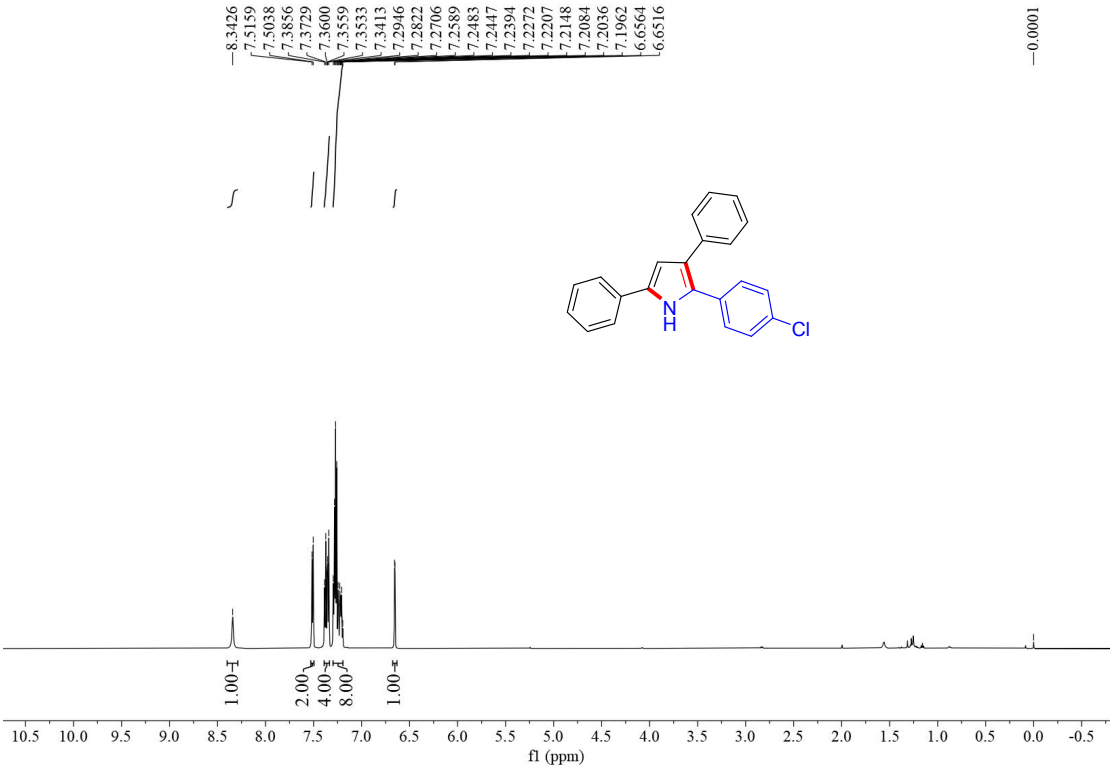
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3h



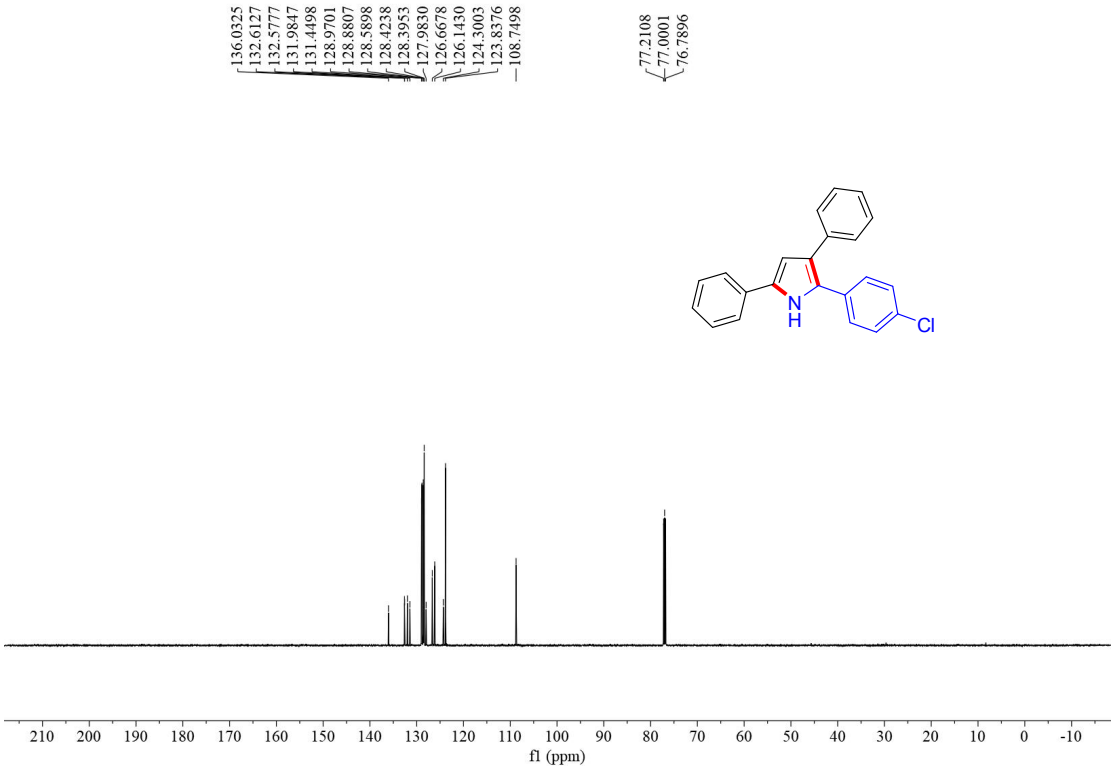
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3h



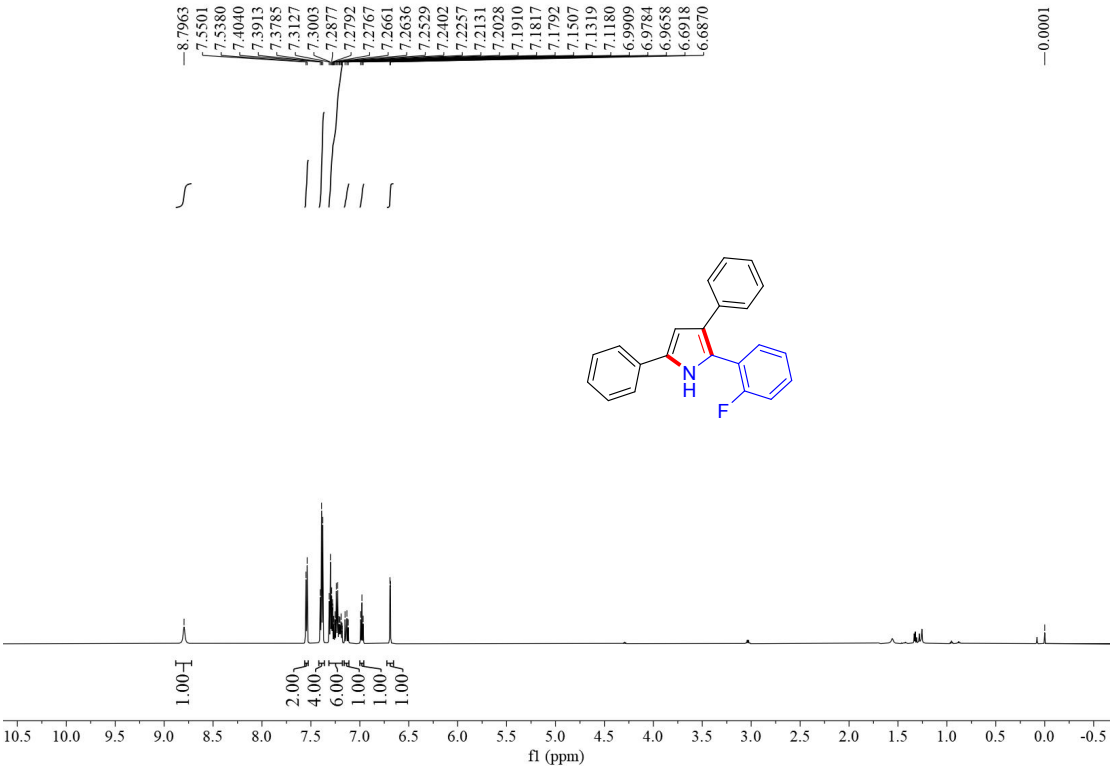
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3i



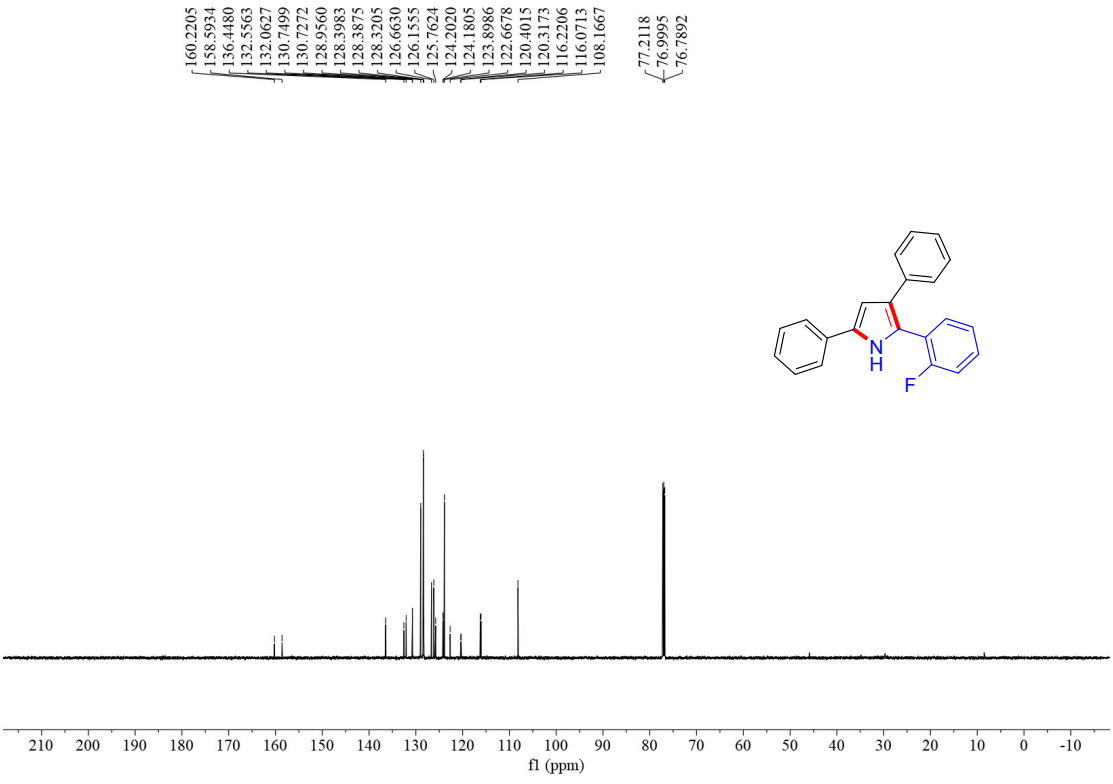
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3i



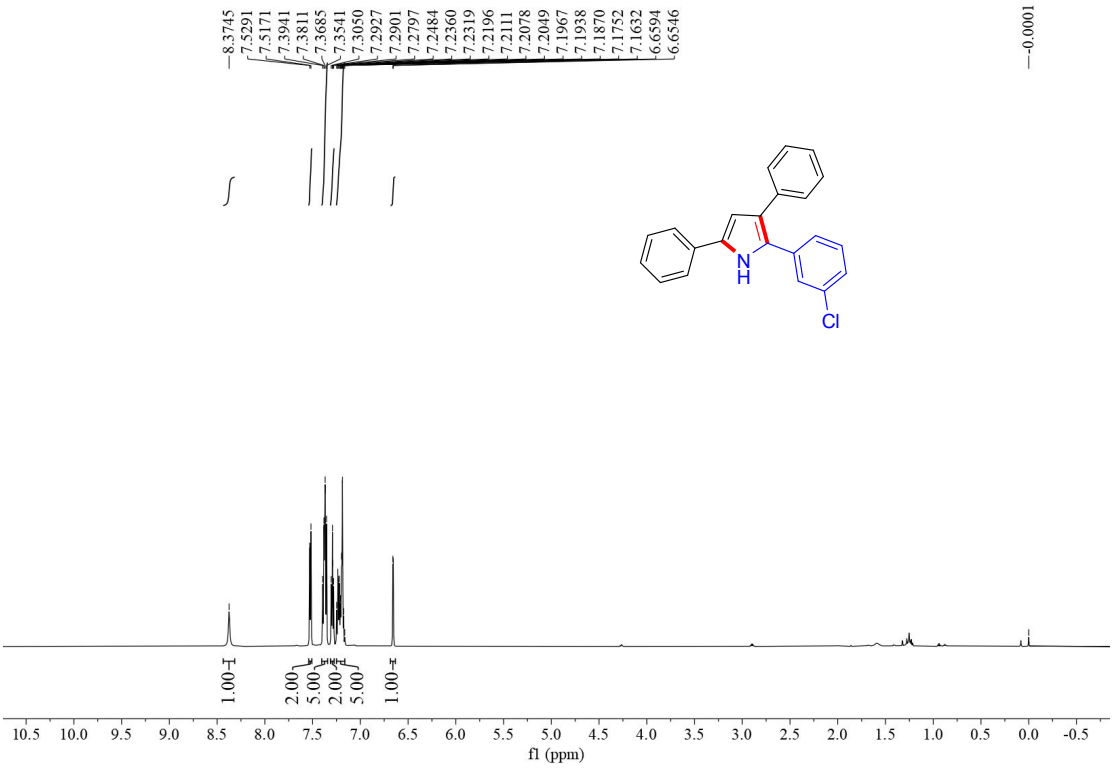
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3j



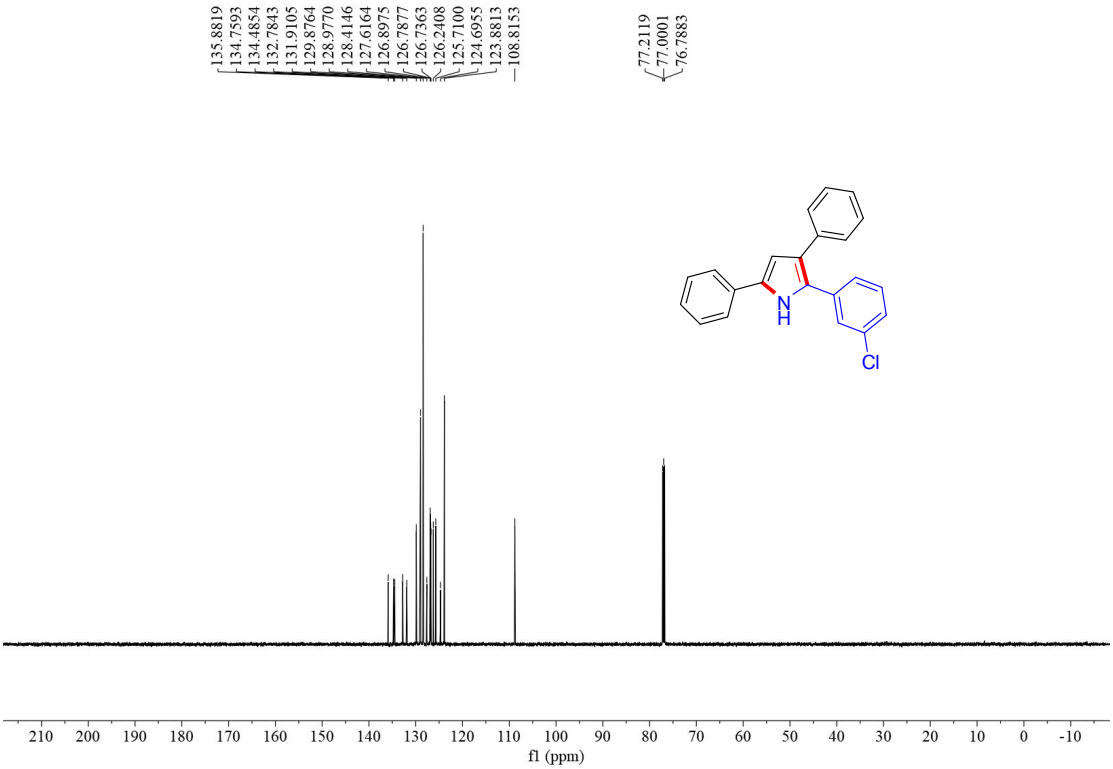
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3j



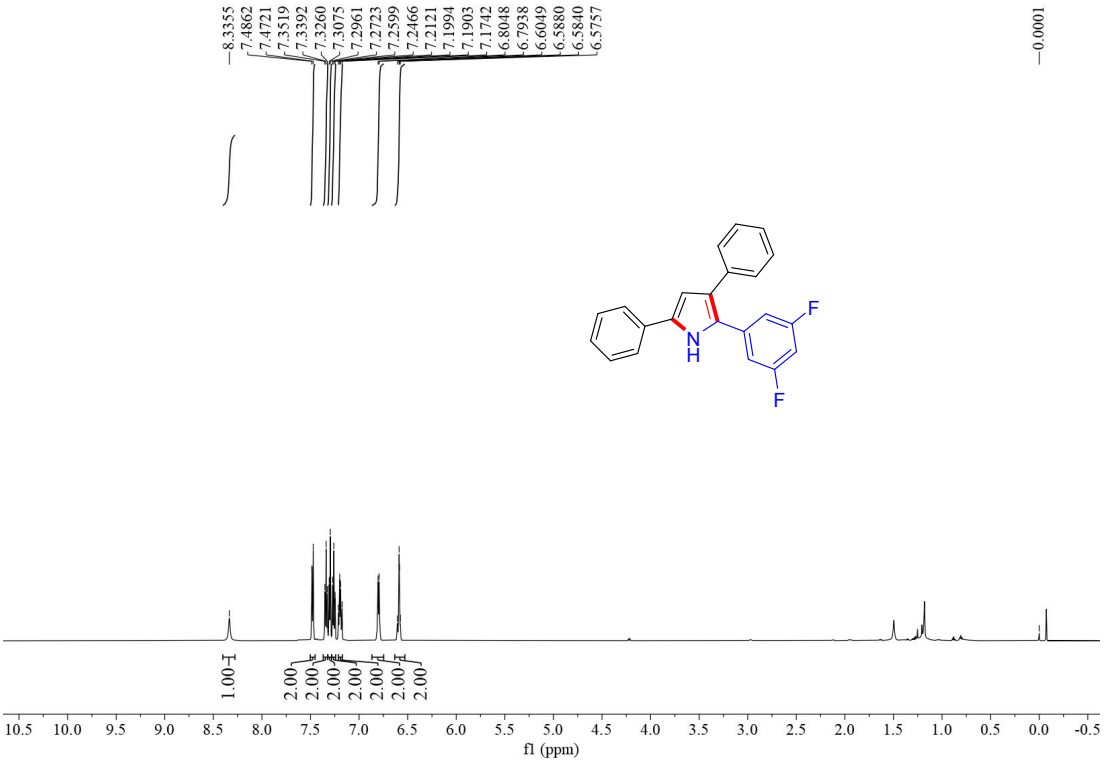
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3k



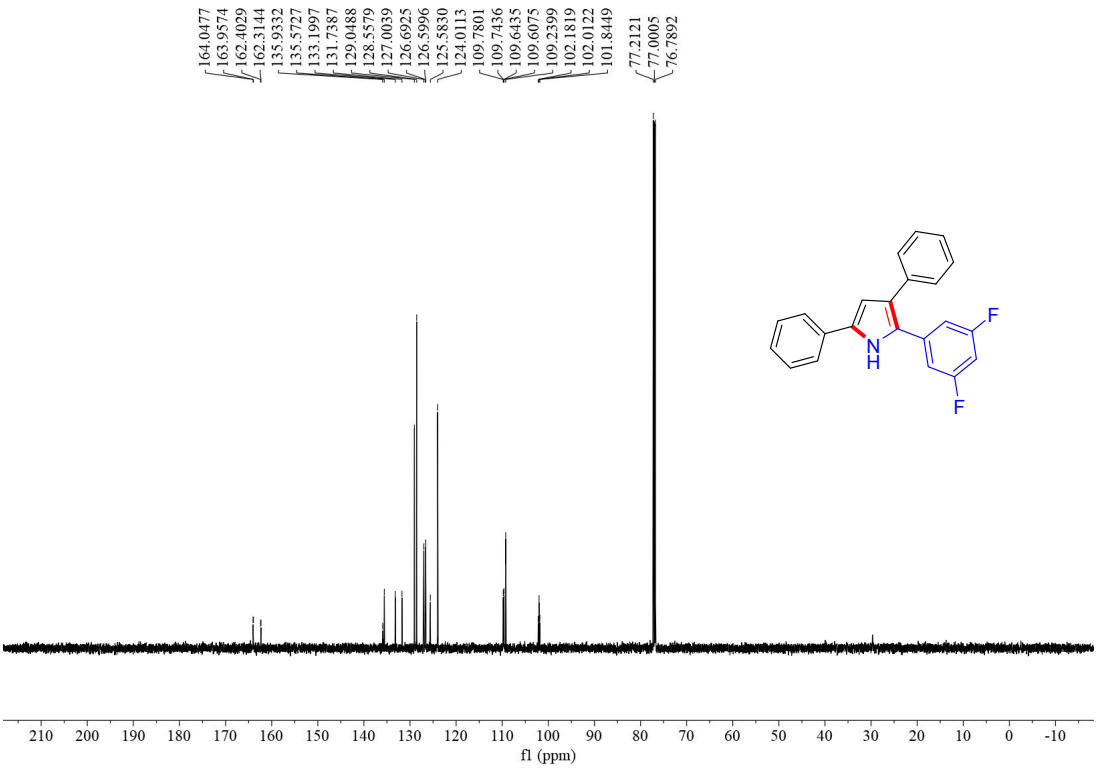
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3k



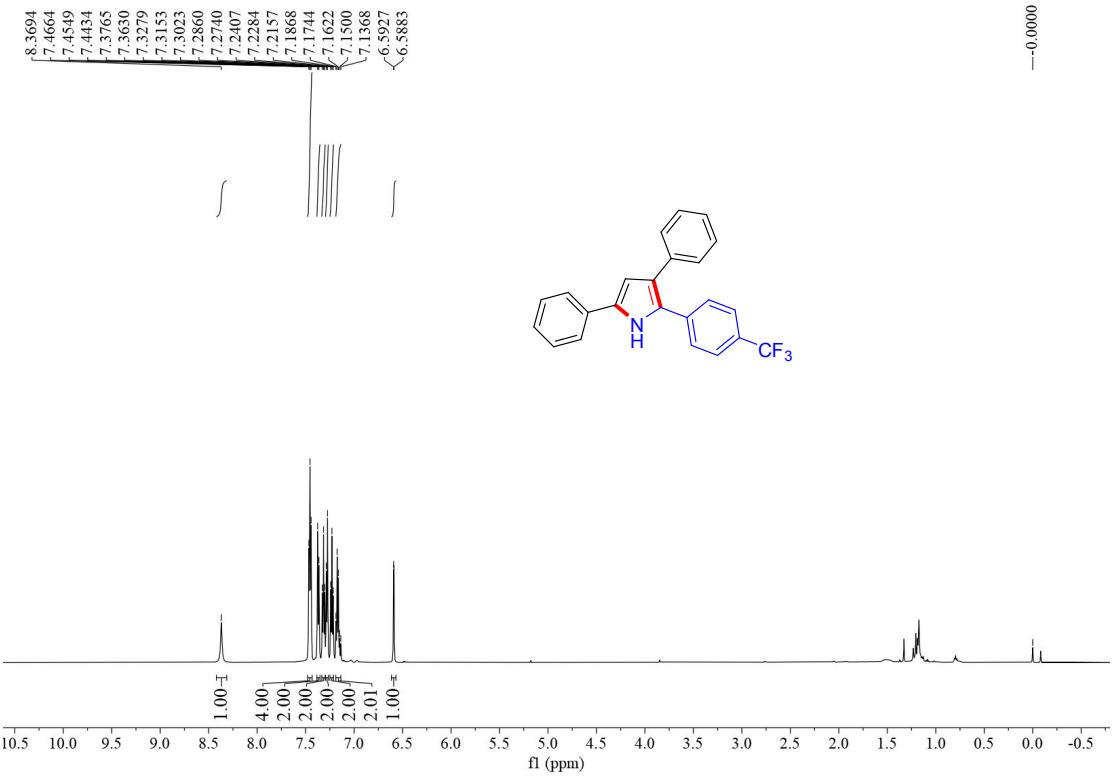
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3l



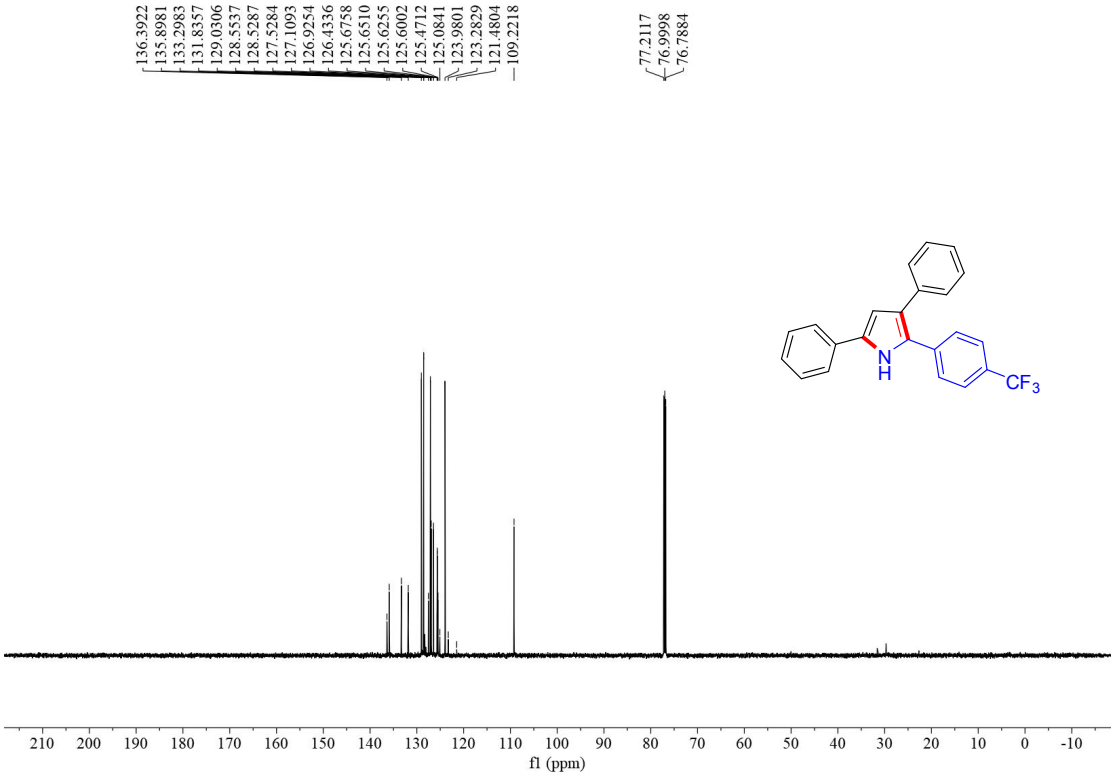
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3l



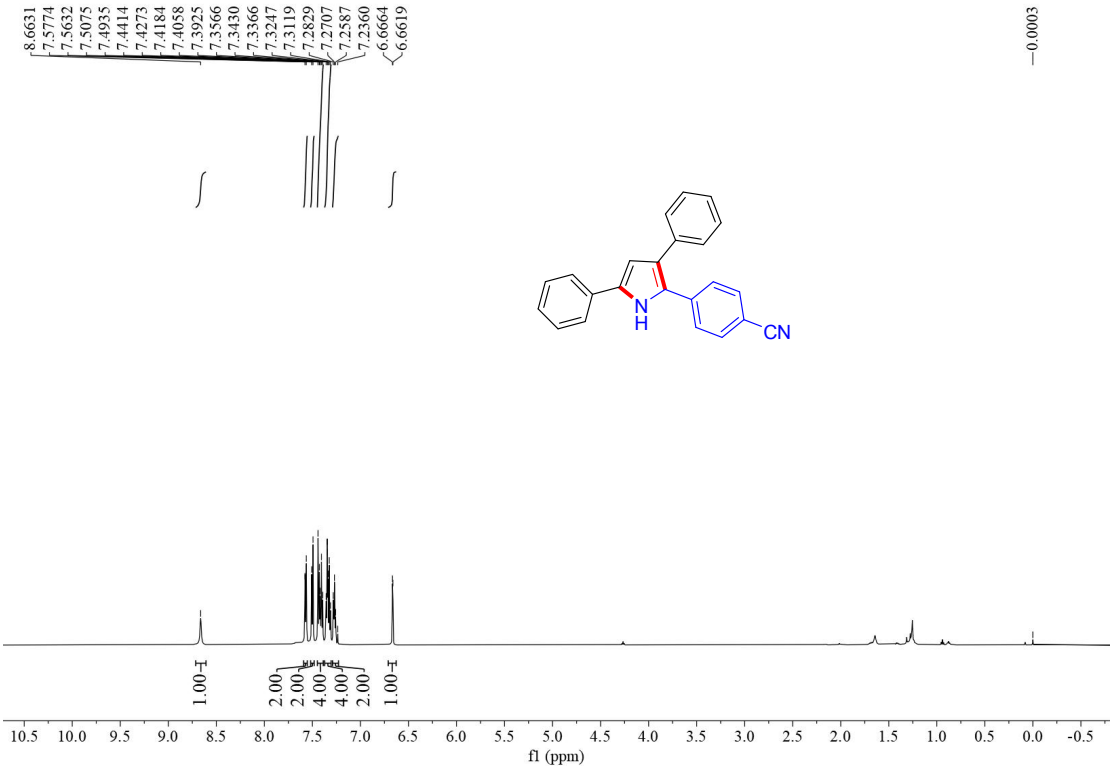
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3m



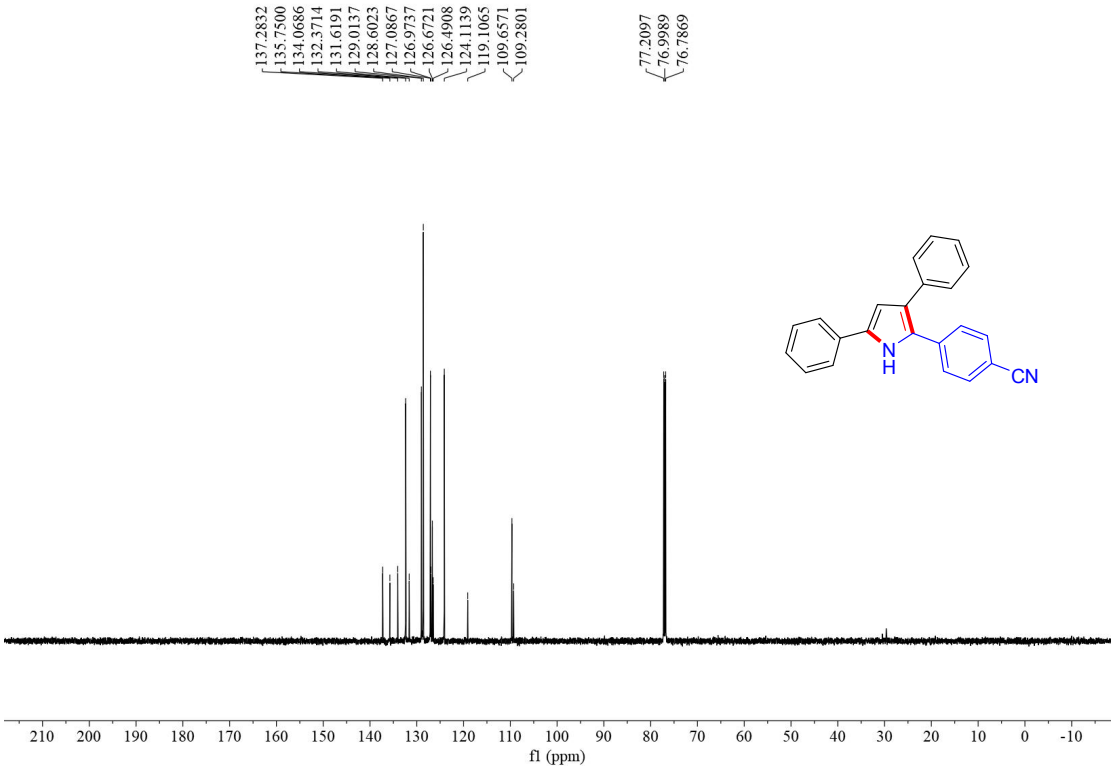
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3m



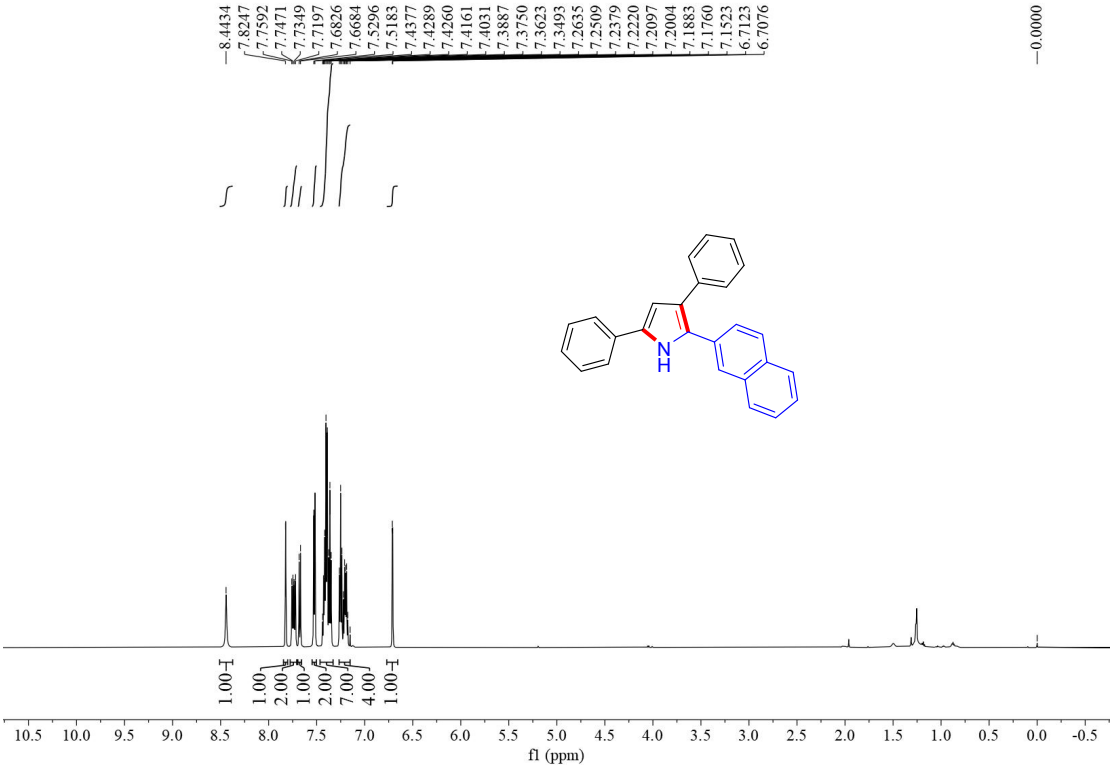
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3n



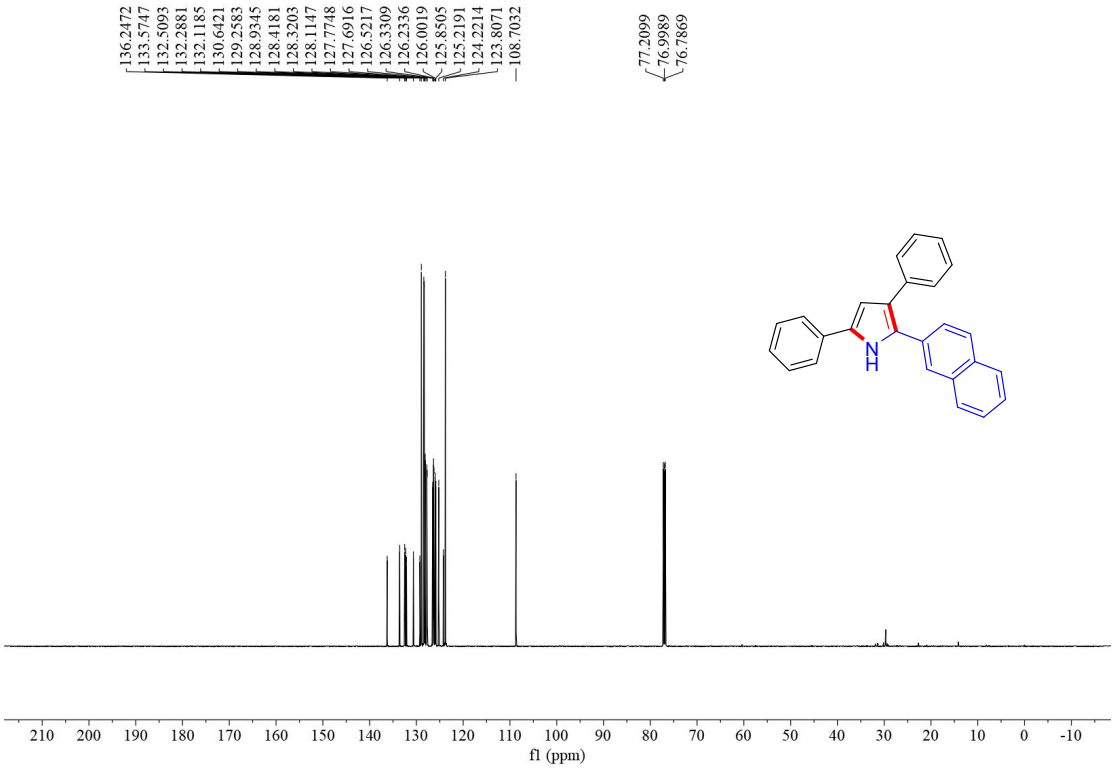
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3n



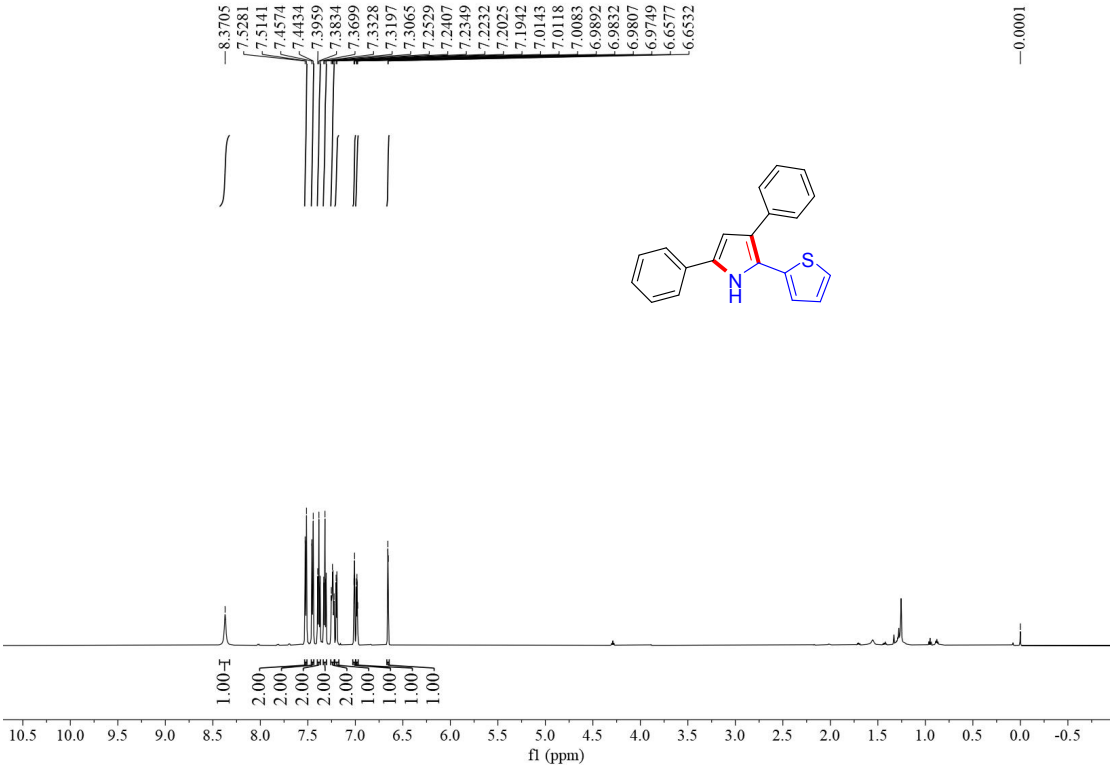
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3o



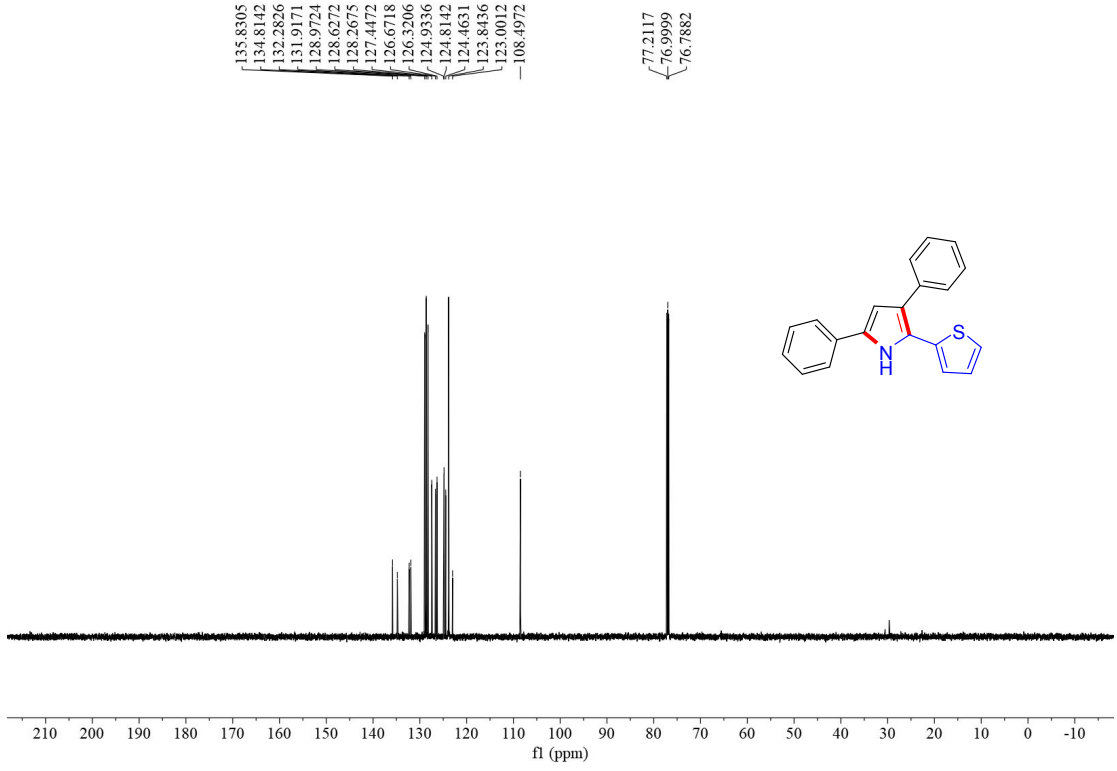
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3o



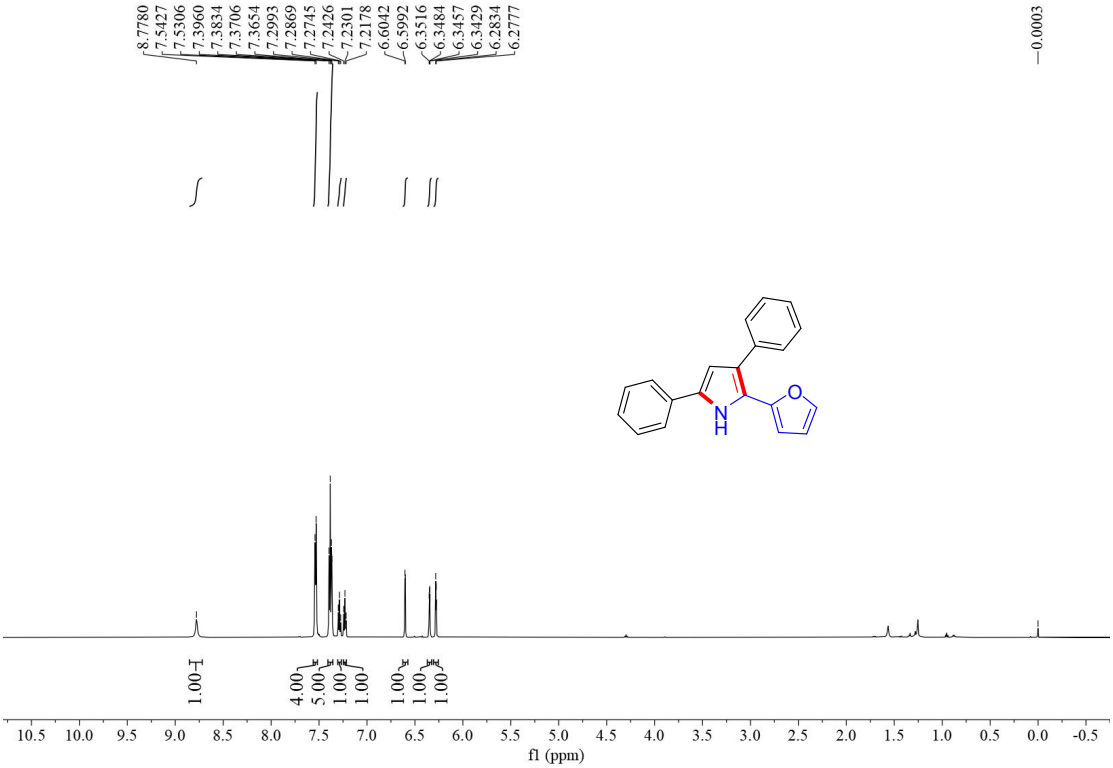
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3p



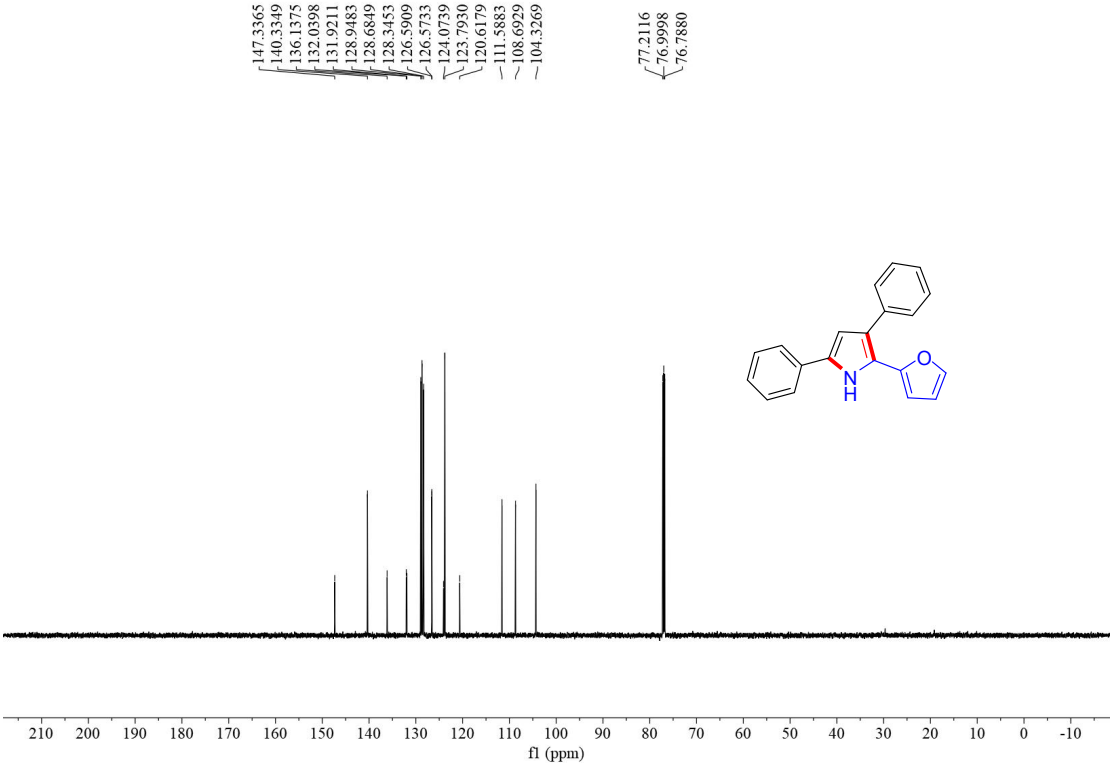
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3p



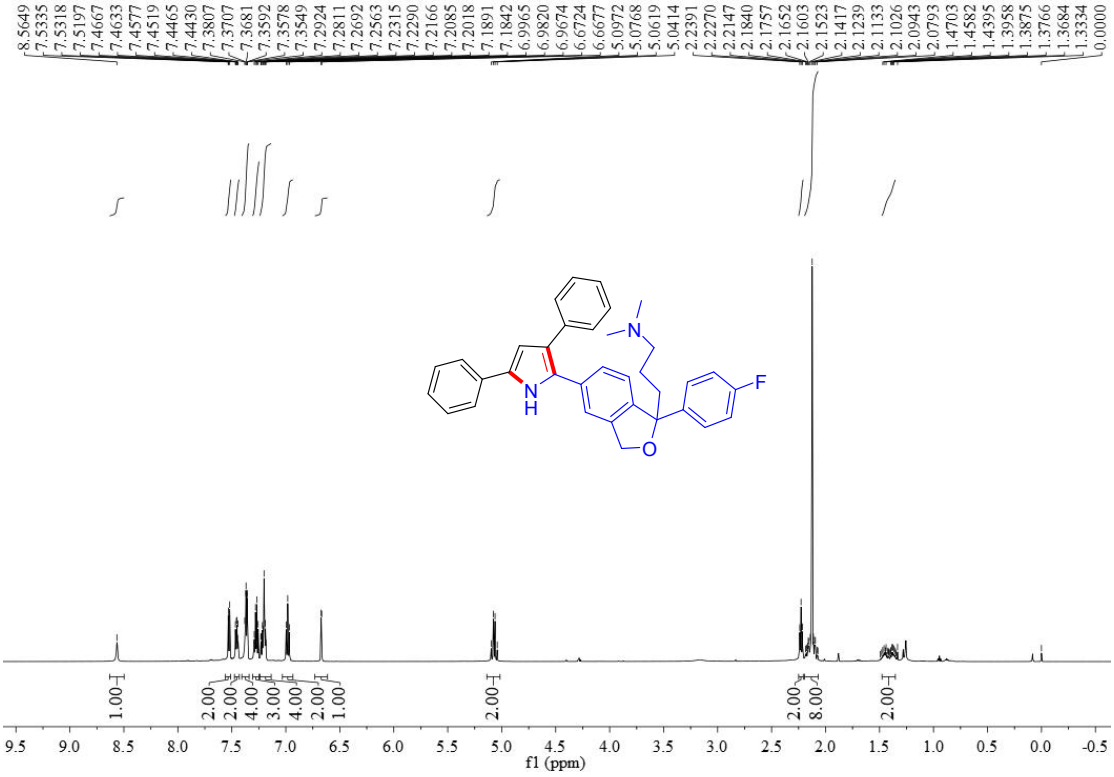
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3q



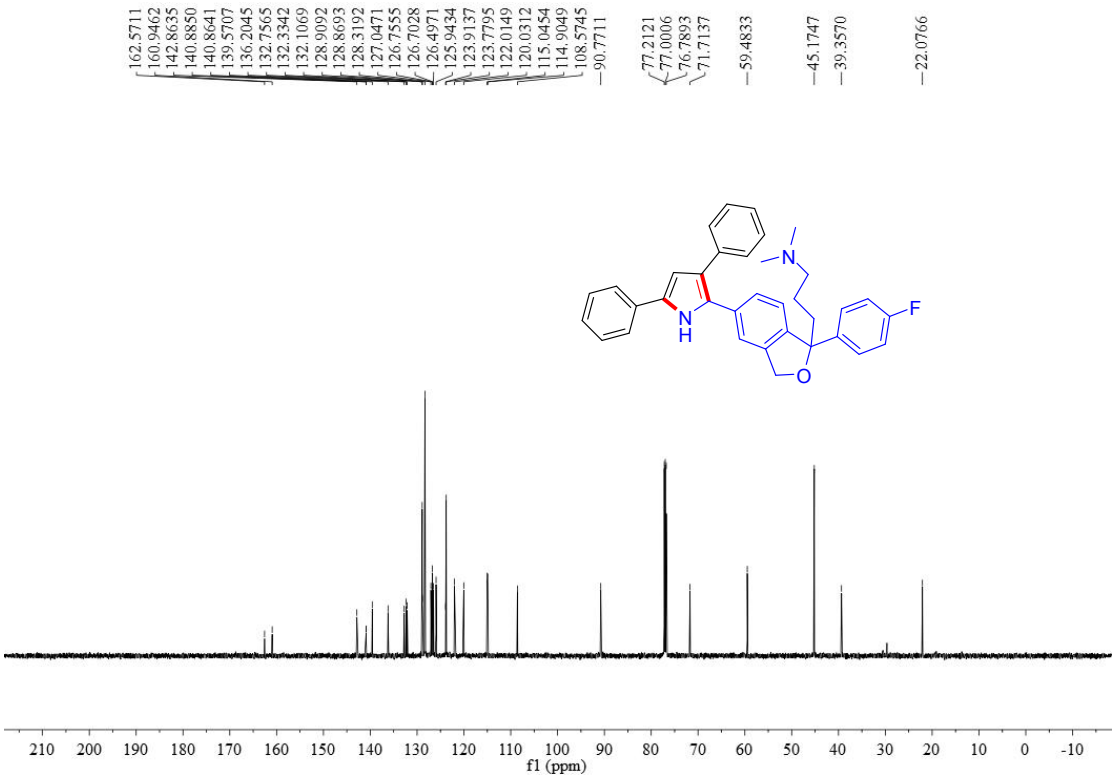
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3q



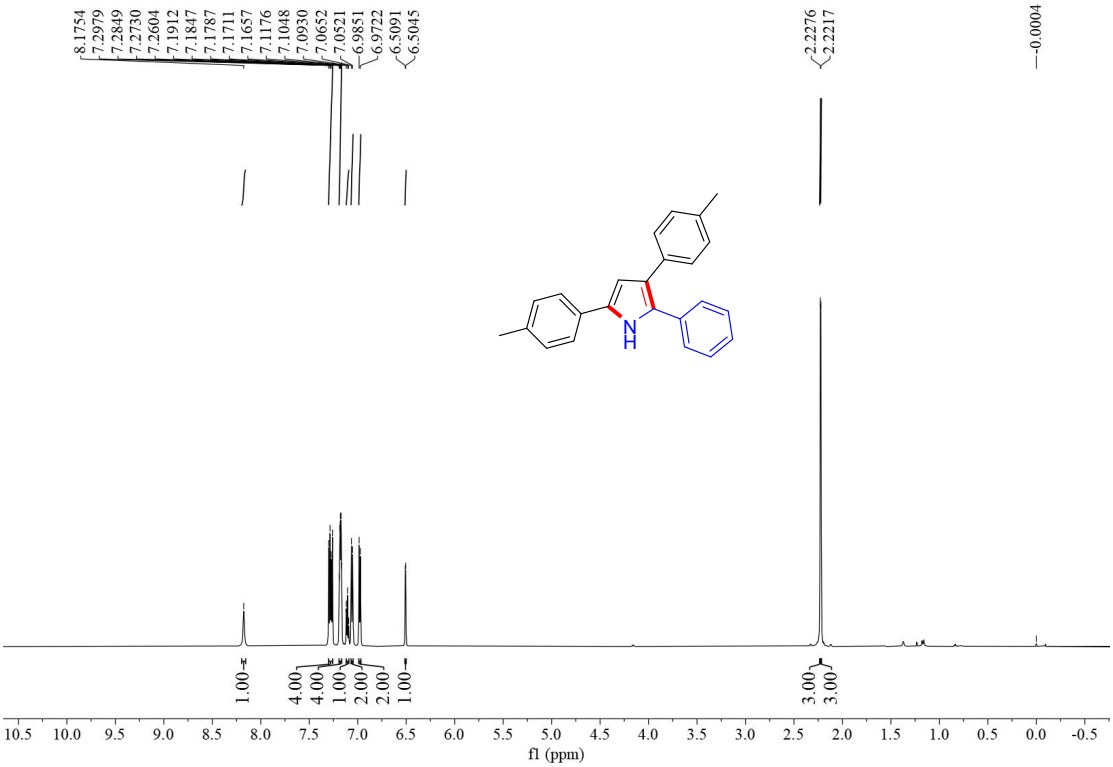
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3r



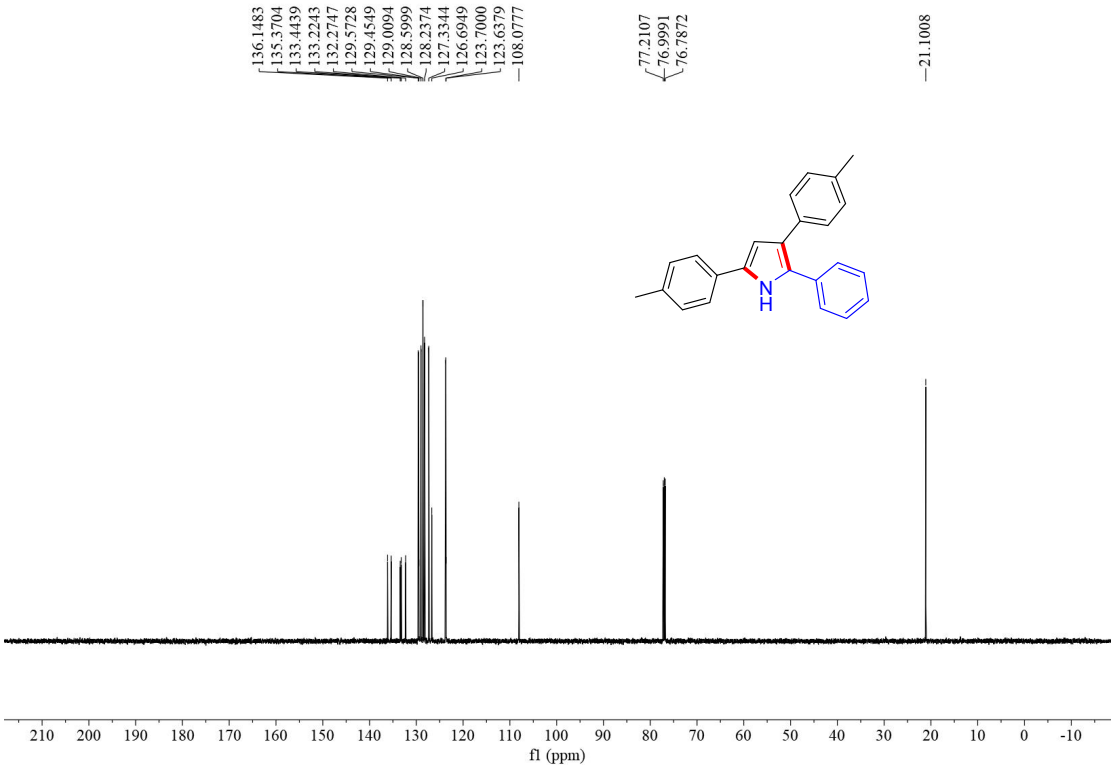
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3r



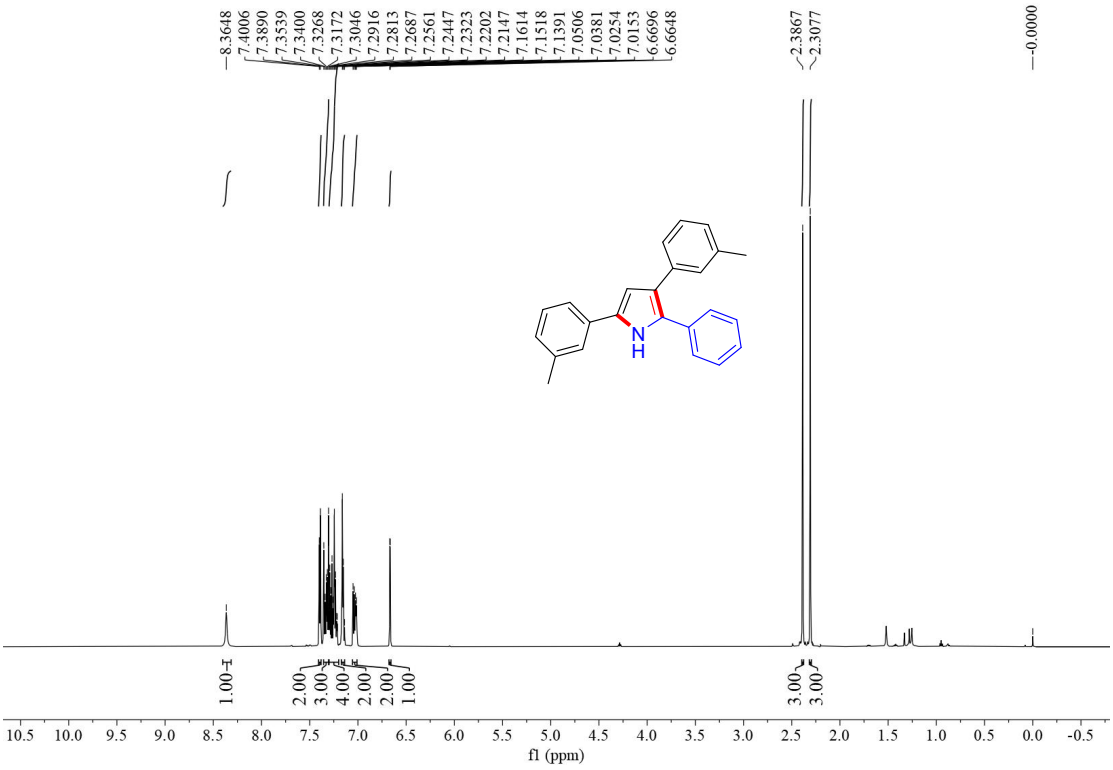
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3s



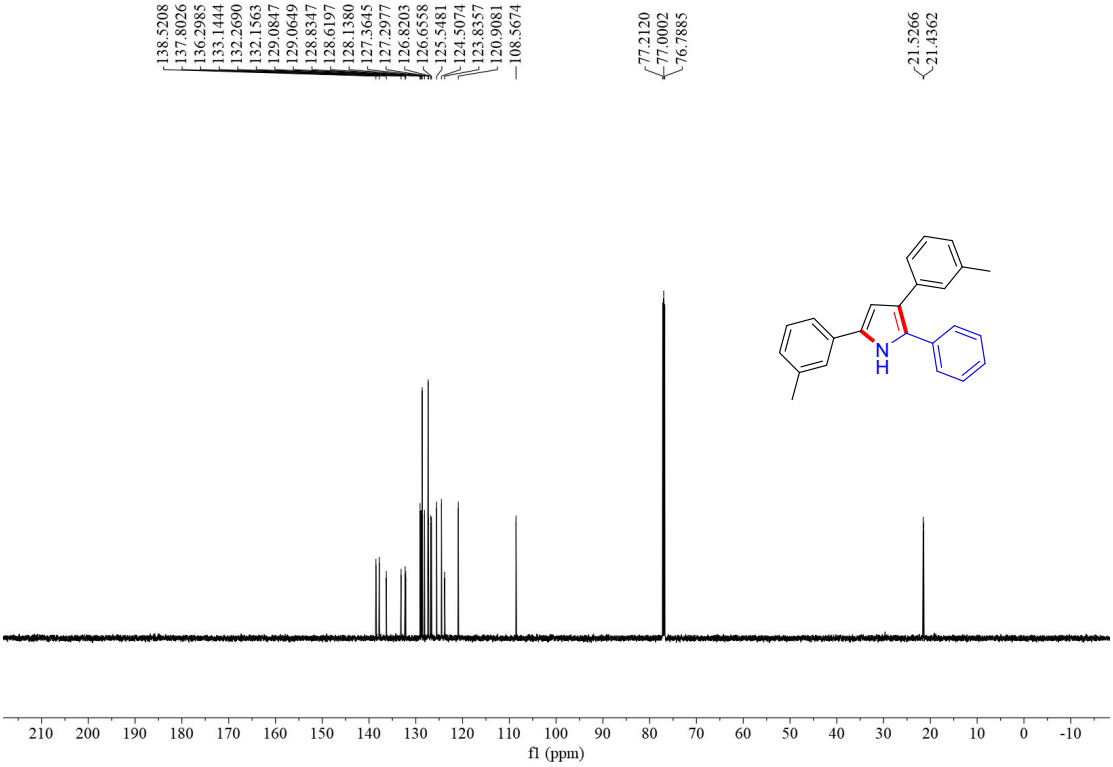
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3s



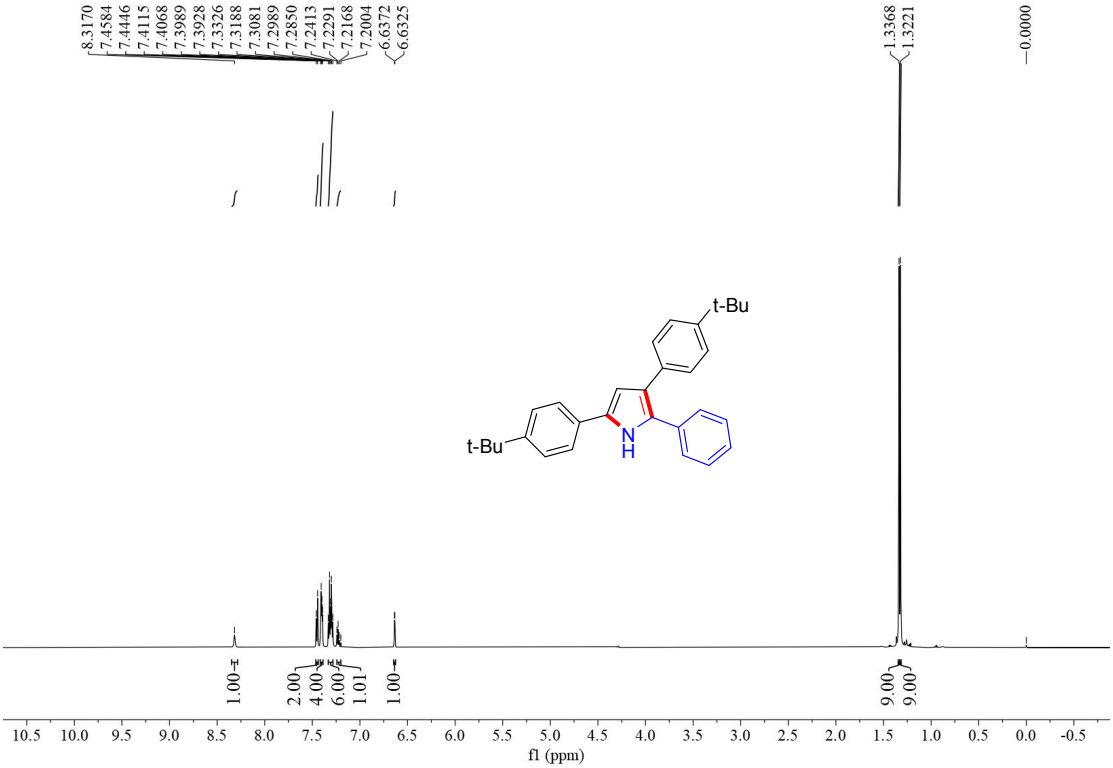
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3t



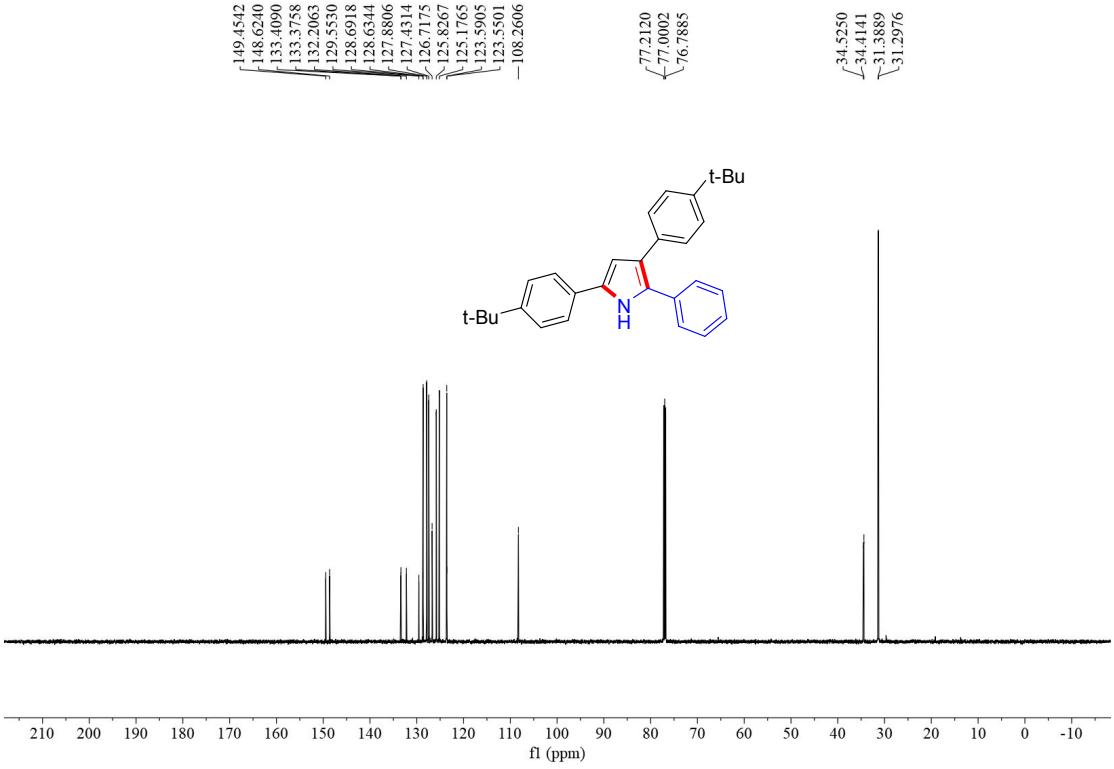
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3t



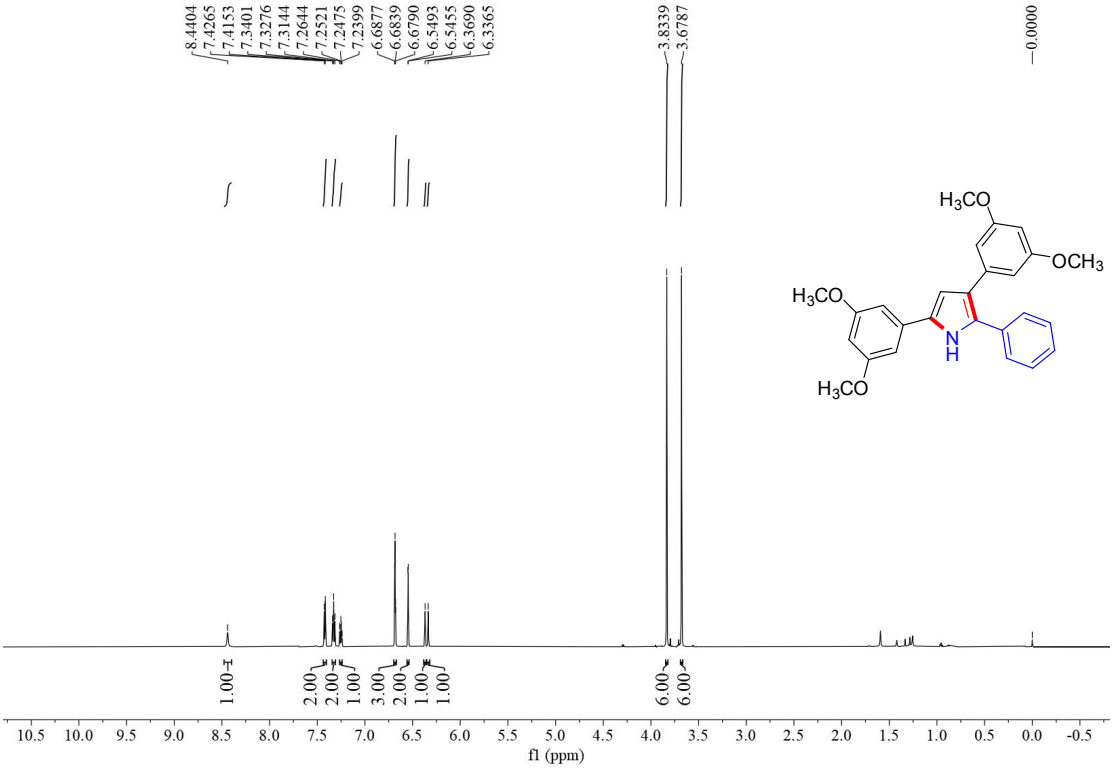
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3u



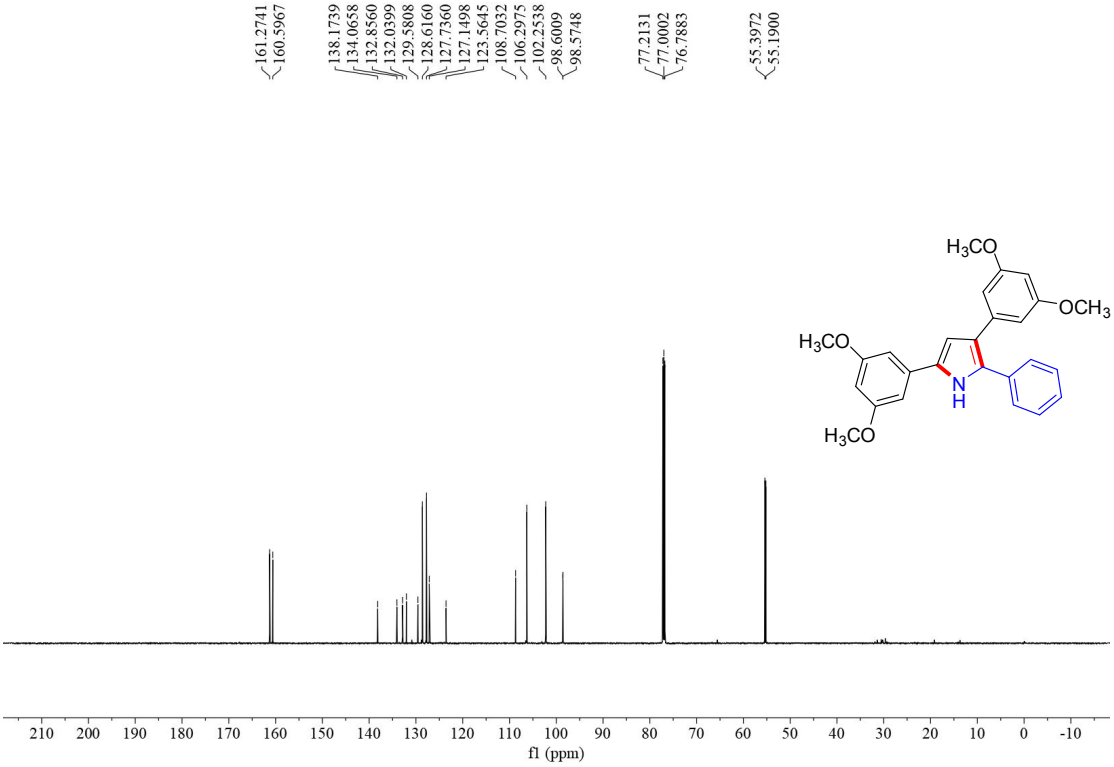
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3u



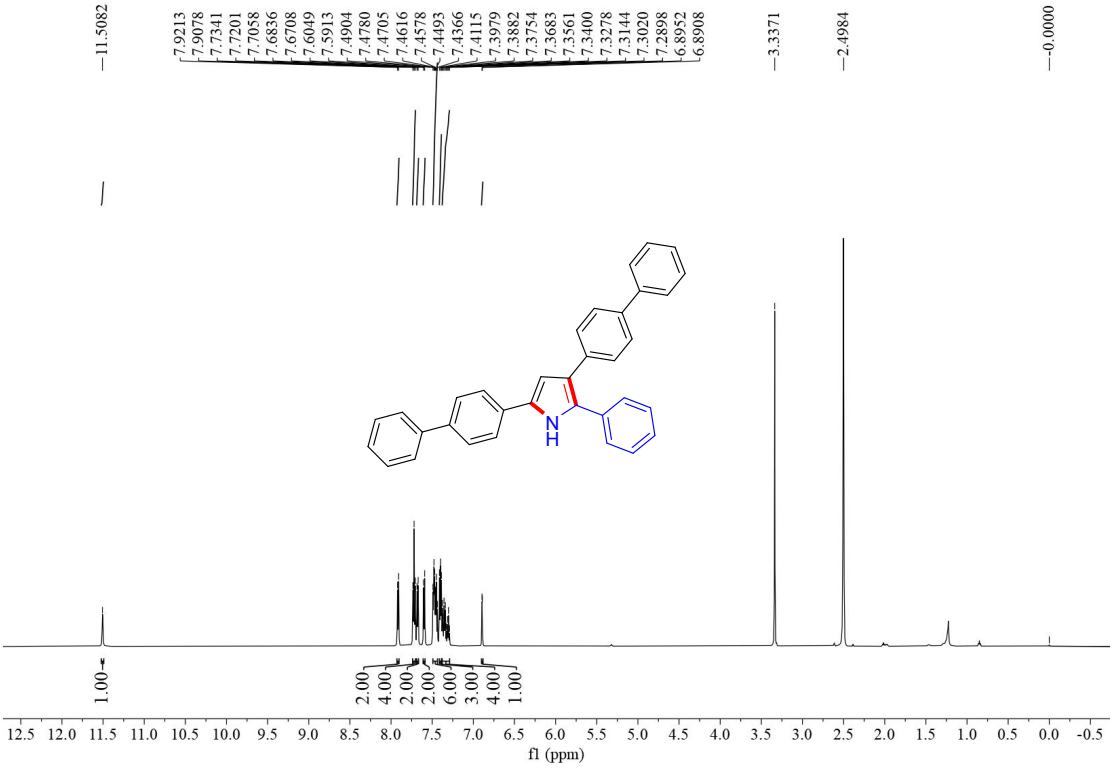
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3v



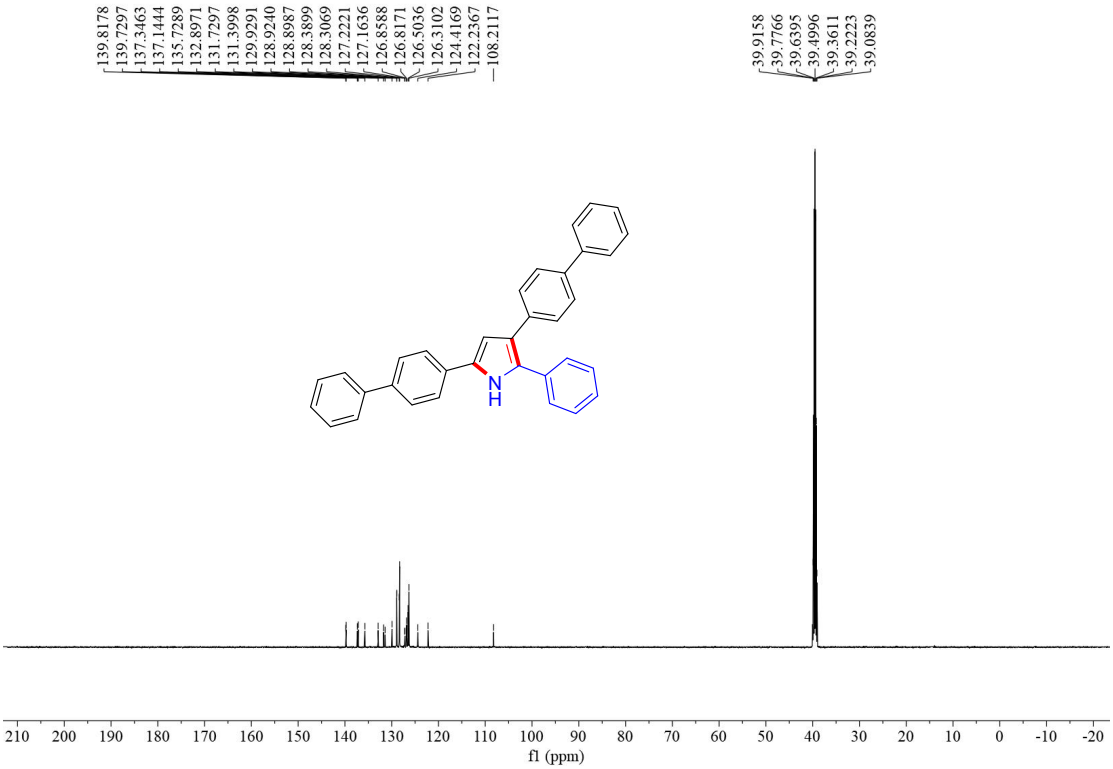
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3v



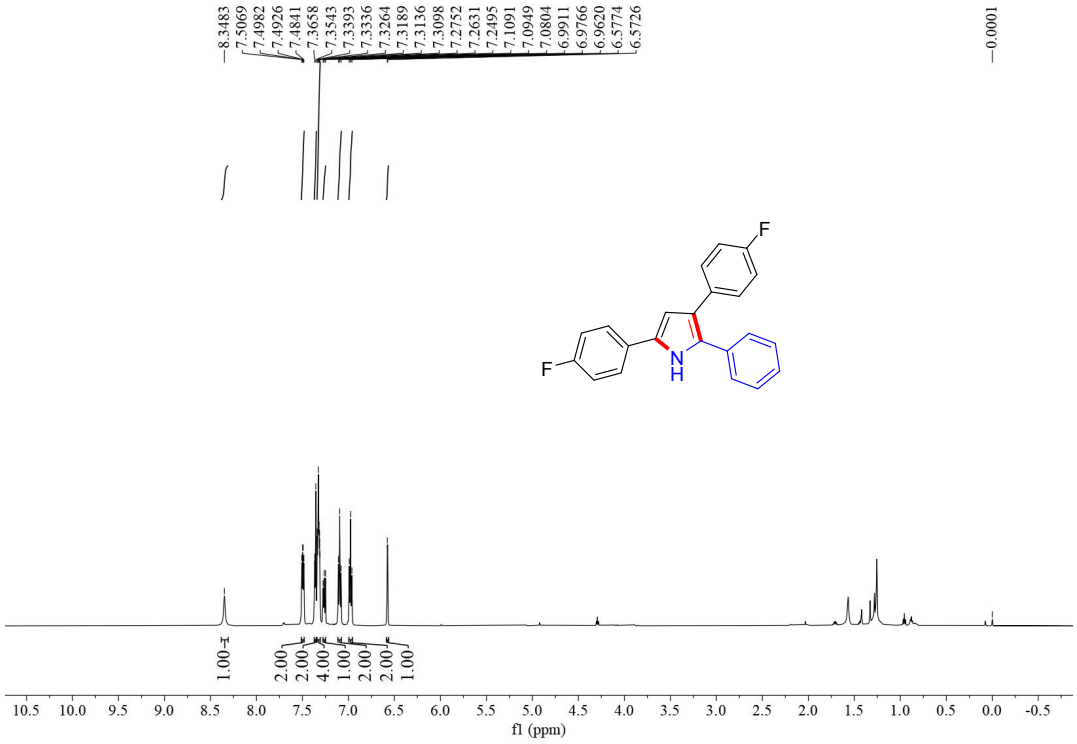
^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound 3w



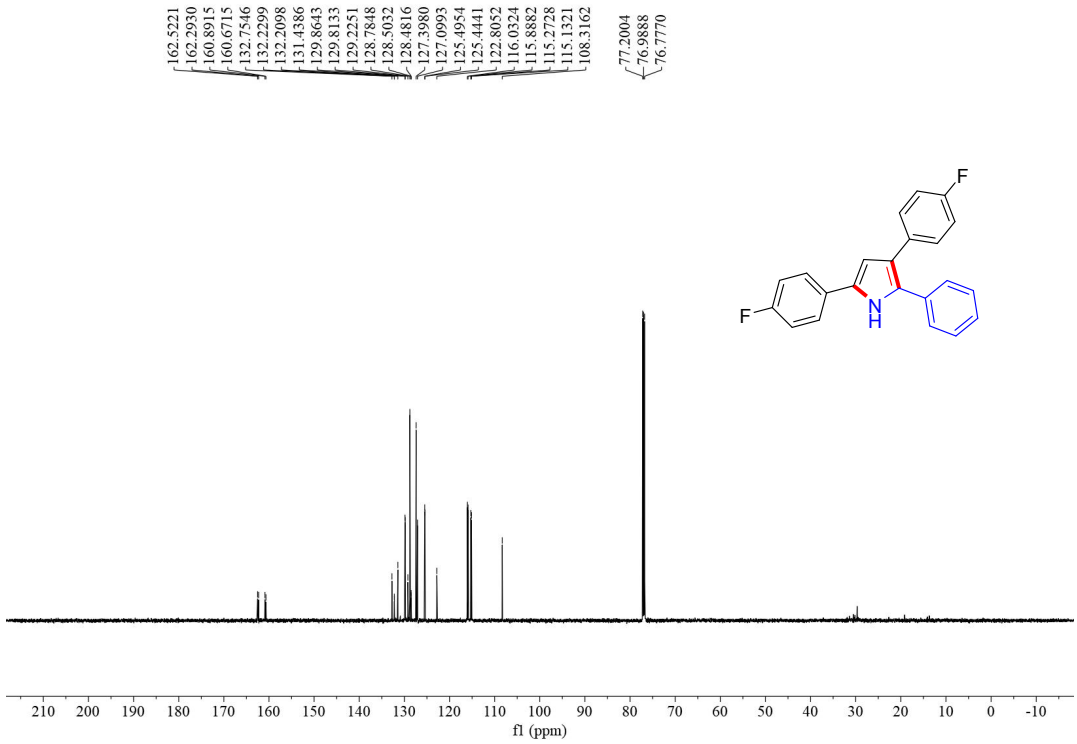
^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound 3w



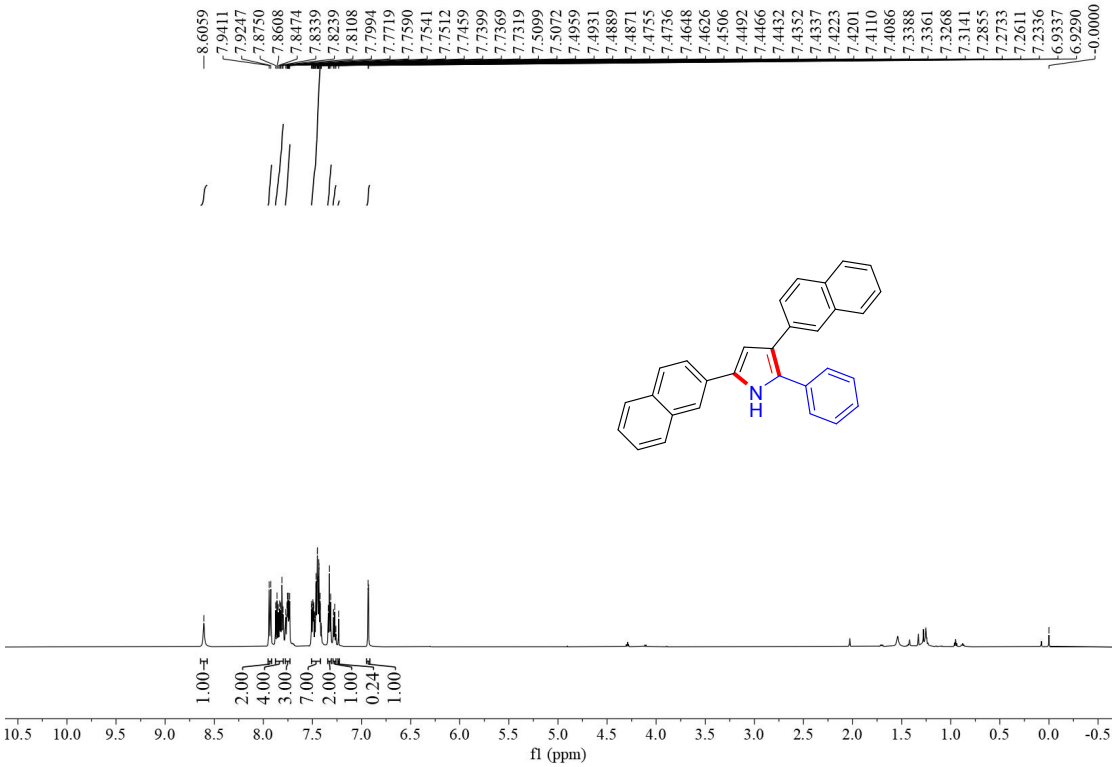
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3x



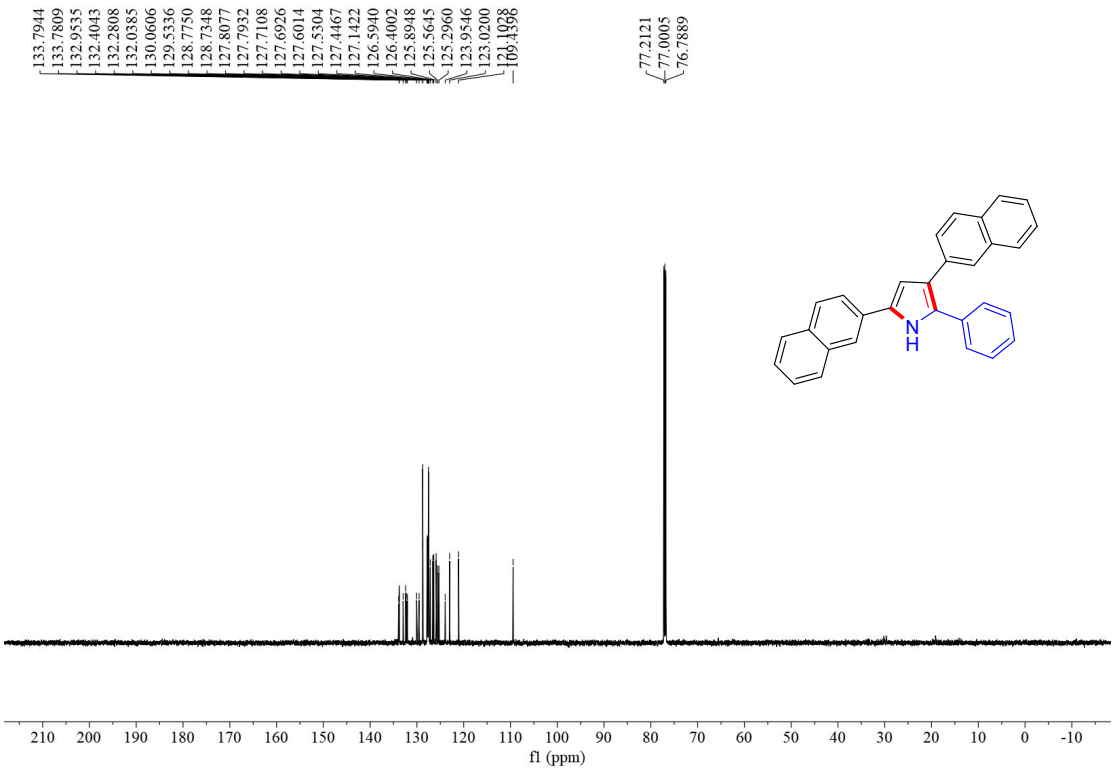
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3x



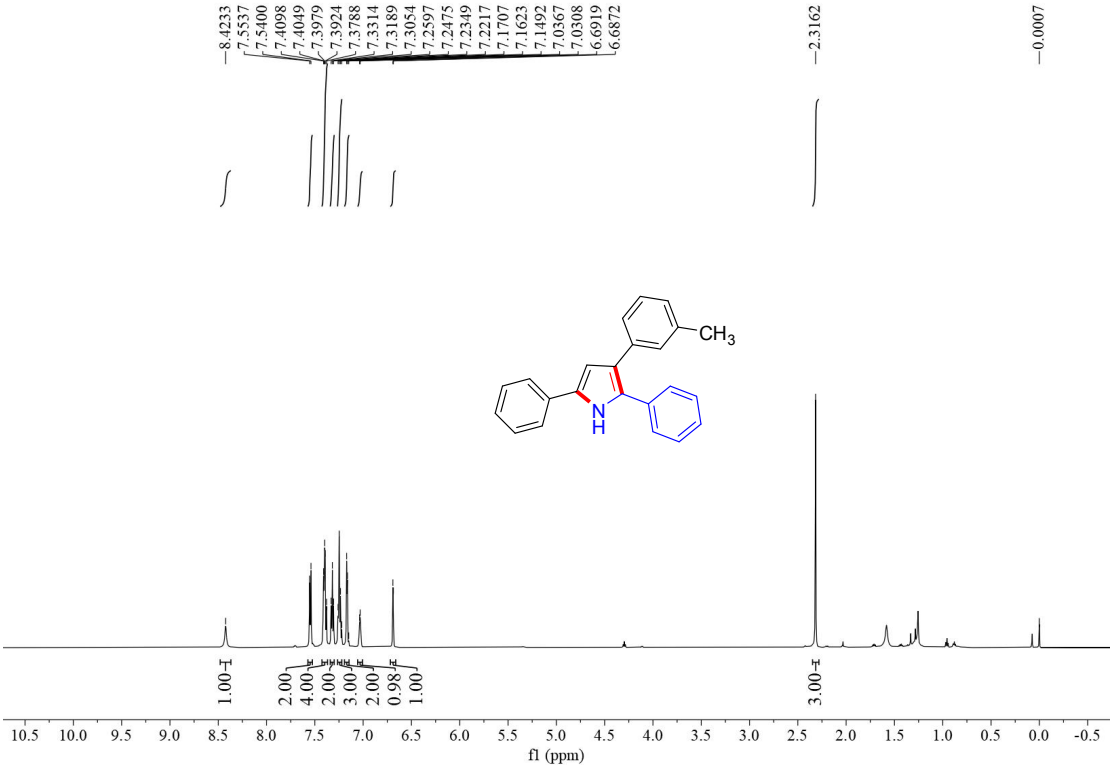
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3y



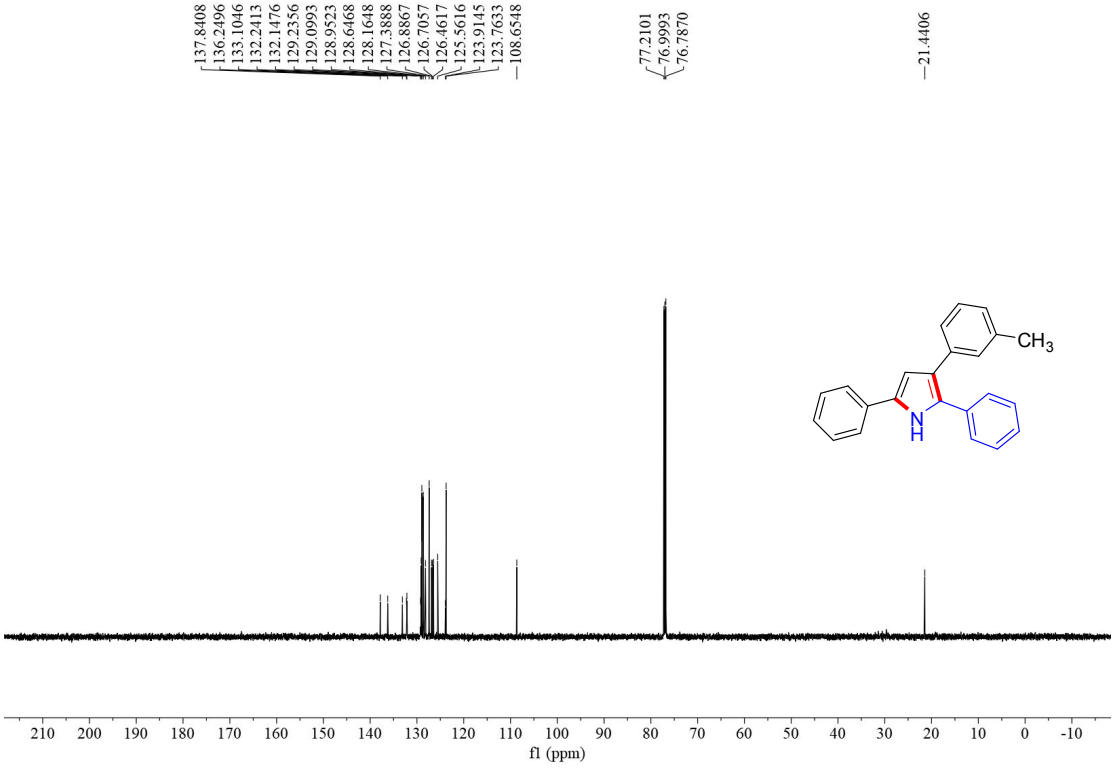
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3y



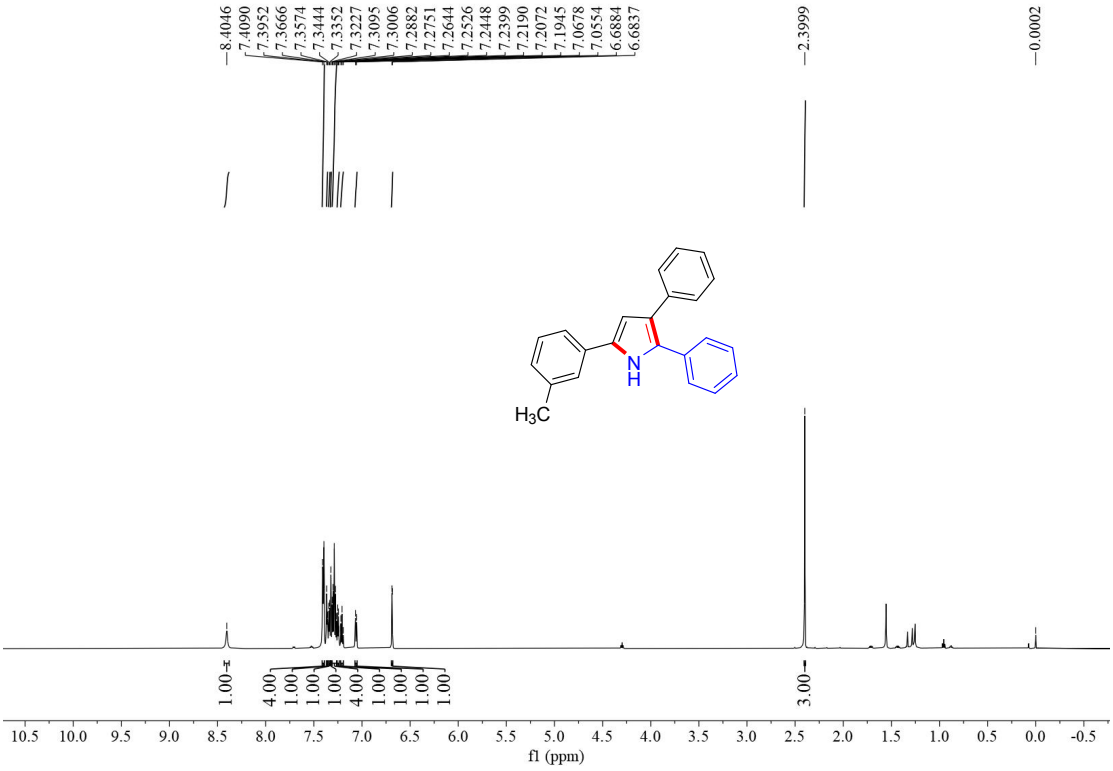
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3aa



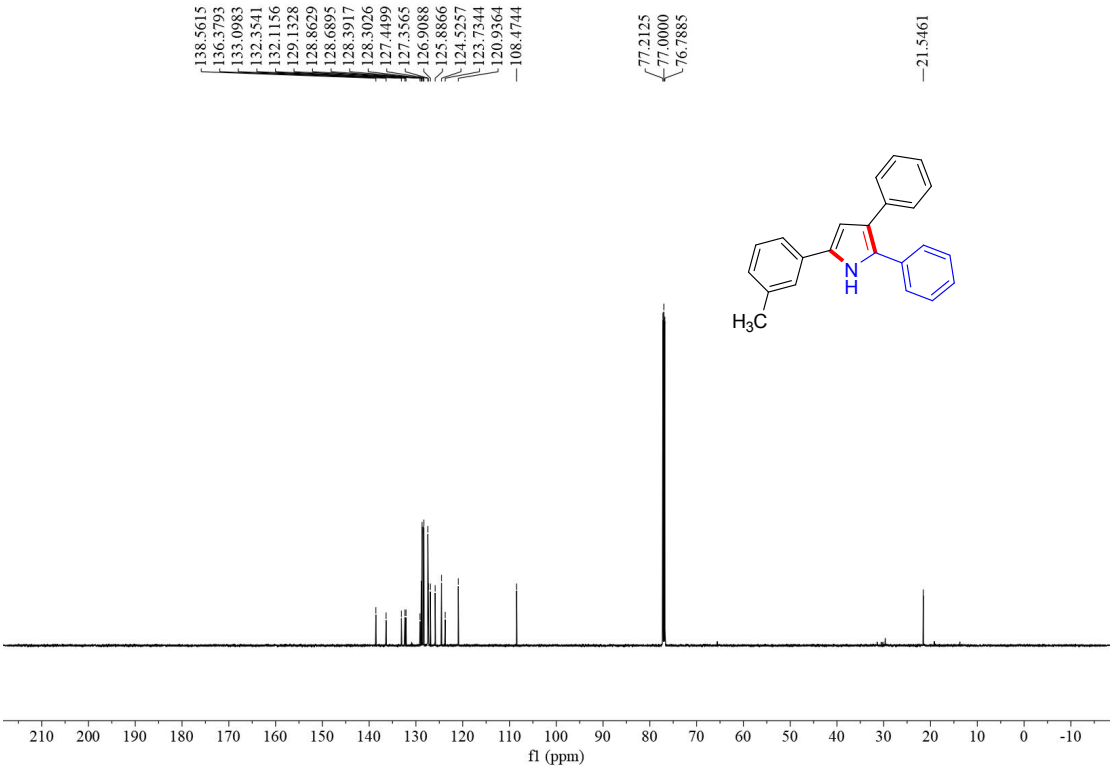
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3aa



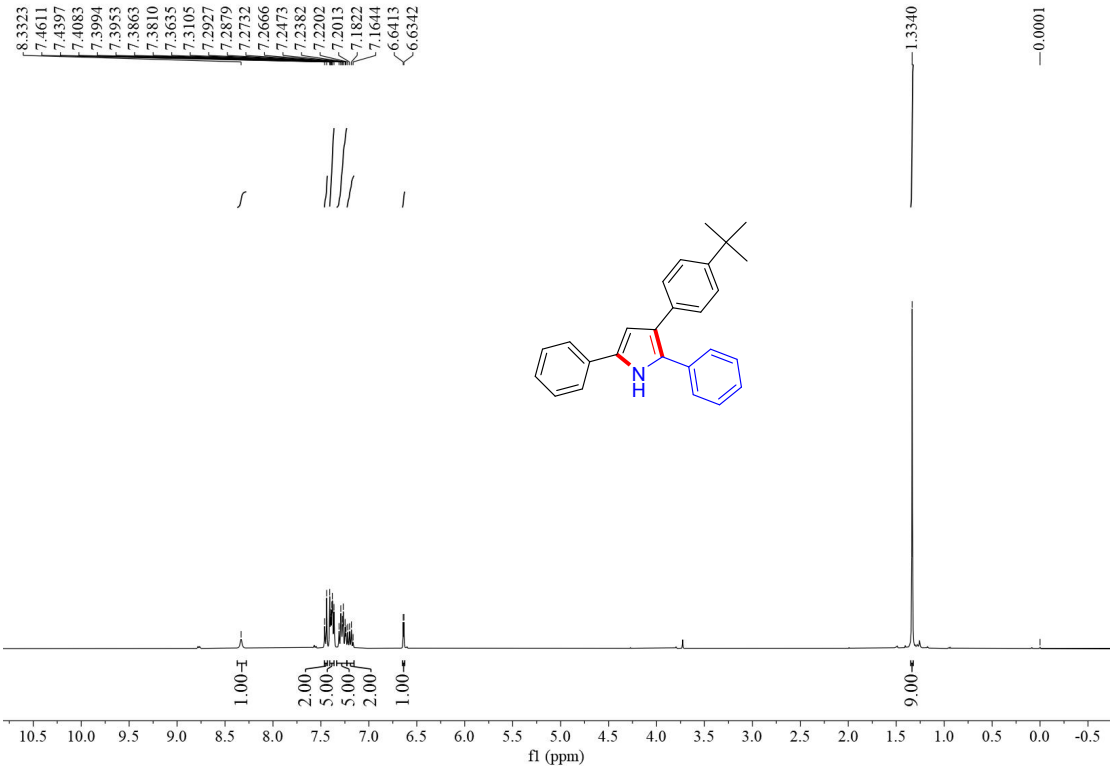
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3aa'



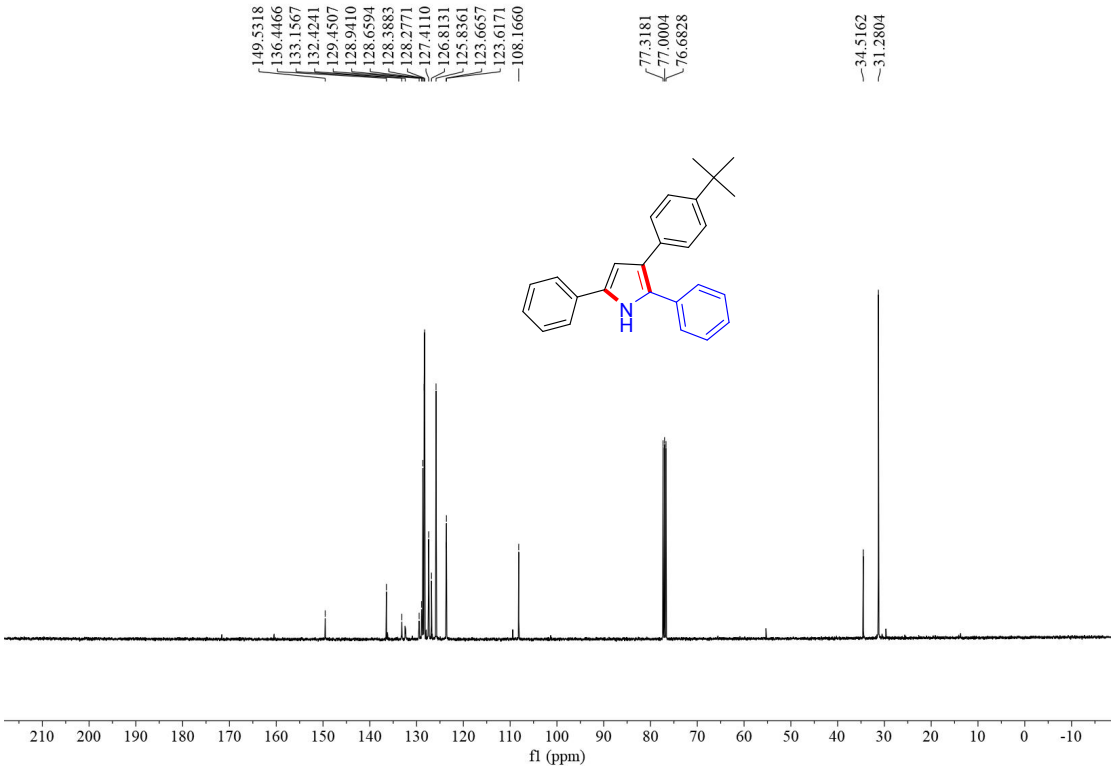
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3aa'



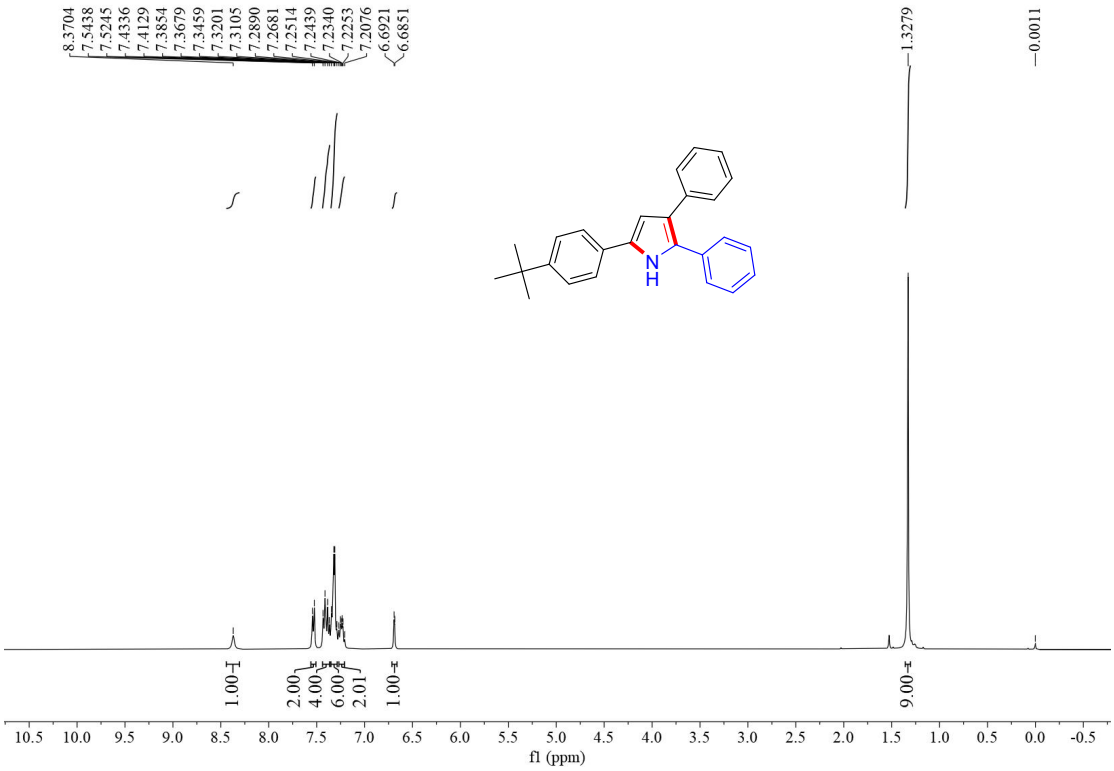
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3ba



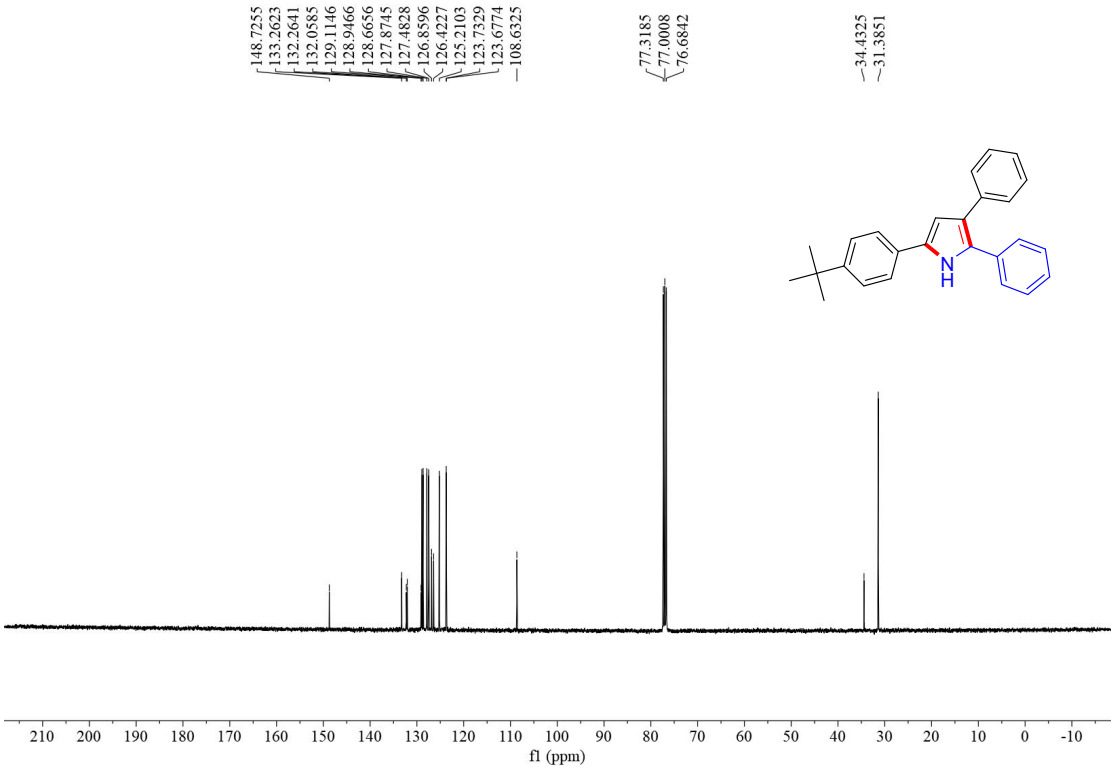
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3ba



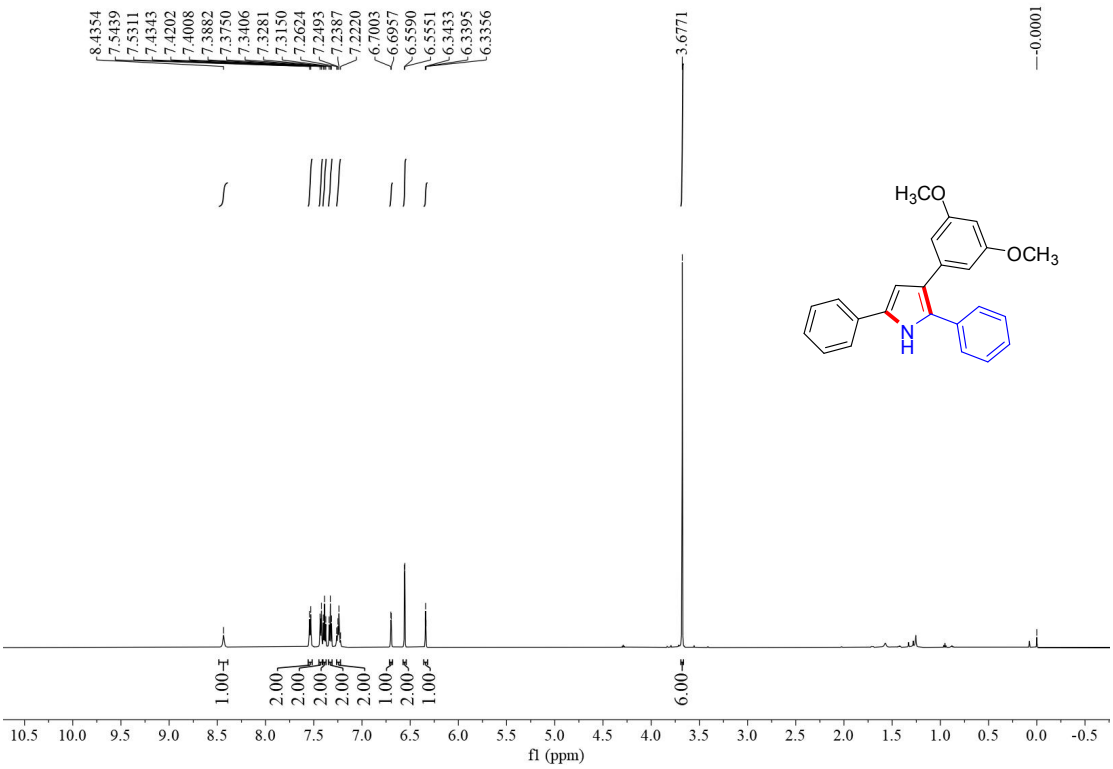
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3ba'



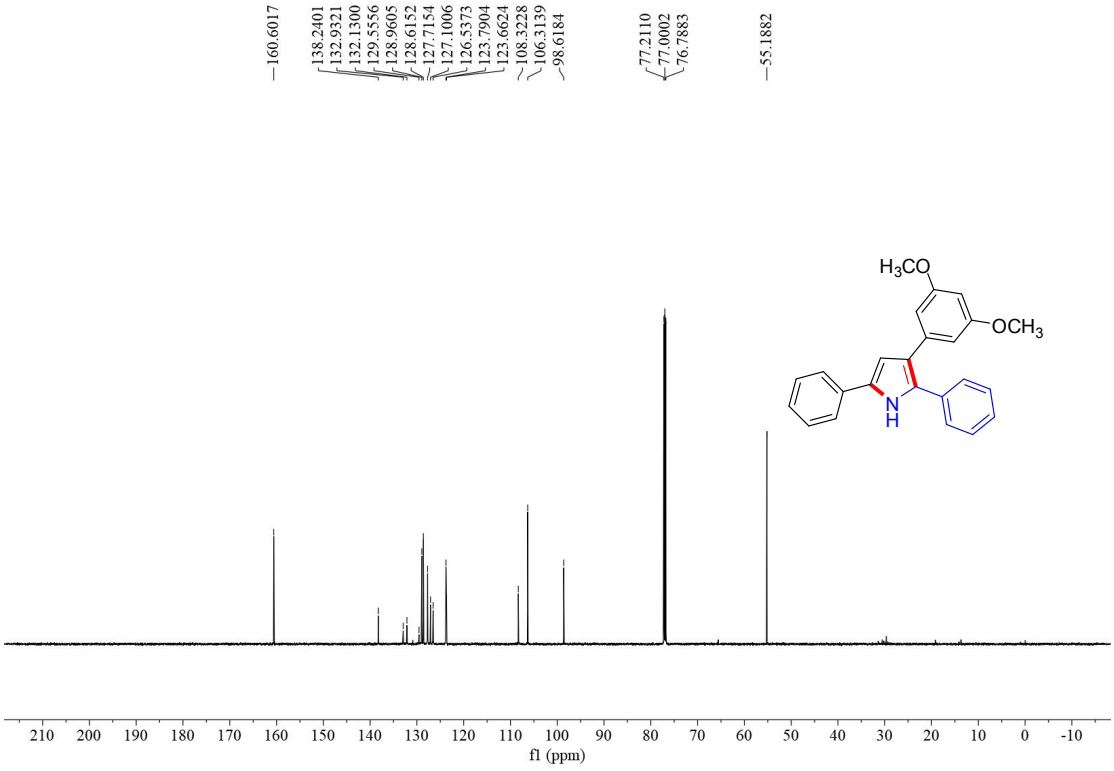
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3ba'



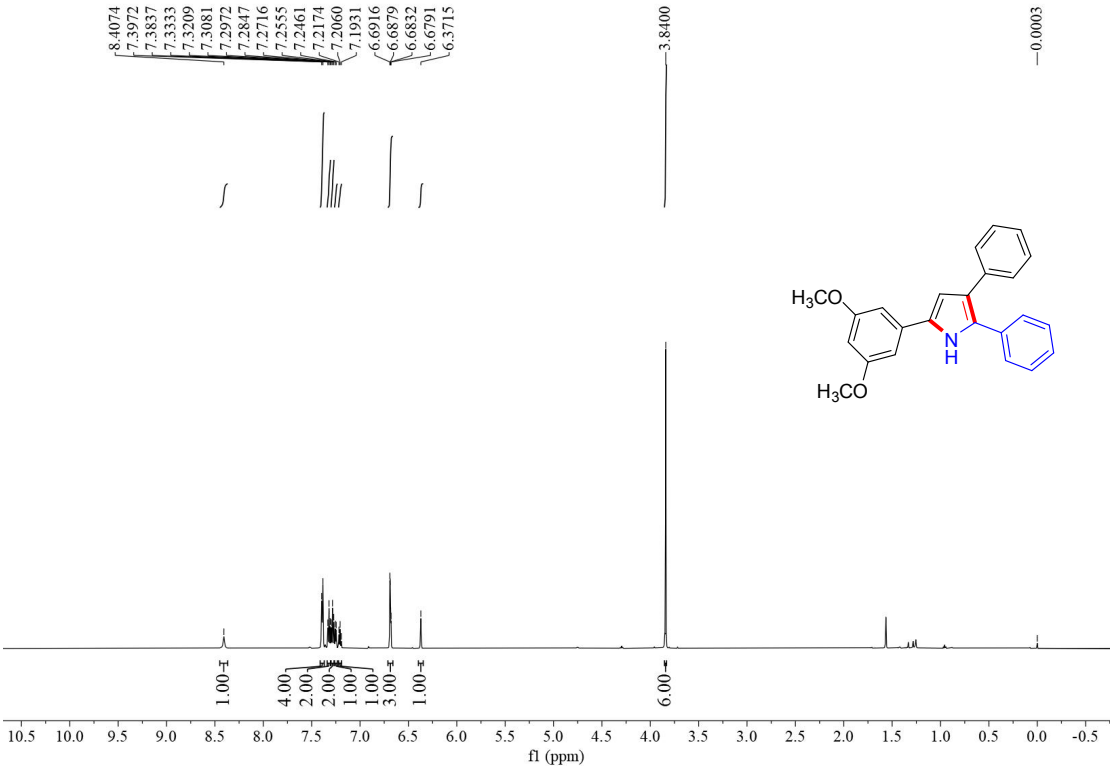
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3ca



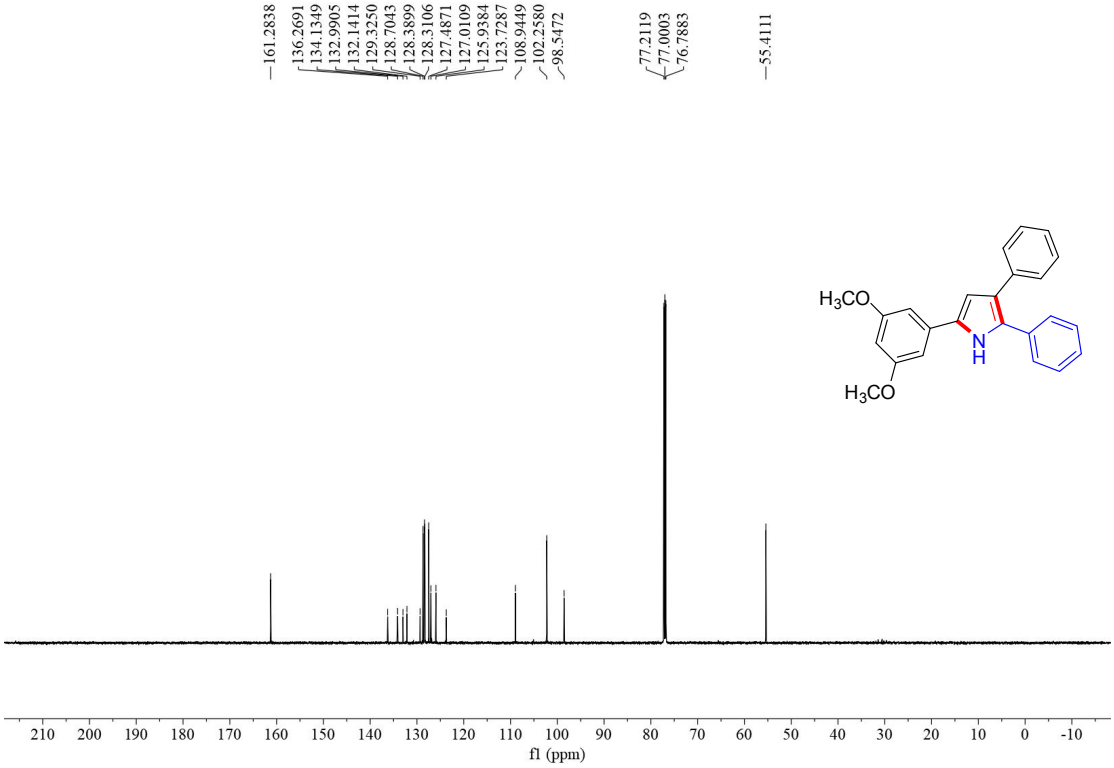
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3ca



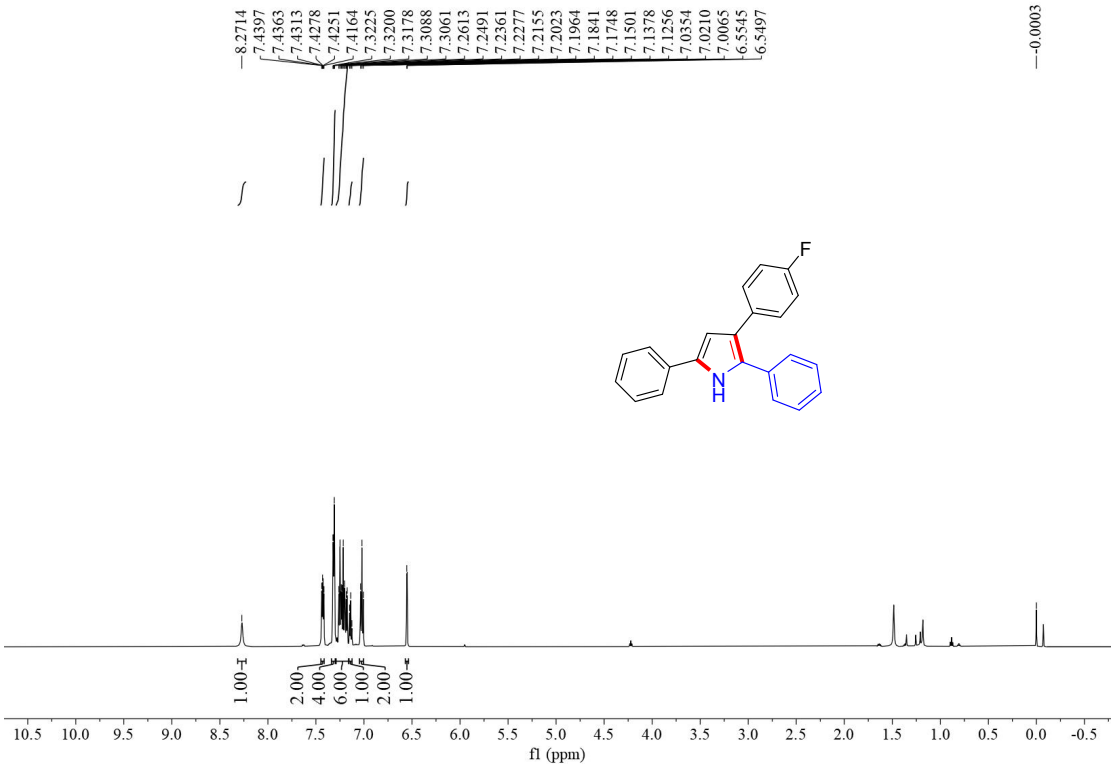
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3ca'



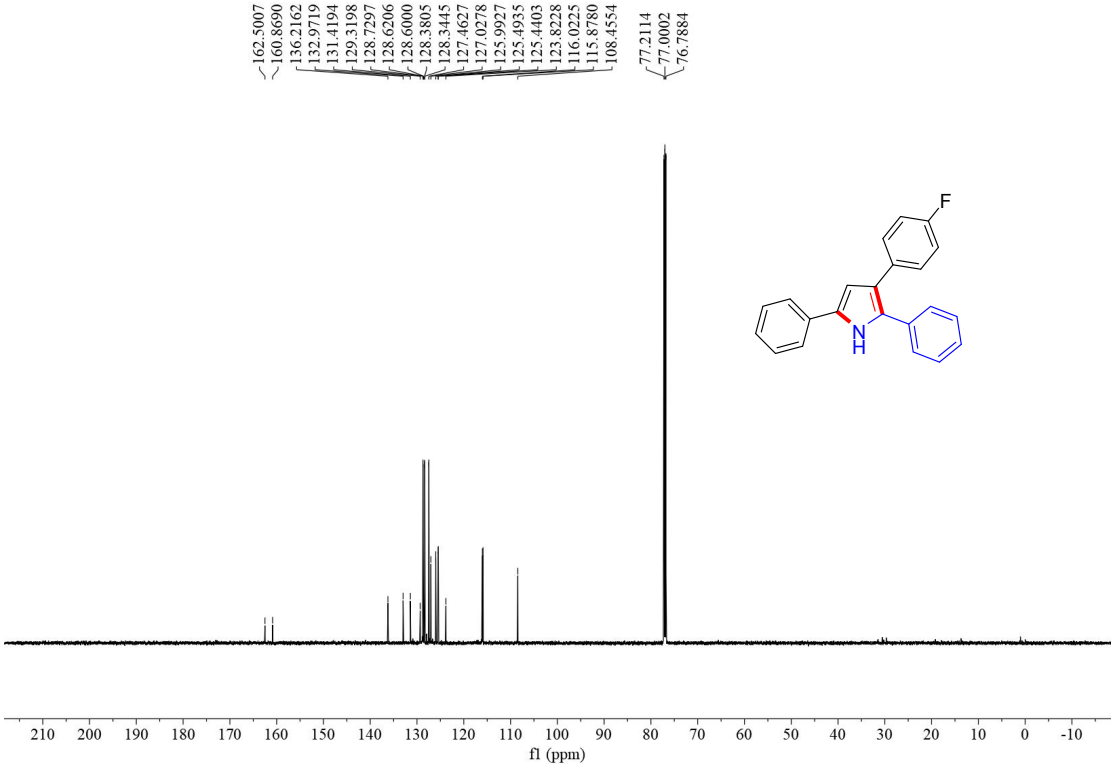
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3ca'



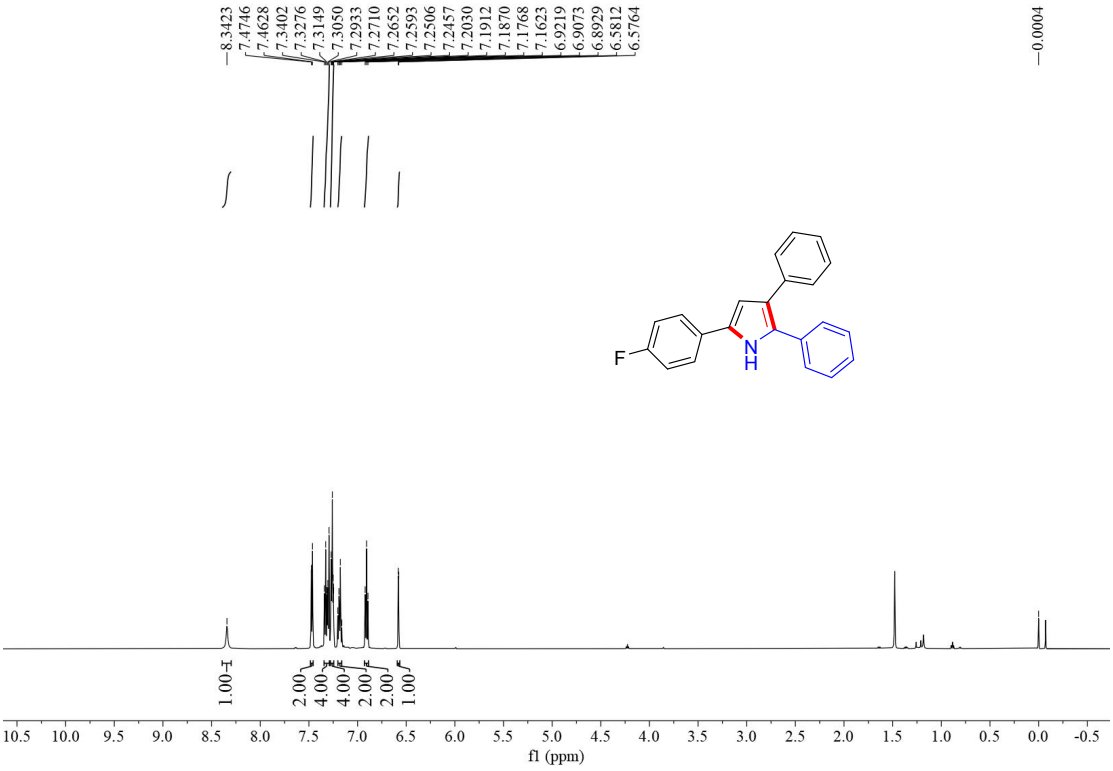
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3da



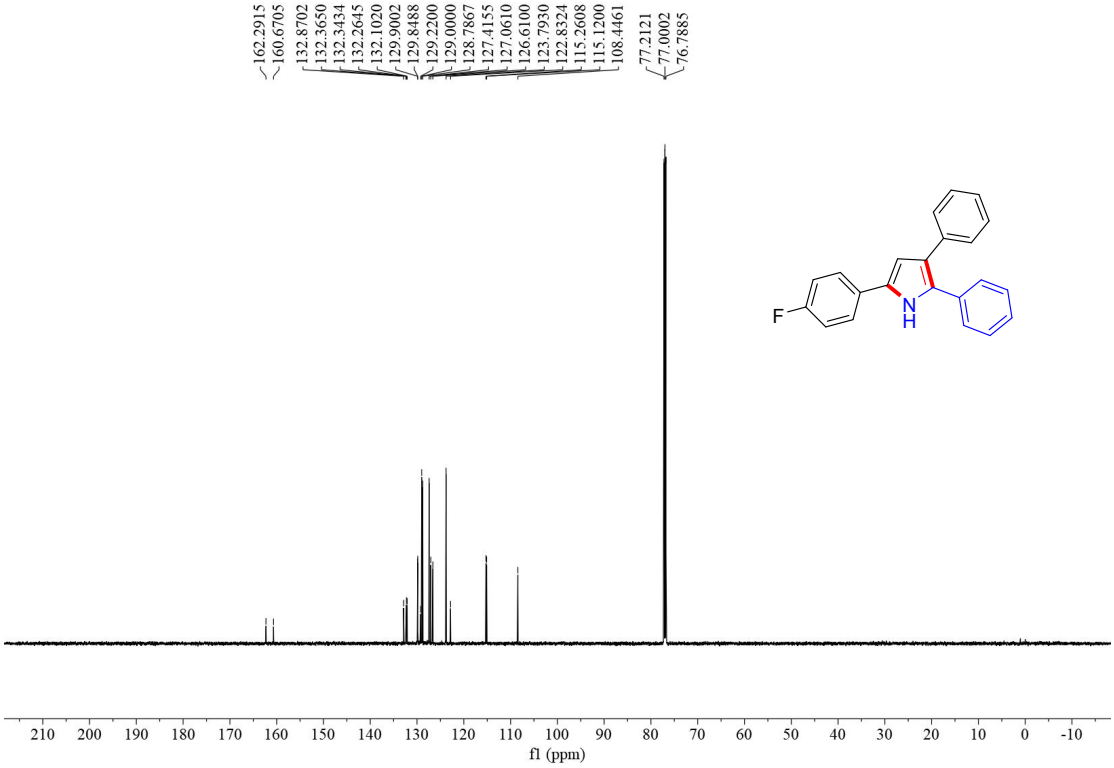
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3da



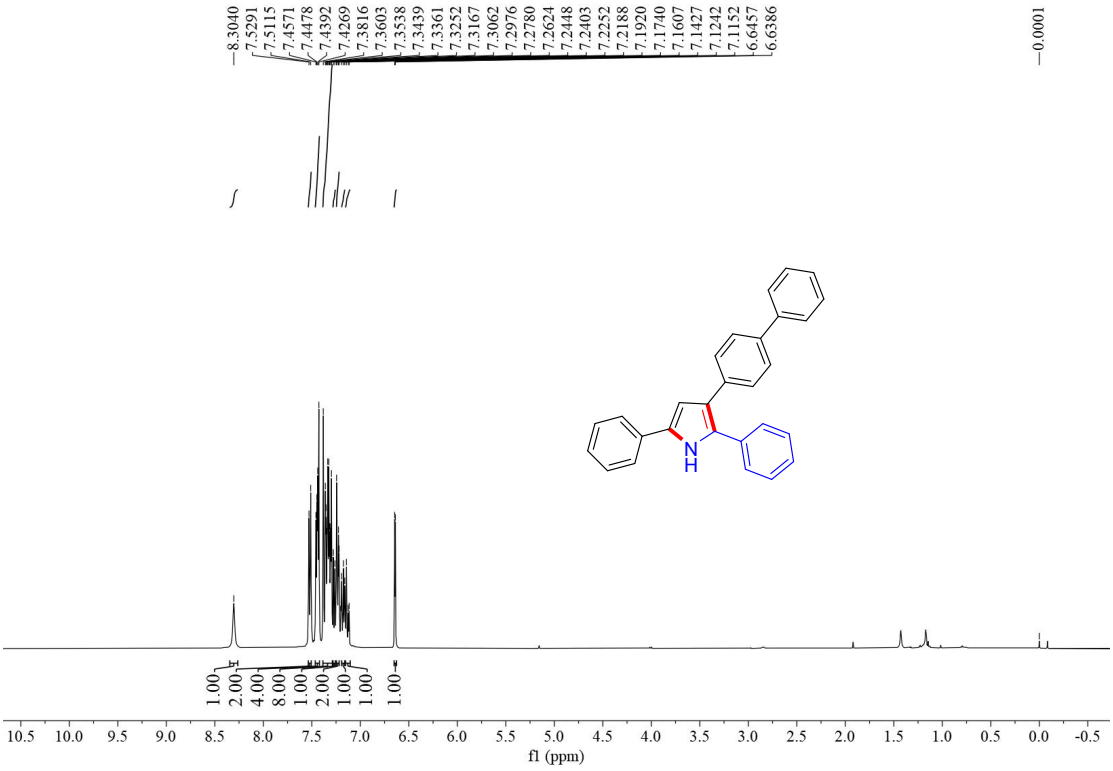
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3da'



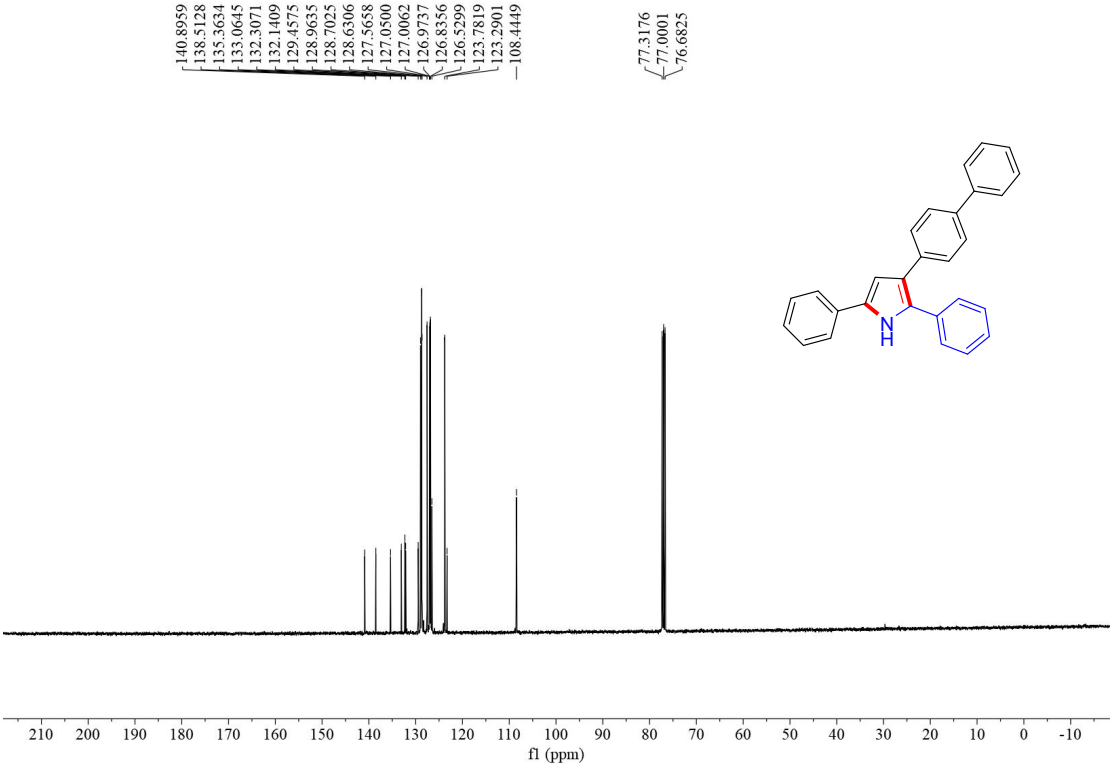
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3da'



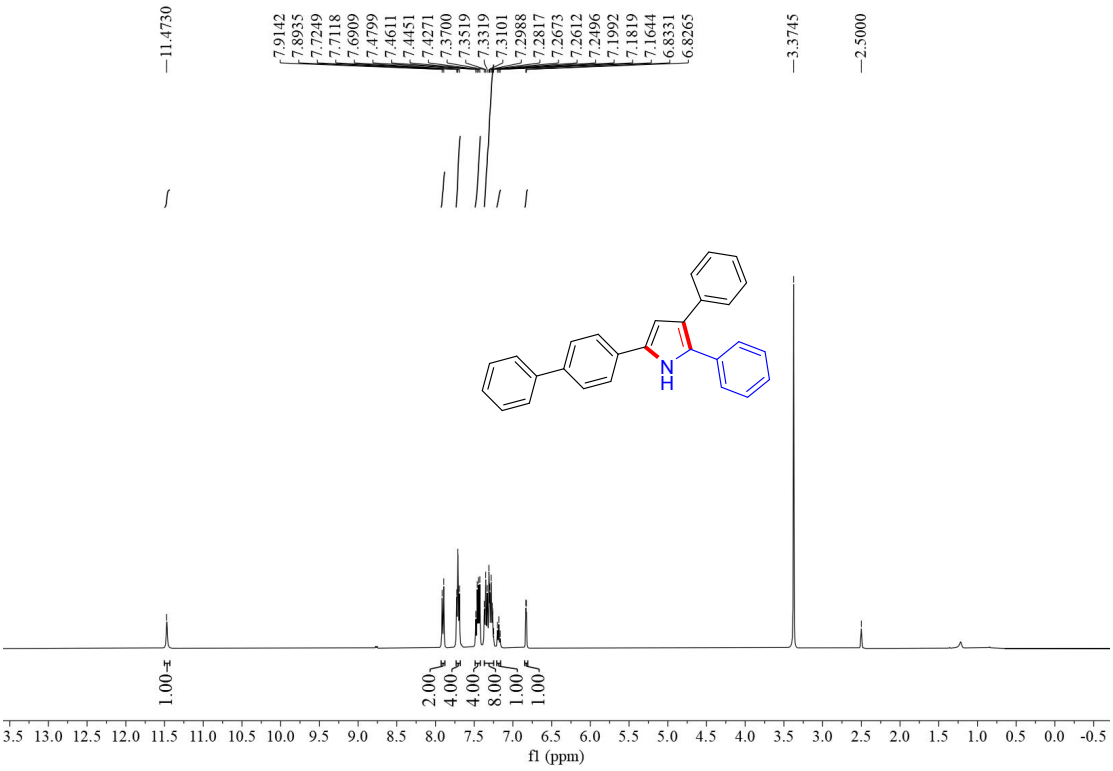
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3ea



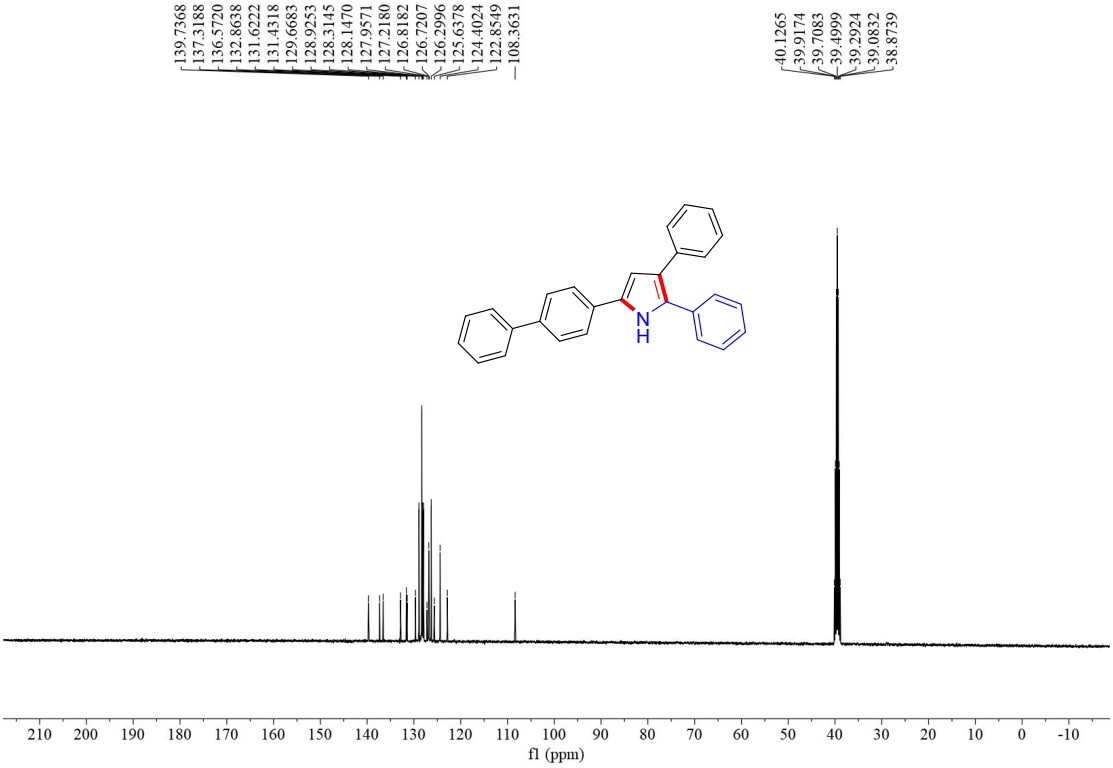
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3ea



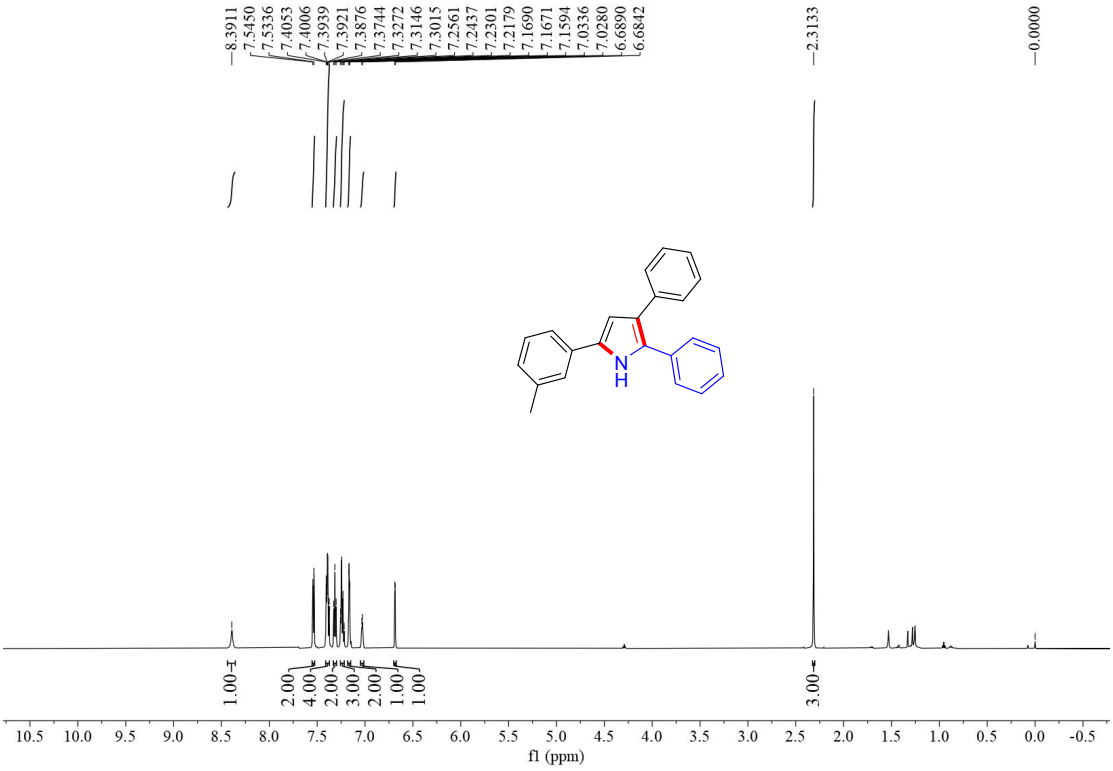
^{1}H NMR (400 MHz,DMSO-d_6) spectrum of compound 3ea'



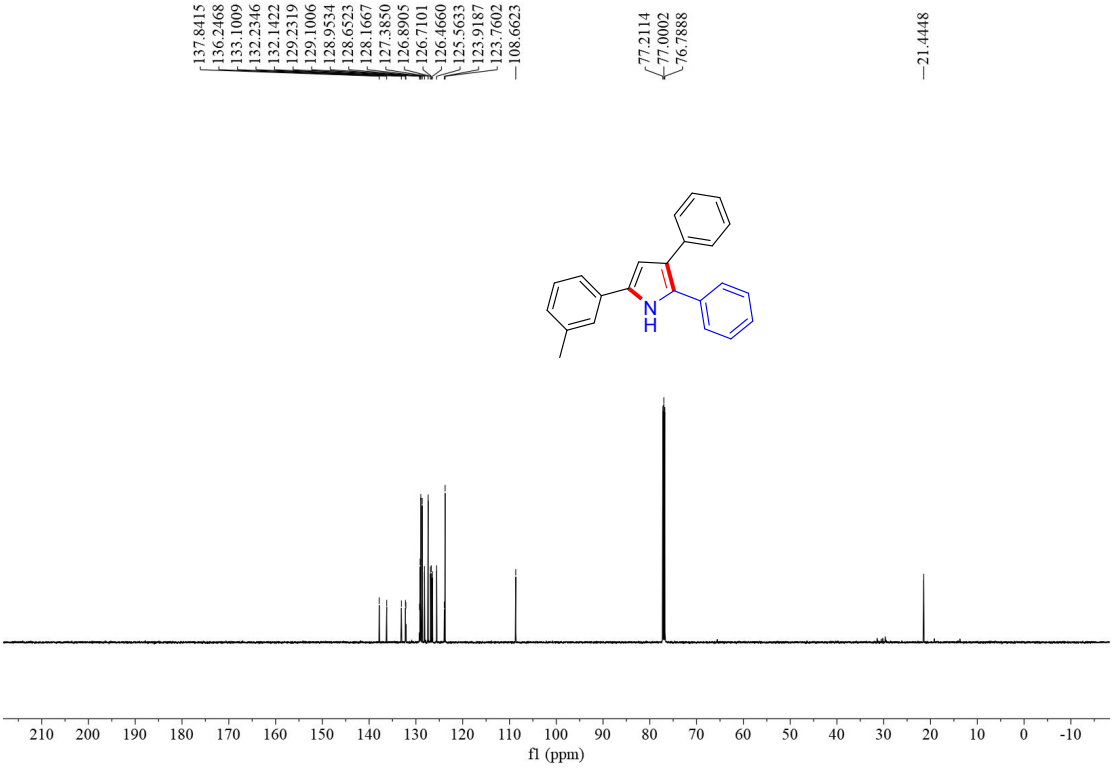
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound 3ea'



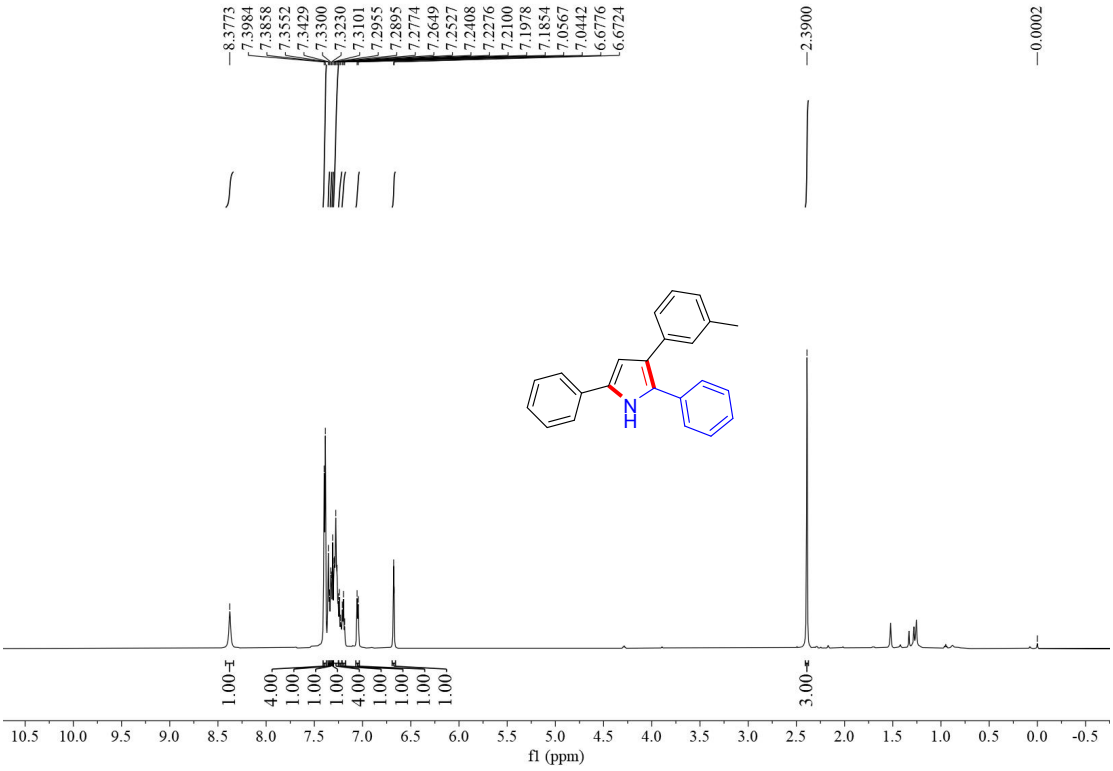
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3ab



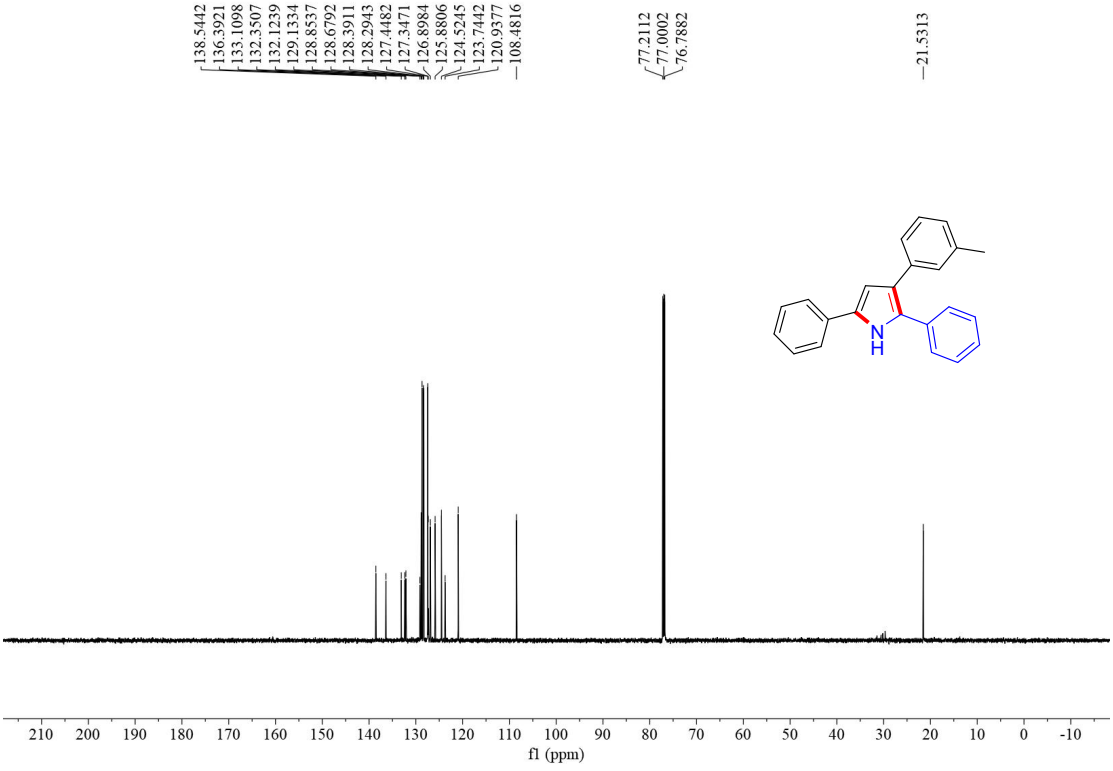
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3ab



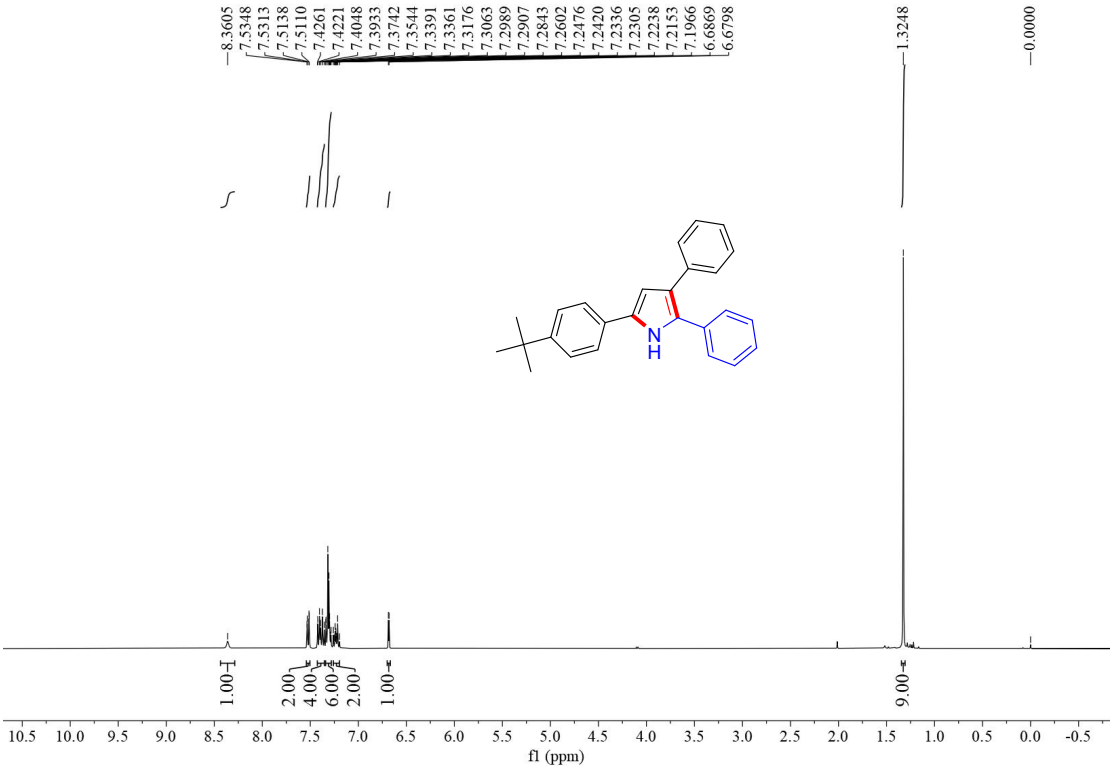
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3ab'



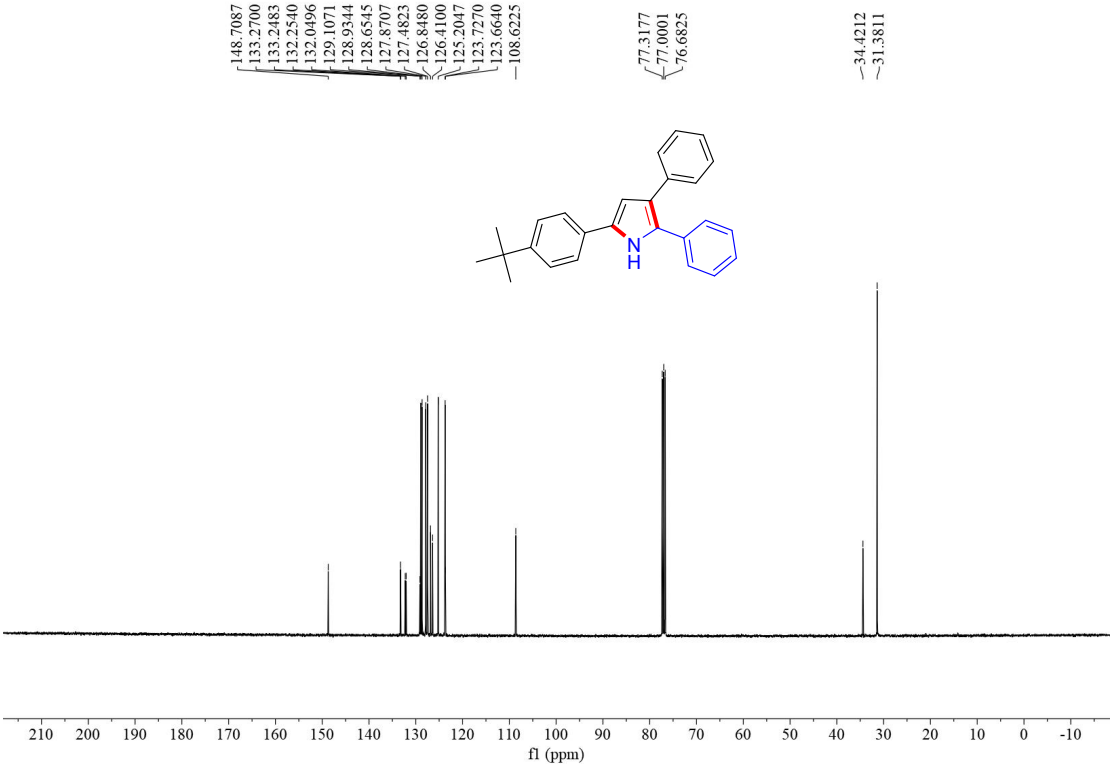
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3ab'



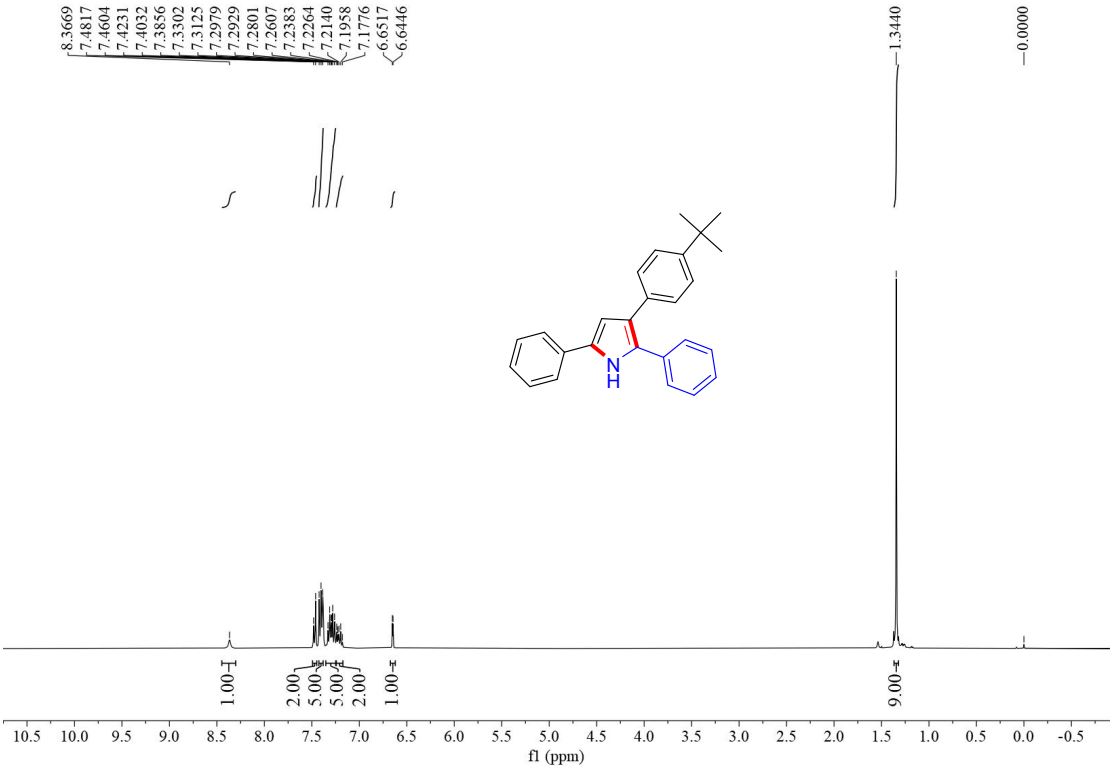
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3ac



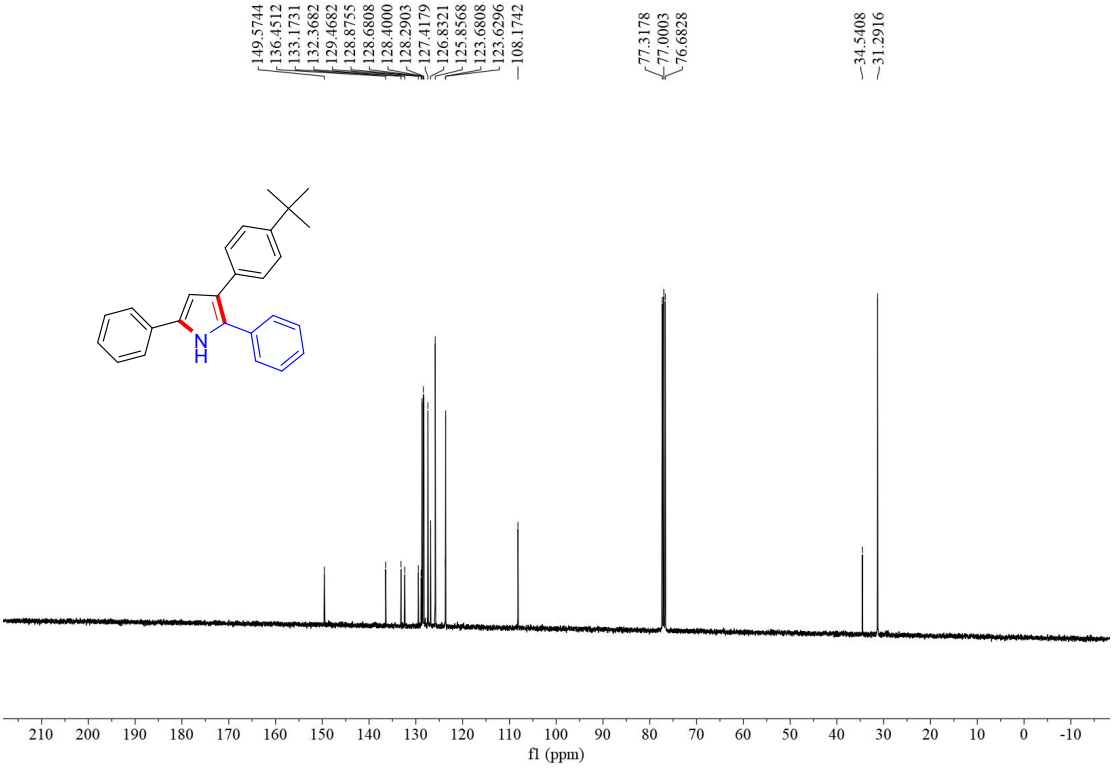
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3ac



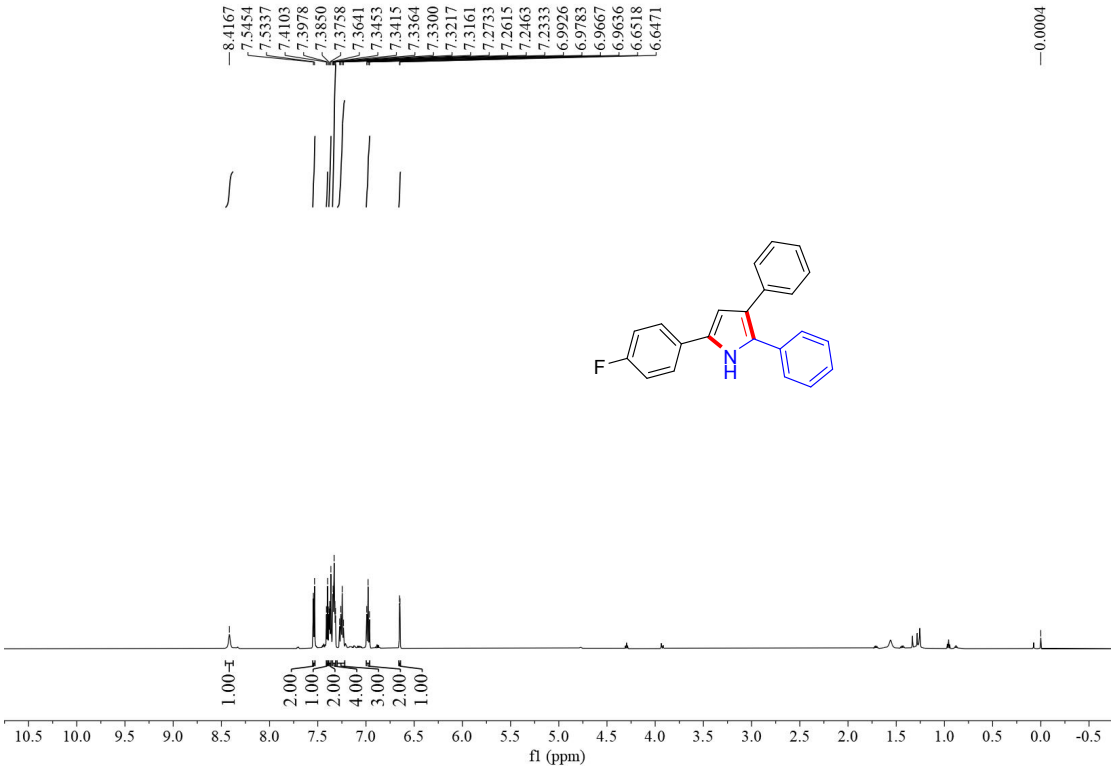
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3ac'



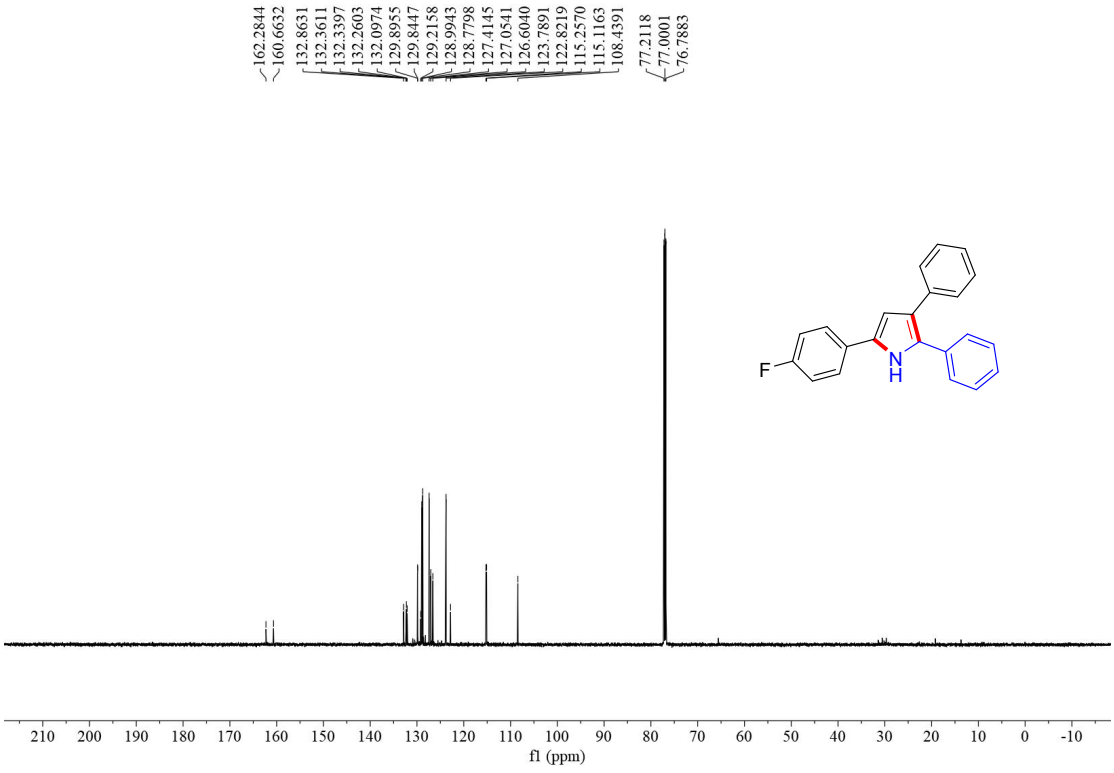
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3ac'



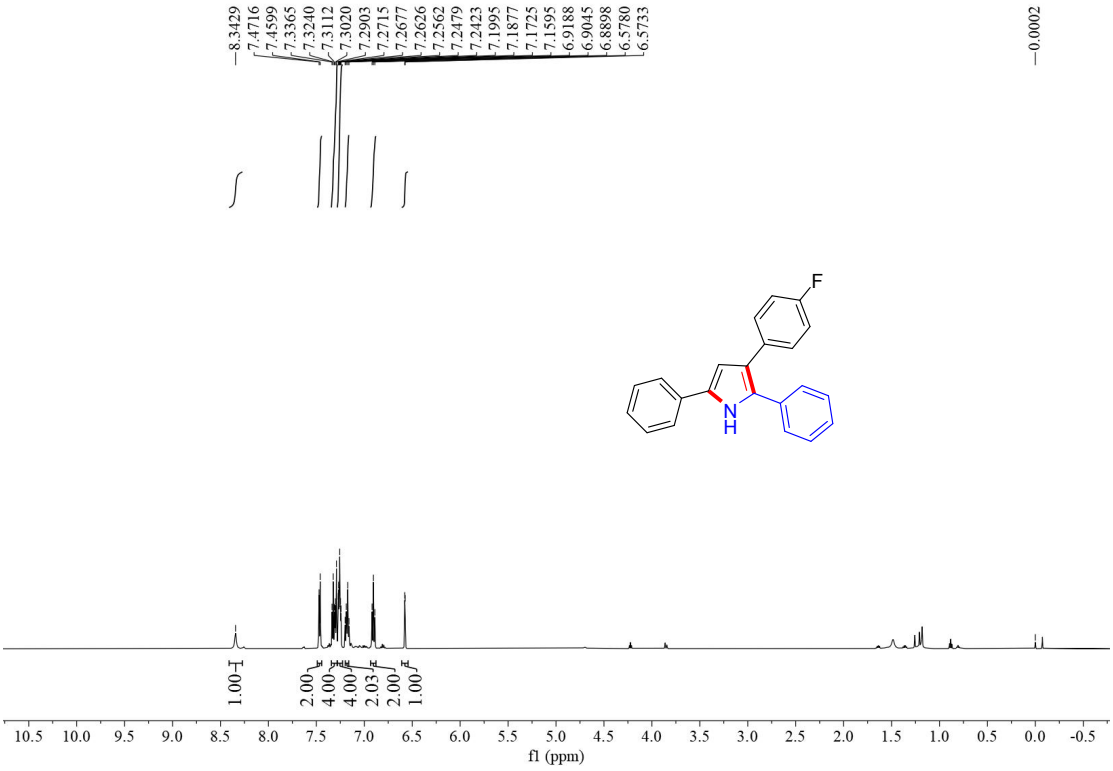
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3ad



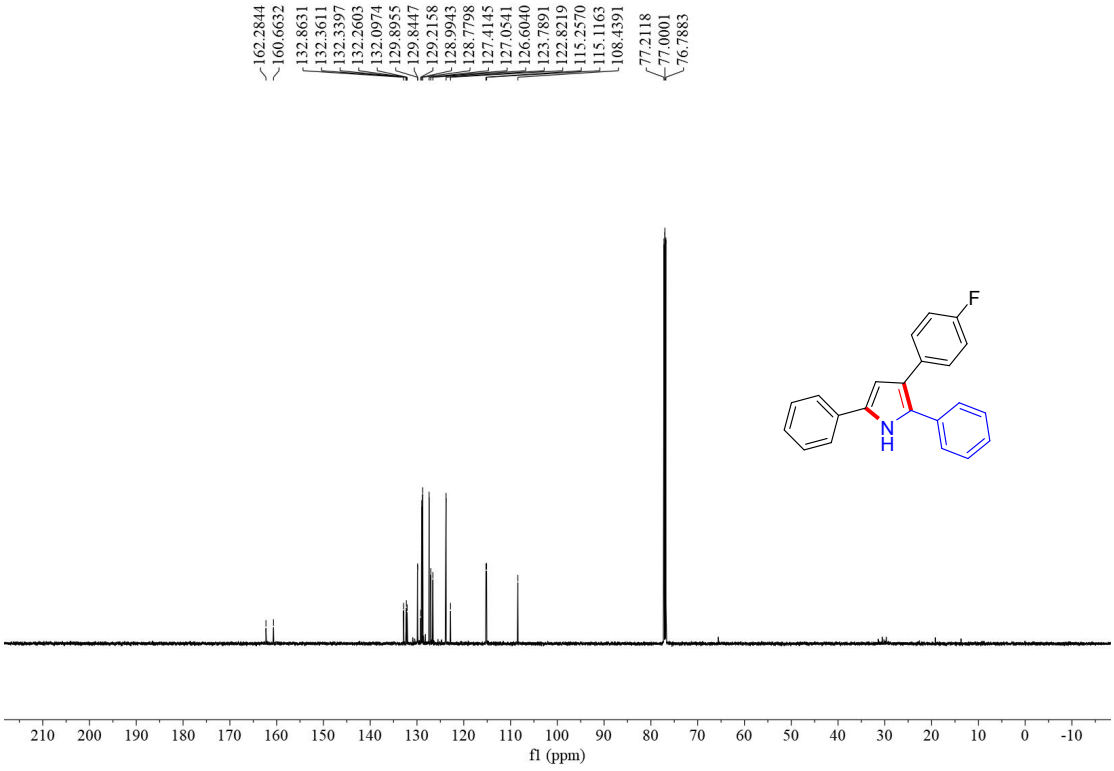
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3ad



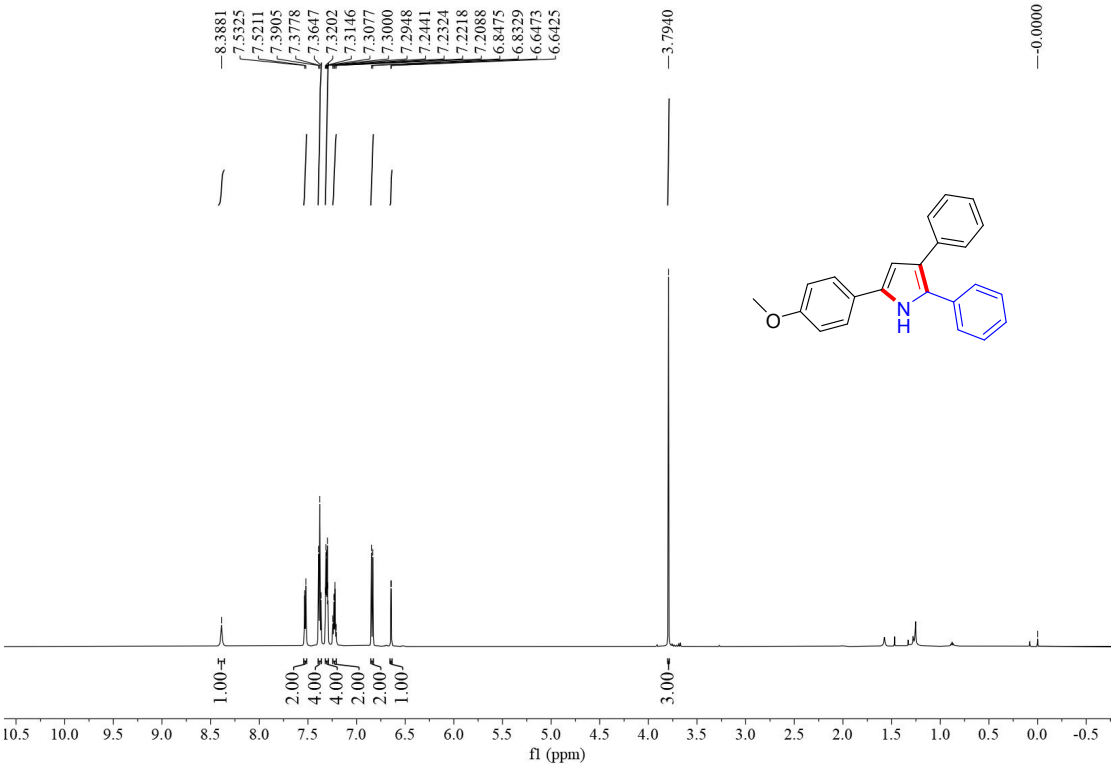
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3ad'



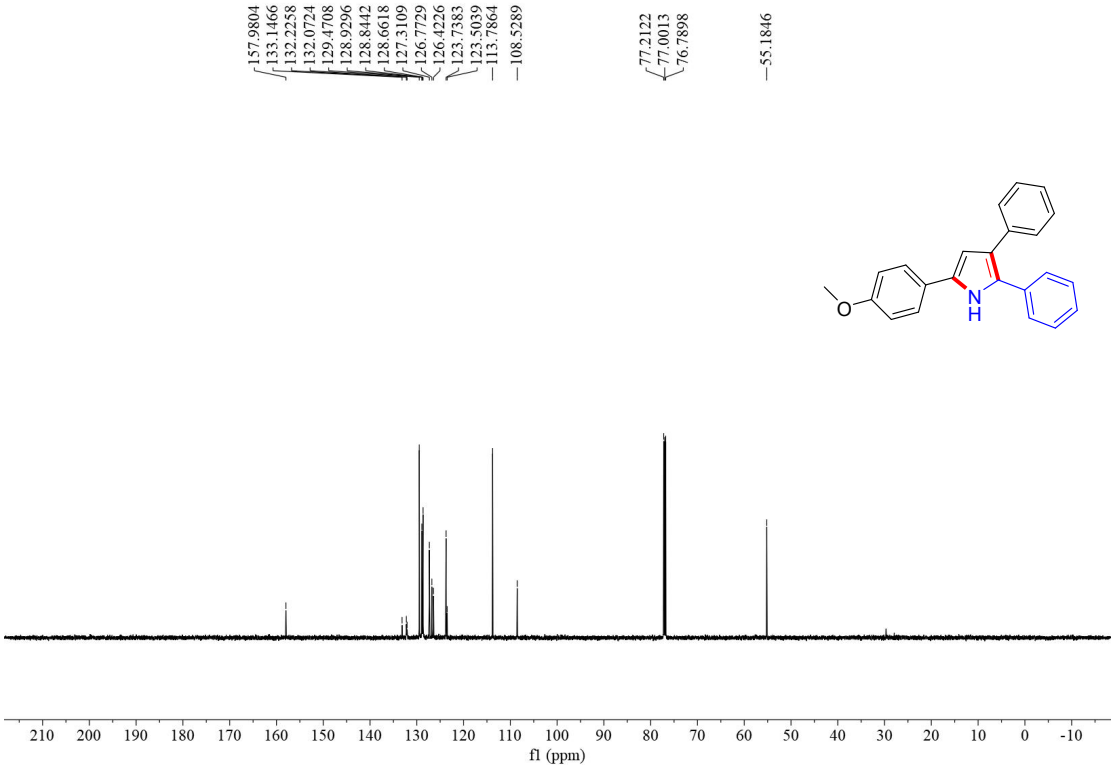
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3ad'



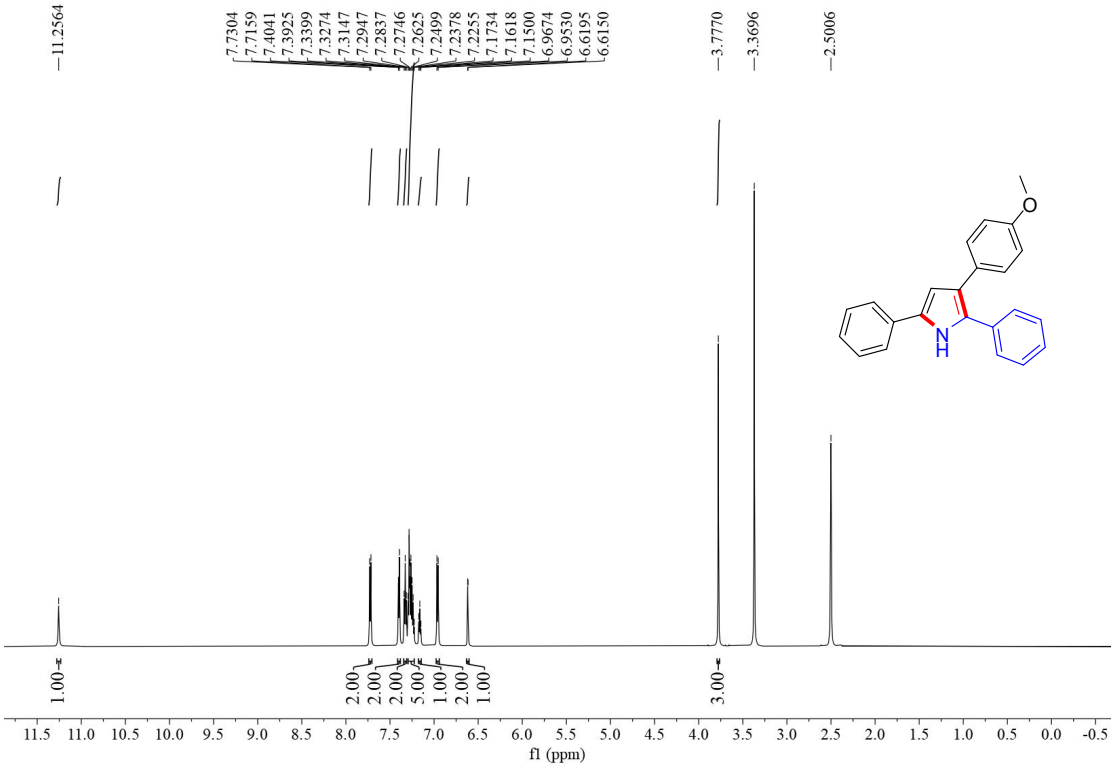
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound 3ae



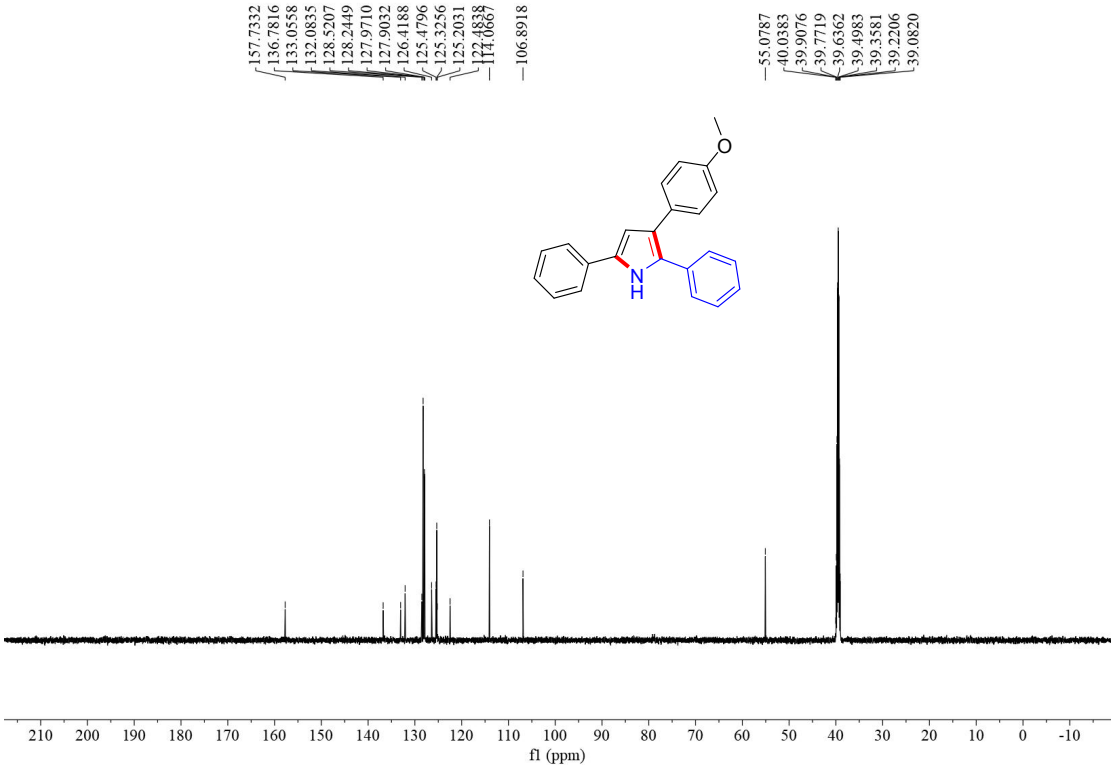
^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound 3ae



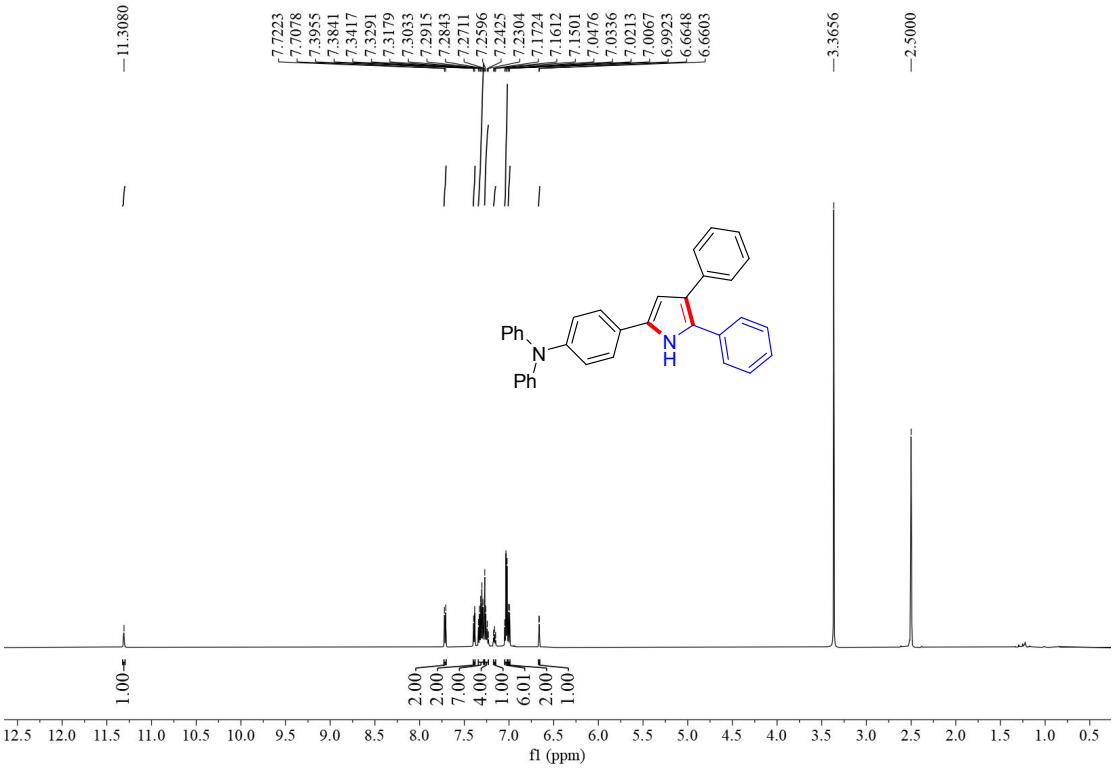
^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound 3ae'



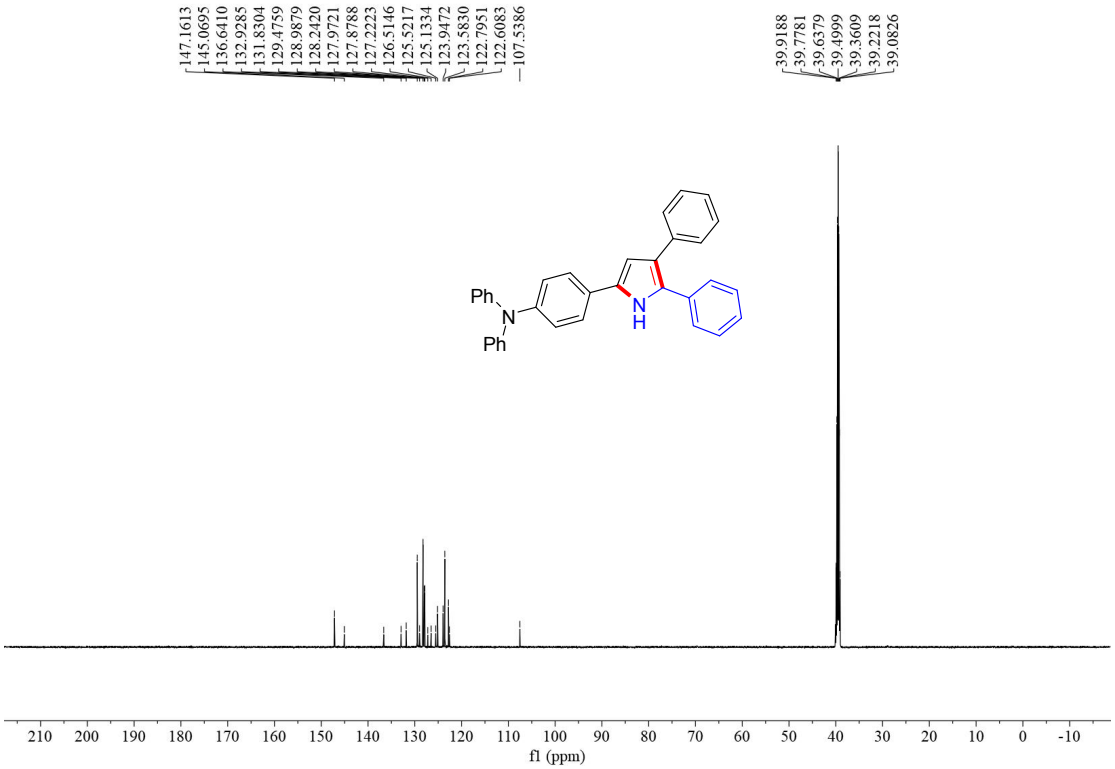
^{13}C NMR (150 MHz, DMSO-d*6*) spectrum of compound 3ae'



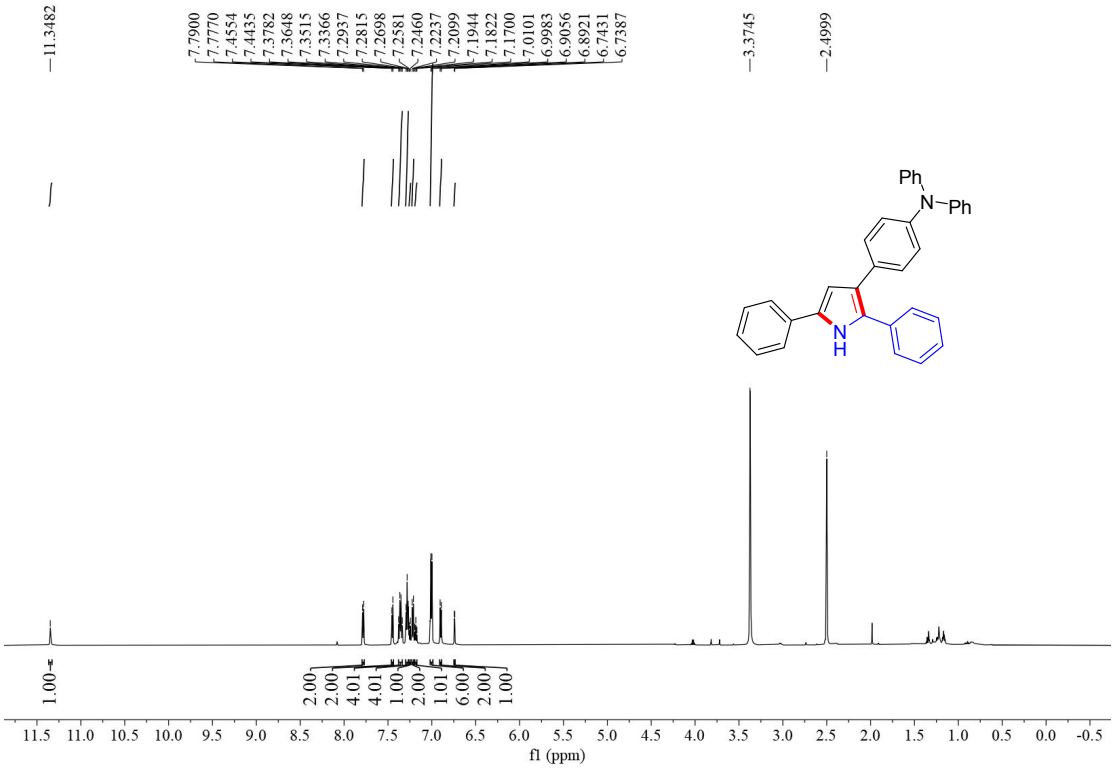
^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound 3af



^{13}C NMR (150 MHz, DMSO-d*6*) spectrum of compound 3af



^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound 3af'



^{13}C NMR (150 MHz, DMSO-d*6*) spectrum of compound 3af'