Supporting Information

Aromatization as the driving force for single electron transfer towards C–C cross-coupling reactions

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1. General Considerations:

All starting compounds employed in this study were procured from commercial suppliers and were used without further purification. All chemicals were purchased from Sigma Aldrich, Avra, TCI, Alfa Aeaser, GLR innovations. Glasswares were dried overnight at 160 °C. Benzene was dried by heating over sodium with benzophenone as indicator. Solvents such as ether, acetone were used as received from the commercial suppliers. For thin layer chromatography (TLC), silica-coated aluminium foils with fluorescent indicator 254 nm (from Merck) were used. Column chromatography was performed using SD Fine silica gel 60-120 mesh using a gradient of ethyl acetate and hexane as mobile phase. High-resolution mass spectra were recorded on a Waters QTOF mass spectrometer. ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz Bruker Biospin Advance III FT-NMR spectrometer. Fluorescence quenching experiments were carried out in a Cary Eclipse Fluorescence Spectrofluorometer. UV-Vis was recorded using Varian Cary 60 (Agilent technologies) spectrophotometer. NMR shifts are reported as delta (δ) units in parts per million (ppm) and coupling constants (J) are reported in Hertz (Hz). The following abbreviations are utilized to describe peak patterns when appropriate: s = singlet, d = doublet, t = triplet, q = quartet and m = multiplet. Chemical shifts (δ) are quoted to the nearest 0.01 ppm relative to tetramethylsilane (δ 0.00 ppm) in $CDCl_3$(δ 7.26 ppm) or $(CD_3)_2SO$ (δ 2.50 ppm). Carbon chemical shifts are internally referenced to the deuterated solvent signals in $CDCl_3$ (δ 77.1 ppm) or $(CD_3)_2SO$ (δ 39.5 ppm). Theoretical calculations were performed using gaussian09.[1]

2. General procedure for synthesis of aryldiazonium tetrafluoroborate.

Substituted diazonium salts were prepared following the reported literature.[2] Substituted aniline (10 mmol) was dissolved in 5 mL distilled water at room temperature. Then 5 mL of 46% hydrofluoroboric acid was added to the mixture at 0-5 ^{o}C. Sodium nitrite (0.7 g) was dissolved in 2 mL of water and cooled down to 0-5 ^{o}C separately. Now this cooled sodium nitrite solution was added dropwise over the course of 10 minutes to the main reaction mixture and the resulting mixture was stirred for 30 min, maintaining the temperature at 0-5 ^{o}C. After that the precipitate was collected by filtration and the residue was washed with ice-cooled distilled water. The precipitate was dissolved in minimum amount of acetone and then diethyl ether was added. The crystals of the respective

diazonium salts were collected from the solution, washed with diethyl ether and dried under vacuum.

3. Reaction procedure for C–H arylation of benzene and mesitylene.

In a Schlenk flask aryldiazonium salt (0.5 mmol), KO^{t}Bu (0.6 mmol) and the initiator molecule (**L1**) (10 mol%) were dried for 30 mins in a Schlenk line. After that DMSO (1 mL) and arene (10 mmol) was added to the reaction mixture under argon atmosphere. The reaction mixture was stirred under visible light irradiation for 10 h in an argon atmosphere at room temperature. After the completion of the reaction, dichloromethane was added to the mixture and extracted. Then the resulting solution was dried over Na_2SO_4, filtered and concentrated under the reduced pressure. Purification by column chromatography with EtOAc/hexane afforded the corresponding product. The biaryl products were fully characterized by ^{1}H and ^{13}C NMR spectroscopies.

4. Reaction procedure for C–H arylation of thiophene and furan.

In a Schlenk flask aryl diazonium salt (0.5 mmol), KO^{t}Bu (0.6 mmol) and the additive ligand (**L1**) (10 mol%) were dried for 30 mins in a Schlenk line. After that DMSO (1 mL) and heteroarene (10 mmol) was added to the reaction mixture under argon atmosphere. The reaction mixture was stirred under visible light irradiation for 10 h in an argon atmosphere at room temperature. After the completion of the reaction, dichloromethane was added to the mixture and extracted. Then the resulting solution was dried over Na_2SO_4, filtered and concentrated under the reduced pressure. Purification by column chromatography with EtOAc/hexane afforded the corresponding product. The biaryl products were fully characterized by ^{1}H and ^{13}C NMR spectroscopies.

5. Reaction procedure for C–H arylation of benzofuran.

In a Schlenk flask aryl diazonium salt (0.5 mmol), KO^{t}Bu (0.6 mmol) and the additive ligand (**L1**) (10 mol%) were dried for 30 mins in a well-equipped Schlenk line. After that DMSO (1 mL) and benzofuran (5 mmol) was added to the reaction mixture under argon atmosphere. The reaction mixture was stirred under visible light irradiation for 10 h in an argon atmosphere at room temperature. After the completion of the reaction, dichloro methane was added to the mixture and extracted. Then the resulting solution was dried over Na_2SO_4, filtered and concentrated under the reduced pressure. Purification by column

chromatography with EtOAc/hexane afforded the corresponding product. The biaryl products were fully characterized by ^{1}H and ^{13}C NMR spectroscopies.

6. Control experiments:

6.1. Radical quenching experiment:

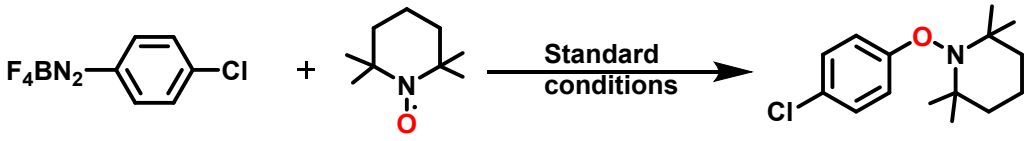
In a Schlenk flask aryl diazonium salt (0.5 mmol), KO^{t}Bu (0.6 mmol) and additive (10 mol%) were dried for 30 mins in a well-equipped Schlenk line. After that DMSO (1mL) and benzene (10 mmol) were added to the reaction mixture and different amount of TEMPO was added in the reaction mixture at argon atmosphere. The reaction mixture was stirred under visible light irradiation for 10 h under an argon atmosphere at room temperature.

Table S1: Yield of the product with different loading of TEMPO:

S.No	TEMPO equivalence	Yield (%)
1.	0.6 equiv	15
2.	1 equiv	trace

6.2. Trapping of intermediate:

In a Schlenk flask aryl diazonium salt (0.5 mmol), KO^{t}Bu (0.6 mmol) and additive (10 mol%) were dried for 30 mins in a well-equipped Schlenk line. After that DMSO (1 mL) was added dropwise to the reaction mixture and TEMPO (0.6 mmol) was added in the reaction mixture under argon atmosphere. The reaction mixture was stirred for 10 h under visible light irradiation at room temperature. The desired intermediate was characterised by ESI-MS. (M+H = 268.1453).



(M+H = 268.1453)

6.3. ICP-MS Analysis of KO^{t}Bu:

This analysis was conducted on Agilent's 7700X instrument, following a method AOAC 999.10. The contents of transition metal elements (Cu, Pd, Ni, Co and Fe) were found to be less than detection limit (0.1 ppm).

Table S2: ICP-MS analysis on the contents (in ppm) of transition metals in KO^{t}Bu

Entry	Parameter	Results	
		Result-1	**Result-2**
1.	Copper	BDL (MDL: 0.1 mg/kg)	BDL (MDL: 0.1 mg/kg)
2.	Palladium	BDL (MDL: 0.1 mg/kg)	BDL (MDL: 0.1 mg/kg)
3.	Iron	2.26 mg/kg	2.26 mg/kg
4.	Nickel	BDL (MDL: 0.1 mg/kg)	BDL (MDL: 0.1 mg/kg)
5.	Cobalt	BDL (MDL: 0.1 mg/kg)	BDL (MDL: 0.1 mg/kg)

BDL: Below Detection Limit, MDL: Method Detection Limit

7. The UV-visible absorption experiment:

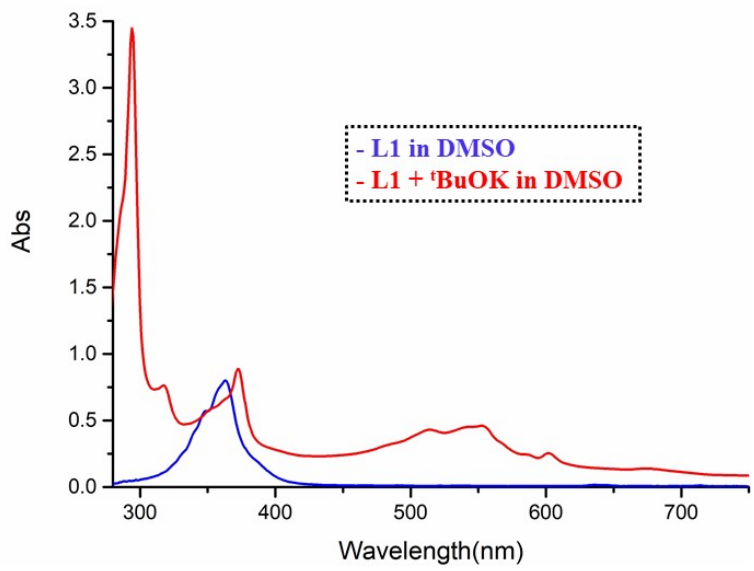


Figure S1. UV-visible spectra of **L1** (blue) and **L1**+ KO^{t}Bu (red) mixture in DMSO.

8. Fluorescence quenching experiment and Stern-Volmer plot:

Fluorescence quenching experiments were performed using a PerkinElmer LS 55 Fluorescence Spectrometer. In each experiment, measurement was carried out mixing 10^{-6} M solution of **L1** and KO^{t}Bu in DMSO with appropriate amount of quencher in a screw-capped air-tight quartz cuvette. The sample solutions were previously degassed with argon. The solution was irradiated at 470 nm, and the emission intensity was traced at 579 nm. Plots

were derived according to the Stern-Volmer equation and K_{sv} was calculated. Stern-Volmer equation is the following

$$I_0/I = 1 + K_{sv}[Q]$$

Where I_0 is the fluorescence intensity without the quencher, I is the intensity with the quencher, [Q] is the concentration of added quencher and K_{sv} is the Stern-Volmer quenching constant.

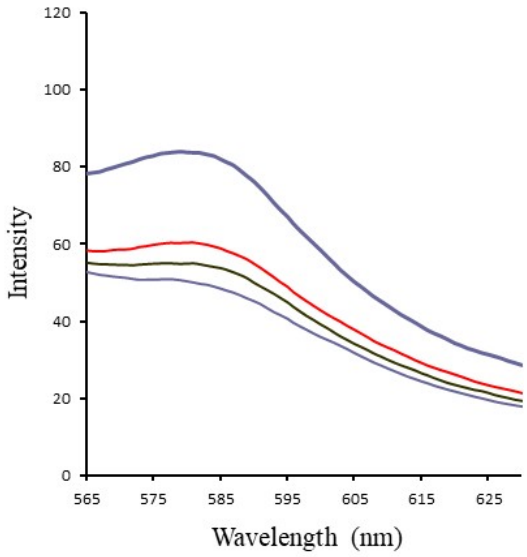
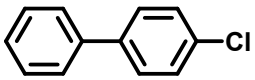


Figure S2. Emission spectra of **L1** and KO^{t}Bu mixture in DMSO with different amount of 4-chlorobenzene diazonium tetrafluoroborate.

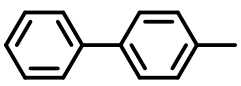
9. Analytical data:

4-chlorophenylbenzene (2a) :[2]



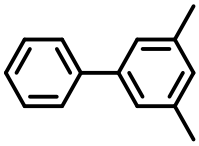
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (m, 4H), 7.42 (m, 5H).^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 139.8, 133.5, 129.0, 129.0, 128.5, 127.7, 127.1.

4-methylphenylbenzene (2b):[3]



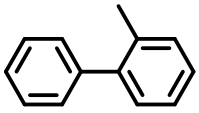
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 7.8 Hz, 2H), 7.63 (d, J = 7.8 Hz, 2H), 7.55 (t, J = 7.7 Hz, 2H), 7.48 – 7.42 (m, 1H), 7.38 (d, J = 7.8 Hz, 2H), 2.52 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 141.3, 138.4, 137.3, 137.1, 131.3, 129.6, 128.8, 127.1, 127.1, 21.2.

3,5-dimethylphenylbenzene (2c):[4]



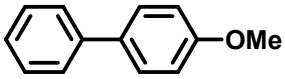
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (t, *J* = 5.6 Hz, 2H), 7.51 (q, *J* = 5.9 Hz, 2H), 7.46 – 7.38 (m, 1H), 7.32 (d, *J* = 6.4 Hz, 2H), 7.10 (s, 1H), 2.49 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.6, 141.4, 138.4, 129.0, 128.8, 127.3, 127.2, 125.2, 21.5.

2-methylphenylbenzene (2d):[16]



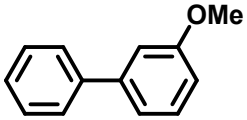
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.44 (m, 2H), 7.39 (m, 3H), 7.33 – 7.28 (m, 4H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 135.5, 130.4, 129.9, 129.3, 128.2, 127.4, 126.9, 125.9, 76.8, 20.6.

4-methoxyphenylbenzene (2e):[2]



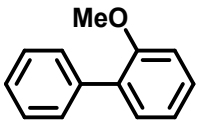
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.8 Hz, 4H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.35 – 7.28 (m, 1H), 6.99 (d, *J* = 8.7 Hz, 2H), 3.86 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 140.9, 133.9, 128.8, 128.2, 126.8, 126.7, 114.3, 55.4.

3-methoxyphenylbenzene (2f): [16]



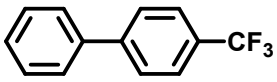
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 7.2, 1.3 Hz, 2H), 7.50 – 7.42 (m, 2H), 7.37 (td, *J* = 7.5, 7.1, 3.7 Hz, 2H), 7.21 (dt, *J* = 7.7, 1.3 Hz, 1H), 7.18 – 7.13 (m, 1H), 6.92 (ddd, *J* = 8.2, 2.6, 1.0 Hz, 1H), 3.88 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 142.9, 141.2, 129.9, 128.9, 127.6, 127.3, 119.8, 113.0, 112.8, 55.4.

2-methoxyphenylbenzene (2g): [4]



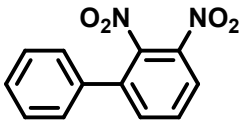
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.4 Hz, 2H), 7.48 (t, *J* = 8.0 Hz, 2H), 7.39 (t, *J* = 7.1 Hz, 3H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.05 (d, *J* = 8.7 Hz, 1H), 3.86 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 156.5, 138.6, 131.0, 130.8, 129.7, 128.7, 128.1, 127.0, 120.9, 111.3, 55.6.

4-trifluoromethylphenylbenzene (2h):[5]



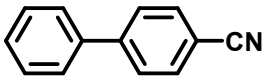
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (s, 4H), 7.61 (d, *J* = 7.1 Hz, 2H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 139.9, 129.1, 128.3, 127.6, 127.4, 125.8 (q, *J*=3.7 Hz), 123.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.4.

2,4-dinitrophenylbenzene (2i): [19]



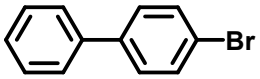
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 2.3 Hz, 1H), 8.47 (dd, *J* = 8.6, 2.3 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.49 (d, *J* = 6.7 Hz, 3H), 7.37 – 7.32 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 147.0, 142.4, 135.3, 133.4, 129.7, 129.2, 127.8, 126.6, 119.8.

4-cyanophenylbenzene (2j):[6]



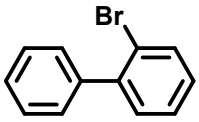
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (q, *J* = 8.0 Hz, 4H), 7.59 (d, *J* = 7.6 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.43 (t, *J* = 7.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 139.3, 132.7, 129.2, 128.8, 127.9, 127.4, 119.1, 111.0.

4-bromophenylbenzene (2k):[5]



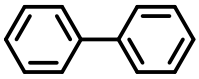
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.53 (m, 4H), 7.45 (td, *J* = 8.6, 2.2 Hz, 4H), 7.40 – 7.35 (m, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 140.1, 132.0, 129.0, 128.9, 127.8, 127.1, 121.7.

4-bromophenylbenzene (2l): [19]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.3 Hz, 1H), 7.50 – 7.43 (m, 5H), 7.39 (d, *J* = 6.8 Hz, 2H), 7.27 – 7.22 (m, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 141.2, 133.2, 131.4, 129.5, 128.8, 128.1, 127.7, 127.5, 122.7.

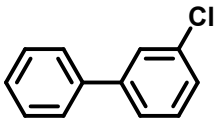
Biphenyl (2m): [2]



^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.62 (d, 2H, *J* = 8 Hz), 7.46 (t, 4H, *J* = 8Hz), 7.37 (t,

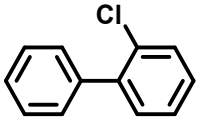
1H, *J*= 8 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 128.9, 127.4, 127.3.

3-chlorophenylbenzene (2n):[24]



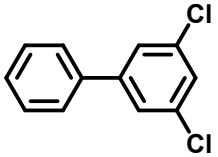
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.56 (m, 3H), 7.48 (t, *J* = 7.5 Hz, 3H), 7.43 – 7.33 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 139.9, 134.8, 130.1, 129.0, 128.0, 127.4, 127.4, 127.2, 125.4.

2-chlorophenylbenzene (2o):[17]



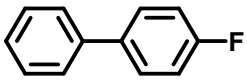
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.49 (m, 5H), 7.49 – 7.31 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 139.5, 132.6, 131.5, 130.0, 129.6, 128.6, 128.2, 127.7, 126.9.

3,5-dichloro-1,1'-biphenyl (2p):[20]



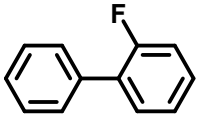
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.52 (m, 2H), 7.49 – 7.39 (m, 5H), 7.35 (t, *J* = 1.9 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 138.6, 135.4, 129.1, 128.6, 127.2, 127.16, 125.7.

4-fluorophenylbenzene (2q):[2]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dt, *J* = 9.2, 2.6 Hz, 4H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.37 (t, *J* = 7.3 Hz, 1H), 7.15 (t, *J* = 8.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6 (d, J=247.4 Hz), 140.37, 137.4 (d, J=3 Hz), 129.0, 128.8 (d, J=8 Hz), 127.4, 127.2, 115.7 (d, J=21.2 Hz).

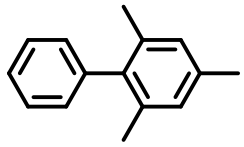
4-fluorophenylbenzene (2r):[24]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dt, *J* = 8.2, 1.5 Hz, 2H), 7.41 (m, 3H), 7.36 – 7.31 (m, 1H), 7.31 – 7.24 (m, 1H), 7.17 (td, *J* = 7.5, 1.3 Hz, 1H), 7.12 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9 (d, J=248.3 Hz), 136.0, 130.9 (d, J=5 Hz), 129.3, 129.2 (d, J=3 Hz), 129.1 (d,

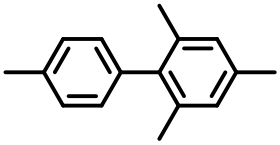
J=8.1 Hz), 128.6, 127.8, 124.4 (d, J=5 Hz), 116.2 (d, J=23.2 Hz).

2-Phenylmesitylene (3a):[2]



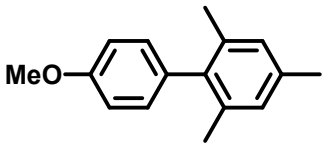
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (t, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.22 (d, *J* = 6.8 Hz, 2H), 7.03 (s, 2H), 2.42 (s, 3H), 2.09 (s, 6H).^{13}C NMR (100 MHz, $CDCl_3$) δ 141.2, 139.2, 136.7, 136.1, 129.4, 128.5, 128.2, 126.6, 21.2, 20.9.

1-Methyl-4-mesitylbenzene (3b):[7]



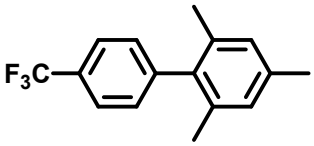
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 7.6 Hz, 2H), 7.03 (d, *J* = 7.8 Hz, 2H), 6.94 (s, 2H), 2.40 (s, 3H), 2.33 (s, 3H), 2.01 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 138.1, 136.6, 136.3, 136.1, 129.3, 129.2, 128.1, 21.4, 21.2, 20.9.

1-Methoxy-4-mesitylbenzene (3c):[2]



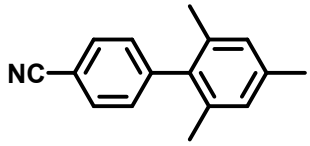
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 – 7.03 (m, 2H), 6.99 – 6.92 (m, 4H), 3.86 (s, 3H), 2.33 (s, 3H), 2.01 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 138.8, 136.6, 133.4, 130.4, 128.2, 113.9, 55.3, 21.2, 20.9.

1-Trifluoromethyl-4-mesitylbenzene (3d):[8]



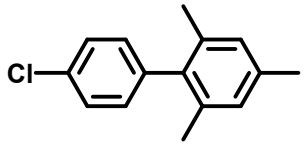
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 6.99 (s, 2H), 2.37 (s, 3H), 2.02 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.2, 137.8, 137.4, 135.8, 129.9, 129.2, 128.9, 128.4, 125.5 (q, *J*=3.7 Hz), 21.2, 20.8.

1-Cyano-4-mesitylbenzene (3e):[9]



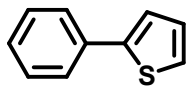
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 8.3 Hz, 2H), 6.98 (s, 2H), 2.36 (s, 3H), 1.99 (s, 6H).^{13}C NMR (100 MHz, $CDCl_3$) δ 146.5, 137.7, 137.2, 135.4, 132.4, 130.4, 128.4, 110.7, 21.2, 20.7.

1-Chloro-4-mesitylbenzene (3f):[2]



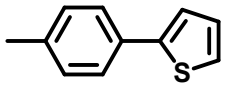
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.98 (s, 2H), 2.37 (s, 3H), 2.04 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.6, 137.9, 137.0, 136.0, 132.6, 130.9, 128.77, 128.3, 21.2, 20.8.

2-(phenyl) thiophene (4a):[10]



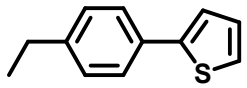
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.1 Hz, 2H), 7.35 – 7.25 (m, 3H), 7.09 (q, *J* = 3.1, 1.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 134.5, 129.0, 128.1, 127.6, 126.1, 124.9, 123.2.

2-(4-methylphenyl) thiophene (4b):[11]



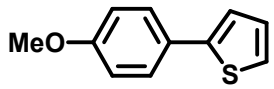
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.7 Hz, 2H), 7.28 (dd, *J* = 11.1, 4.2 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 2H), 7.09 (t, *J* = 4.4 Hz, 1H), 2.39 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 137.5, 131.8, 129.7, 128.1, 126.0, 124.4, 122.7, 21.3.

2-(4-ethylphenyl) thiophene (4c):[13]



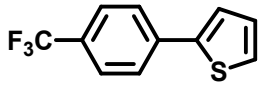
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.9 Hz, 2H), 7.29 (dt, *J* = 18.2, 6.4 Hz, 4H), 7.11 (d, *J* = 4.2 Hz, 1H), 2.71 (d, *J* = 7.8 Hz, 2H), 1.31 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 143.8, 132.0, 128.5, 128.4, 128.0, 126.5, 126.1, 124.4, 122.7, 28.7, 15.7.

2-(4-methoxyphenyl) thiophene (4d):[22]



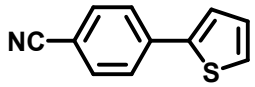
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.54 (m, 2H), 7.25 – 7.20 (m, 2H), 7.07 (dd, *J* = 5.1, 3.6 Hz, 1H), 6.96 – 6.90 (m, 2H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 144.4, 128.0, 127.4, 127.3, 124.0, 122.2, 114.4, 55.5.

2-(4-trifluoromethylphenyl) thiophene (4e):[22]



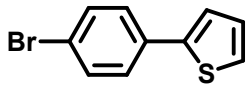
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.9 Hz, 2H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.40 (dd, *J* = 3.7, 1.2 Hz, 1H), 7.37 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.12 (dd, *J* = 5.1, 3.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 128.5, 126.7, 126.4, 126.0 (q, *J*=3,7 Hz), 124.6.

2-(4-cyanophenyl) thiophene (4f): [23]



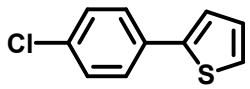
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.63 (m, 4H), 7.43 – 7.38 (m, 2H), 7.13 (dd, *J* = 5.1, 3.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.2, 138.7, 128.7, 127.2, 126.2, 125.2, 119.0, 110.6, 77.5, 76.8.

2-(4-bromophenyl) thiophene (4g):[7]



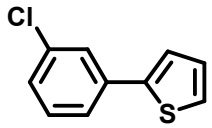
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 4H), 7.30 (dd, *J* = 4.5, 1.6 Hz, 2H), 7.09 (d, *J* = 4.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.1, 128.4, 127.6, 125.4, 123.6, 121.4.

2-(4-chlorophenyl)thiophene (4h):[7]



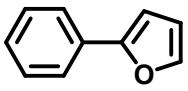
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.54 (m, 2H), 7.41 – 7.36 (m, 2H), 7.35 – 7.31 (m, 2H), 7.12 (dd, *J* = 5.1, 3.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.1, 133.2, 132.9, 129.0, 128.2, 127.6, 127.1, 125.2, 123.5.

2-(3-chlorophenyl)thiophene (4i):[24]



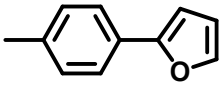
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.26 – 7.23 (m, 2H), 7.23 – 7.15 (m, 2H), 7.05 – 7.01 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 136.2, 134.9, 128.2, 127.5, 126.0, 125.7, 124.2, 124.0.

2-phenyl furan (5a): [10]



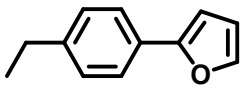
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.6 Hz, 2H), 7.53 (s, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.32 (t, *J* = 6.9 Hz, 1H), 6.72 (d, *J* = 3.4 Hz, 1H), 6.53 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 142.1, 131.0, 128.8, 127.4, 123.9, 111.7, 105.1.

2-(4-methylphenyl) furan (5b): [12]



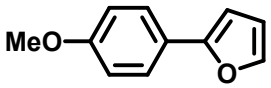
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.1 Hz, 2H), 7.45 (d, *J* = 1.8 Hz, 1H), 7.19 (d, *J* = 7.9 Hz, 2H), 6.59 (d, *J* = 3.3 Hz, 1H), 6.46 (m, 1H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.3, 141.8, 137.3, 129.5, 128.4, 123.9, 111.7, 104.3, 21.4.

2-(4-ethylphenyl) thiophene (5c): [13]



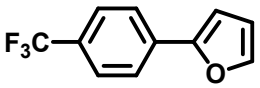
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.58 (m, 2H), 7.45 (d, *J* = 1.0 Hz, 1H), 7.22 (d, *J* = 8.6 Hz, 2H), 6.60 (d, *J* = 4.2 Hz, 1H), 6.46 (m, 1H), 2.67 (m, 2H), 1.26 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.3, 143.7, 141.8, 128.6, 128.3, 124.0, 111.7, 104.4, 28.8, 15.7.

2-(4-methoxyphenyl) furan (5d): [10]



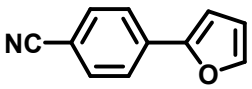
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.62 (m, 2H), 7.46 (dd, *J* = 1.8, 0.8 Hz, 1H), 6.95 (d, *J* = 8.9 Hz, 2H), 6.54 (dd, *J* = 3.3, 0.8 Hz, 1H), 6.47 (dd, *J* = 3.3, 1.8 Hz, 1H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 154.1, 141.5, 125.3, 124.1, 114.2, 111.6, 103.5, 55.4.

2-(4-trifluoromethylphenyl) furan (5e):[12]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.1 Hz, 2H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 1.8 Hz, 1H), 6.77 (d, *J* = 3.4 Hz, 1H), 6.52 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.6, 143.2, 134.1, 129.2, 128.9, 125.8(q, *J*=3.7 Hz), 125.7, 123.9, 112.1, 107.1.

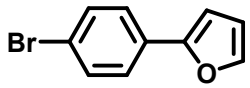
2-(4-cyanophenyl) furan (5f):[12]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.3 Hz, 2H), 7.65 (d, *J* = 8.6 Hz, 2H), 7.54 (s, 1H), 6.81 (d, *J* = 3.5 Hz, 1H), 6.53 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 143.8, 134.8,

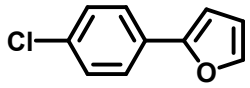
132.7, 124.1, 112.4, 110.4, 108.3.

2-(4-bromophenyl) furan (5g):[7]



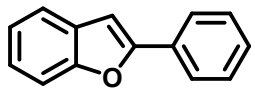
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (m, 4H), 7.50 (d, *J* = 1.8 Hz, 1H), 6.66 (m, 1H), 6.50 (dd, *J* = 3.4, 1.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 142.4, 131.8, 129.8, 125.3, 121.1, 111.9, 105.6.

2-(4-chlorophenyl) furan (5h):[12]



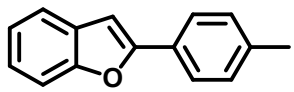
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.58 (m, 2H), 7.47 (s, 1H), 7.37 – 7.33 (m, 2H), 6.64 (t, *J* = 2.5 Hz, 1H), 6.48 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 142.4, 133.1, 129.5, 129.0, 125.1, 111.9, 105.6.

2-phenyl benzofuran (6a):[15]



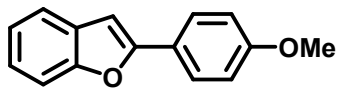
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.1 Hz, 2H), 7.60 (d, *J* = 6.8 Hz, 1H), 7.54 (d, *J* = 8.8 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.39 – 7.34 (m, 1H), 7.30 (td, *J* = 8.1, 7.6, 1.5 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.04 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.3, 154.9, 138.7, 129.6, 129.5, 127.9, 125.0, 124.1, 123.0, 120.9, 111.2, 100.7, 21.6.

2-(4-methylphenyl)benzofuran (6b):[15]



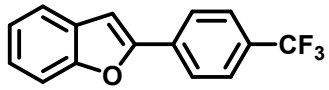
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.60 – 7.56 (m, 1H), 7.53 (d, *J* = 8.7 Hz, 1H), 7.31 – 7.21 (m, 4H), 6.98 (s, 1H), 2.41 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 156.3, 154.9, 138.7, 129.6, 129.5, 127.9, 125.0, 124.1, 123.0, 120.9, 111.2, 100.7, 21.6.

2-(4-methoxyphenyl)benzofuran (6c):[15]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.77 (m, 2H), 7.58 – 7.54 (m, 1H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.28 – 7.20 (m, 2H), 7.02 – 6.96 (m, 2H), 6.90 (s, 1H), 3.87 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 156.2, 154.8, 129.6, 126.6, 123.9, 123.5, 123.0, 120.7, 114.4, 111.1, 99.8, 55.5.

2-(4-trifluoromethylphenyl)benzofuran (6d):[14]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.9 Hz, 2H), 7.70 (d, *J* = 8.1 Hz, 2H), 7.62 (d, *J* = 6.5 Hz, 1H), 7.55 (d, *J* = 9.0 Hz, 1H), 7.36 – 7.31 (m, 1H), 7.29 – 7.24 (m, 1H), 7.14 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 154.3, 133.8, 130.1, 129.0, 125.9 (q, J=3.7 Hz), 125.2, 125.1, 123.4, 121.4, 111.5, 103.4.

10. ^{1}H and ^{13}C Spectra of synthesized molecules:

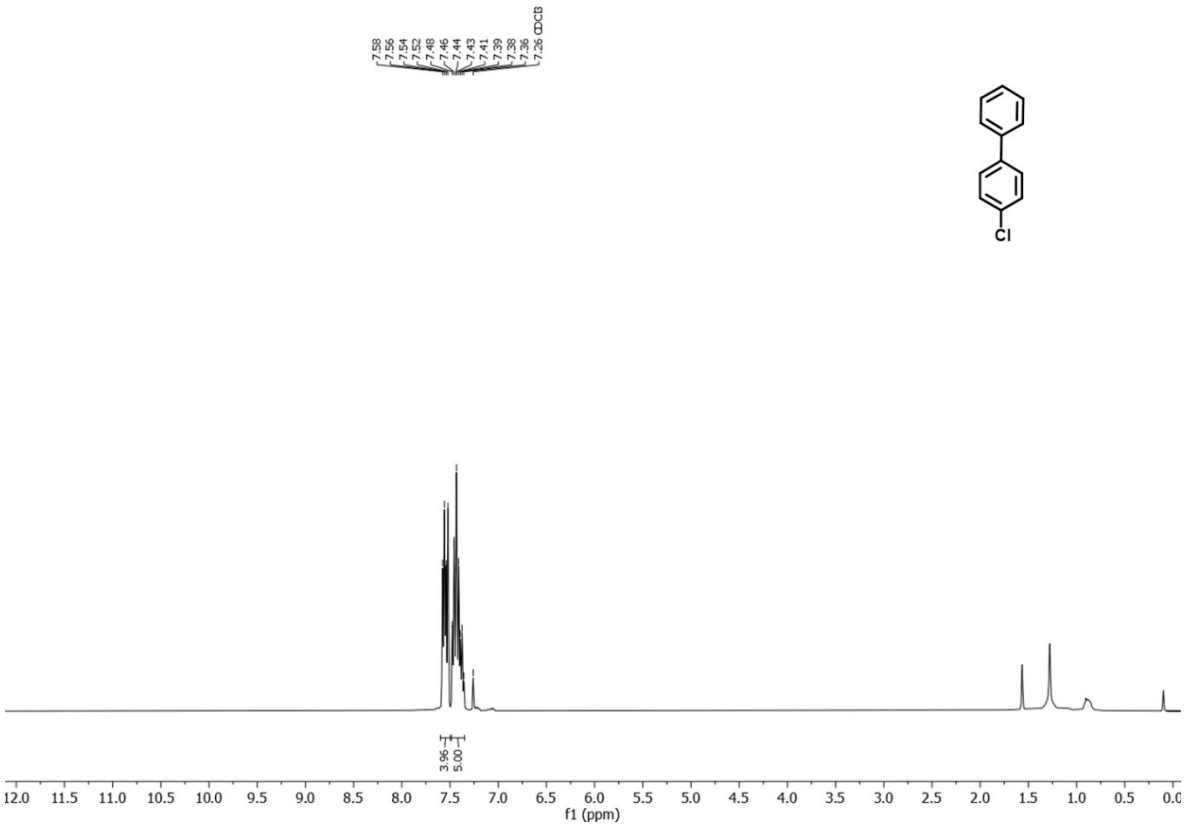


Figure S3. ^{1}H NMR spectrum (400 MHz) of **2a** in $CDCl_3$.

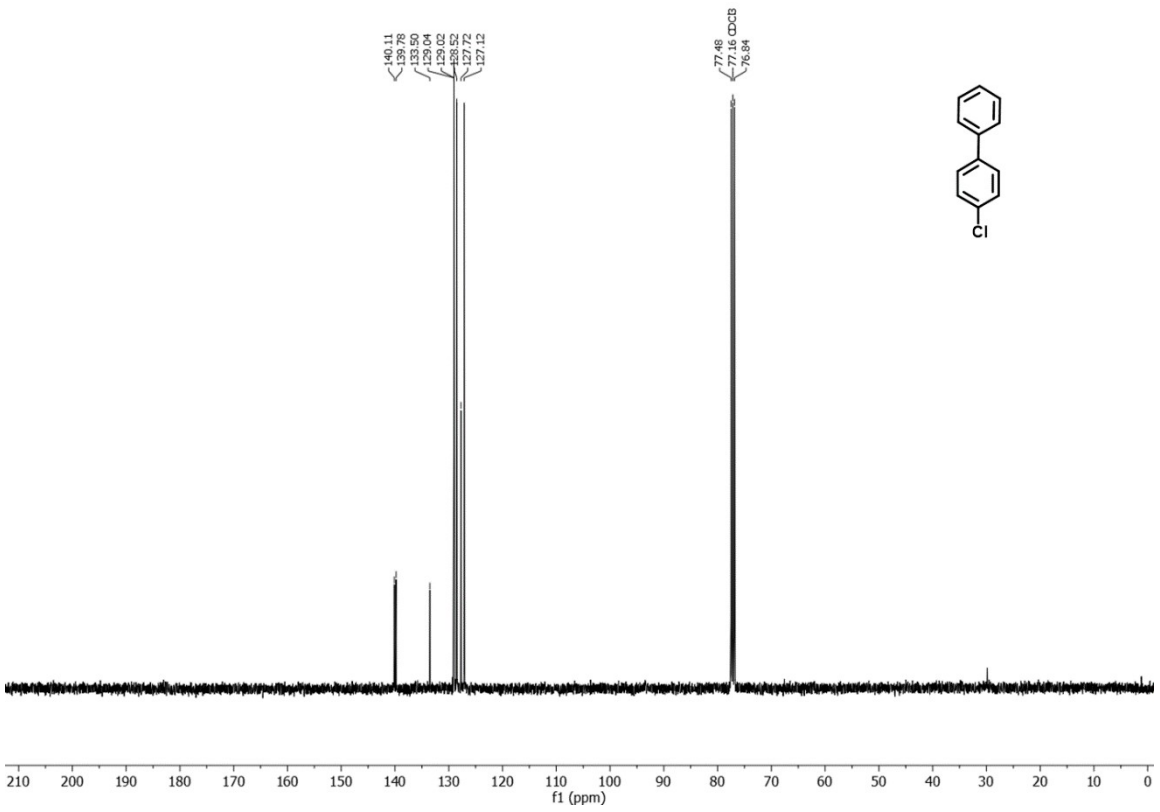


Figure S4. ^{13}C NMR spectrum (100 MHz) of **2a** in $CDCl_3$.

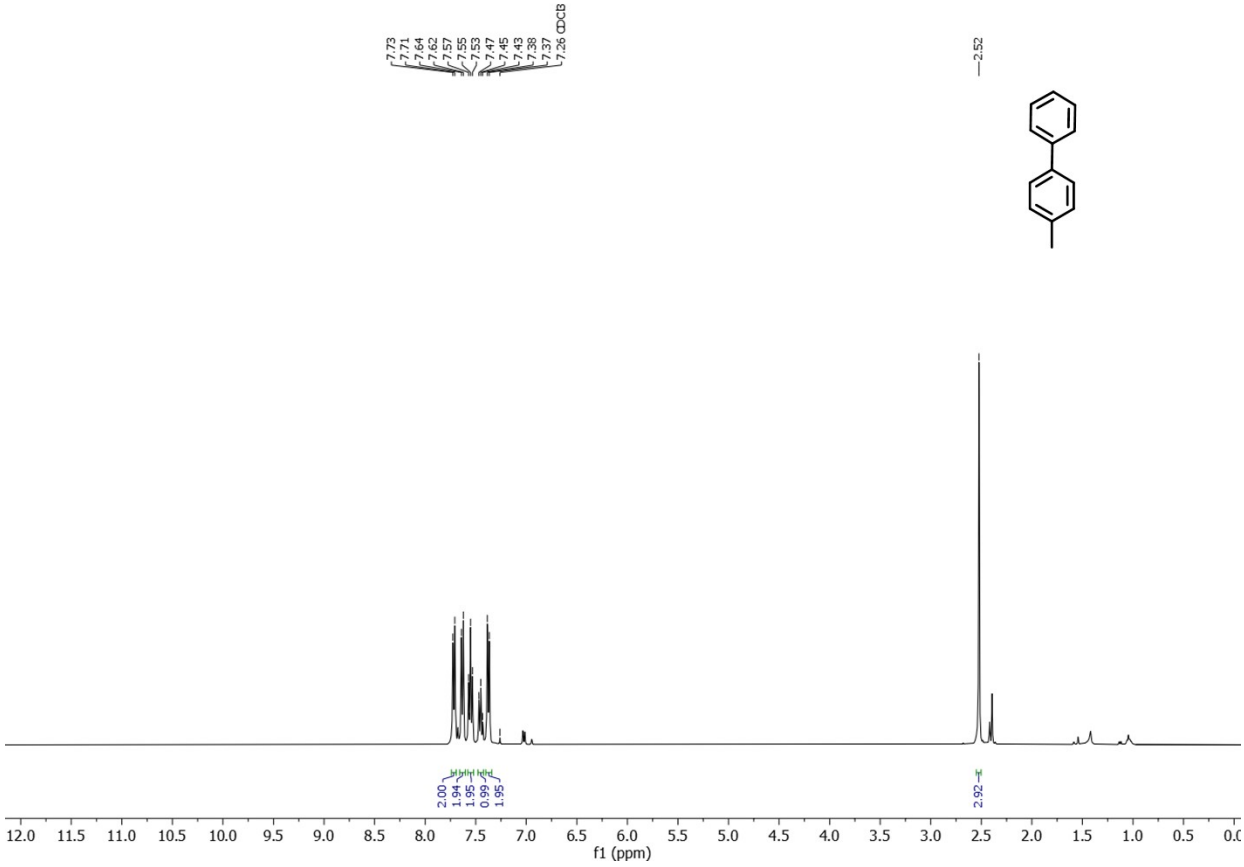


Figure S5. ^{1}H NMR spectrum (400 MHz) of **2b** in $CDCl_3$.

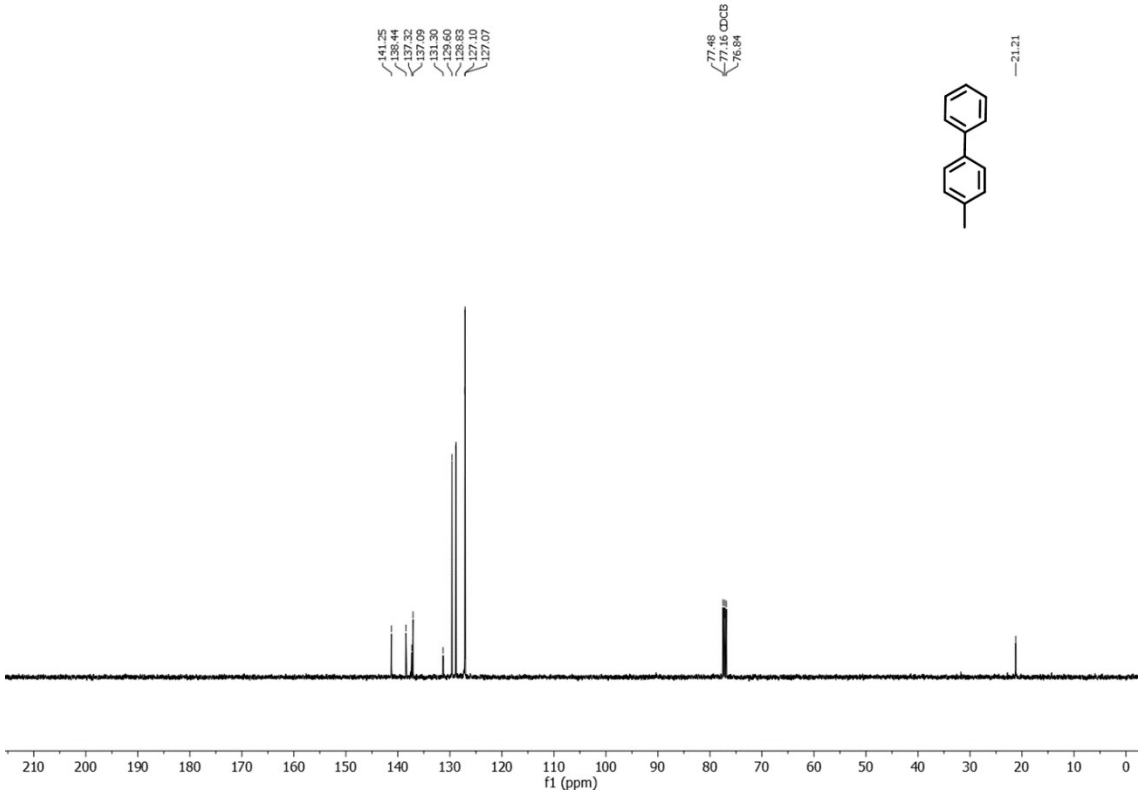


Figure S6. ^{13}C NMR spectrum (100 MHz) of **2b** in $CDCl_3$.

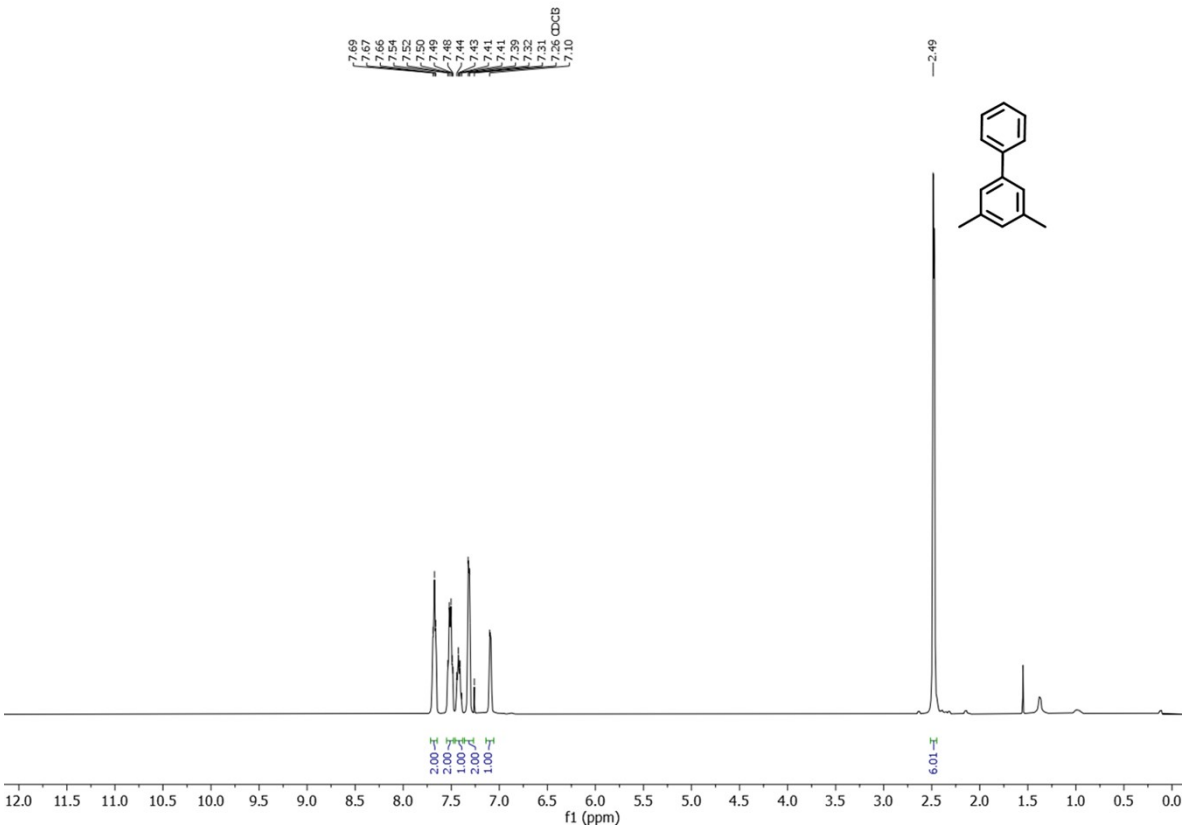


Figure S7. ^{1}H NMR spectrum (400 MHz) of **2c** in $CDCl_3$.

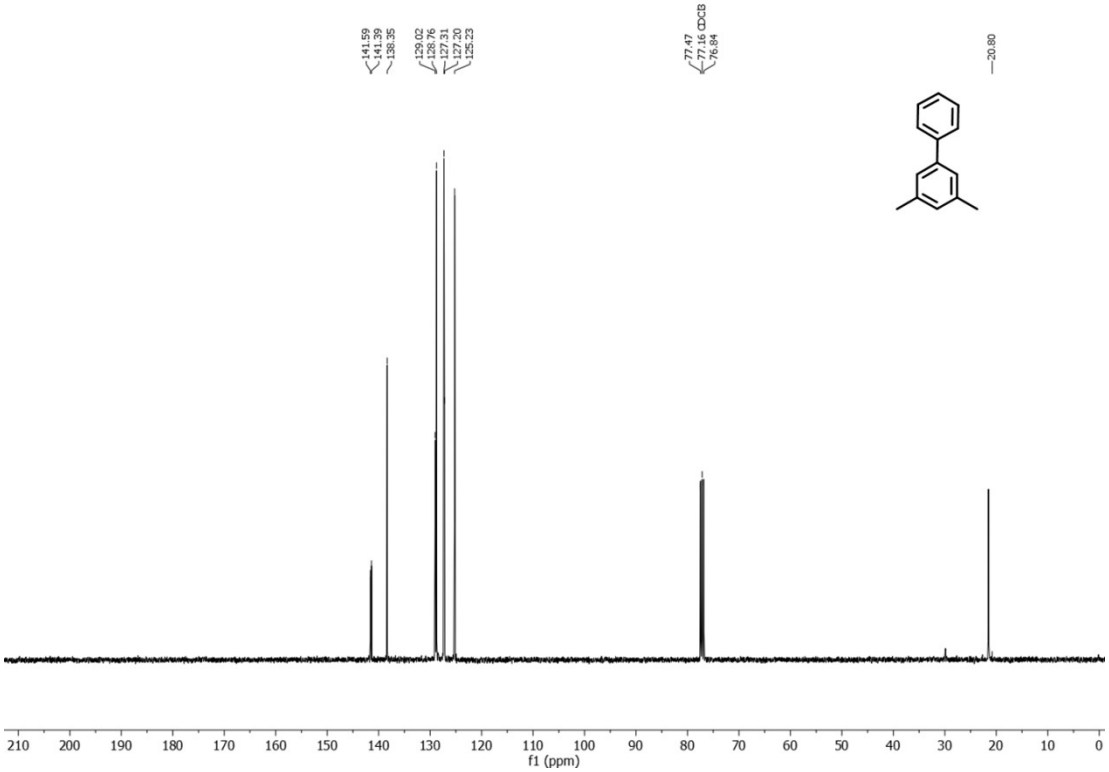


Figure S8. ^{13}C NMR spectrum (100 MHz) of **2c** in $CDCl_3$.

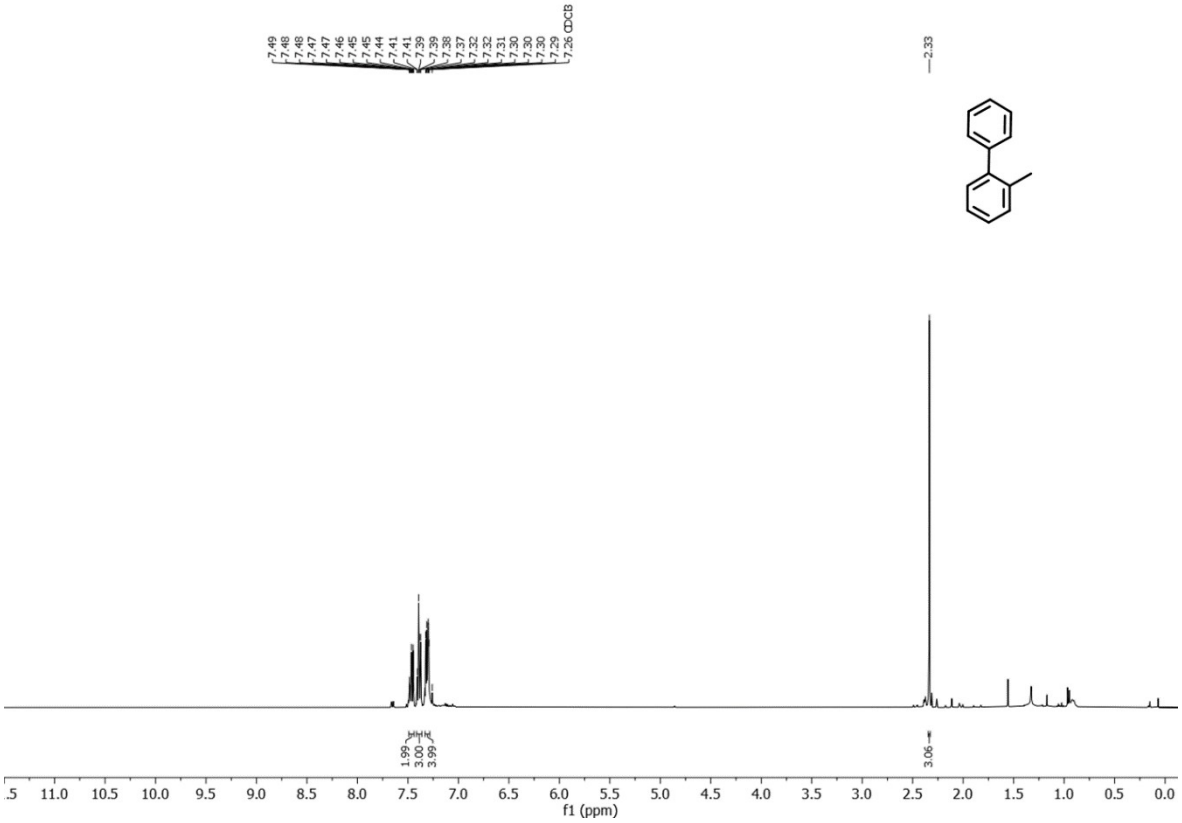


Figure S9. ^{1}H NMR spectrum (400 MHz) of **2d** in $CDCl_3$.

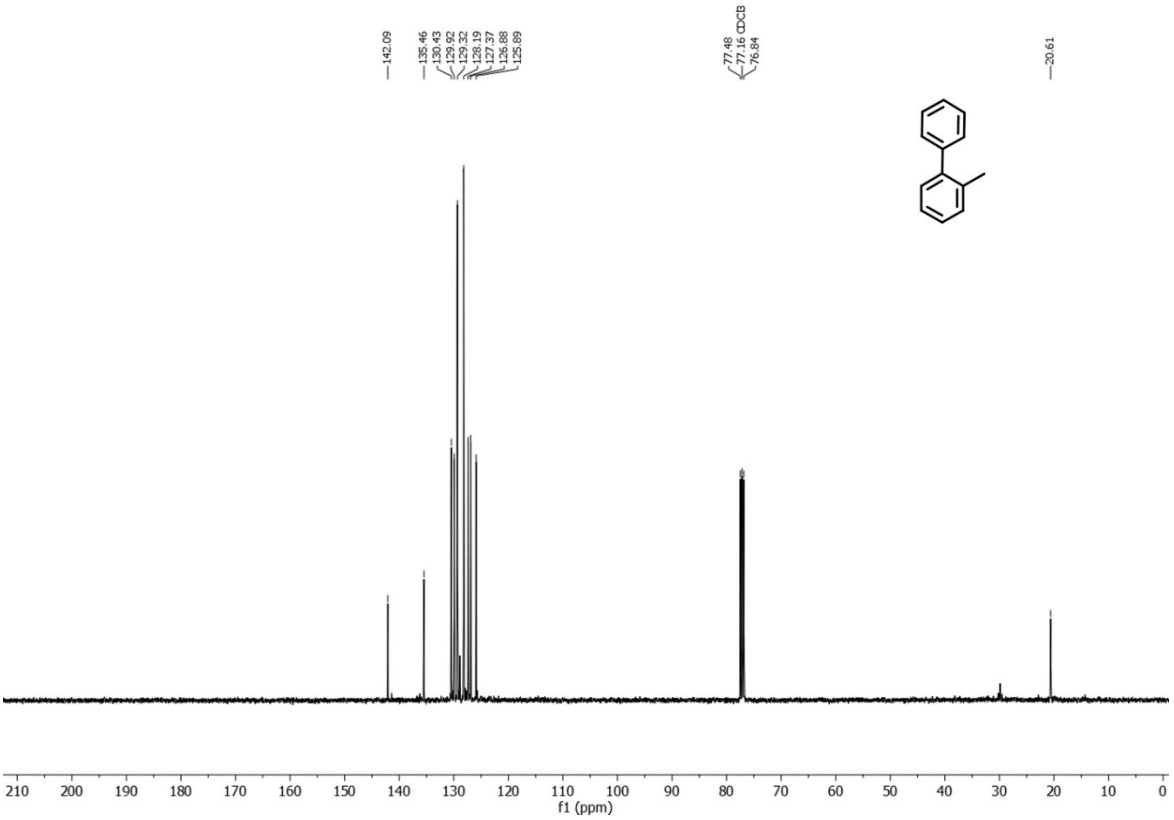


Figure S10. ^{13}C NMR spectrum (100 MHz) of **2d** in $CDCl_3$.

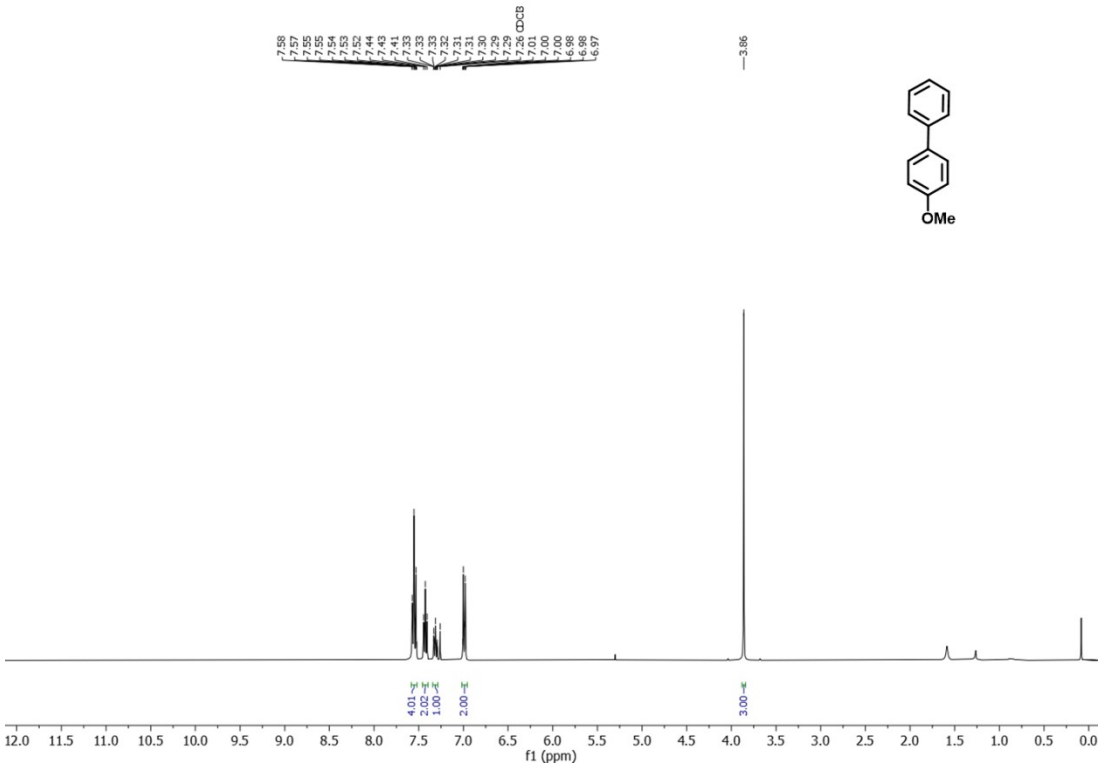


Figure S11. ^{1}H NMR spectrum (400 MHz) of **2e** in $CDCl_3$.

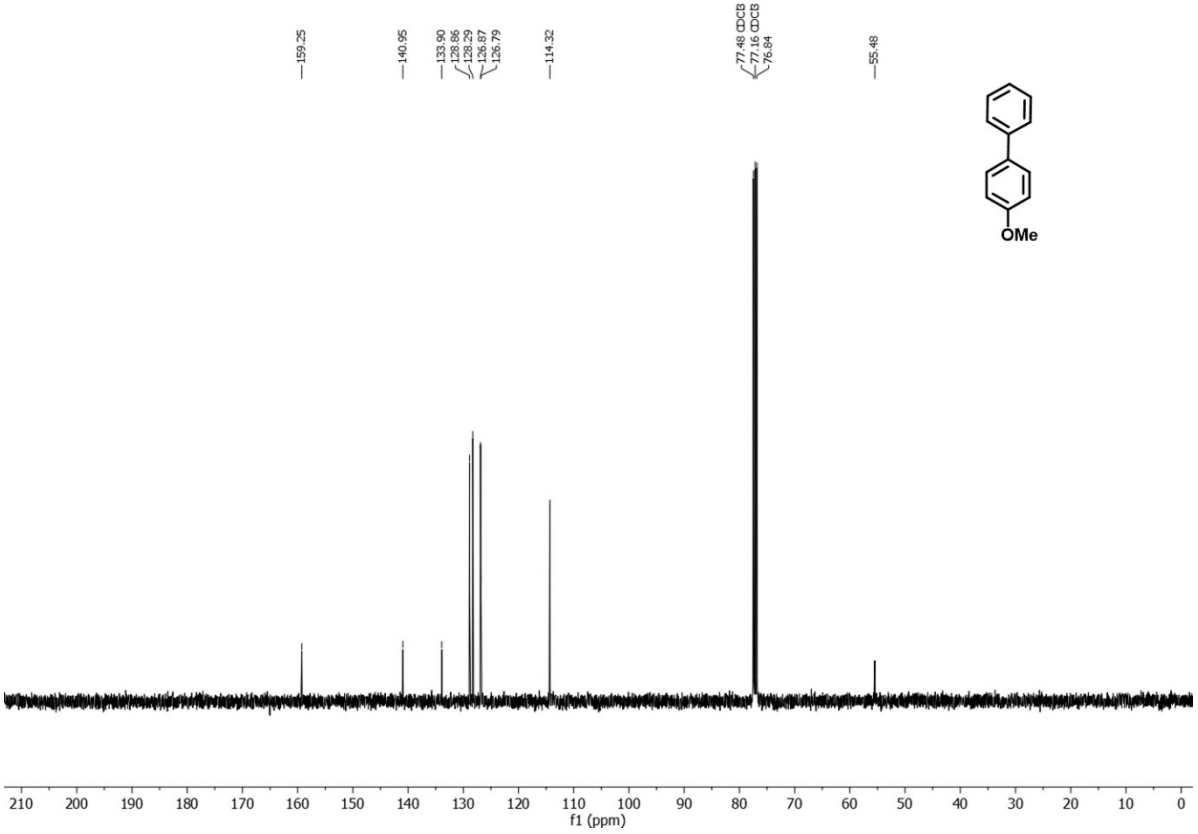


Figure S12. ^{13}C NMR spectrum (100 MHz) of **2e** in $CDCl_3$.

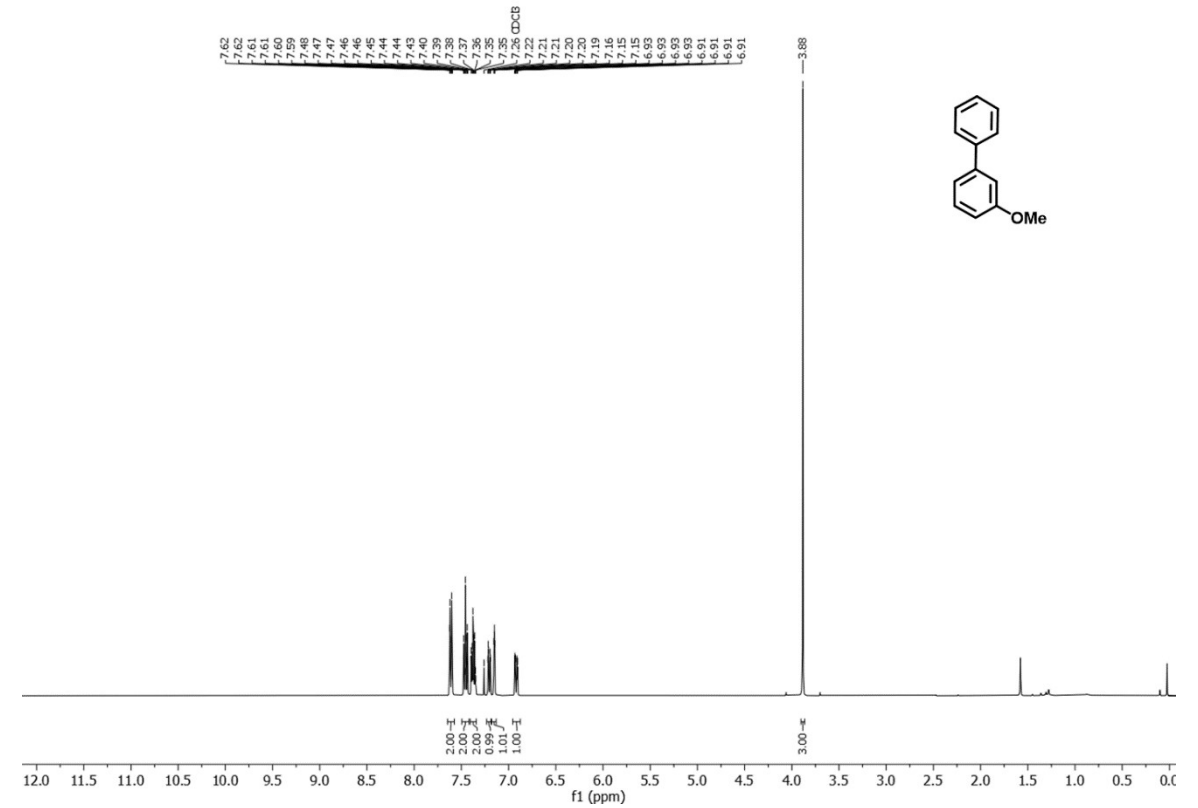


Figure S13. ^{1}H NMR spectrum (400 MHz) of **2f** in $CDCl_3$.

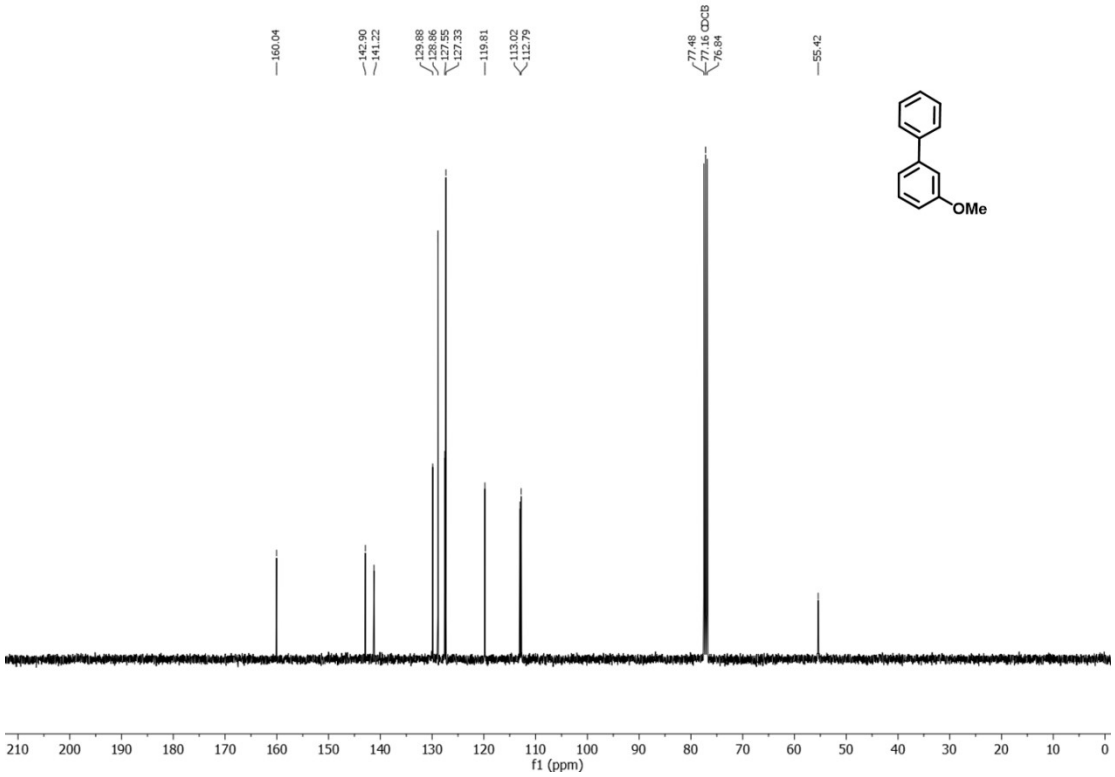


Figure S14. ^{13}C NMR spectrum (100 MHz) of **2f** in $CDCl_3$.

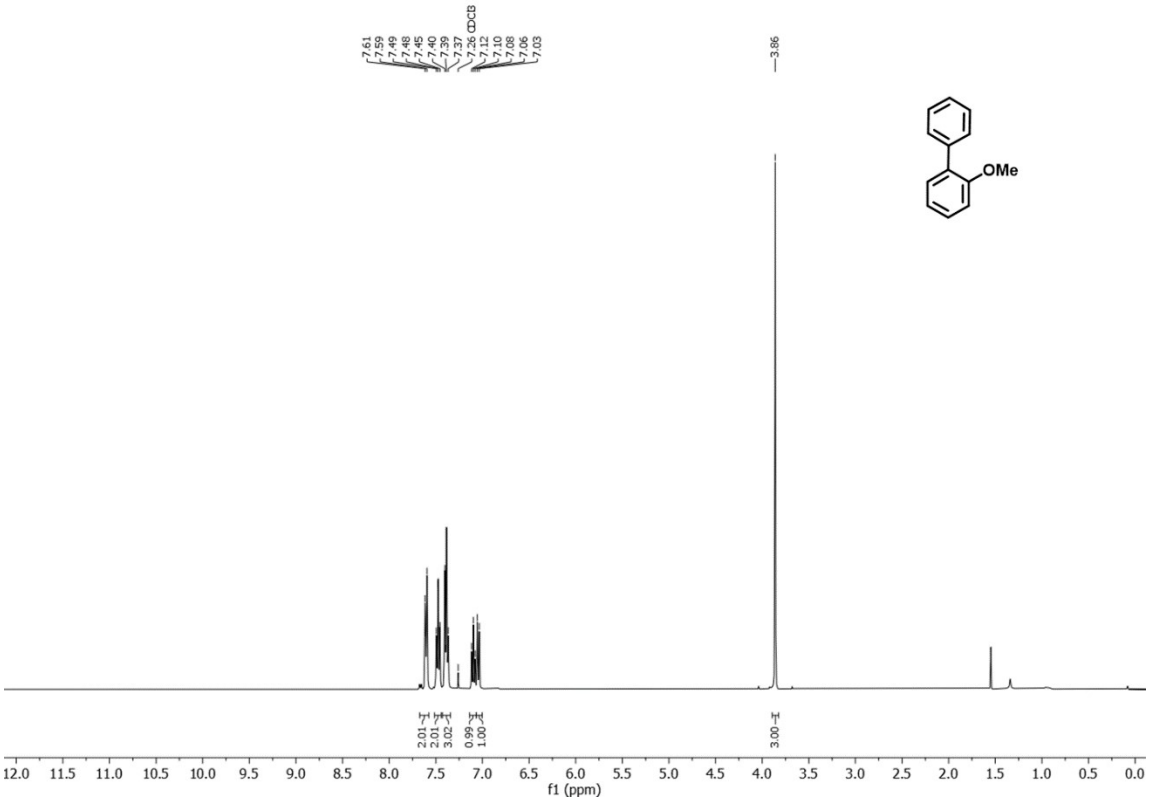


Figure S15. ^{1}H NMR spectrum (400 MHz) of **2g** in $CDCl_3$.

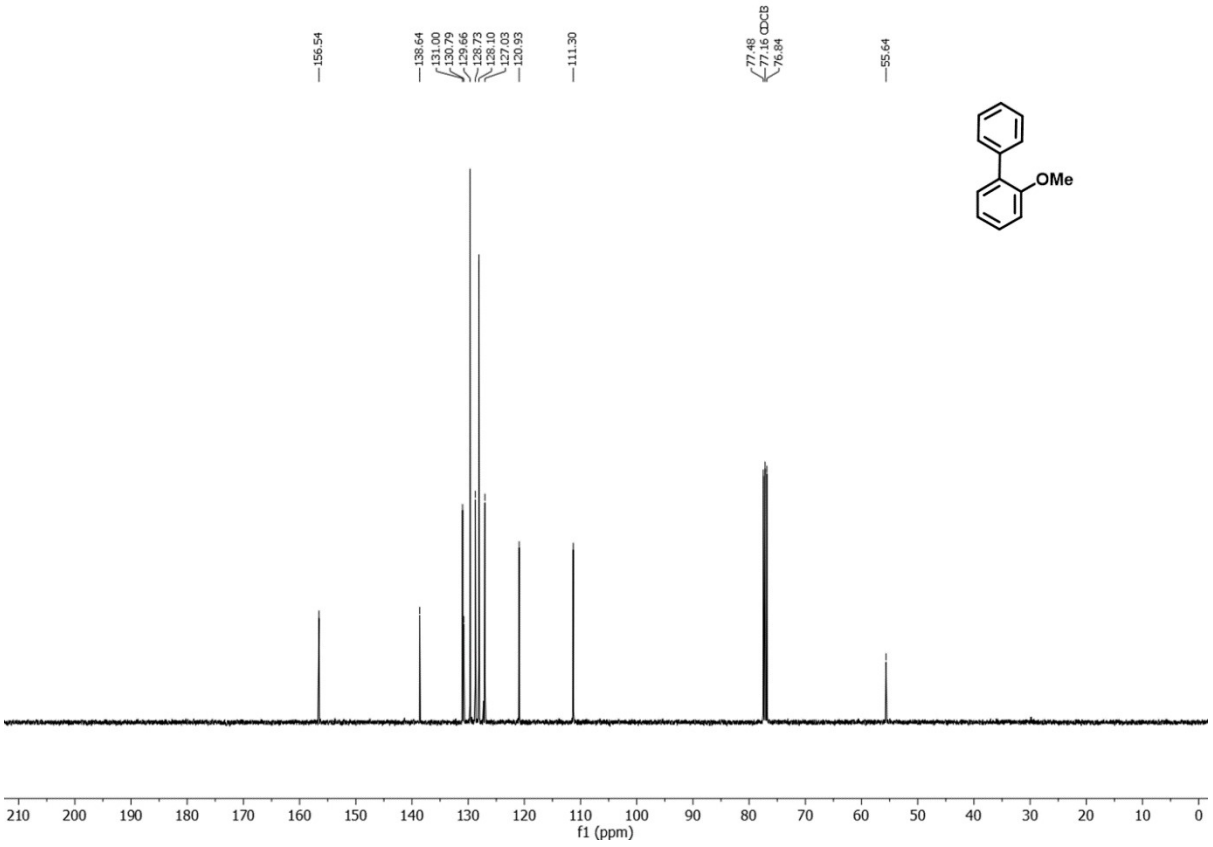


Figure S16. ^{13}C NMR spectrum (100 MHz) of **2g** in $CDCl_3$.

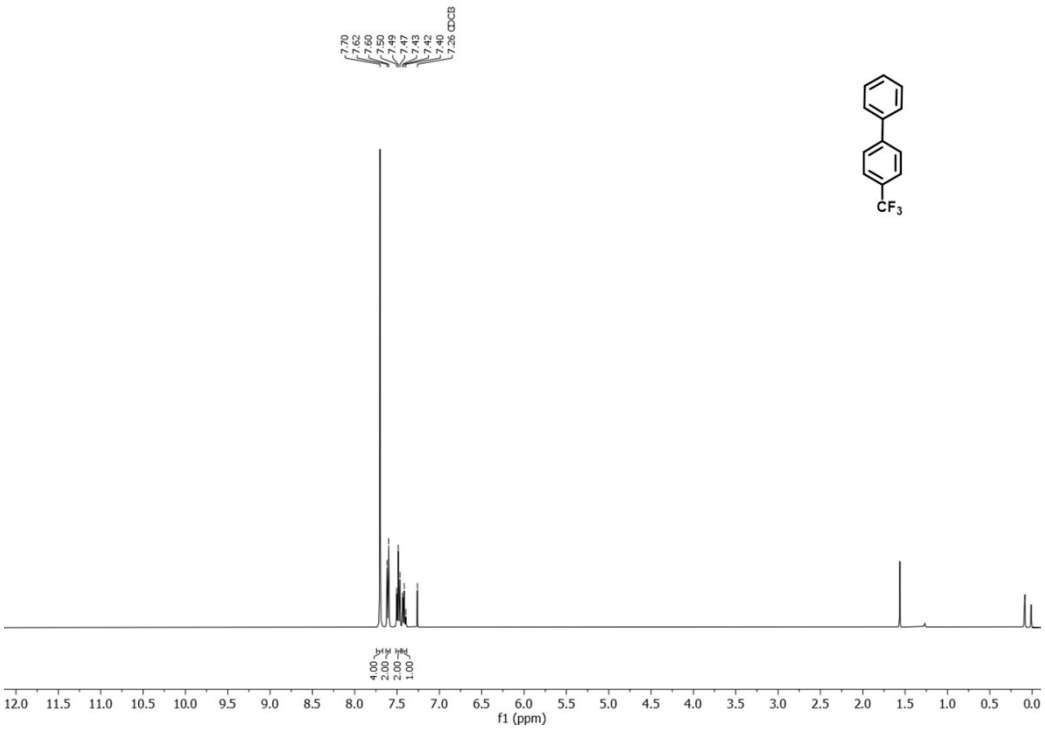


Figure S17. ^{1}H NMR spectrum (400 MHz) of **2h** in $CDCl_3$.

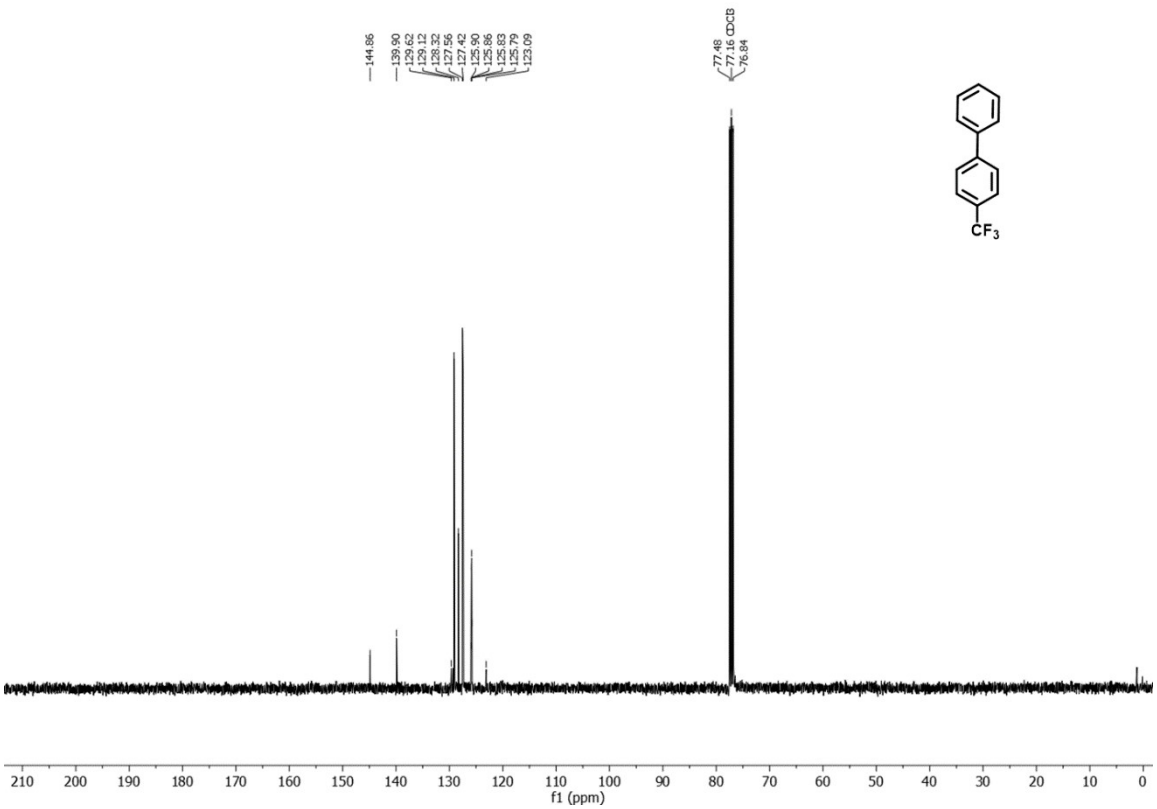


Figure S18. ^{13}C NMR spectrum (100 MHz) of **2h** in $CDCl_3$.

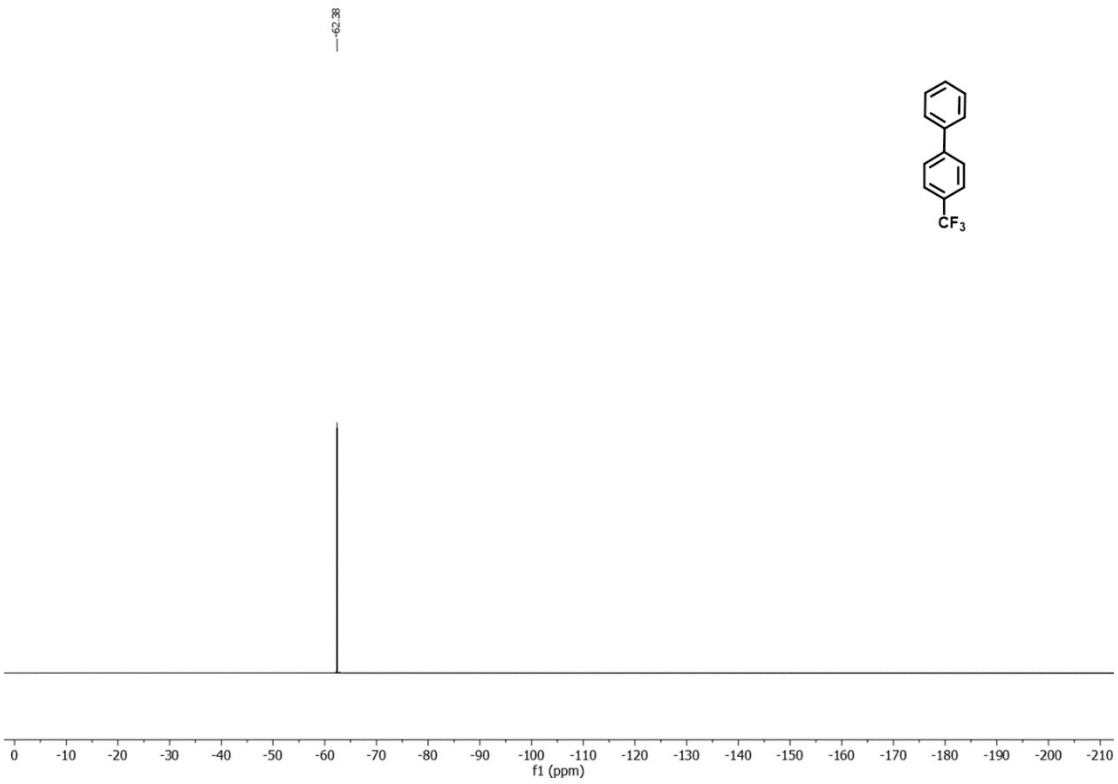


Figure S19. ^{19}F NMR spectrum (376 MHz) of **2h** in $CDCl_3$.

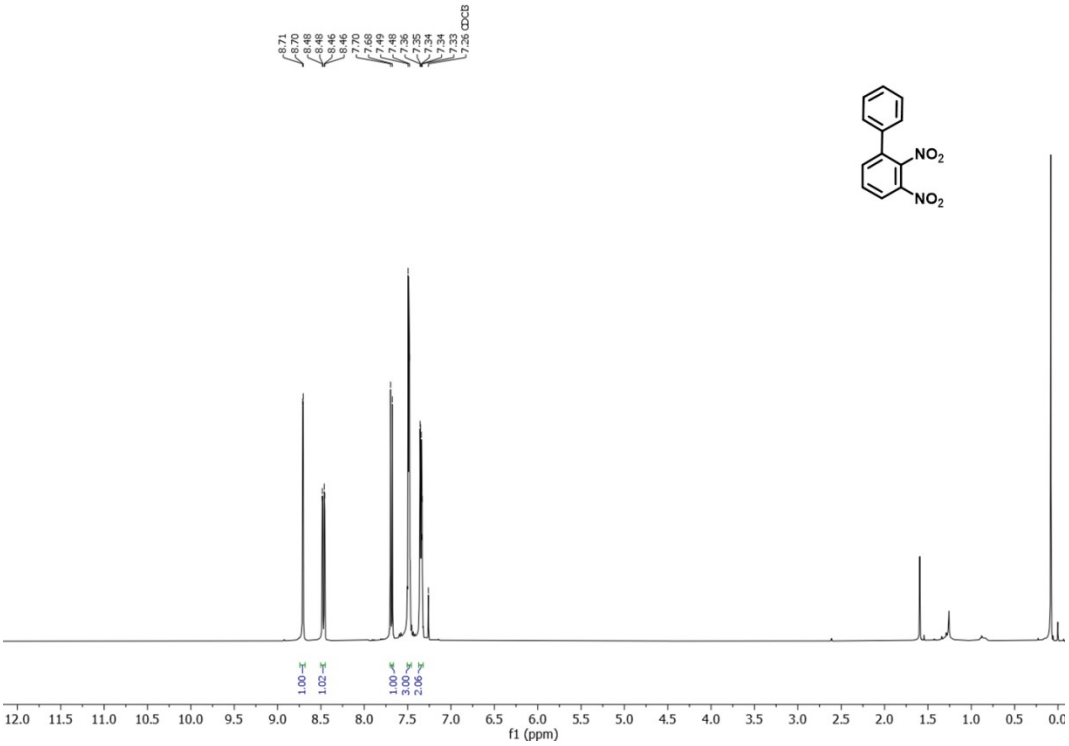


Figure S20. ^{1}H NMR spectrum (400 MHz) of **2i** in $CDCl_3$.

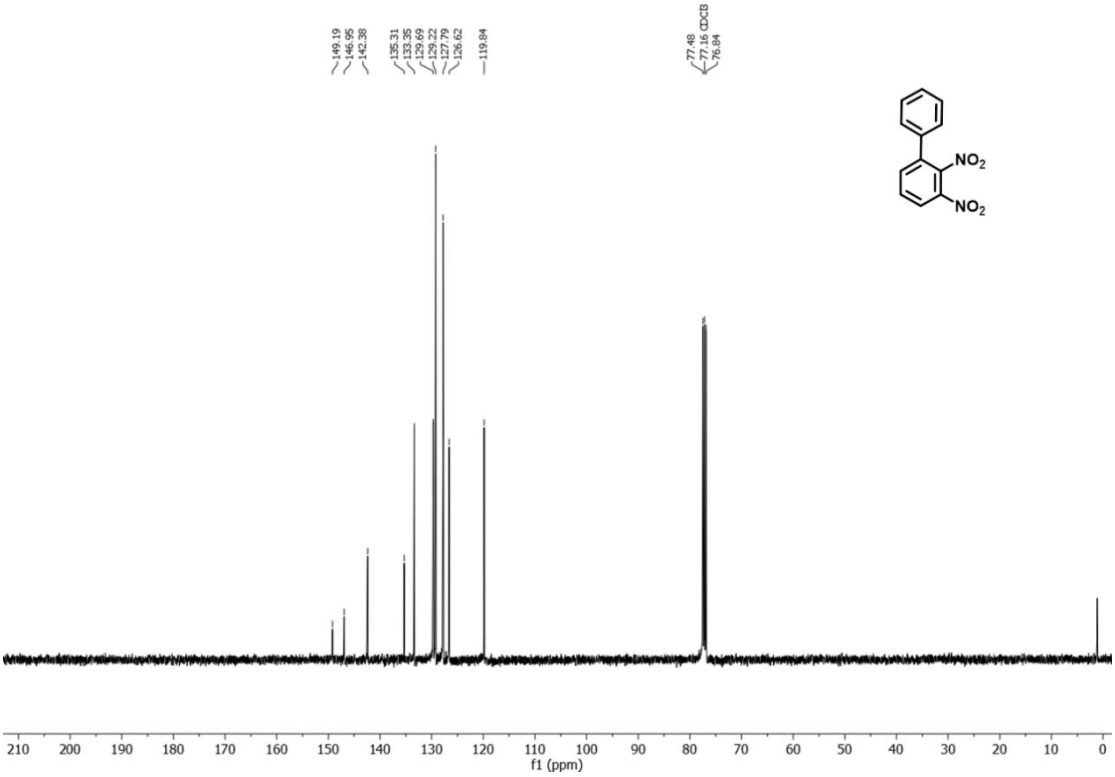


Figure S21. ^{13}C NMR spectrum (100 MHz) of **2i** in $CDCl_3$.

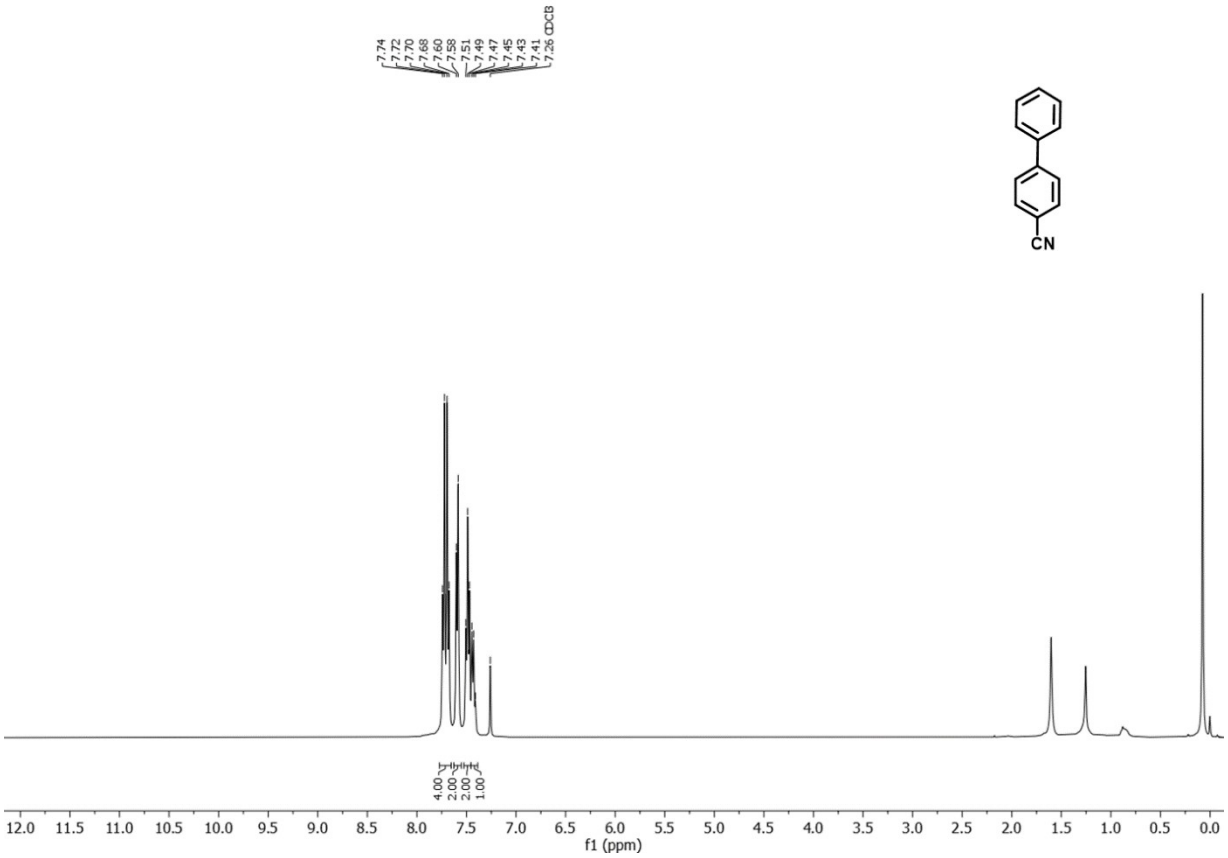


Figure S22. ^{1}H NMR spectrum (400 MHz) of **2j** in $CDCl_3$.

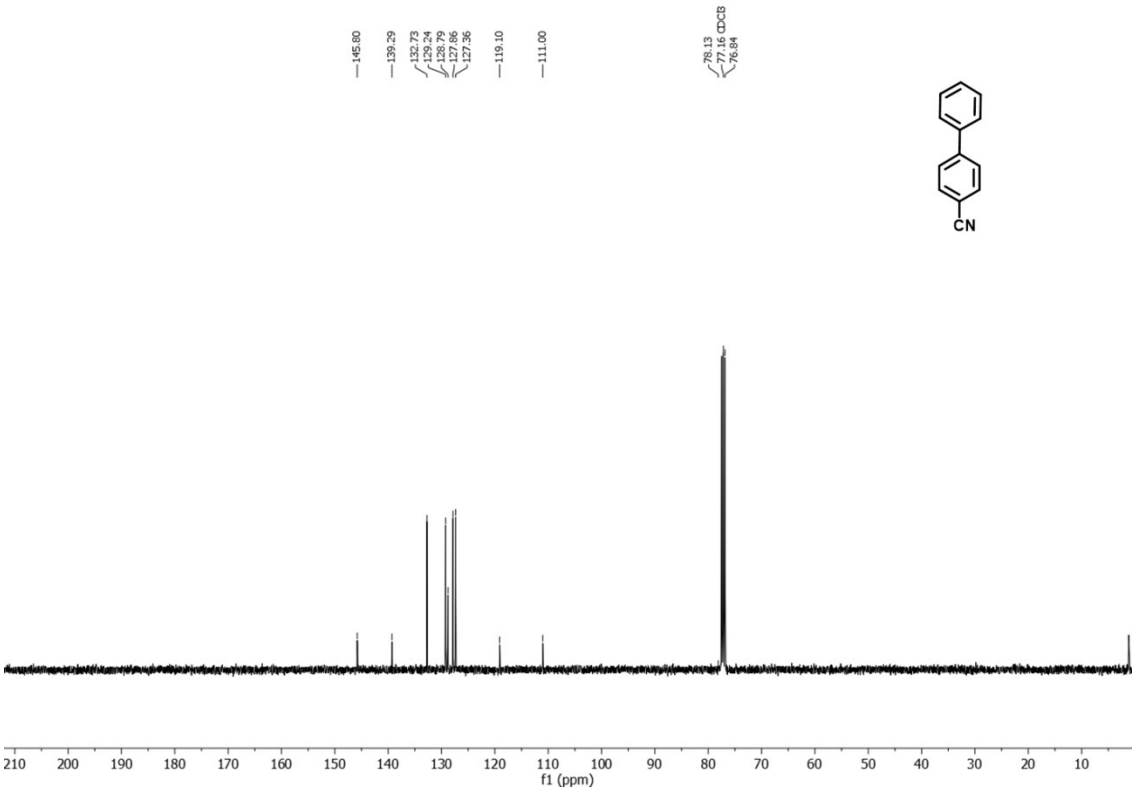


Figure S23. ^{13}C NMR spectrum (100 MHz) of **2j** in $CDCl_3$.

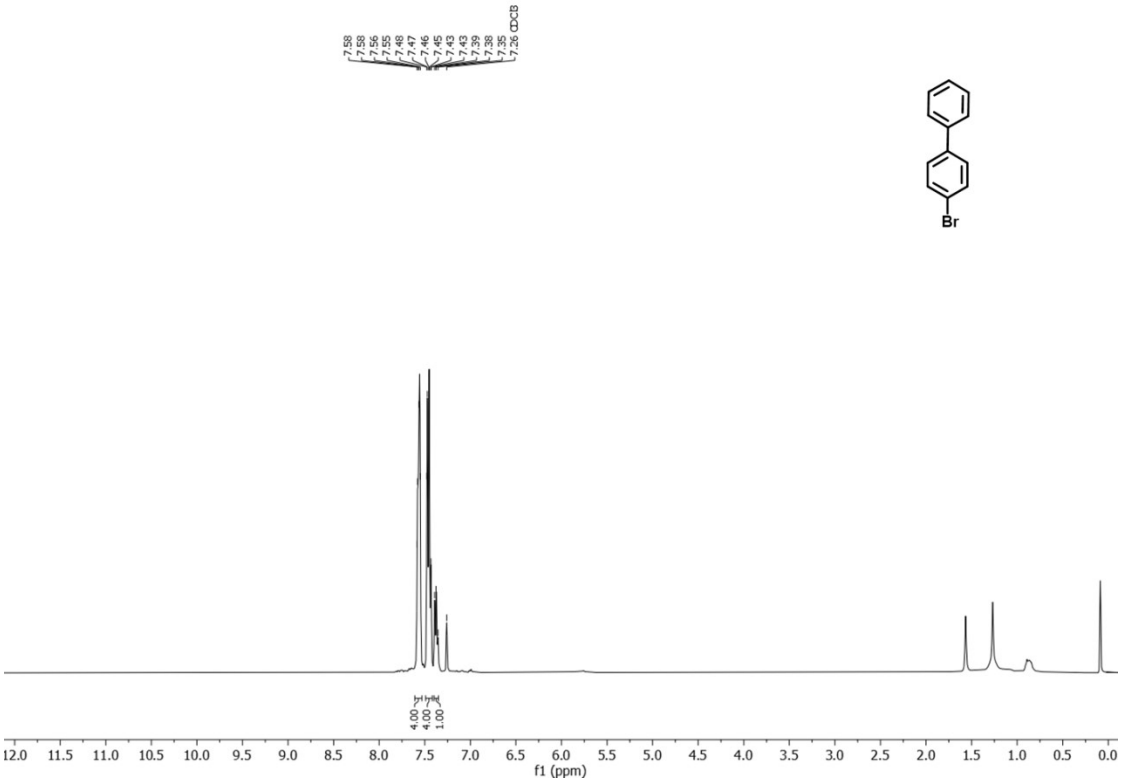


Figure S24. ^{1}H NMR spectrum (400 MHz) of **2k** in $CDCl_3$.

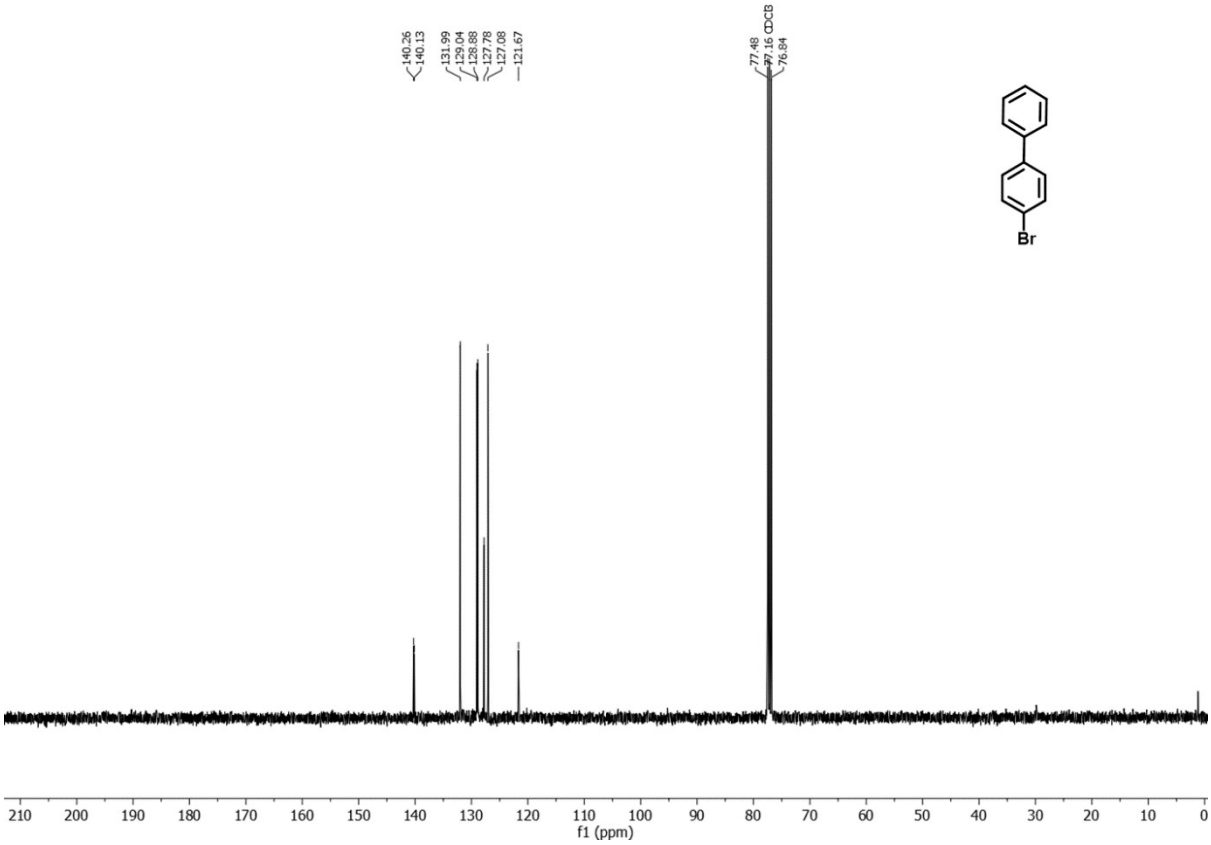


Figure S25. ^{13}C NMR spectrum (100 MHz) of **2k** in $CDCl_3$.

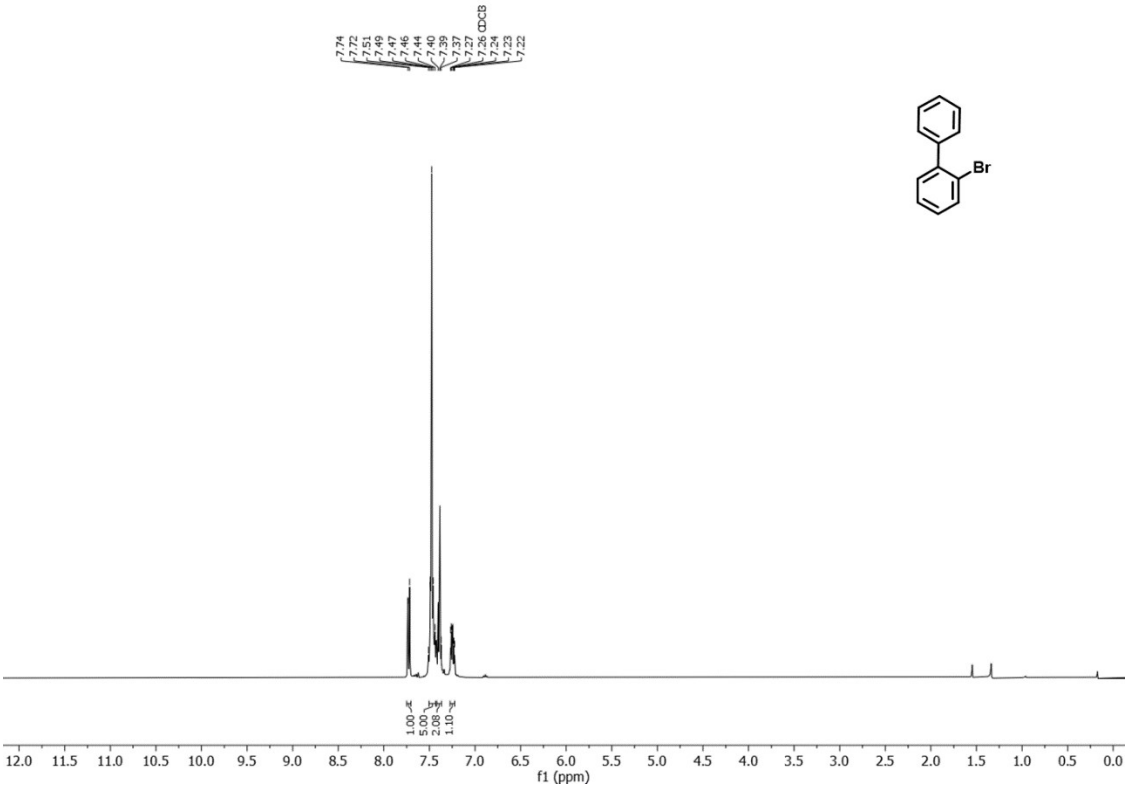


Figure S26. ^{1}H NMR spectrum (400 MHz) of **2l** in $CDCl_3$.

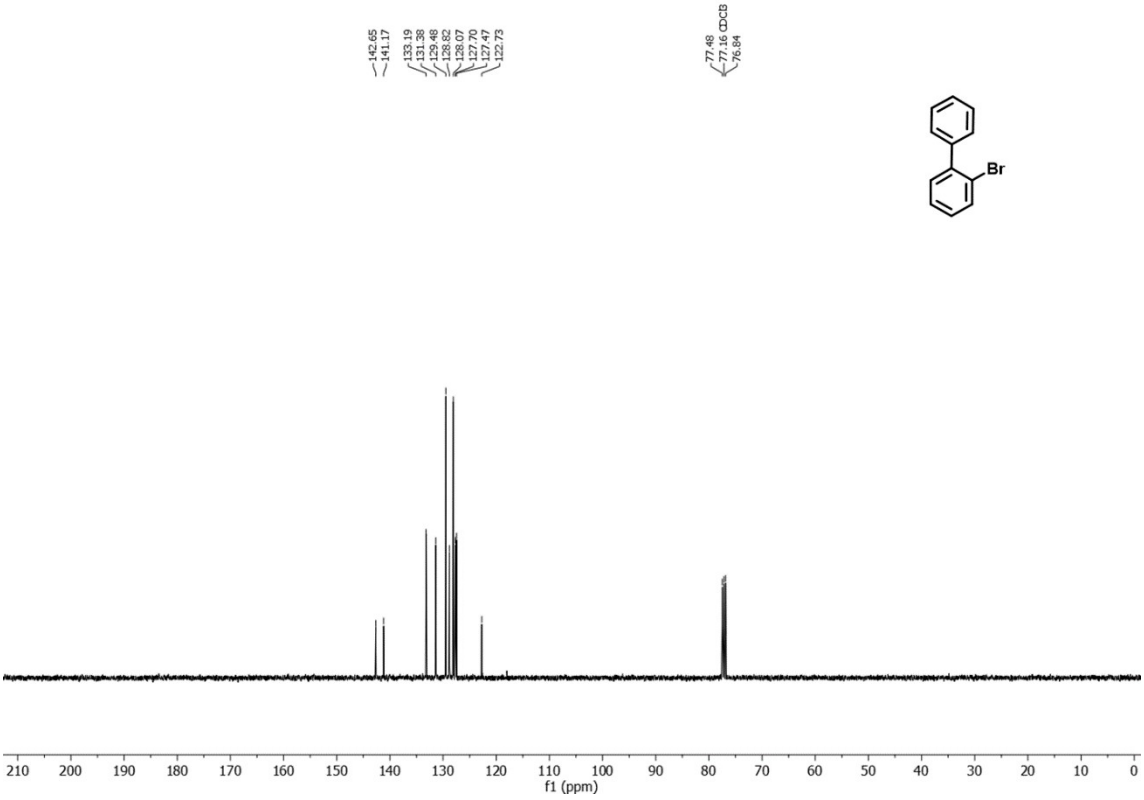


Figure S27. ^{13}C NMR spectrum (100 MHz) of **2l** in $CDCl_3$.

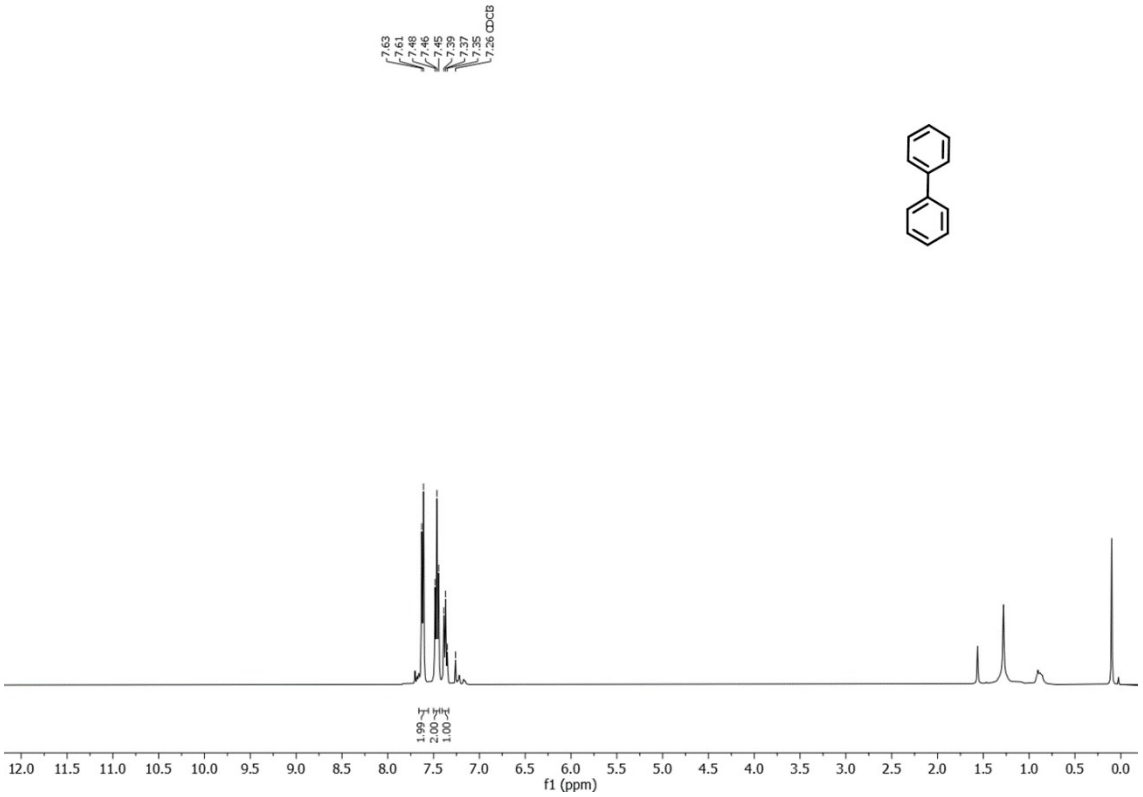


Figure S28. ^{1}H NMR spectrum (400 MHz) of **2m** in $CDCl_3$.

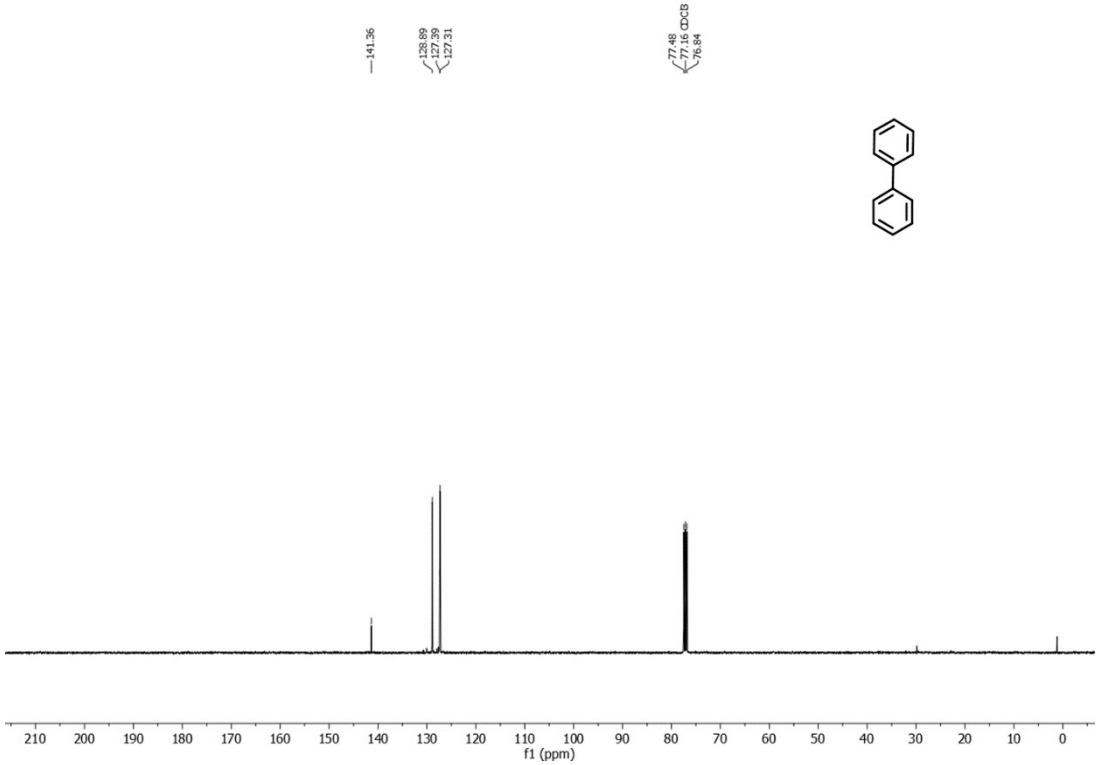


Figure S29. ^{13}C NMR spectrum (100 MHz) of **2m** in $CDCl_3$.

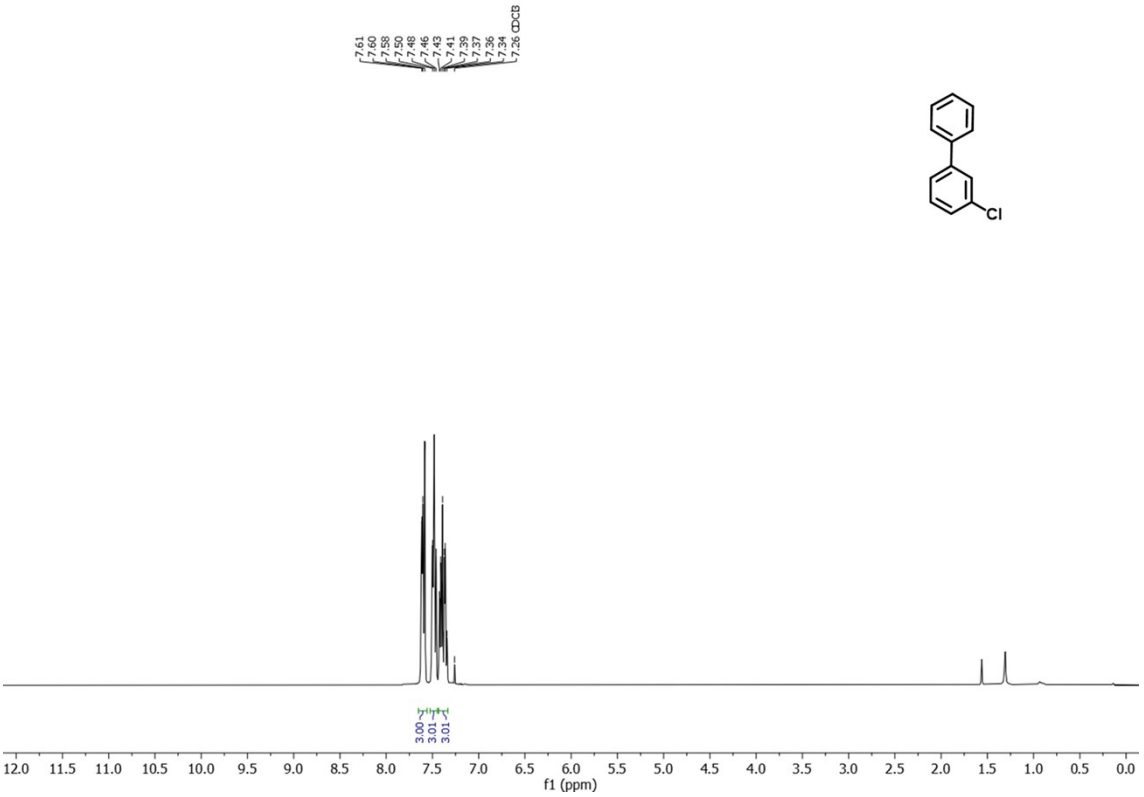


Figure S30. ^{1}H NMR spectrum (400 MHz) of **2n** in $CDCl_3$.

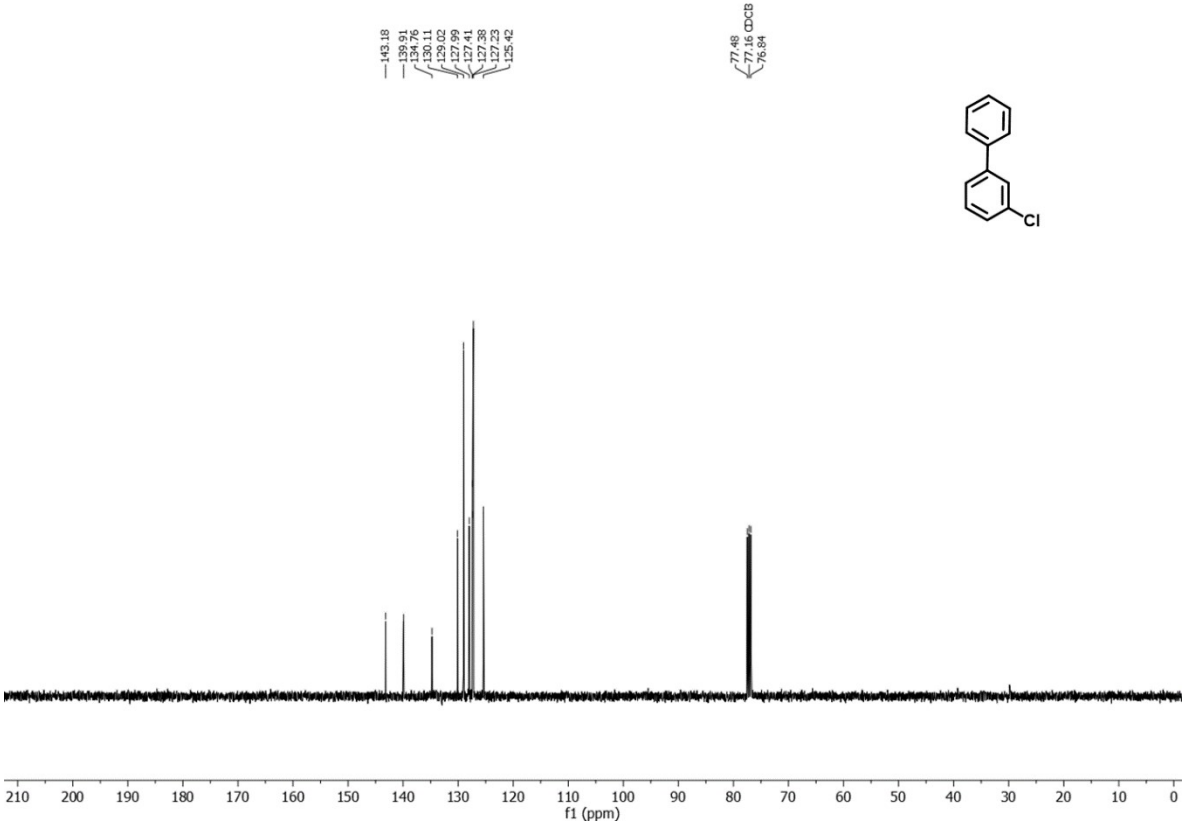


Figure S31. ^{13}C NMR spectrum (100 MHz) of **2n** in $CDCl_3$.

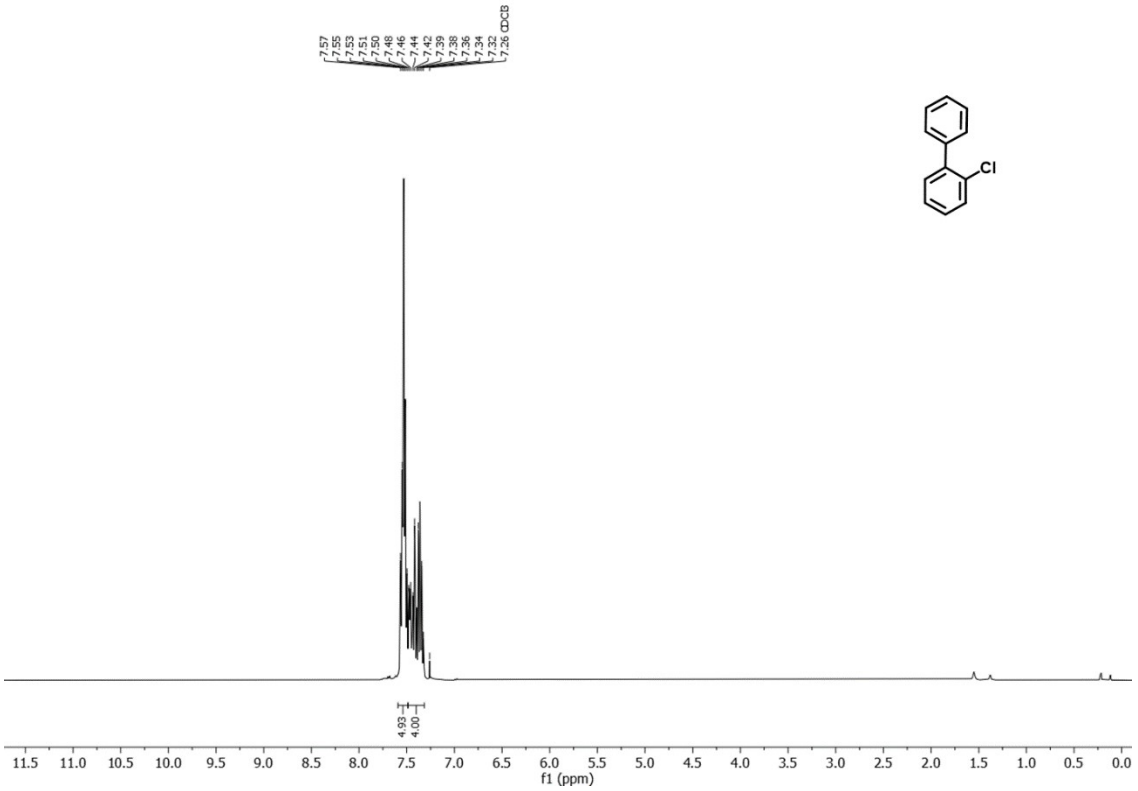


Figure S32. ^{1}H NMR spectrum (400 MHz) of **2o** in $CDCl_3$.

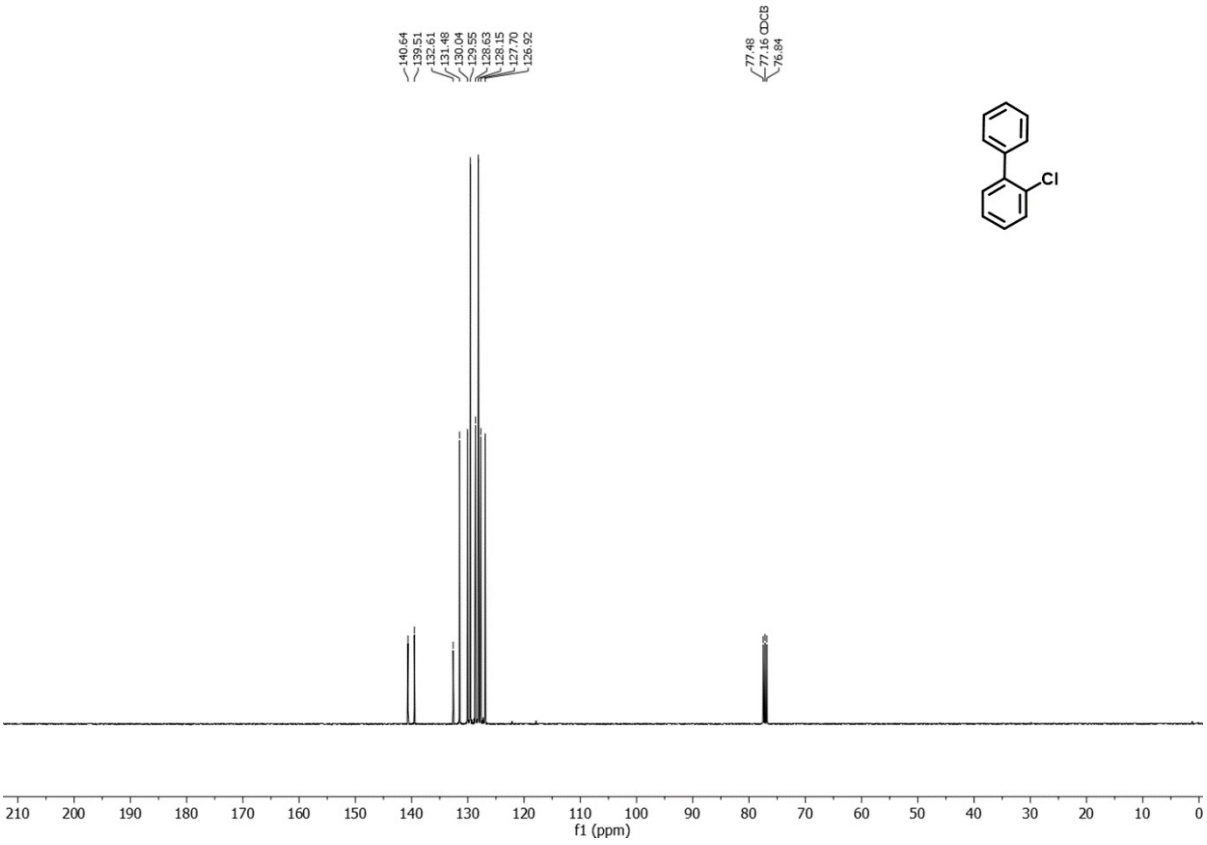


Figure S33. ^{13}C NMR spectrum (100 MHz) of **2o** in $CDCl_3$.

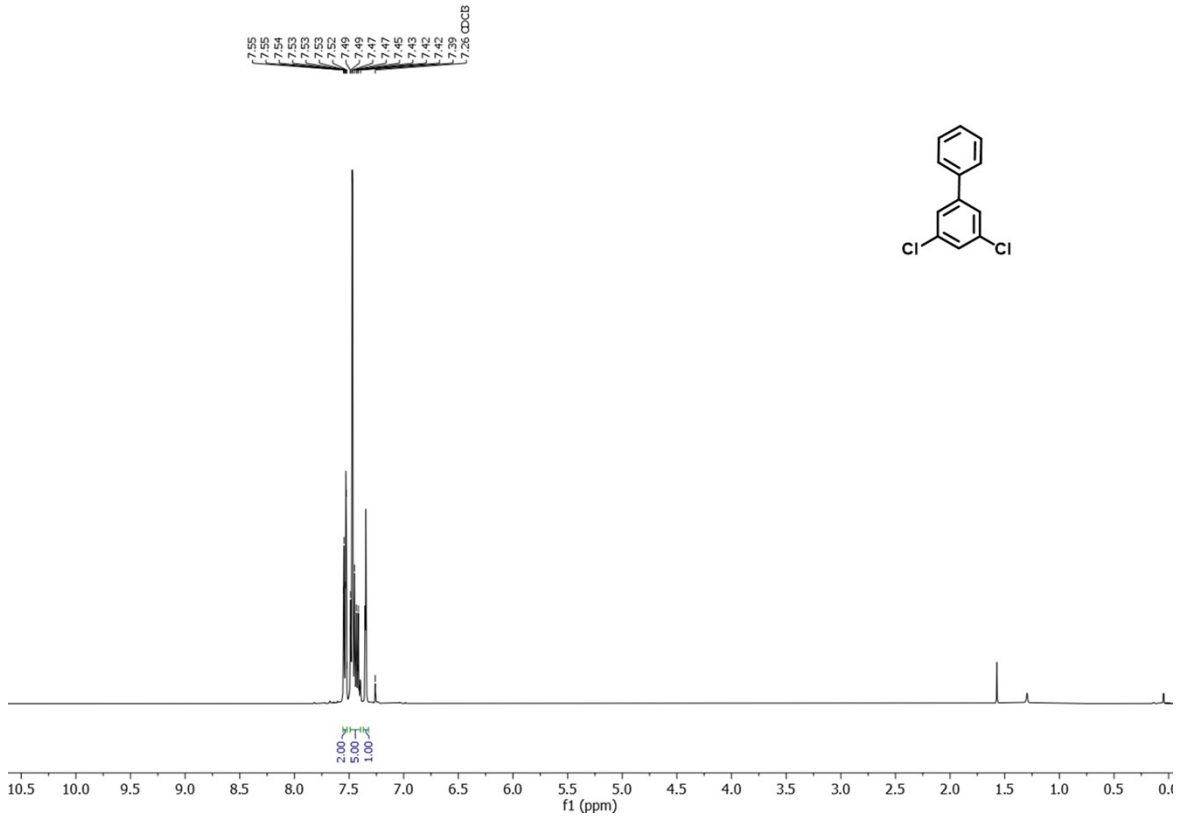


Figure S34. ^{1}H NMR spectrum (400 MHz) of **2p** in $CDCl_3$.

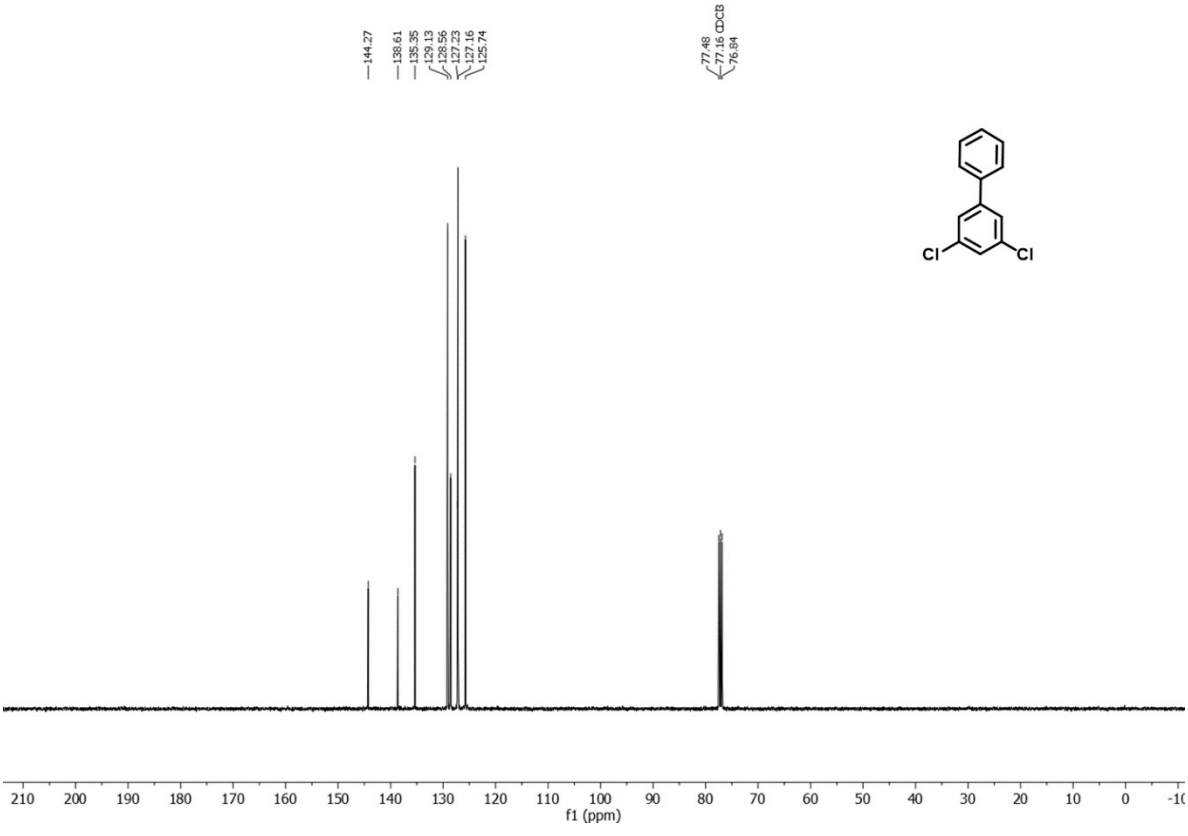


Figure S35. ^{13}C NMR spectrum (100 MHz) of **2p** in $CDCl_3$.

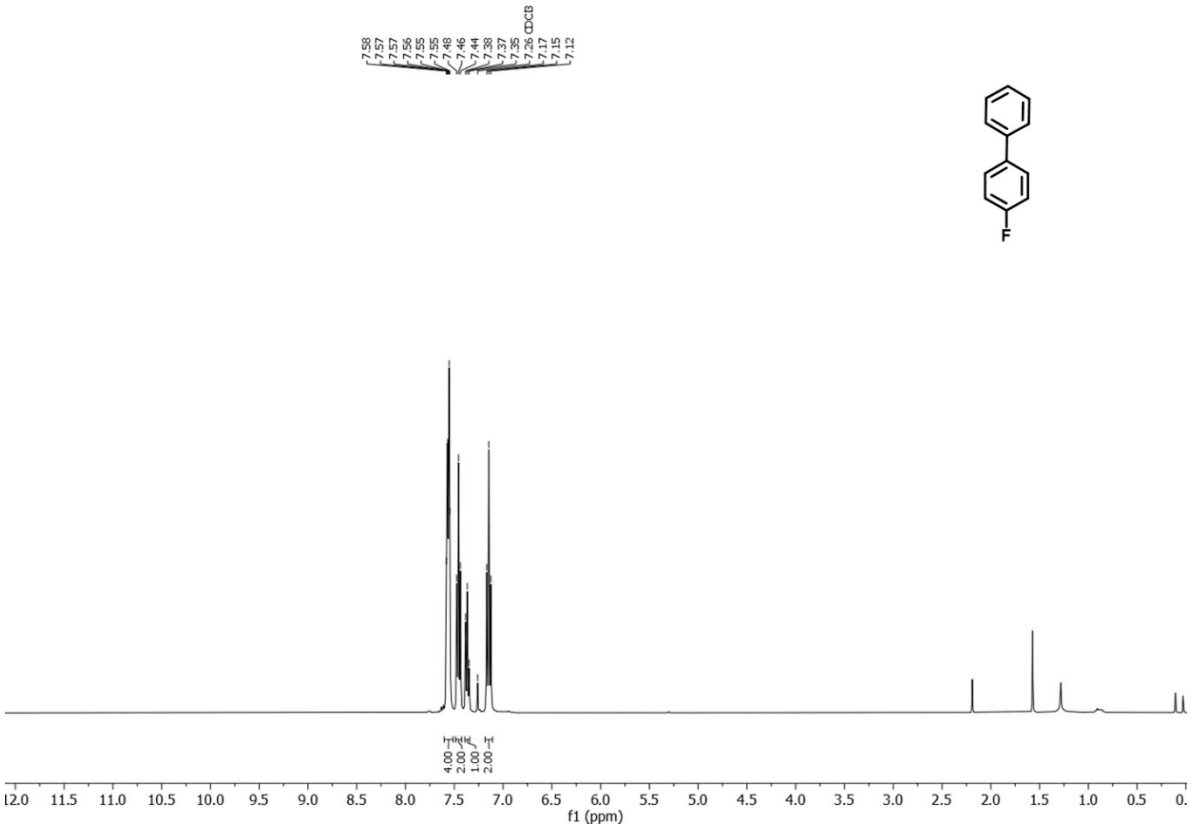


Figure S36. ^{1}H NMR spectrum (400 MHz) of **2q** in $CDCl_3$.

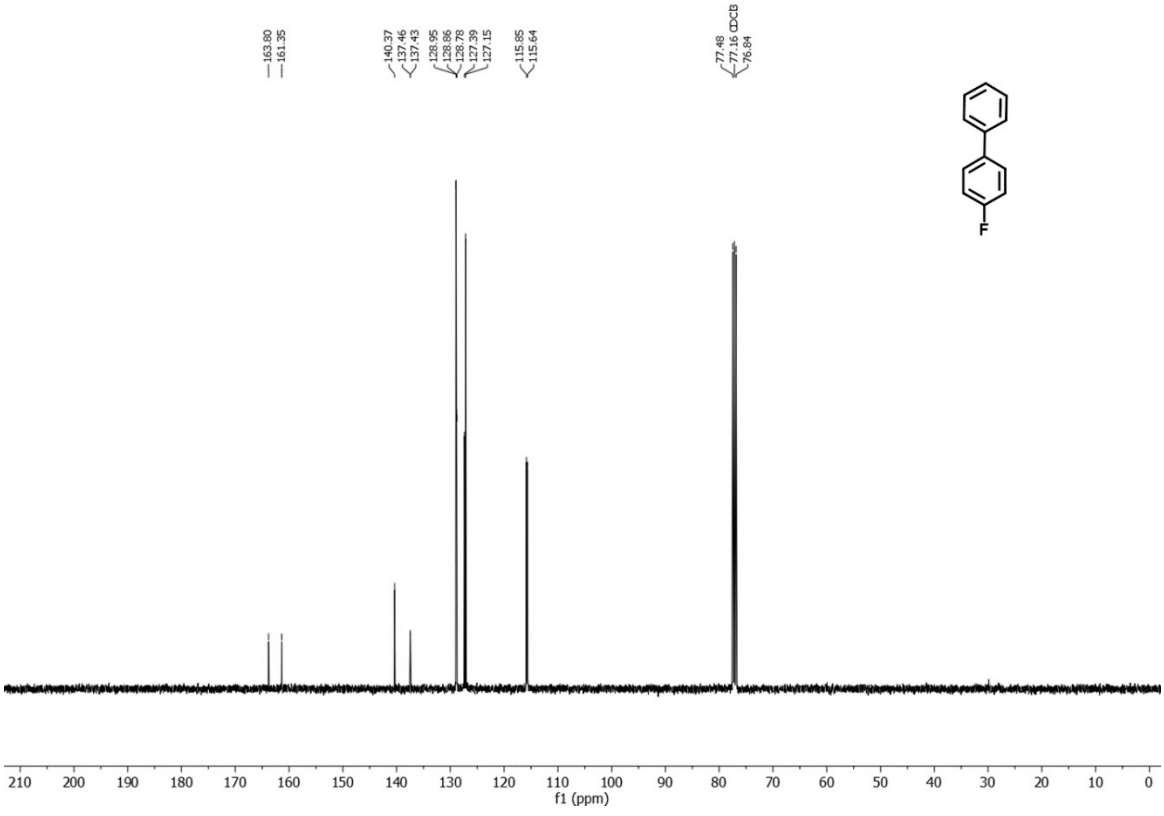


Figure S37. ^{13}C NMR spectrum (100 MHz) of **2q** in $CDCl_3$.

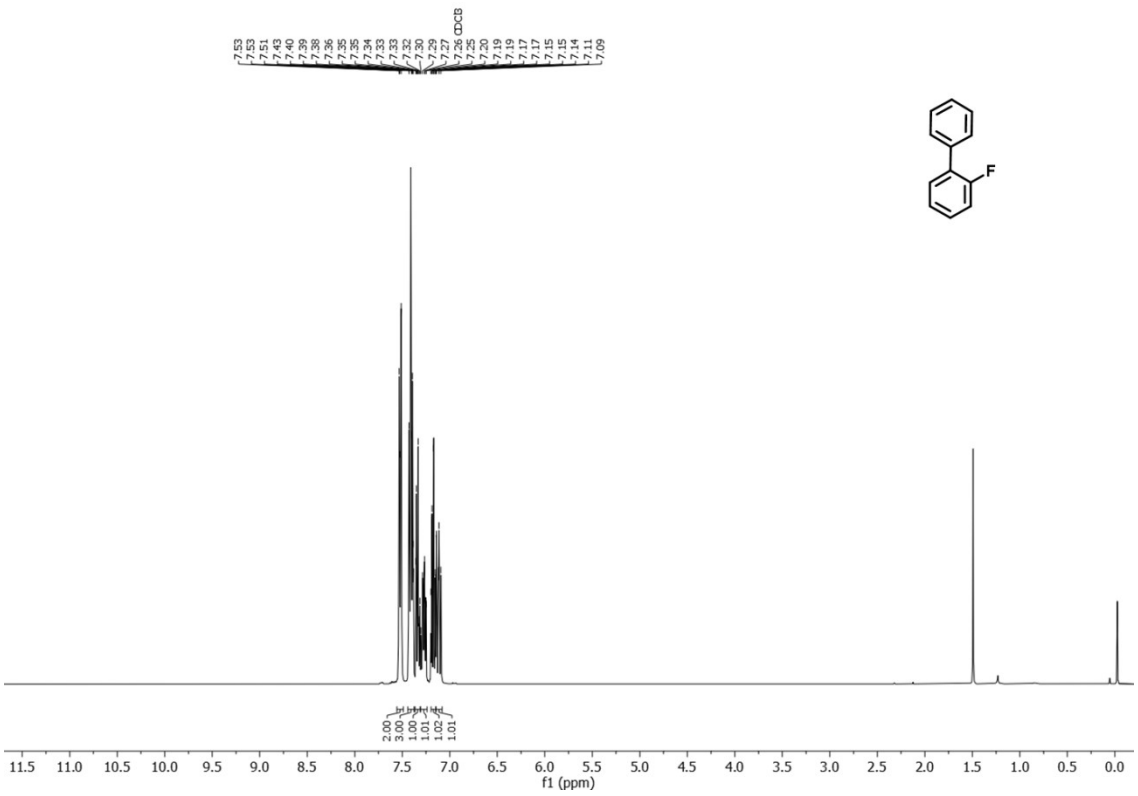


Figure S38. ^{1}H NMR spectrum (400 MHz) of **2r** in $CDCl_3$.

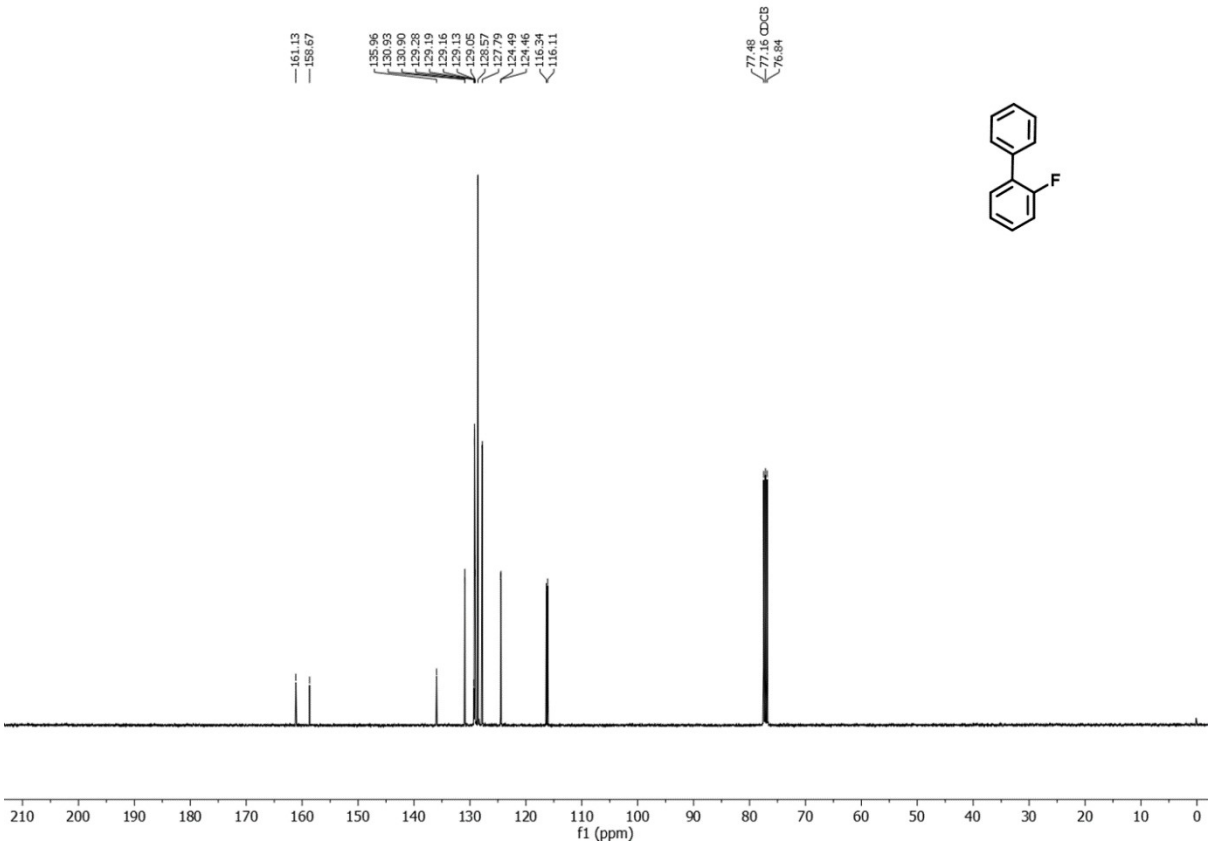


Figure S39. ^{13}C NMR spectrum (100 MHz) of **2r** in $CDCl_3$.

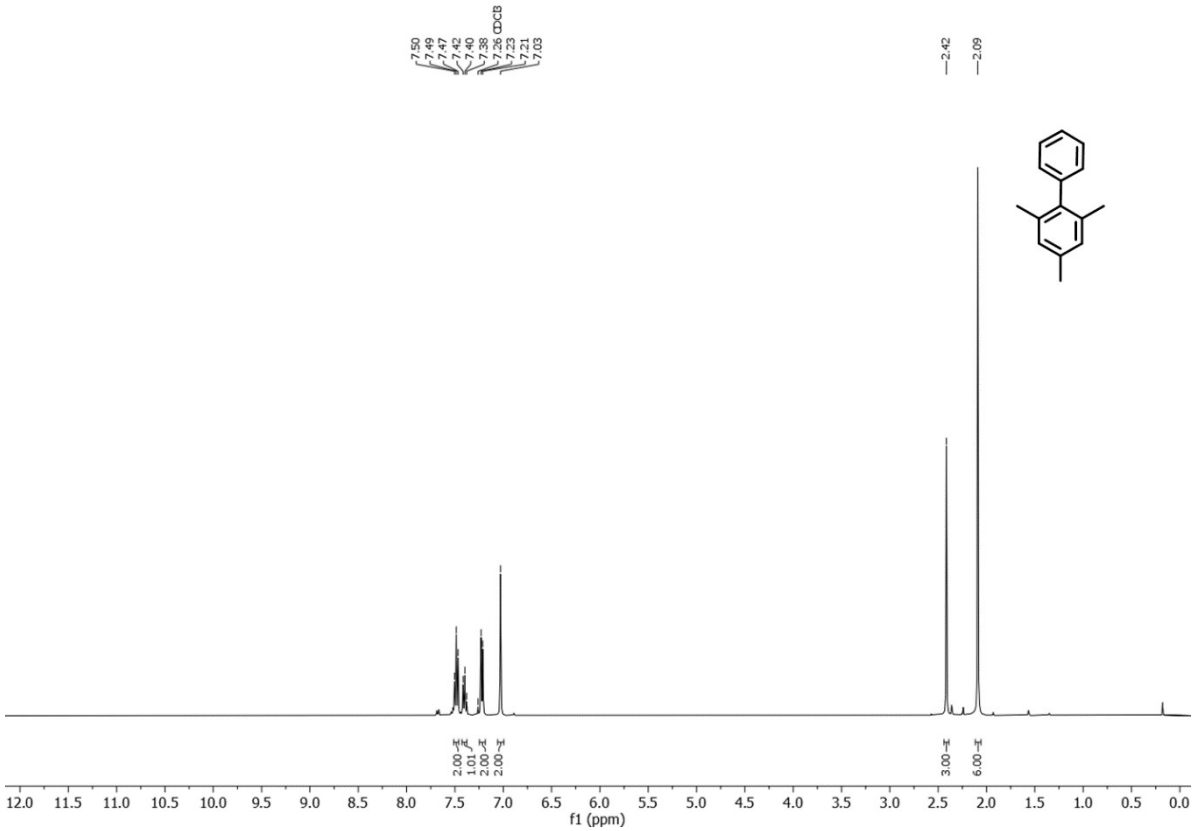


Figure S40. ^{1}H NMR spectrum (400 MHz) of **3a** in $CDCl_3$.

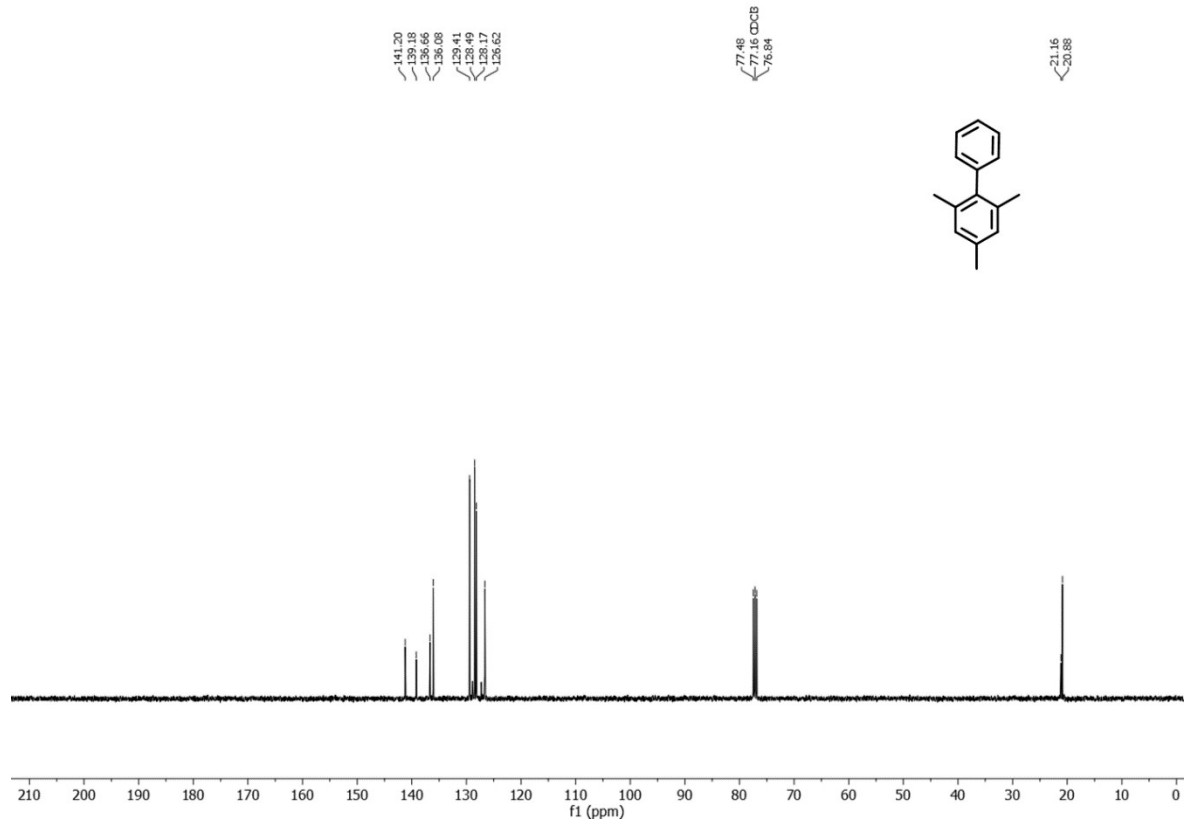


Figure S41. ^{13}C NMR spectrum (100 MHz) of **3a** in $CDCl_3$.

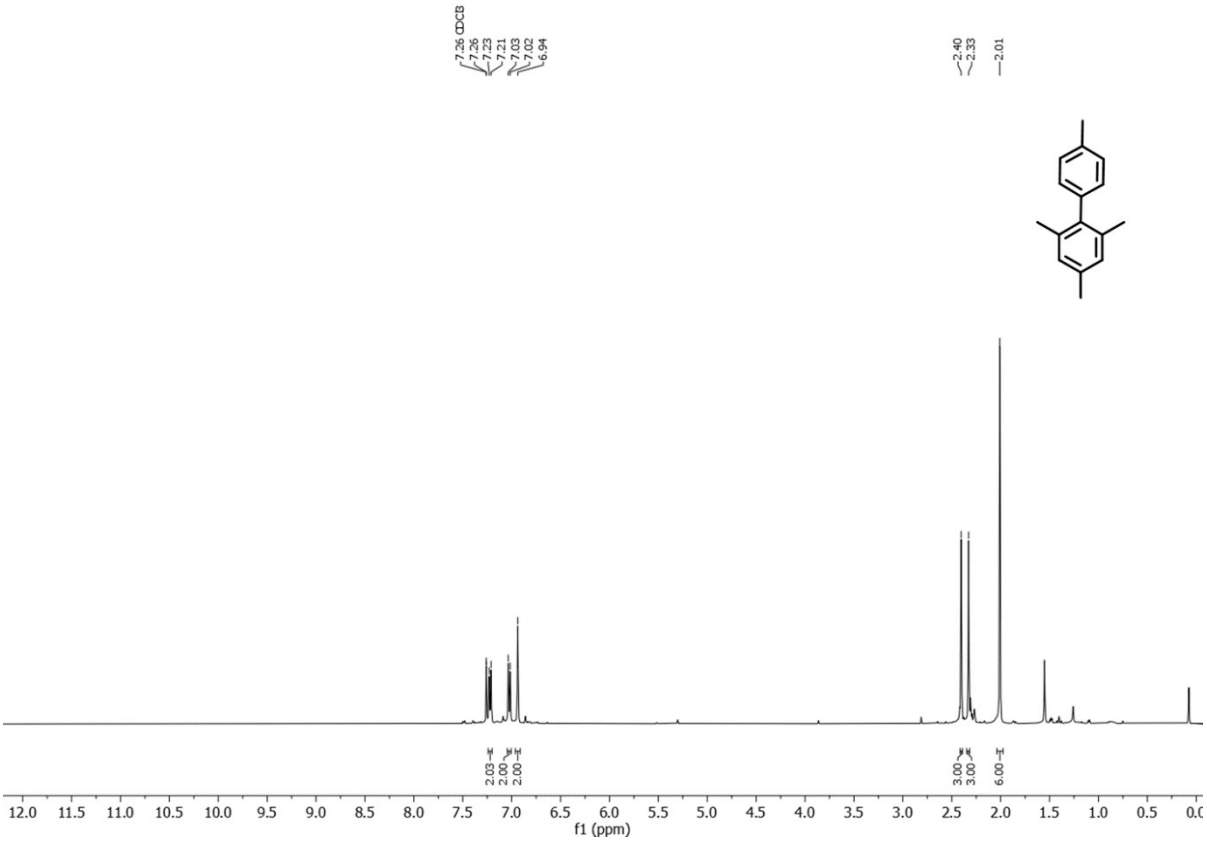


Figure S42. ^{1}H NMR spectrum (400 MHz) of **3b** in $CDCl_3$.

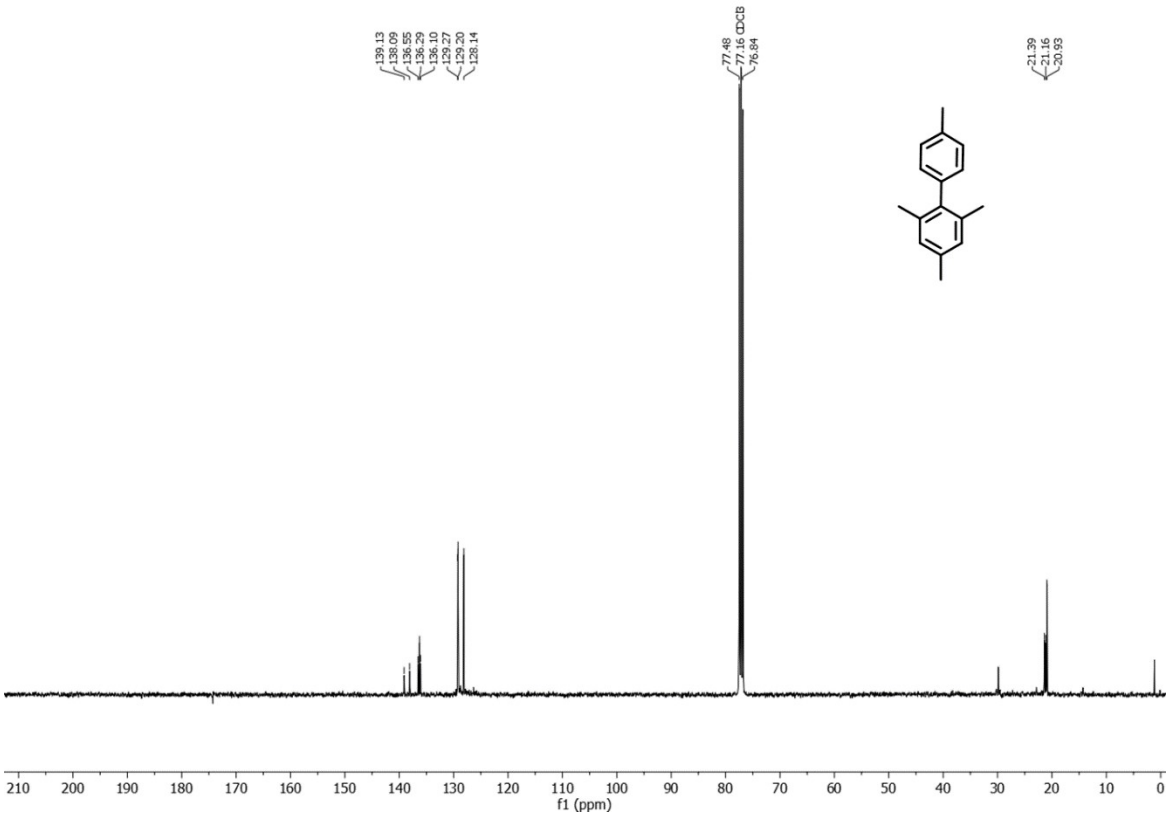


Figure S43. ^{13}C NMR spectrum (100 MHz) of **3b** in $CDCl_3$.

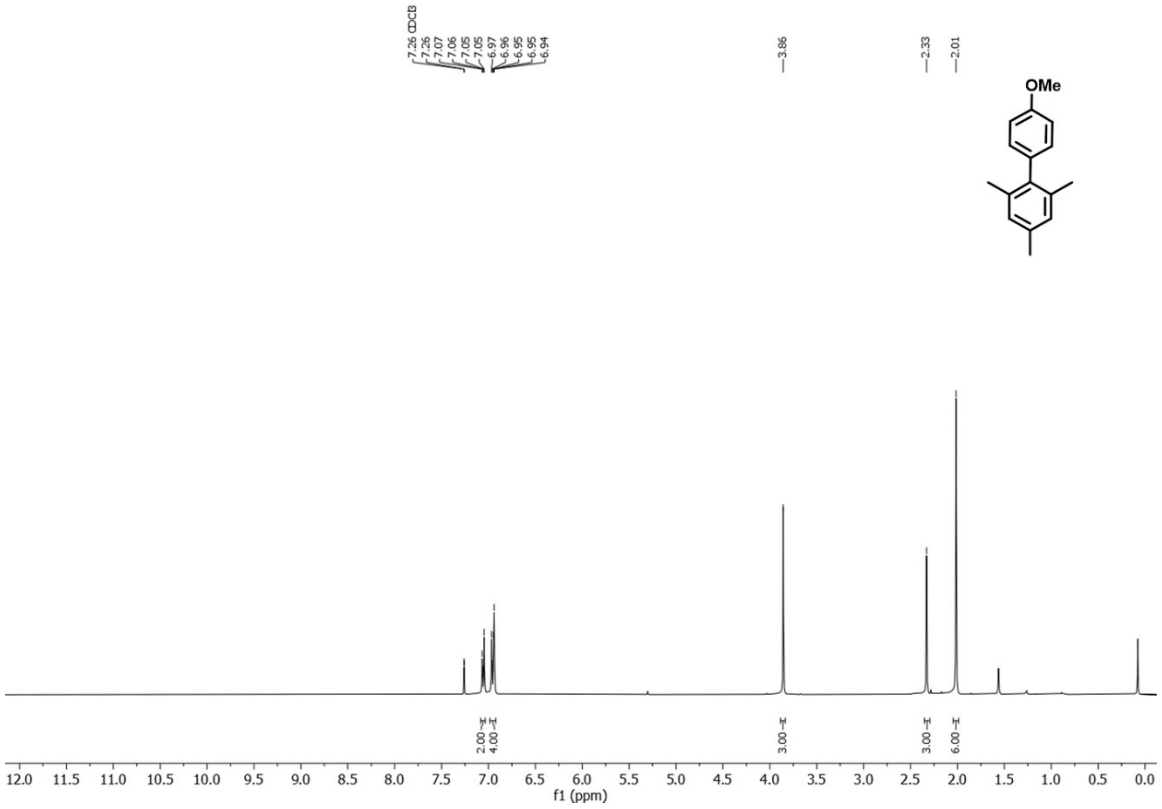


Figure S44. ^{1}H NMR spectrum (400 MHz) of **3c** in $CDCl_3$.

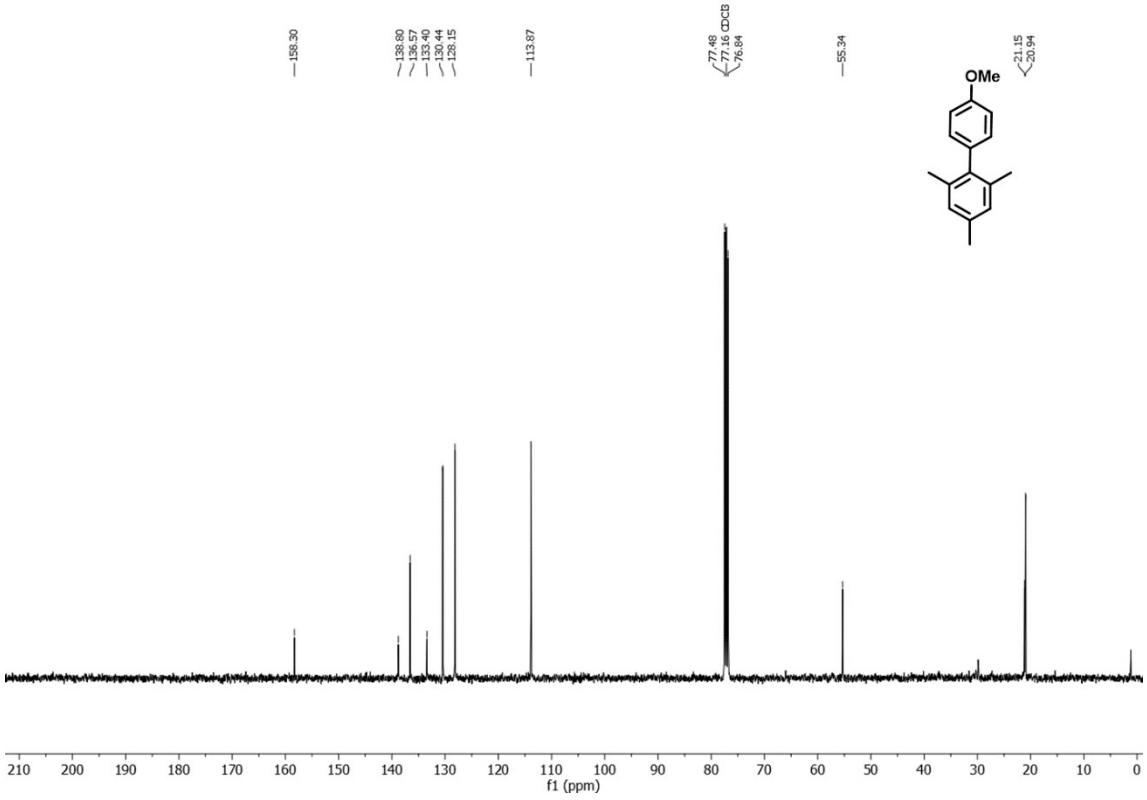


Figure S45. ^{13}C NMR spectrum (100 MHz) of **3c** in $CDCl_3$.

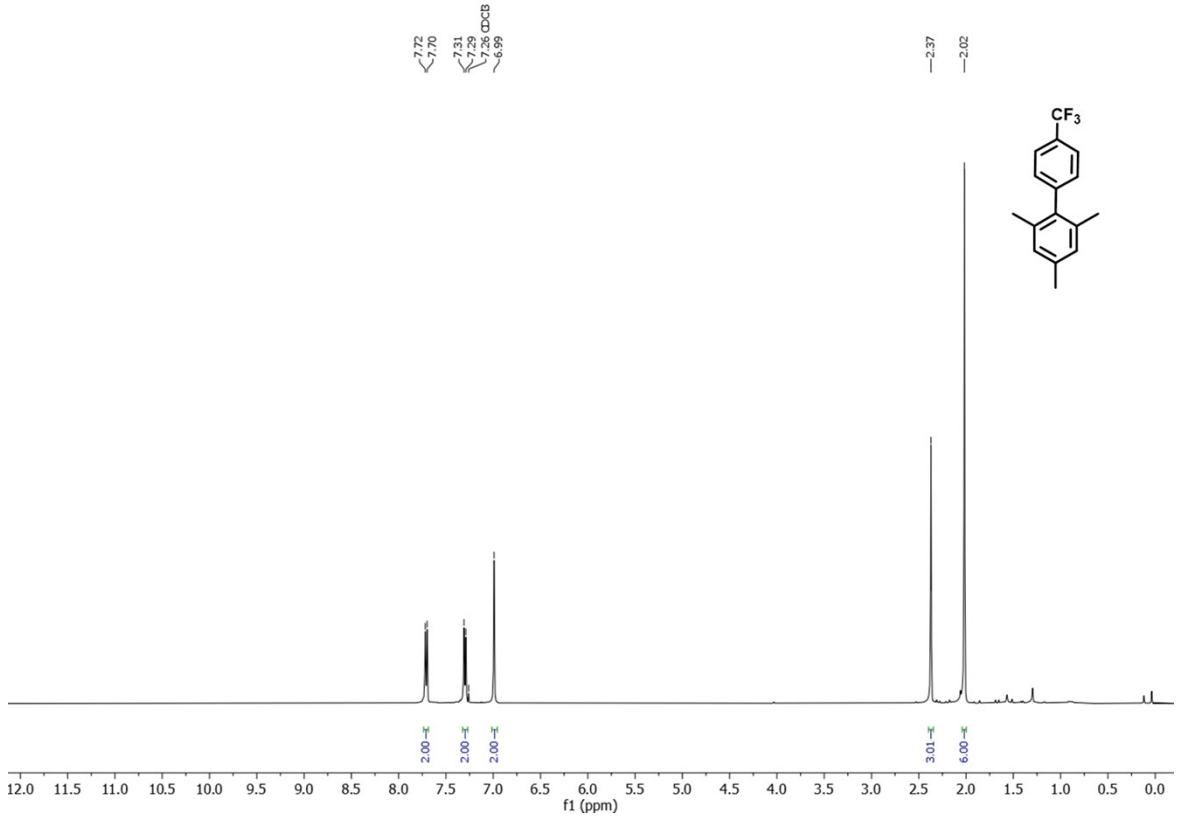


Figure S46. ^{1}H NMR spectrum (400 MHz) of **3d** in $CDCl_3$.

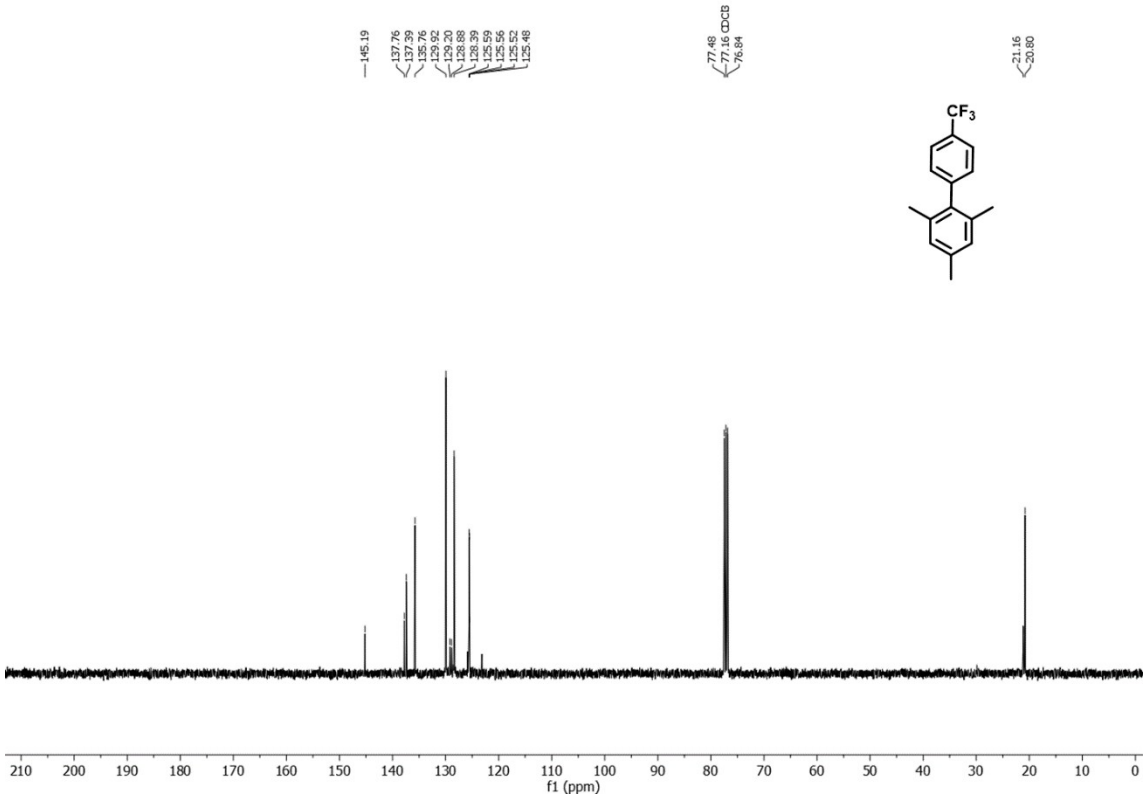


Figure S47. ^{13}C NMR spectrum (100 MHz) of **3d** in $CDCl_3$.

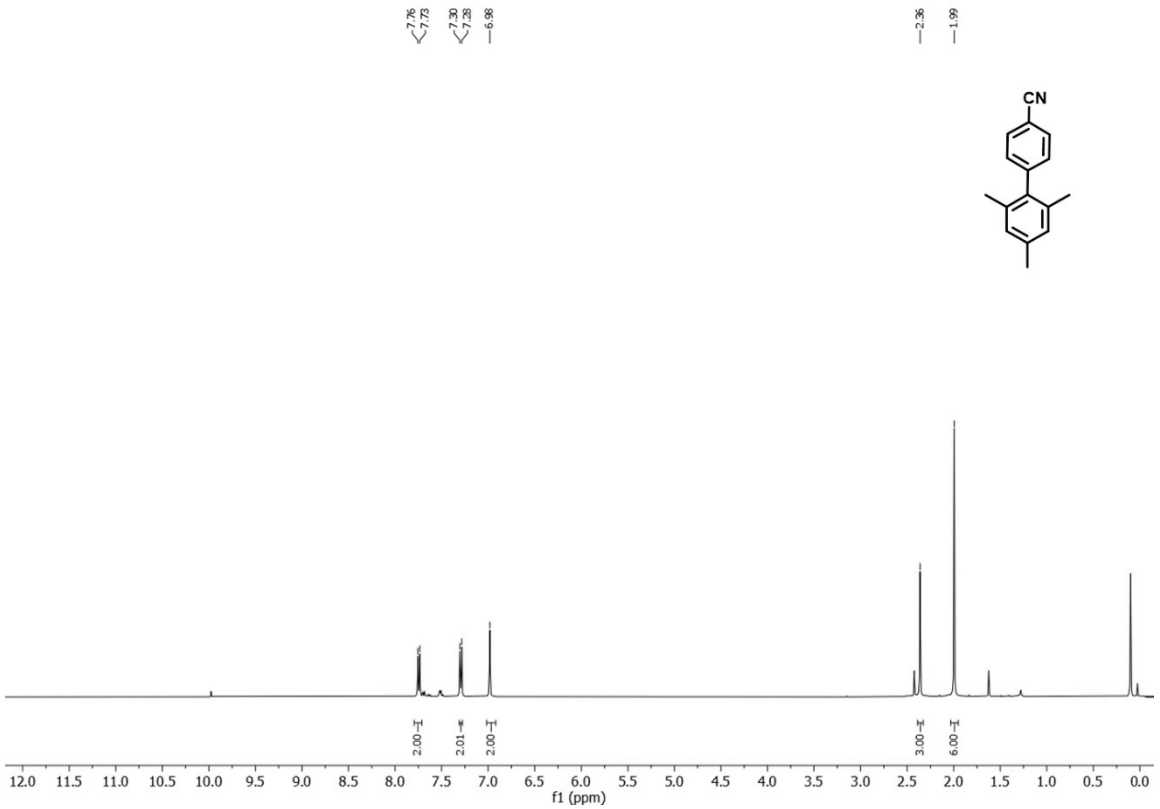


Figure S48. ^{1}H NMR spectrum (400 MHz) of **3e** in $CDCl_3$.

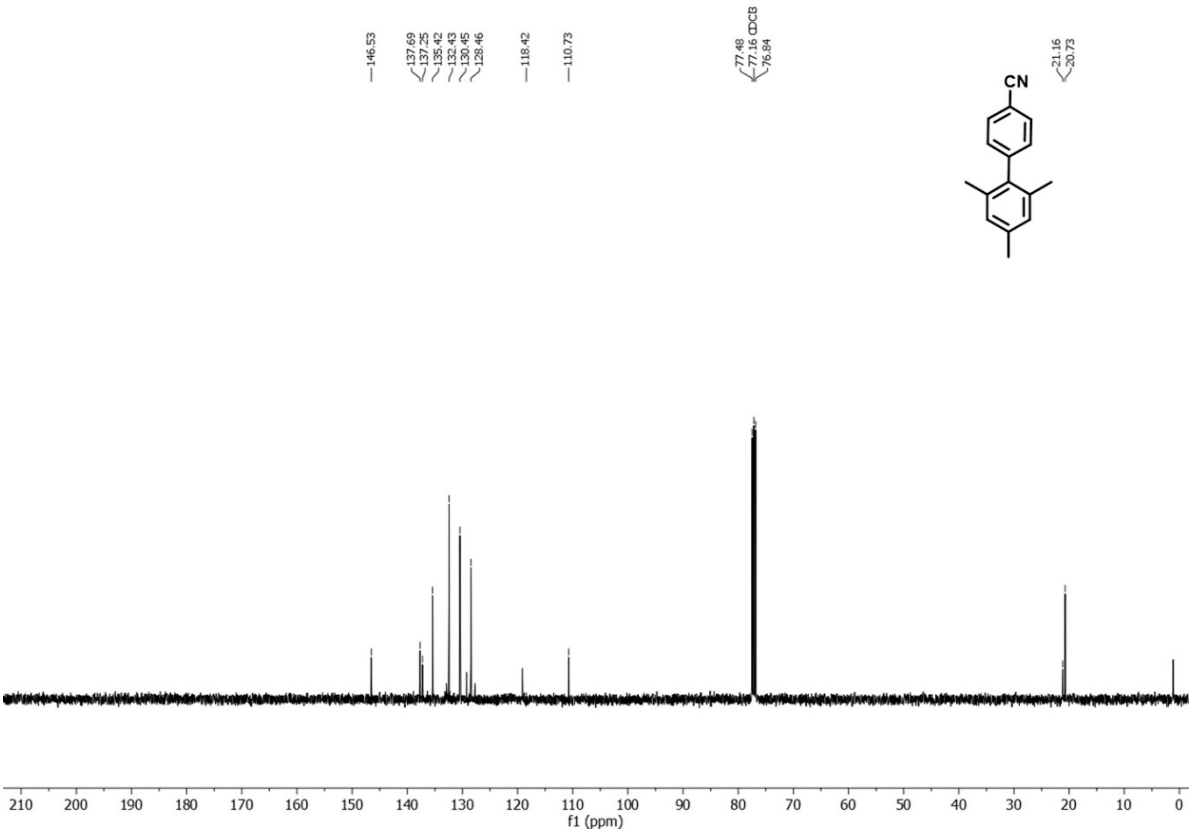


Figure S49. ^{13}C NMR spectrum (100 MHz) of **3e** in $CDCl_3$.

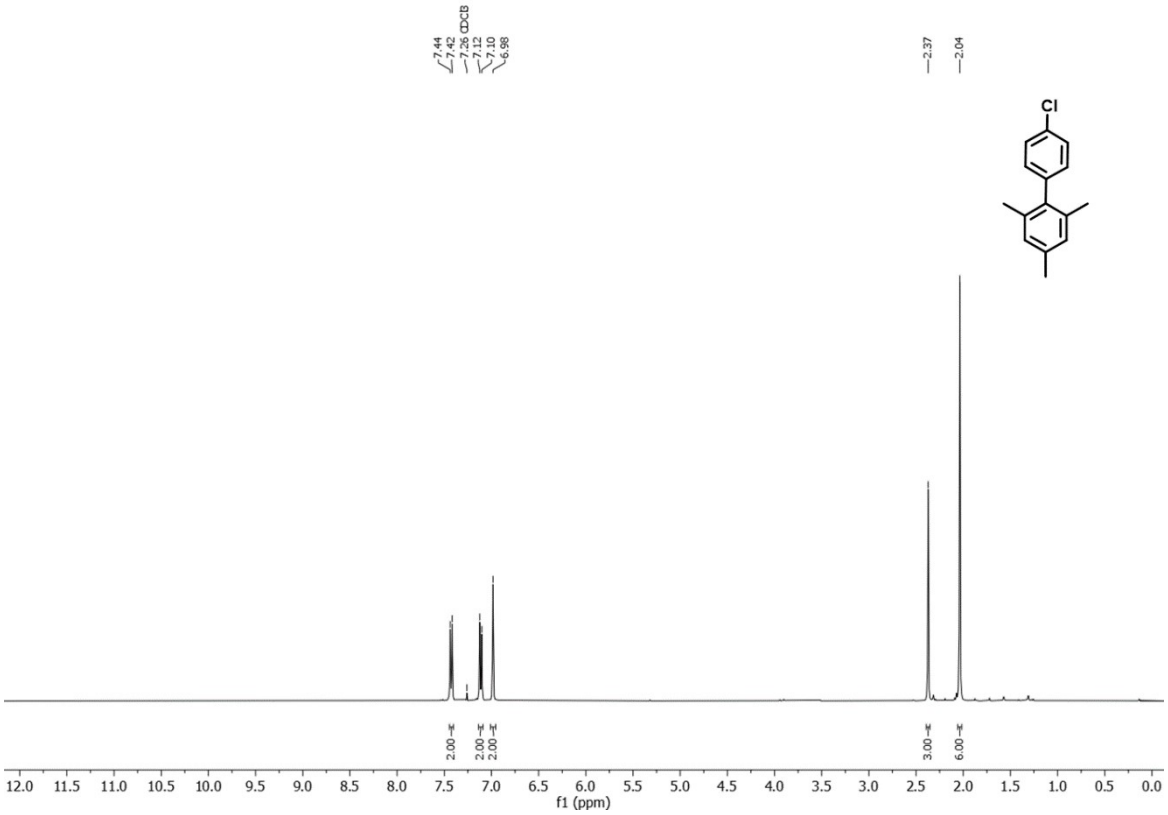


Figure S50. ^{1}H NMR spectrum (400 MHz) of **3f** in $CDCl_3$.

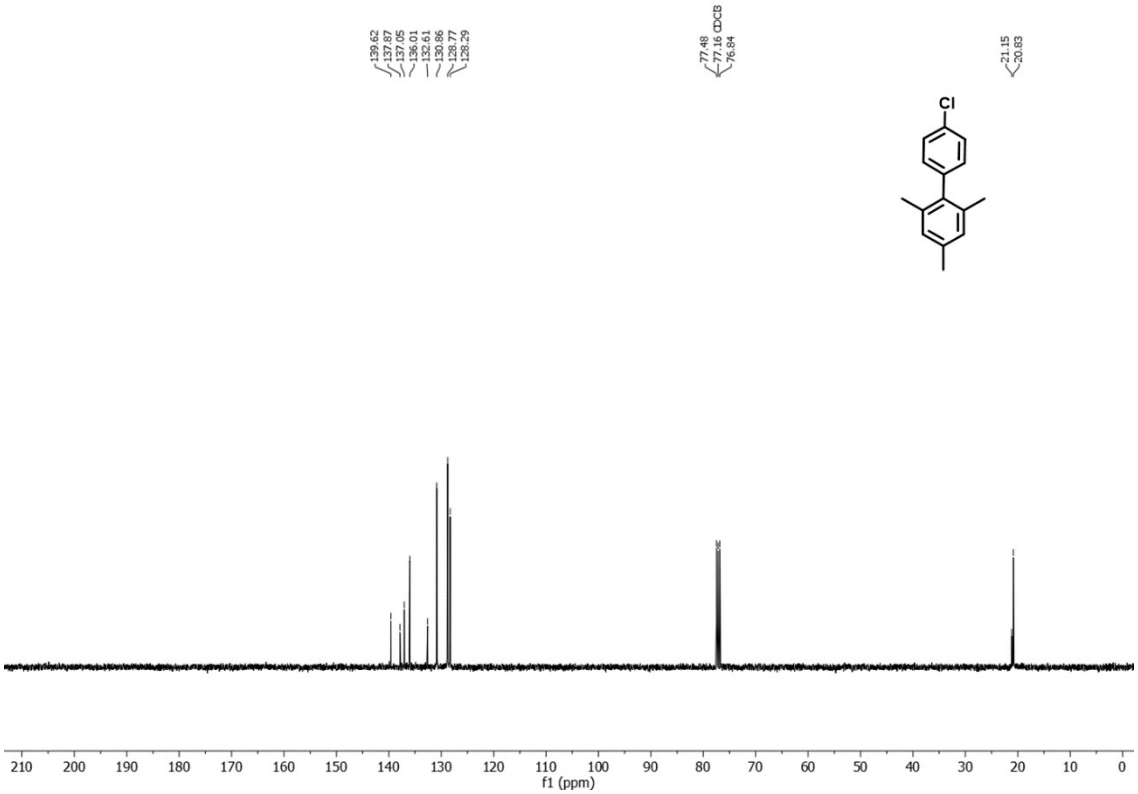


Figure S51. ^{13}C NMR spectrum (100 MHz) of **3f** in $CDCl_3$.

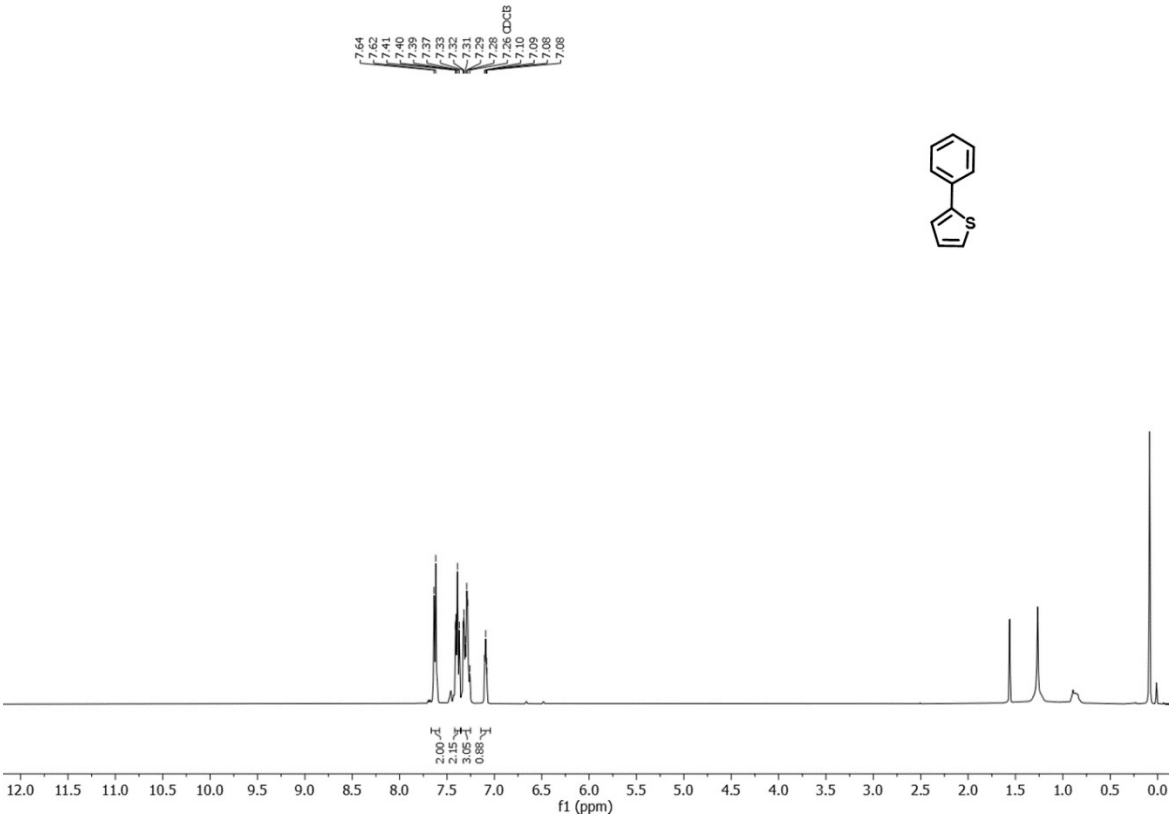


Figure S52. ^{1}H NMR spectrum (400 MHz) of **4a** in $CDCl_3$.

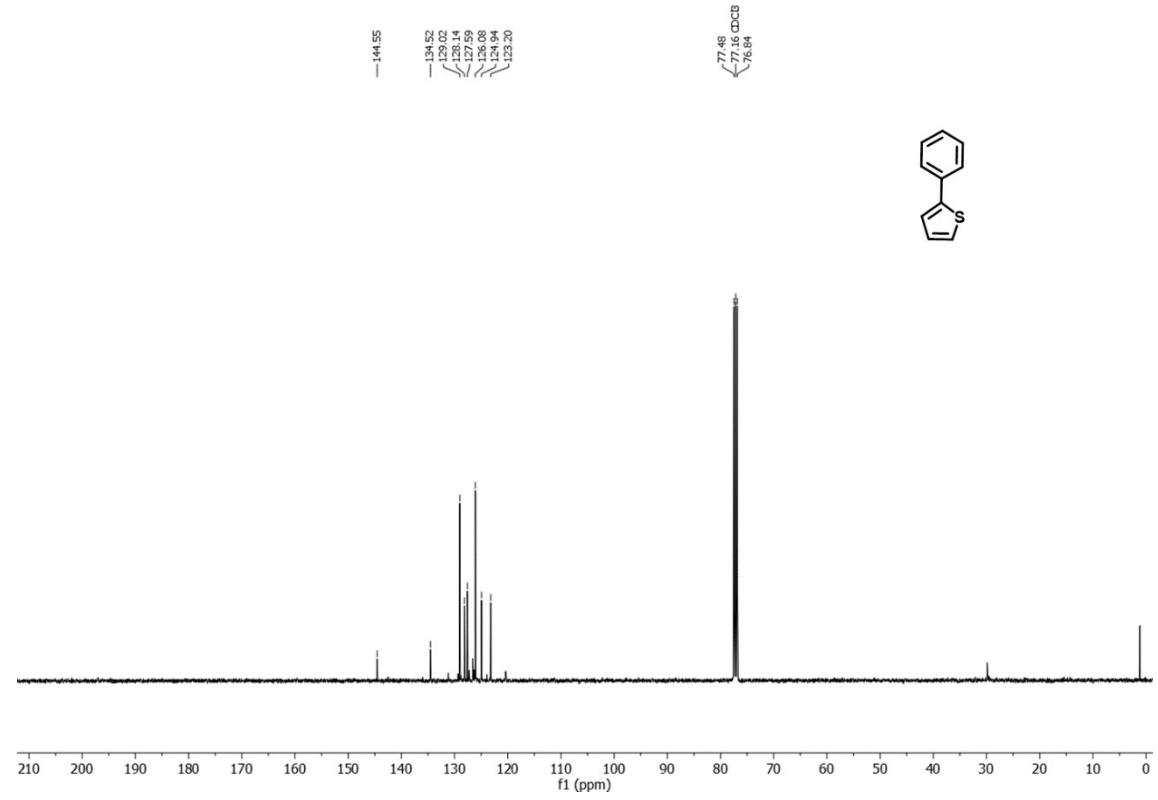


Figure S53. ^{13}C NMR spectrum (100 MHz) of **4a** in $CDCl_3$.

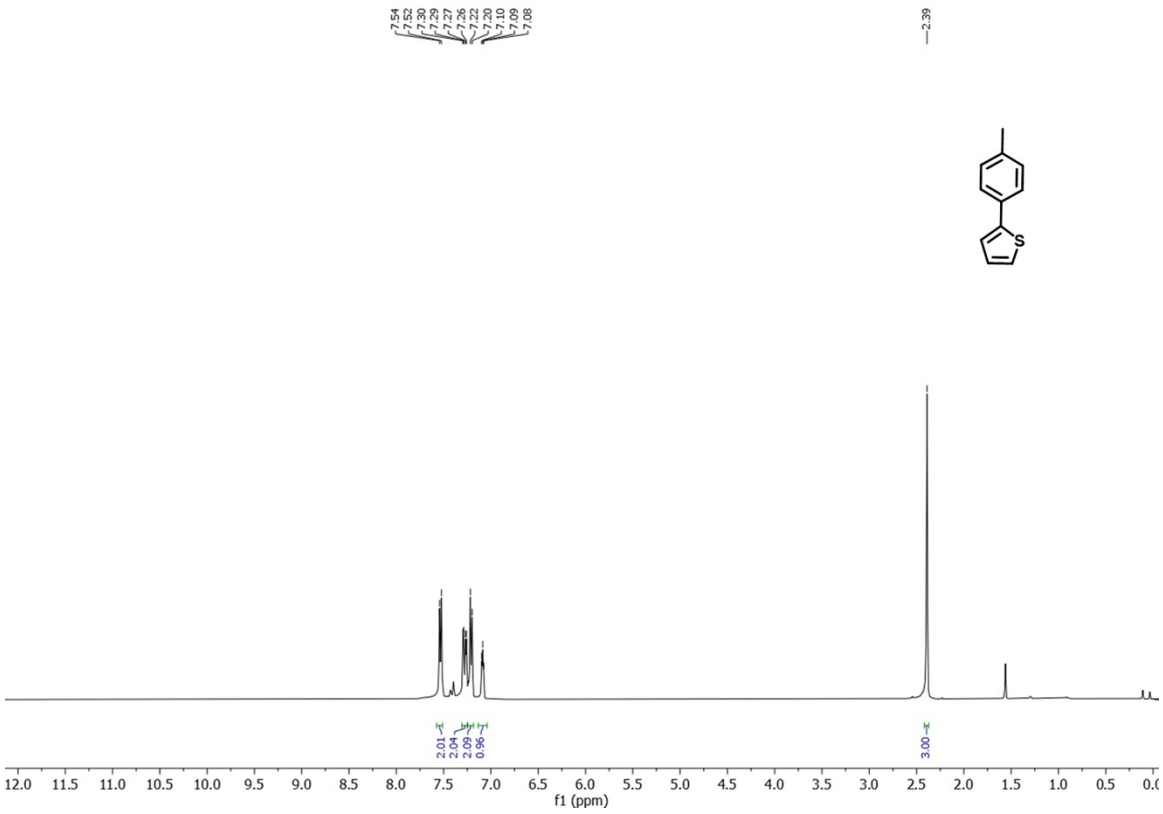


Figure S54. ^{1}H NMR spectrum (400 MHz) of **4b** in $CDCl_3$.

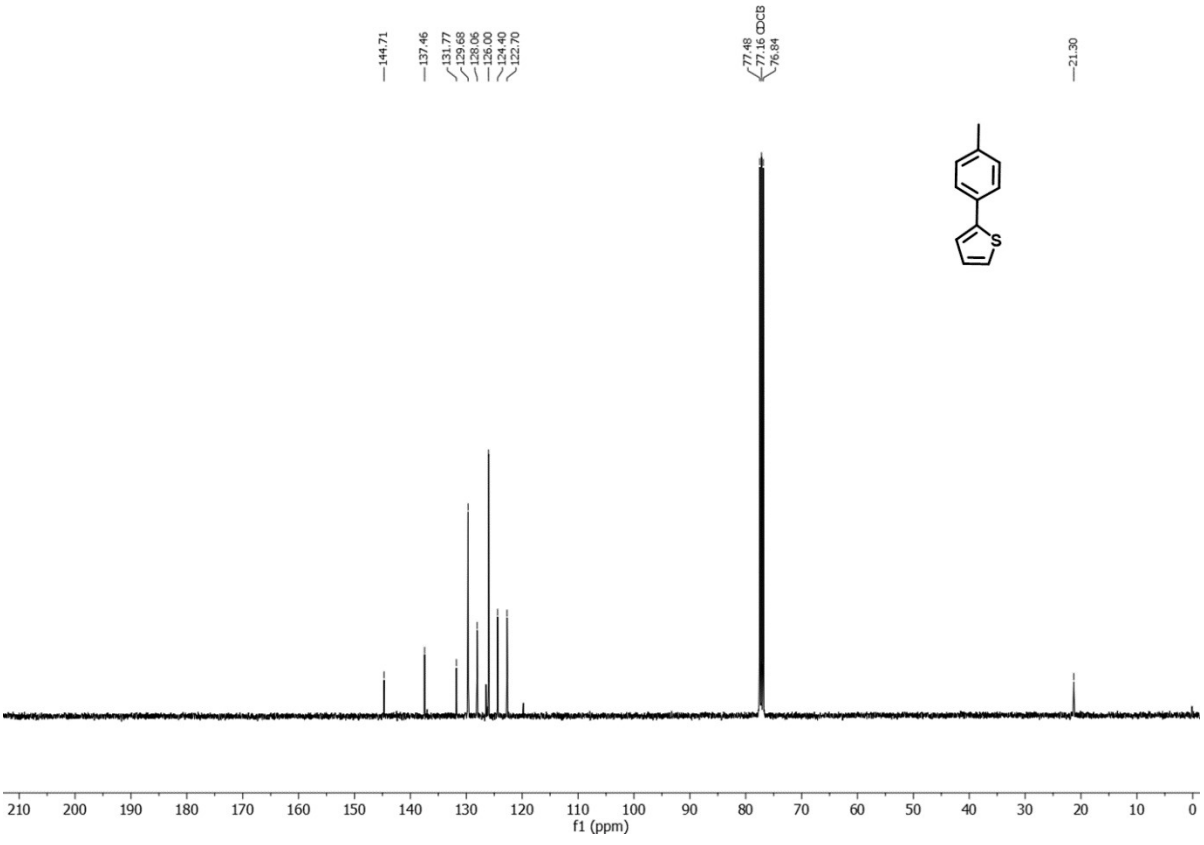


Figure S55. ^{13}C NMR spectrum (100 MHz) of **4b** in $CDCl_3$.

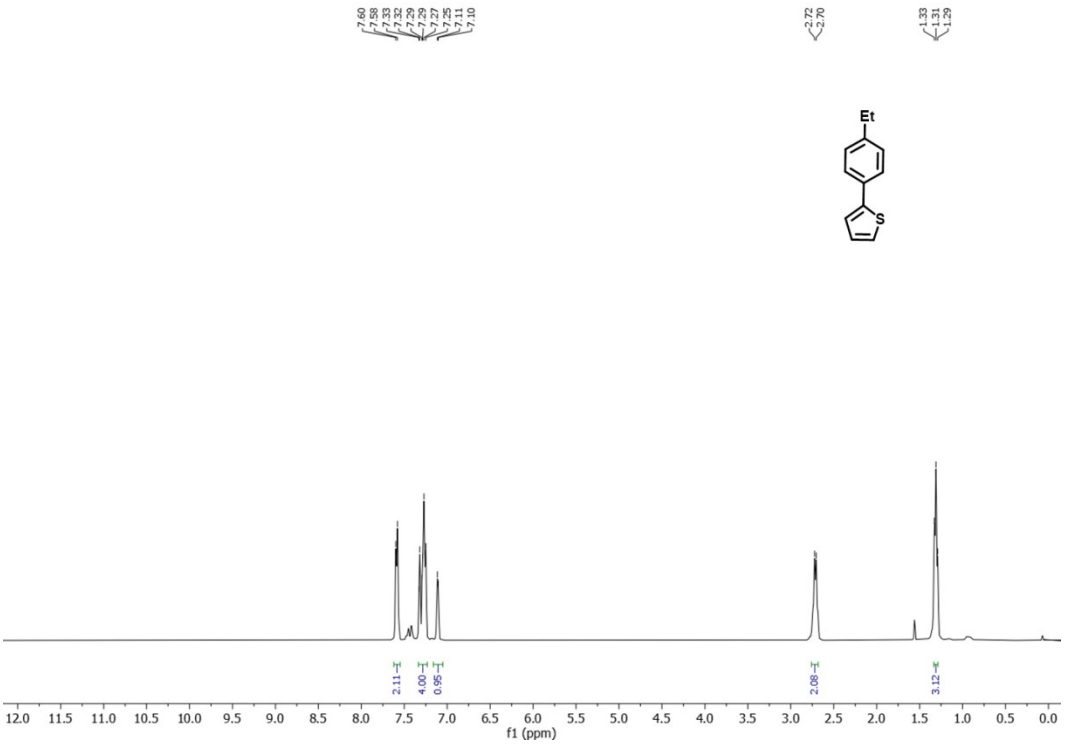


Figure S56. ^{1}H NMR spectrum (400 MHz) of **4c** in $CDCl_3$.

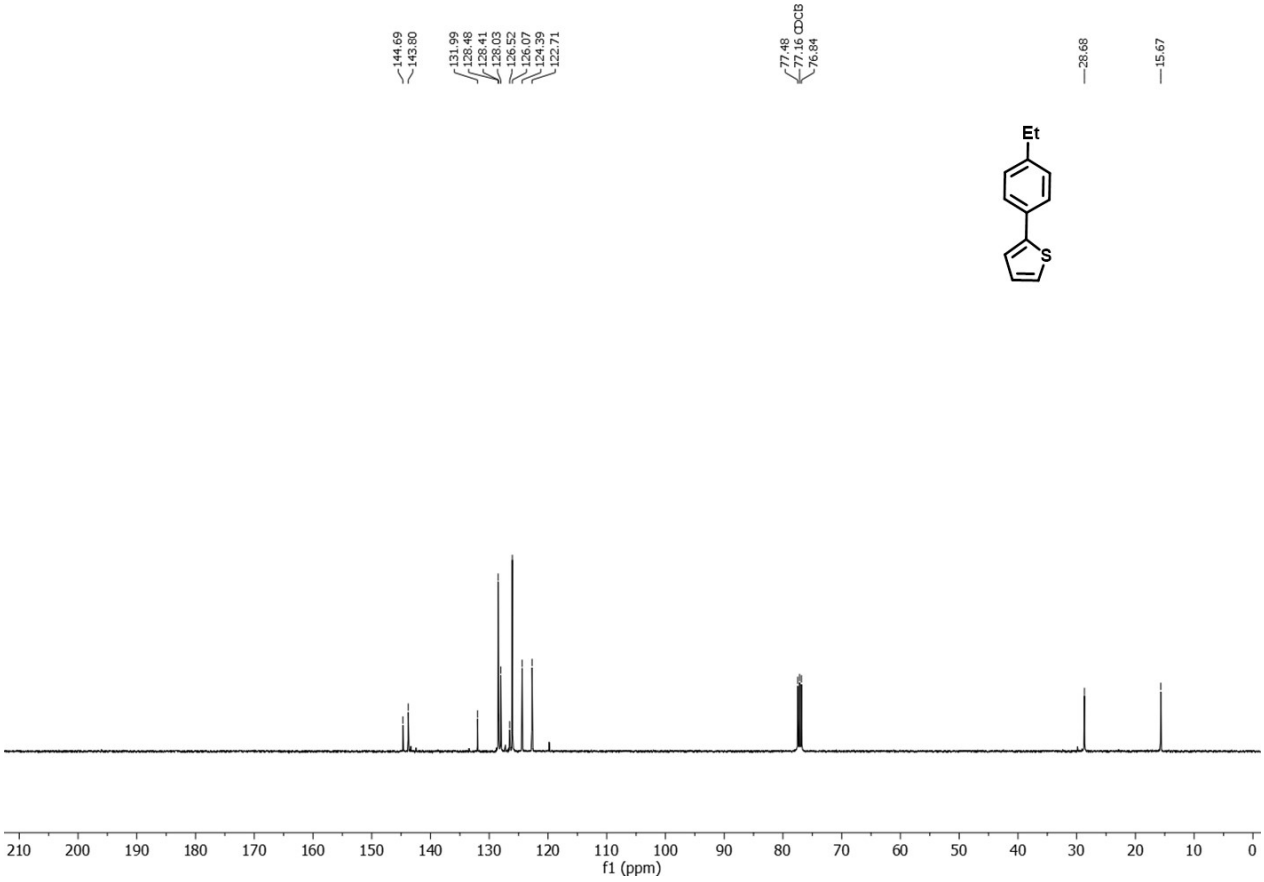


Figure S57. ^{13}C NMR spectrum (100 MHz) of **4c** in $CDCl_3$.

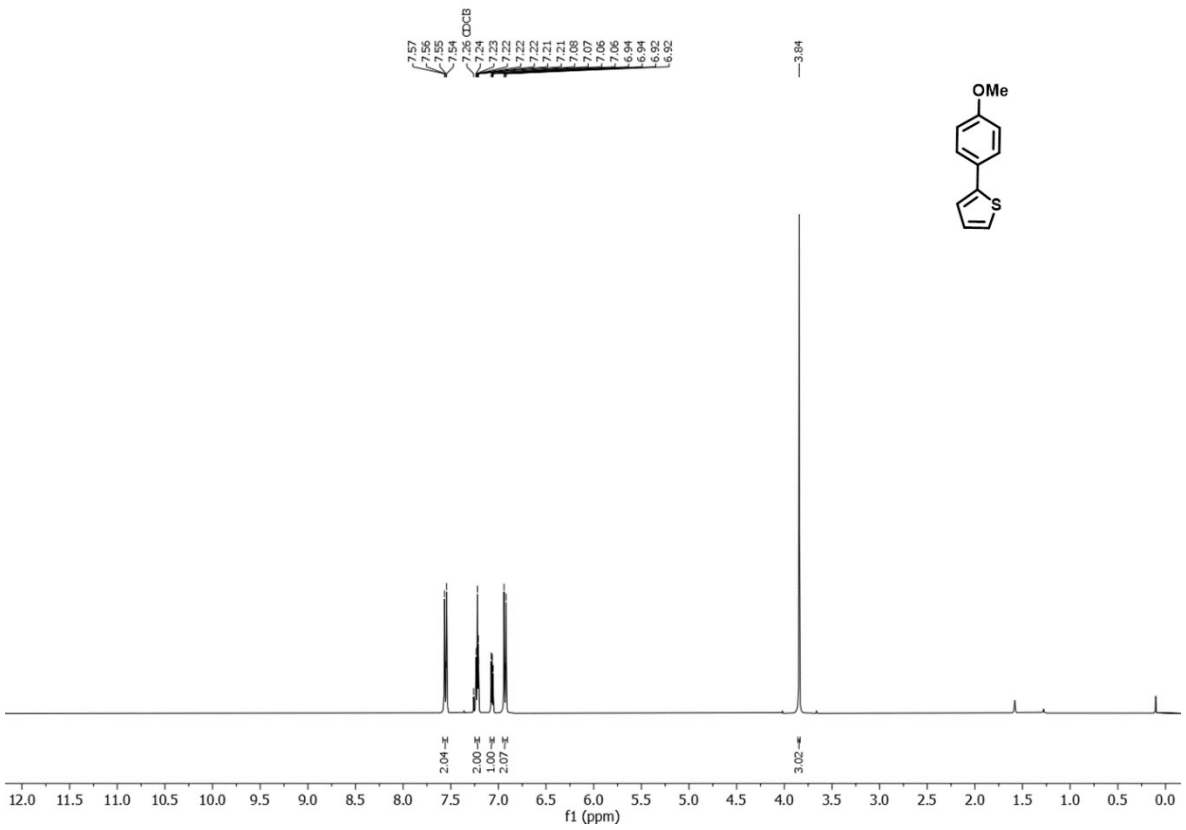


Figure S58. ^{1}H NMR spectrum (400 MHz) of **4d** in $CDCl_3$.

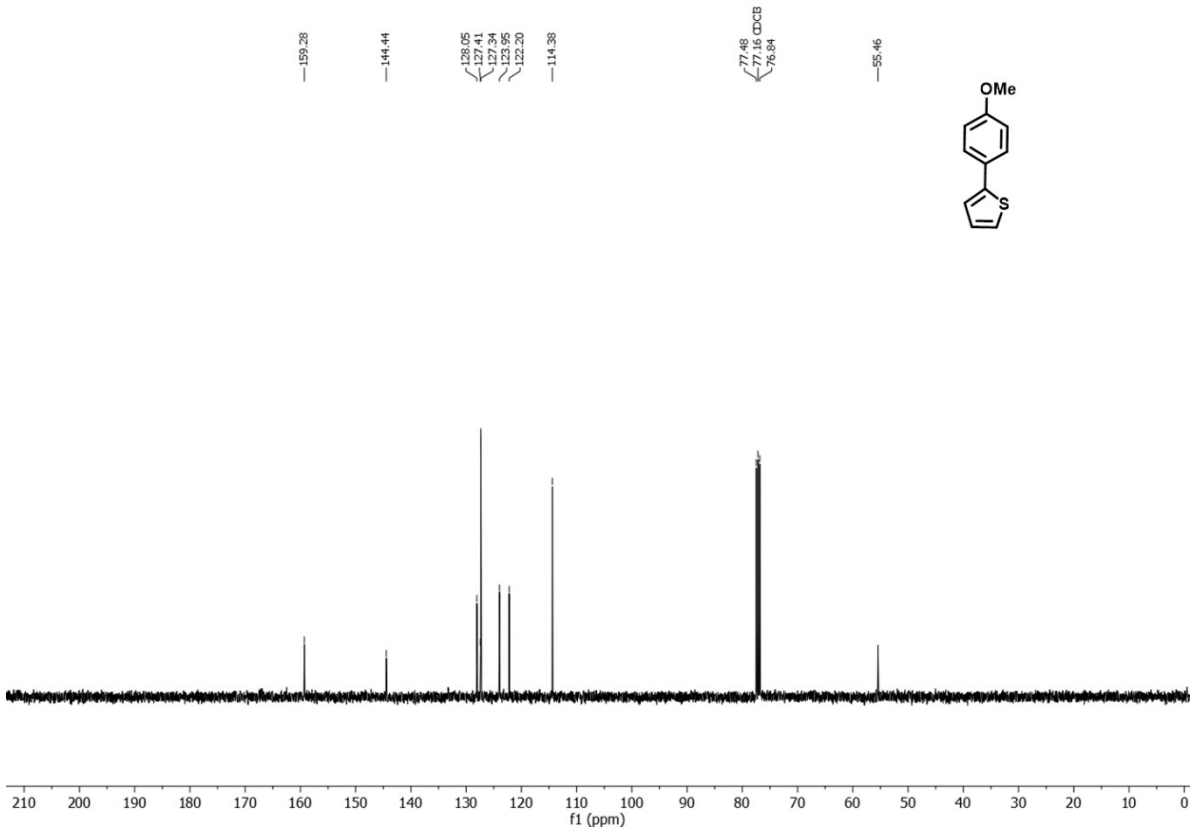


Figure S59. ^{13}C NMR spectrum (100 MHz) of **4d** in $CDCl_3$.

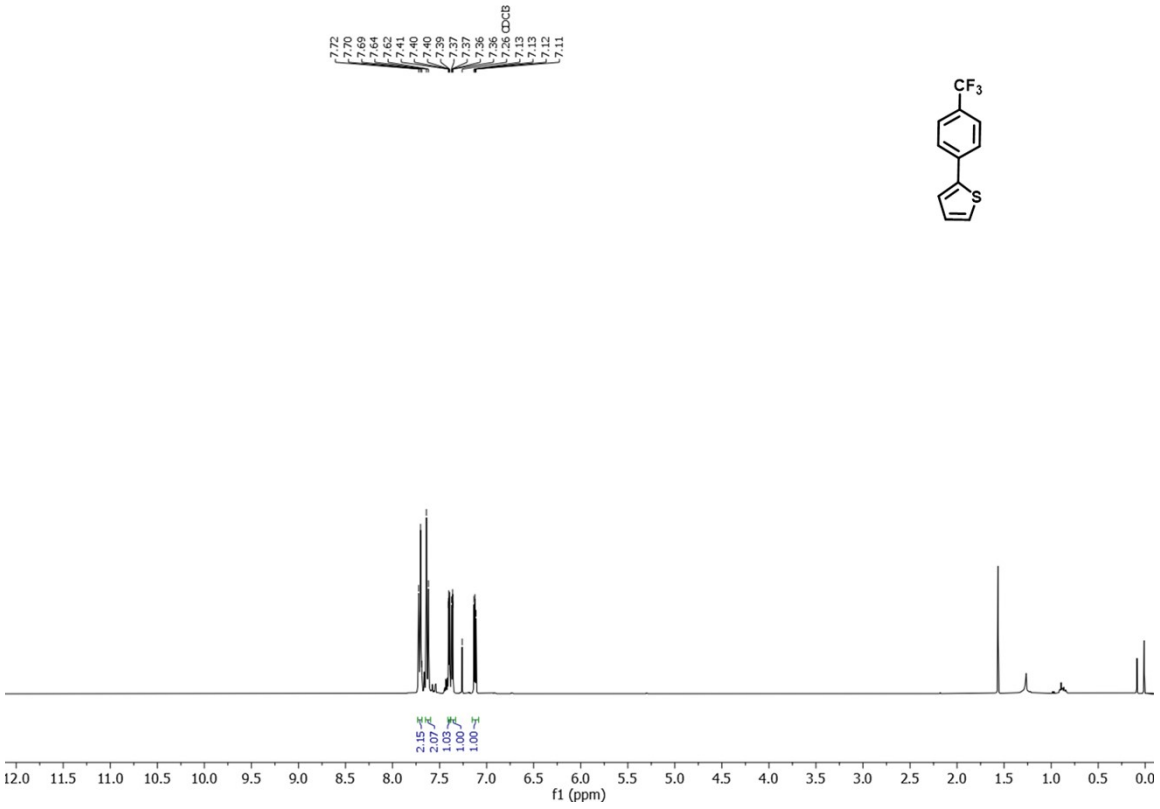


Figure S60. ^{1}H NMR spectrum (400 MHz) of **4e** in $CDCl_3$.

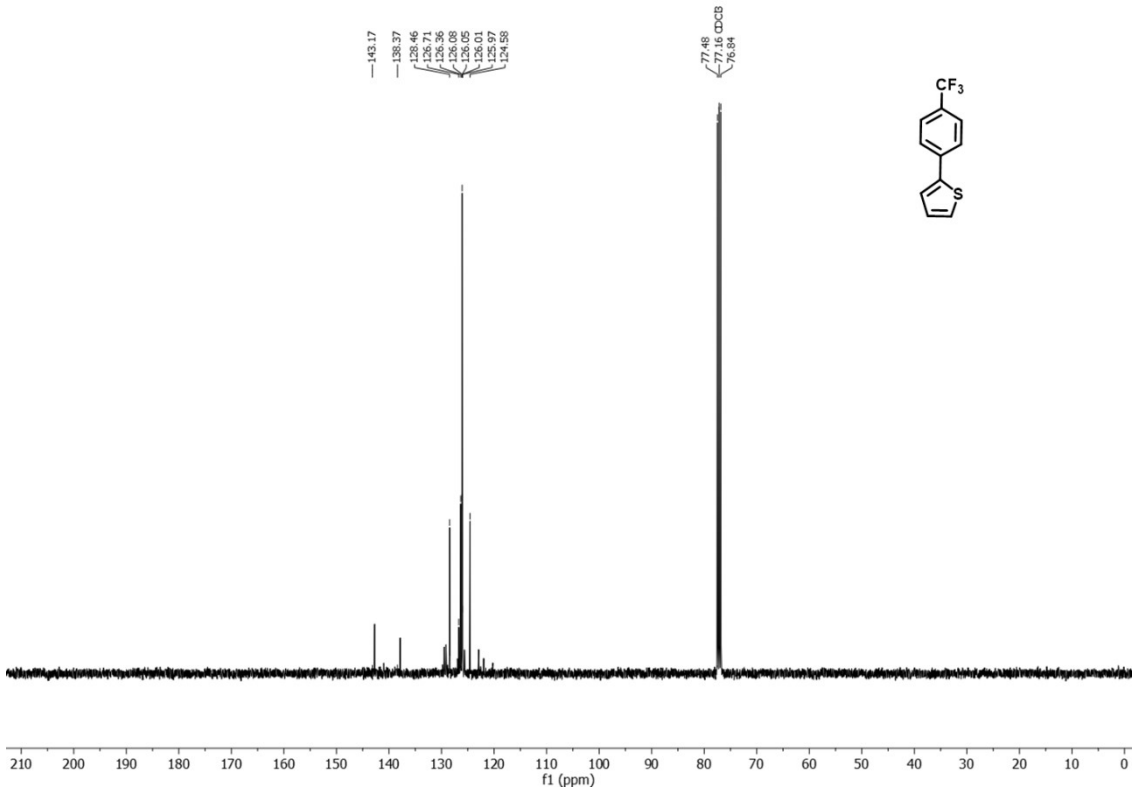


Figure S61. ^{13}C NMR spectrum (100 MHz) of **4e** in $CDCl_3$.

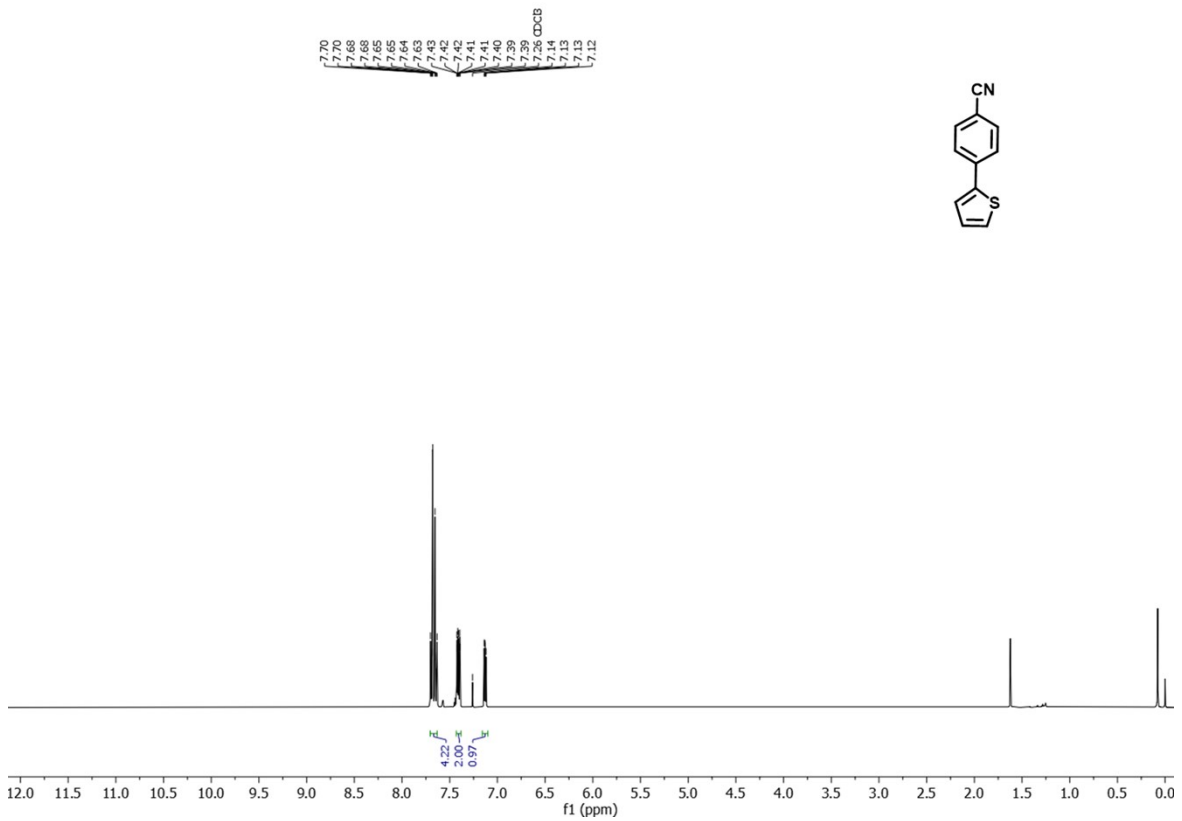


Figure S62. ^{1}H NMR spectrum (400 MHz) of **4f** in $CDCl_3$.

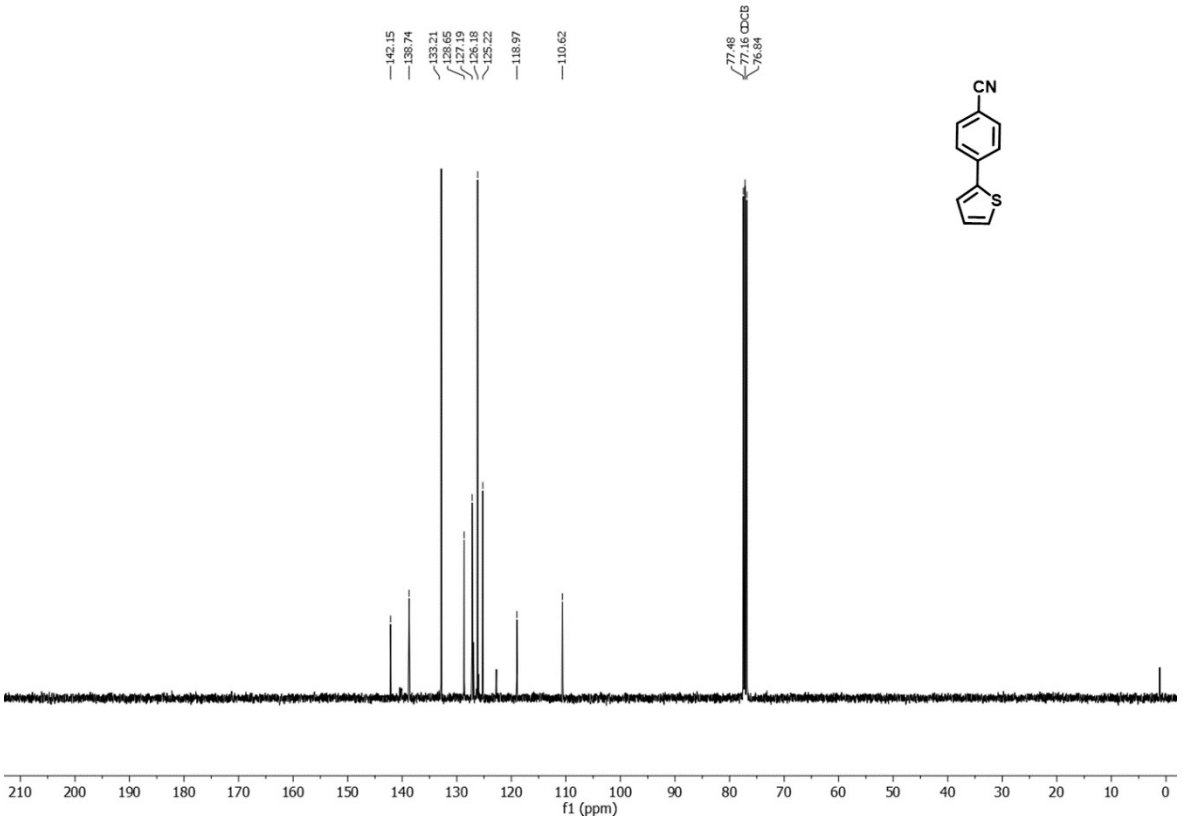


Figure S63. ^{13}C NMR spectrum (100 MHz) of **4f** in $CDCl_3$.

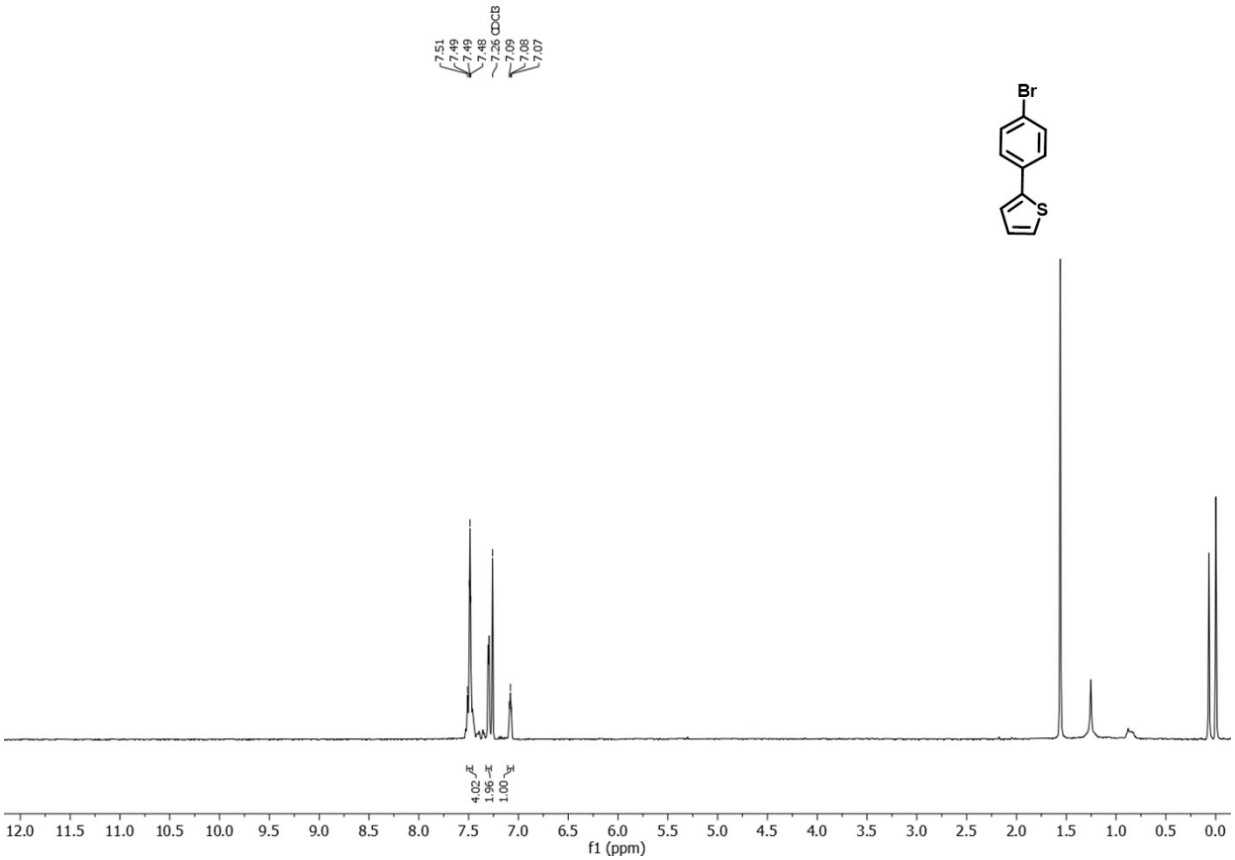


Figure S64. ^{1}H NMR spectrum (400 MHz) of **4g** in $CDCl_3$.

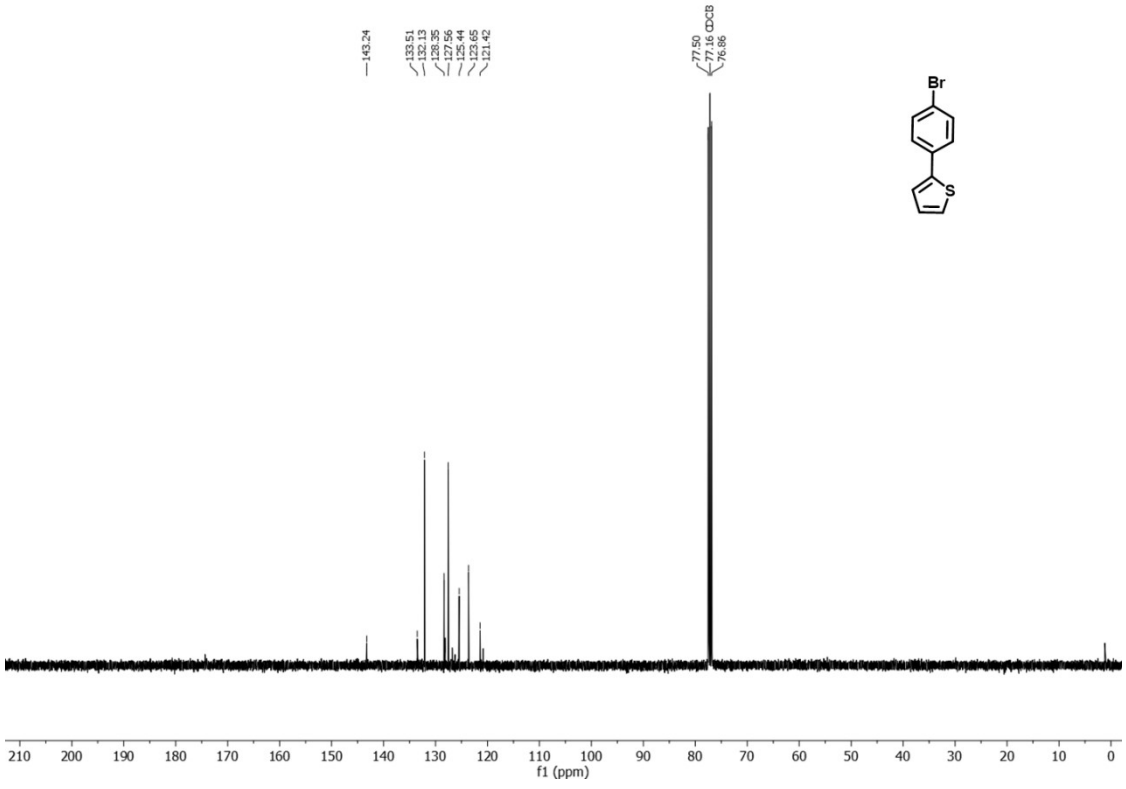


Figure S65. ^{13}C NMR spectrum (100 MHz) of **4g** in $CDCl_3$.

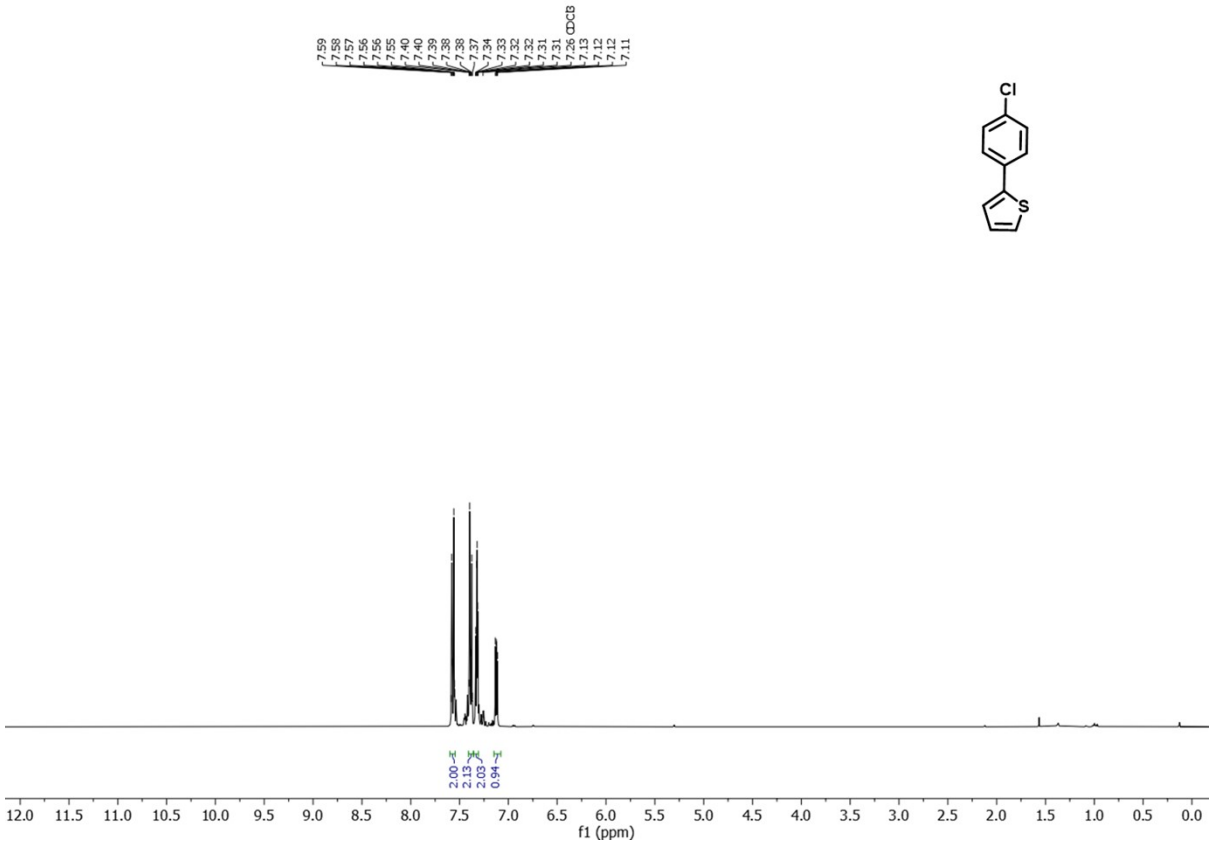


Figure S66. ^{1}H NMR spectrum (400 MHz) of **4h** in $CDCl_3$.

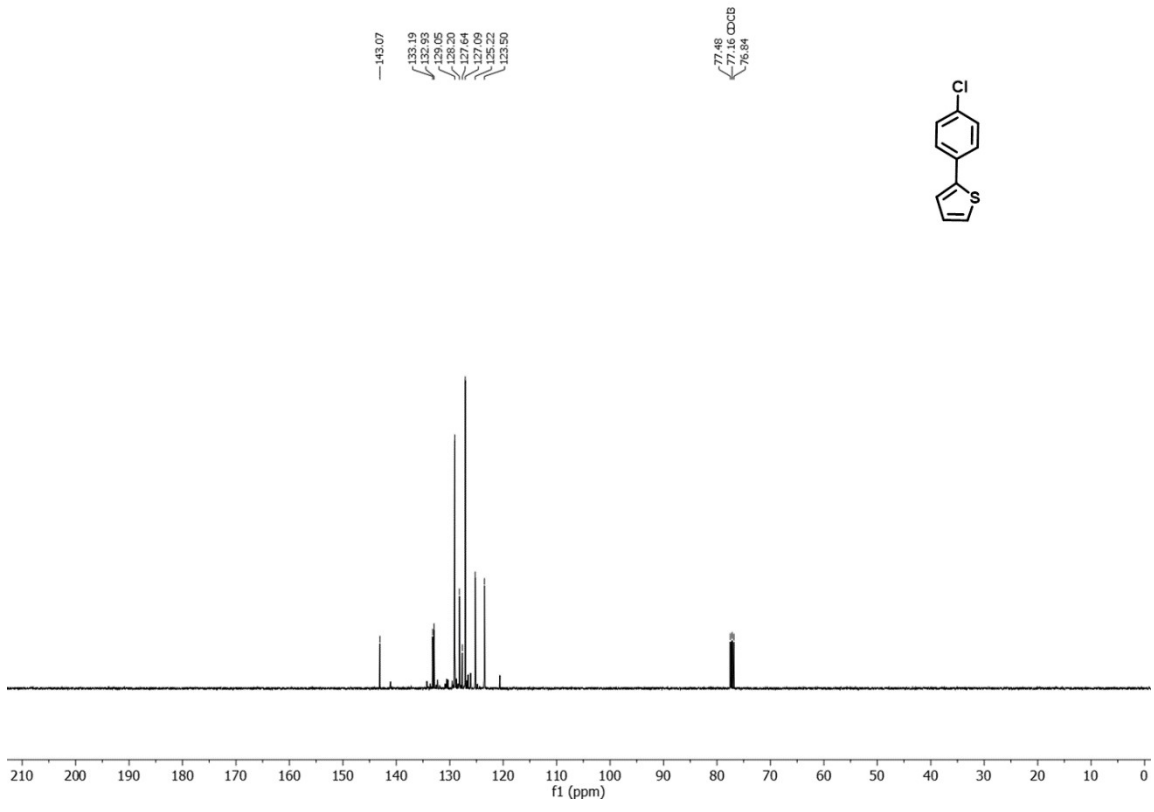


Figure S67. ^{13}C NMR spectrum (100 MHz) of **4h** in $CDCl_3$.

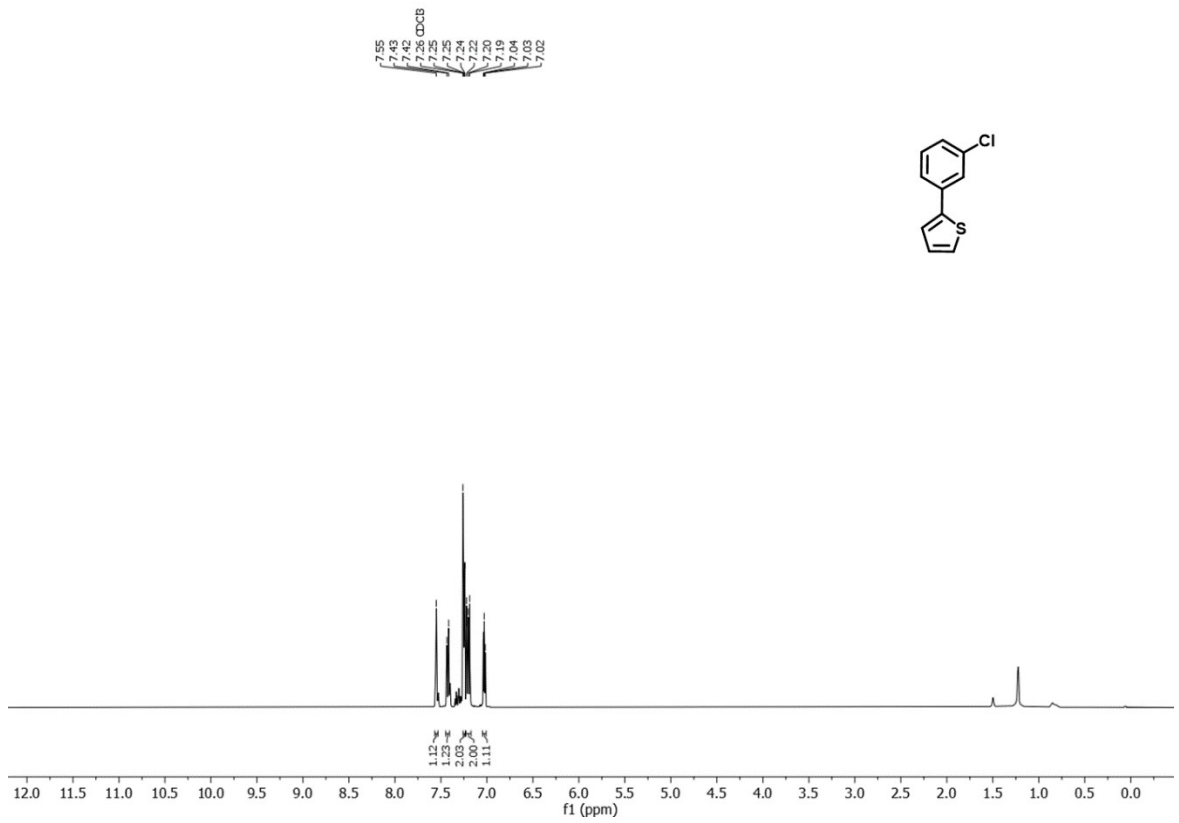


Figure S68. ^{1}H NMR spectrum (400 MHz) of **4i** in $CDCl_3$.

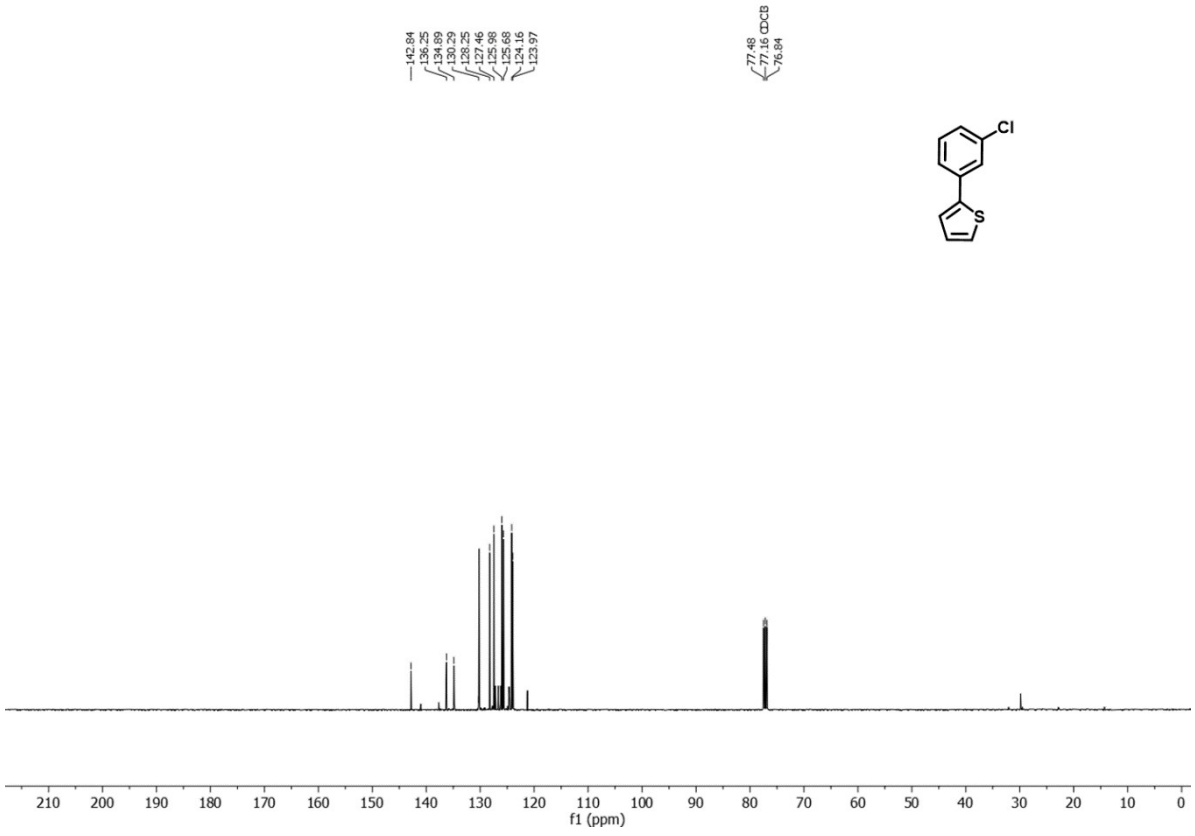


Figure S69. ^{13}C NMR spectrum (100 MHz) of **4i** in $CDCl_3$.

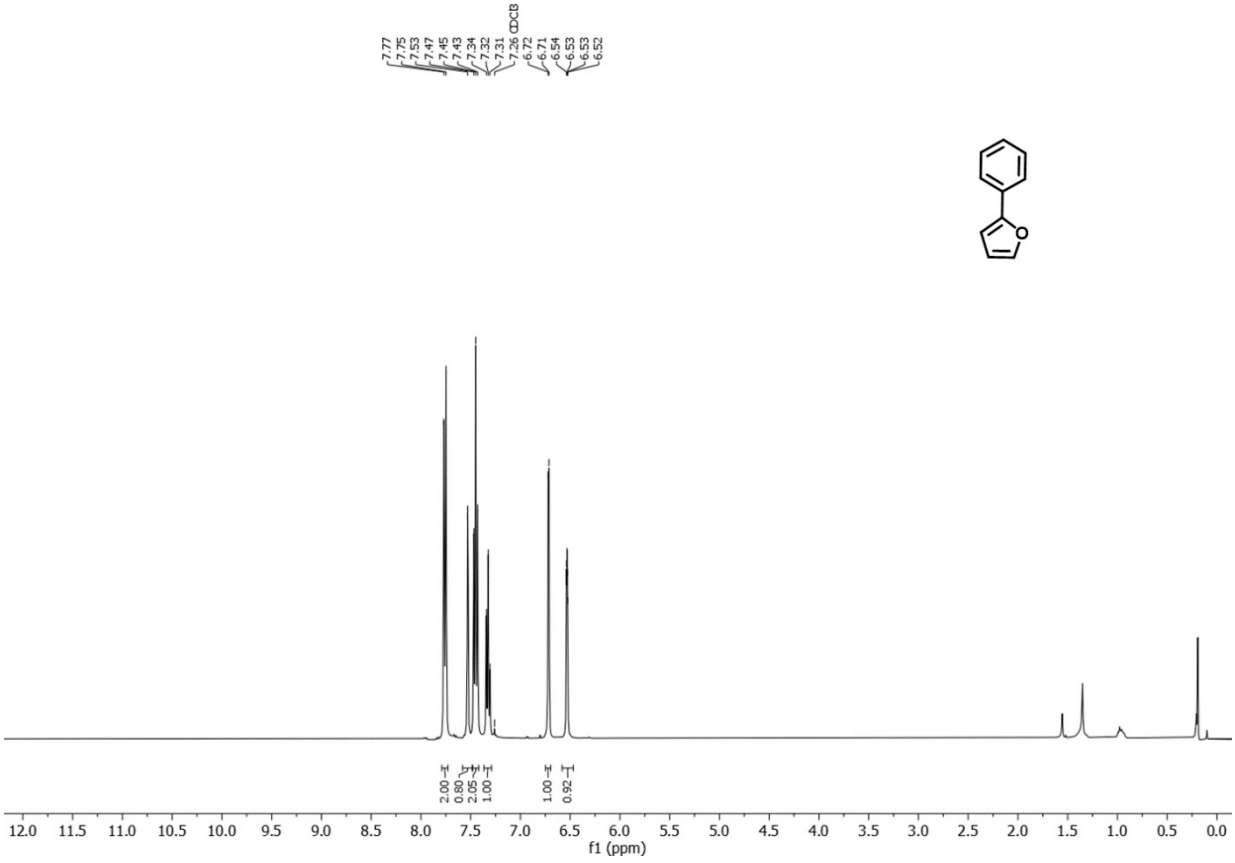


Figure S70. ^{1}H NMR spectrum (400 MHz) of **5a** in $CDCl_3$.

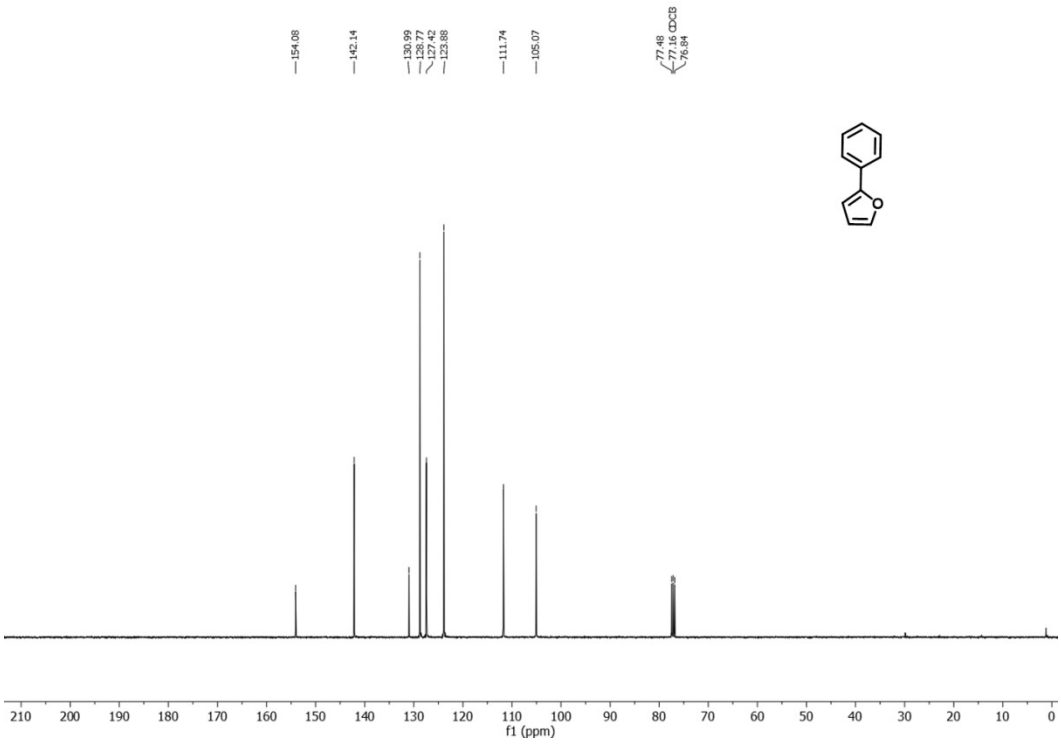


Figure S71. ^{13}C NMR spectrum (100 MHz) of **5a** in $CDCl_3$.

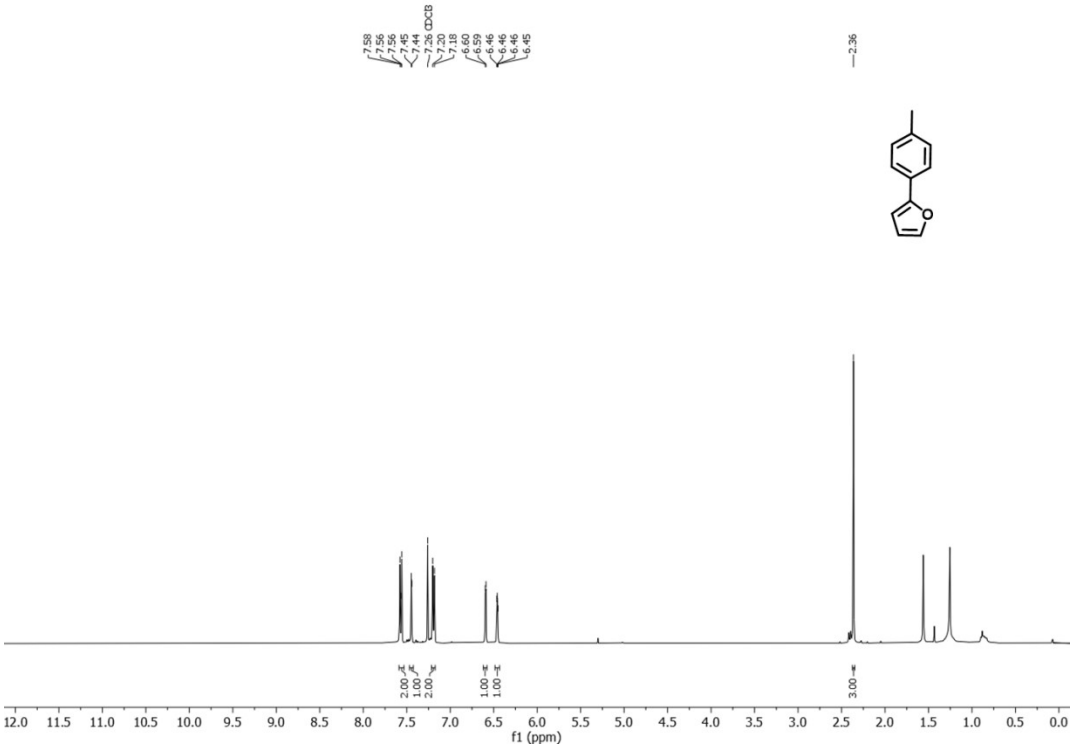


Figure S72. ^{1}H NMR spectrum (400 MHz) of **5b** in $CDCl_3$.

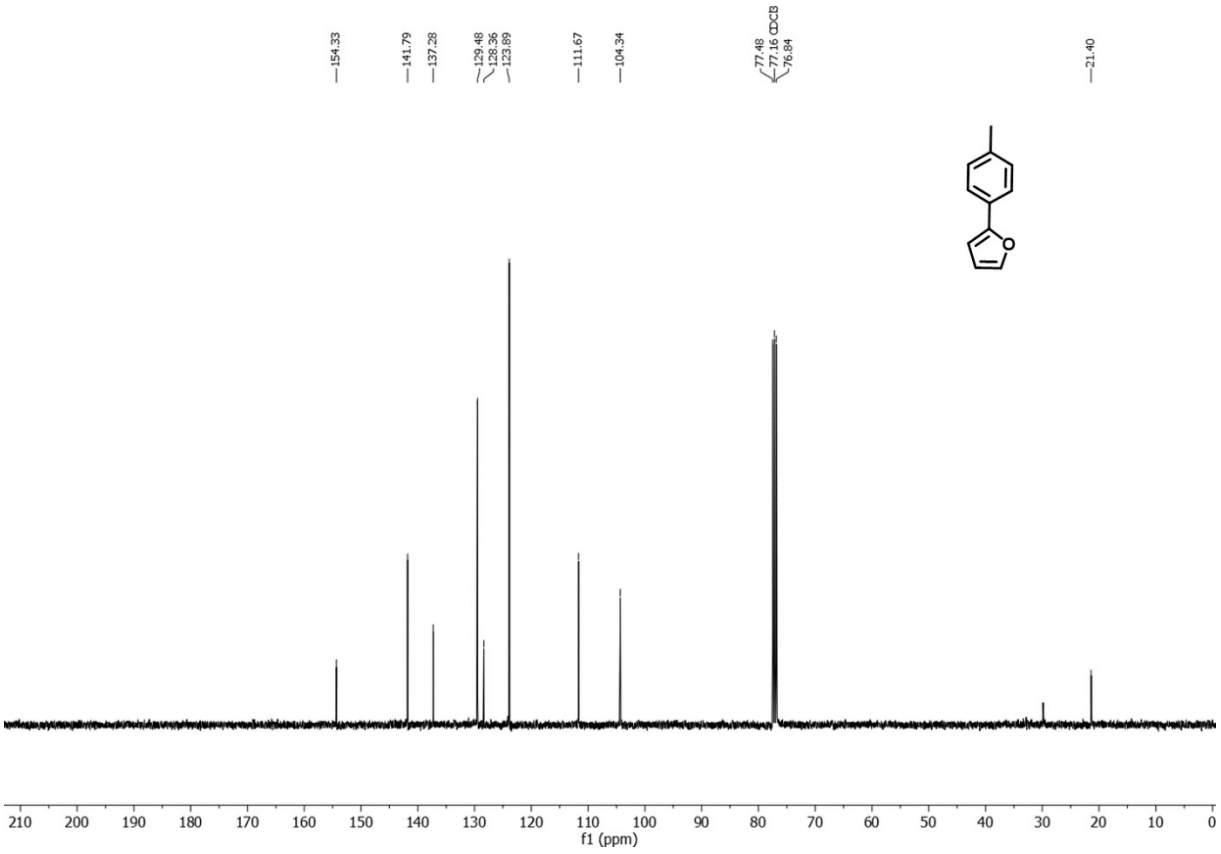


Figure S73. ^{13}C NMR spectrum (100 MHz) of **5b** in $CDCl_3$.

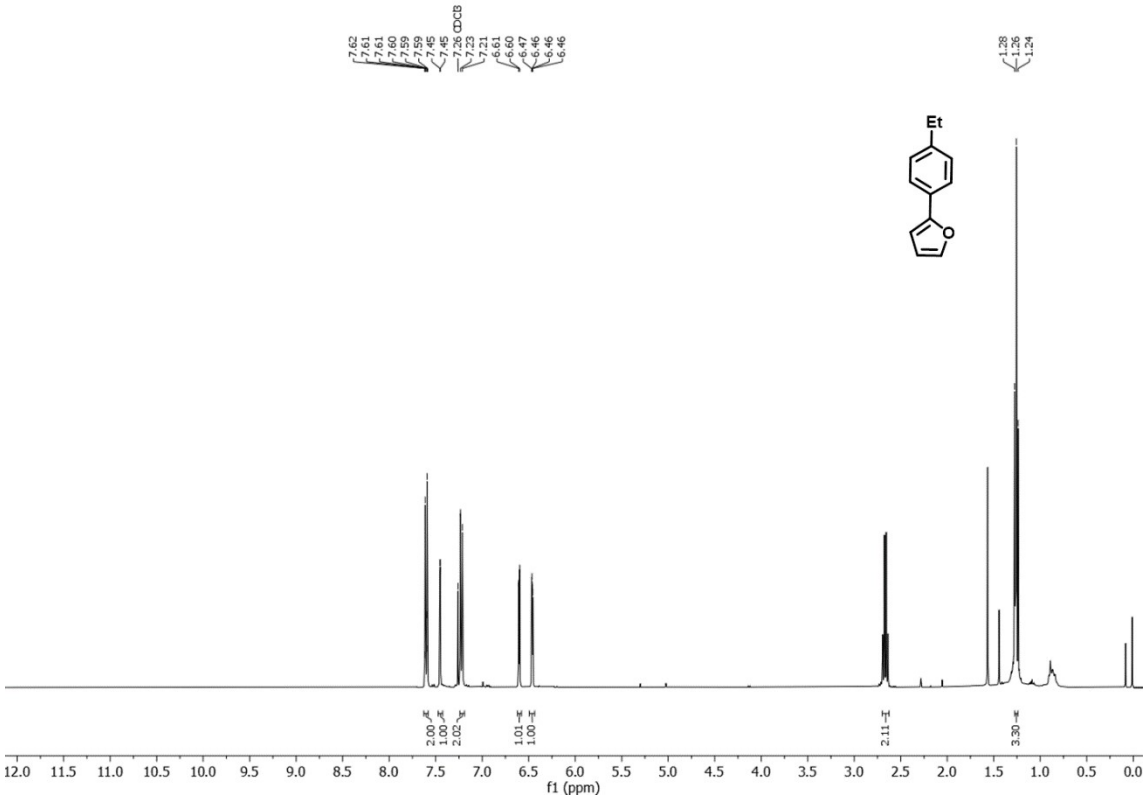


Figure S74. ^{1}H NMR spectrum (400 MHz) of **5c** in $CDCl_3$.

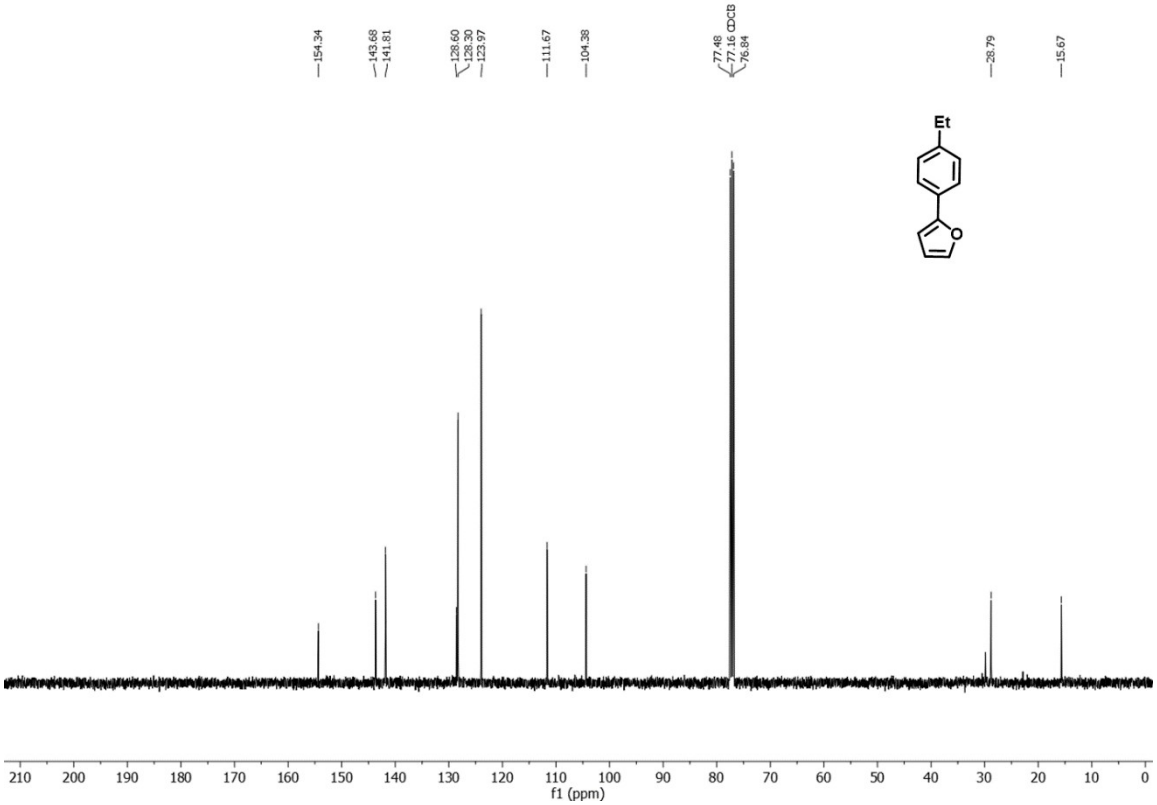


Figure S75. ^{13}C NMR spectrum (100 MHz) of **5c** in $CDCl_3$.

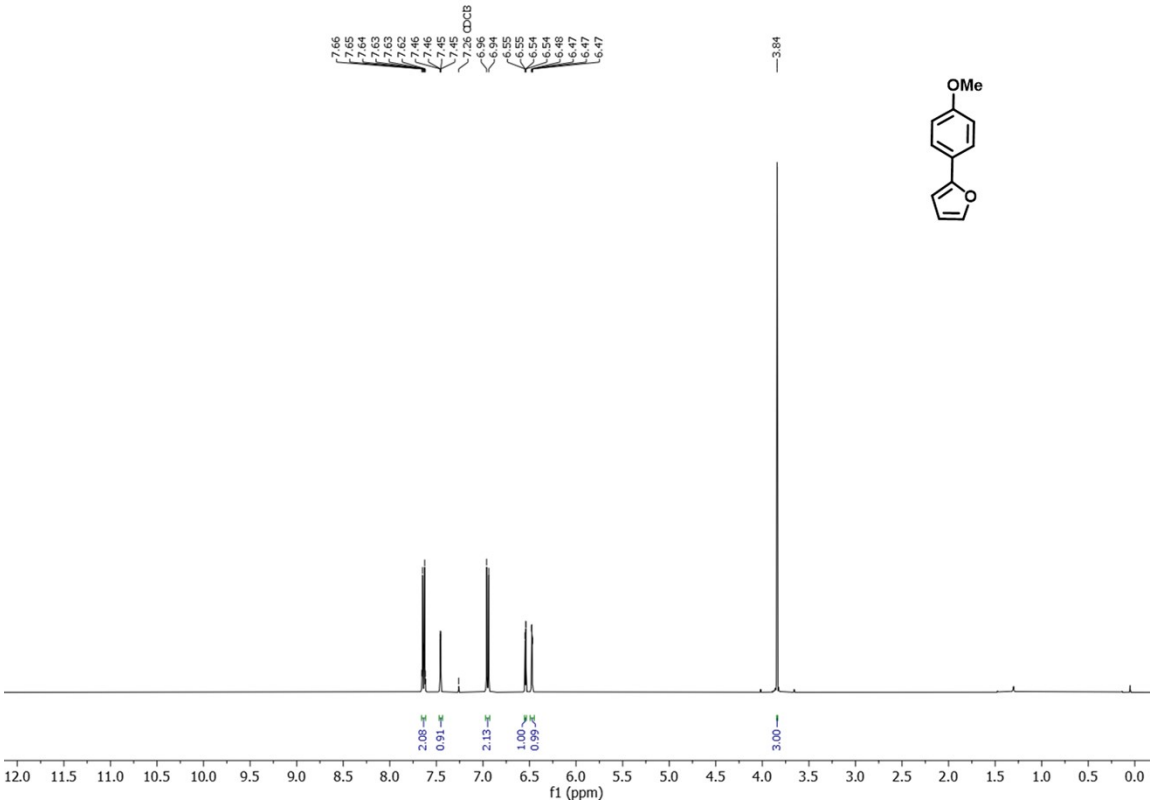


Figure S76. ^{1}H NMR spectrum (400 MHz) of **5d** in $CDCl_3$.

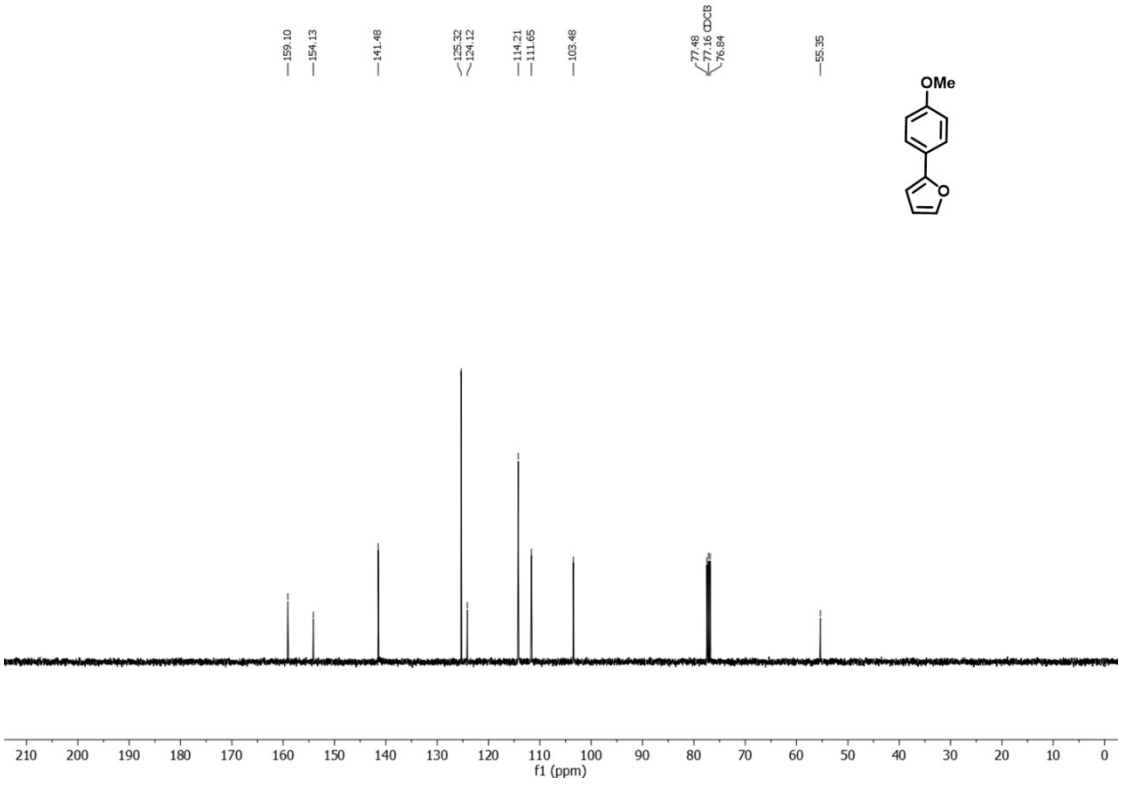


Figure S77. ^{13}C NMR spectrum (100 MHz) of **5d** in $CDCl_3$.

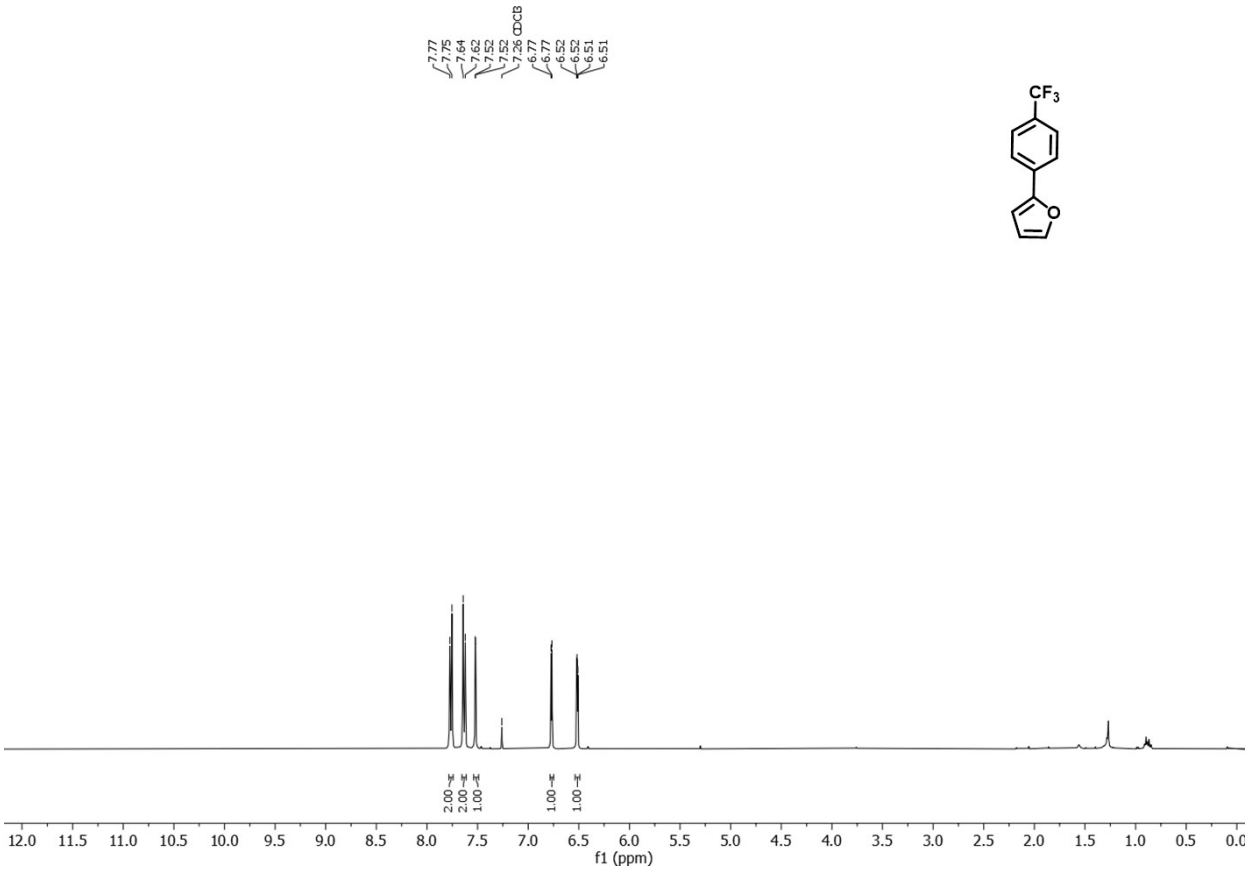


Figure S78. ^{1}H NMR spectrum (400 MHz) of **5e** in $CDCl_3$.

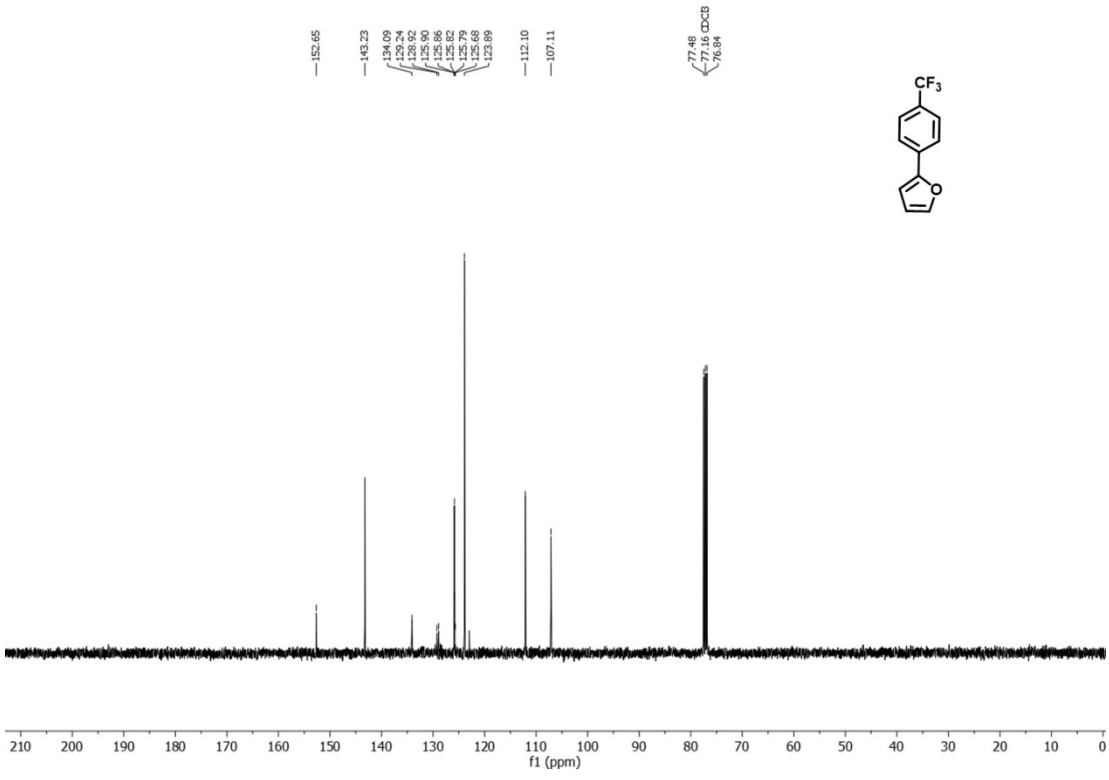


Figure S79. ^{13}C NMR spectrum (100 MHz) of **5e** in $CDCl_3$.

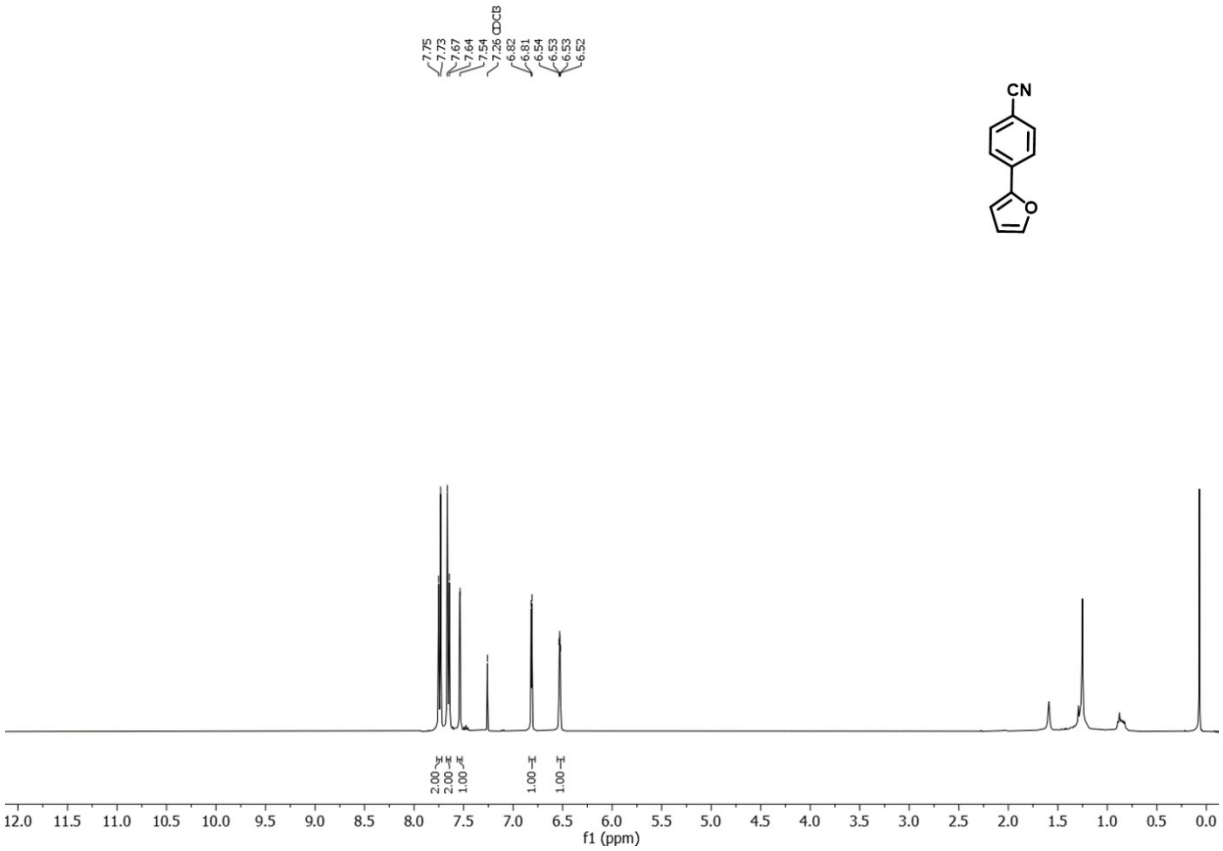


Figure S80. ^{1}H NMR spectrum (400 MHz) of **5f** in $CDCl_3$.

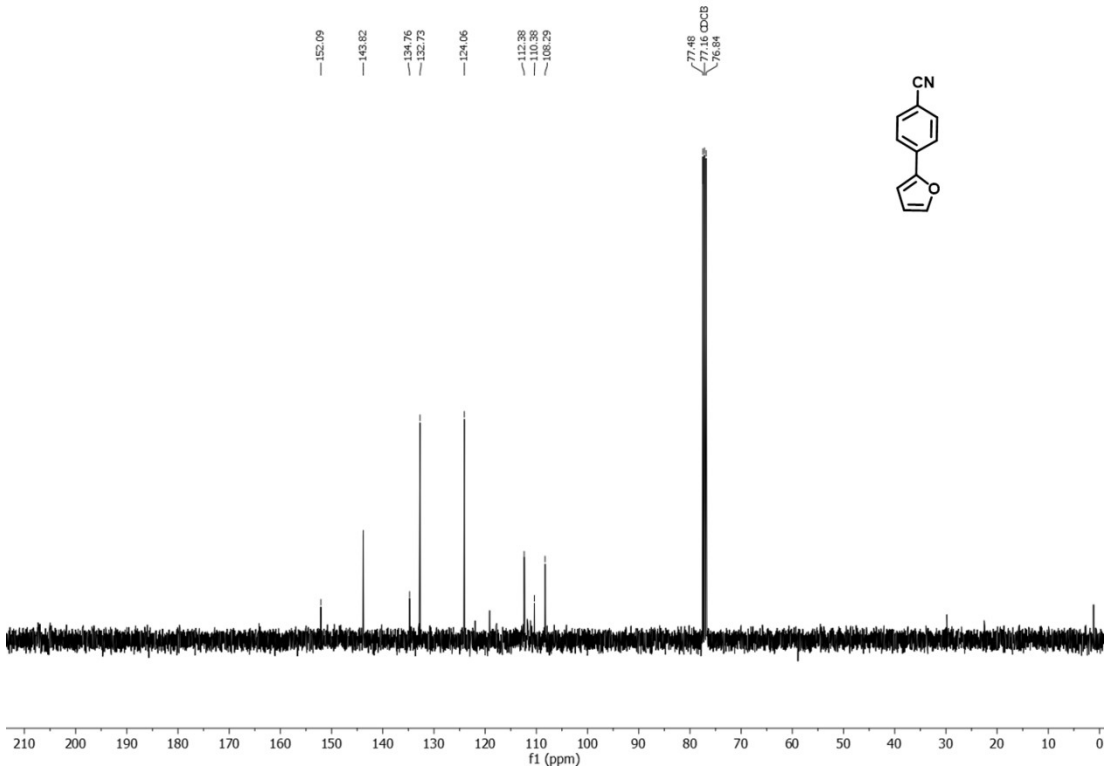


Figure S81. ^{13}C NMR spectrum (100 MHz) of **5f** in $CDCl_3$.

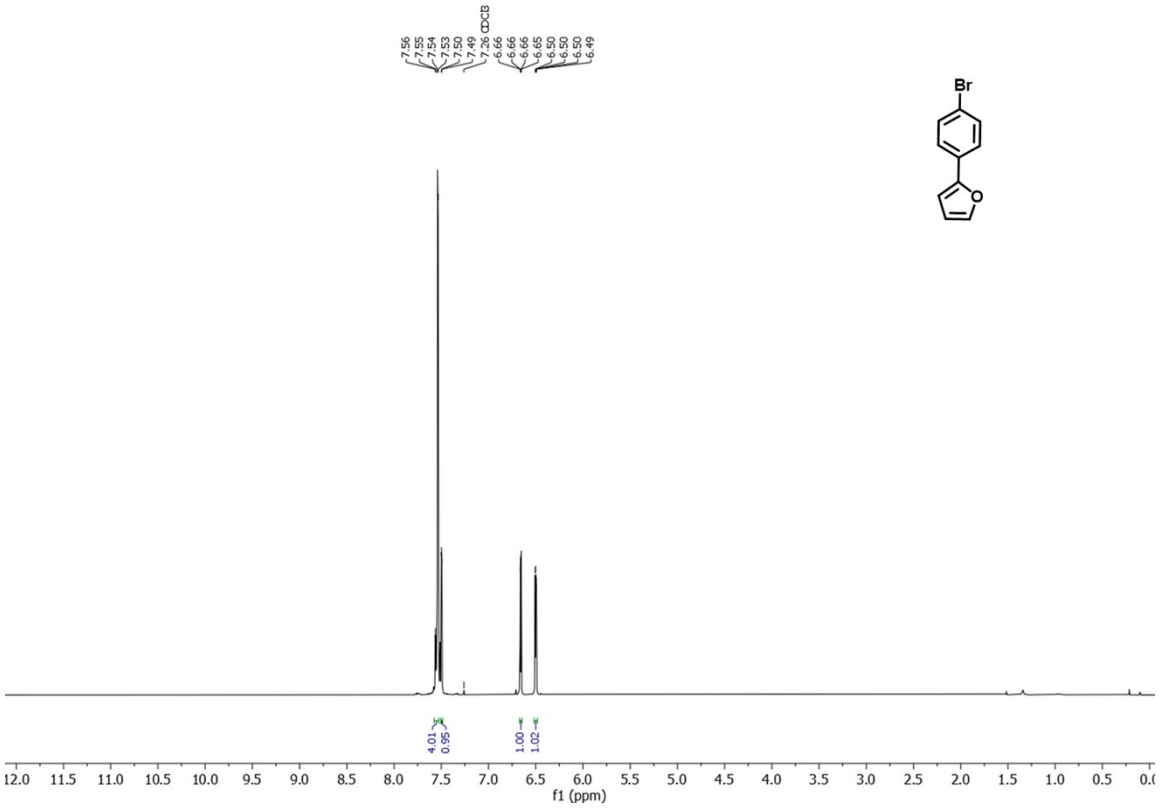


Figure S82. ^{1}H NMR spectrum (400 MHz) of **5g** in $CDCl_3$.

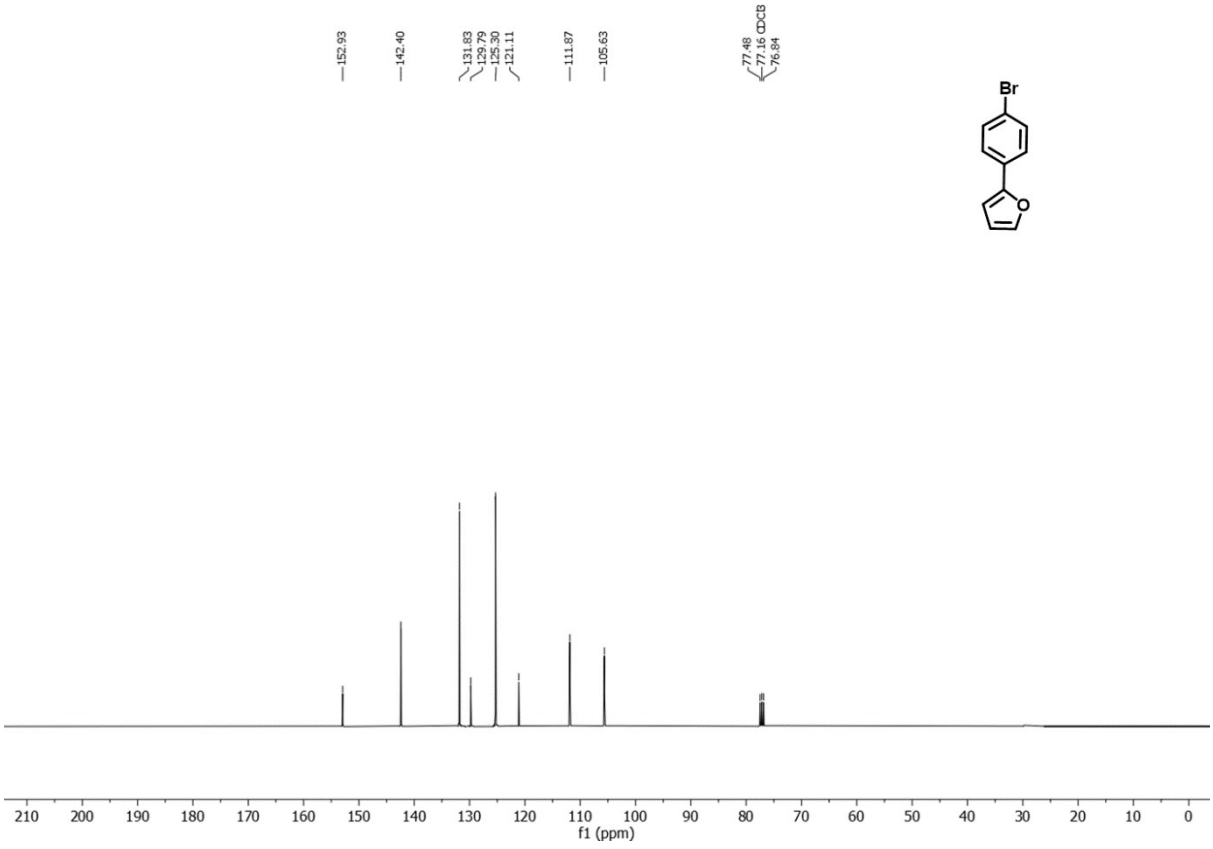


Figure S83. ^{13}C NMR spectrum (100 MHz) of **5g** in $CDCl_3$.

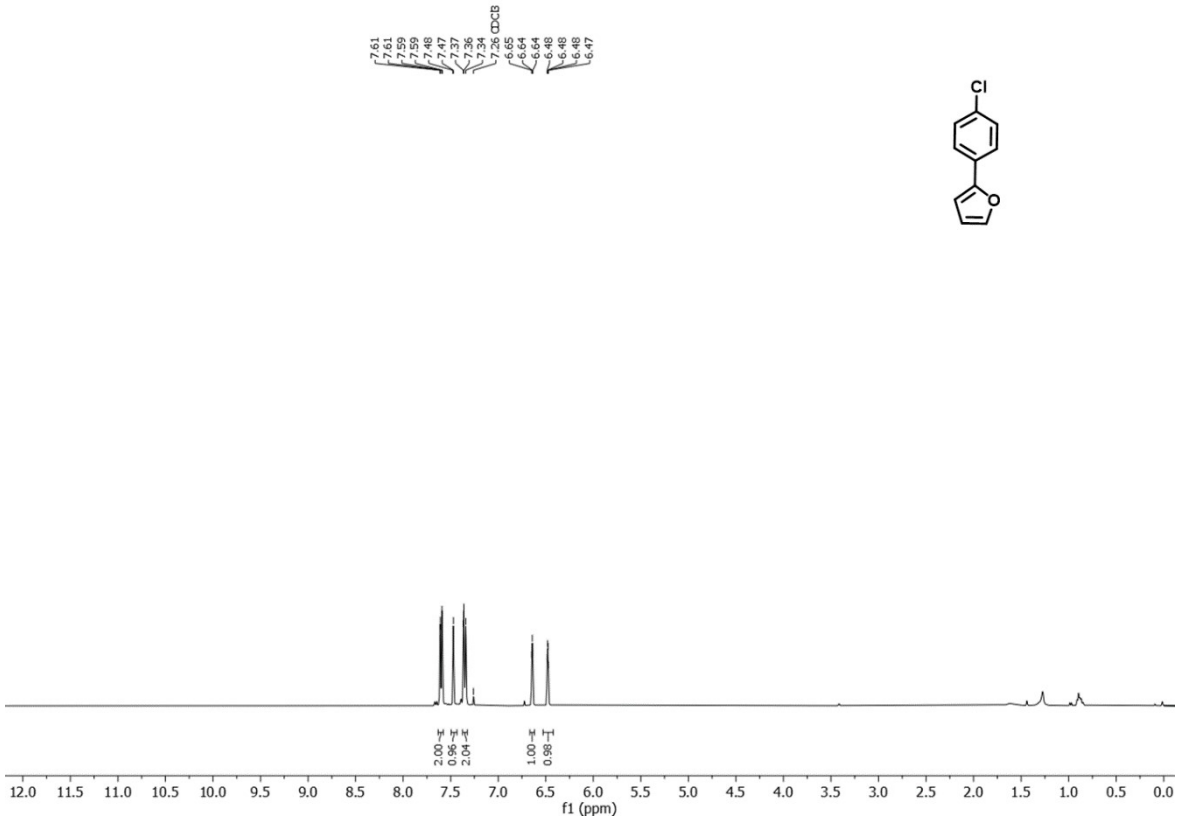


Figure S84. ^{1}H NMR spectrum (400 MHz) of **5h** in $CDCl_3$.

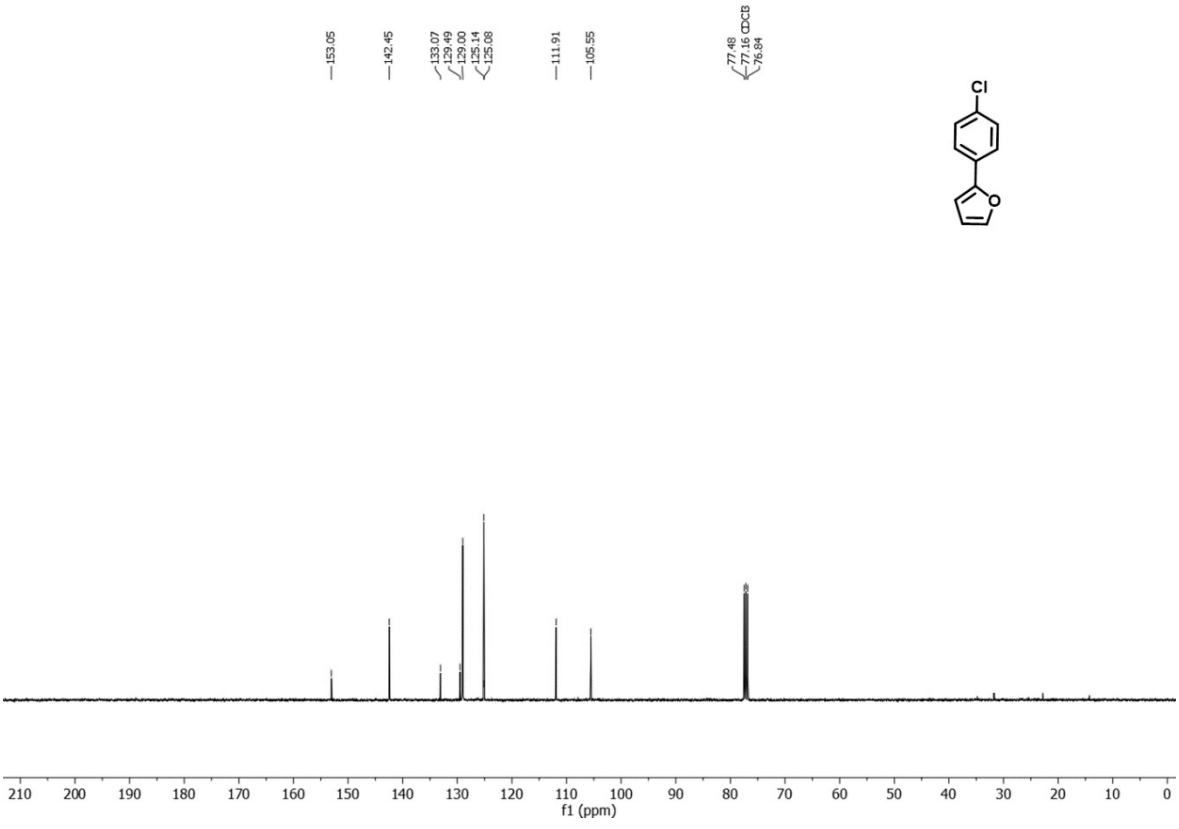


Figure S85. ^{13}C NMR spectrum (100 MHz) of **5h** in $CDCl_3$.

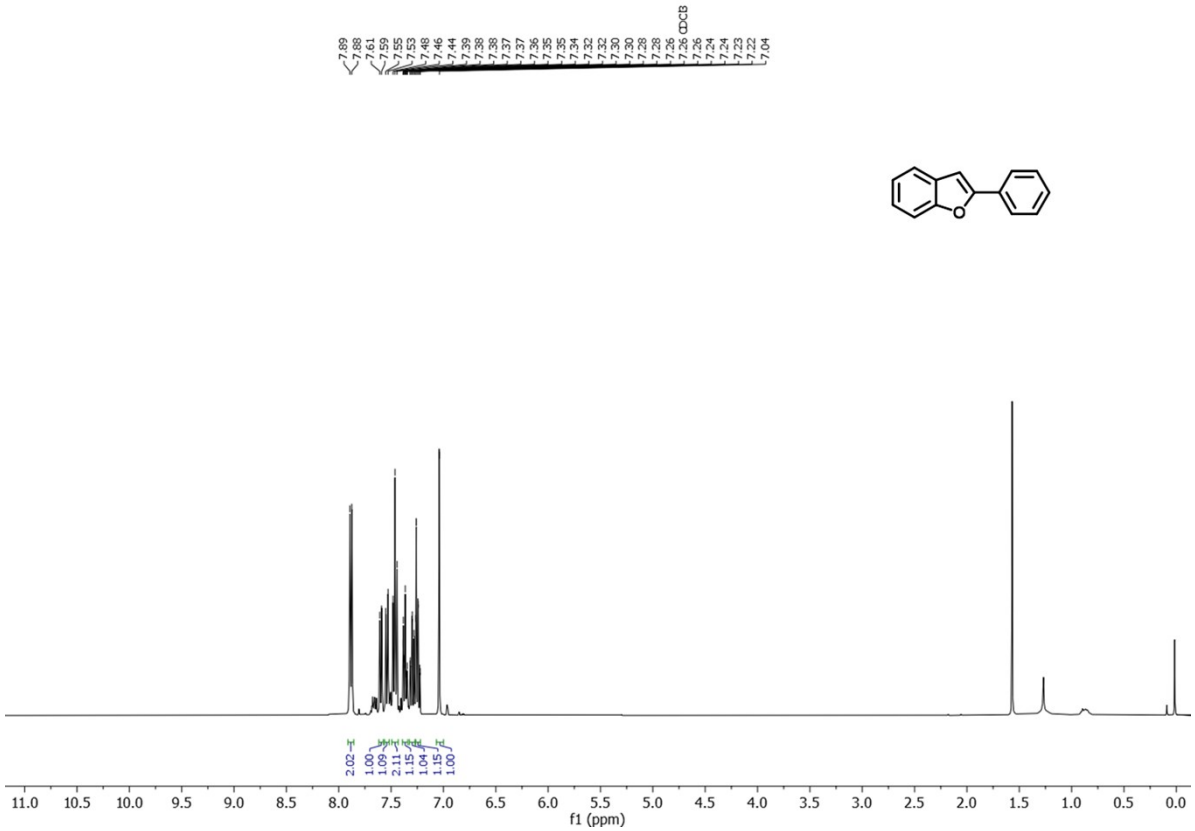


Figure S86. ^{1}H NMR spectrum (400 MHz) of **6a** in $CDCl_3$.

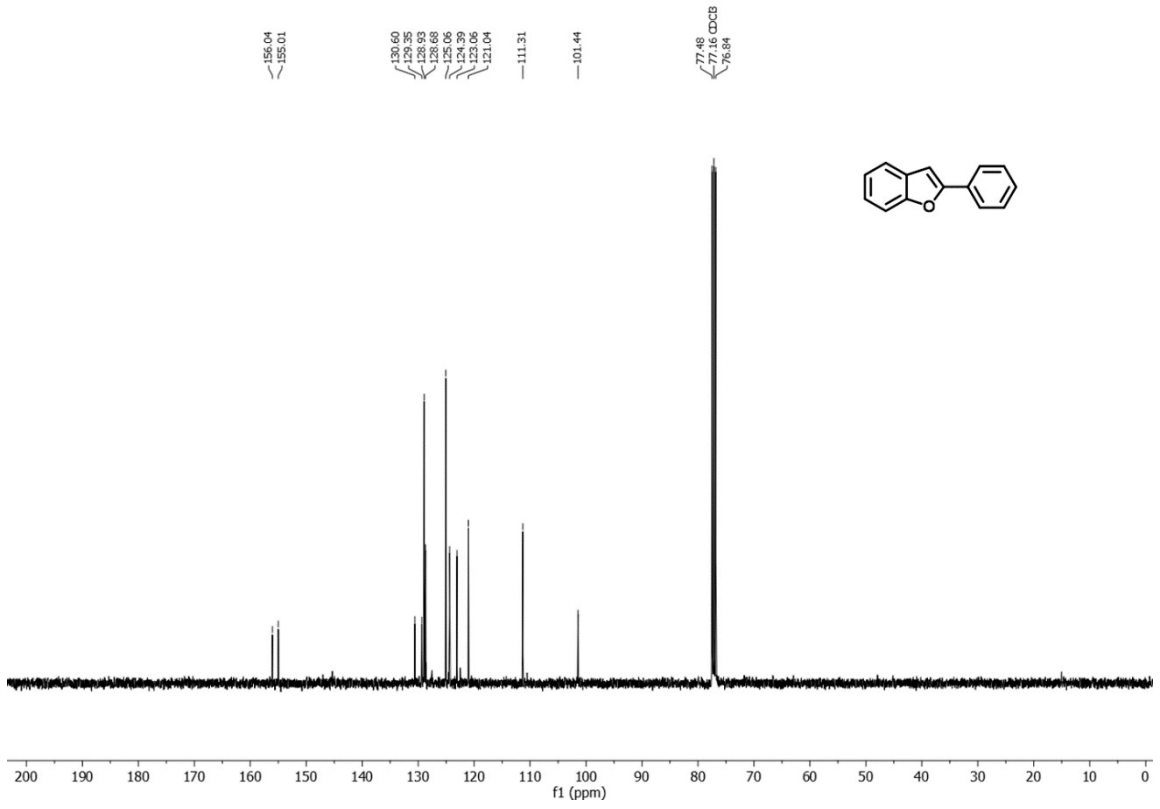


Figure S87. ^{13}C NMR spectrum (100 MHz) of **6a** in $CDCl_3$.

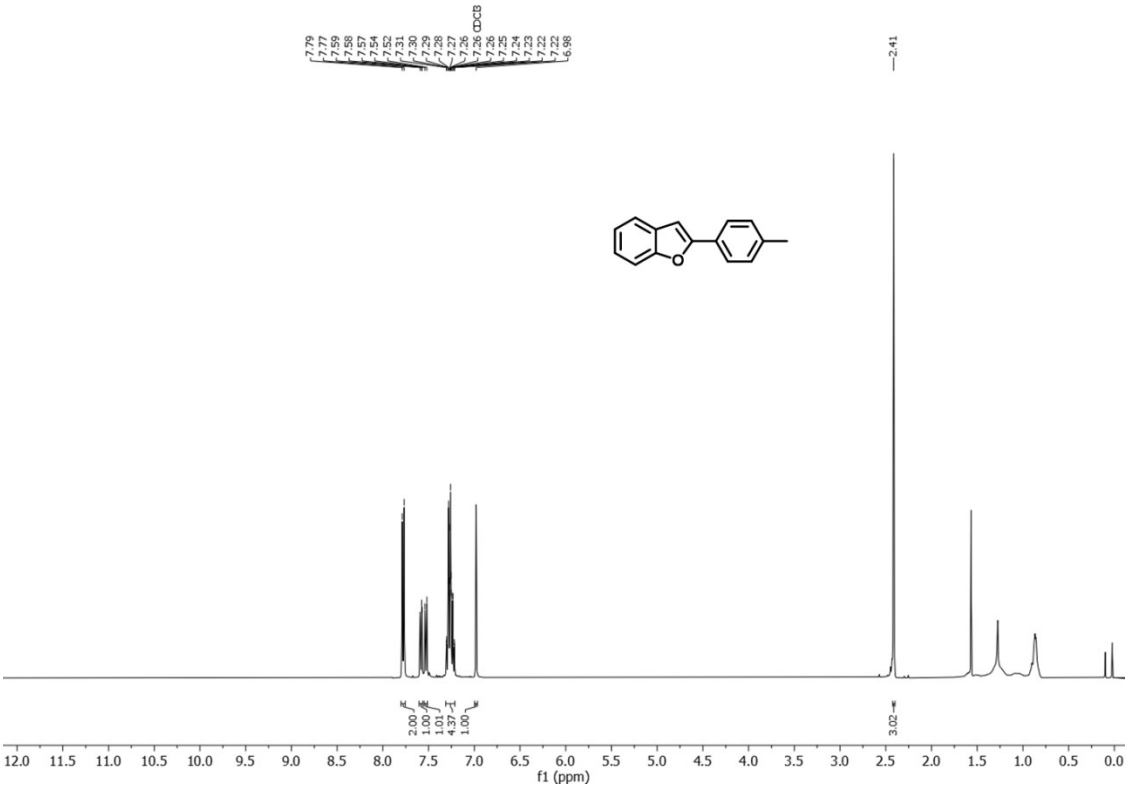


Figure S88. ^{1}H NMR spectrum (400 MHz) of **6b** in $CDCl_3$.

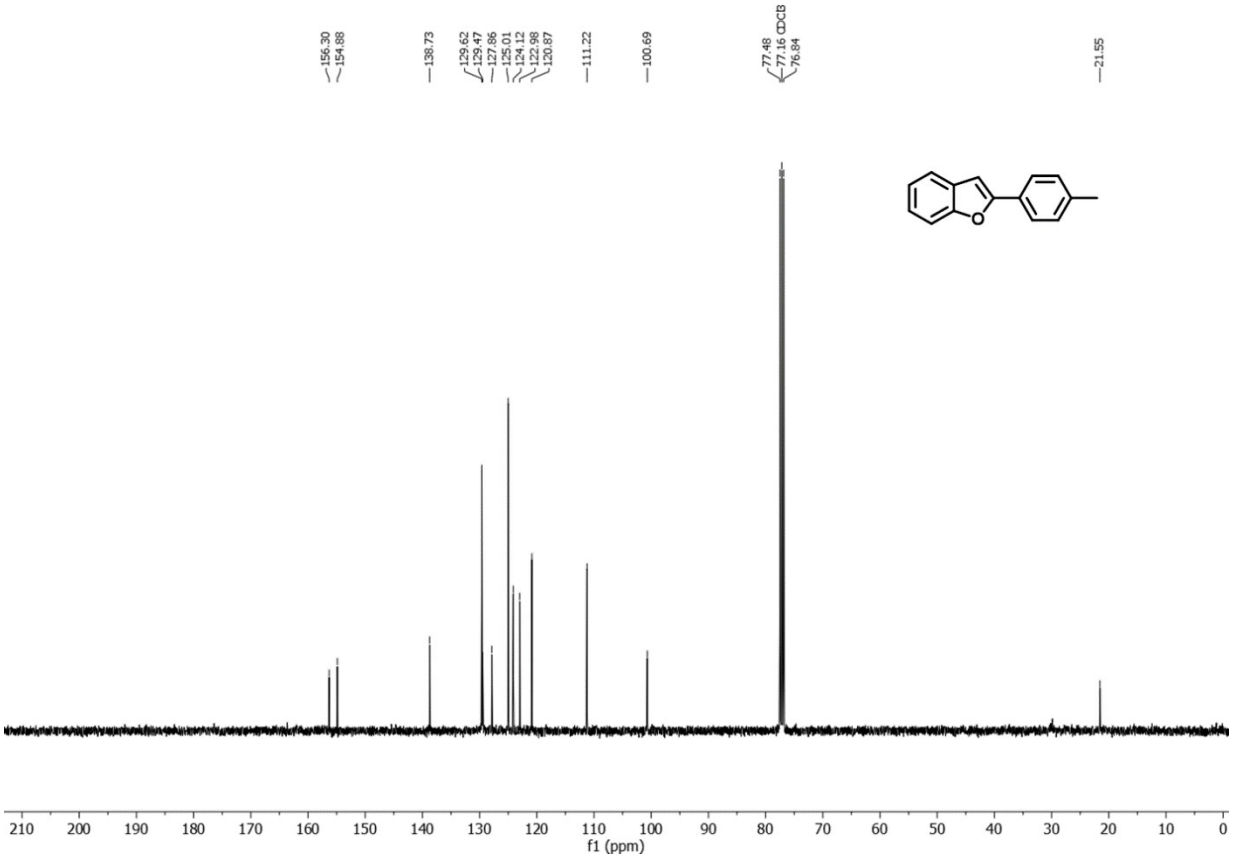


Figure S89. ^{13}C NMR spectrum (100 MHz) of **6b** in $CDCl_3$.

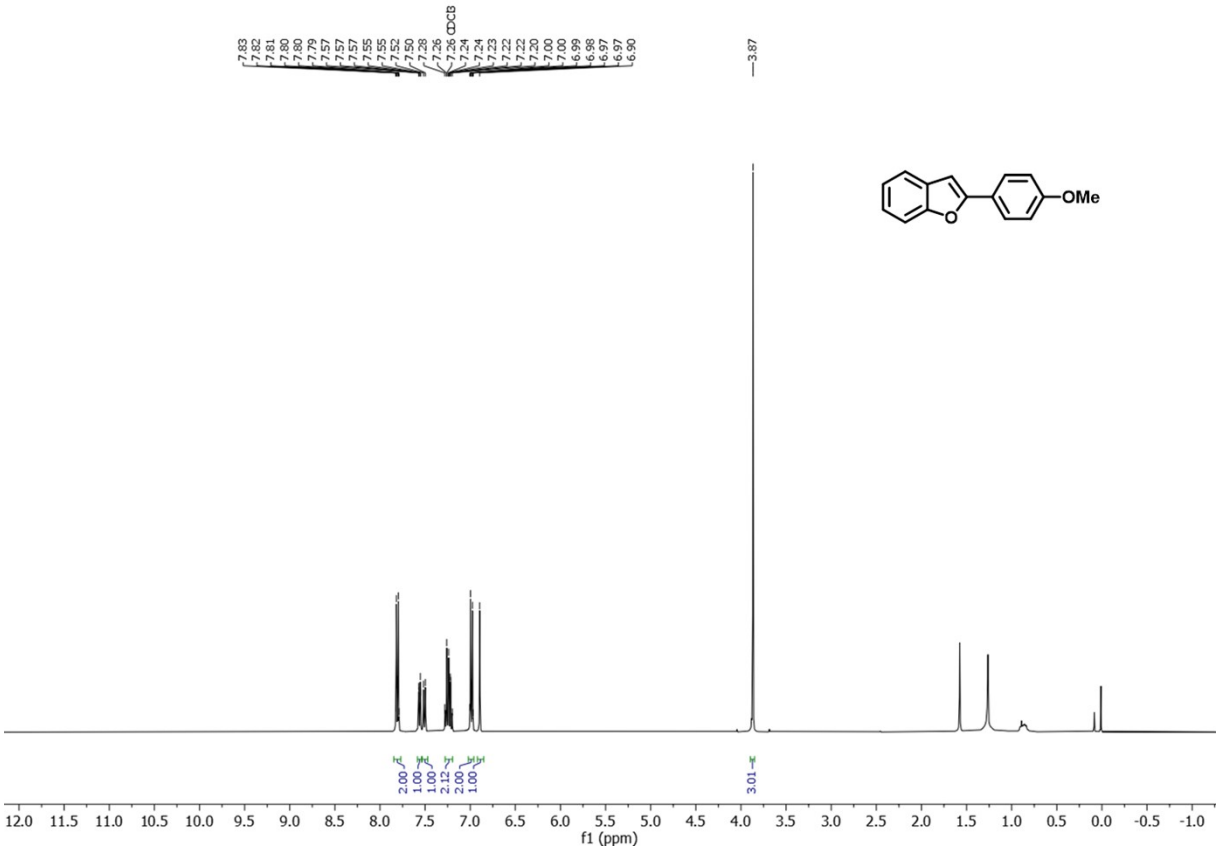


Figure S90. ^{1}H NMR spectrum (400 MHz) of **6c** in $CDCl_3$.

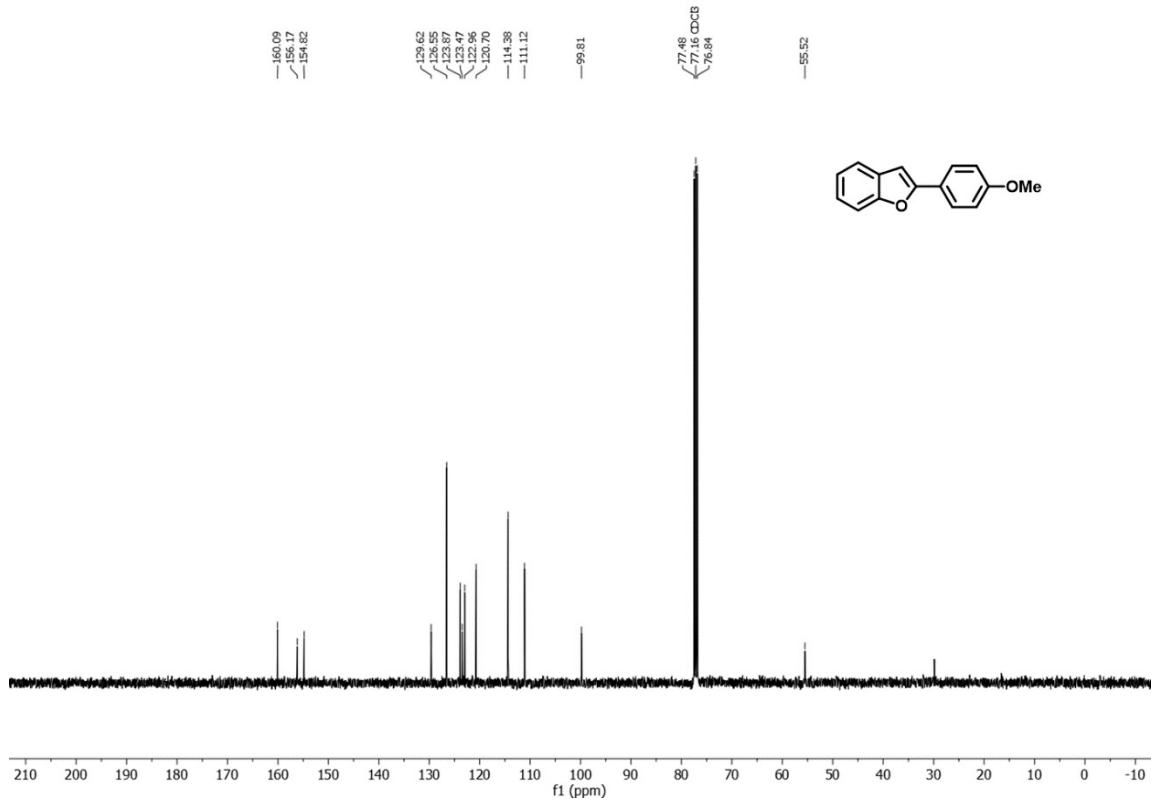


Figure S91. ^{13}C NMR spectrum (100 MHz) of **6c** in $CDCl_3$.

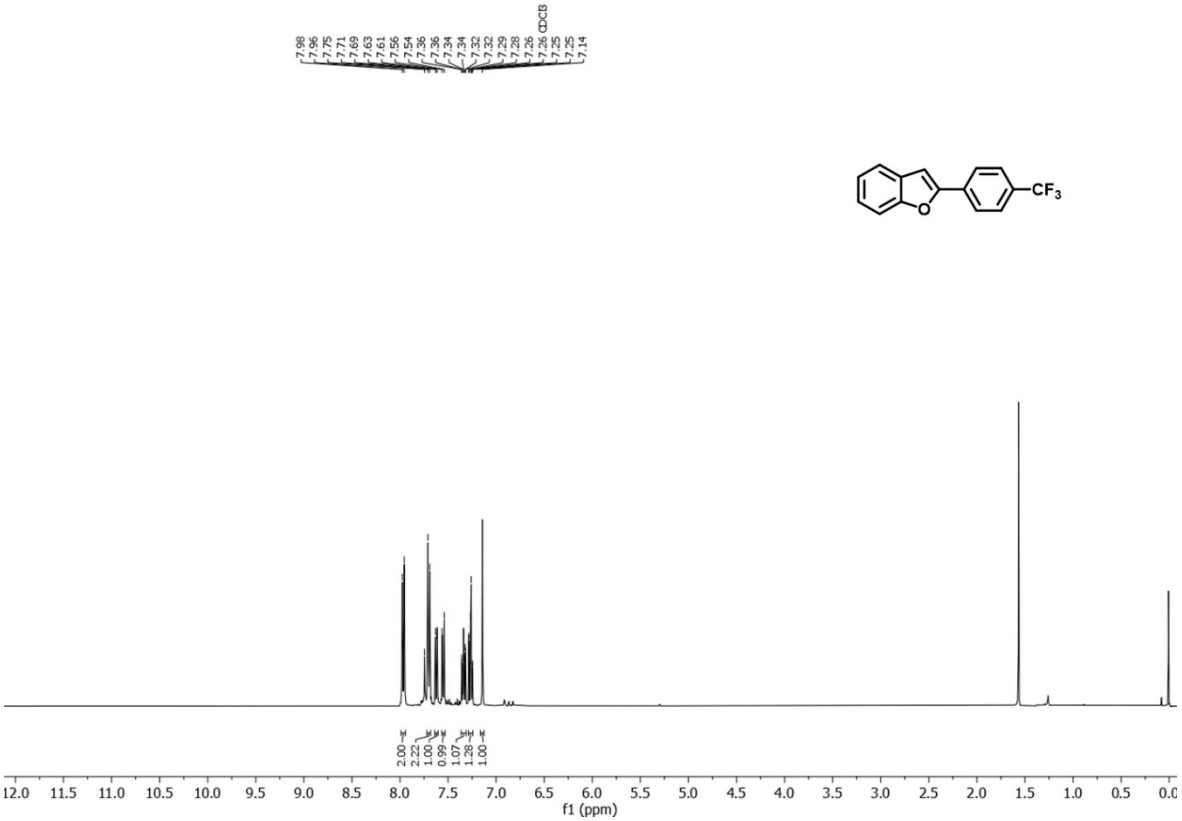


Figure S92. ^{1}H NMR spectrum (400 MHz) of **6d** in $CDCl_3$.

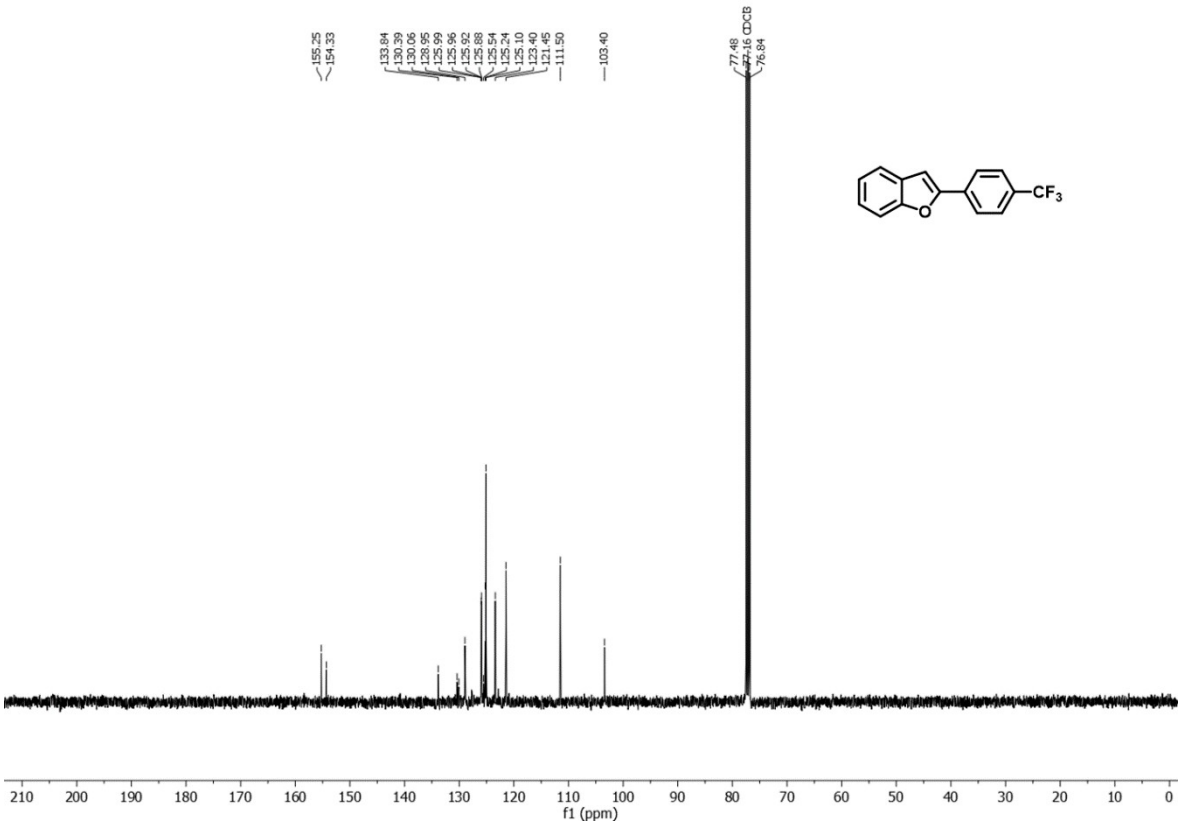


Figure S93. ^{13}C NMR spectrum (100 MHz) of **6d** in $CDCl_3$.

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