Electronic Supporting Information

Deciphering Single Electron Transfer Ability of Fluorene Under Photoredox Conditions

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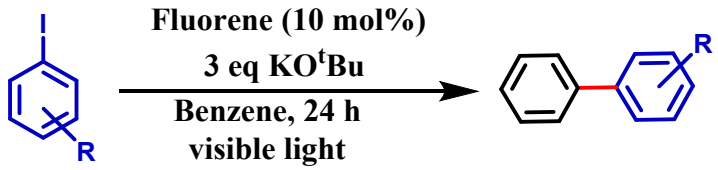
1. General considerations:

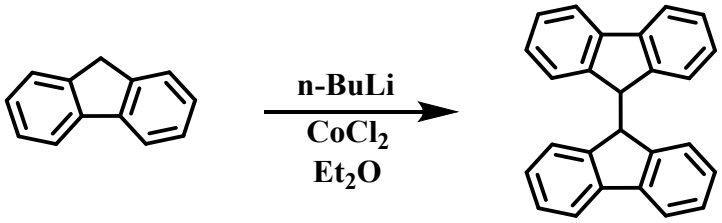
All starting compounds employed in this study were procured from commercial suppliers and were used without further purification. All chemicals were purchased from Sigma Aldrich, Avra, TCI, Alfa Aesar, GLR innovations. Glassware was dried overnight at 160 °C before use. Benzene was dried by heating over sodium with benzophenone as an 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 size) using a gradient of ethyl acetate and hexane as mobile phase. GC-MS measurements were done on Agilent 5977B GC/MSD instrument. ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz Bruker Biospin Advance III FT-NMR spectrometer. The electrochemical measurements were performed using CHI-610 electrochemical workstation from CH Instruments (USA). Fluorescence quenching experiments were carried out in a Cary Eclipse Fluorescence Spectrofluorometer. Photo-luminescent lifetime data were collected using a Fluorolog-3 spectrofluorophotometer (Horiba Jobin Yvon, NJ) equipped with a single photon counting module in multi-channel scaler mode. The lifetime was determined using the decay analysis software package, DAS v6.1. 1. The photochemical reactions were conducted with eplite 50 W white LED. Reaction tube was kept 7-8 cm away from the light source. UV-Vis spectra were 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 with respect to residual proton peak for $CDCl_3$(δ 7.26 ppm). Carbon chemical shifts are internally referenced with respect to the deuterated solvent resonance for $CDCl_3$ (δ 77.1 ppm).

2. General procedure for the synthesis of C–C cross-coupling reaction of aryl halides with benzene.



In a pressure tube, aryl iodide (0.5 mmol), KO^{t}Bu (1.5 mmol) and fluorene (10 mol%) were taken in a glove box. After that dry benzene (2 mL) was added to the reaction mixture and the tube was closed properly. The reaction mixture was stirred under visible light irradiation for 24 h 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 reduced pressure. Subsequent purification by column chromatography with EtOAc/hexane combination as the eluent afforded the corresponding product. The biaryl products were fully characterized by ^1H and ^{13}C NMR spectroscopies.

3. Synthetic procedure of 9H,9'H-9,9'-bifluorene (1c).



1c was synthesized following literature procedure.[1] A 100 mL oven-dried Schlenk flask was charged with 1.0 g (4.5 mmol) of fluorene under nitrogen flow. The solid was then dissolved in 40 mL of diethyl ether and cooled to -78 °C. A syringe was used to add 4 mL (5 mmol) of 1.6 M n-butyllithium in hexanes to the cooled solution, then allowed to stir at ambient temperature for 2.5 h upon which the solution turned red. The red solution was again cooled to -78 °C before the addition of 0.6 g (4.5 mmol) of cobalt(II) chloride. After 1 h of stirring at ambient temperature, saturated solutions of NaCl (10 mL) and NH_4Cl (10 mL) were added. The aqueous layer was extracted with 3 × 15 mL portions of dichloromethane, and magnesium sulfate was added to the organic phase. After filtration, solvent was removed under vacuum and the resulting solid was washed with pentane and ether to give 482 mg (65% yield) of 9H,9'H-9,9'-bifluorene (**1c**). The authenticity of the product was confirmed by ^1H and ^{13}C NMR spectroscopies. ^1H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 7.6 Hz, 4H), 7.29 (d, J = 8.7 Hz, 4H), 7.09 (t, J = 7.0 Hz, 4H), 6.96 (d, J = 7.8 Hz,

4H), 4.85 (s, 2H).[13]C NMR (100 MHz, $CDCl_3$) δ 144.8, 141.6, 127.4, 126.8, 124.2, 119.8, 49.9. Spectroscopic data matched with literature report.[2]

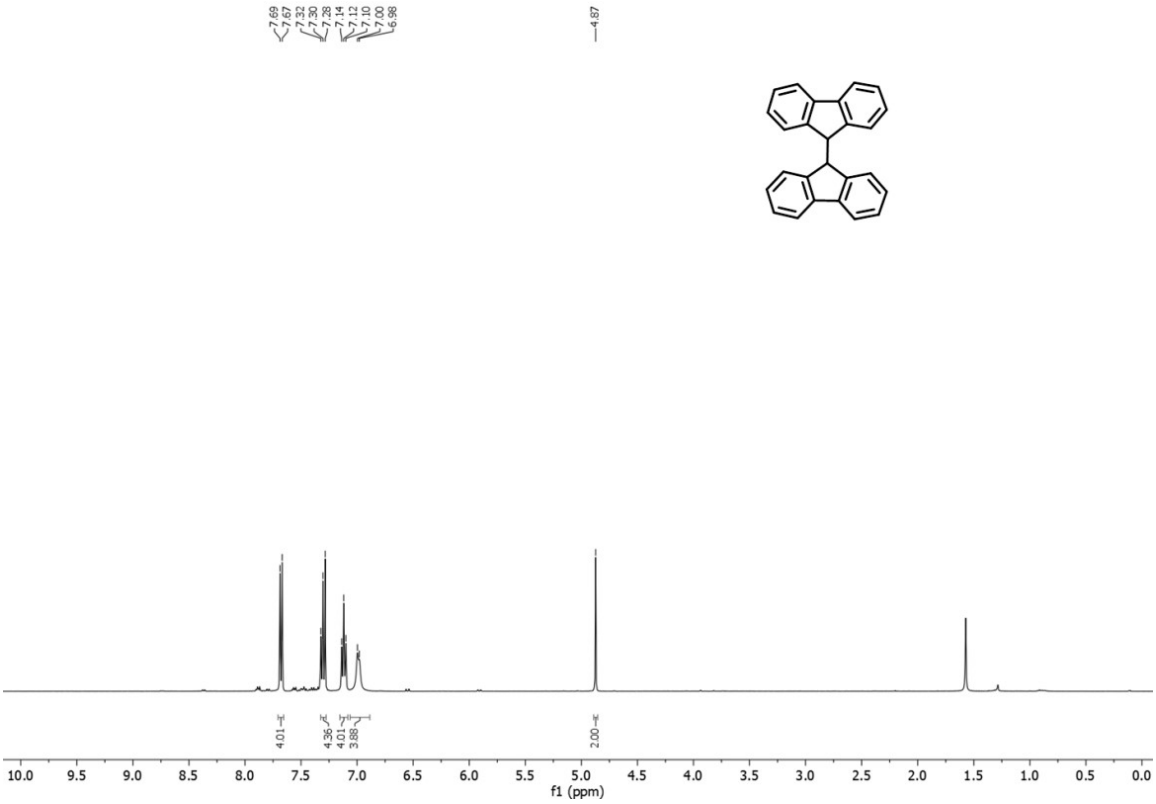


Figure S1. [1]H NMR spectrum (400 MHz) of **1c** in $CDCl_3$.

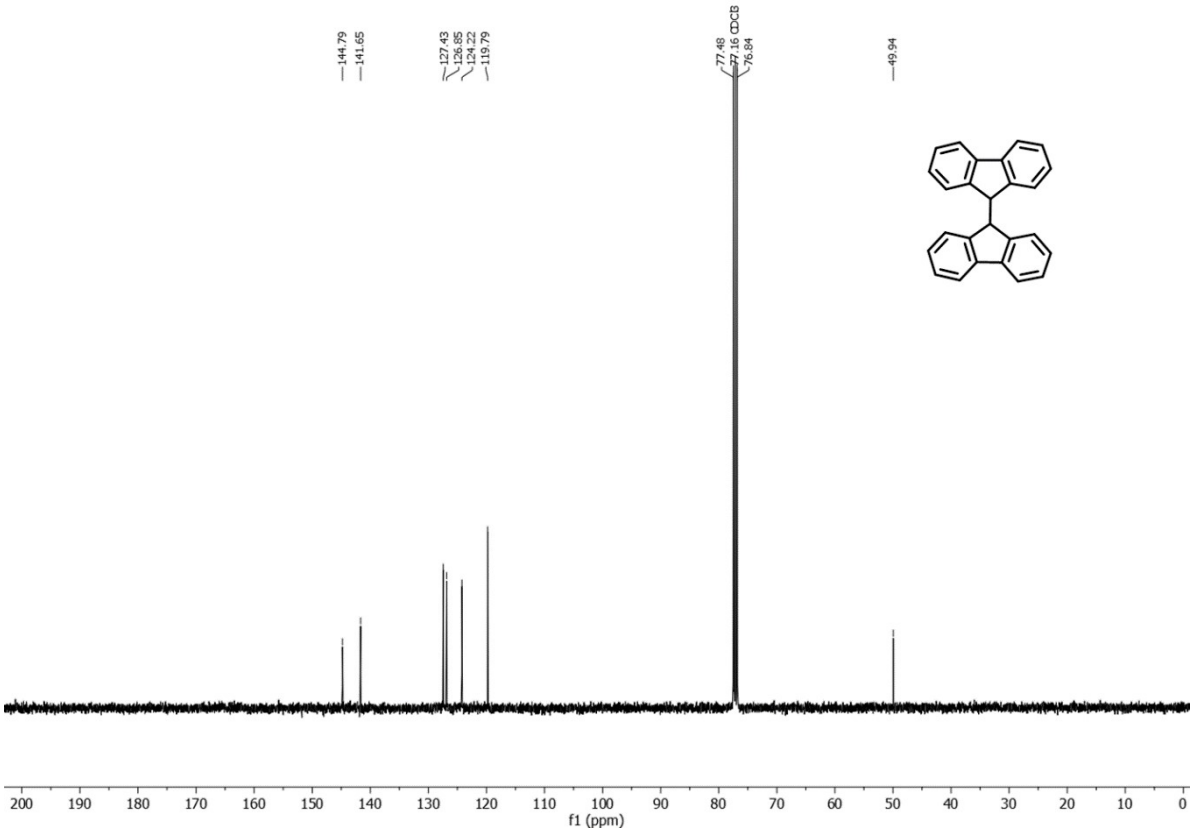
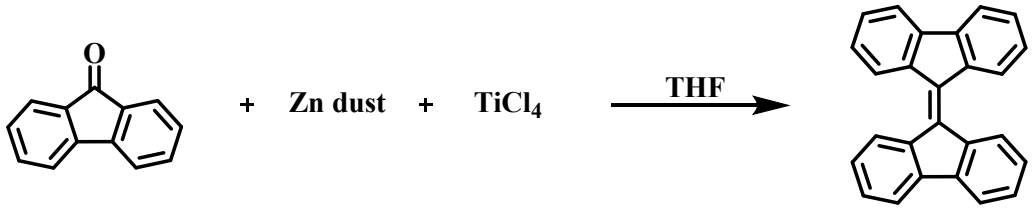


Figure S2. ^{13}C NMR spectrum (100 MHz) of **1c** in $CDCl_3$.

4. Synthetic procedure of 9,9'-bifluorenylidene(1g).



1g was synthesized following literature procedure.[3] In an oven-dry 250 mL round bottom flask, zinc dust (74 mmol) and $TiCl_4$ (37.5 mmol) were added in 40 mL dry THF solvent under N_2 atmosphere at 0 °C. Then, the mixture was transferred to the 20 mL THF solutions of fluorenone (10 mmol) via cannula. After that the reaction mixture was refluxed for 24 h, then the reaction mixture was cooled and quenched with a saturated aqueous solution of NH_4Cl. The organic products were extracted in ethyl acetate. The organic layer was dried over anhydrous $MgSO_4$, filtered, and concentrated in vacuo. The crude product was purified by column chromatography to give the desired product **1g** in 983 mg (60% yield) as a red solid. The authenticity of the product was confirmed by ^1H NMR and ^{13}C NMR spectroscopies. ^1H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, J = 7.8 Hz, 4H),

7.71 (d, J = 7.5 Hz, 4H), 7.36 – 7.31 (m, 4H), 7.24 – 7.18 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 138.4, 129.3, 127.0, 126.9, 120.0. Spectroscopic data matched with literature report.[4]

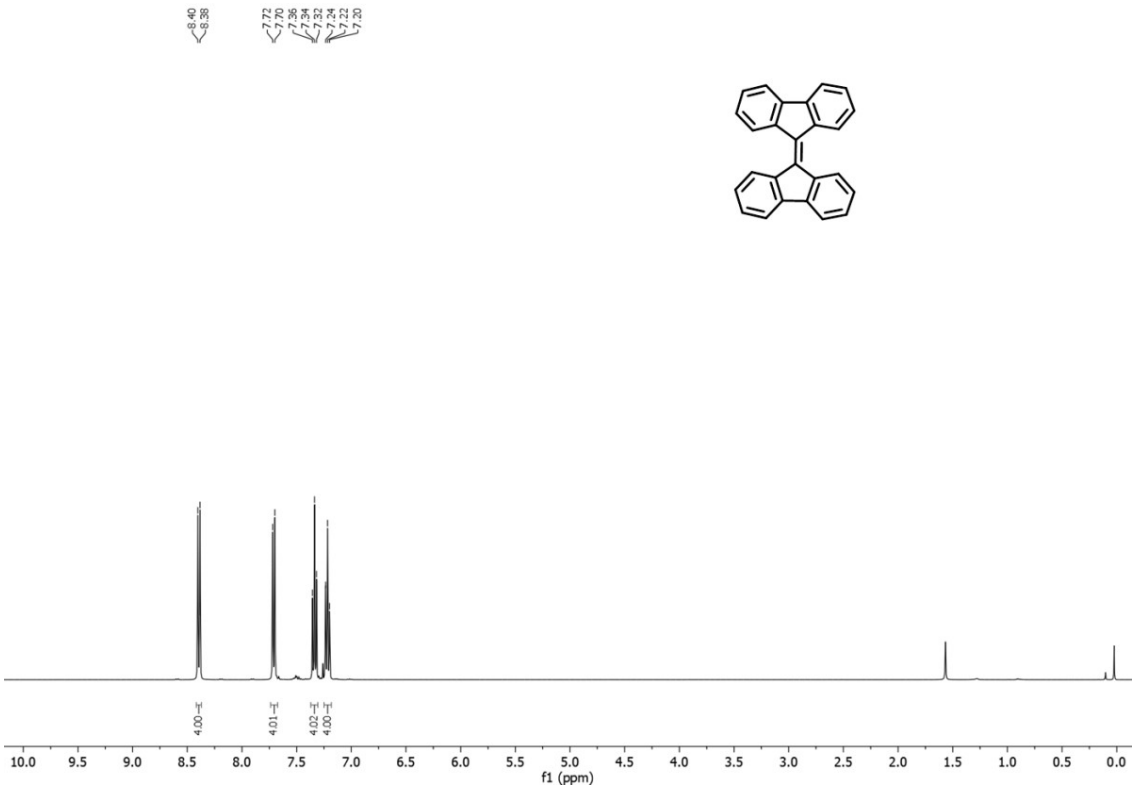


Figure S3. ^{1}H NMR spectrum (400 MHz) of **1g** in $CDCl_3$.

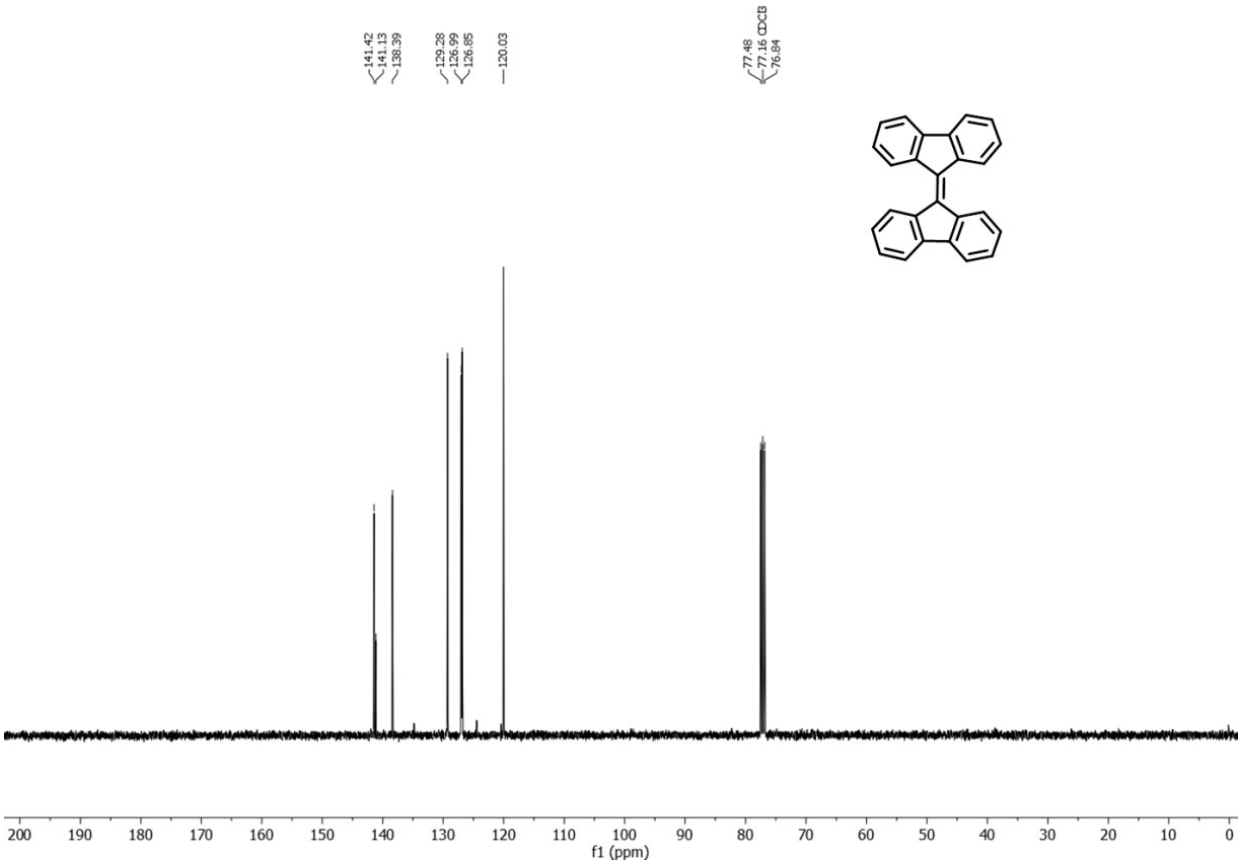
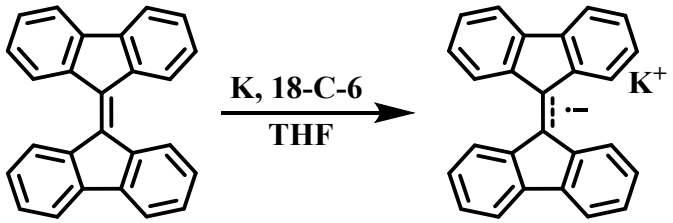


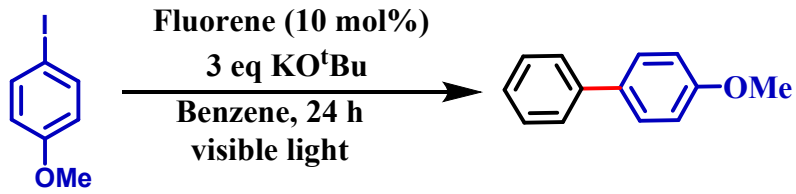
Figure S4. ^{13}C NMR spectrum (100 MHz) of **1g** in $CDCl_3$.

5. Synthesis of 9,9'-bifluorenylidenyl radical anion.



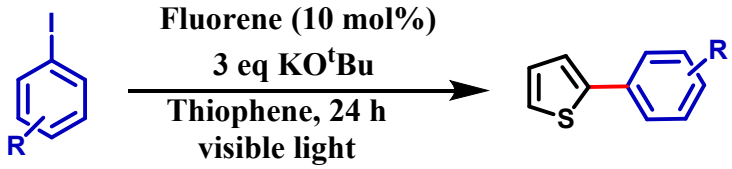
In a glove box, 9,9'-bifluorenylidene (2 mmol) was dissolved in THF (3 mL) giving an intense yellow color. Then potassium (2.1 mmol) and 18-crown-6 (2.1 mmol) were added to the solution. The reaction mixture was stirred at room temperature for 5 minutes during which a dark brown colored solution ensued. The reaction mixture was dried further to isolate **1f**.

6. Gram-scale synthesis of 3g



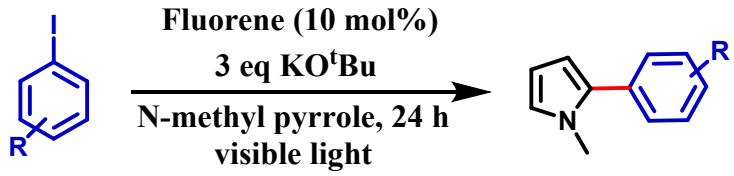
In a sealed tube, 4-iodoanisole (4.3 mmol, 1 g), KO^{t}Bu (12.9 mmol, 1.4 g) and fluorene (10 mol%) were taken in a glove box. After that dry benzene (16 mL) was added to the reaction mixture and the tube was closed properly. The reaction mixture was stirred under visible light irradiation for 24 h at 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 reduced pressure. Subsequent purification by column chromatography with EtOAc/hexane combination as the eluent afforded the corresponding product in 56 % isolated yield. The biaryl product was fully characterized by ^1H and ^{13}C NMR spectroscopies.

7. C-C cross coupling reaction of 4-iodo anisole with thiophene as a coupling partner



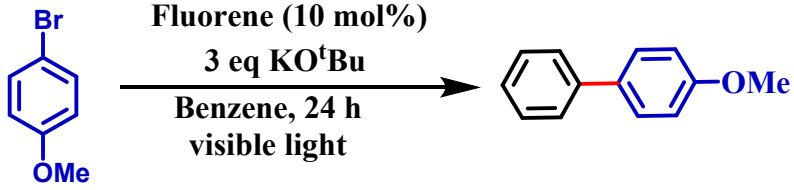
In a sealed tube, aryl iodide (0.5 mmol), KO^{t}Bu (1.5 mmol) and fluorene (10 mol%) were taken in a glove box. After that dry thiophene (1.5 mL) was added to the reaction mixture and the tube was closed properly. The reaction mixture was stirred under visible light irradiation for 24 h at room temperature. 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 reduced pressure. Subsequent purification by column chromatography with EtOAc/hexane combination as the eluent afforded the corresponding product. The hetero-biaryl products were fully characterized by ^1H and ^{13}C NMR spectroscopies.

8. C-C cross coupling reaction of 4-iodo anisole with N-methyl pyrrole as a coupling partner



In a sealed tube, aryl iodide (0.5 mmol), KO^{t}Bu (1.5 mmol) and fluorene (10 mol%) were taken in a glove box. After that dry N-methyl pyrrole (1.5 mL) was added to the reaction mixture and the tube was closed properly. The reaction mixture was stirred under visible light irradiation for 24 h 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 reduced pressure. Subsequent purification by column chromatography with EtOAc/hexane combination as the eluent afforded the corresponding product. The hetero-biaryl products were fully characterized by ^1H and ^{13}C NMR spectroscopies.

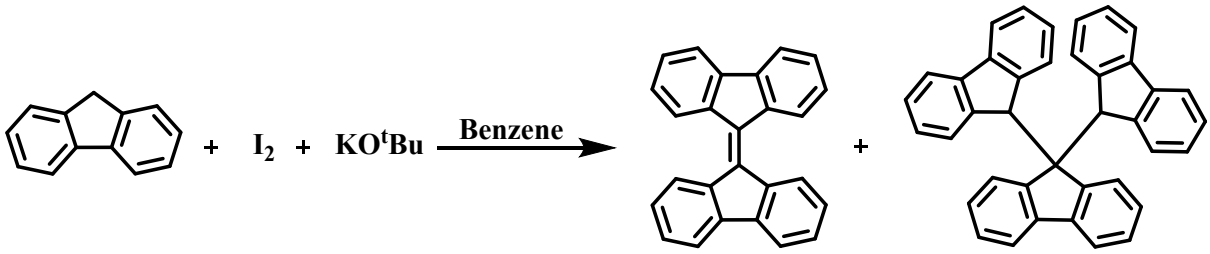
9. C-C cross coupling reaction of 4-bromo anisole with benzene as a coupling partner



In a sealed tube, 4-bromoanisole (0.5 mmol), KO^{t}Bu (1.5 mmol) and fluorene (10 mol%) were taken in a glove box. After that dry benzene (2 mL) was added to the reaction mixture and the tube was closed properly. The reaction mixture was stirred under visible light irradiation for 24 h 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 reduced pressure. Subsequent purification by column chromatography with EtOAc/hexane combination as the eluent afforded the corresponding product in 55 % isolated yield. The biaryl product was fully characterized by ^1H and ^{13}C NMR spectroscopies.

10. Mechanistic investigations:

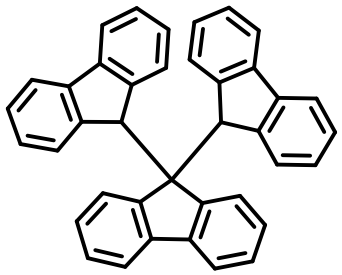
10.1. Reaction of fluorene with I_2 in the presence of KO^{t}Bu



1 **1g** (40%) **1h** (14%)

In an oven-dried Schlenk flask, **1** (1 mmol), KO^{t}Bu (1.5 mmol) and I_2 (2 mmol) were mixed under inert atmosphere. After that dry benzene (2 mL) was added to the reaction mixture. The reaction mixture was stirred under visible light irradiation for 24 h under inert 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 **1g** (40%) and **1h** (14%).

9H,9''H-9,9':9',9''-terfluorene (1h):



1h was fully characterized by ^{1}H and ^{13}C NMR spectroscopies. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 7.5 Hz, 2H), 7.87 – 7.79 (m, 2H), 7.62 – 7.52 (m, 4H), 7.43 (d, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 7.7 Hz, 2H), 7.11 (t, *J* = 8.0 Hz, 2H), 6.96 (t, *J* = 7.0 Hz, 2H), 6.88 – 6.80 (m, 2H), 6.51 (t, *J* = 8.2 Hz, 2H), 6.30 (d, *J* = 7.7 Hz, 2H), 5.41 (s, 2H), 5.35 (d, *J* = 7.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.3,144.3, 143.9, 143.7, 141.7, 141.0, 136.2, 128.1, 127.6, 127.4, 126.9, 126.8, 126.0, 124.6, 123.6, 120.4, 119.3, 118.8. Spectroscopic data matched with literature report.[5]

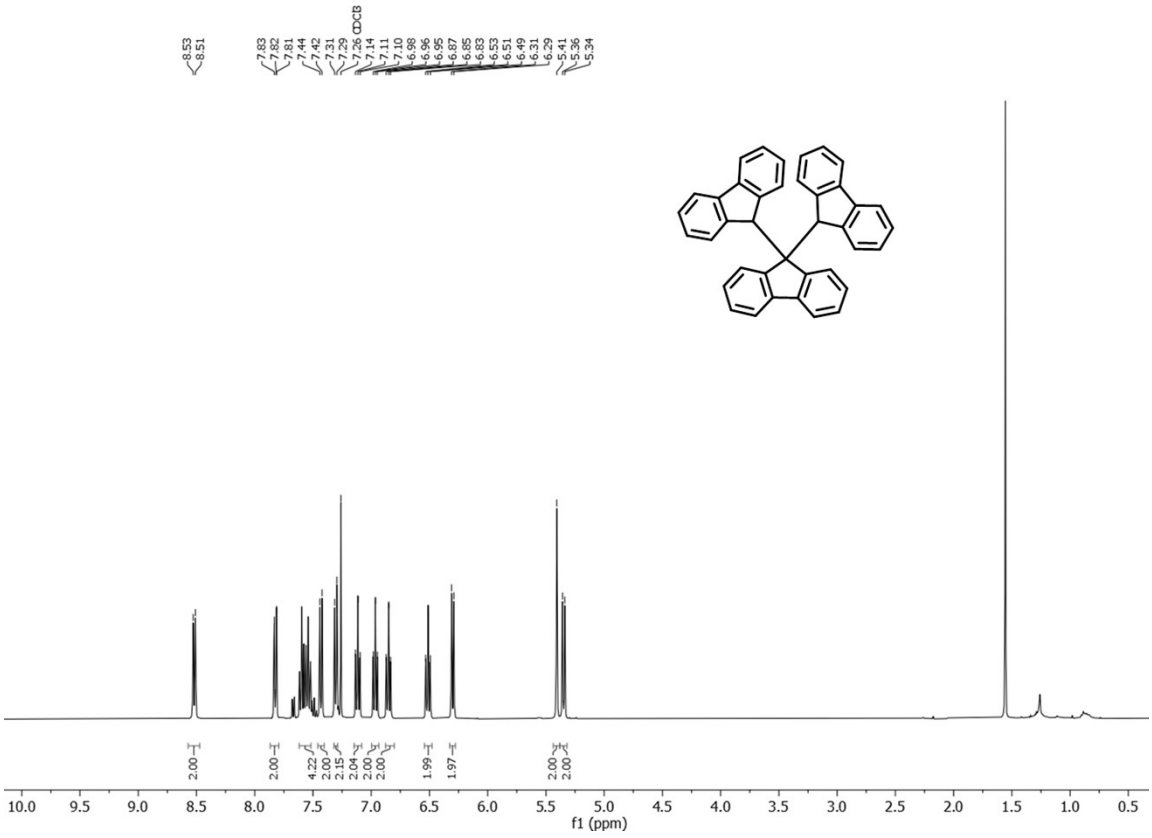


Figure S5. ^{1}H NMR spectrum (400 MHz) of **1h** in $CDCl_3$. Adventitious moisture was from the NMR solvent.

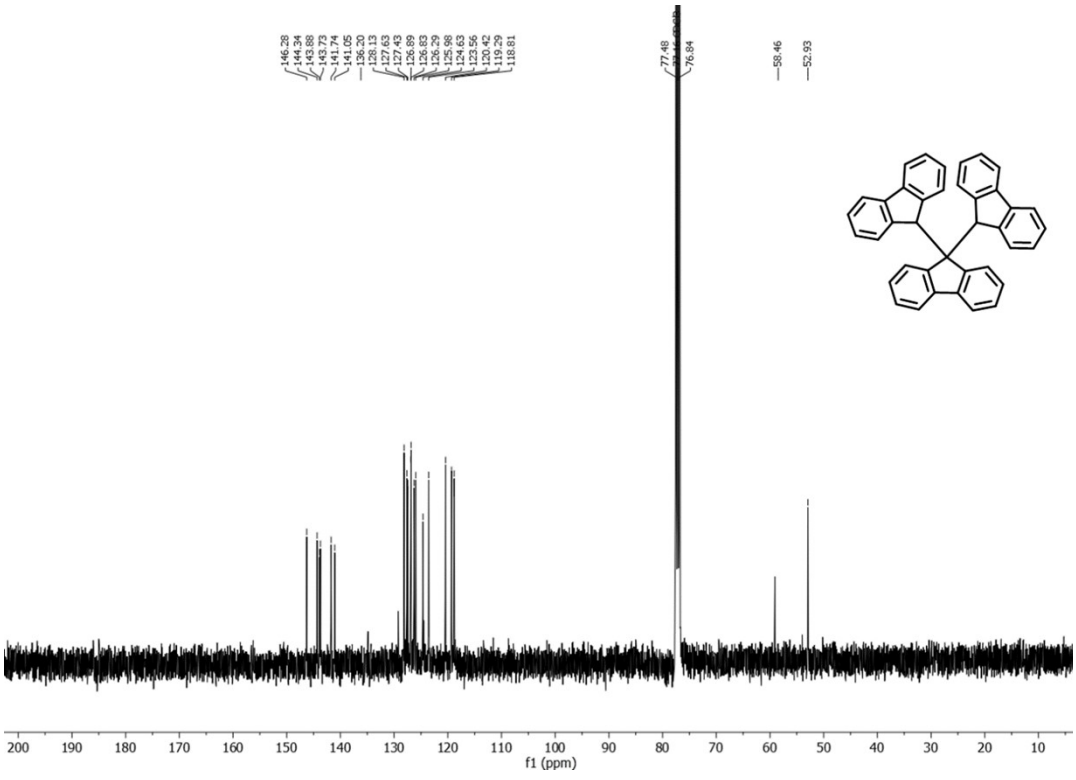
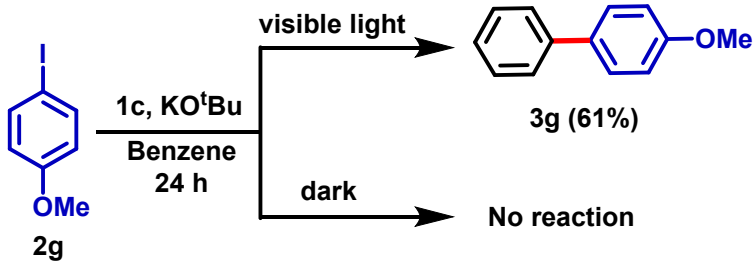


Figure S6. ^{13}C NMR spectrum (100 MHz) of **1h** in $CDCl_3$.

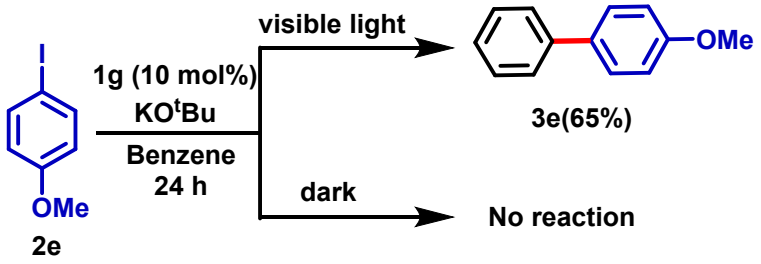
10.2. C-C cross-coupling reaction taking 9H,9'H-9,9'-bifluorene(1c) as initiator



In a pressure tube 4-iodoanisole (0.5 mmol), KO^{t}Bu (1.5 mmol) and **1c** (10 mol%) were charged in a glove box. After that dry benzene (2 mL) was added to the reaction mixture and the tube was securely closed. The reaction mixture was stirred under visible light irradiation for 24 h in N_2 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. Further purification by column chromatography with EtOAc/hexane combination as the eluent afforded the corresponding product in 61% yield. The biaryl product (**3g**) was fully characterized by ^{1}H and ^{13}C NMR spectroscopies.

When the same reaction was repeated under dark condition, no product was isolated.

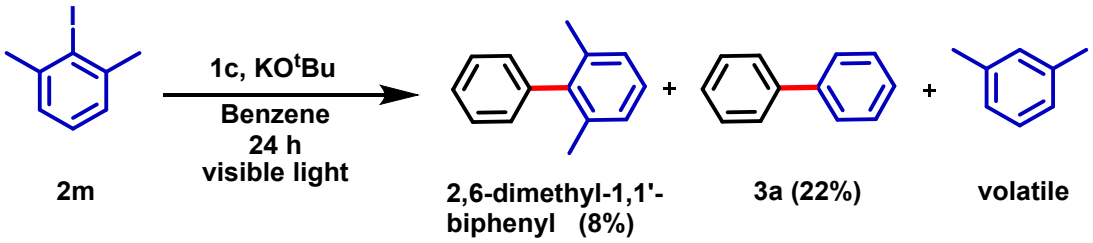
10.3. C-C cross-coupling reaction taking 9,9'-bifluorenylidene(1g)



Inside the glove box, a pressure tube was charged with 4-iodoanisole (0.5 mmol), KO^{t}Bu (1.5 mmol) and **1g** (10 mol%). After that dry benzene (2 mL) was added to the reaction mixture and the tube was closed properly. The reaction mixture was stirred under visible light irradiation for 24 h under N_2 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. Further purification by column chromatography with hexane afforded the corresponding product in 64% yield. The biaryl products were fully characterized by ^{1}H and ^{13}C NMR spectroscopies.

When the same reaction was repeated under dark condition, no product was isolated.

10.4. C-C cross-coupling reaction taking 2,6-dimethyl iodobenzene



Inside a glove box, a pressure tube was charged with 2,6-dimethyl iodobenzene (0.5 mmol), KO^{t}Bu (1.5 mmol) and fluorene (10 mol%). After that dry benzene (2 mL) was added to the reaction mixture and the tube was tightly closed. The reaction mixture was stirred under visible light irradiation for 24 h 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 reduced pressure. Purification of the crude mixture by column chromatography with hexane afforded 2,6-dimethyl-1,1'-biphenyl (8%) and **3a** (22%) in overall 30% yield. The biaryl products were fully characterized by ^{1}H and ^{13}C NMR spectroscopies.

10.5. Electron paramagnetic resonance spectroscopy

In a solution of **1g** (0.05 mmol, 17 mg) in toluene, KO^{t}Bu (0.07 mmol, 8 mg) was added. The reaction mixture was irradiated with visible light. The light exposure was continued for 5 minutes during which the yellow color of the solution was changed to dark brown. The X-band EPR measurement of this solution was carried out at room temperature. A sharp signal at g = 2.004 was observed, which indicated the formation of an organic radical anion.

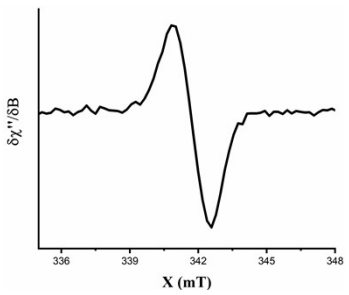


Figure S7. X-band (9.32 GHz) EPR signal of **1f** obtained from **1g** and KO^{t}Bu mixture after shining visible light.

10.6. Radical quenching experiment:

To a solution of fluorene (0.1 mmol), KO^{t}Bu (1.5 mmol), 4-iodoanisole (0.5 mmol) in benzene (2 mL), TEMPO (1 equiv, 0.5 mmol) were added. The reaction mixture was stirred for 24 h under visible light irradiation. The reaction was quenched fully and no desired biaryl product was obtained. The TEMPO-adduct was detected by mass spectrometry (M+H = 264.1927).

11. Cyclic voltammetry:

We attempted to evaluate the oxidation potential of **1a** by cyclic voltammetry. To prepare **1a**, 3.5 mg of fluorene and 3 mg of KH (30 % w/w in mineral oil) were taken in 1 mL of dry THF and stirred for 10 min. Then the solution was filtered through PTFE filter. Then 19 mL THF solution of 0.1 M (nBu$_4$N)PF$_6$ was added to the filtrate as the supporting electrolyte. To evaluate the ground-state oxidation, a three-electrode set-up was used where glassy carbon was the working electrode, a Pt wire as the counter and Ag/AgCl containing 1M KCl solution as the reference electrode, respectively. The shown voltammogram (Figure S8A) was collected with a scan rate of 100 mV sec^{-1}. The peak positions for the anodic and cathodic waves were internally referenced with respect to Fc$^+$/Fc couple.

Furthermore, CV data for **1g** was collected by dissolving it (4 mg) in 15 mL THF with a 0.1 M (nBu$_4$N)PF$_6$ solution as the supporting electrolyte. The shown voltammogram (Figure S8b) was collected with a scan rate of 100 mV sec^{-1}. The peak positions for the anodic and cathodic waves were internally referenced with respect to Fc$^+$/Fc couple.

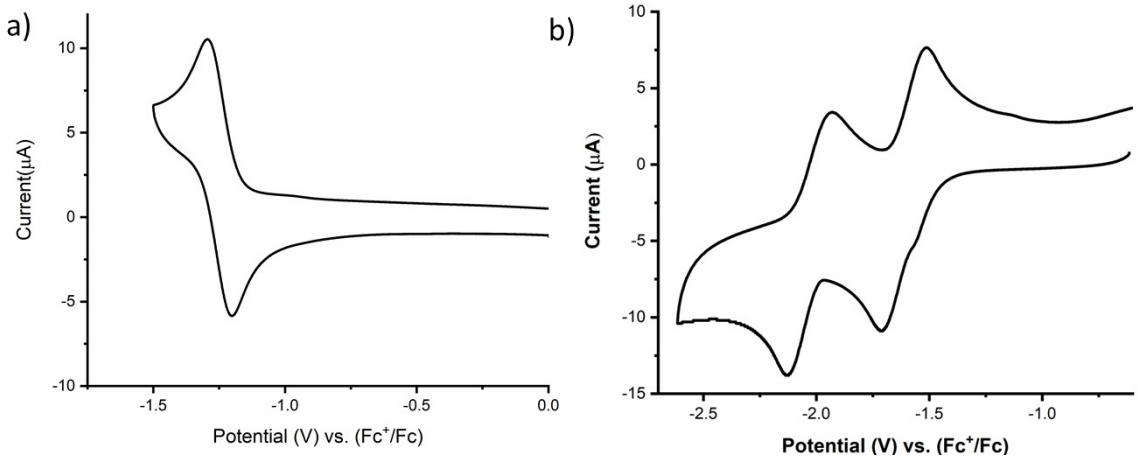


Figure S8. (a) Cyclic voltammogram of **1a**. (b) Cyclic voltammogram of **1g.**

12. The UV-Visible absorption experiments:

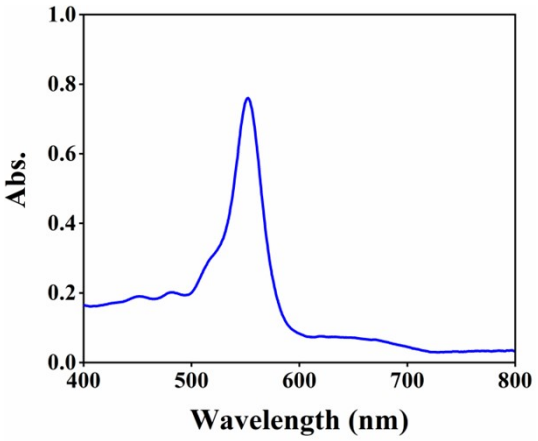


Figure S9. UV-visible spectra of **1a** in MeCN.

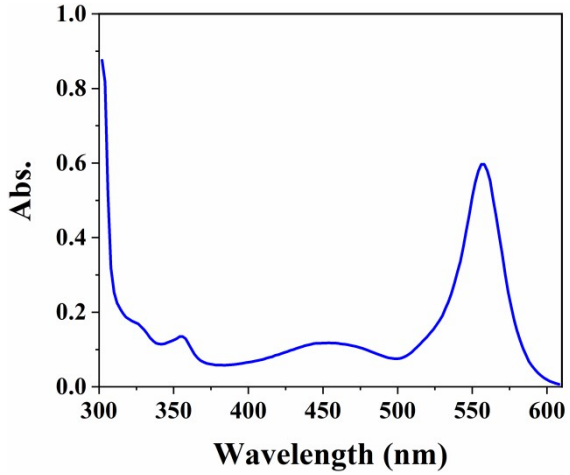


Figure S10. UV-visible spectra of **1d** in THF.

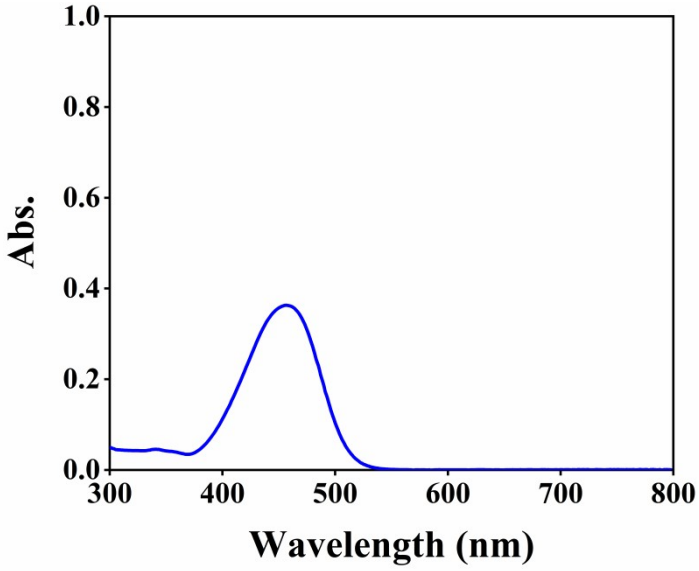


Figure S11. UV-visible spectra of **1g** in THF.

13. Fluorescence quenching experiment and Stern-Volmer plot:

In this experiment, measurements were carried out on a 10^{-6} M solution of **1a** in MeCN with appropriate amount of quencher in quartz cuvette. The sample solutions were previously degassed with argon. The solution was irradiated at 515 nm, and the emission intensity was examined at 571 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 in the presence of the quencher, [Q] is the concentration of added quencher and K_{SV} is the Stern-Volmer quenching constant.

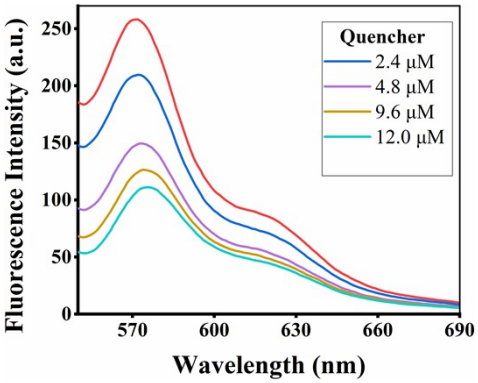


Figure S12. Emission spectra of **1a** in MeCN with different amounts of 4-iodo anisole added as quencher.

The ground-state oxidation potential for **1a** was measured vs. Fc^+/Fc and then converted to a value vs. SCE using the conversion $E^o_{1/2}$ (Fc^+/Fc) = +0.400 V vs. SCE. The ground state oxidation potential of the fluorene carbanion was measured electrochemically to be -1.4 V (vs SCE). The excited-state potential was estimated through modification of the ground state potential by $E_{o,o}$. The excited-state potential was calculated to be -3.6 V.

14. Computational data:

All calculations were carried out using Density Functional Theory as implemented in the Gaussian09[6] quantum chemistry programs. The geometries of stationary points were optimized with the B3LYP density functional theory. We used 6-31G(d) basis set for elements H, C. Harmonic force constants were computed at the optimized geometries to characterize the stationary points as minima. Spin density of the radical was visualized

through Gaussview.

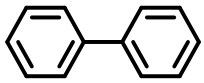
Coordinates:

1f

0 2
C -4.00267700 2.46740500 -1.28110300
C -2.73257900 2.94453000 -1.65401700
C -1.58946600 2.18672100 -1.43922100
C -1.70672600 0.92846300 -0.82186700
C -2.99838500 0.43715800 -0.48069000
C -4.13991800 1.20886800 -0.70465300
H -4.88162600 3.07815400 -1.46514900
H -2.64785300 3.91711300 -2.13104800
H -0.61659700 2.55042600 -1.76056800
H -5.12558900 0.82719800 -0.44790900
C -1.43703000 -1.22669000 -0.01008300
C -0.99627300 -2.43931900 0.56401600
C -1.92442200 -3.30616500 1.13629000
C -3.29313800 -2.99302100 1.16308900
C -3.74390700 -1.78702400 0.62935400
C -2.82953900 -0.90282800 0.05861600
H 0.05408100 -2.72136000 0.53315600
H -1.58274900 -4.24908400 1.55527100
H -3.99856800 -3.69007300 1.60523900
H -4.80024500 -1.53081600 0.67198800
C -0.70679900 -0.08128600 -0.52946300
C 0.70645200 0.08162300 -0.52965300
C 1.70632400 -0.92810800 -0.82229100
C 1.43676300 1.22693300 -0.01019100
C 1.58899900 -2.18628400 -1.43982600
C 2.99803600 -0.43688600 -0.48114500
C 0.99604600 2.43940400 0.56427200
C 2.82927100 0.90303100 0.05834400
C 2.73207300 -2.94409200 -1.65480100
H 0.61610300 -2.54991200 -1.76117600
C 4.13953400 -1.20860800 -0.70529600
C 1.92425000 3.30612800 1.13662600
H -0.05433700 2.72135400 0.53370500
C 3.74370600 1.78712100 0.62917100
C 4.00221700 -2.46705700 -1.28190200
H 2.64728800 -3.91660100 -2.13197200
H 5.12523500 -0.82699200 -0.44858400
C 3.29298600 2.99300300 1.16318900
H 1.58261000 4.24892900 1.55589800
H 4.80004600 1.53089800 0.67165900
H 4.88113500 -3.07780500 -1.46610300
H 3.99845500 3.68997100 1.60540800
K 0.00146400 -0.00102800 2.28103100

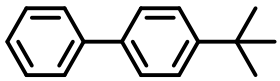
15. Analytical data:

Biphenyl (3a) :



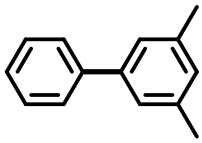
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 61 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.43 – 7.35 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 128.9, 127.4, 127.3. Spectroscopic data matched with the literature.[7]

4-(tert-butyl)-1,1'-biphenyl (3b) :



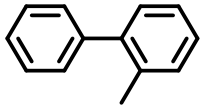
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a white solid (yield: 63 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.3 Hz, 2H), 7.66 (d, *J* = 8.2 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.53 (t, *J* = 7.7 Hz, 2H), 7.43 (t, *J* = 7.3 Hz, 1H), 1.49 (s, 9H).^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 141.2, 138.5, 128.8, 127.2, 127.1, 126.9, 125.8, 34.6, 31.5. Spectroscopic data matched with the literature.[8]

3,5-dimethyl-1,1'-biphenyl (3c) :



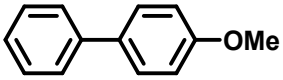
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a yellow oil (yield: 65 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.5 Hz, 7H), 7.58 – 7.52 (m, 9H), 7.49 – 7.43 (m, 4H), 7.36 (s, 8H), 7.13 (s, 3H), 2.52 (s, 30H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 141.4, 141.2, 138.2, 128.9, 128.6, 127.2, 127.1, 125.1, 21.4. Spectroscopic data matched with the literature.[9]

2-methyl-1,1'-biphenyl (3d) :



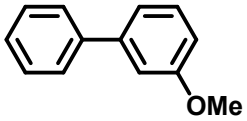
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 59 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.49 (m, 2H), 7.44 (d, *J* = 8.1 Hz, 3H), 7.41 – 7.33 (m, 4H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 135.4, 130.4, 129.9, 129.3, 128.2, 127.4, 126.9, 125.9, 20.6. Spectroscopic data matched with the literature.[10]

4-methoxy-1,1'-biphenyl (3e) :



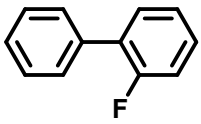
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a white solid (yield: 75 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.47 (m, 4H), 7.39 (t, *J* = 7.1 Hz, 2H), 7.29 (d, *J* = 8.8 Hz, 1H), 6.95 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 140.9, 133.9, 128.8, 128.3, 126.8, 126.8, 114.3, 55.4. Spectroscopic data matched with the literature.[7]

3-methoxy-1,1'-biphenyl (3f) :



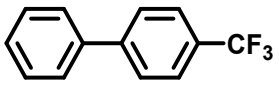
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a white solid (yield: 66 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.6 Hz, 2H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.40 – 7.35 (m, 2H), 7.21 (d, *J* = 7.6 Hz, 1H), 7.16 (s, 1H), 6.92 (dd, *J* = 8.2, 2.7 Hz, 1H), 3.89 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 142.9, 141.2, 129.9, 128.9, 127.6, 127.3, 119.8, 113.0, 112.8, 55.4. Spectroscopic data matched with the literature.[10]

2-fluoro-1,1'-biphenyl (3g) :



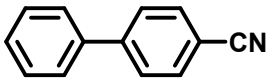
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a white solid (yield: 71 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.4 Hz, 2H), 7.50 – 7.44 (m, 3H), 7.42 – 7.30 (m, 2H), 7.25 – 7.14 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 158.7, 136.0, 130.9, 130.9, 129.3, 129.2, 129.2, 129.1, 129.1, 128.6, 127.8, 124.5, 124.5, 116.3, 116.1. Spectroscopic data matched with the literature.[11]

4-(trifluoromethyl)-1,1'-biphenyl (3h) :



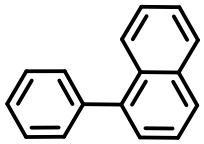
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a white solid (yield: 80 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (s, 4H), 7.64 (d, *J* = 7.7 Hz, 2H), 7.52 (t, *J* = 7.5 Hz, 2H), 7.46 (d, *J* = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 139.9, 129.1, 128.3, 127.6, 127.4, 125.9, 125.9, 125.8, 125.8, 123.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.33. Spectroscopic data matched with the literature.[12]

[1,1'-biphenyl]-4-carbonitrile (3i) :



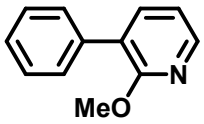
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a white solid (yield: 78 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.66 (m, 4H), 7.59 (dd, *J* = 6.9, 1.6 Hz, 2H), 7.51 – 7.46 (m, 2H), 7.46 – 7.40 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 139.3, 132.7, 129.2, 128.8, 127.9, 127.4, 119.1, 111.0. Spectroscopic data matched with the literature.[13]

1-phenylnaphthalene (3j) :



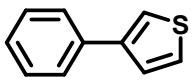
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a white solid (yield: 51 mg, 50%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 – 7.92 (m, 2H), 7.90 (d, *J* = 8.3 Hz, 1H), 7.61 – 7.50 (m, 6H), 7.47 (dd, *J* = 5.4, 1.6 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 140.8, 140.3, 133.9, 131.7, 130.1, 128.3, 127.7, 127.3, 127.0, 126.1, 125.8, 125.4. Spectroscopic data matched with the literature.[14]

2-methoxy-3-phenylpyridine (3k) :



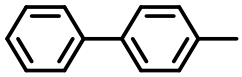
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless oil (yield: 55 mg, 59%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 5.0, 1.9 Hz, 1H), 7.62 (dd, *J* = 14.6, 7.1 Hz, 3H), 7.46 (t, *J* = 7.4 Hz, 2H), 7.39 (t, *J* = 7.3 Hz, 1H), 6.99 (dd, *J* = 7.3, 5.0 Hz, 1H), 4.02 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 145.8, 138.6, 136.8, 129.2, 128.3, 127.6, 124.7, 117.2. Spectroscopic data matched with the literature.[15]

3-phenylthiophene (3l) :



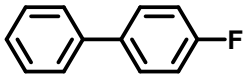
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 45 mg, 56%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.3 Hz, 2H), 7.53 – 7.41 (m, 5H), 7.37 (t, *J* = 7.4 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 142.4, 135.9, 128.9, 127.2, 126.6, 126.4, 126.3, 120.4. Spectroscopic data matched with the literature.[14]

4-methyl-1,1'-biphenyl (3m) :



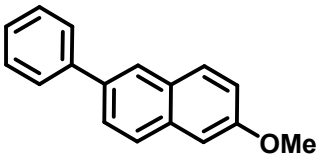
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a yellow oil (yield: 53 mg, 63%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 7.9 Hz, 2H), 7.50 (d, *J* = 7.7 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.26 (d, *J* = 7.7 Hz, 2H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 141.3, 138.5, 137.2, 129.6, 128.8, 127.1, 127.1, 21.2. Spectroscopic data matched with the literature.[21]

4-fluoro-1,1'-biphenyl (3n) :



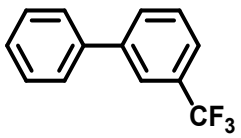
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a white solid (yield: 71 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.4 Hz, 2H), 7.50 – 7.44 (m, 3H), 7.42 – 7.30 (m, 2H), 7.25 – 7.14 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 158.7, 136.0, 130.9, 130.9, 129.3, 129.2, 129.2, 129.1, 129.1, 128.6, 127.8, 124.5, 124.5, 116.3, 116.1. Spectroscopic data matched with the literature.[11]

2-methoxy-6-phenylnaphthalene (3o) :



The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a white solid (yield: 53 mg, 45%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 1.8 Hz, 1H), 7.84 – 7.79 (m, 2H), 7.75 – 7.69 (m, 3H), 7.52 – 7.46 (m, 2H), 7.41 – 7.35 (m, 1H), 7.23 – 7.16 (m, 2H), 3.95 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.9, 141.3, 136.5, 133.9, 129.8, 129.3, 128.9, 127.4, 127.3, 127.2, 126.2, 125.7, 119.3, 105.6. Spectroscopic data matched with the literature.[22]

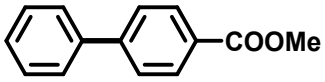
3-(trifluoromethyl)-1,1'-biphenyl (3p) :



The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a white solid (yield: 82 mg, 74%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 (d, *J* = 2.0 Hz, 1H), 7.78 (dt, *J* = 7.6, 1.8 Hz, 1H), 7.65 – 7.60 (m, 3H), 7.57 (t, *J* = 7.7 Hz, 1H), 7.51 – 7.46 (m, 2H), 7.44 – 7.39 (m, 1H). ^{13}C NMR (100 MHz,

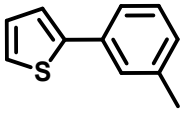
Chloroform-*d*) δ 142.1, 139.9, 130.6, 129.4, 129.1, 128.2, 127.3, 124.1, 124.0. Spectroscopic data matched with the literature.[21]

methyl [1,1'-biphenyl]-4-carboxylate (3q) :



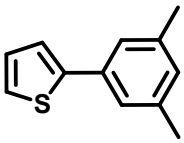
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 59 mg, 70%). Spectroscopic data matched with the literature.[24] ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 7.0 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 3.94 (s, 3H).^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.2, 145.8, 140.1, 130.2, 129.1, 129.0, 128.3, 127.4, 127.2, 52.3.

2-(3-methylphenyl)thiophene (4a) :



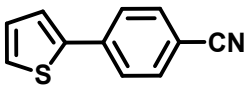
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 53 mg, 61%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 (d, *J* = 7.3 Hz, 2H), 7.35 – 7.26 (m, 3H), 7.15 – 7.07 (m, 2H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 144.7, 138.6, 134.4, 128.9, 128.4, 128.1, 126.8, 124.8, 123.2, 123.1, 21.6. Spectroscopic data matched with the literature.[25]

2-(3,5-dimethylphenyl)thiophene (4b) :



The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 56 mg, 59%).^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 (d, *J* = 4.7 Hz, 1H), 7.27 (d, *J* = 5.1 Hz, 3H), 7.08 (dd, *J* = 5.1, 3.6 Hz, 1H), 6.95 (s, 1H), 2.37 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 144.8, 138.5, 134.3, 129.3, 127.9, 124.6, 123.9, 122.9, 21.4. Spectroscopic data matched with the literature.[26]

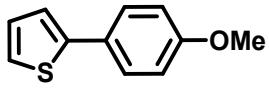
2-(4-cyanophenyl)thiophene (4c) :



The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 63 mg, 68%).^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 (q, *J* = 8.7 Hz, 4H), 7.43 – 7.37 (m, 2H), 7.13 (dd, *J* = 5.1, 3.7 Hz, 1H).

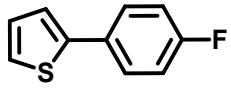
^{13}C NMR (100 MHz, Chloroform-*d*) δ 142.1, 138.7, 128.6, 127.2, 126.2, 125.2, 118.9, 110.6. Spectroscopic data matched with the literature.[17]

2-(4-methoyphenyl)thiophene (4d) :



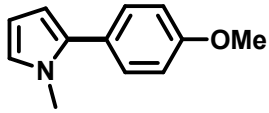
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 53 mg, 56%).^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 – 7.53 (m, 2H), 7.25 – 7.20 (m, 2H), 7.07 (dd, *J* = 5.1, 3.6 Hz, 1H), 6.95 – 6.91 (m, 2H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 159.3, 144.4, 128.0, 127.4, 127.3, 123.9, 122.2, 114.4. Spectroscopic data matched with the literature.[16]

2-(4-fluorophenyl)thiophene (4e) :



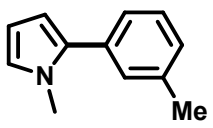
The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 60 mg, 67%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.55 (m, 2H), 7.28 (d, *J* = 5.1 Hz, 1H), 7.26 (d, *J* = 3.6 Hz, 1H), 7.13 – 7.06 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.6, 161.2, 143.4, 130.8, 128.2, 127.8, 127.7, 124.9, 123.2, 116.0, 115.8. Spectroscopic data matched with the literature.[25]

2-(4-methoxyphenyl)-1-methyl-1H-pyrrole (5a) :



The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 51 mg, 54%). Spectroscopic data matched with the literature.[18] ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 (d, *J* = 8.6 Hz, 2H), 6.96 (d, *J* = 8.7 Hz, 2H), 6.74- 6.69 (m, 1H), 6.21 (t, *J* = 3.1 Hz, 1H), 6.18 (dd, *J* = 3.4, 1.8 Hz, 1H), 3.86 (s, 3H), 3.65 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 158.7, 134.5, 130.1, 126.0, 123.1, 113.9, 108.1, 107.7, 55.4, 35.0.

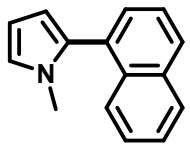
1-methyl-2-(m-tolyl)-1H-pyrrole (5b) :



The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 45 mg, 52%). Spectroscopic data

matched with the literature.[19] ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 (t, *J* = 7.5 Hz, 1H), 7.25 – 7.18 (m, 2H), 7.13 (d, *J* = 7.3 Hz, 1H), 6.71 (s, 1H), 6.21 (d, *J* = 2.9 Hz, 2H), 3.67 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 138.1, 134.9, 133.4, 129.6, 128.3, 127.7, 125.9, 123.6, 108.6, 107.8.

1-methyl-2-(naphthalen-1-yl)-1H-pyrrole (5c) :



The compound was purified by column chromatography (silica gel 60–120 mesh) with hexane to give the product as a colourless solid (yield: 52 mg, 50%). Spectroscopic data matched with the literature.[20] ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (t, *J* = 7.6 Hz, 2H), 7.73 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.49 (dq, *J* = 15.9, 7.8 Hz, 4H), 6.83 (s, 1H), 6.32 (t, *J* = 3.0 Hz, 1H), 6.28 (s, 1H), 3.40 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 133.8, 133.4, 132.3, 131.4, 128.9, 128.3, 128.3, 126.4, 126.4, 126.0, 125.3, 122.6, 110.1, 107.7, 34.6.

16. ^{1}H and ^{13}C NMR spectra of compounds.

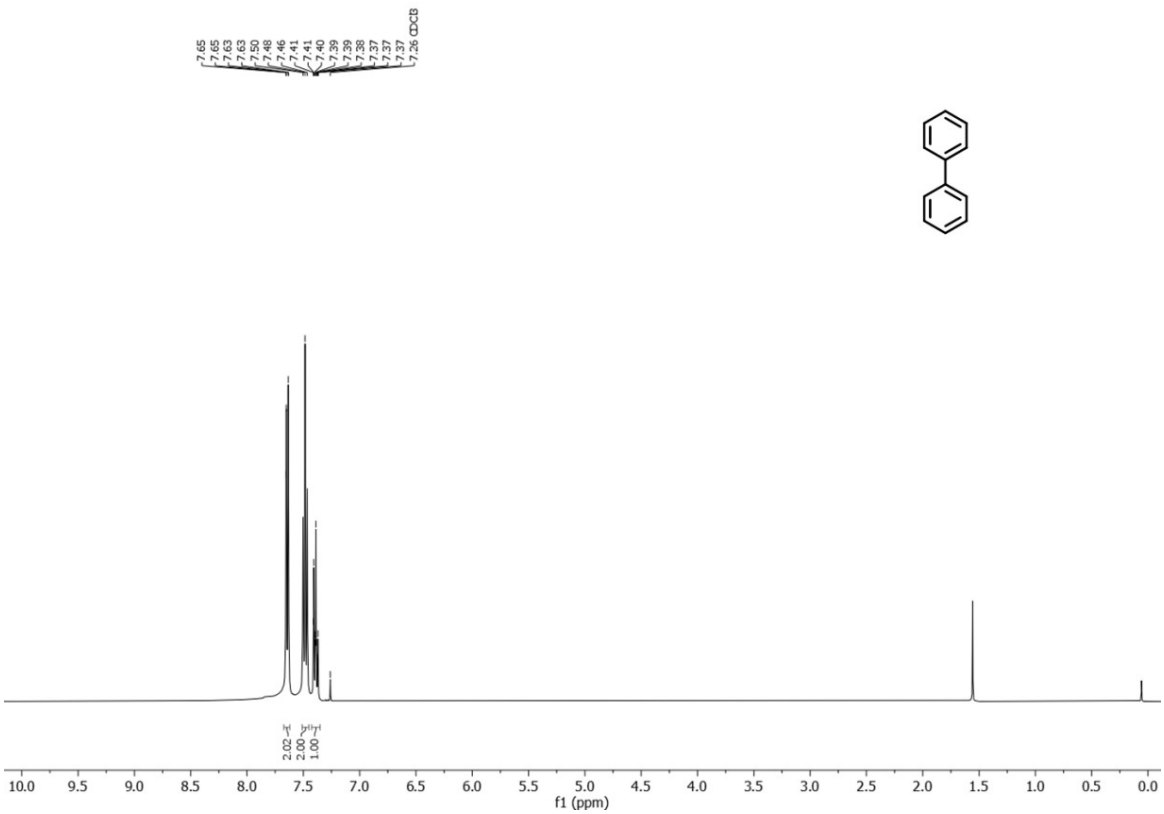


Figure S13. ^{1}H NMR spectrum (400 MHz) of **3a** in $CDCl_3$.

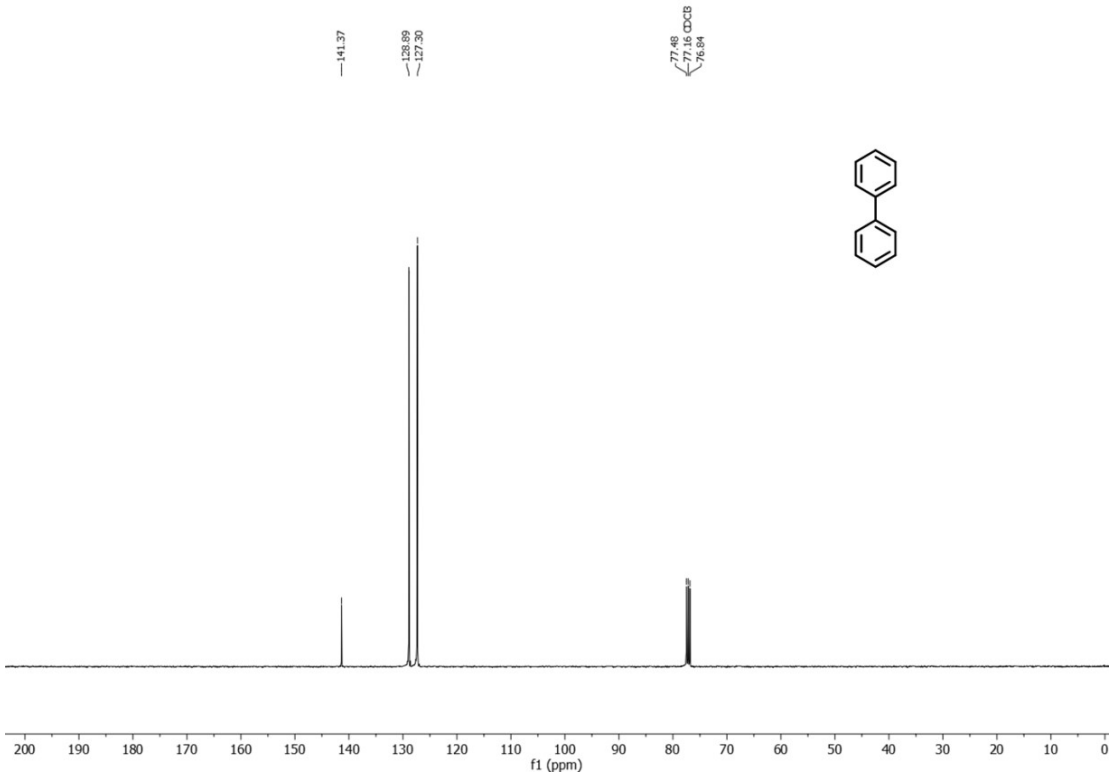


Figure S14. ^{13}C NMR spectrum (100 MHz) of **3a** in $CDCl_3$.

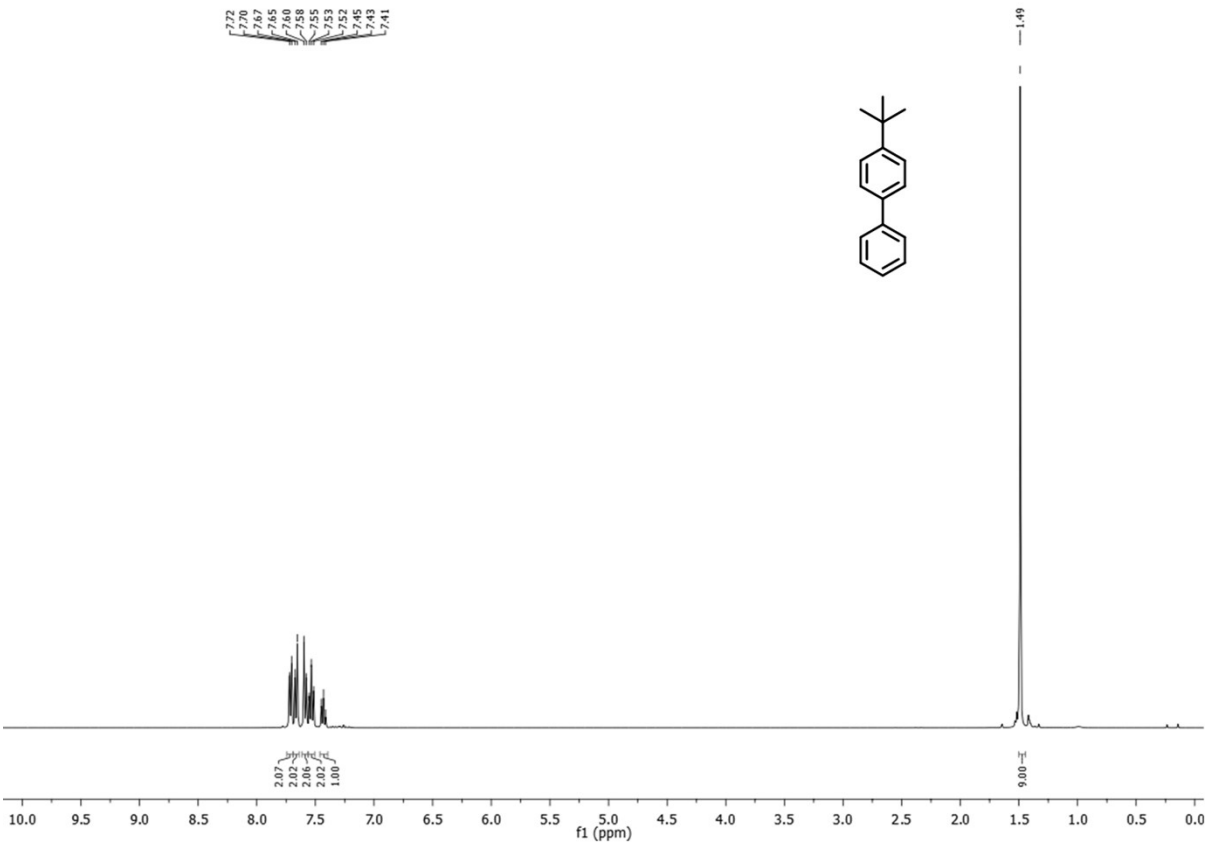


Figure S15. ^{1}H NMR spectrum (400 MHz) of **3b** in $CDCl_3$.

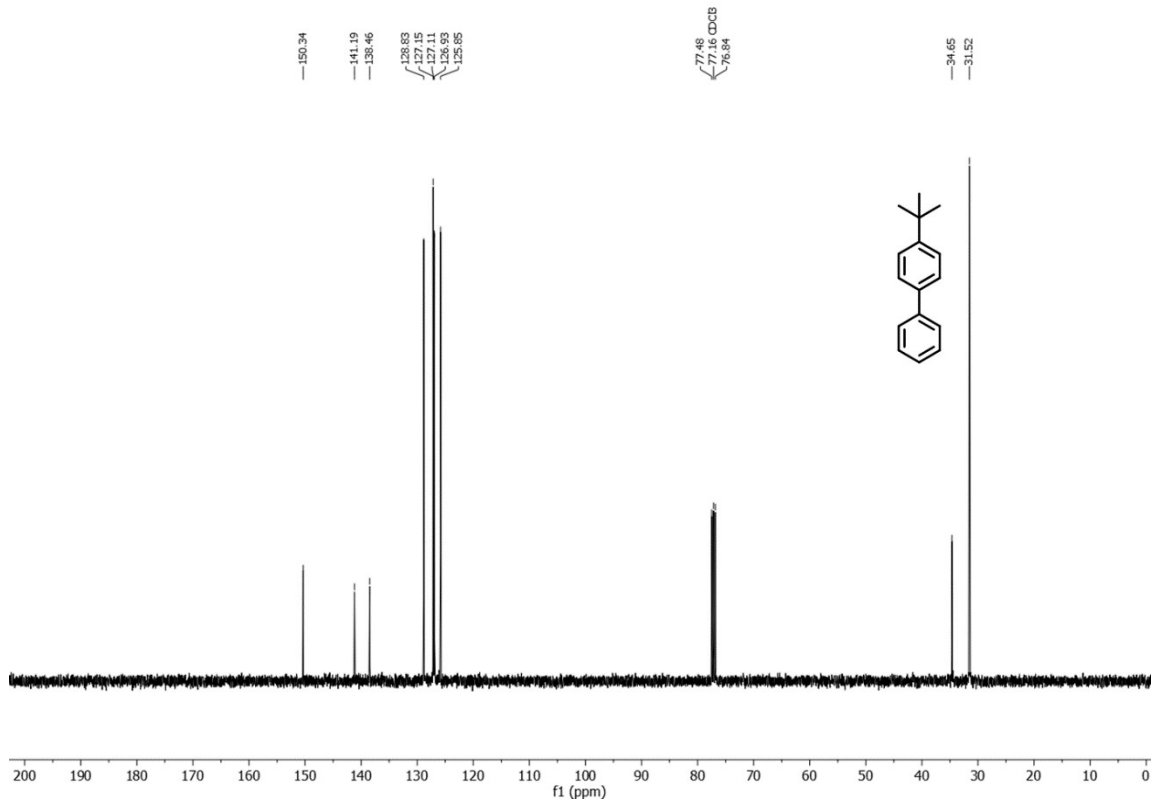


Figure S16. ^{13}C NMR spectrum (100 MHz) of **3b** in $CDCl_3$.

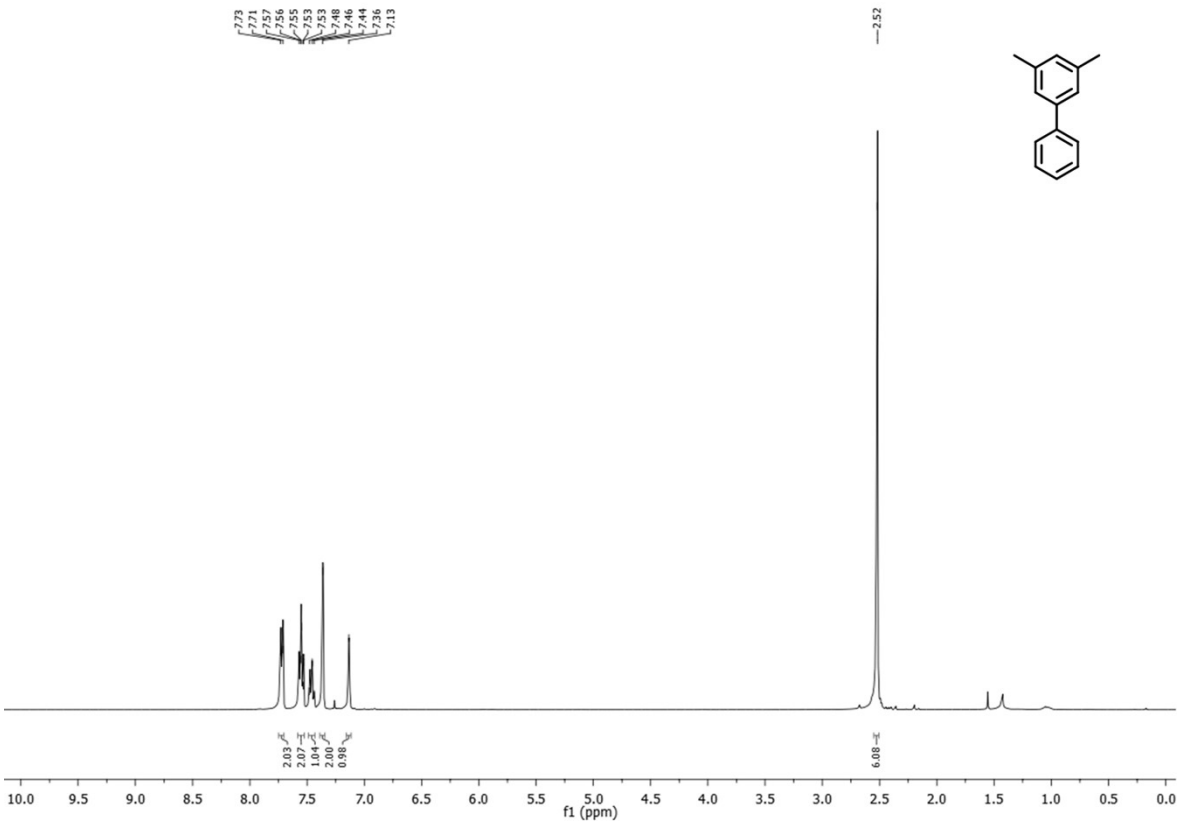


Figure S17. ^{1}H NMR spectrum (400 MHz) of **3c** in $CDCl_3$.

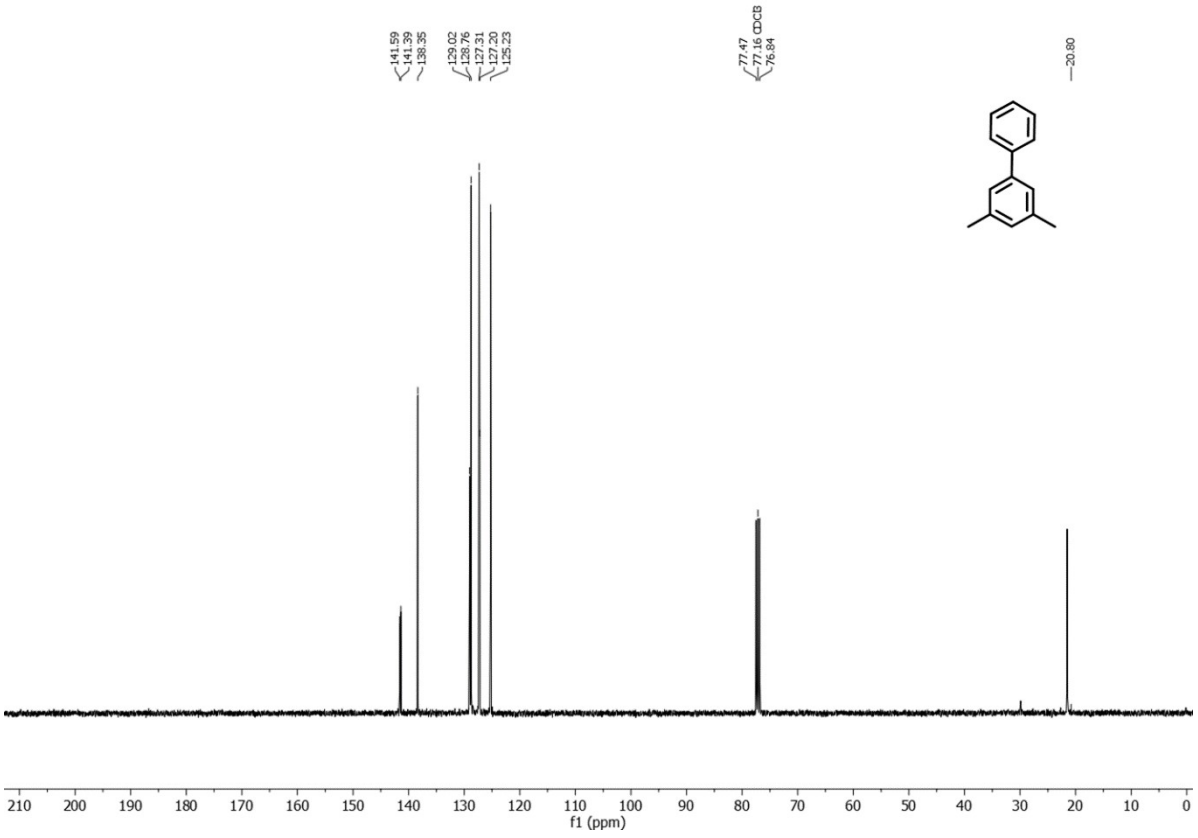


Figure S18. ^{13}C NMR spectrum (100 MHz) of **3c** in $CDCl_3$.

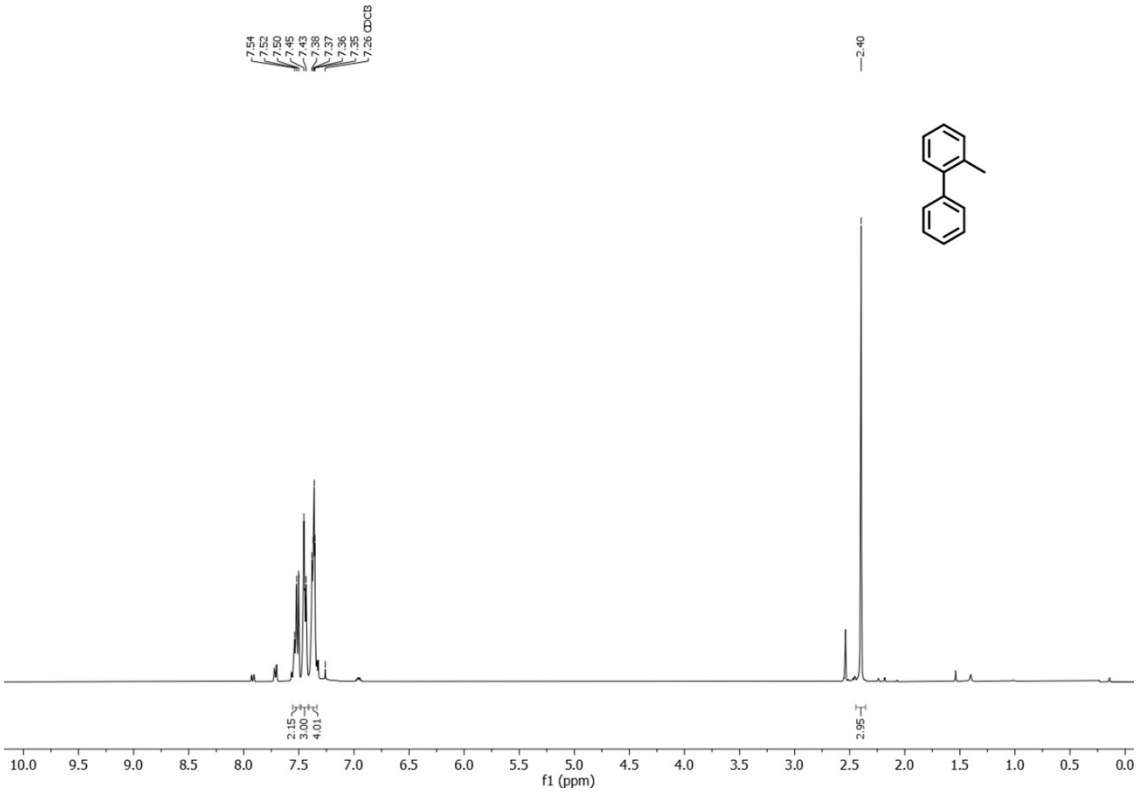


Figure S19. ^{1}H NMR spectrum (400 MHz) of **3d** in $CDCl_3$.

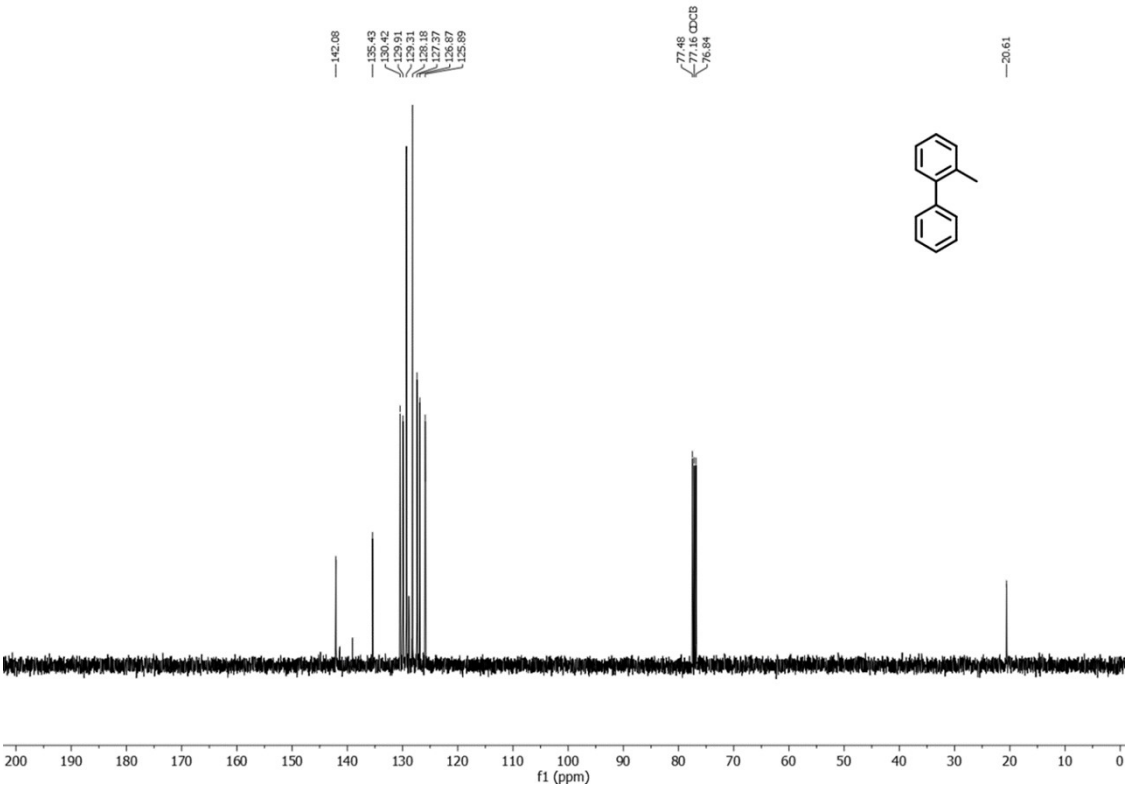


Figure S20. ^{13}C NMR spectrum (100 MHz) of **3d** in $CDCl_3$.

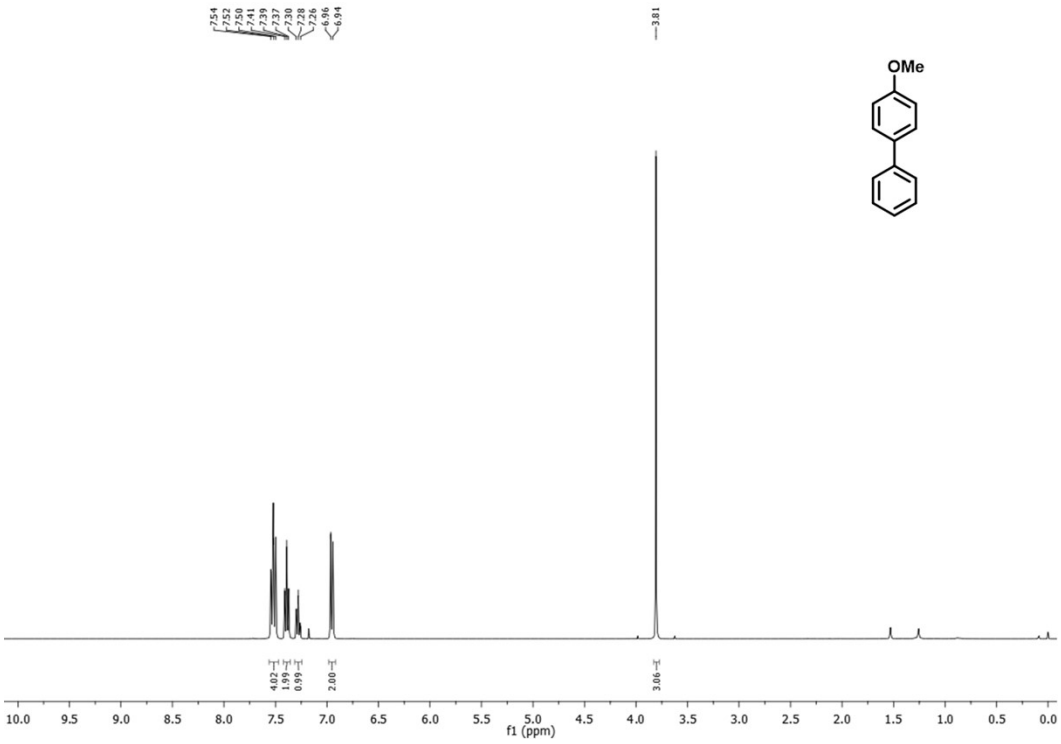


Figure S21. ^{1}H NMR spectrum (400 MHz) of **3e** in $CDCl_3$.

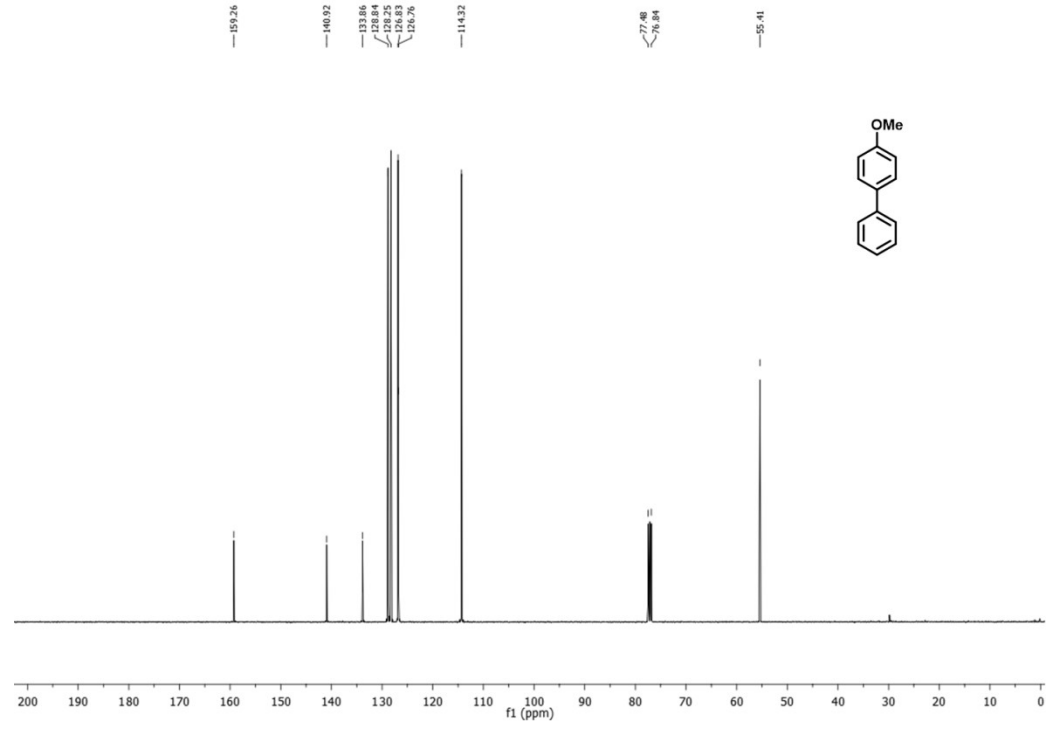


Figure S22. ^{13}C NMR spectrum (100 MHz) of **3e** in $CDCl_3$.

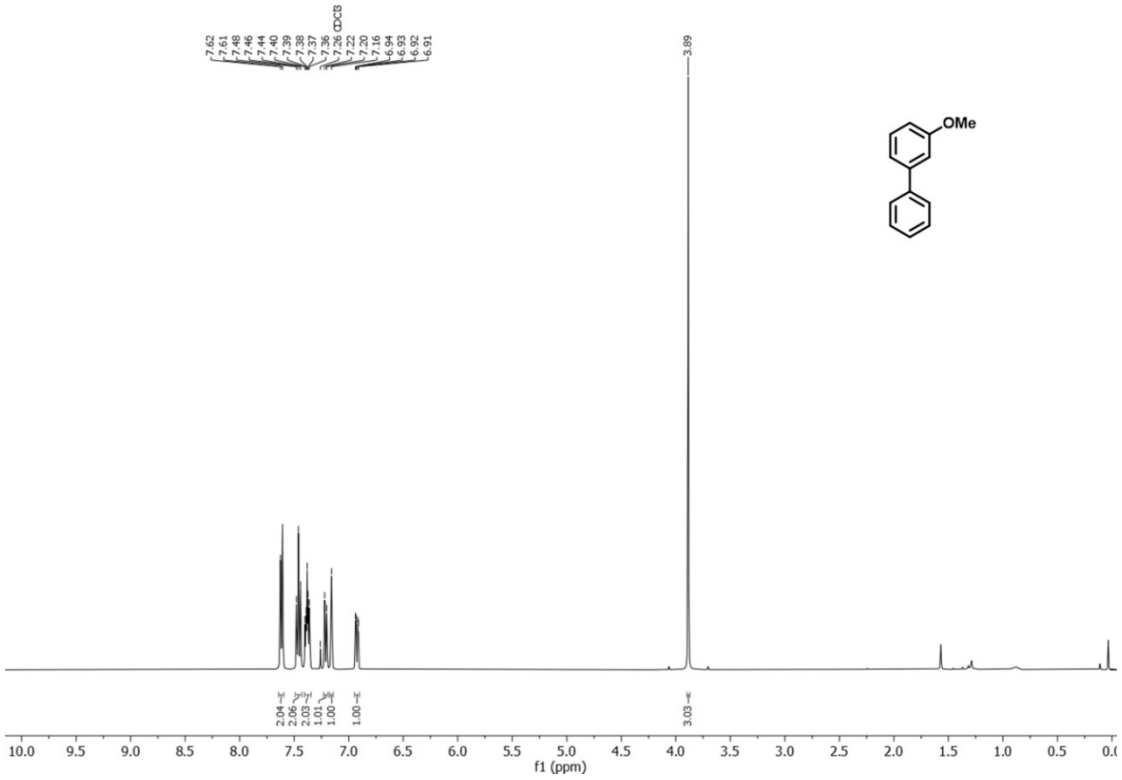


Figure S23. ^{1}H NMR spectrum (400 MHz) of **3f** in $CDCl_3$.

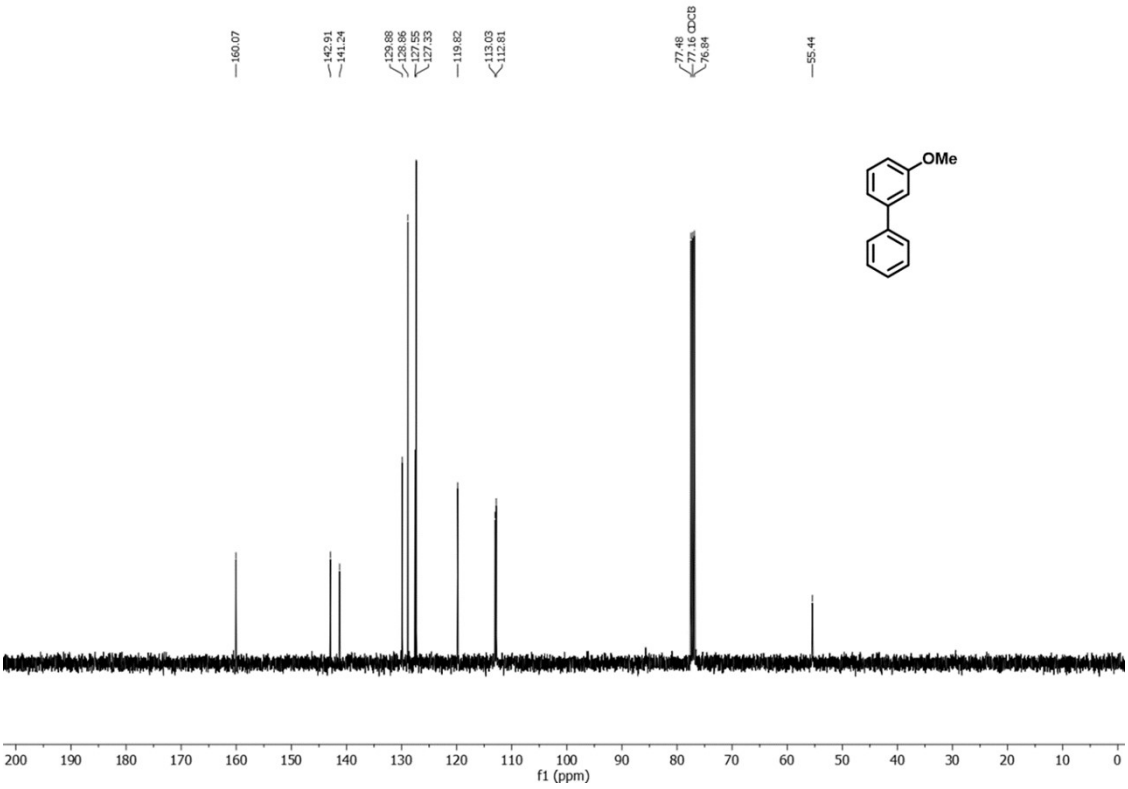


Figure S24. ^{13}C NMR spectrum (100 MHz) of **3f** in $CDCl_3$.

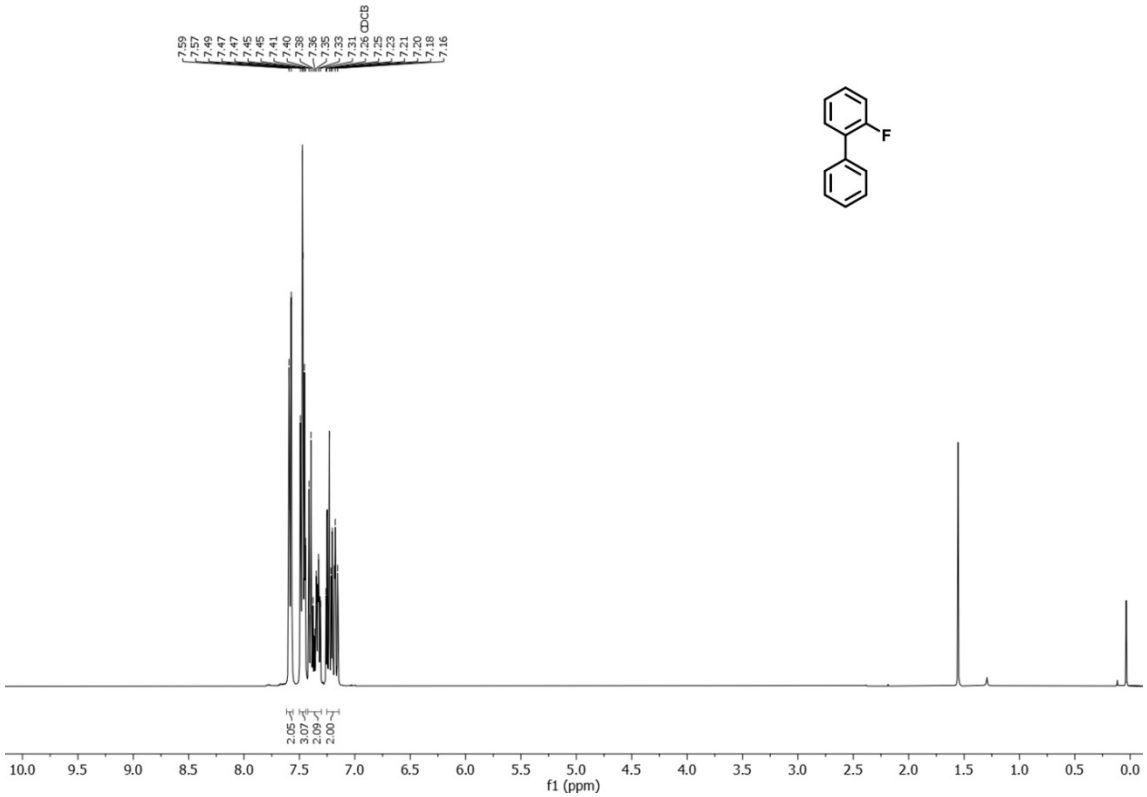


Figure S25. ^{1}H NMR spectrum (400 MHz) of **3g** in $CDCl_3$.

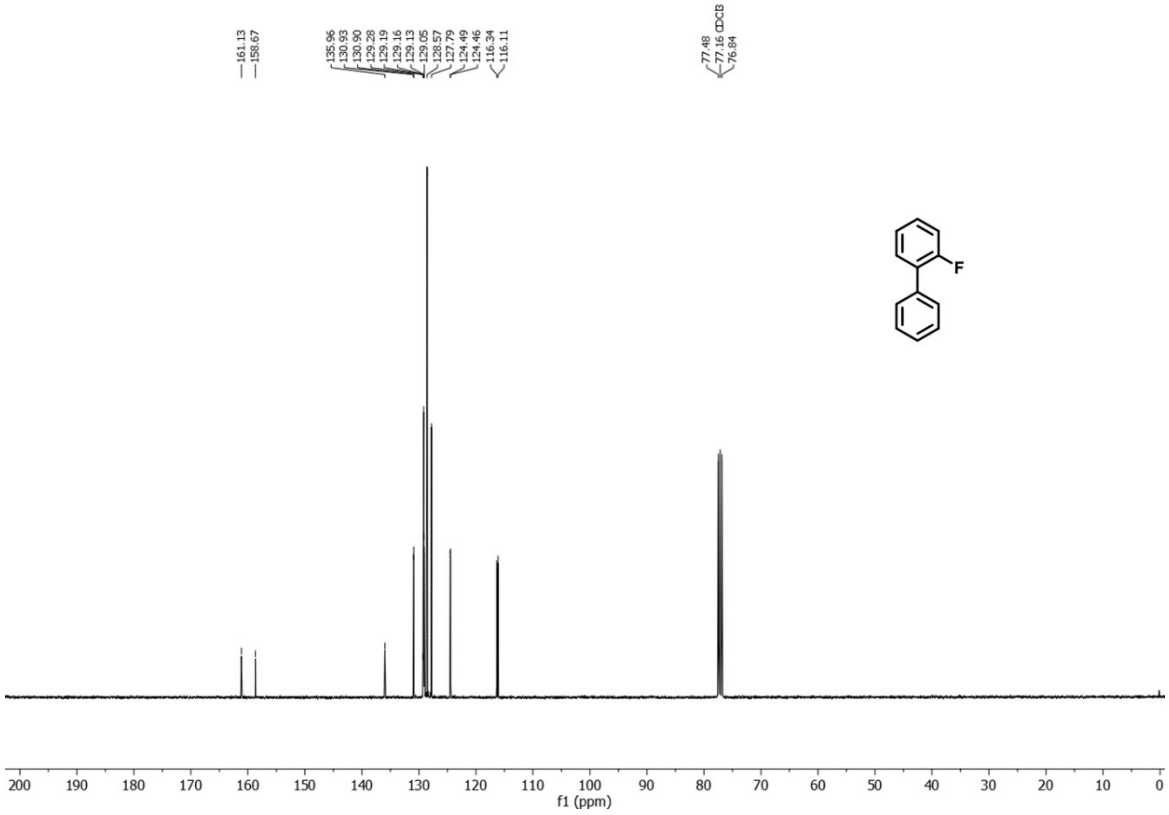


Figure S26. ^{13}C NMR spectrum (100 MHz) of **3g** in $CDCl_3$.

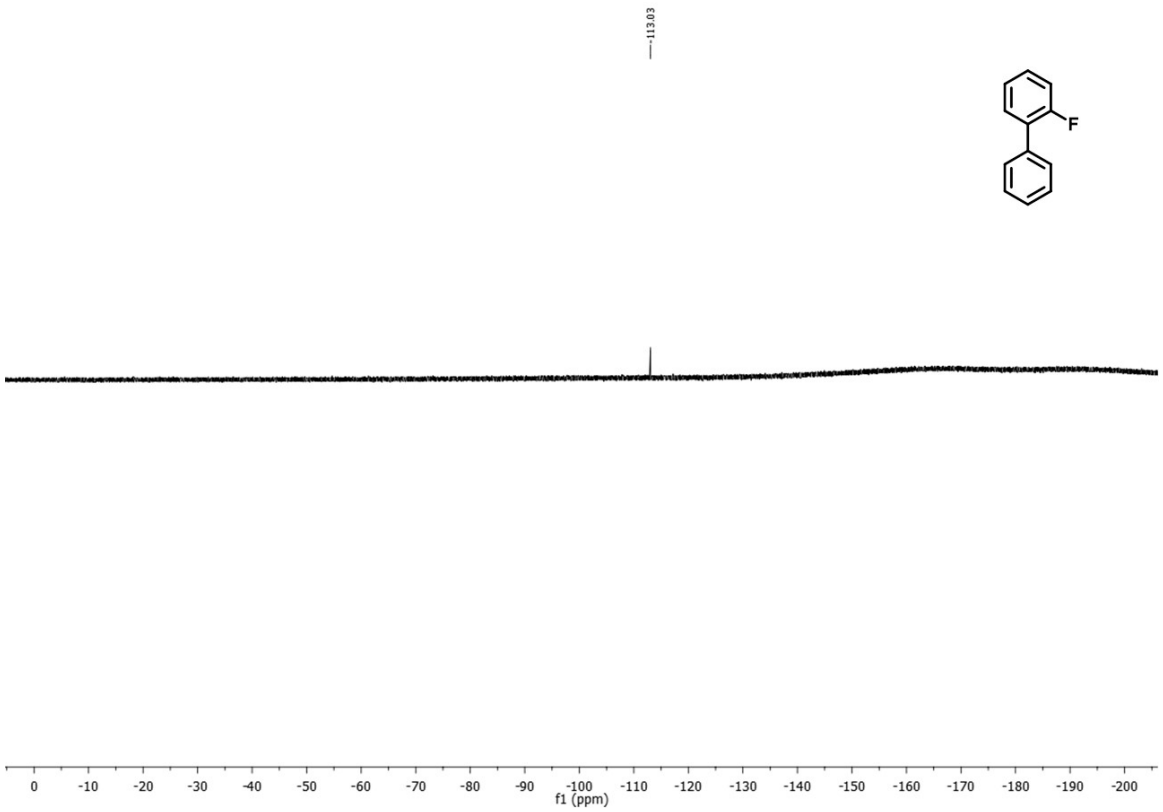


Figure S27. ^{19}F NMR spectrum (100 MHz) of **3g** in $CDCl_3$.

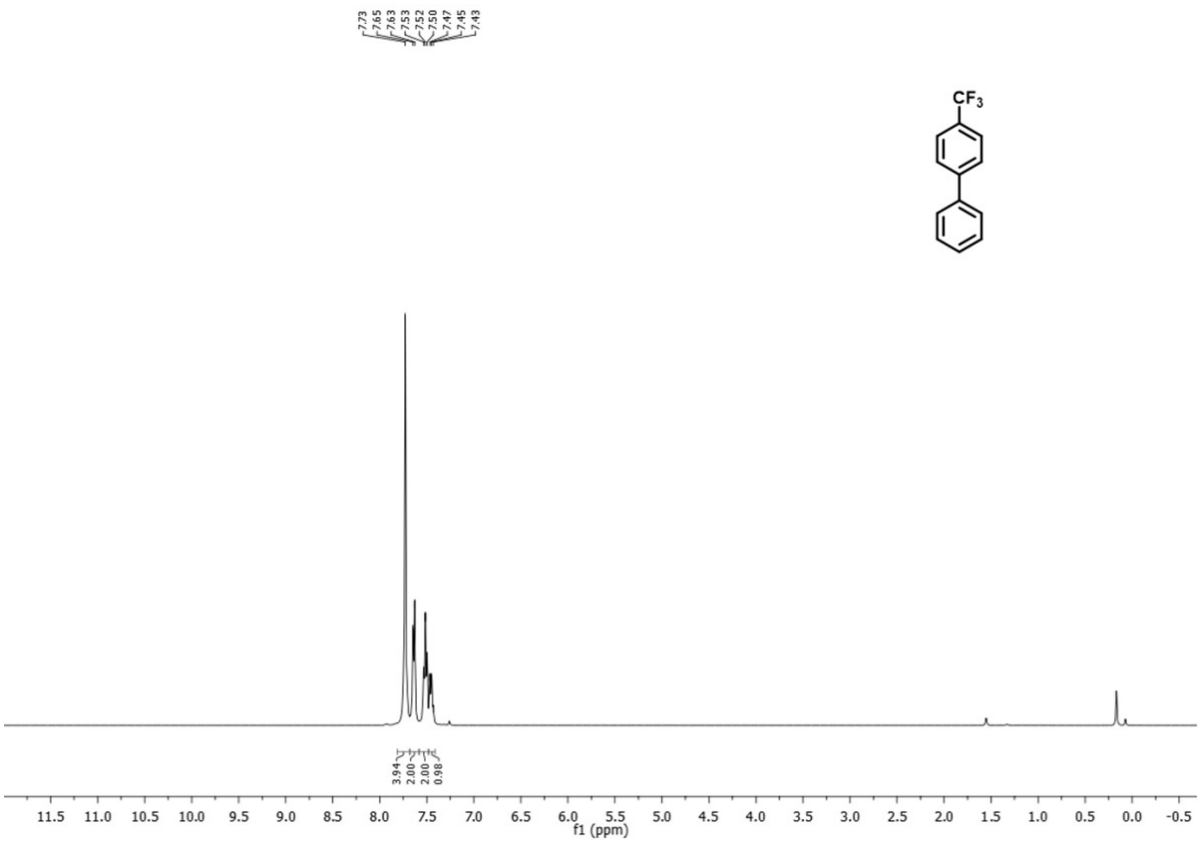


Figure S28. ^{1}H NMR spectrum (400 MHz) of **3h** in $CDCl_3$.

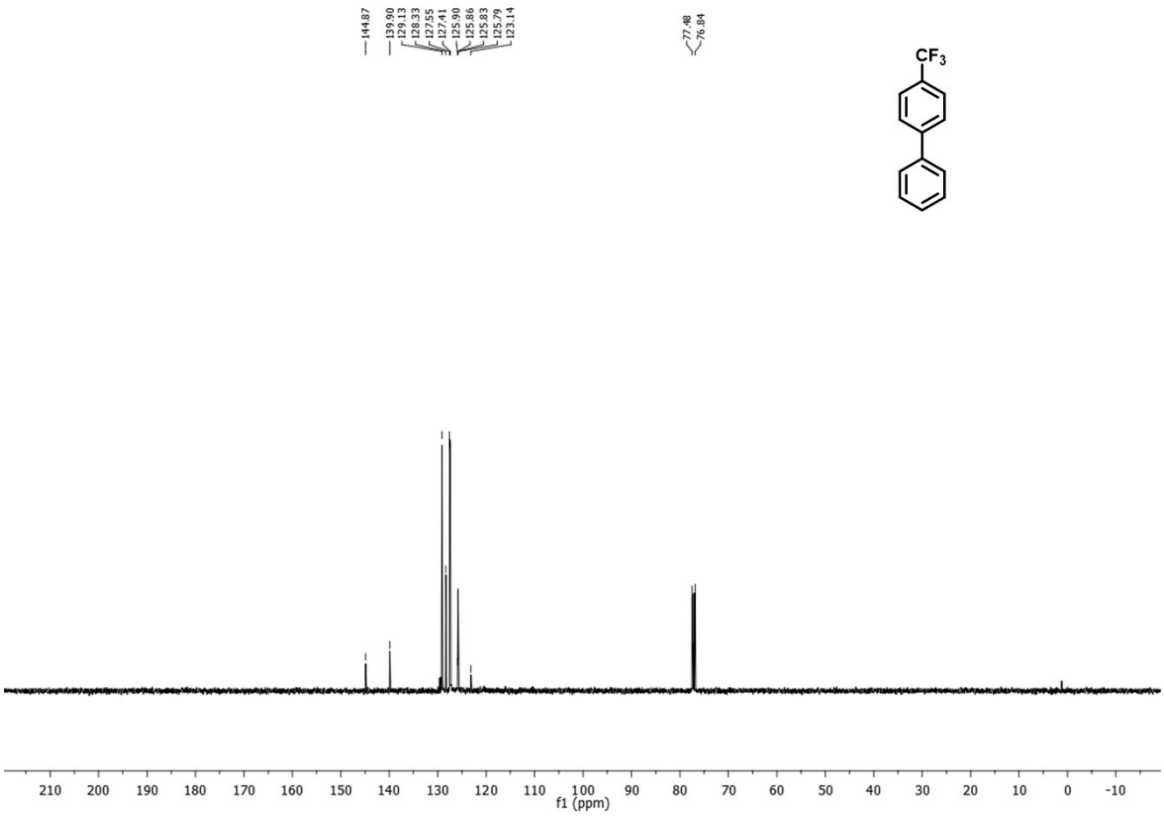


Figure S29. ^{13}C NMR spectrum (100 MHz) of **3h** in $CDCl_3$.

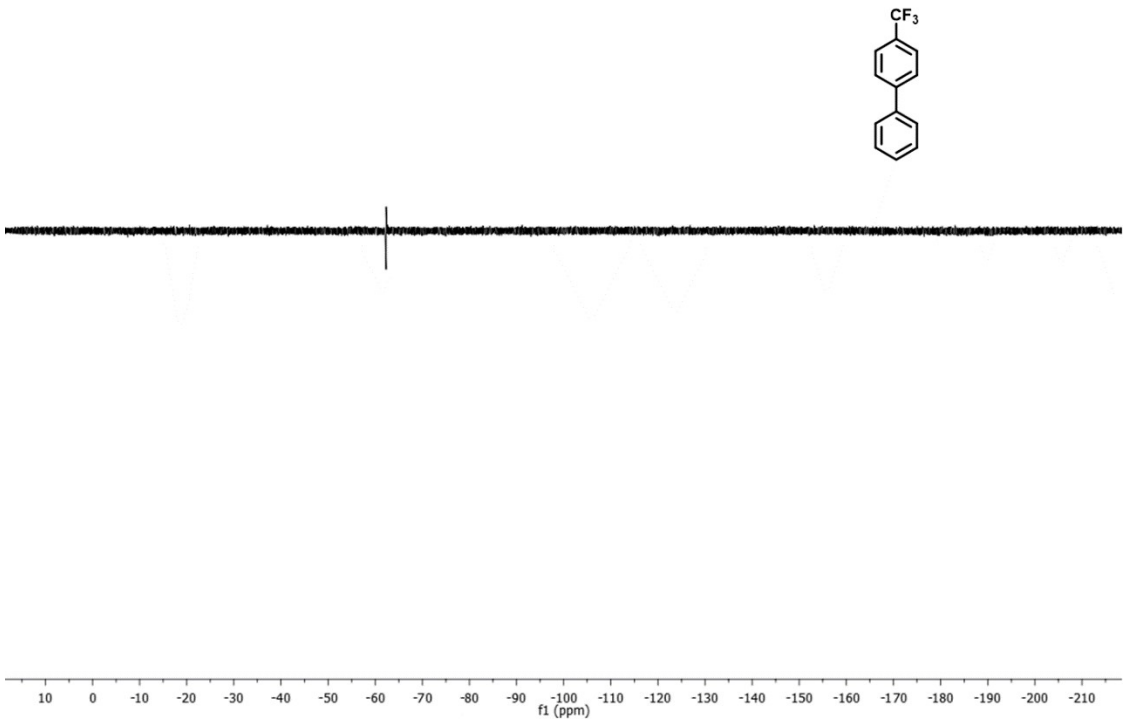


Figure S30. ^{19}F NMR spectrum (100 MHz) of **3h** in $CDCl_3$.

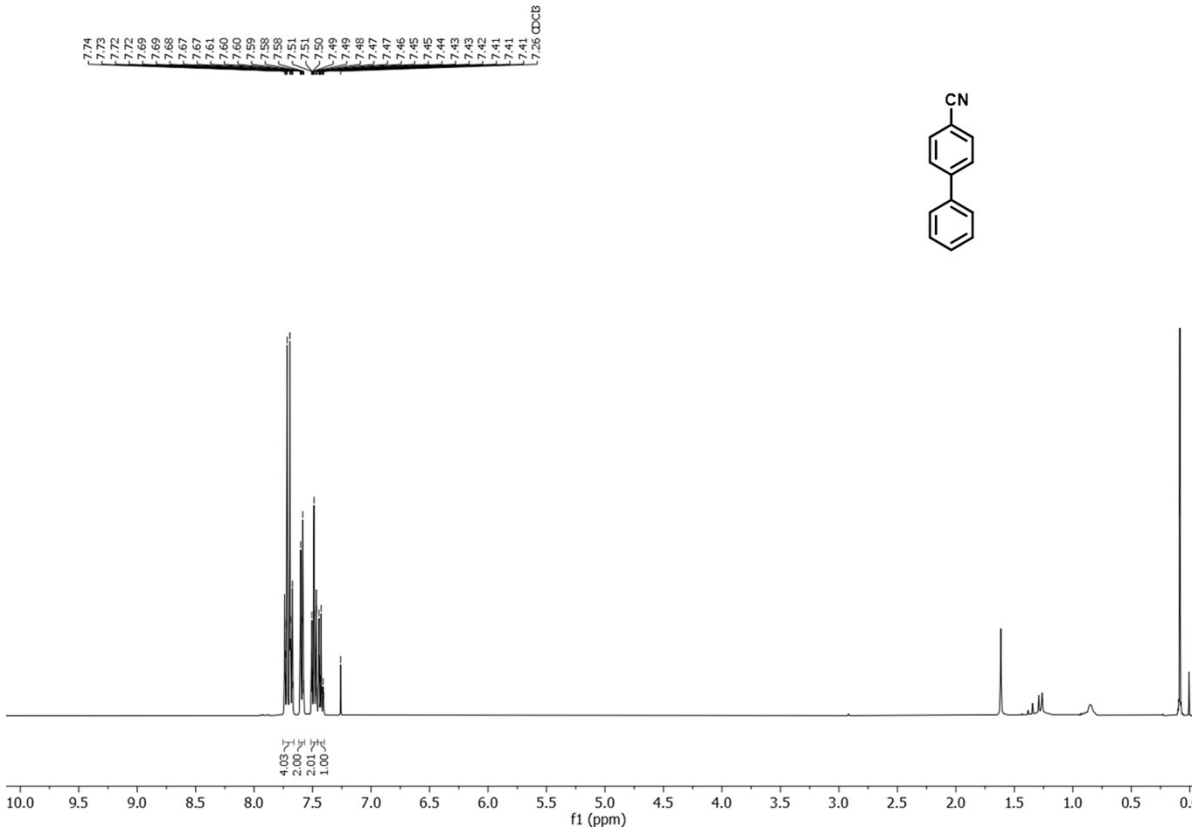


Figure S31. ^{1}H NMR spectrum (400 MHz) of **3i** in $CDCl_3$.

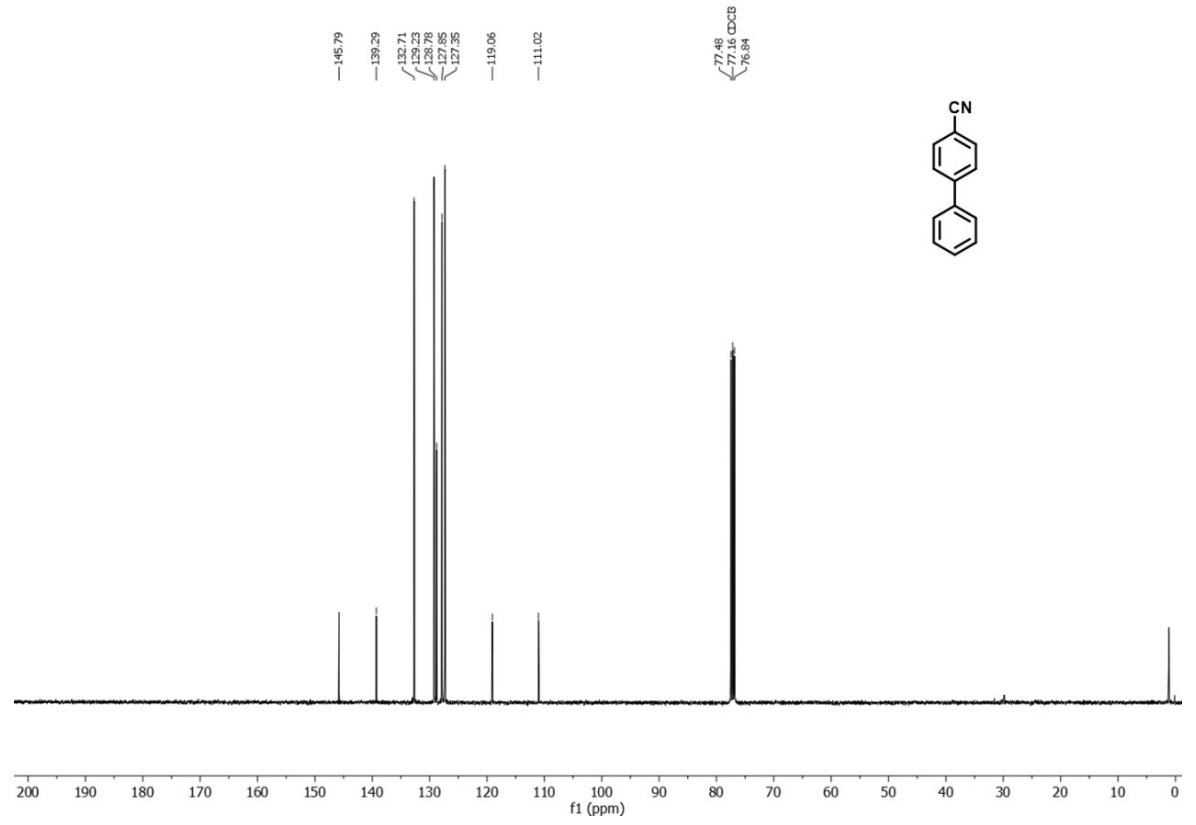


Figure S32. ^{13}C NMR spectrum (100 MHz) of **3i** in $CDCl_3$.

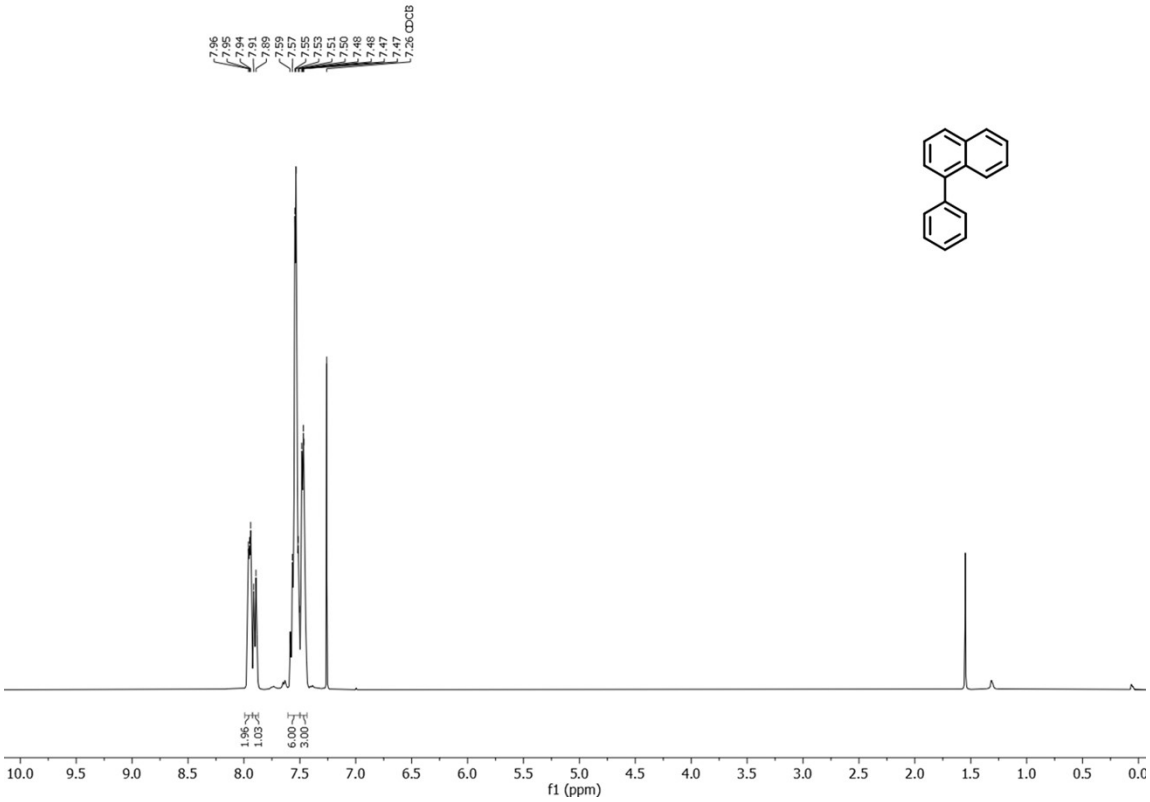


Figure S33. ^{1}H NMR spectrum (400 MHz) of **3j** in $CDCl_3$.

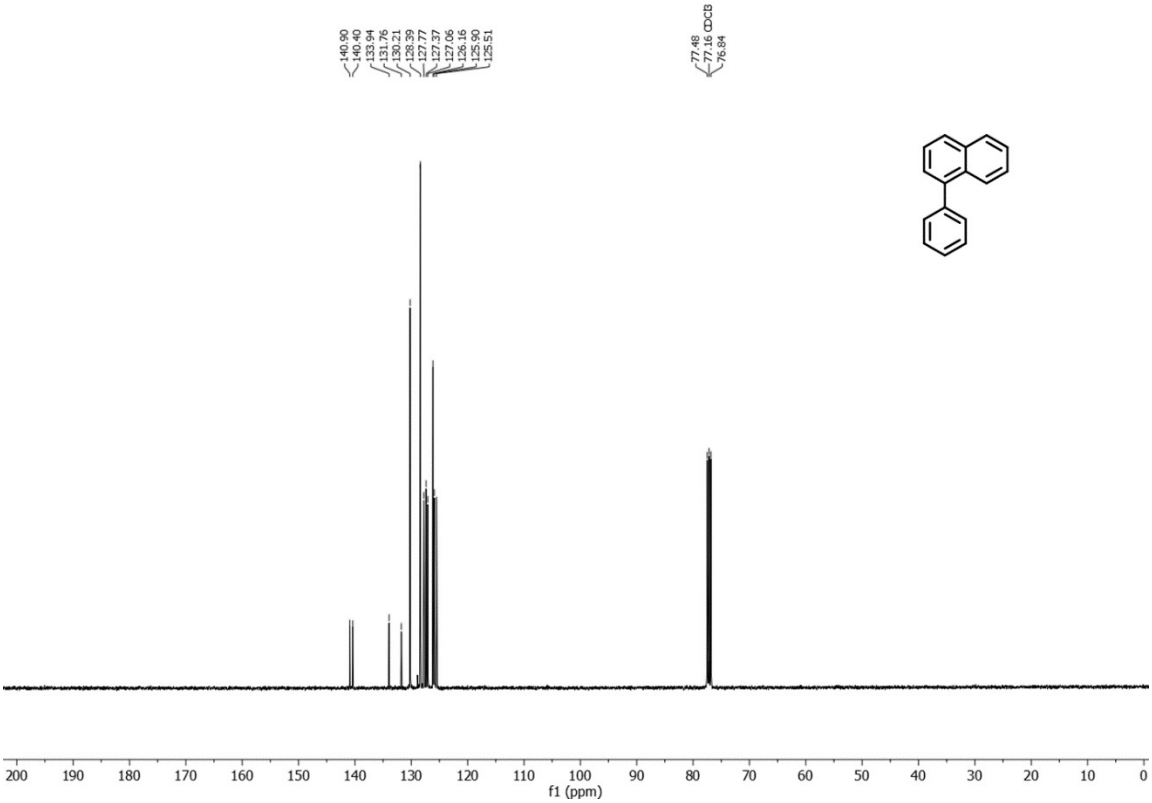


Figure S34. ^{13}C NMR spectrum (100 MHz) of **3j** in $CDCl_3$.

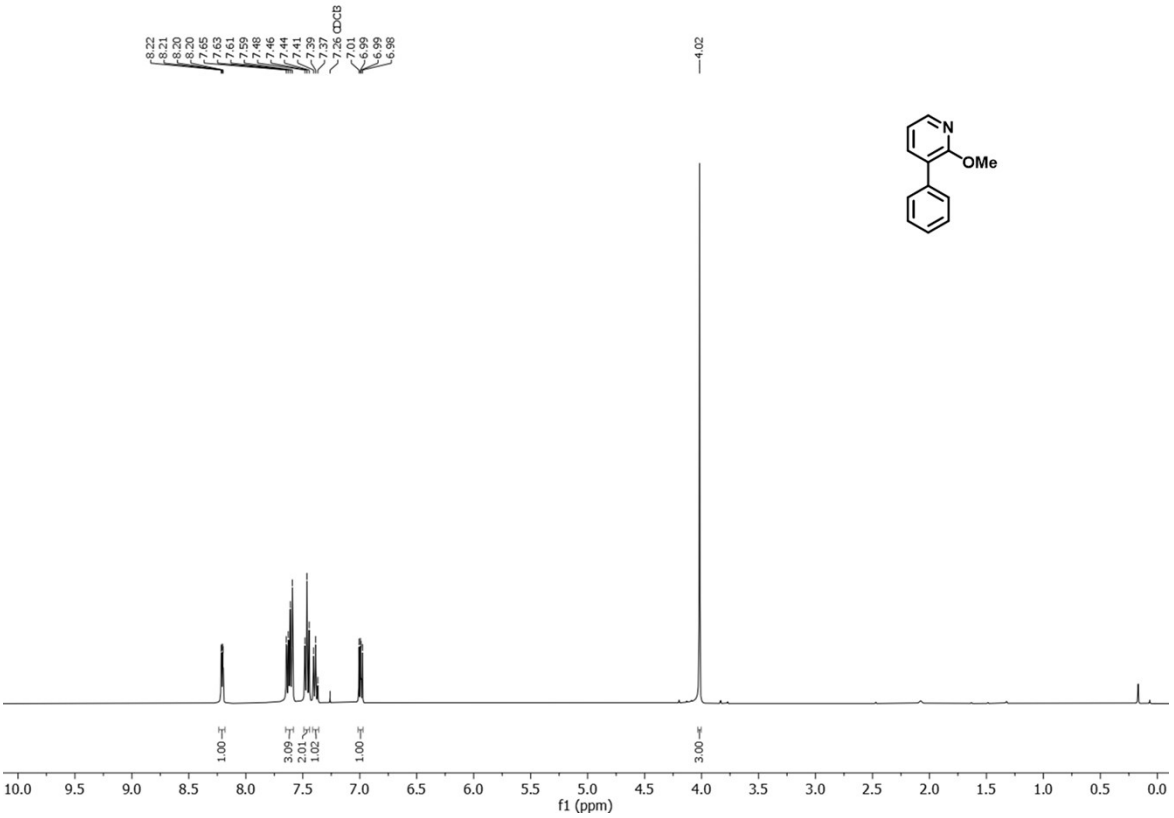


Figure S35. ^{1}H NMR spectrum (400 MHz) of **3k** in $CDCl_3$.

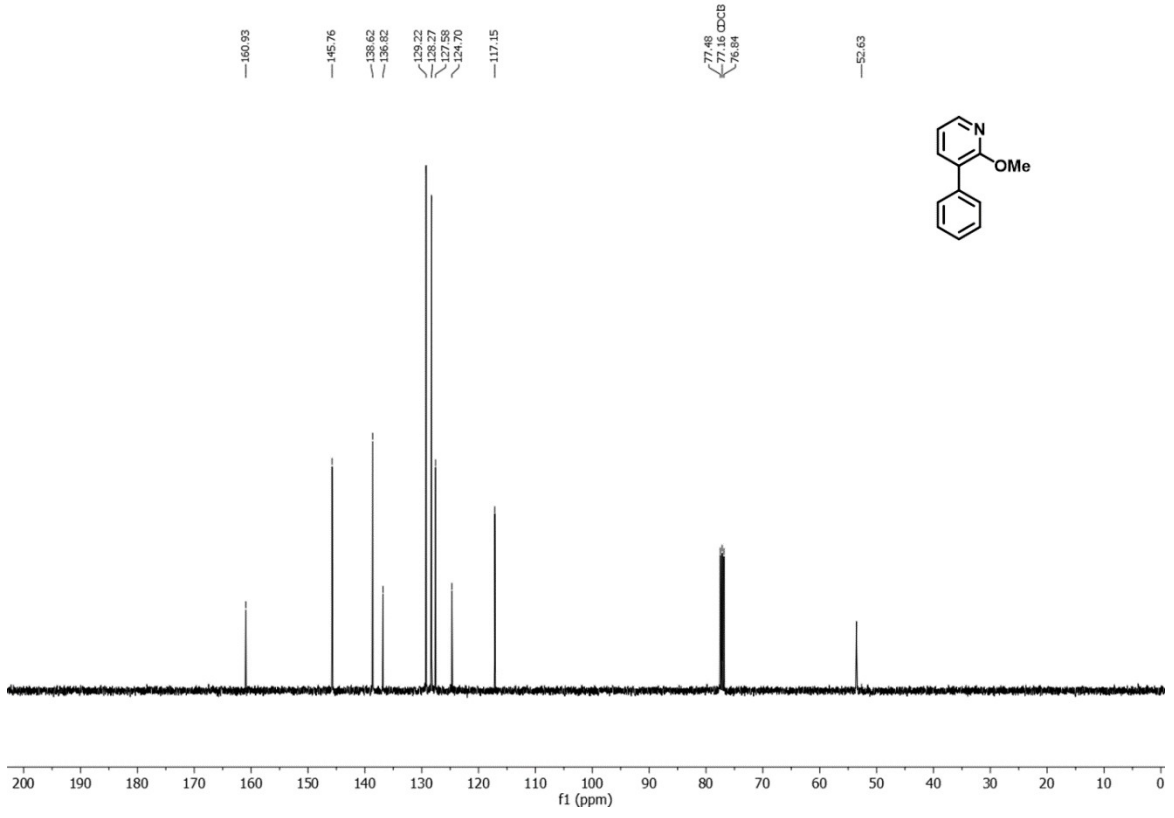


Figure S36. ^{13}C NMR spectrum (100 MHz) of **3k** in $CDCl_3$.

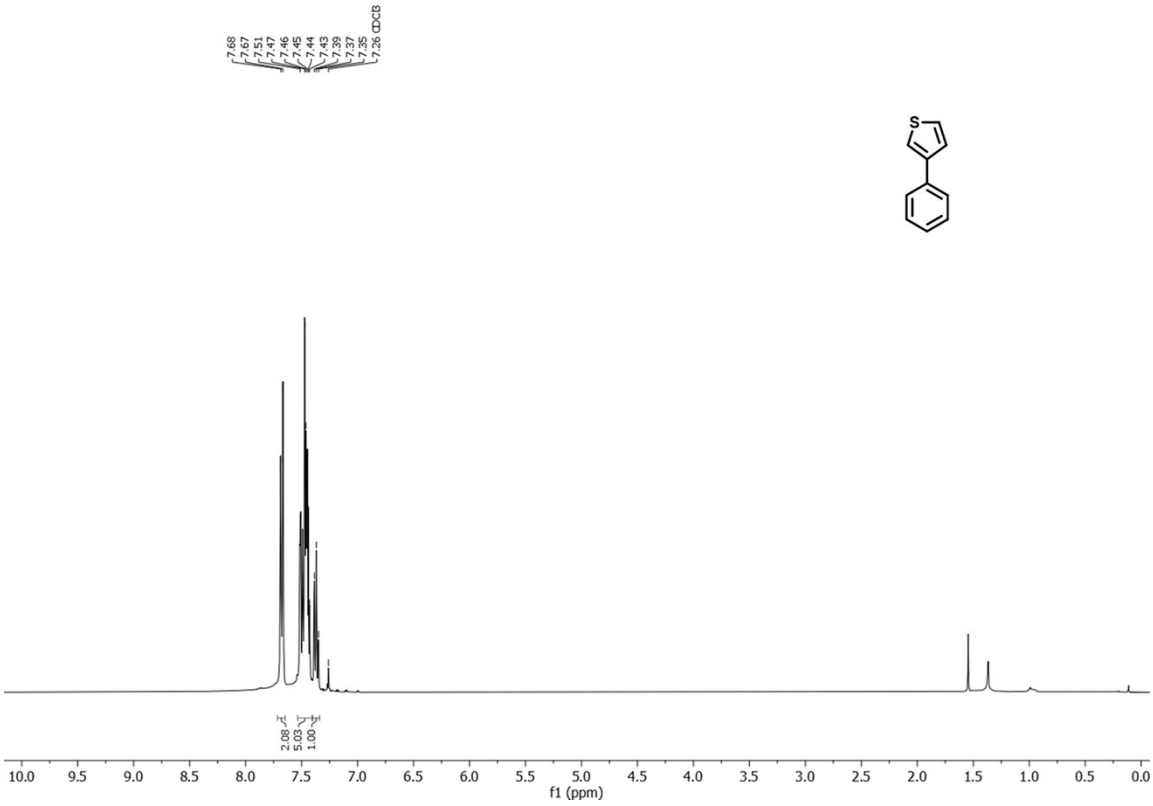


Figure S37. ^{1}H NMR spectrum (400 MHz) of **3l** in $CDCl_3$.

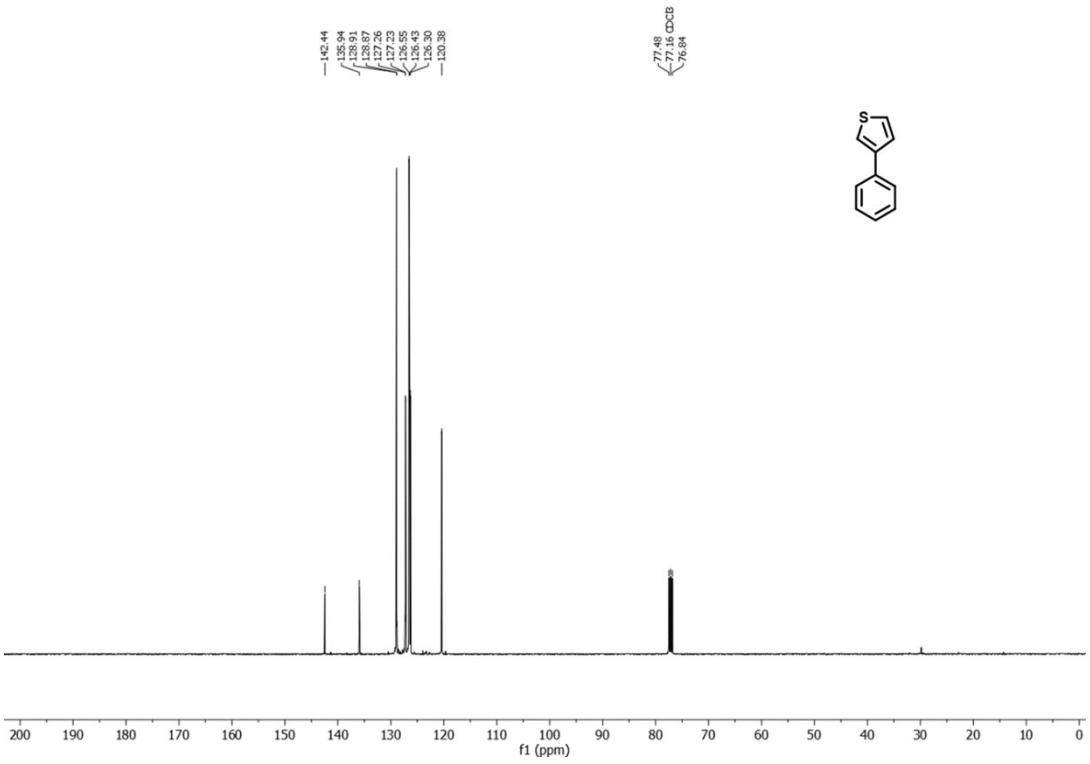


Figure S38. ^{13}C NMR spectrum (100 MHz) of **3l** in $CDCl_3$.

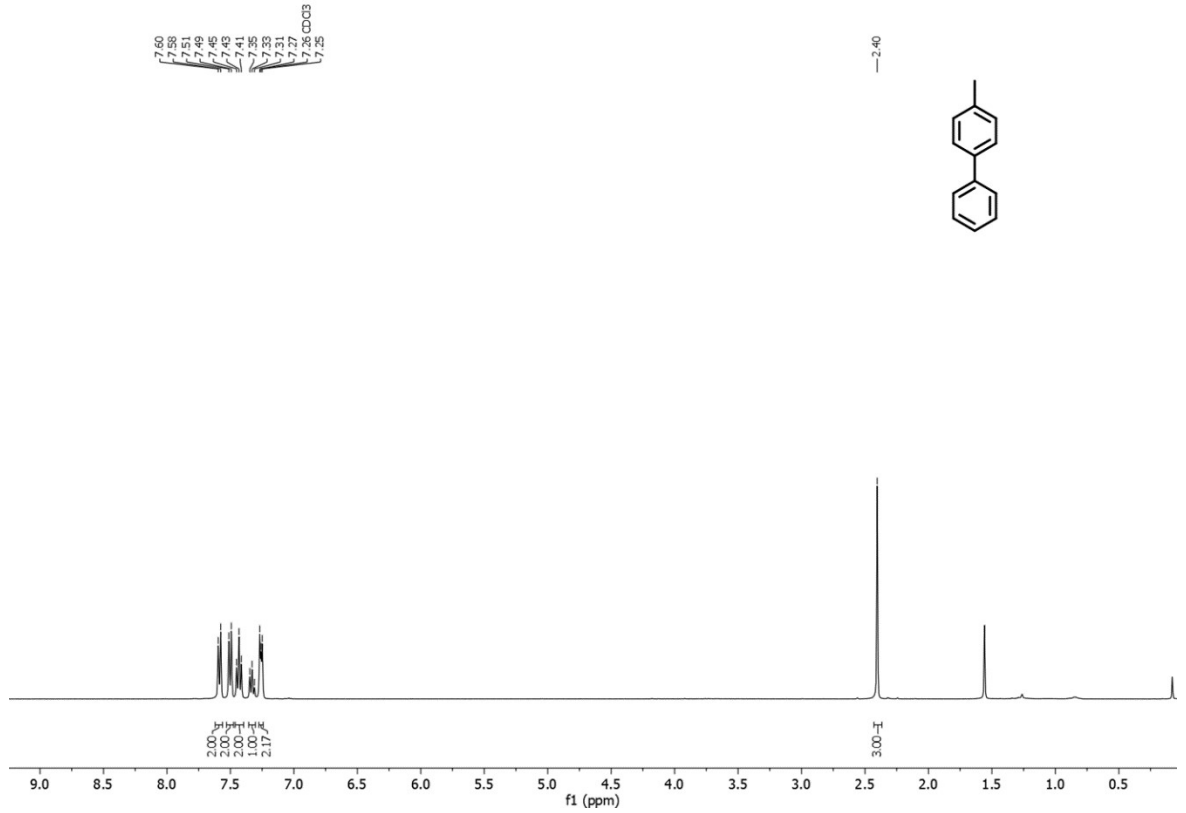


Figure S39. ^{1}H NMR spectrum (400 MHz) of **3m** in $CDCl_3$.

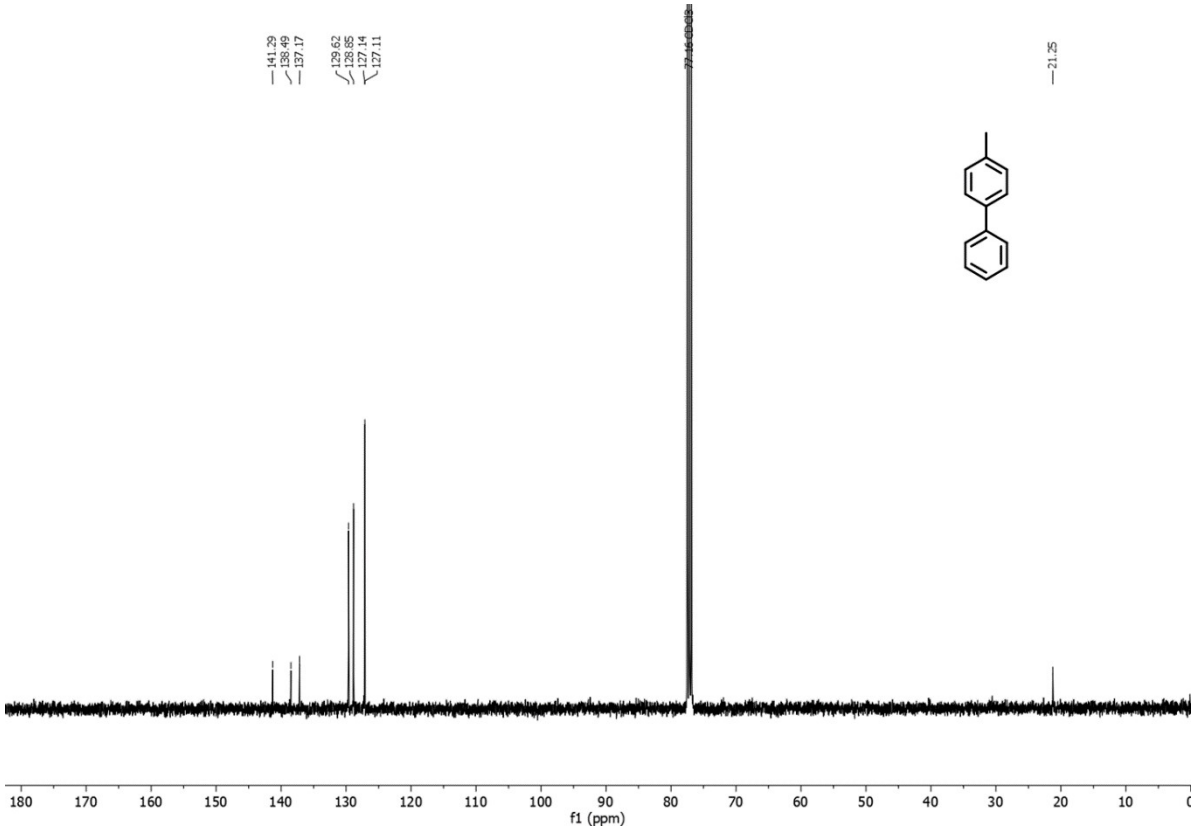


Figure S40. ^{13}C NMR spectrum (100 MHz) of **3m** in $CDCl_3$.

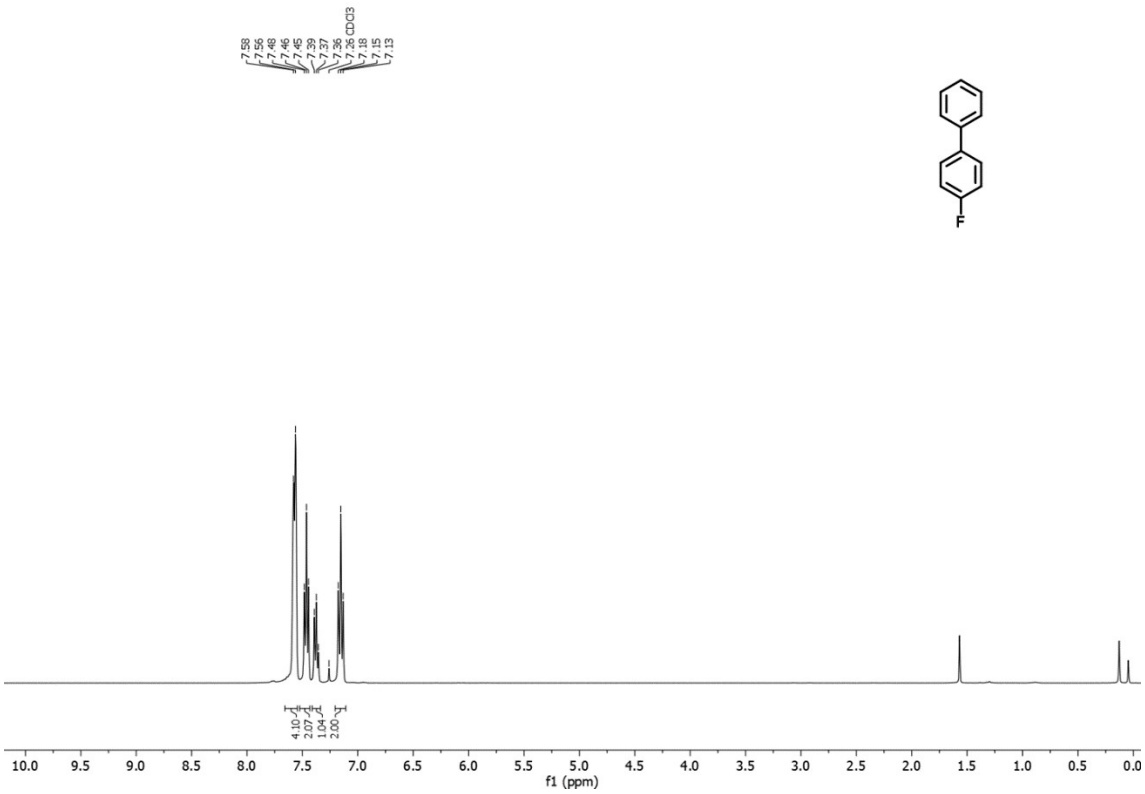


Figure S41. ^{1}H NMR spectrum (400 MHz) of **3n** in $CDCl_3$.

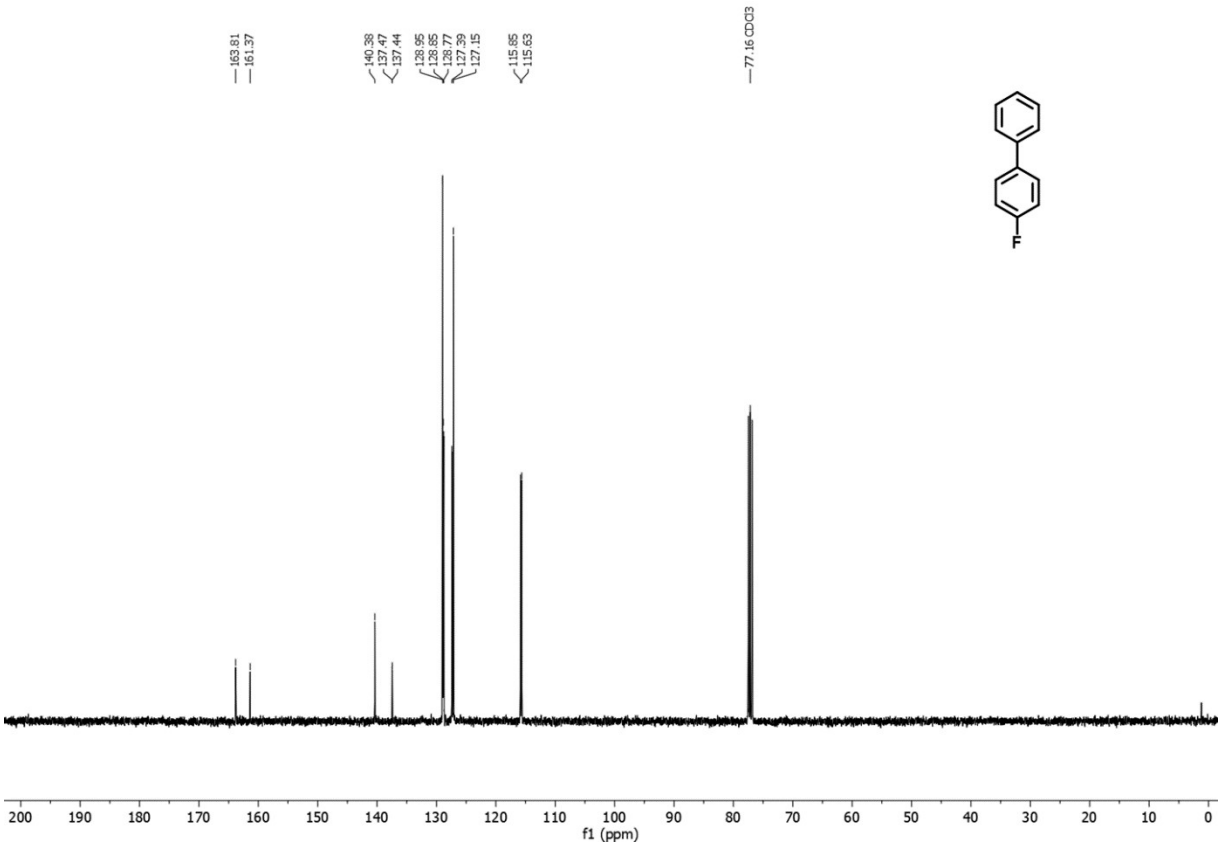


Figure S42. ^{13}C NMR spectrum (100 MHz) of **3n** in $CDCl_3$.

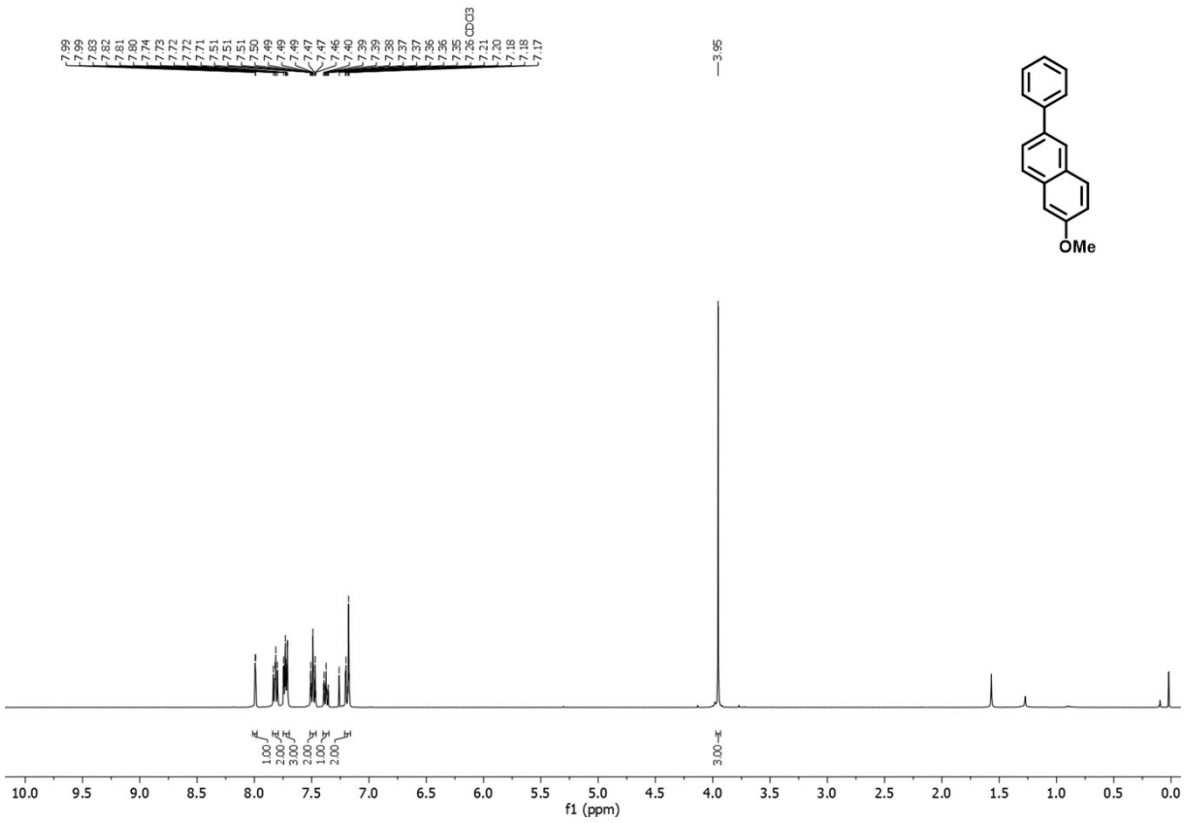


Figure S43. ^{1}H NMR spectrum (400 MHz) of **3o** in $CDCl_3$.

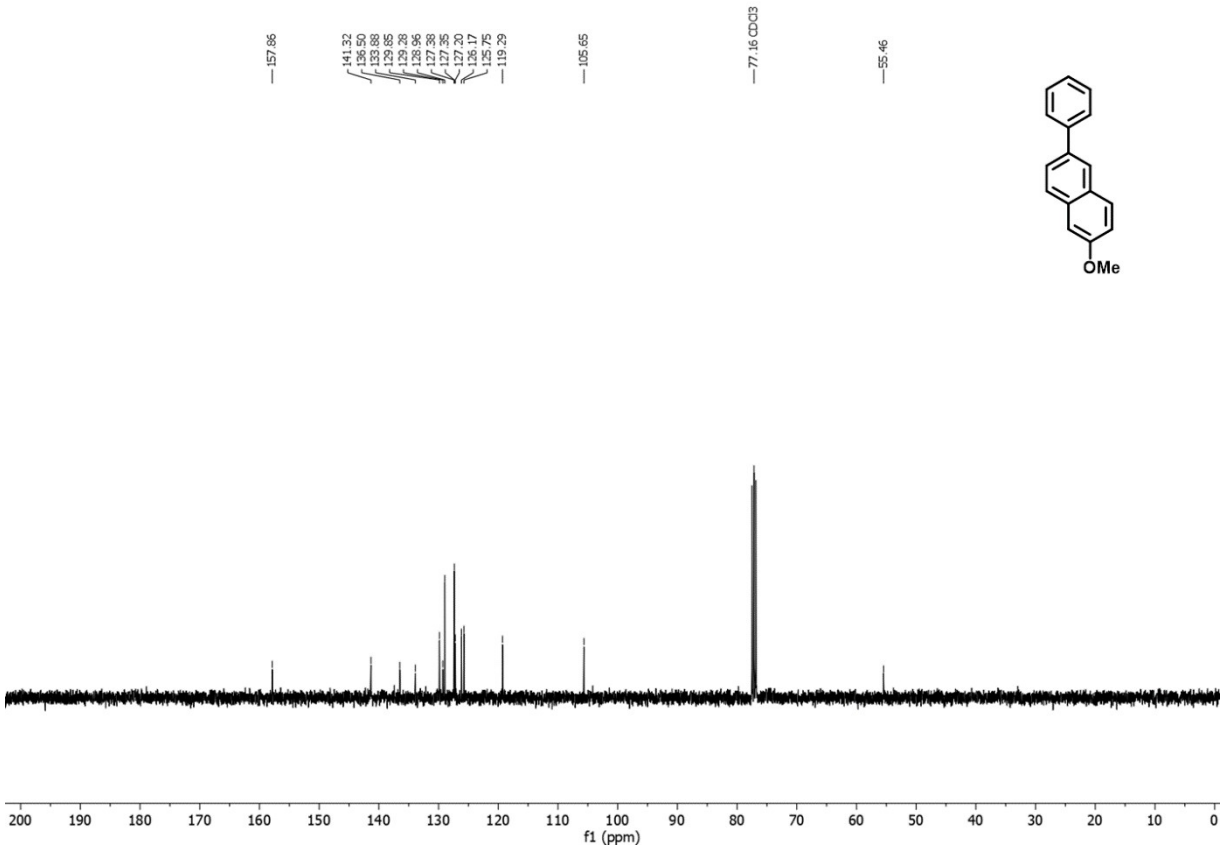


Figure S44. ^{13}C NMR spectrum (100 MHz) of **3o** in $CDCl_3$.

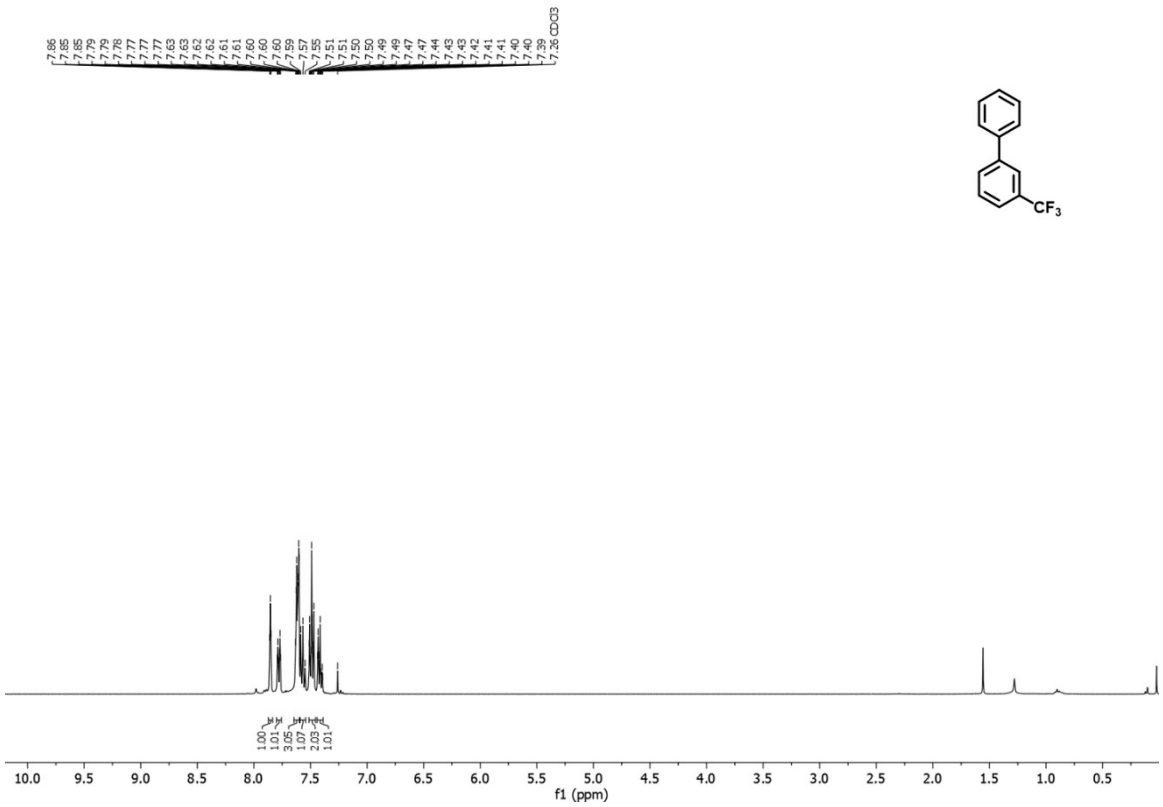


Figure S45. ^{1}H NMR spectrum (400 MHz) of **3p** in $CDCl_3$.

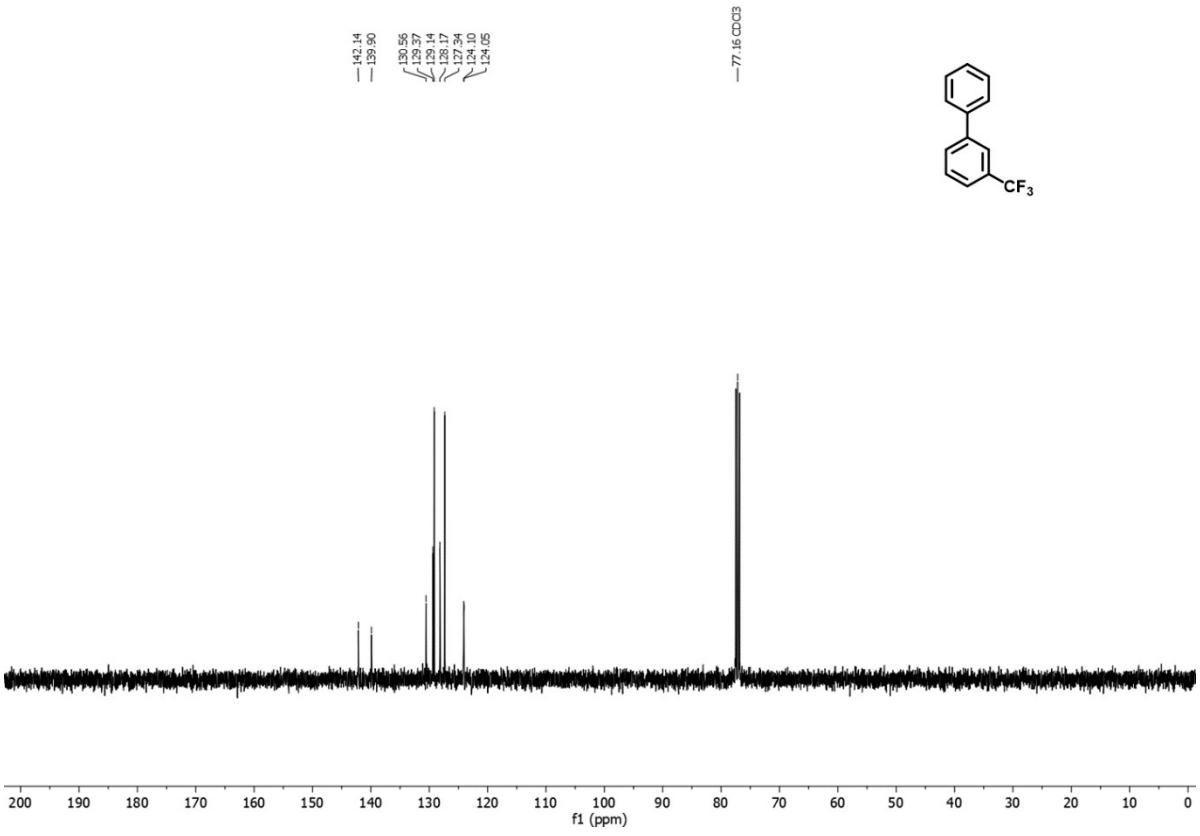


Figure S46. ^{13}C NMR spectrum (100 MHz) of **3p** in $CDCl_3$.

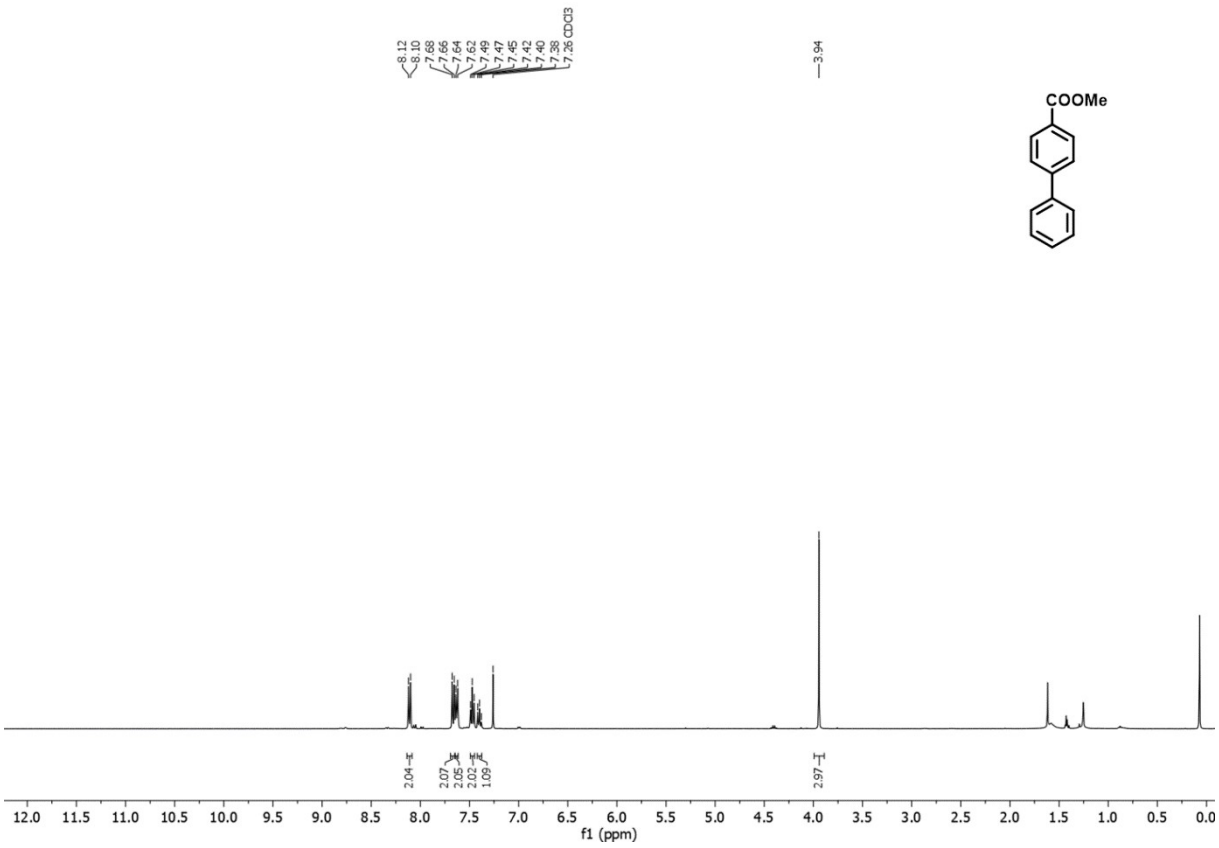


Figure S47. ^{1}H NMR spectrum (400 MHz) of **3q** in $CDCl_3$.

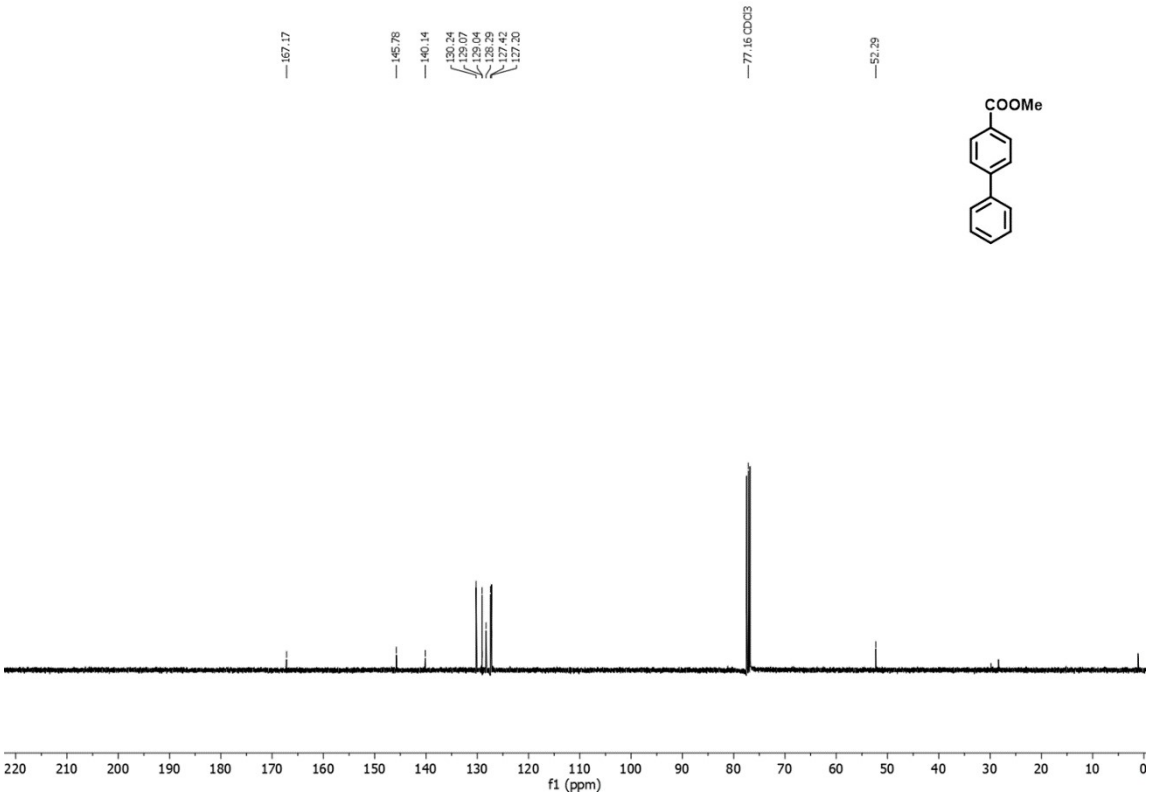


Figure S48. ^{13}C NMR spectrum (100 MHz) of **3q** in $CDCl_3$.

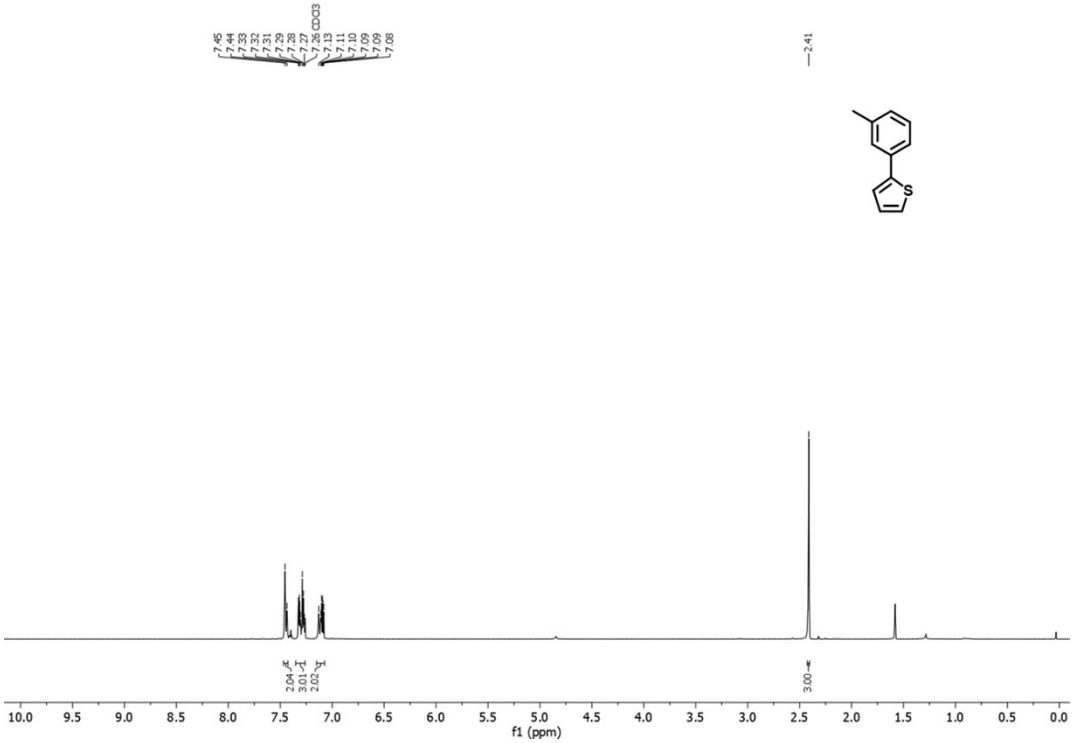


Figure S49. ^{1}H NMR spectrum (400 MHz) of **4a** in $CDCl_3$.

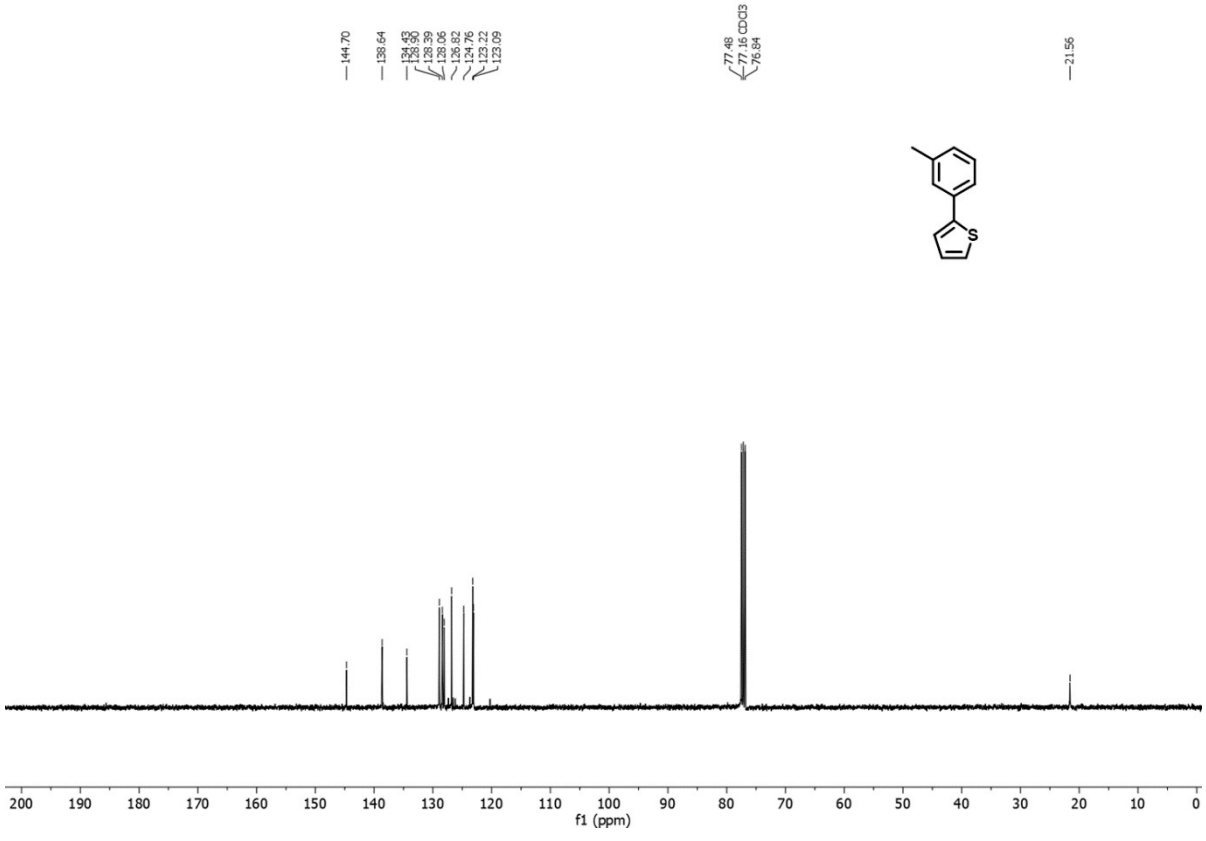


Figure S50. ^{13}C NMR spectrum (100 MHz) of **4a** in $CDCl_3$.

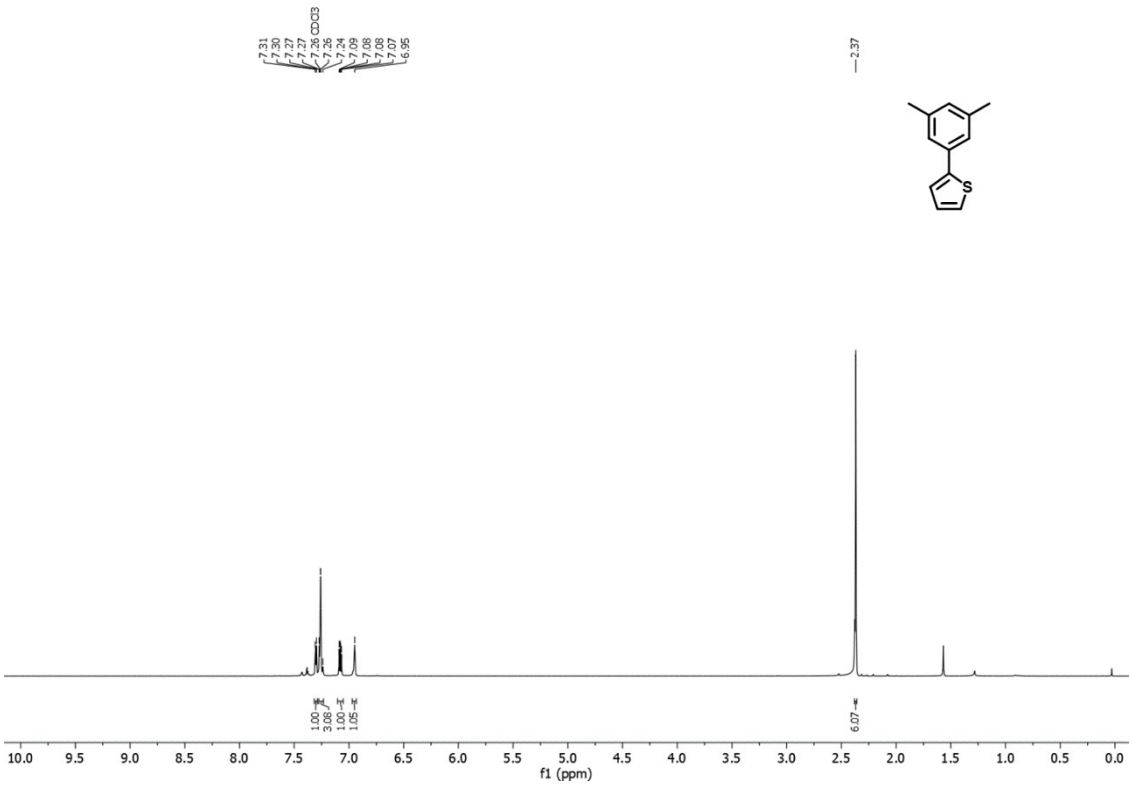


Figure S51. ^{1}H NMR spectrum (400 MHz) of **4b** in $CDCl_3$.

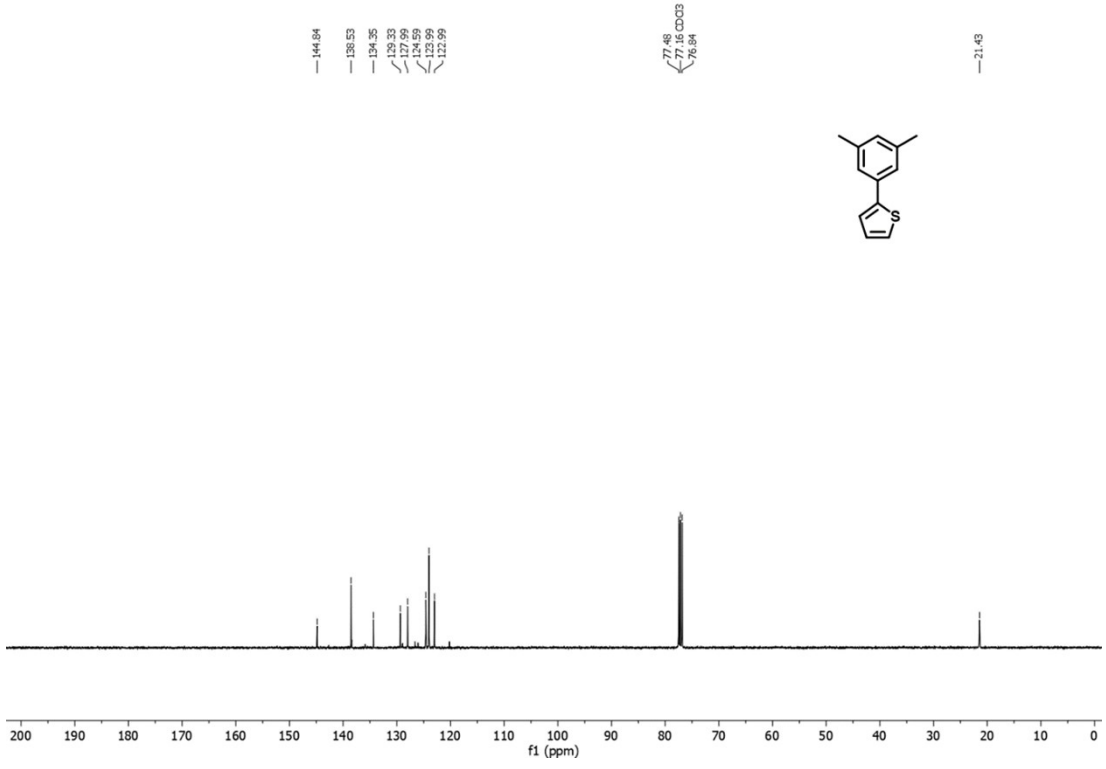


Figure S52. ^{13}C NMR spectrum (100 MHz) of **4b** in $CDCl_3$.

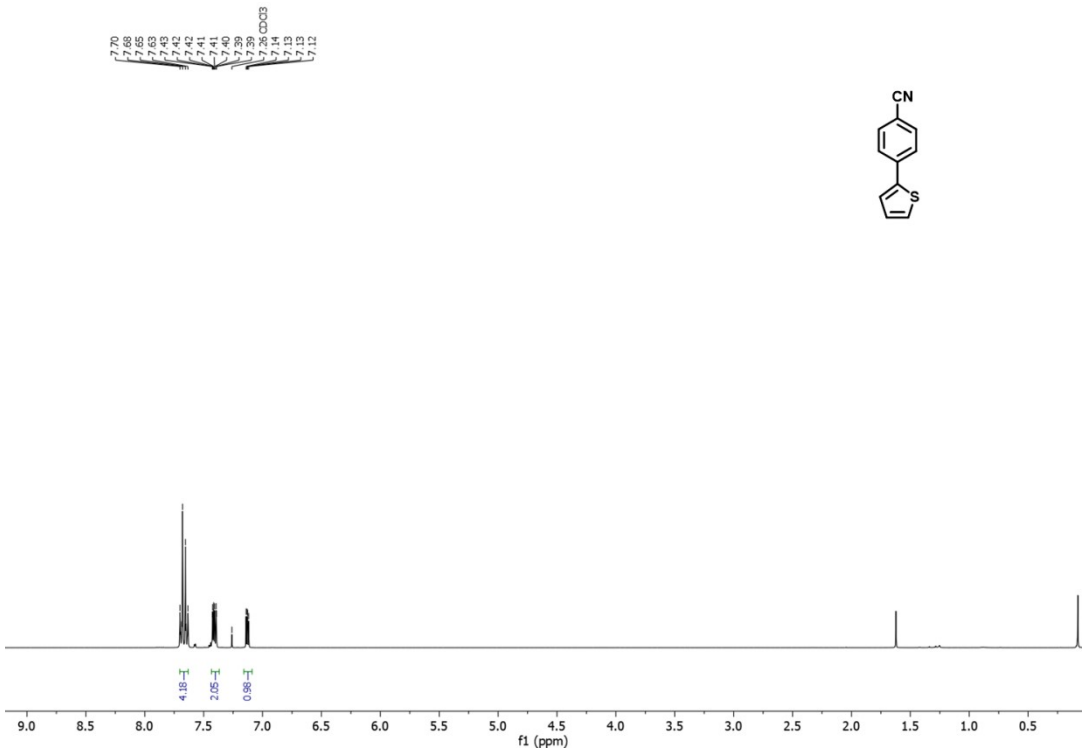


Figure S53. ^{1}H NMR spectrum (400 MHz) of **4c** in $CDCl_3$.

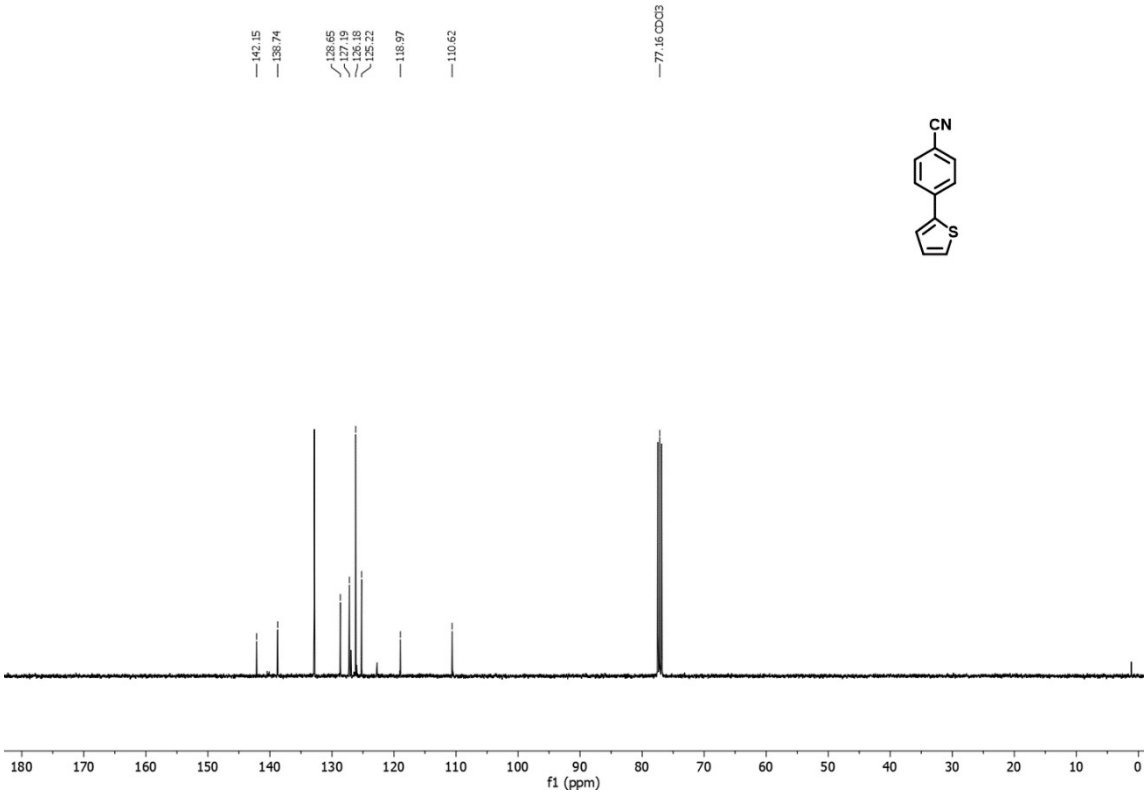


Figure S54. ^{13}C NMR spectrum (100 MHz) of **4c** in $CDCl_3$.

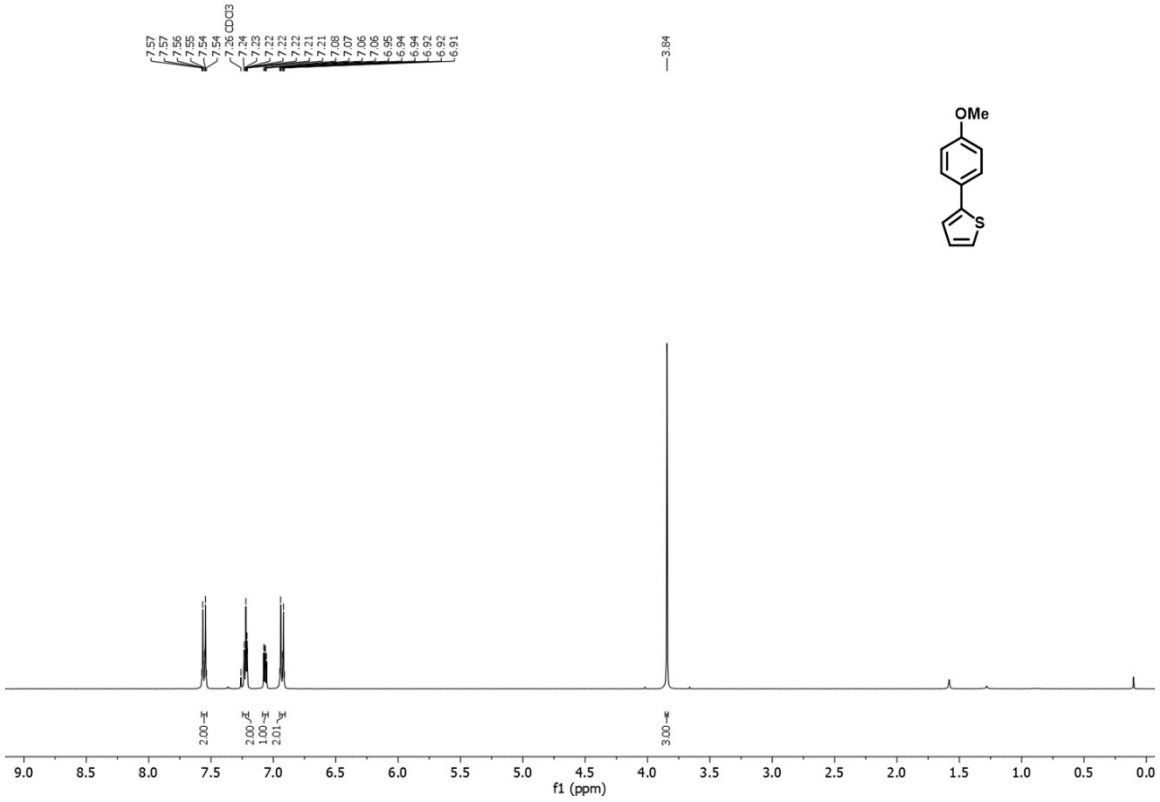


Figure S55. ^{13}C NMR spectrum (100 MHz) of **4d** in $CDCl_3$.

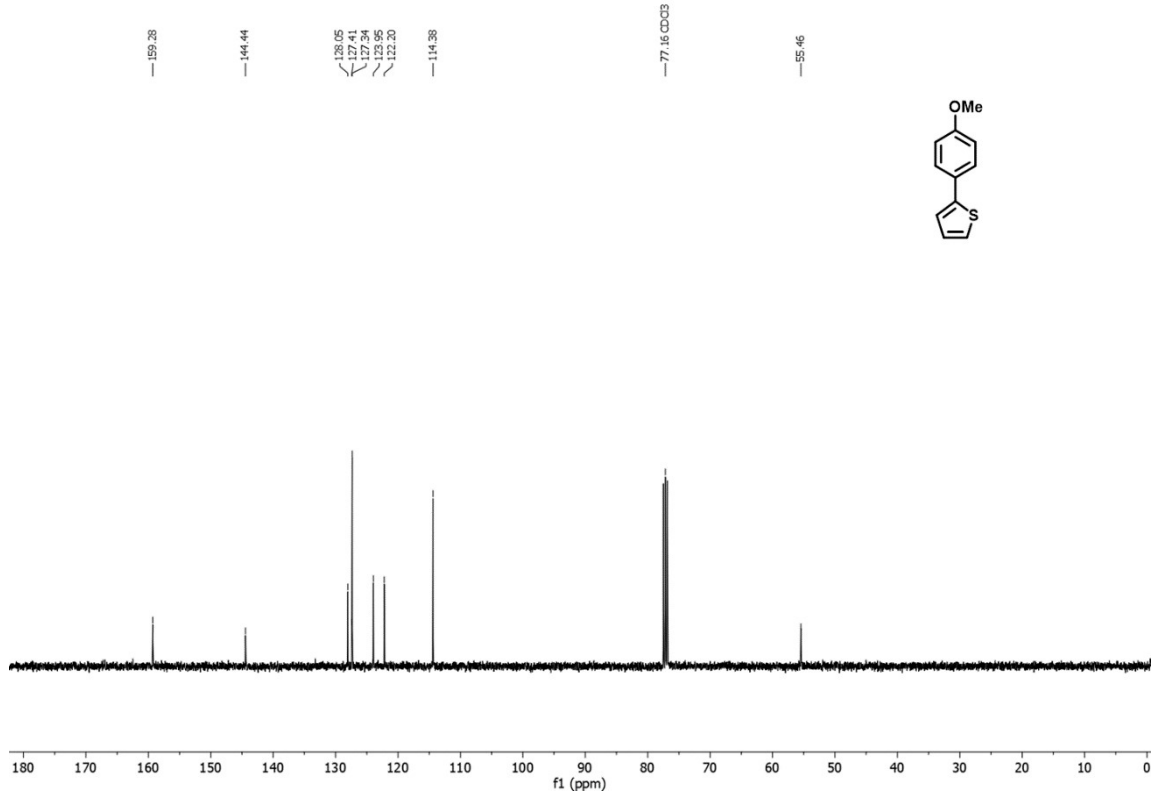


Figure S56. ^{13}C NMR spectrum (100 MHz) of **4d** in $CDCl_3$.

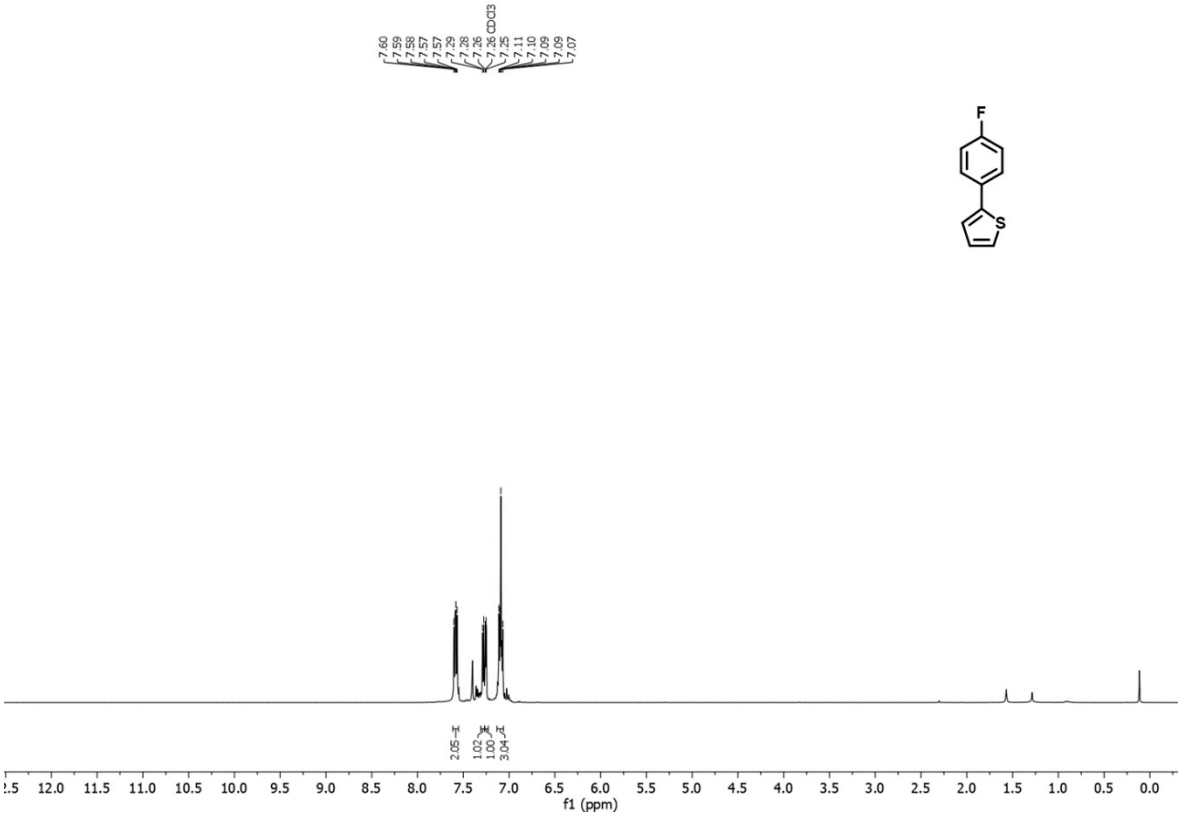


Figure S57. ^{1}H NMR spectrum (400 MHz) of **4e** in $CDCl_3$.

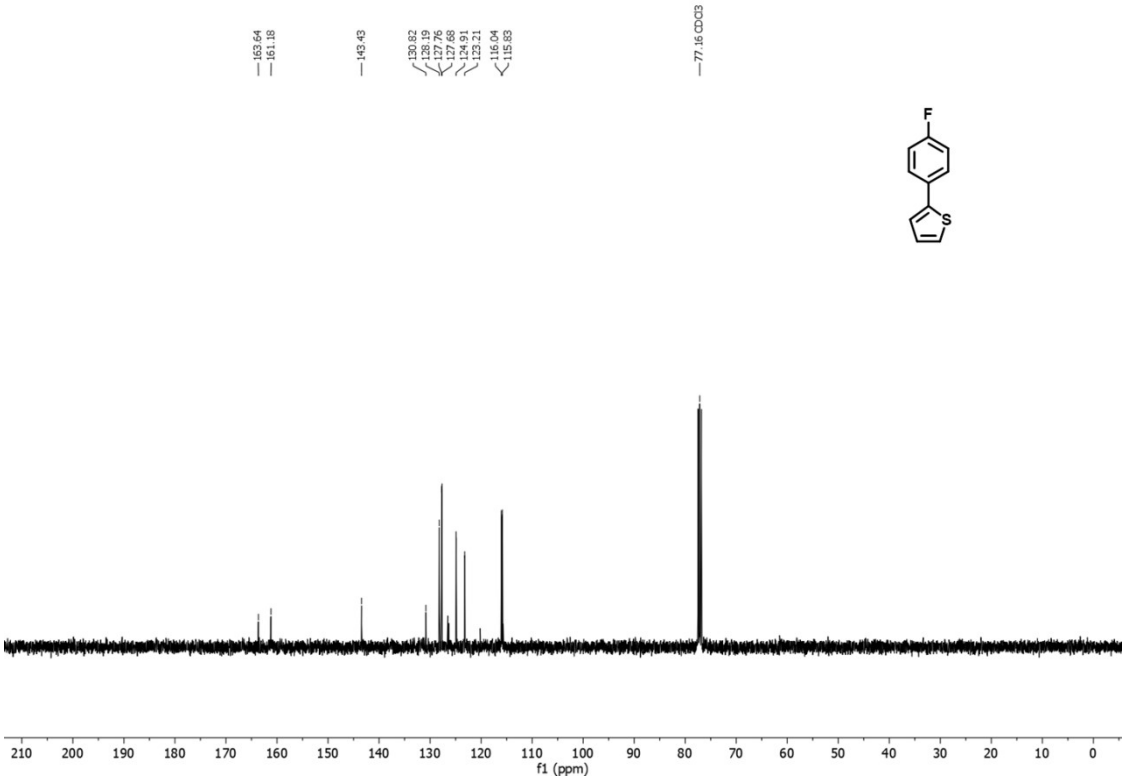


Figure S58. ^{13}C NMR spectrum (100 MHz) of **4e** in $CDCl_3$

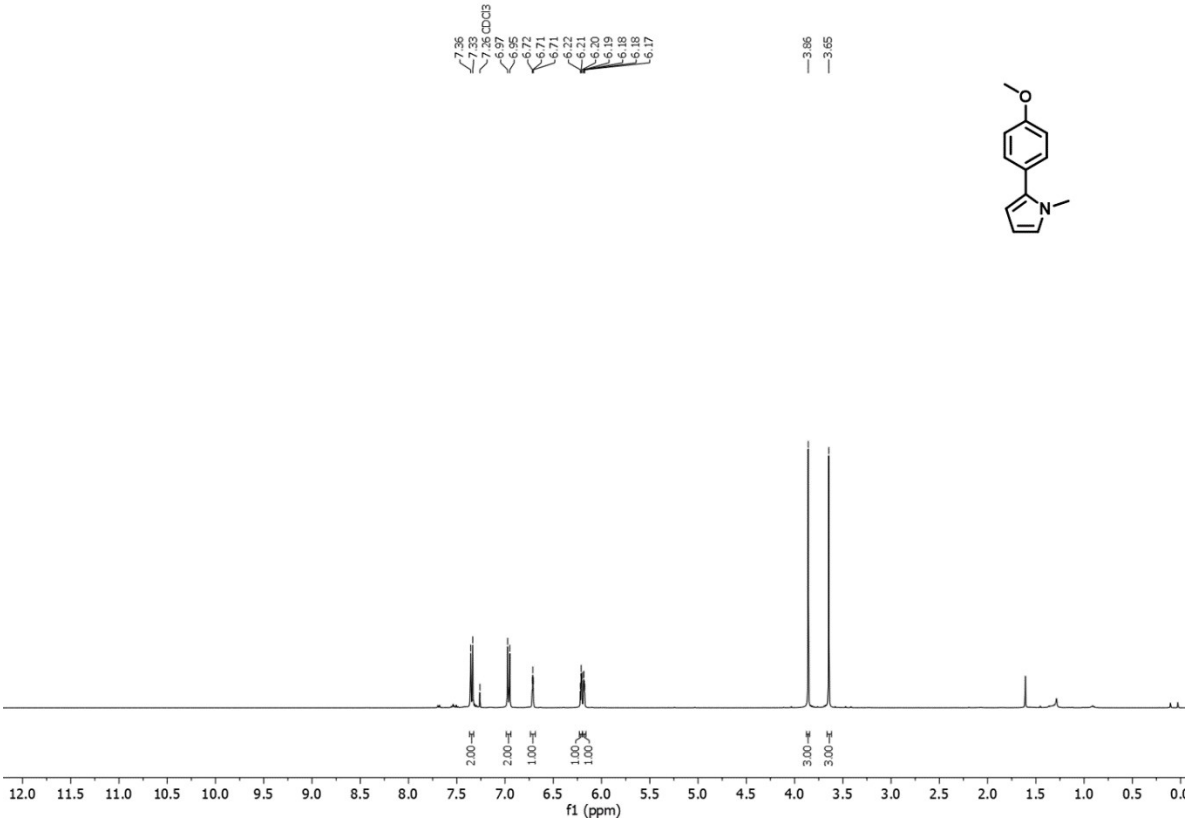


Figure S59. ^{1}H NMR spectrum (400 MHz) of **5a** in $CDCl_3$.

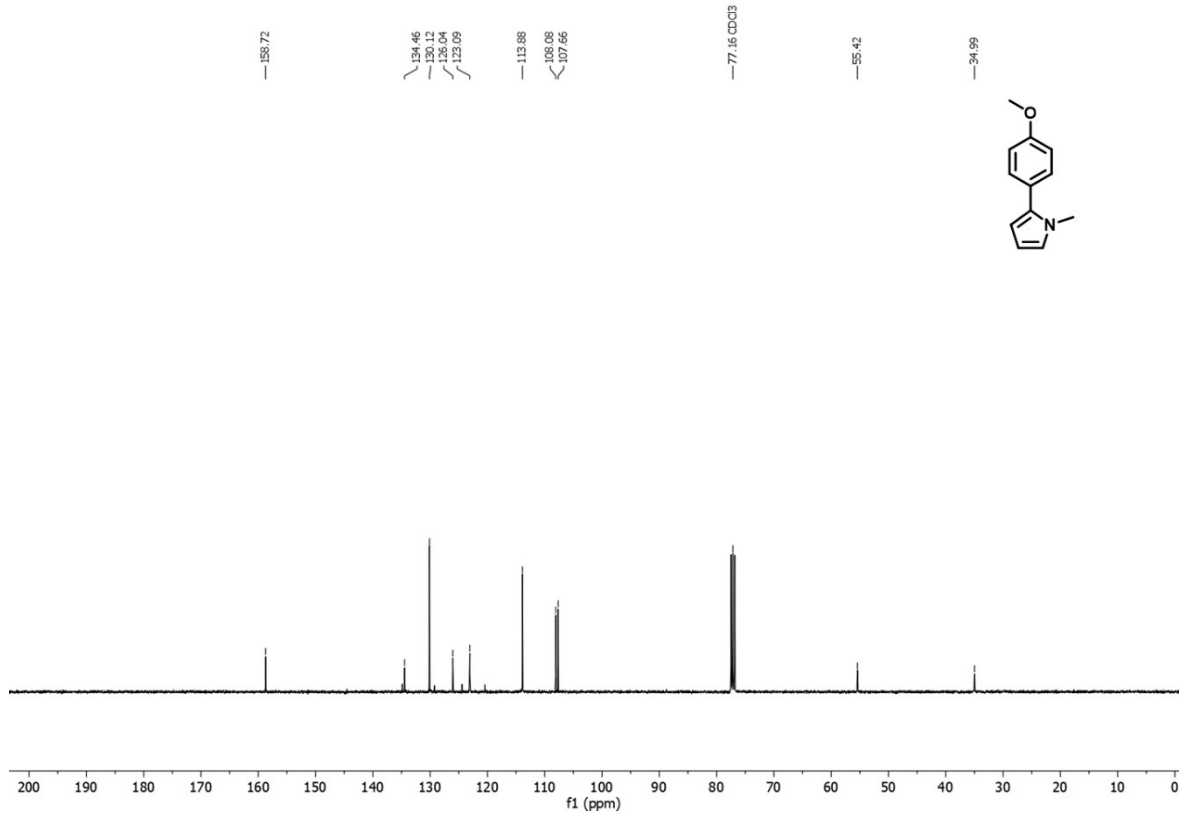


Figure S60. ^{13}C NMR spectrum (100 MHz) of **5a** in $CDCl_3$.

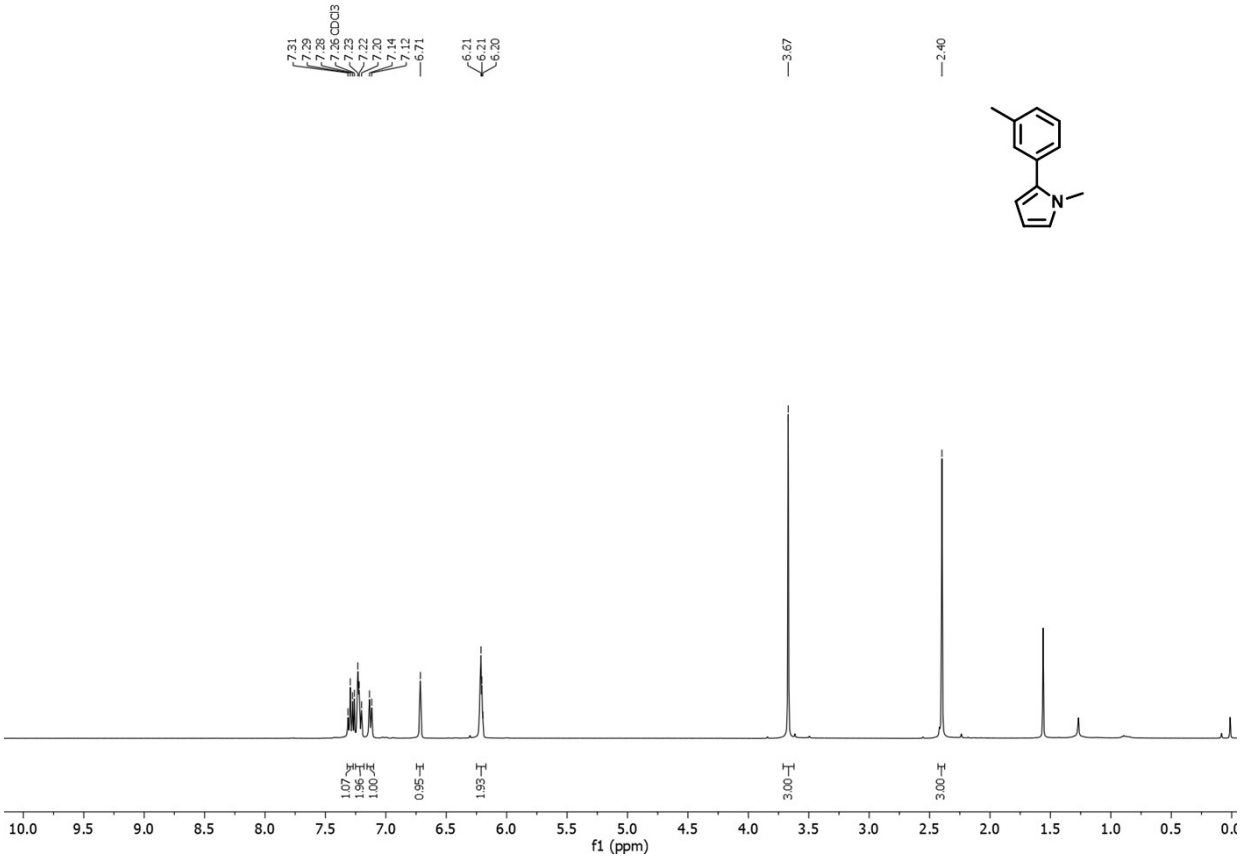


Figure S61. ^{1}H NMR spectrum (400 MHz) of **5b** in $CDCl_3$.

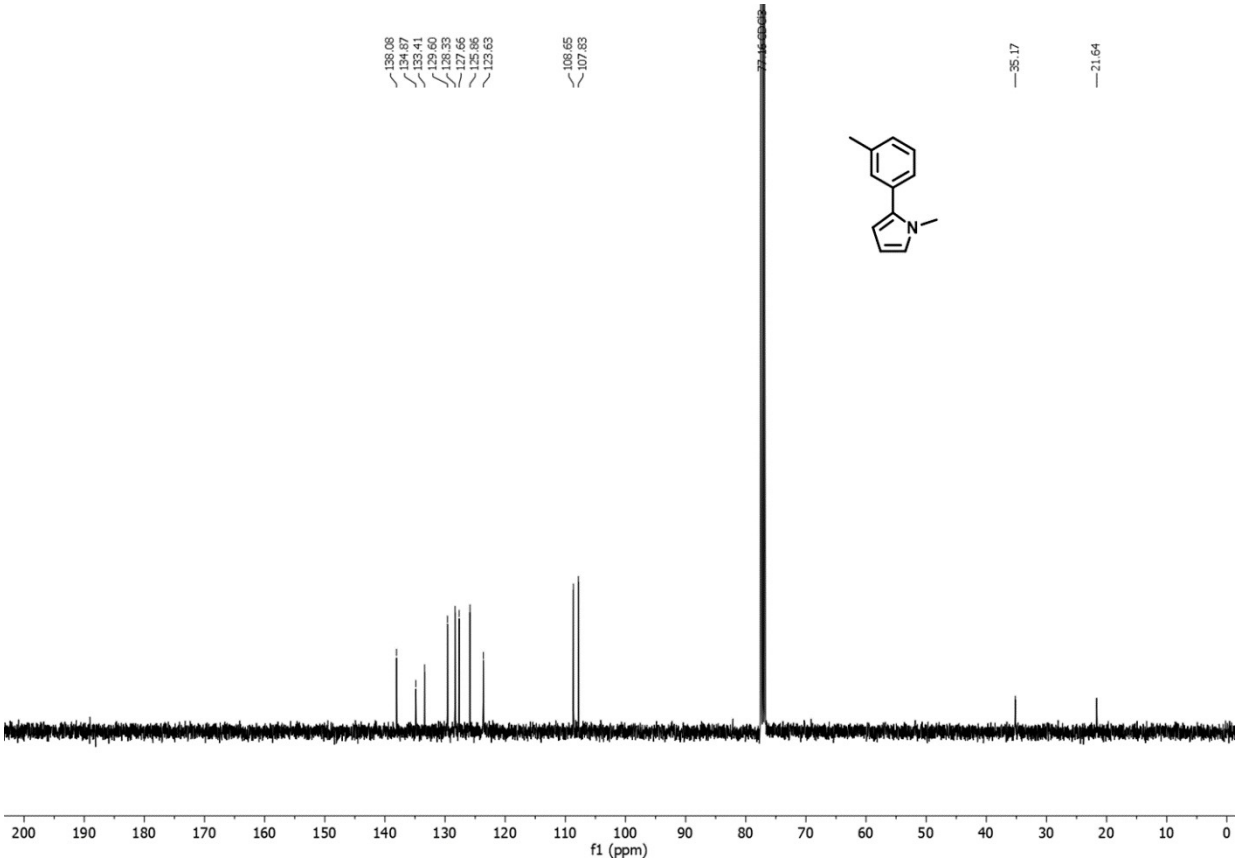


Figure S62. ^{13}C NMR spectrum (100 MHz) of **5b** in $CDCl_3$.

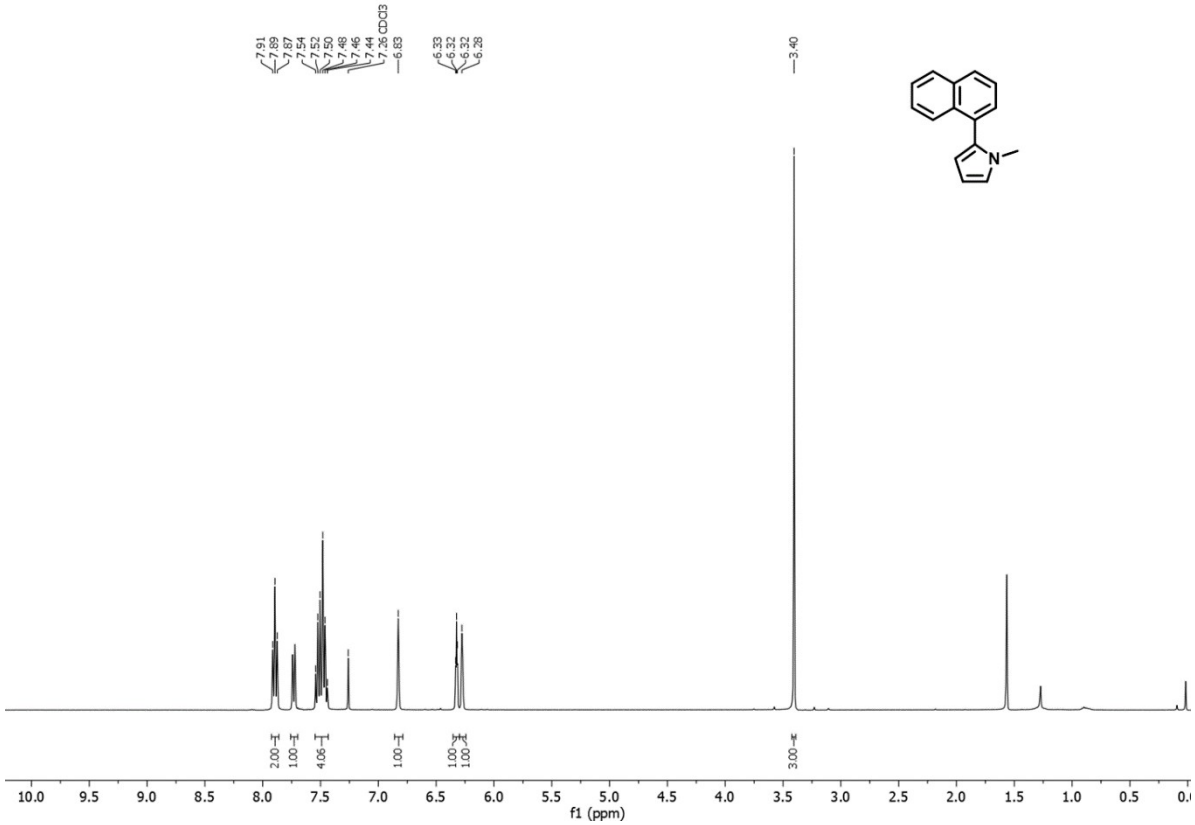


Figure S63. ^{1}H NMR spectrum (400 MHz) of **5c** in $CDCl_3$.

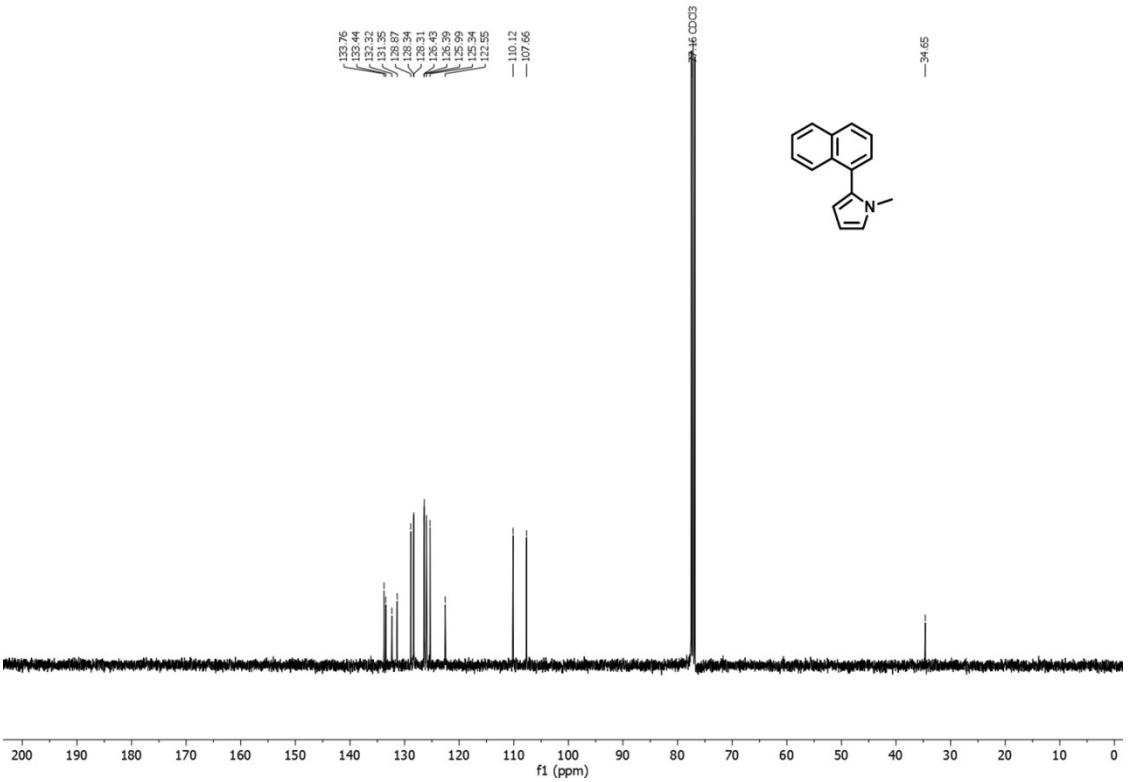


Figure S64. ^{13}C NMR spectrum (100 MHz) of **5c** in $CDCl_3$.

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