

Supplementary Information

Palladium Nanoparticles Supported on β -Cyclodextrin Functionalized Poly(amidoamine)s and Their Application in Suzuki-Miyaura Cross-Coupling Reactions

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General remarks (instrumentation and chemicals)

^1H and ^{13}C NMR spectra were recorded in CDCl_3 on the instrument operated at 500 MHz. Chemical shifts (δ) are given in parts *per* million (ppm) with the residual peak of CHCl_3 at 7.26 and 77.0 ppm as the internal standard. Thin layer chromatography was performed on pre-coated glass-back plates and visualized with UV light at 254 nm. Flash column chromatography was performed with silica gel (200-300 mesh). Commercially the aryl halide, phenyl boronic acid were used directly.

General experimental procedures for cross-coupling reactions

The typically experimental process is as follows: the aryl halide (0.25 mmol), phenyl boronic acid (0.3 mmol) and Na_2CO_3 (0.25 mmol), PPh_3 (0.025 mmol), were placed in a 10 mL Shrek tube with 1 mL of H_2O and the catalyst Pd@PAAs-CD (0.5 mg, 0.2 mol% Pd *per* mol of aryl halide) were added. The reaction mixture was heated to 80 °C and the reaction process was monitored by GC-MS. The reaction mixture was cooled at room temperature for 1 h, and then 3 mL of water was added, extracted with ethyl acetate (3 mL \times 3). The combined organic layers were separated, dried over anhydrous Na_2SO_4 and crude products were obtained by means of rotary evaporator. The product was purified by column chromatography (200-300 mesh silica gels) using a mixture of petroleum ether and ethyl acetate as the eluent to obtain the products.

^1H NMR spectra of EDC-CD and PAAs-CD

One-dimensional NMR spectra were recorded using Bruker AVANCEIII 500 spectrometer with deuterium oxide- d_2 ($\text{D}_2\text{O}-d_2$) and dimethyl sulfoxide ($\text{DMSO}-d_6$) as solvent. The ^1H NMR spectrum from 1-10 ppm of EDC-CD was listed in Figure S1 and ^1H NMR spectrum of PAAs-CD was listed in Figure S2. The difference between branched and linear PAAs from the Figures S1 and S2 can be found.

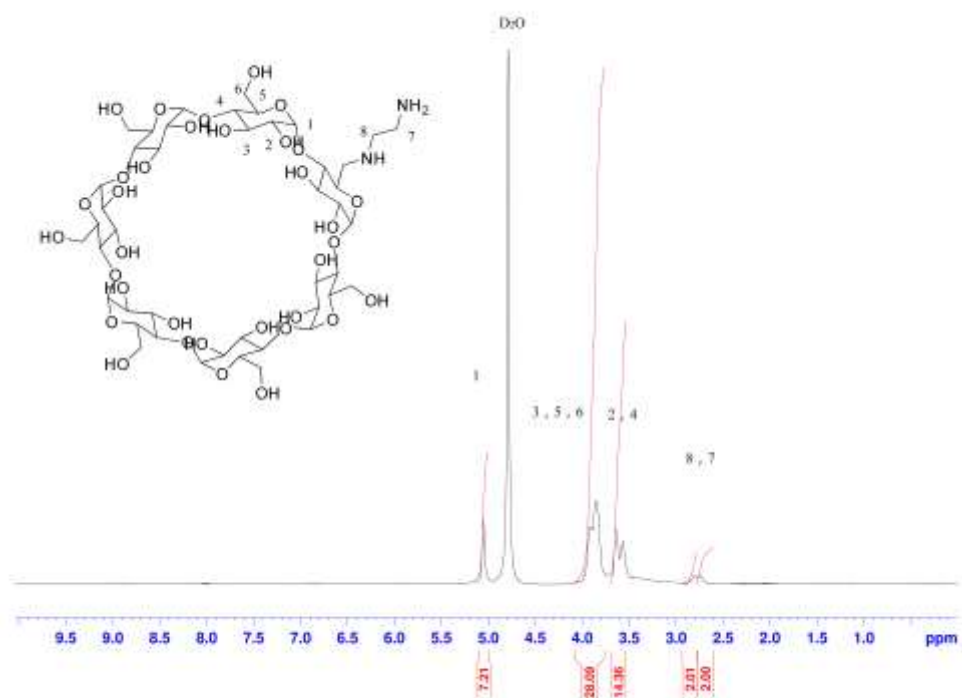


Figure S1. ^1H NMR spectrum (500 MHz, $\text{D}_2\text{O}-d_2$) of EDC-CD.

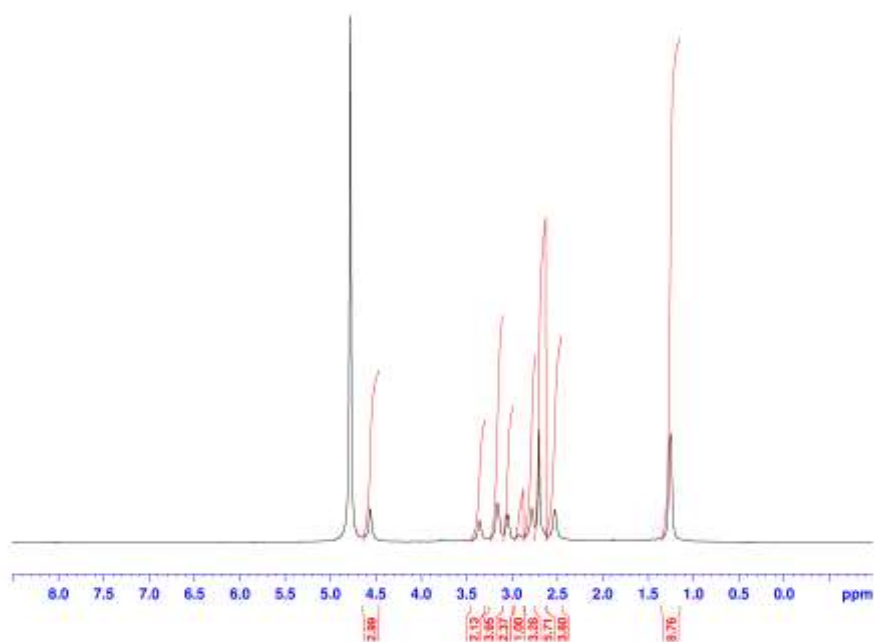


Figure S2. ^1H NMR spectrum of PAAs (sealed with diethylamine). ^1H NMR (400 MHz, $\text{D}_2\text{O}-d_2$) δ 1.18-1.25 (m, 8.7H), 2.52 (s, 3.6H), 2.70 (s, 5.7H), 2.78 (s, 3.2H), 2.92 (s, 1.0H), 3.00-3.10 (br, 3.1H), 3.16 (s, 3.9H), 3.35 (s, 2.1H), 4.56 (s, 2.9H).

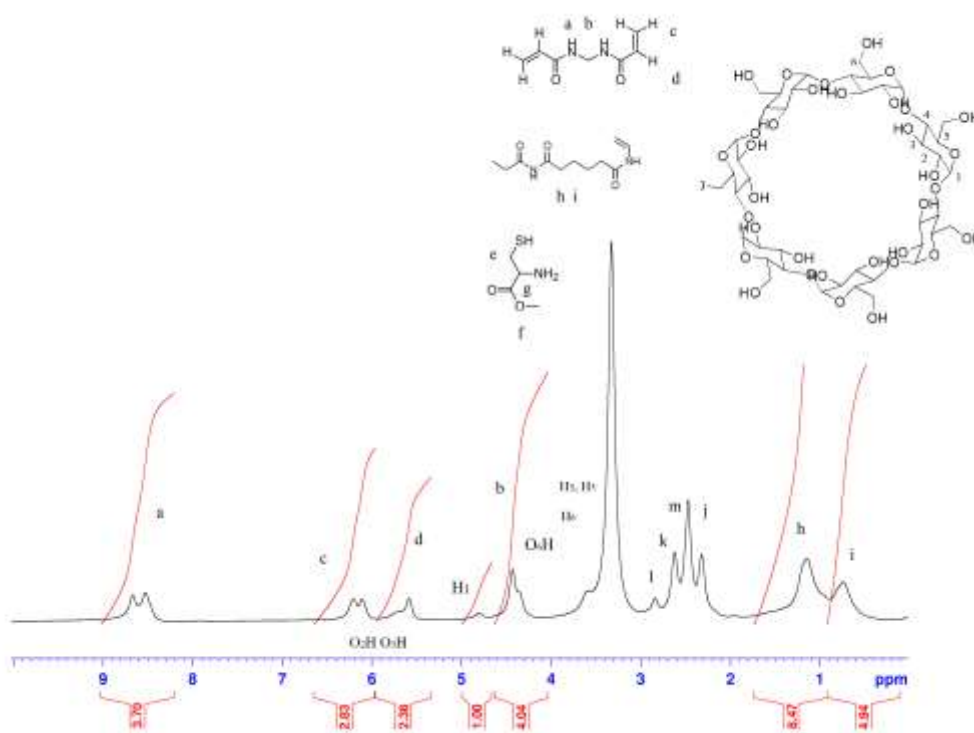


Figure S3. ¹H-NMR spectrum (500 MHz, DMSO-*d*₆) of PAAs-CD.

¹H NMR and ¹³C NMR spectra of coupling product for Suzuki-Miyaura cross coupling reactions

One-dimensional NMR spectra were recorded using Bruker AVANCEIII 500 spectrometer with CDCl₃ as solvent. The full set of ¹H NMR spectra from 1-10 ppm and ¹³C NMR spectra from 0-200 ppm of coupling products were listed below.

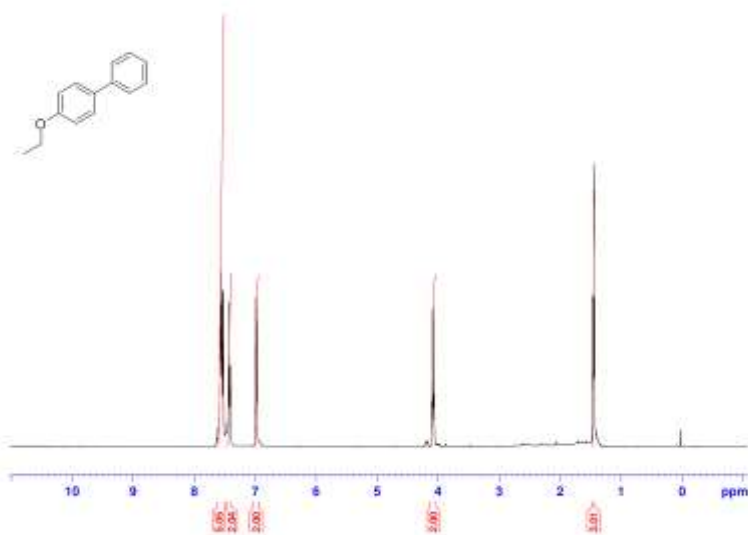


Figure S4. ¹H NMR spectrum (500 MHz, CDCl₃) of 3a.

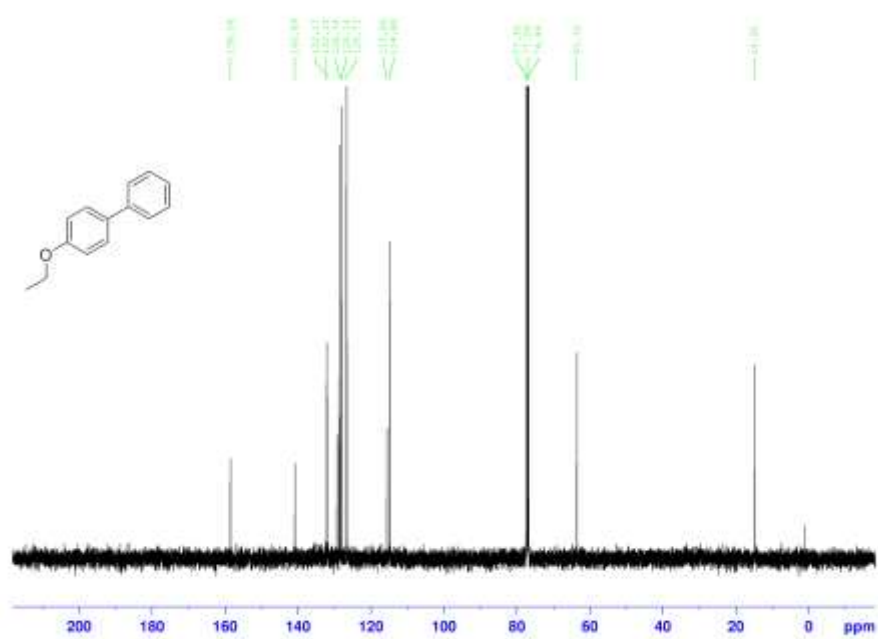


Figure S5. ¹³C NMR spectrum (500 MHz, CDCl₃) of **3a**.

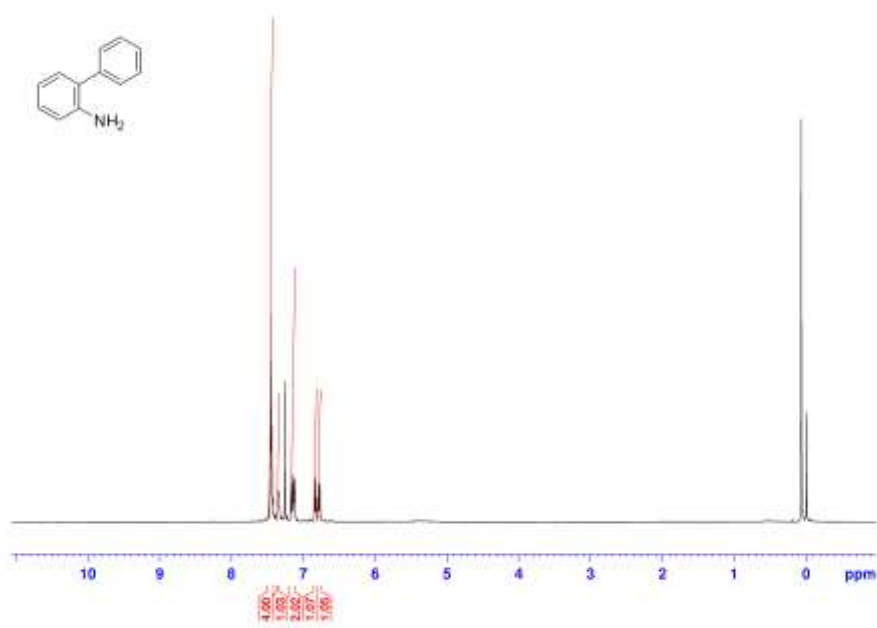


Figure S6. ¹H NMR spectrum (500 MHz, CDCl₃) of **3b**.

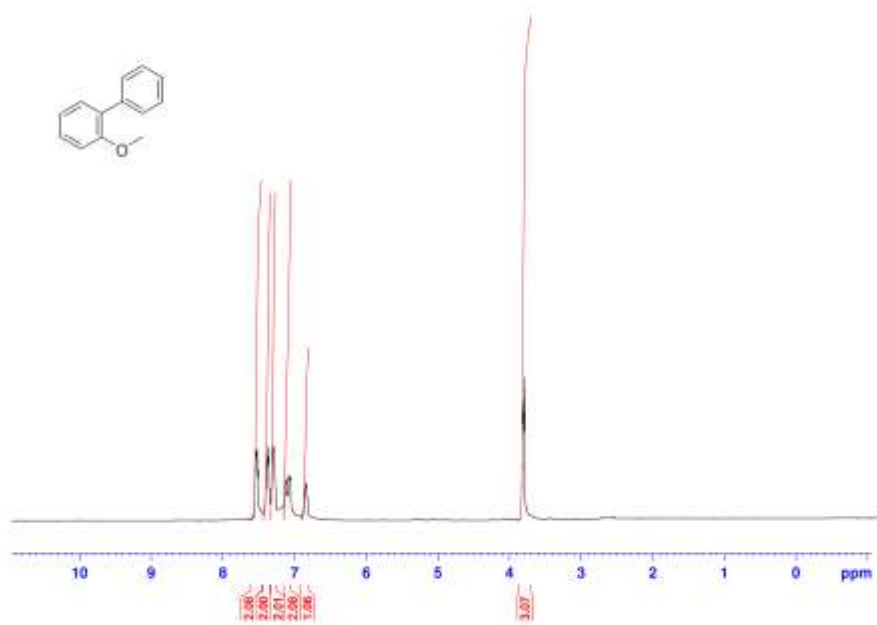


Figure S7. ¹H NMR spectrum (500 MHz, CDCl₃) of **3c**.

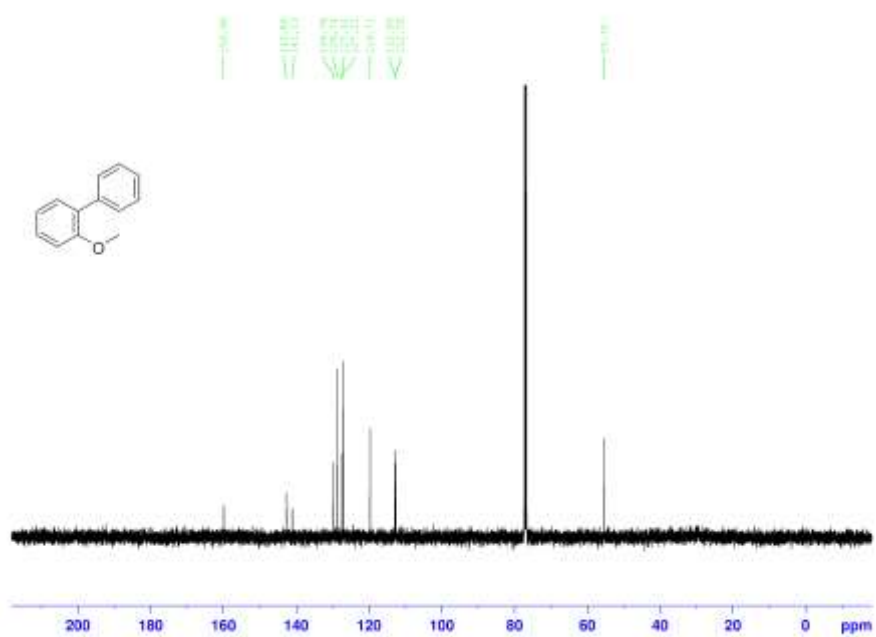


Figure S8. ¹³C NMR spectrum (500 MHz, CDCl₃) of **3c**.

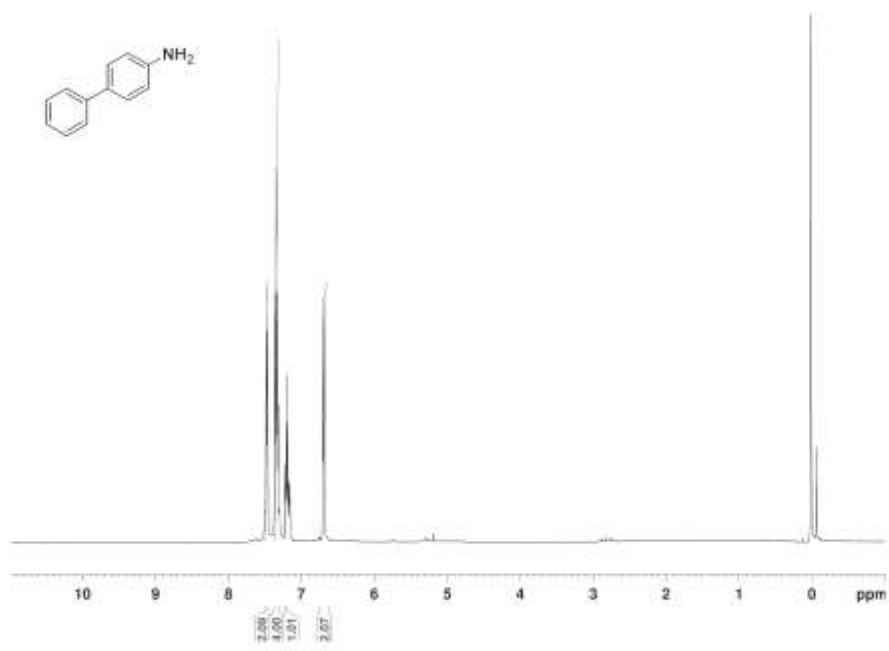


Figure S9. ¹H NMR spectrum (500 MHz, CDCl₃) of **3d**.

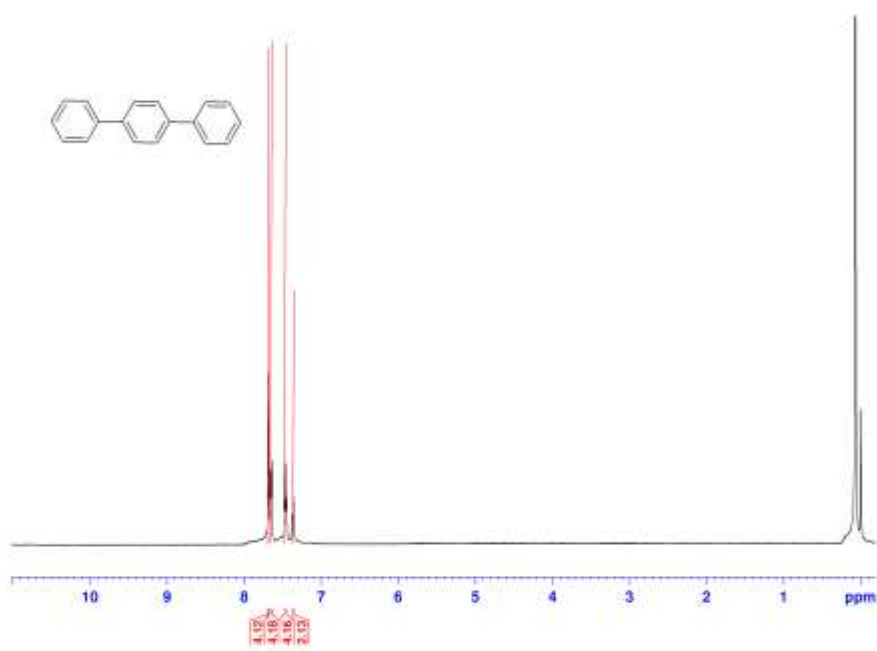


Figure S10. ¹H NMR spectrum (500 MHz, CDCl₃) of **3e**.

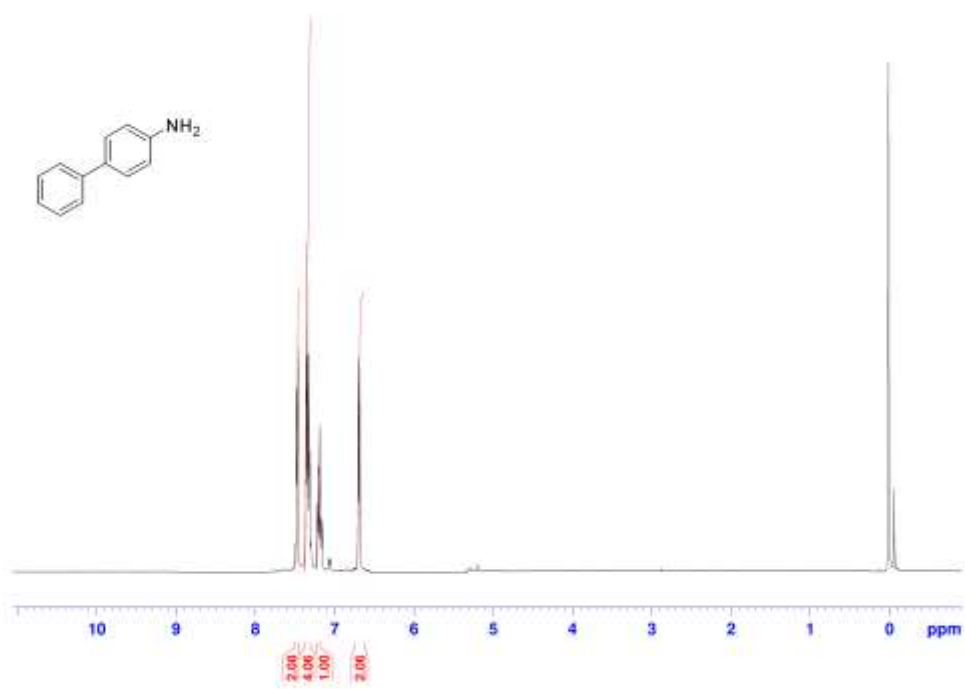


Figure S11. ¹H NMR spectrum (500 MHz, CDCl₃) of **3f**.

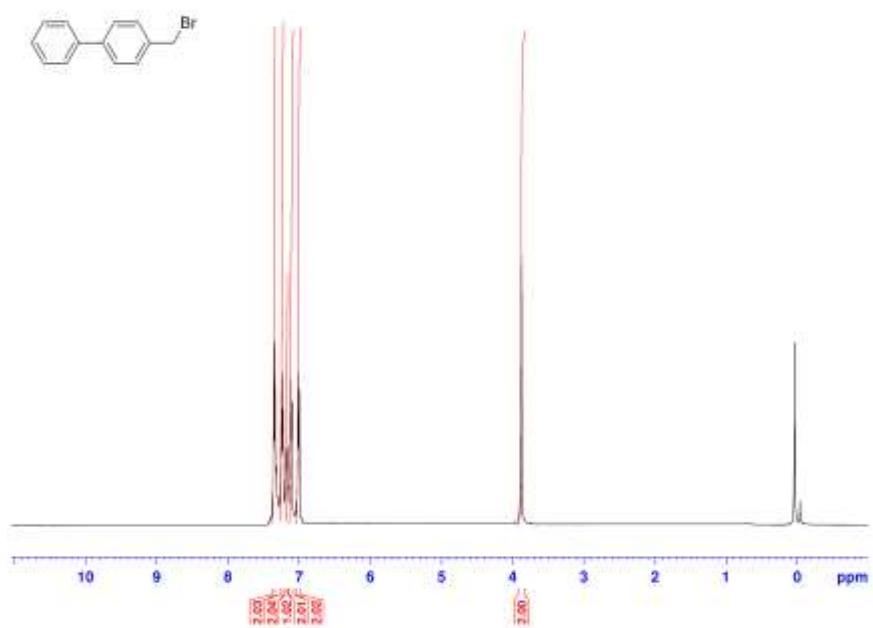


Figure S12. ¹H NMR spectrum (500 MHz, CDCl₃) of **3g**.

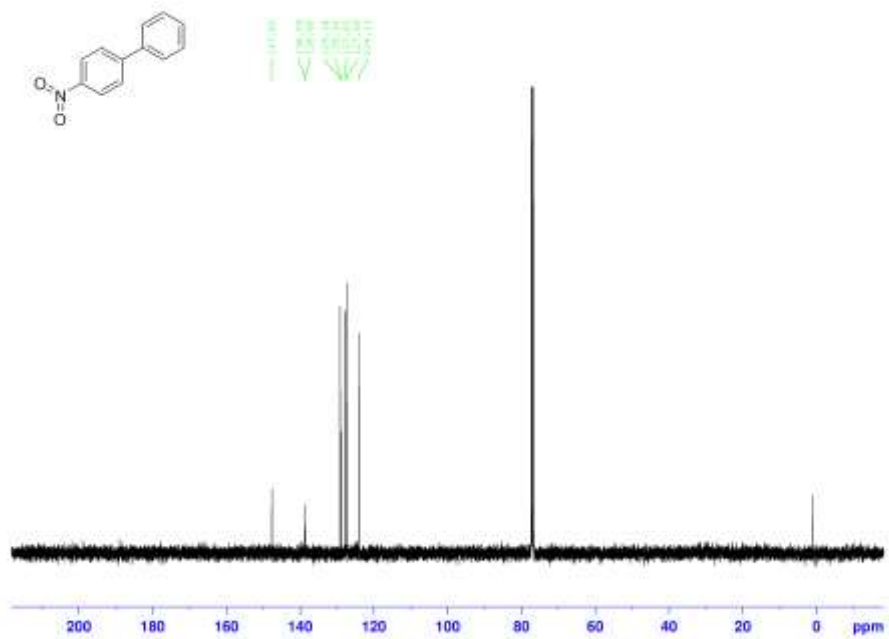


Figure S15. ¹³C NMR spectrum (500 MHz, CDCl₃) of **3h**.

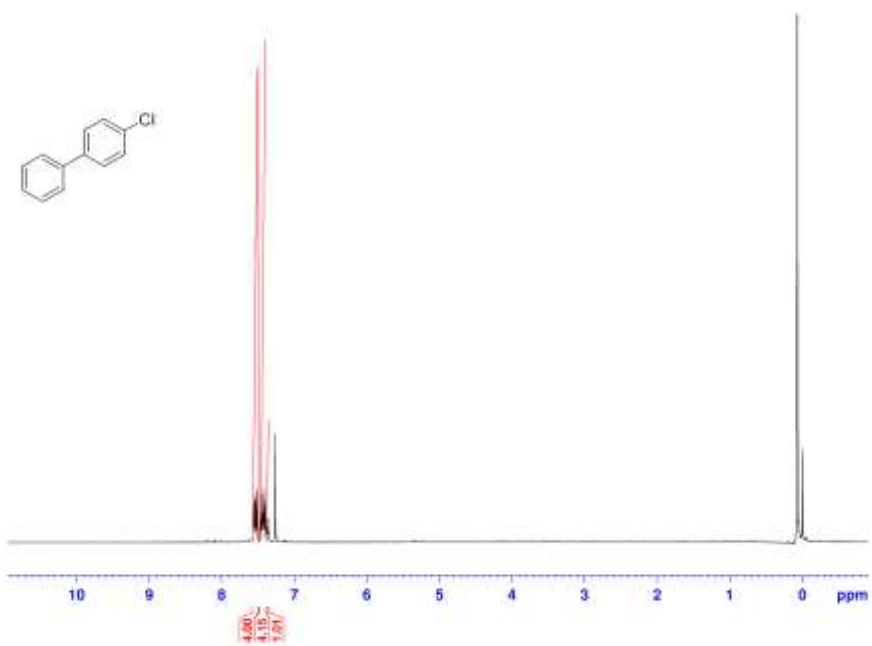


Figure S16. ¹H NMR spectrum (500 MHz, CDCl₃) of **3i**.

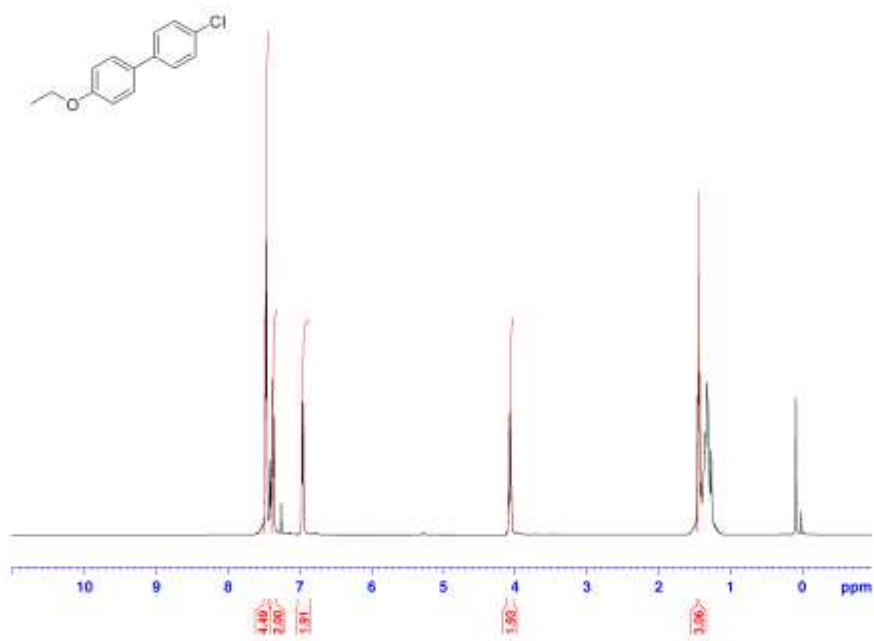


Figure S23. ¹H NMR spectrum (500 MHz, CDCl₃) of 4a.

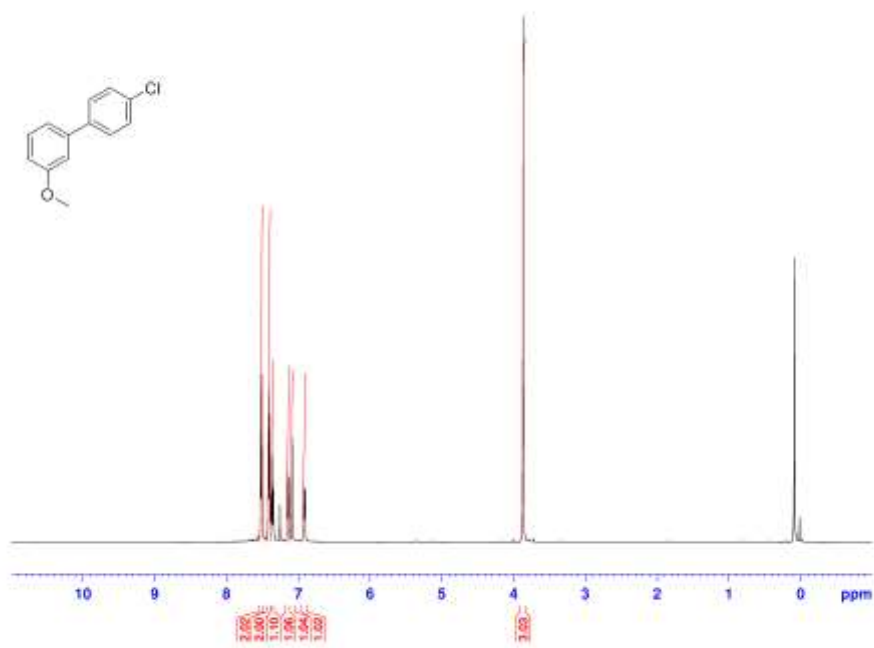


Figure S24. ¹H NMR spectrum of 4c.

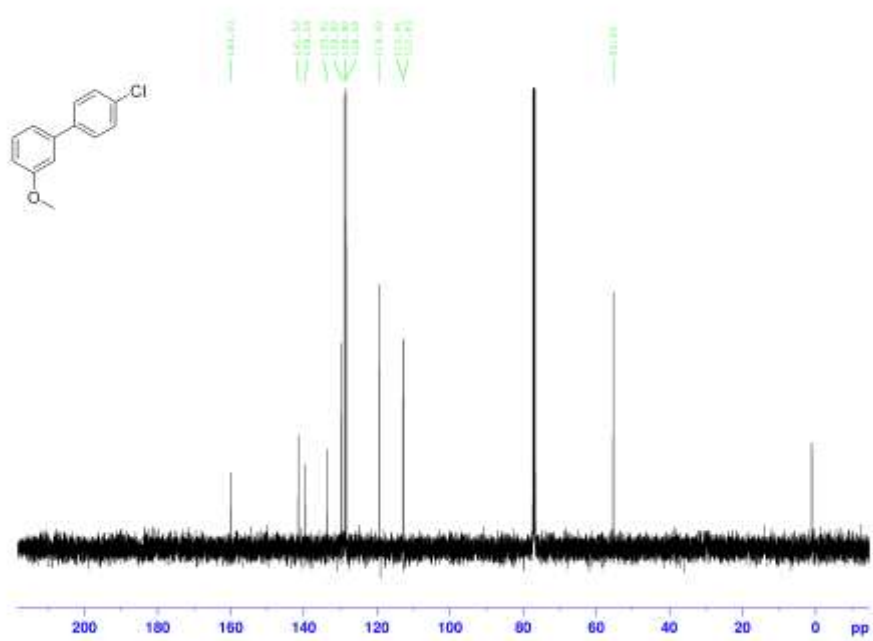


Figure S25. ¹³C NMR spectrum (500 MHz, CDCl₃) of 4c.

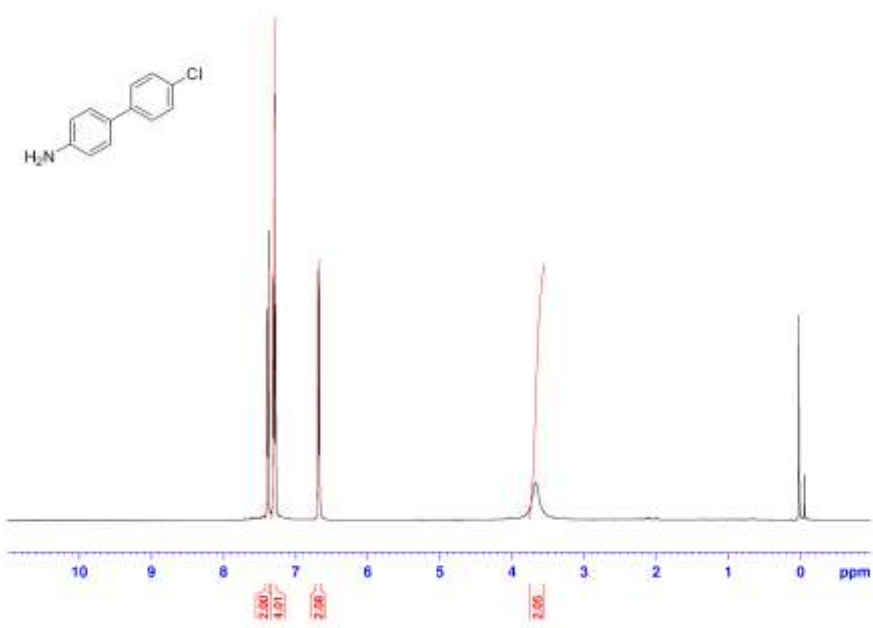


Figure S26. ¹H NMR spectrum (500 MHz, CDCl₃) of 4d.

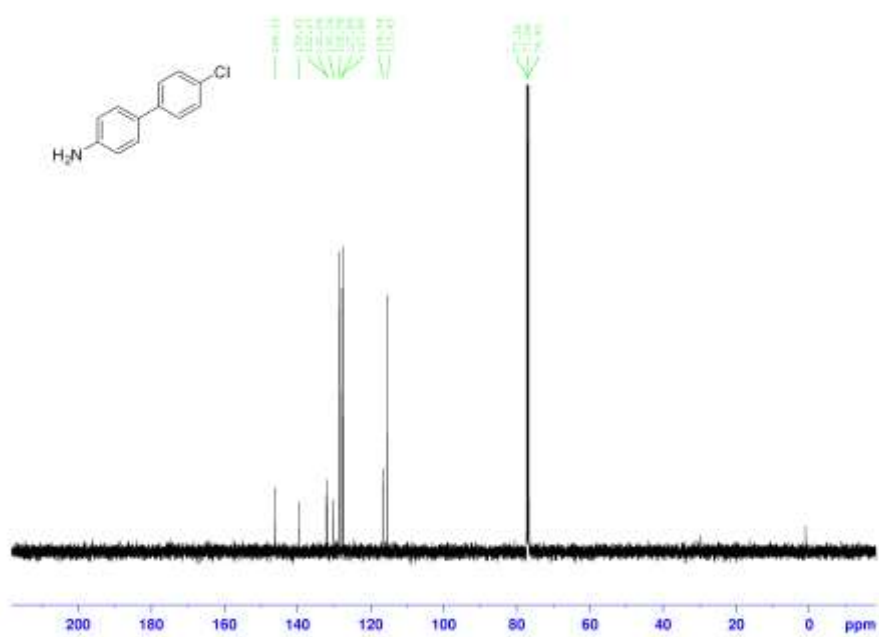


Figure S27. ¹³C NMR spectrum (500 MHz, CDCl₃) of **4d**.

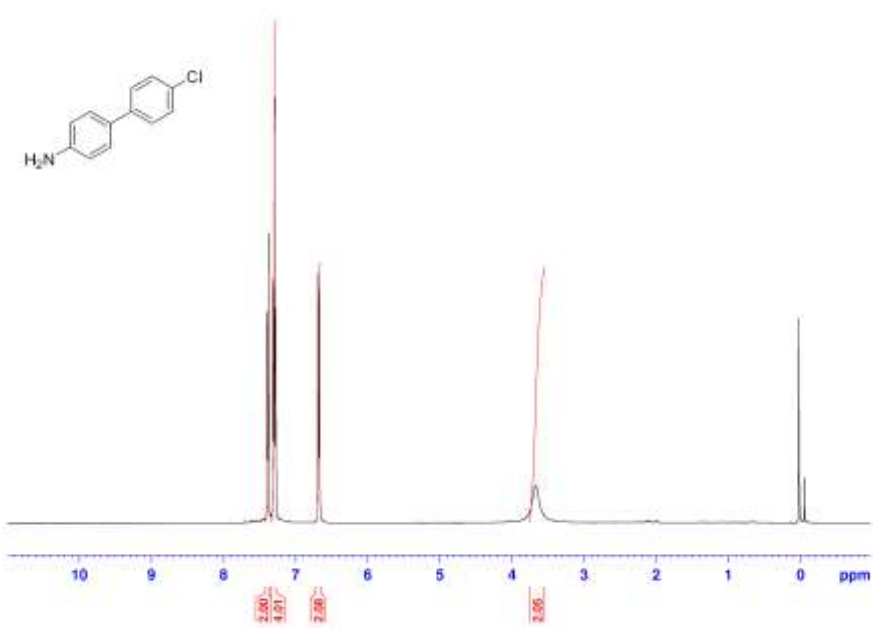


Figure S28. ¹H NMR spectrum (500 MHz, CDCl₃) of **4f**.

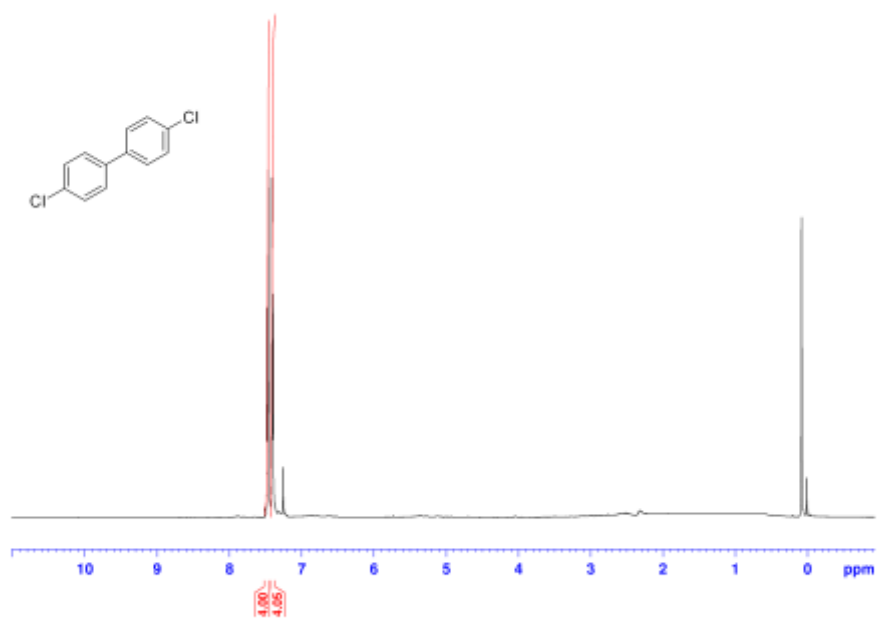


Figure S29. ¹H NMR spectrum (500 MHz, CDCl₃) of 4p.

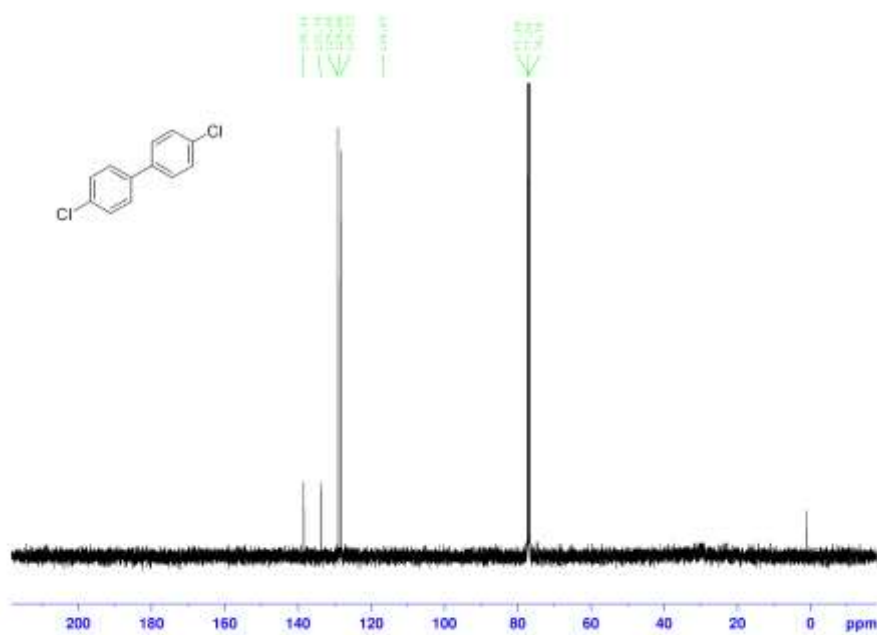


Figure S30. ¹³C NMR spectrum (500 MHz, CDCl₃) of 4p.

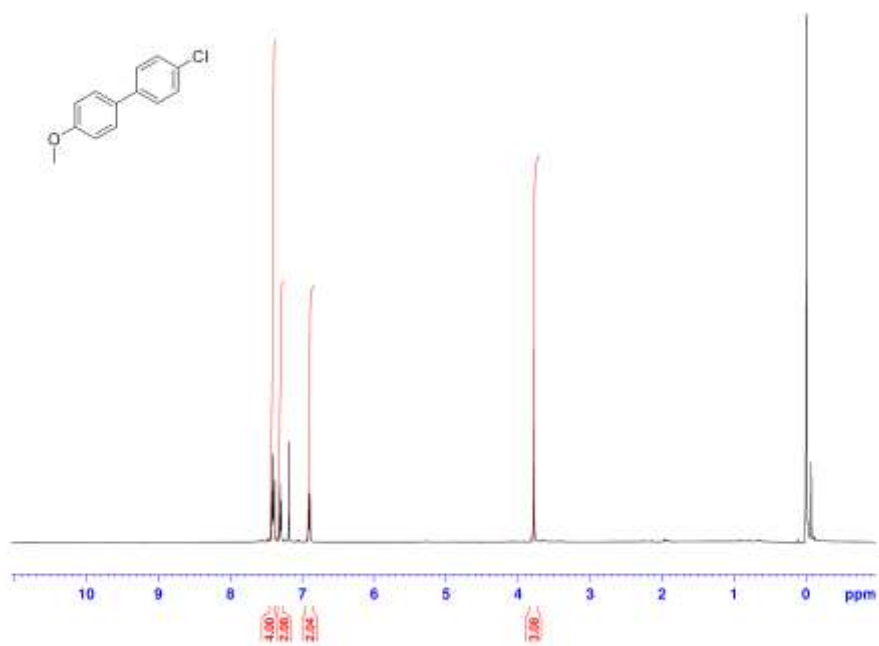


Figure S31. ¹H NMR spectrum (500 MHz, CDCl₃) of **4i**.

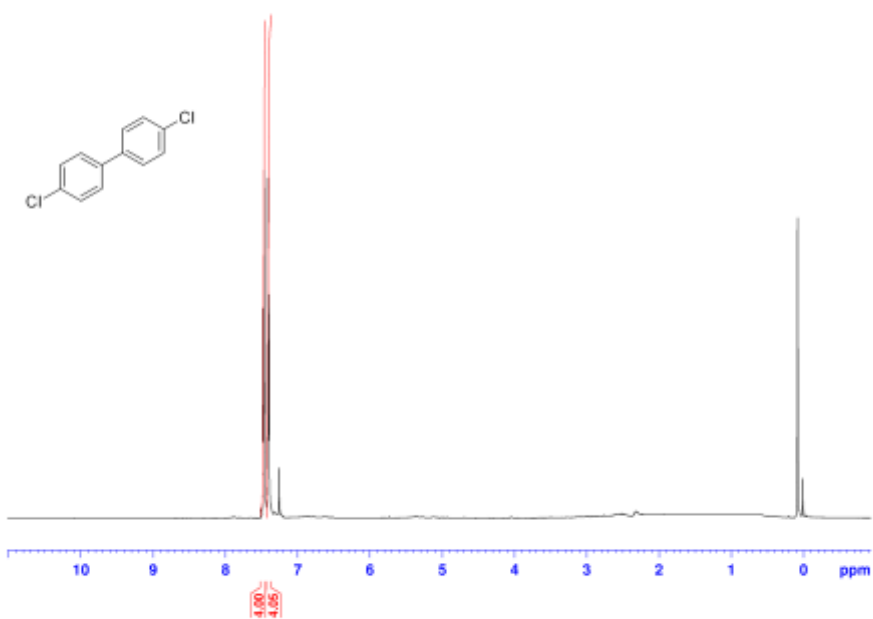


Figure S32. ¹H NMR spectrum (500 MHz, CDCl₃) of **4i**.

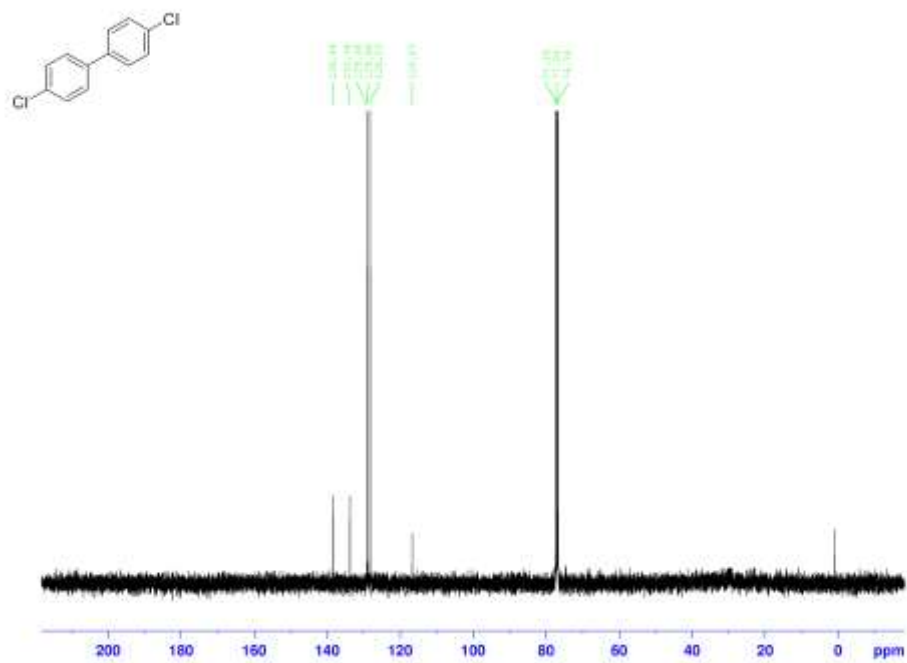


Figure S33. ¹³C NMR spectrum (500 MHz, CDCl₃) of 4i.

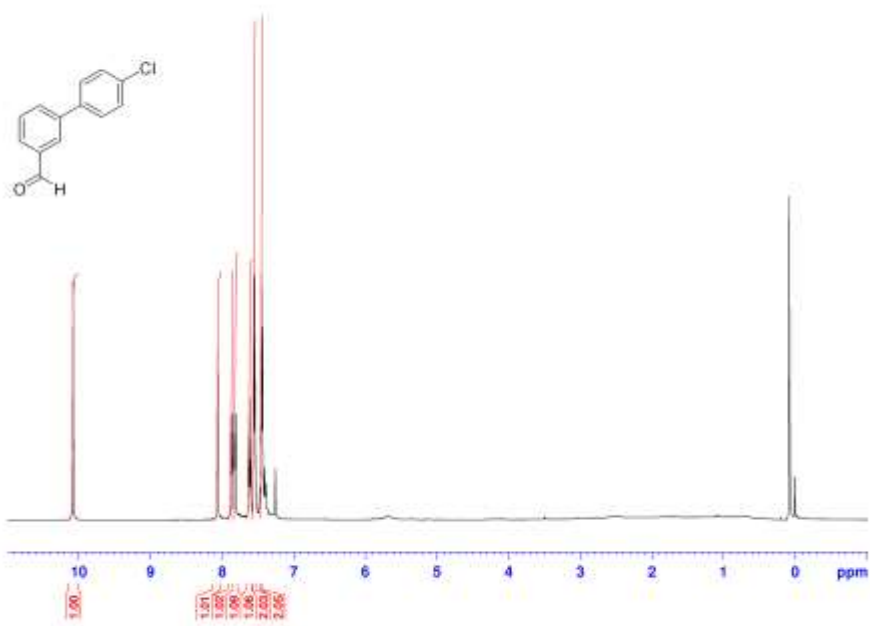


Figure S34. ¹H NMR spectrum (500vMHz, CDCl₃) of 4s.

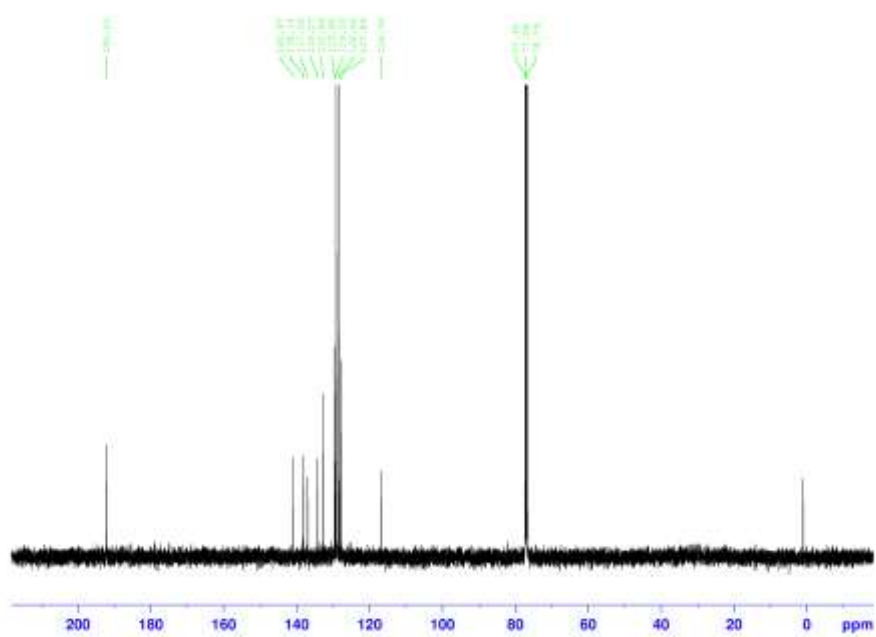


Figure S35. ^{13}C NMR spectrum (500MHz, CDCl_3) of **4s**.

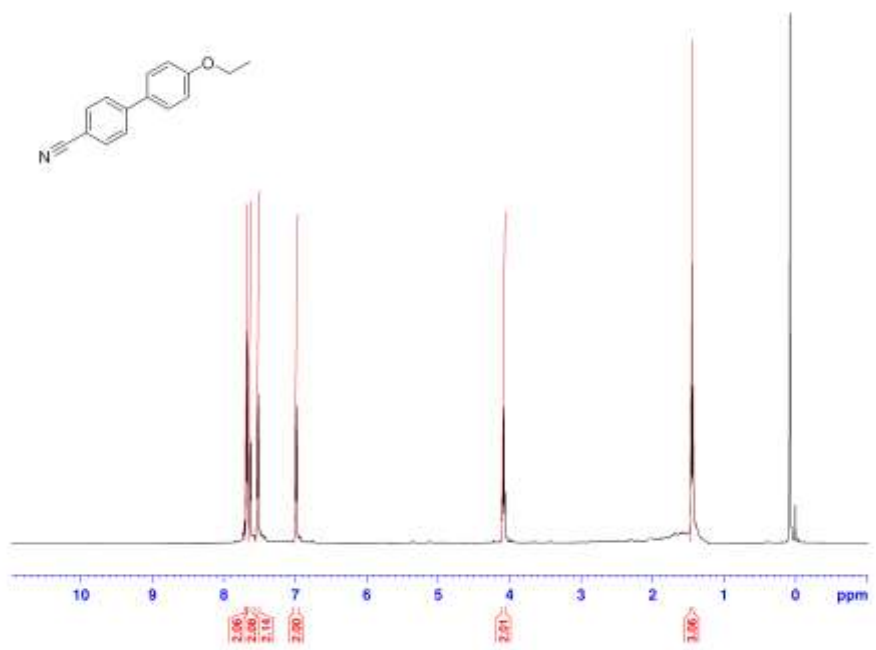


Figure S36. ^1H NMR spectrum (500 MHz, CDCl_3) of **5b**.

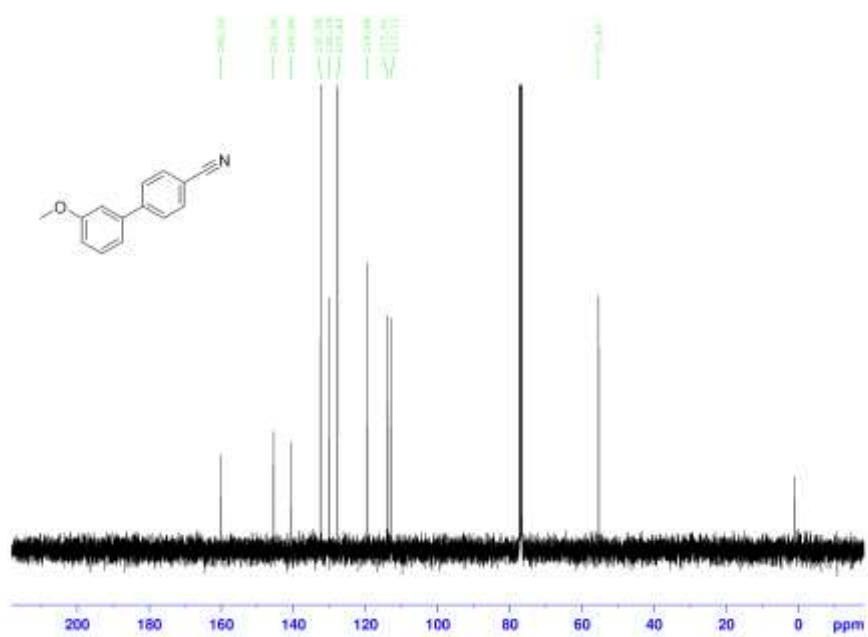


Figure S39. ¹³C NMR spectrum (500 MHz, CDCl₃) of **5c**.

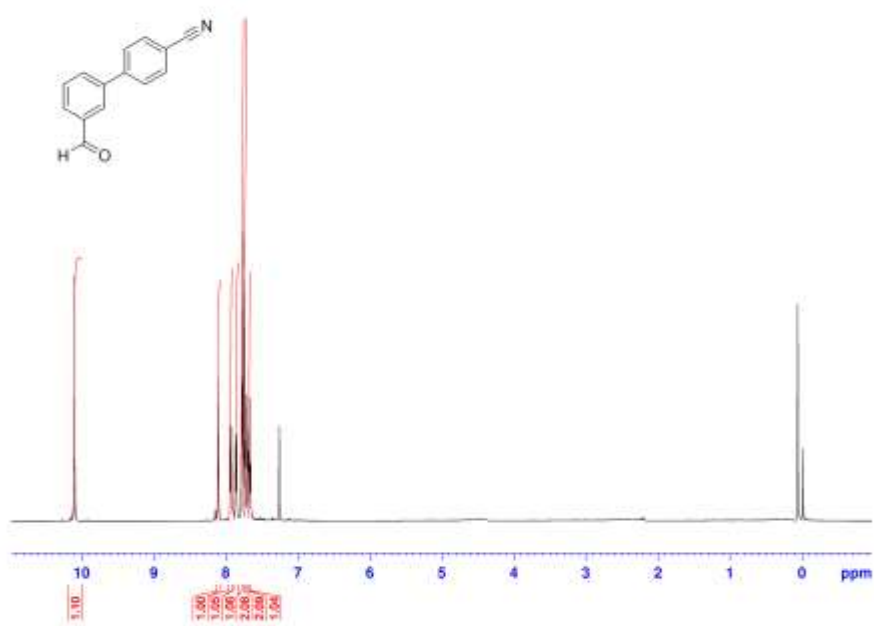


Figure S40. ¹H NMR spectrum (500 MHz, CDCl₃) of **5g**.

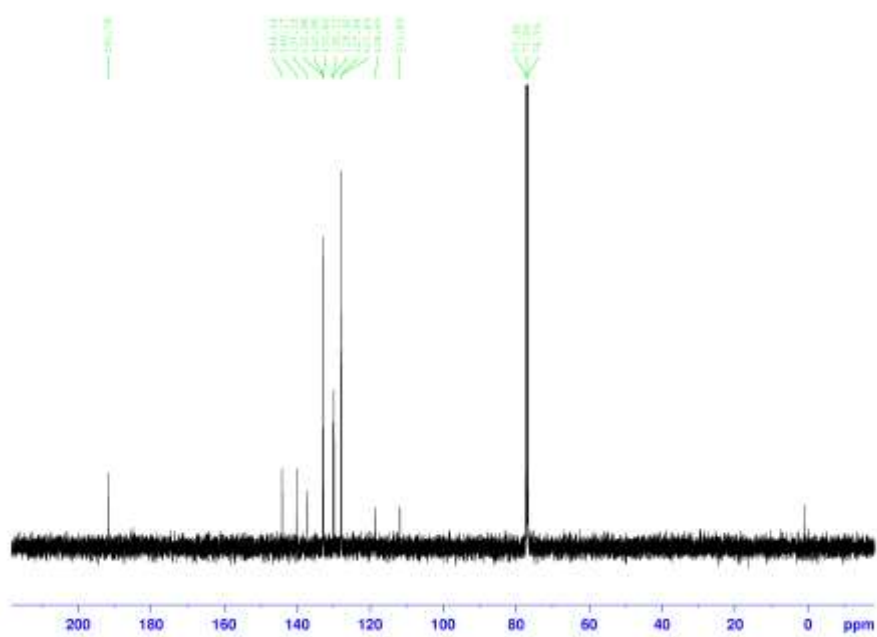


Figure S41. ^{13}C NMR spectrum (500 MHz, CDCl_3) of **5g**.

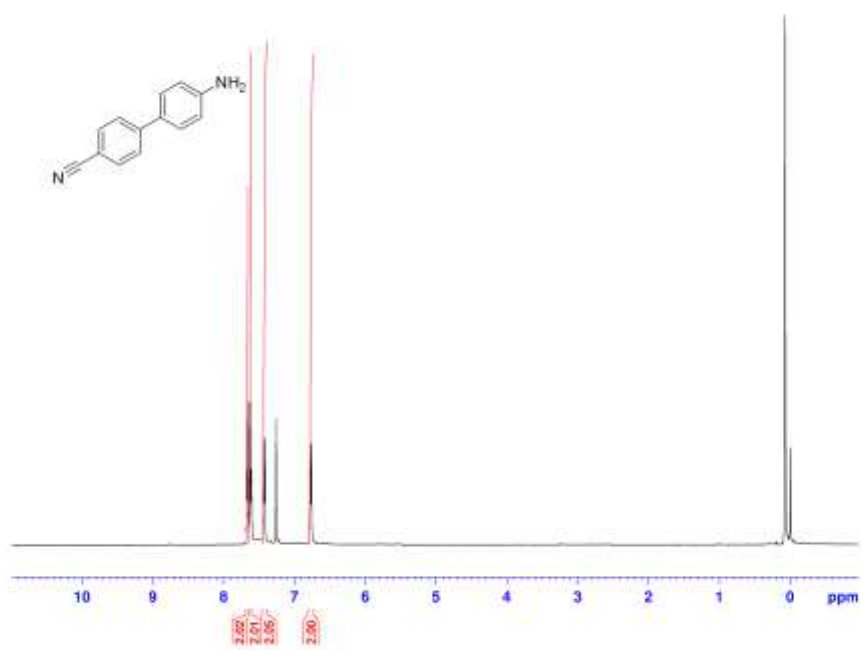


Figure S42. ^1H NMR spectrum (500 MHz, CDCl_3) of **5d**.

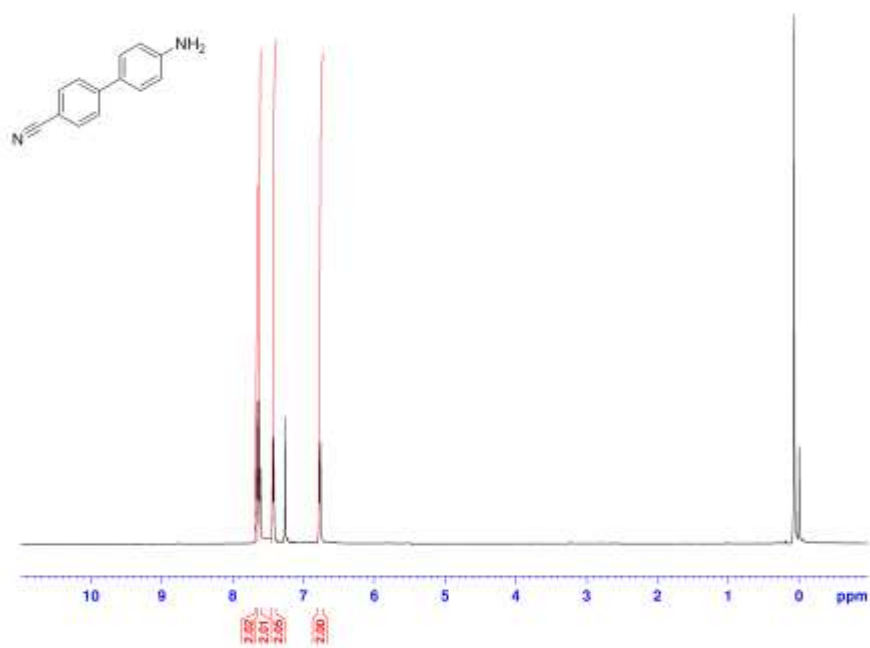


Figure S43. ¹H NMR spectrum (500 MHz, CDCl₃) of **5f**.

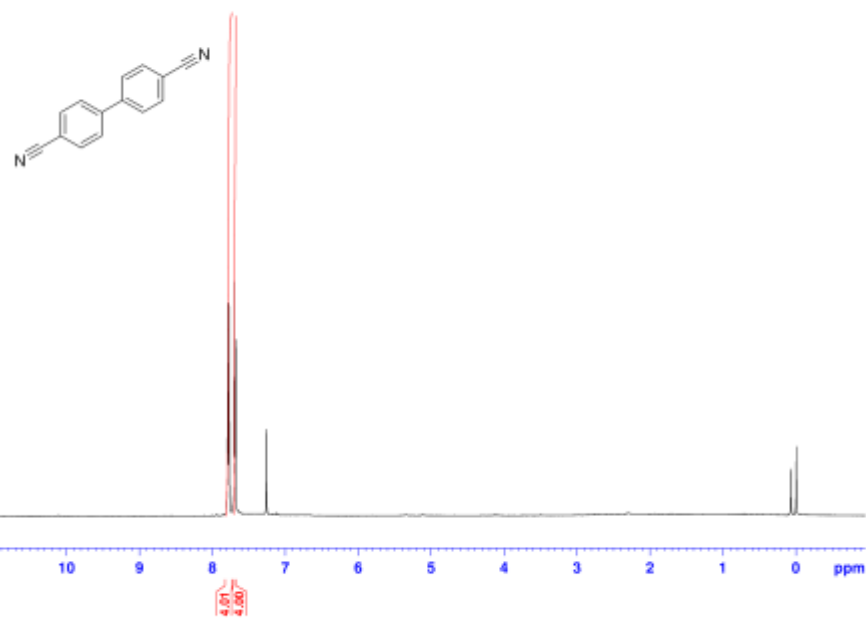


Figure S44. ¹H NMR spectrum (500 MHz, CDCl₃) of **5j**.

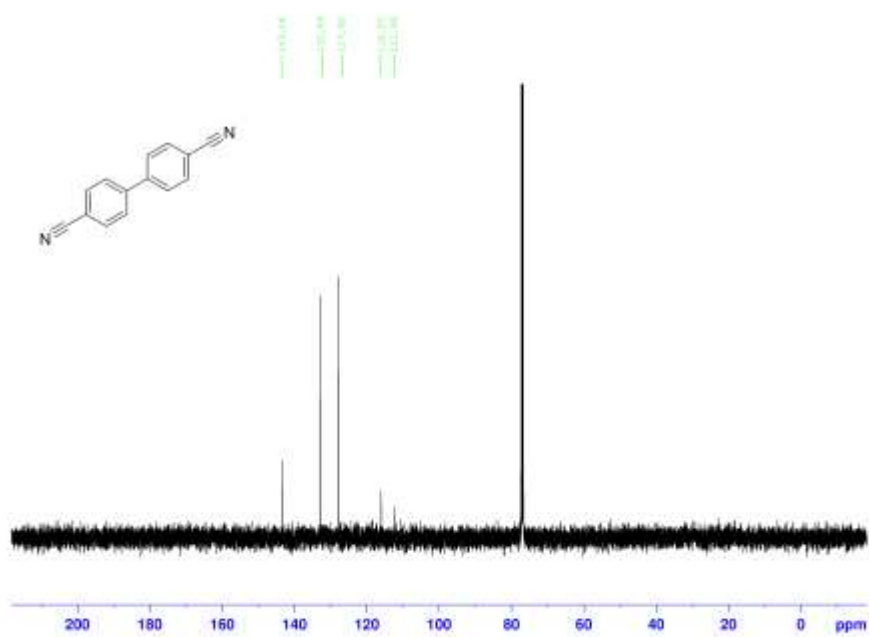


Figure S45. ¹³C NMR spectrum (500 MHz, CDCl₃) of 5j.

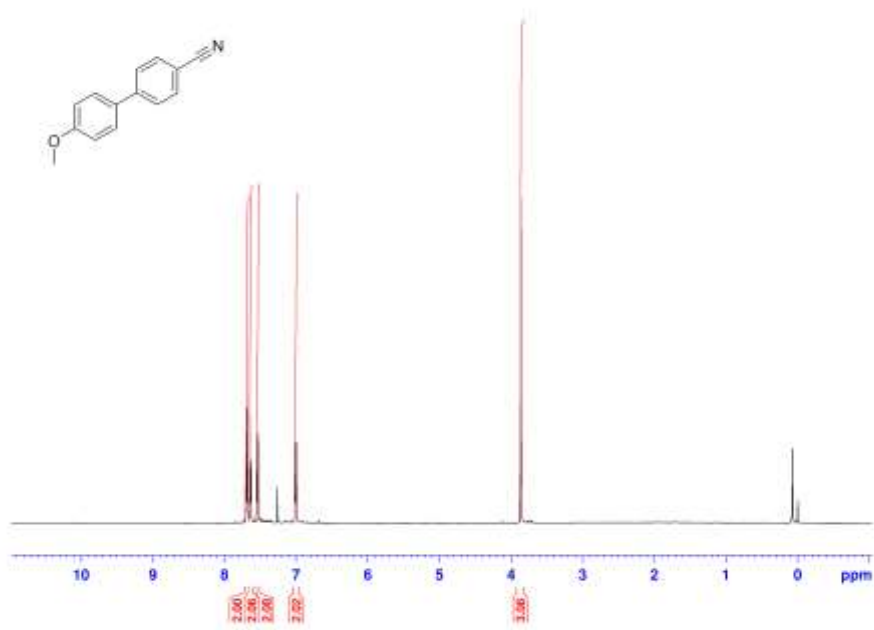


Figure S46. ¹H NMR spectrum (500 MHz, CDCl₃) of 5l.

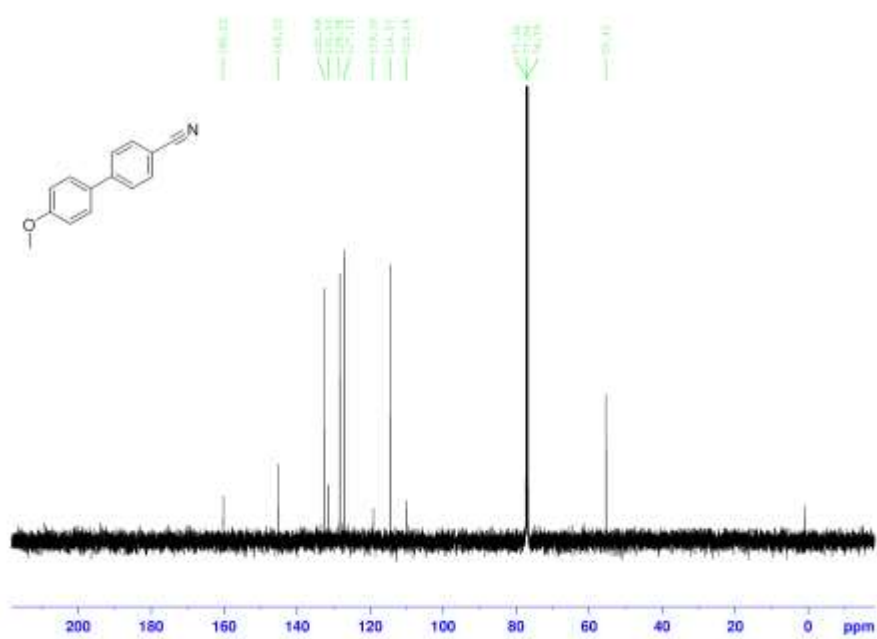


Figure S47. ^{13}C NMR spectrum (500 MHz, CDCl_3) of **51**.