

Crossed McMurry Coupling Reactions for Porphycenic Macrocycles: Non-statistical Selectivity and Rationalisation

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Supporting information

¹H and ¹³C NMR spectra for macrocyclic products and ¹H NMR spectra of crude reaction mixtures.

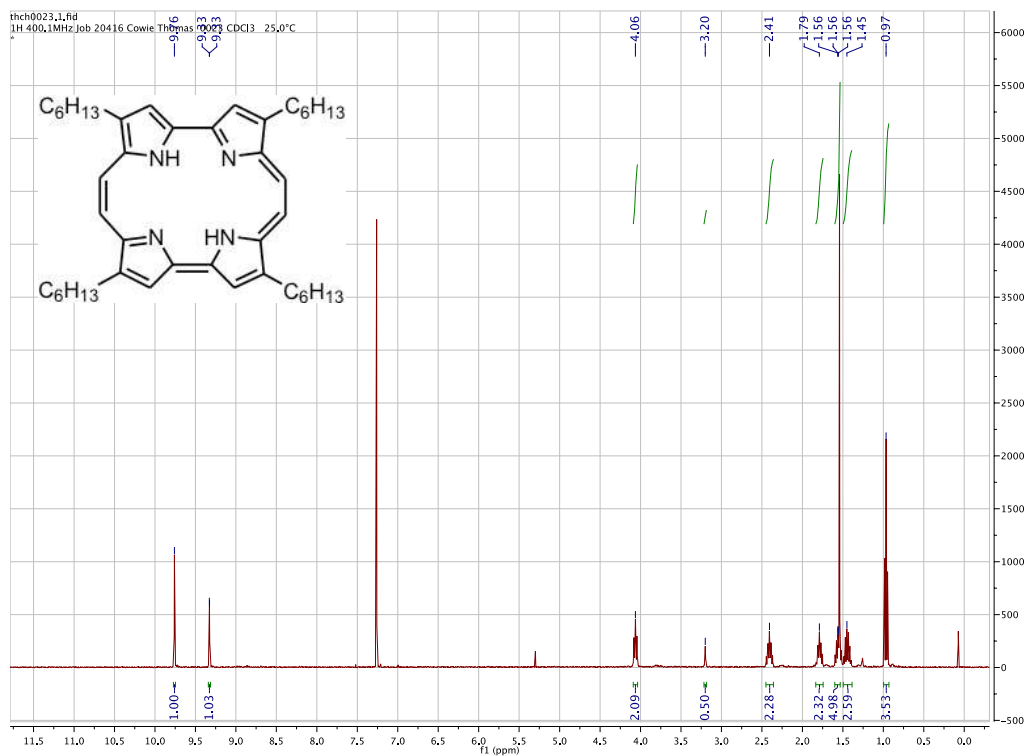


Figure 1. ^1H NMR Spectrum of 11b in CDCl_3

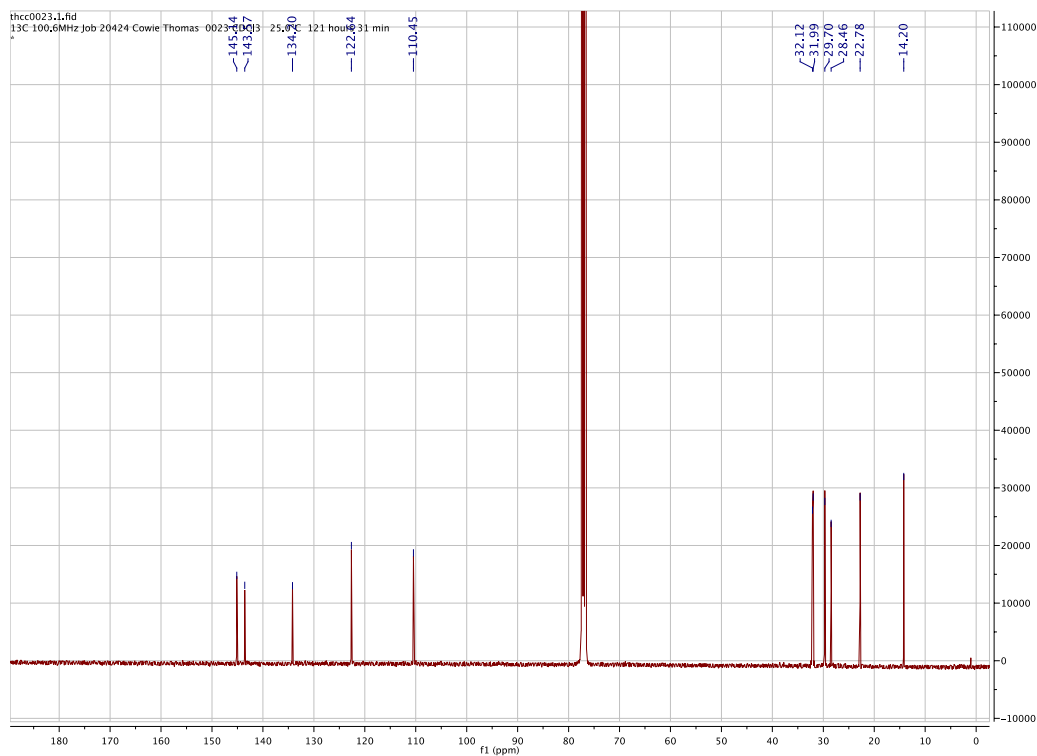


Figure 2. ^{13}C NMR Spectrum of 11b in CDCl_3

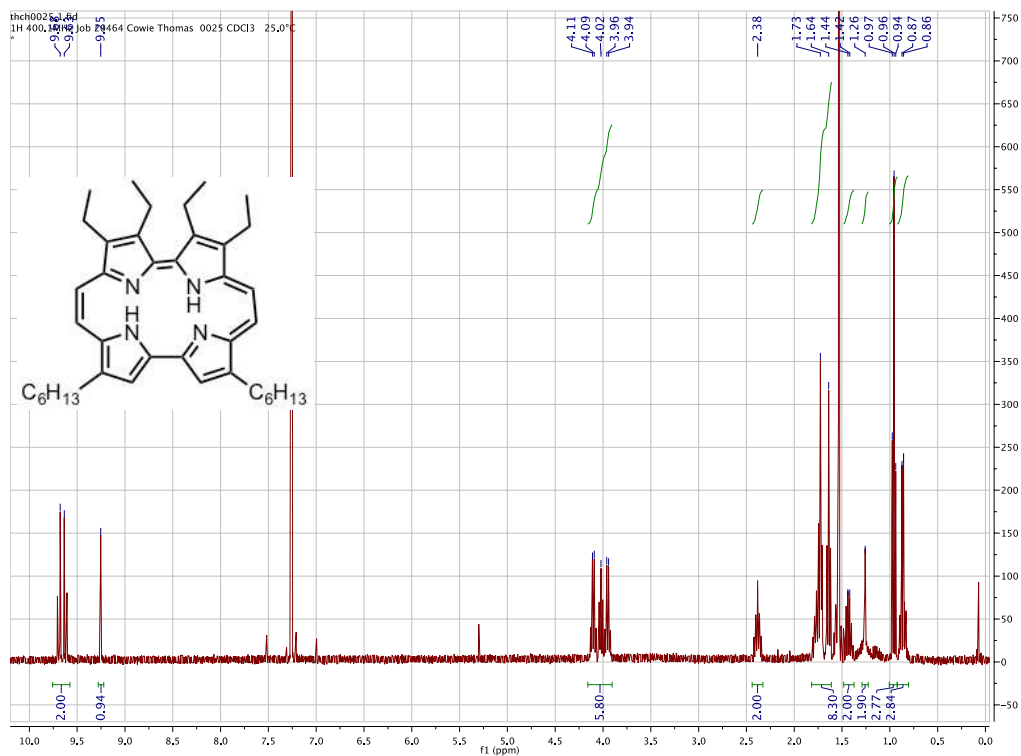


Figure 3. ¹H NMR Spectrum of 11c in CDCl₃

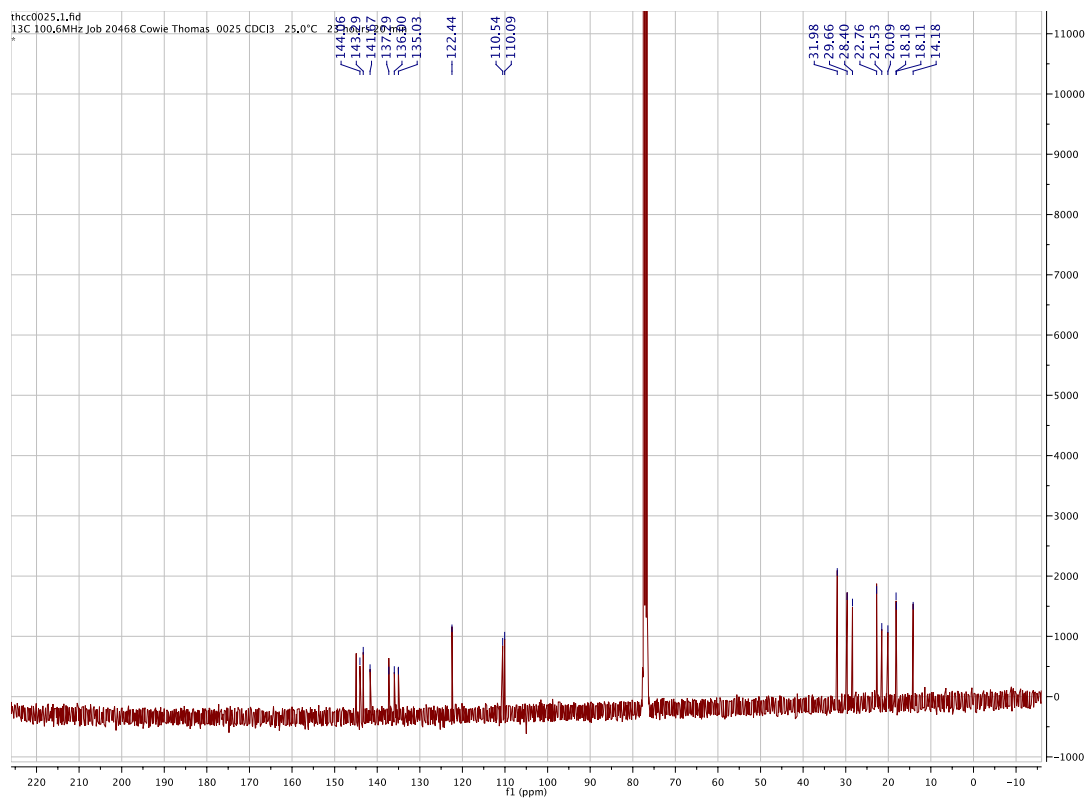


Figure 4. ¹³C NMR Spectrum of 11c in CDCl₃

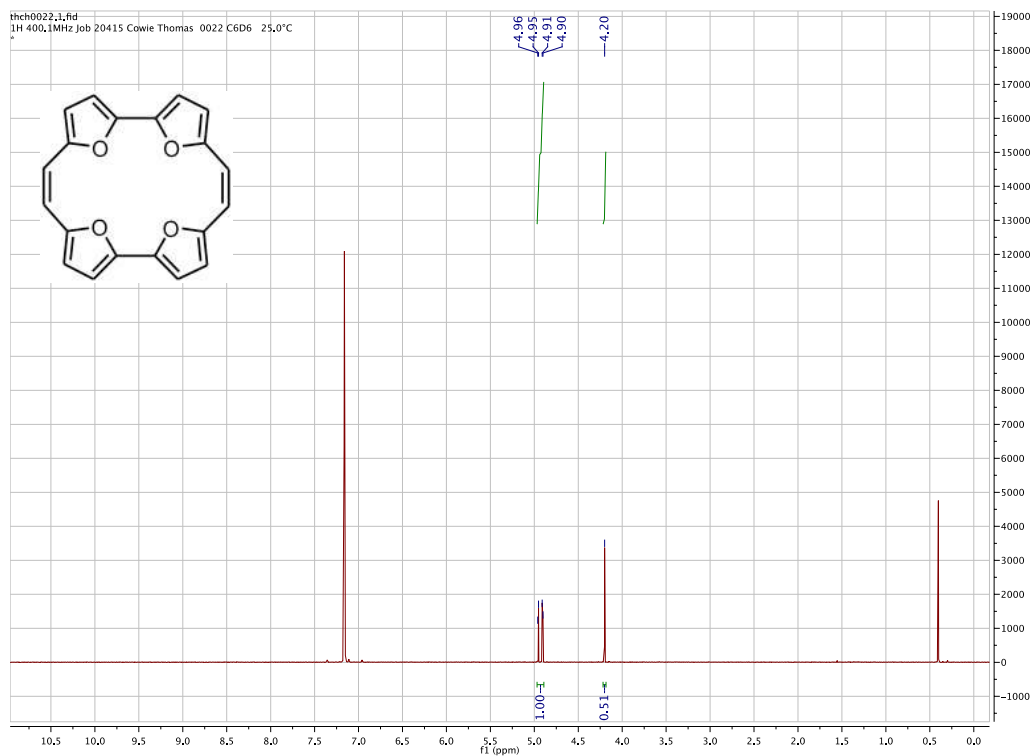


Figure 5. ^1H NMR Spectrum of 12a in C_6D_6

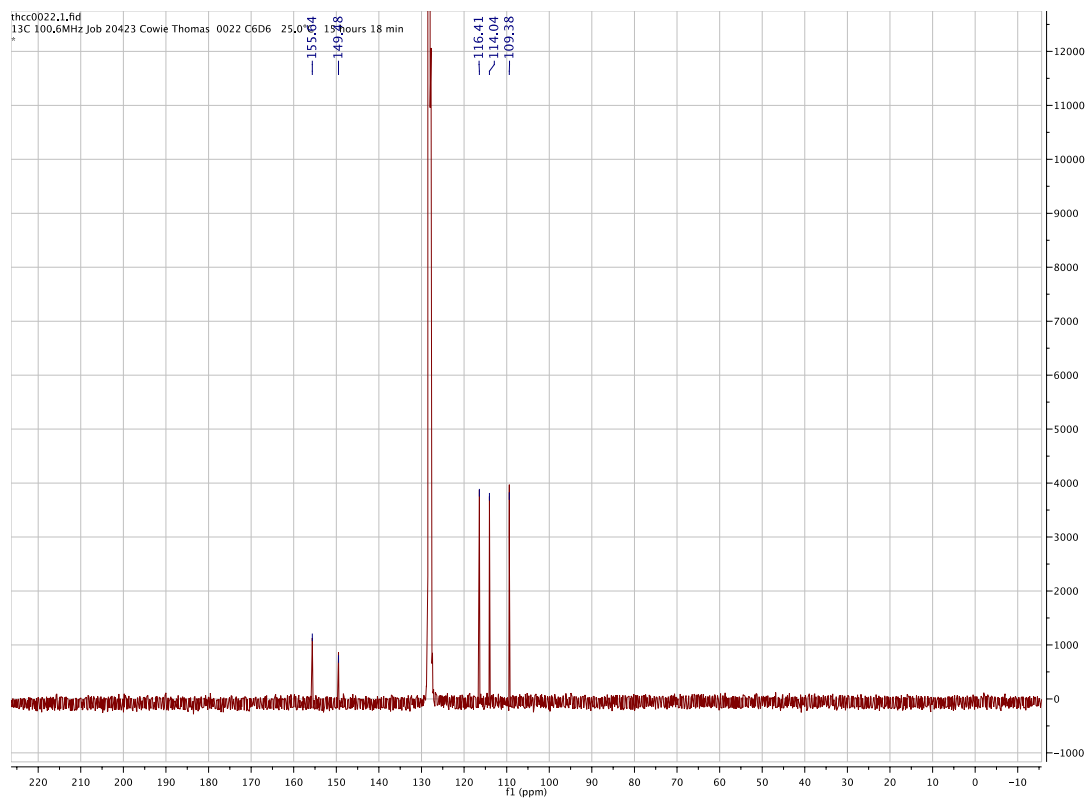


Figure 6. ^{13}C NMR Spectrum of 12a in C_6D_6

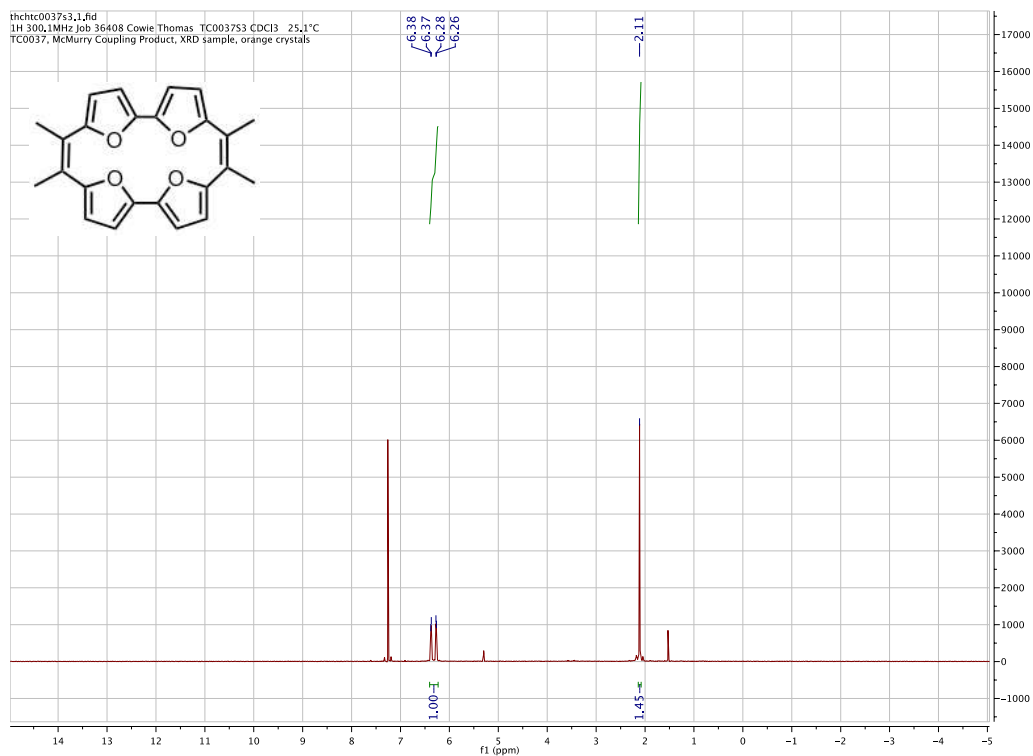


Figure 7. ^1H NMR Spectrum of 12b in CDCl_3

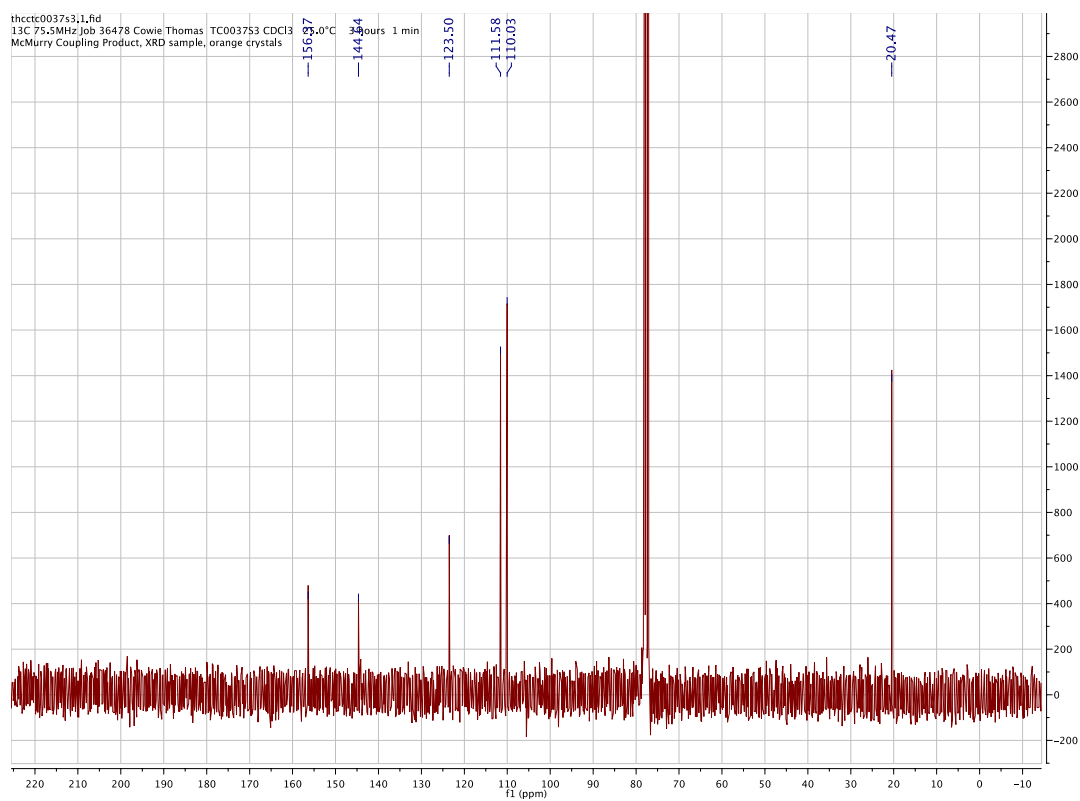


Figure 8. ^{13}C NMR Spectrum of 12b in CDCl_3

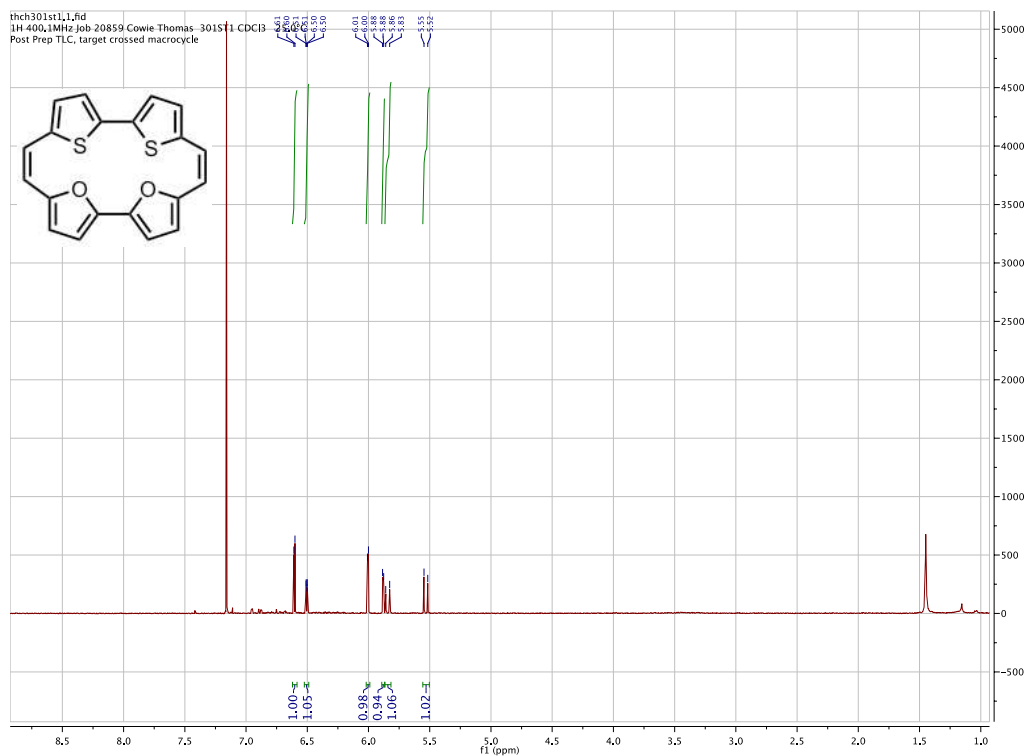


Figure 9. ^1H NMR Spectrum of 16 in CDCl_3

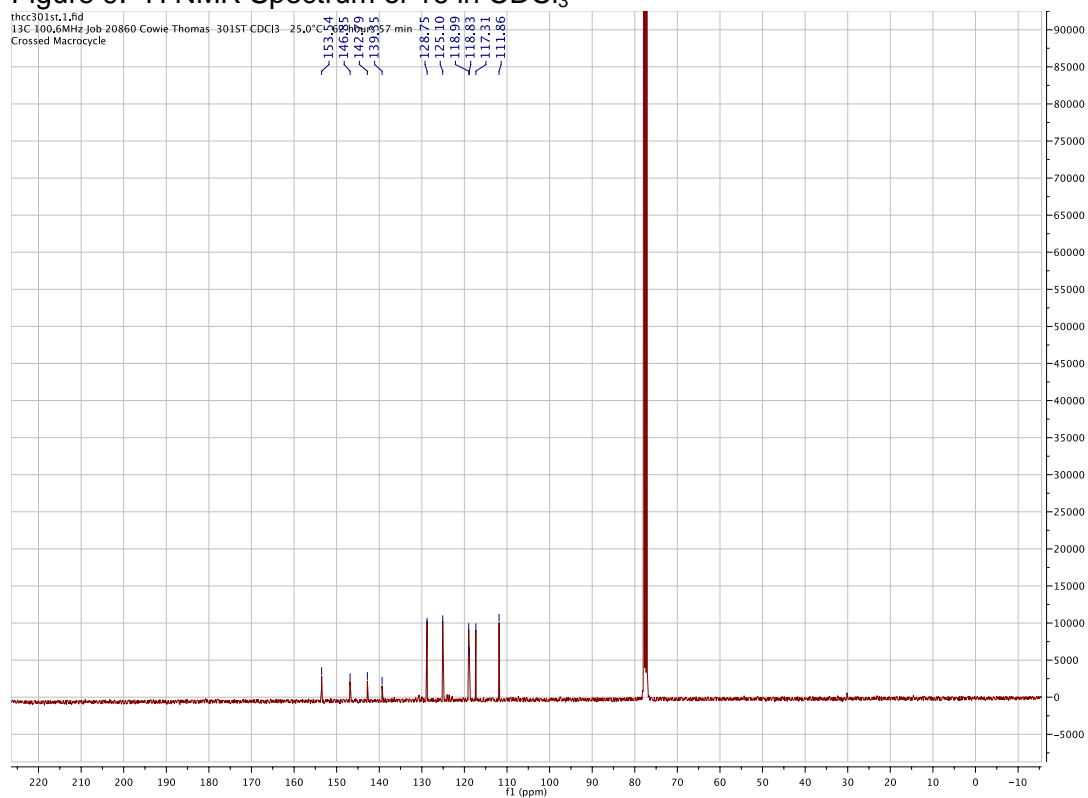


Figure 10. ^{13}C NMR Spectrum of 16 in CDCl_3

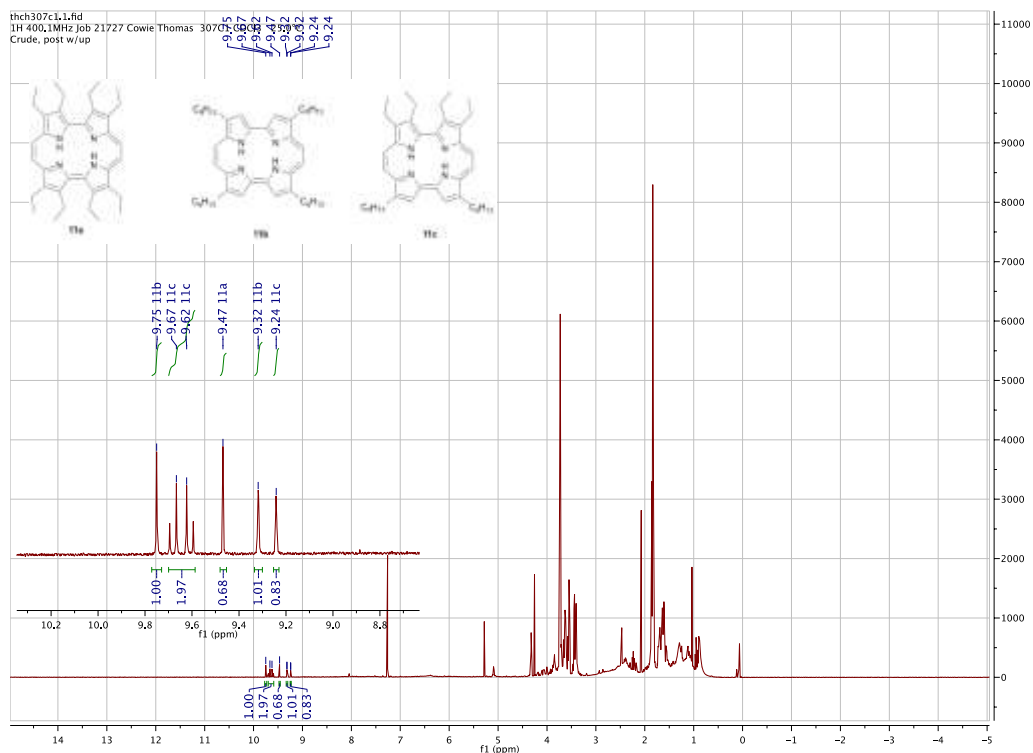


Figure 11. ^1H NMR spectra of crossed McMurry reaction between compound 6 & 7; Ratios of the products are shown, **11a** (20%), **11b** (26%), **11c** (54%, 5% isolated).

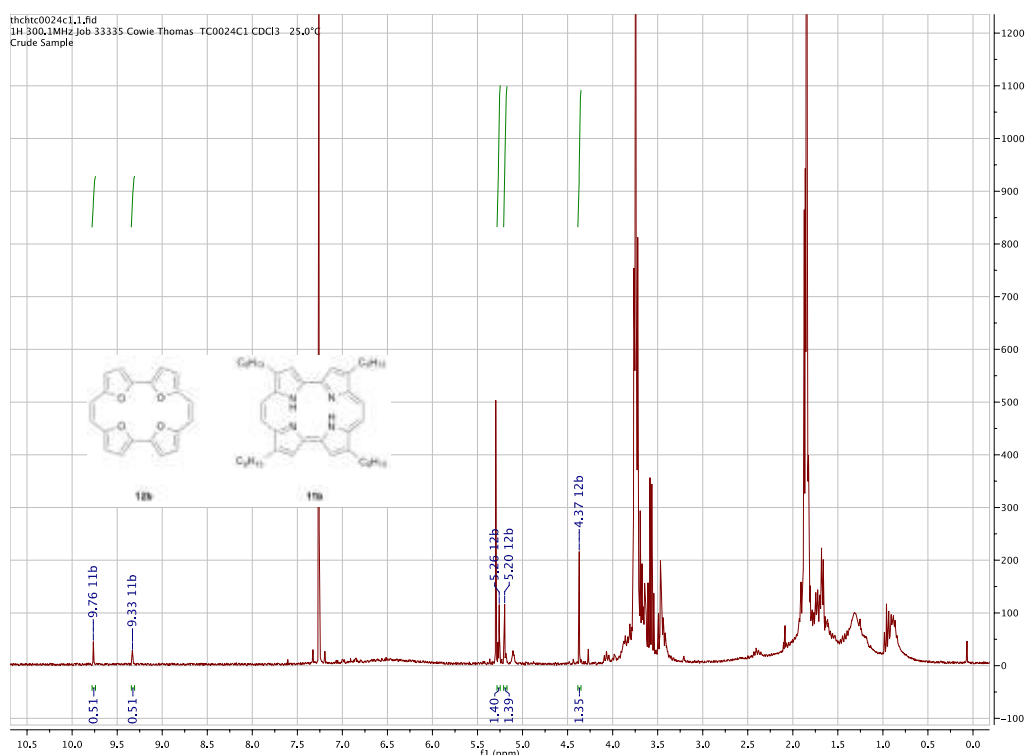


Figure 12. ^1H NMR spectra of crossed McMurry reaction between compound 6 & 9; Ratios of the products are shown, **11b** (27%), **12b** (73%).

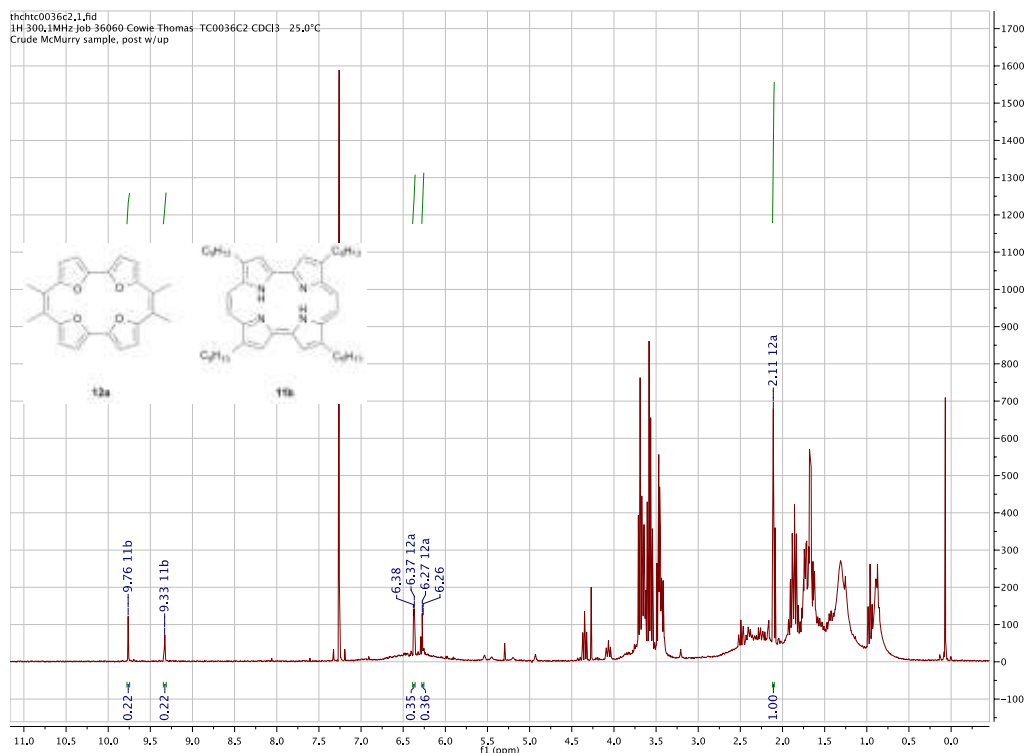


Figure 13. ^1H NMR spectra of crossed McMurry reaction between compound 6 & 10; Ratios of the products are shown, **11b** (41%), **12a** (59%).

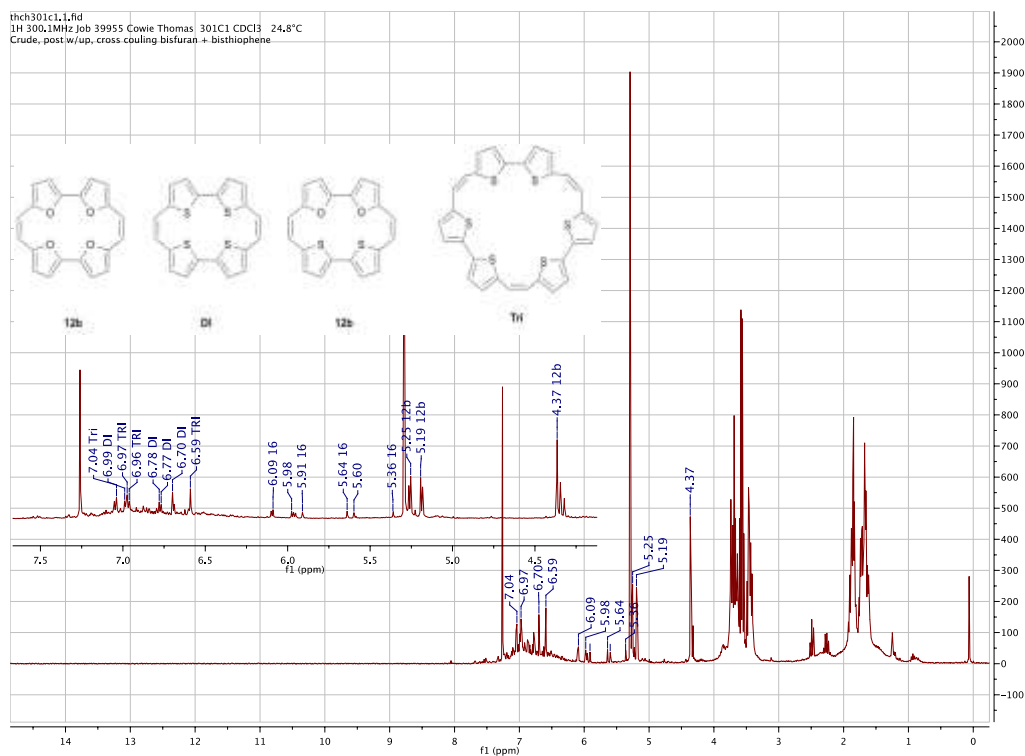


Figure 14. ^1H NMR spectra of crossed McMurry reaction between compound 9 & 15; Ratios of the products are shown, **12b** (45%), Bisthiophene Dimer (**DI**, 17%), Disthiophene Trimer (**TRI**, 14%), **16** (24%, 8% isolated).

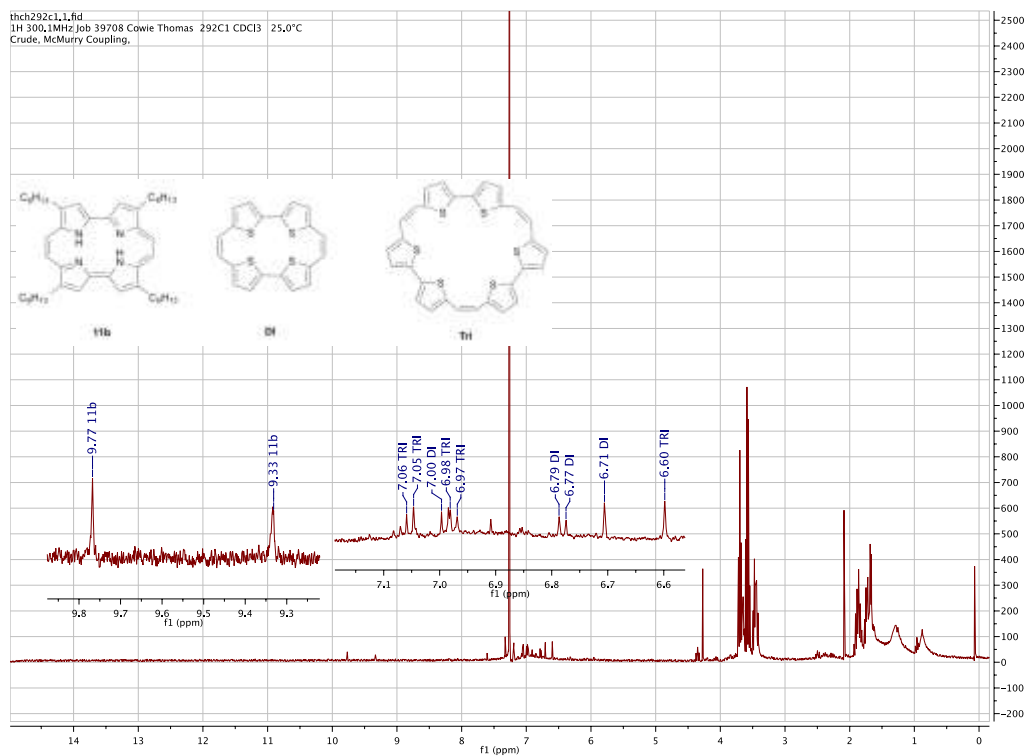


Figure 15. ^1H NMR spectra of crossed McMurry reaction between compound **6** & **15**; Ratios of the products are shown, **11b** (36%), Bithiophene Dimer (**DI**, 47%), Disthiophene Trimer (**TRI**, 18%).