

Supplementary Materials: Chiral Self-Sorting in Truxene-Based Metallacages

Simon Séjourné, Antoine Labrunie, Clément Dalinot, Amina Benchohra, Vincent Carré, Frédéric Aubriet, Magali Allain, Marc Sallé and Sébastien Goeb

| | |
|---|----|
| Figure S1. ^1H NMR spectrum of compound 2 in CDCl_3 | 2 |
| Figure S2. ^{13}C NMR spectrum of compound 2 in CDCl_3 | 2 |
| Figure S3. ^1H NMR spectrum of ligand Trux3Pyr in CDCl_3 | 3 |
| Figure S4. ^{13}C NMR spectrum of ligand Trux3Pyr in CDCl_3 | 3 |
| Figure S5. ^1H COSY NMR spectrum of ligand Trux3Pyr in CDCl_3 | 4 |
| Figure S6. ^1H DOSY NMR spectrum of ligand Trux3Pyr in CDCl_3 | 4 |
| Figure S7. ^1H NMR spectrum of ligand Trux3Pyr in MeOD..... | 5 |
| Figure S8. ^1H COSY NMR spectrum of ligand Trux3Pyr in MeOD..... | 5 |
| Figure S9. ^1H DOSY NMR spectrum of ligand Trux3Pyr in MeOD..... | 6 |
| Figure S10. ^1H NMR spectrum of TruxNaph in MeOD..... | 6 |
| Figure S11. ^1H COSY NMR spectrum of TruxNaph in MeOD..... | 7 |
| Figure S12. ^1H DOSY NMR spectrum of TruxNaph in MeOD..... | 7 |
| Figure S13. ^1H NMR spectrum of TruxTetra in MeOD..... | 8 |
| Figure S14. ^1H COSY NMR spectrum of TruxTetra in MeOD..... | 8 |
| Figure S15. ^1H DOSY NMR spectrum of TruxTetra in MeOD..... | 9 |
| Figure S16. ESI-FTICR HRMS spectrum of TruxNaph in MeOH at $C = 10^{-4}$ M..... | 10 |
| Figure S17. ESI-FTICR HRMS spectrum of TruxTetra in MeOH at $C = 10^{-4}$ M..... | 10 |
| Figure S18. Representation of Bailar twist angles in TruxNaph and TruxTetra | 10 |

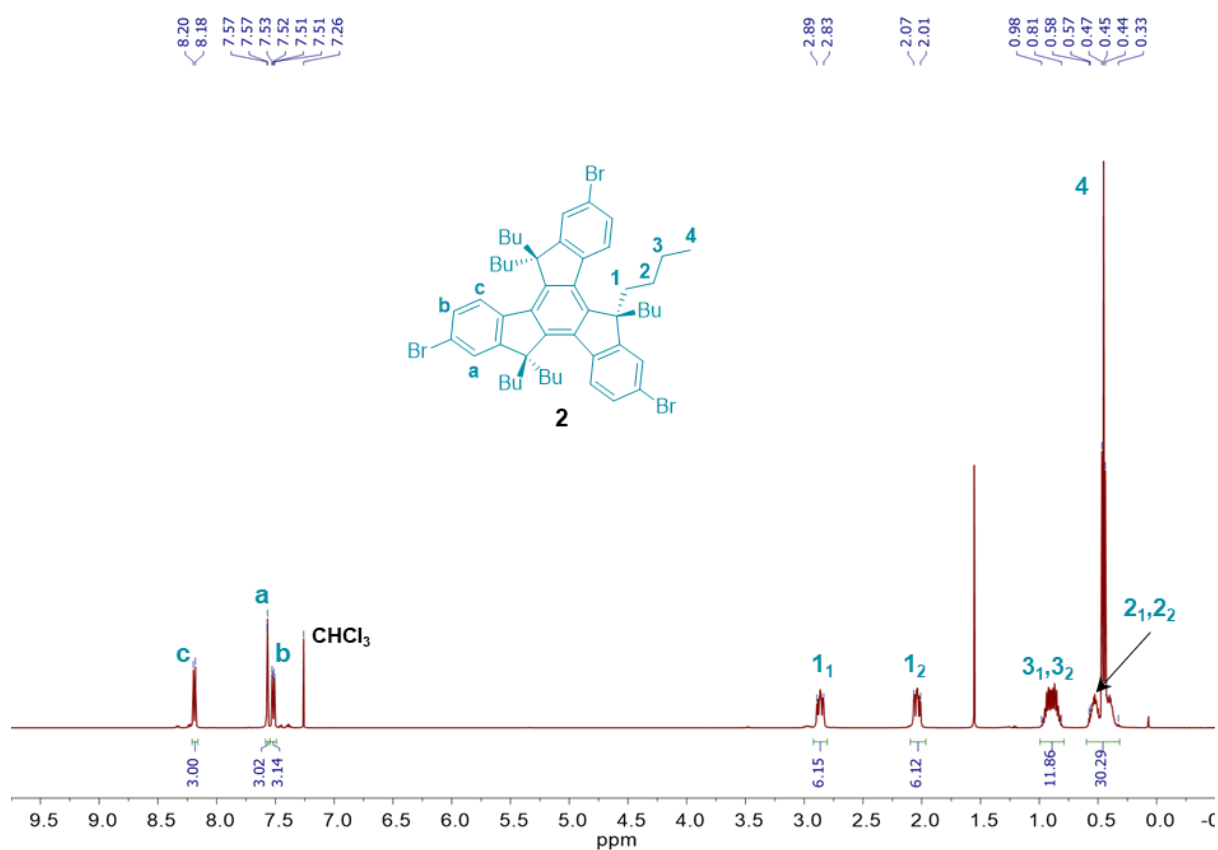


Figure S1. ¹H NMR spectrum of compound **2** in CDCl₃.

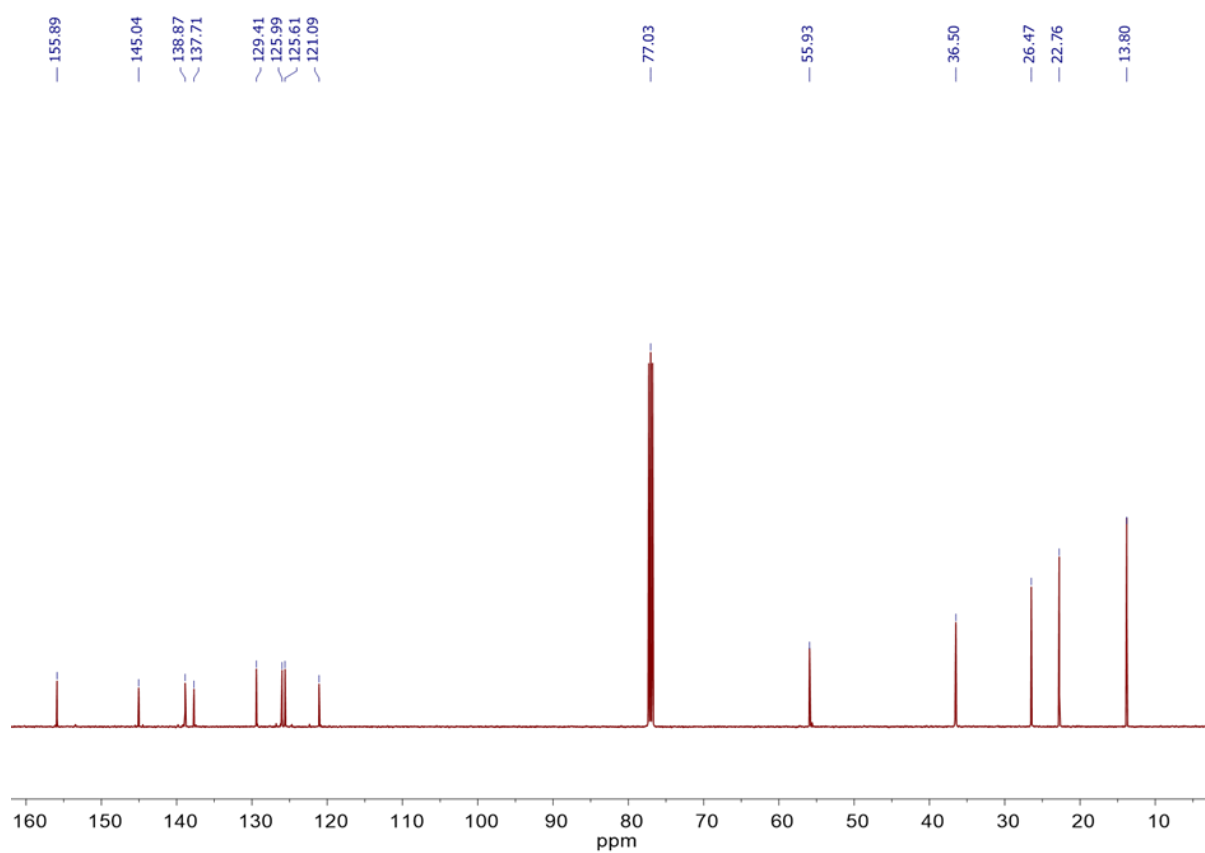


Figure S2. ¹³C NMR spectrum of compound **2** in CDCl₃.

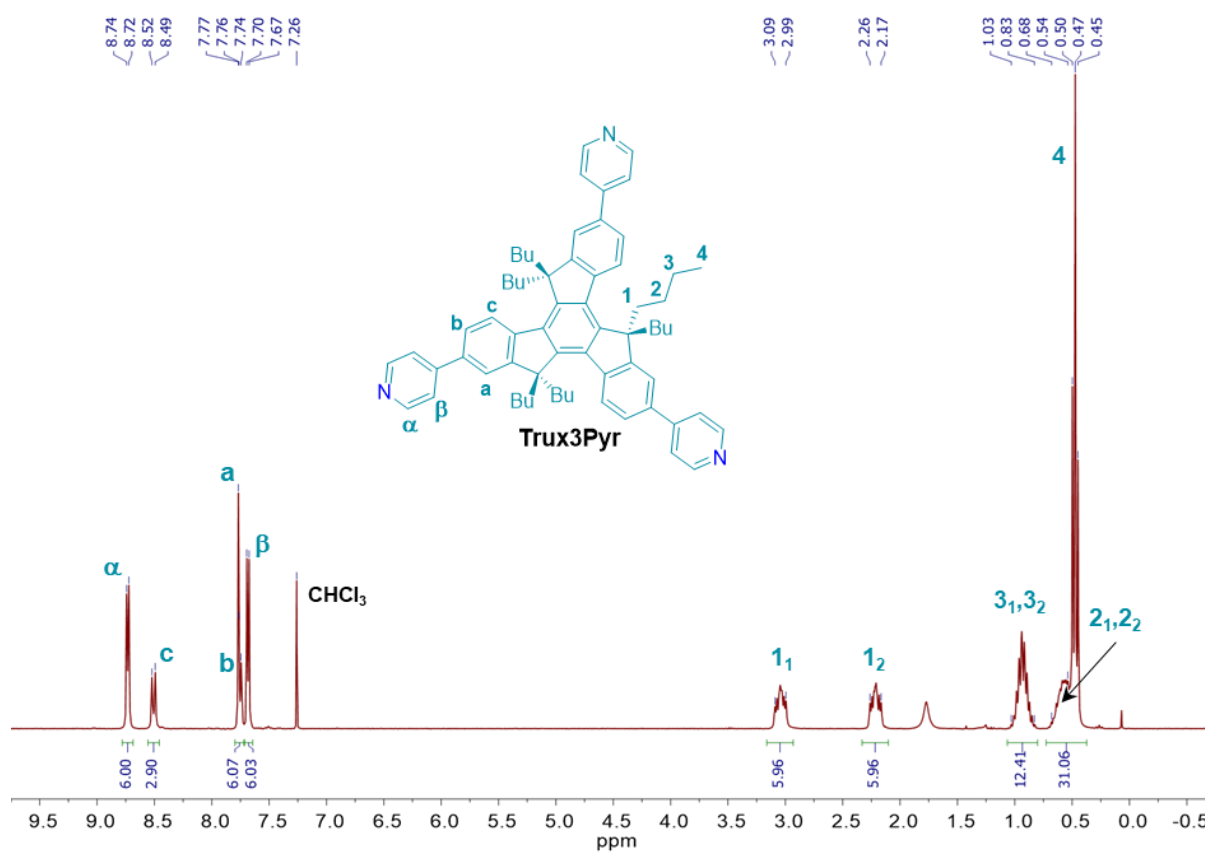


Figure S3. ¹H NMR spectrum of ligand **Trux3Pyr** in CDCl₃.

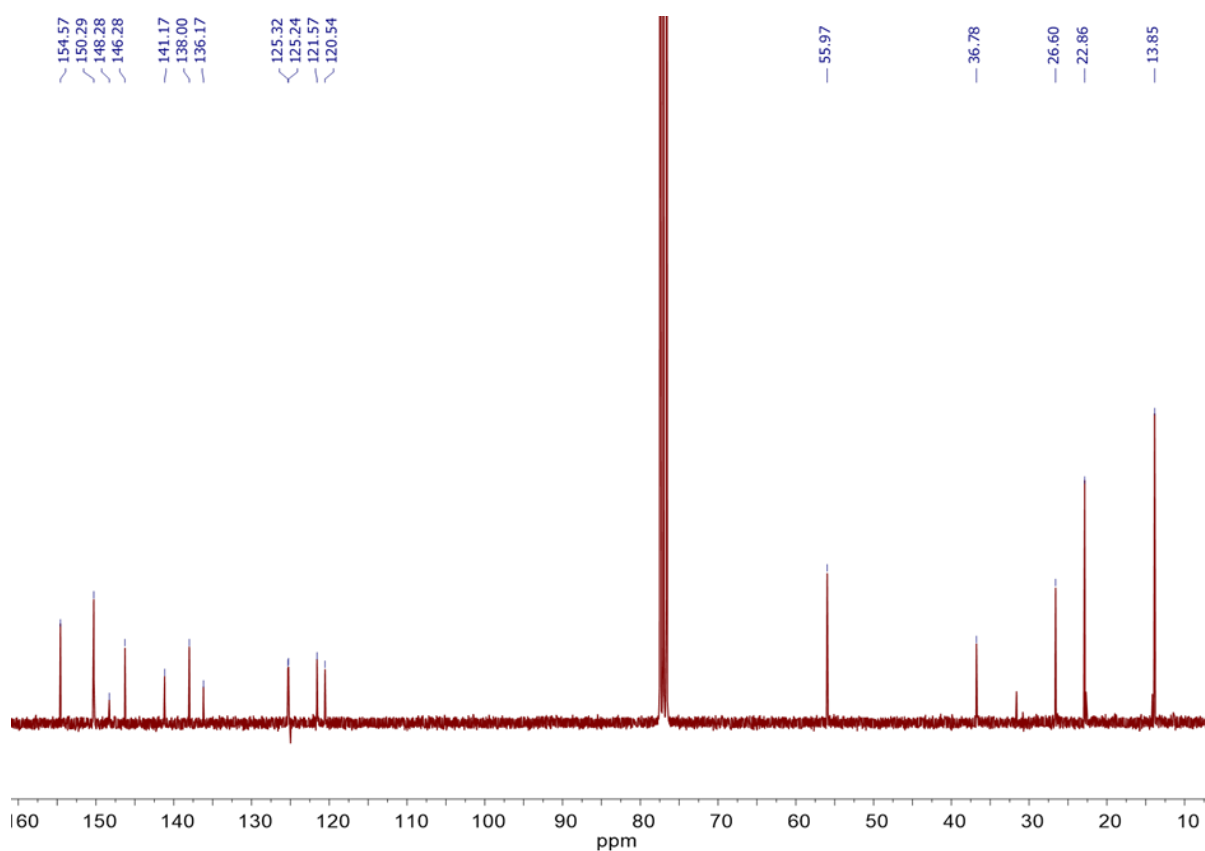


Figure S4. ¹³C NMR spectrum of ligand **Trux3Pyr** in CDCl₃.

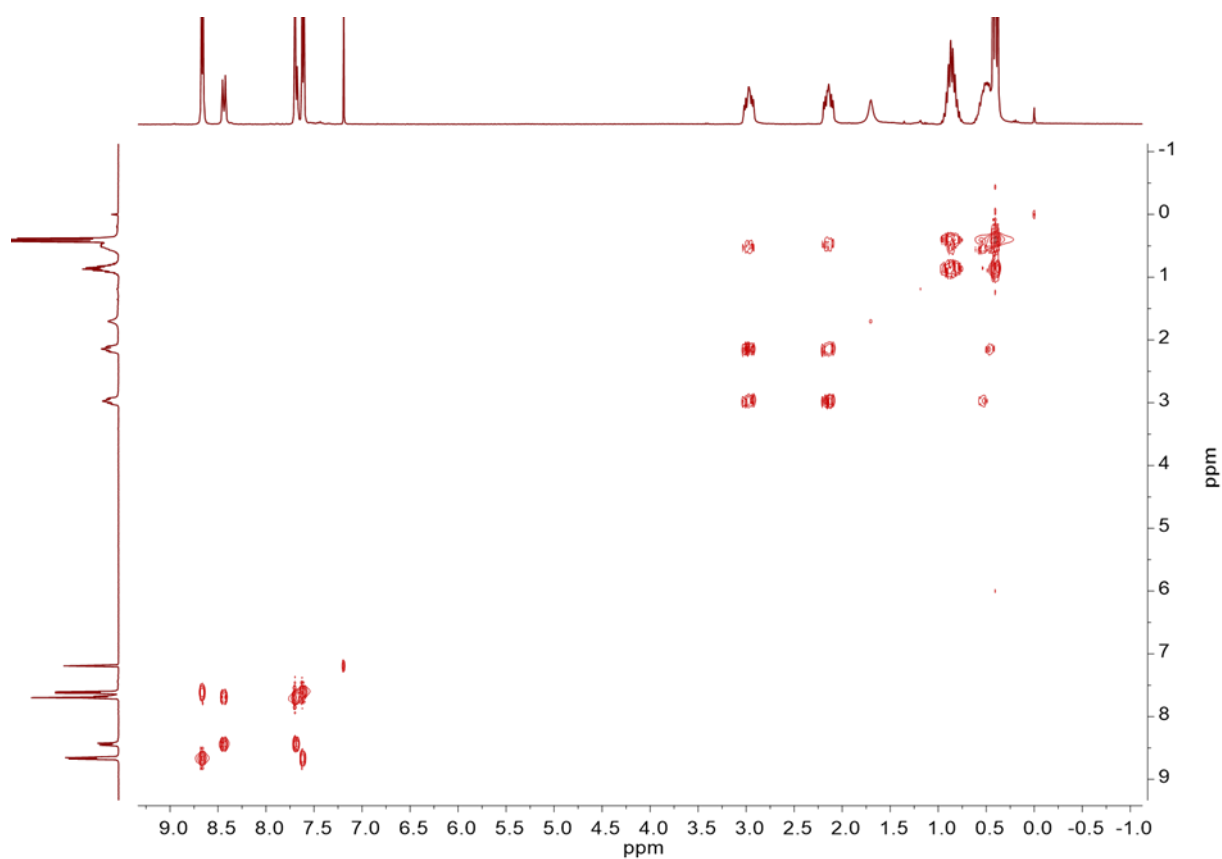


Figure S5. ^1H COSY NMR spectrum of ligand **Trux3Pyr** in CDCl_3 .

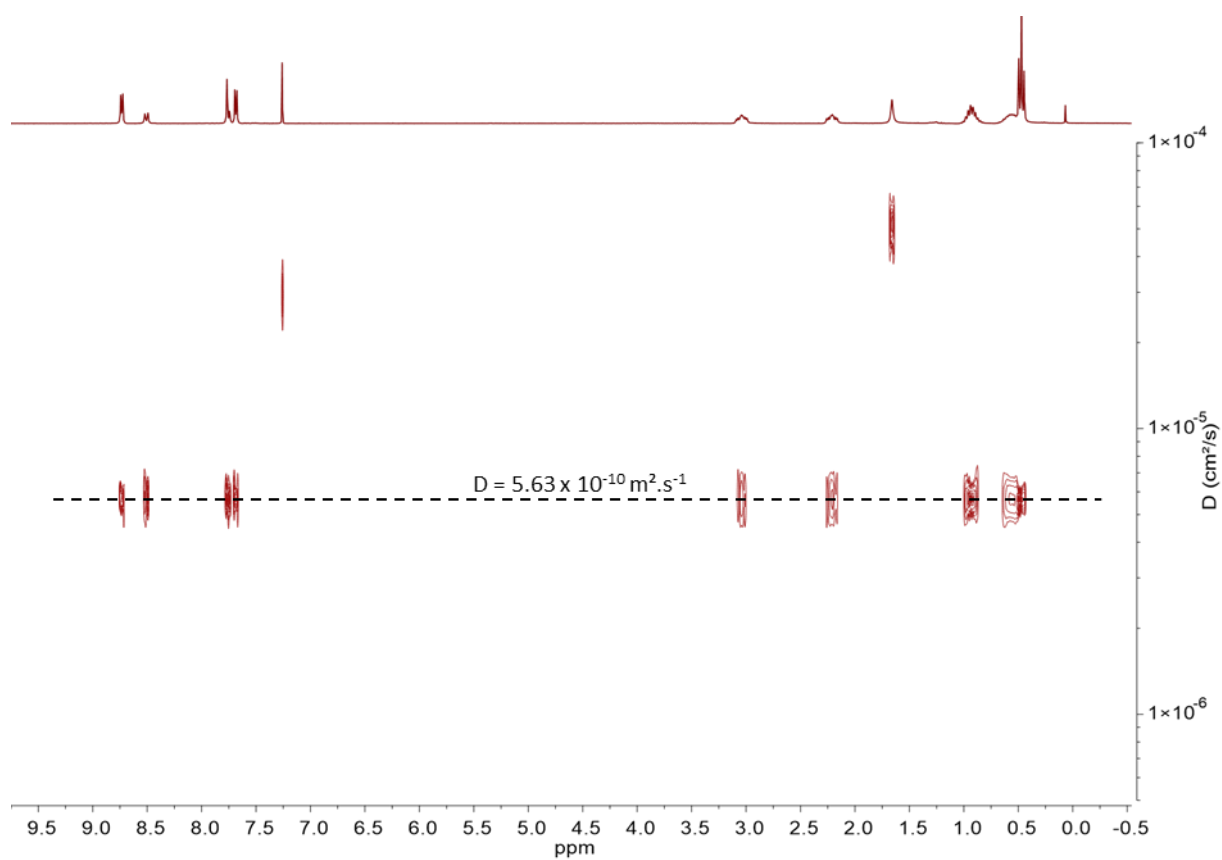


Figure S6. ^1H DOSY NMR spectrum of ligand **Trux3Pyr** in CDCl_3 .

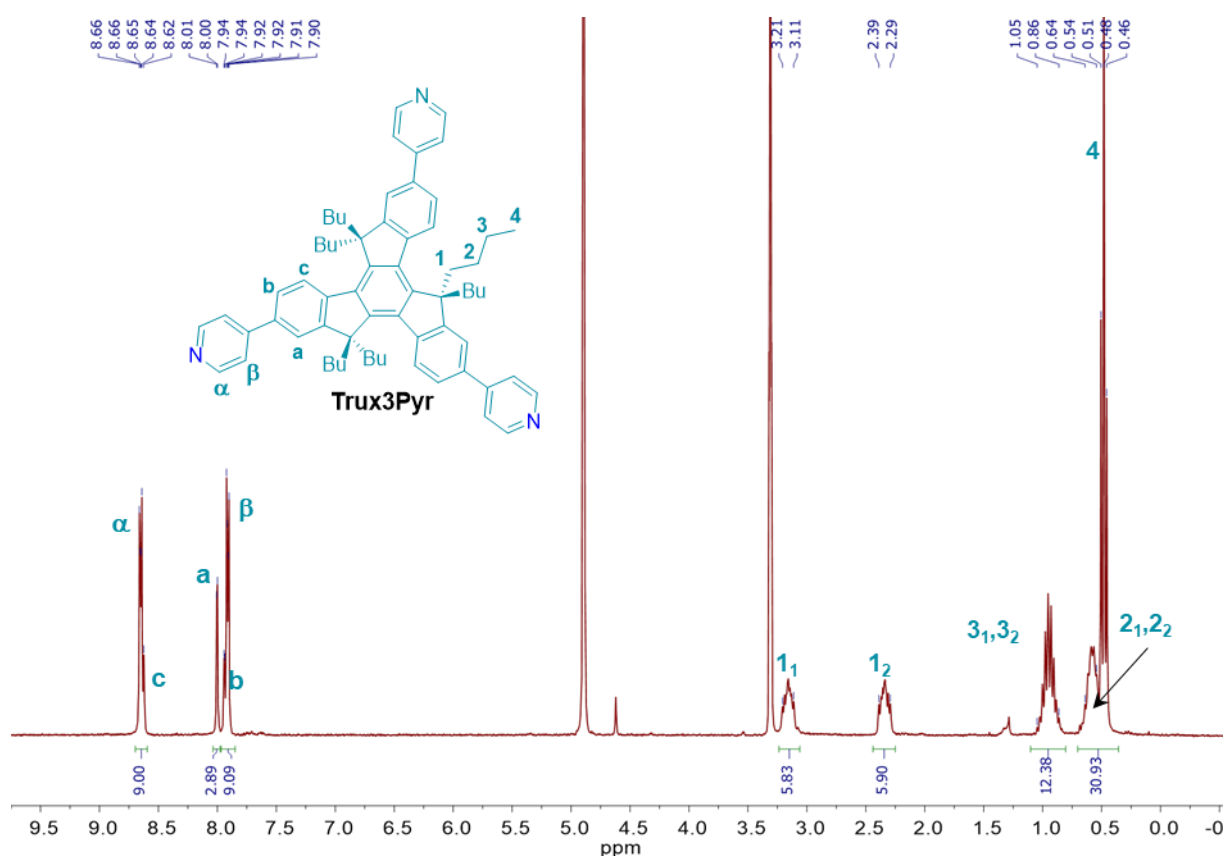


Figure S7. ^1H NMR spectrum of ligand **Trux3Pyr** in MeOD.

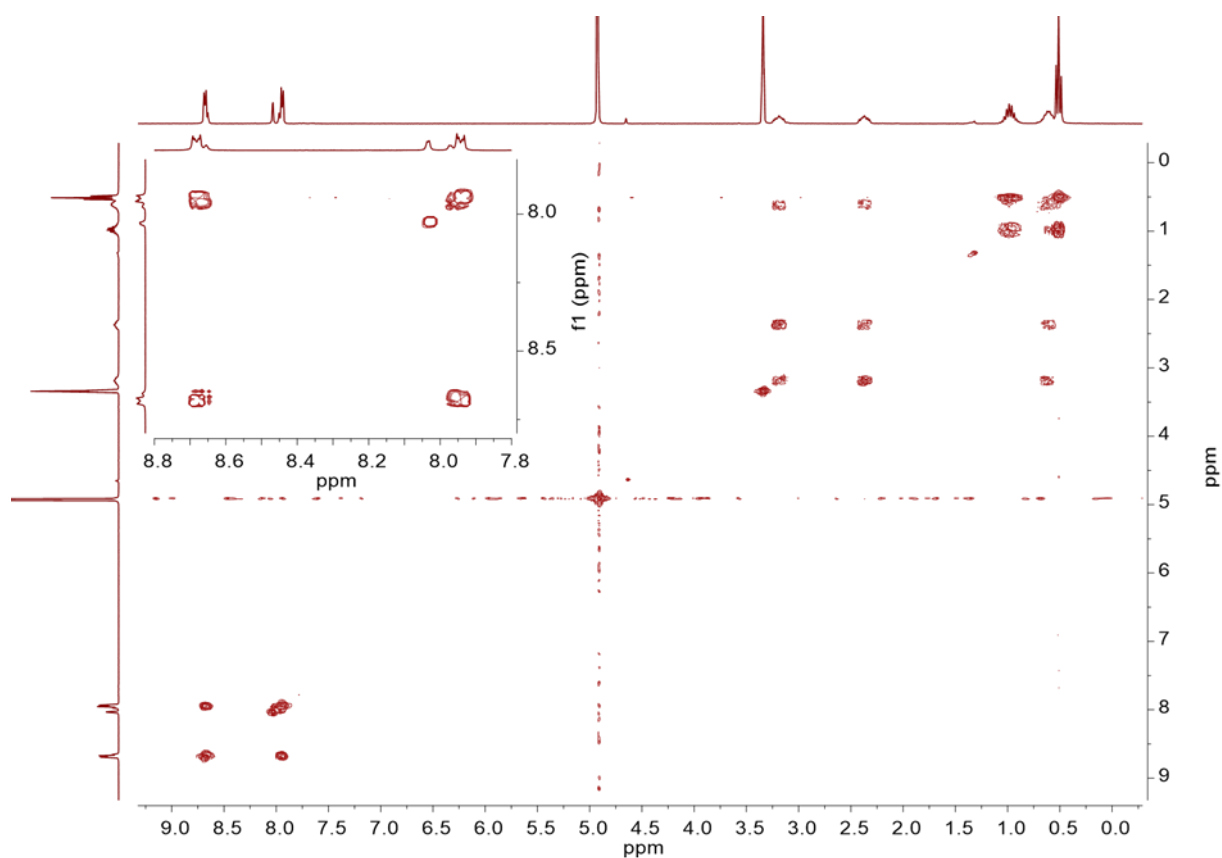


Figure S8. ^1H COSY NMR spectrum of ligand **Trux3Pyr** in MeOD.

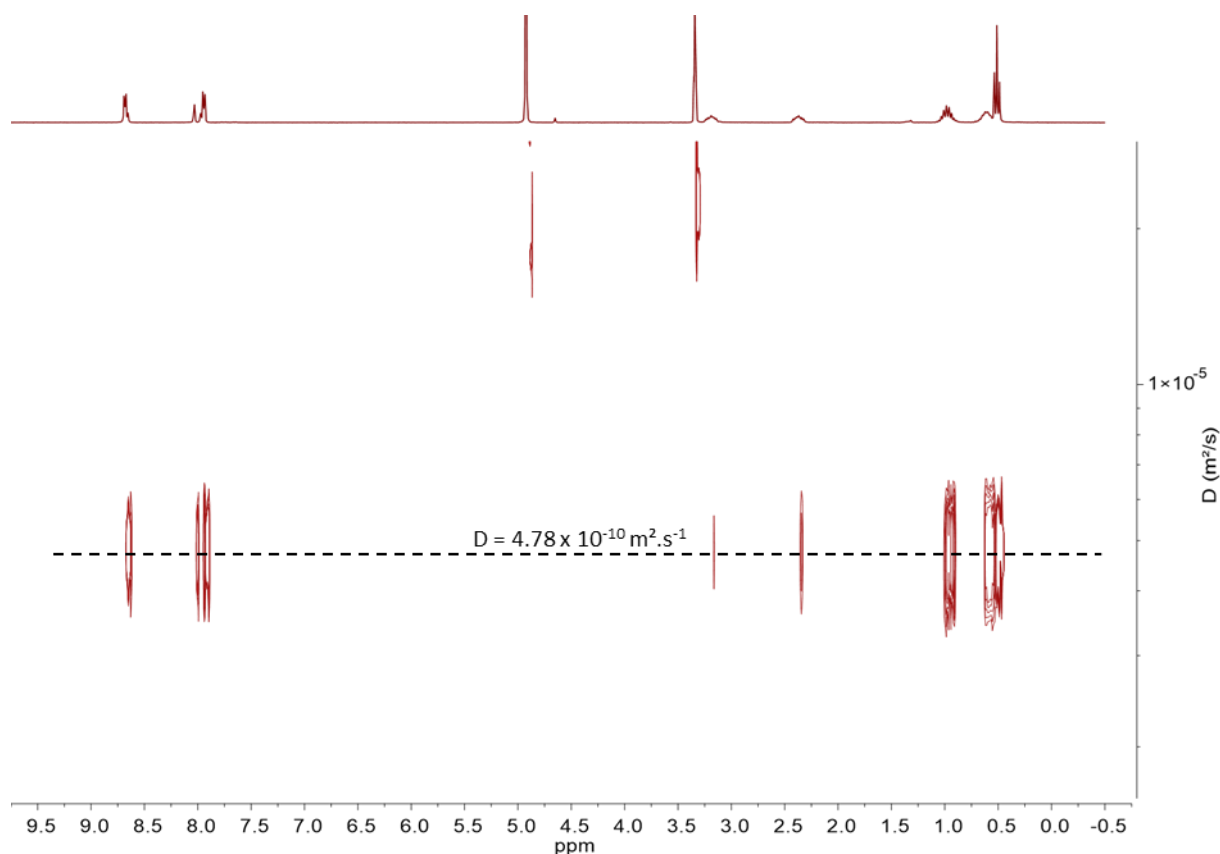


Figure S9. ^1H DOSY NMR spectrum of ligand **Trux3Pyr** in MeOD .

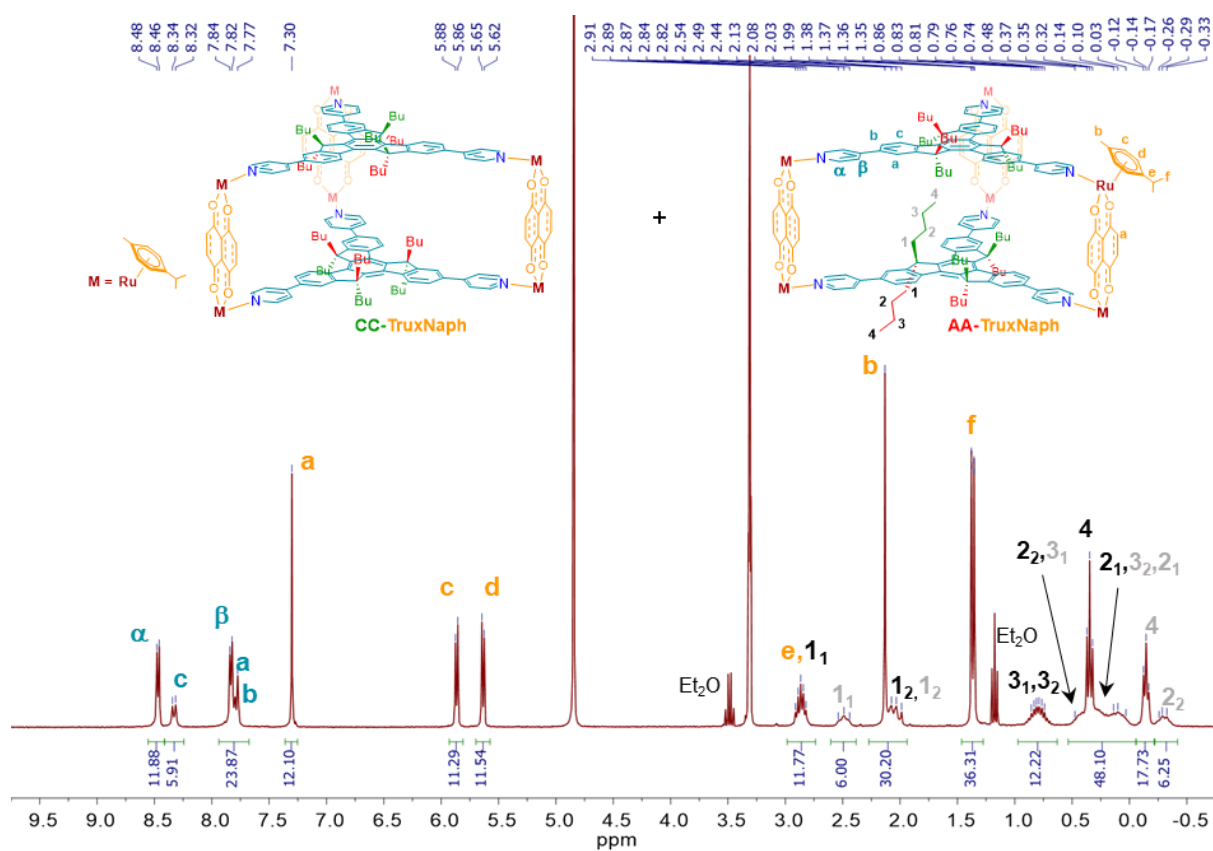


Figure S10. ^1H NMR spectrum of **TruxNaph** in MeOD .

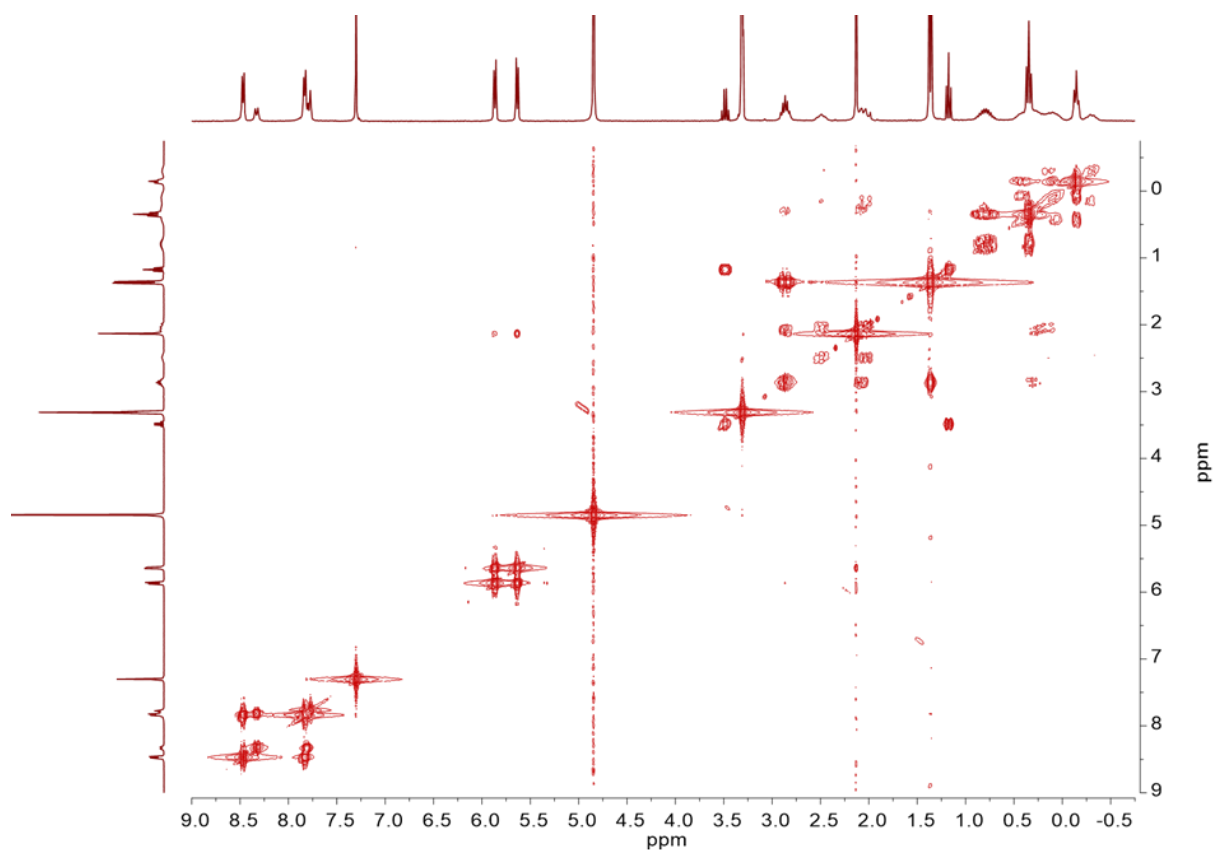


Figure S11. ^1H COSY NMR spectrum of **TruxNaph** in MeOD.

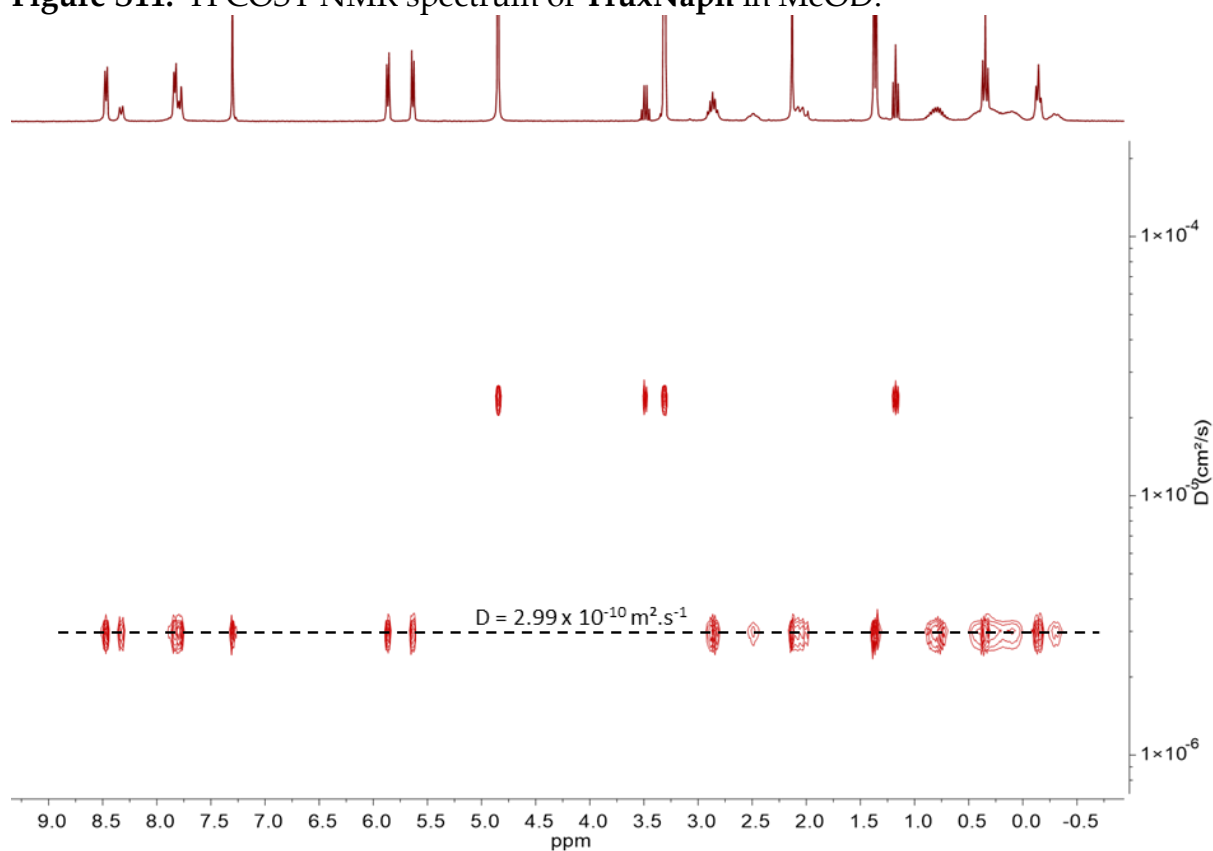


Figure S12. ^1H DOSY NMR spectrum of **TruxNaph** in MeOD.

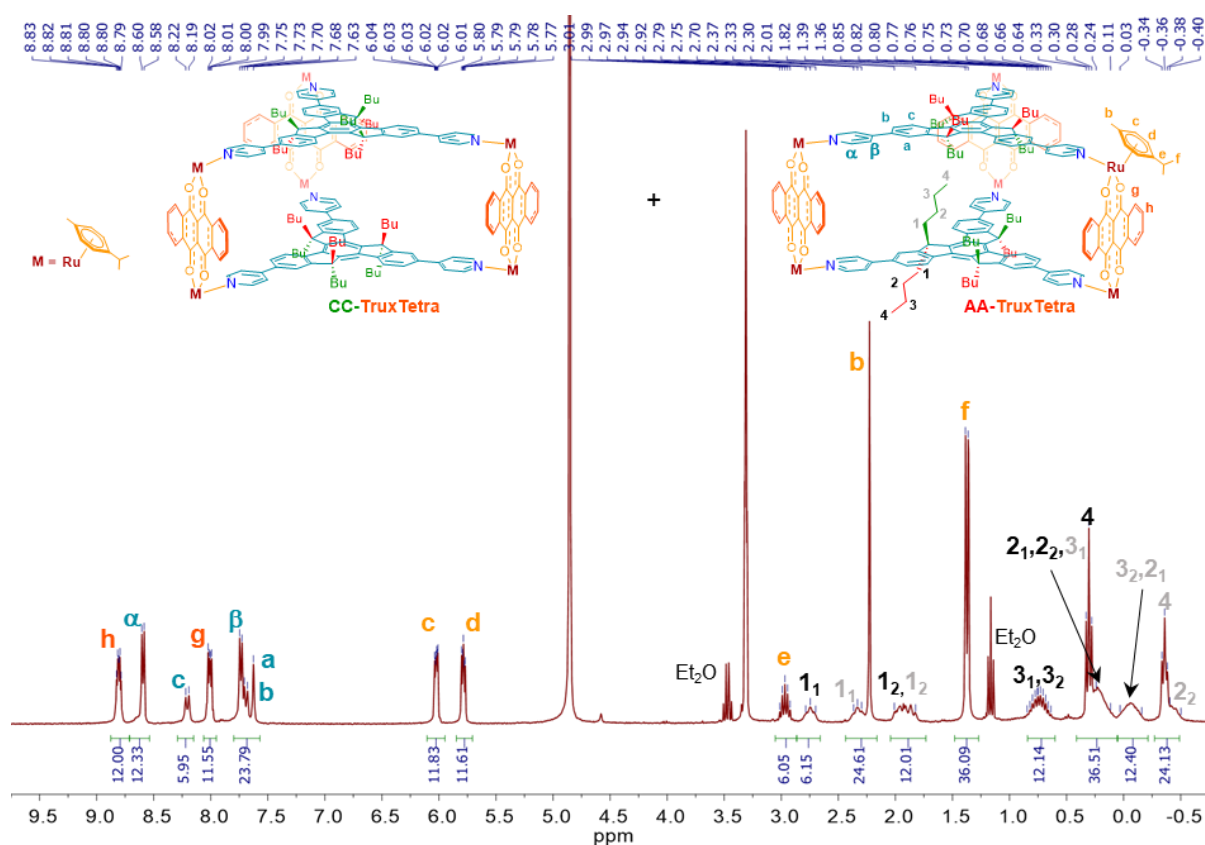


Figure S13. ^1H NMR spectrum of TruxTetra in MeOD.

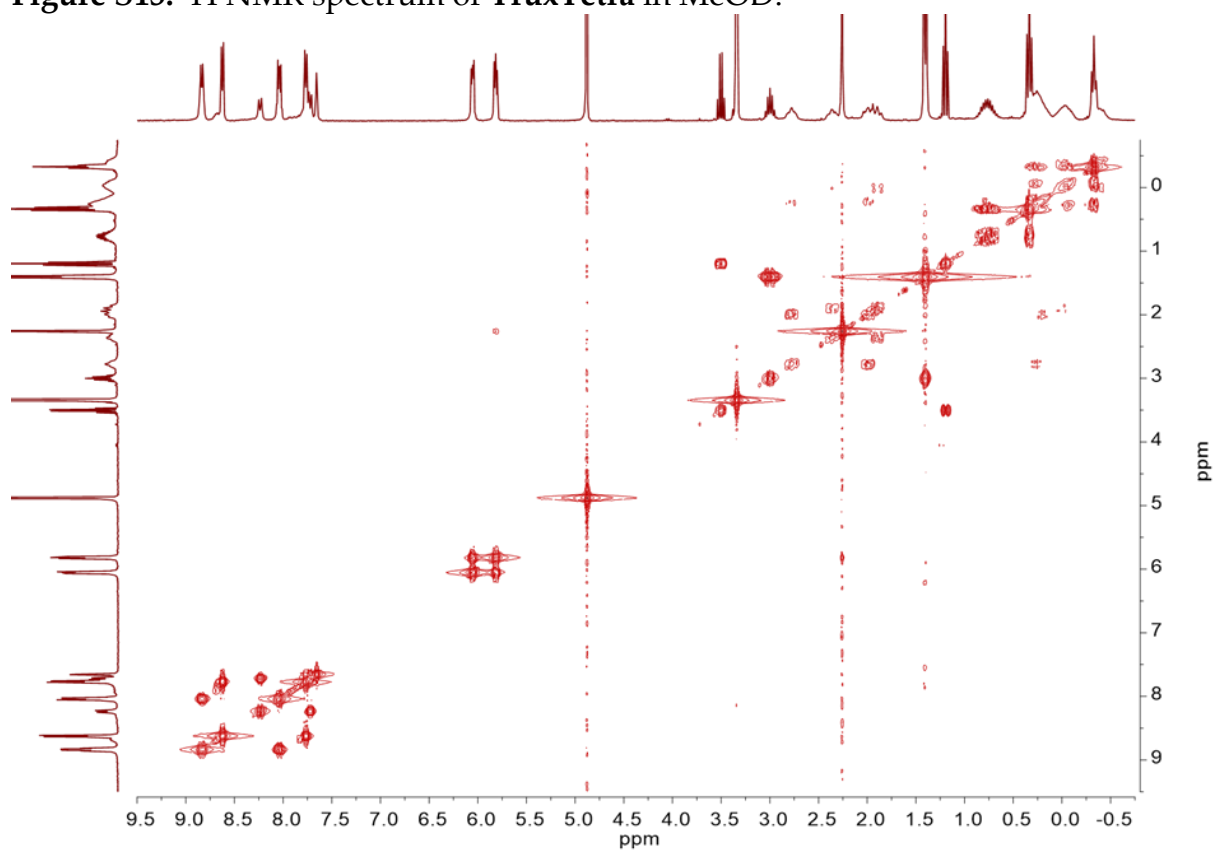


Figure S14. ^1H COSY NMR spectrum of TruxTetra in MeOD.

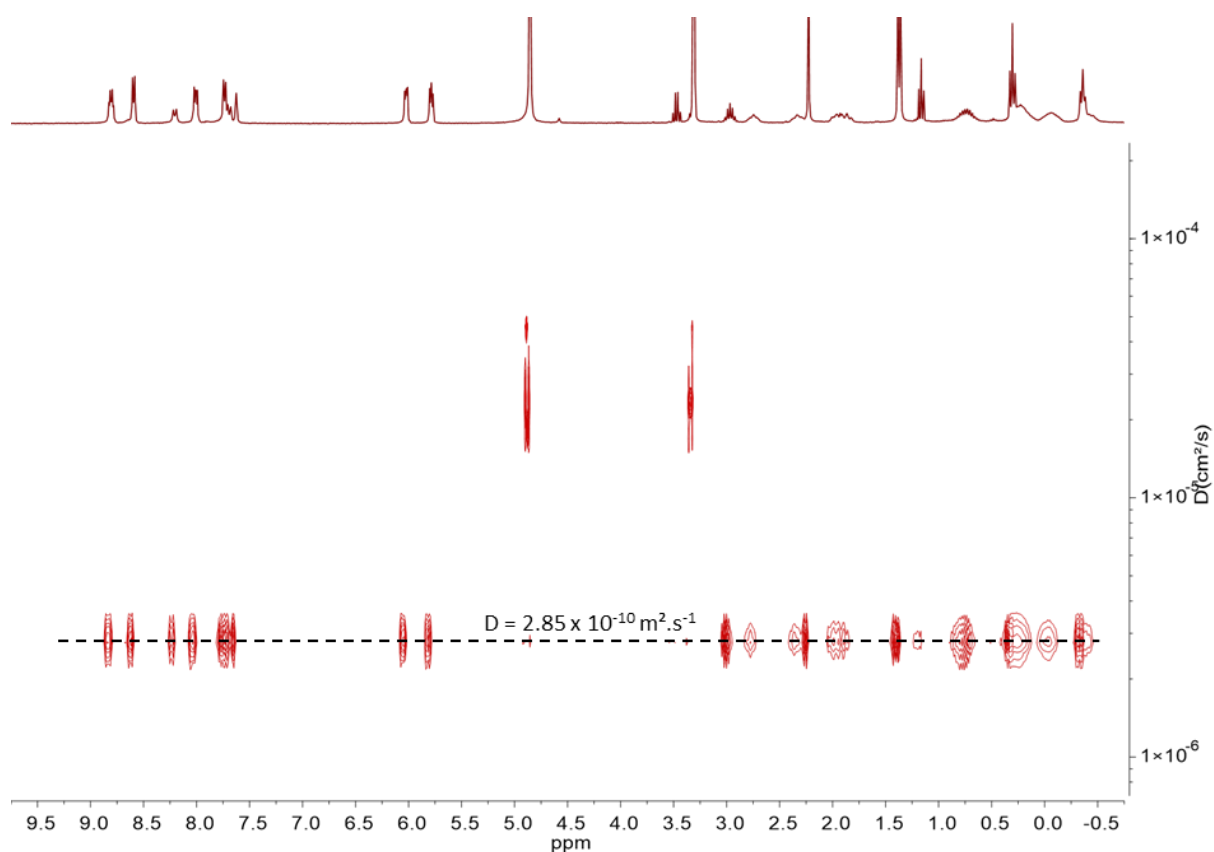


Figure S15. ^1H DOSY NMR spectrum of **TruxTetra** in MeOD.

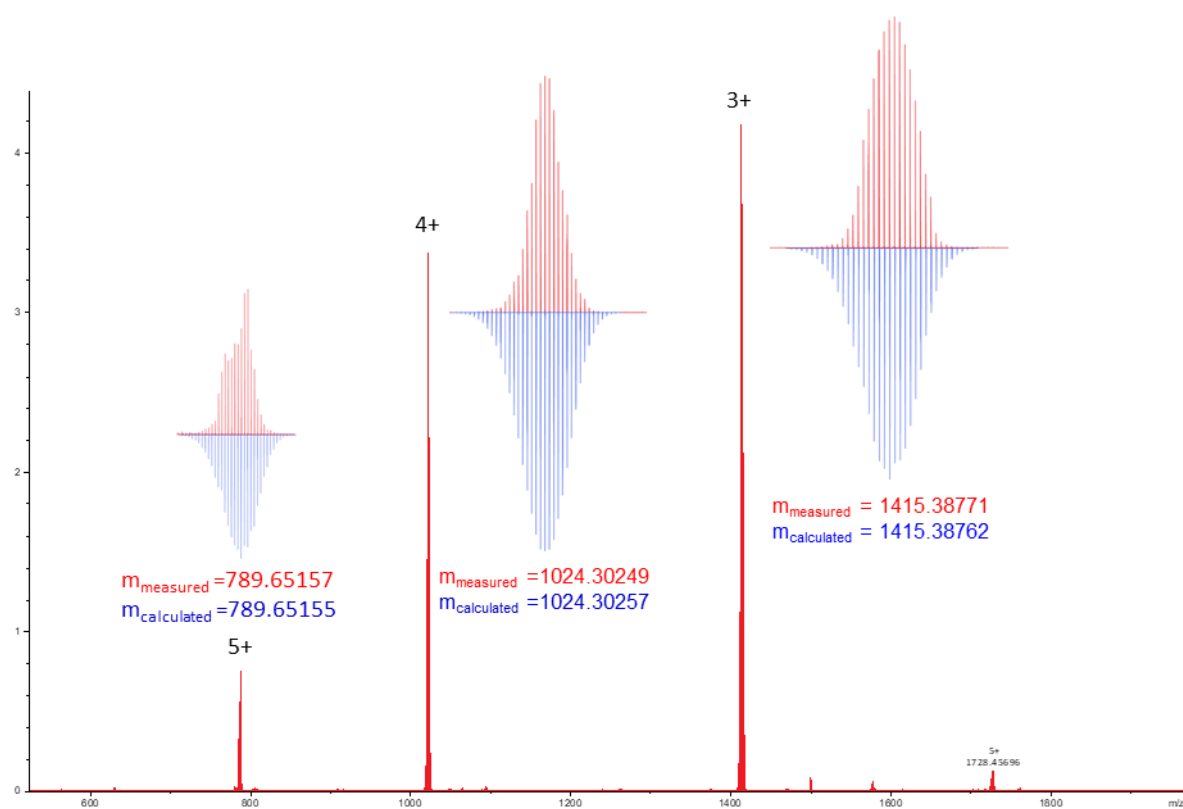
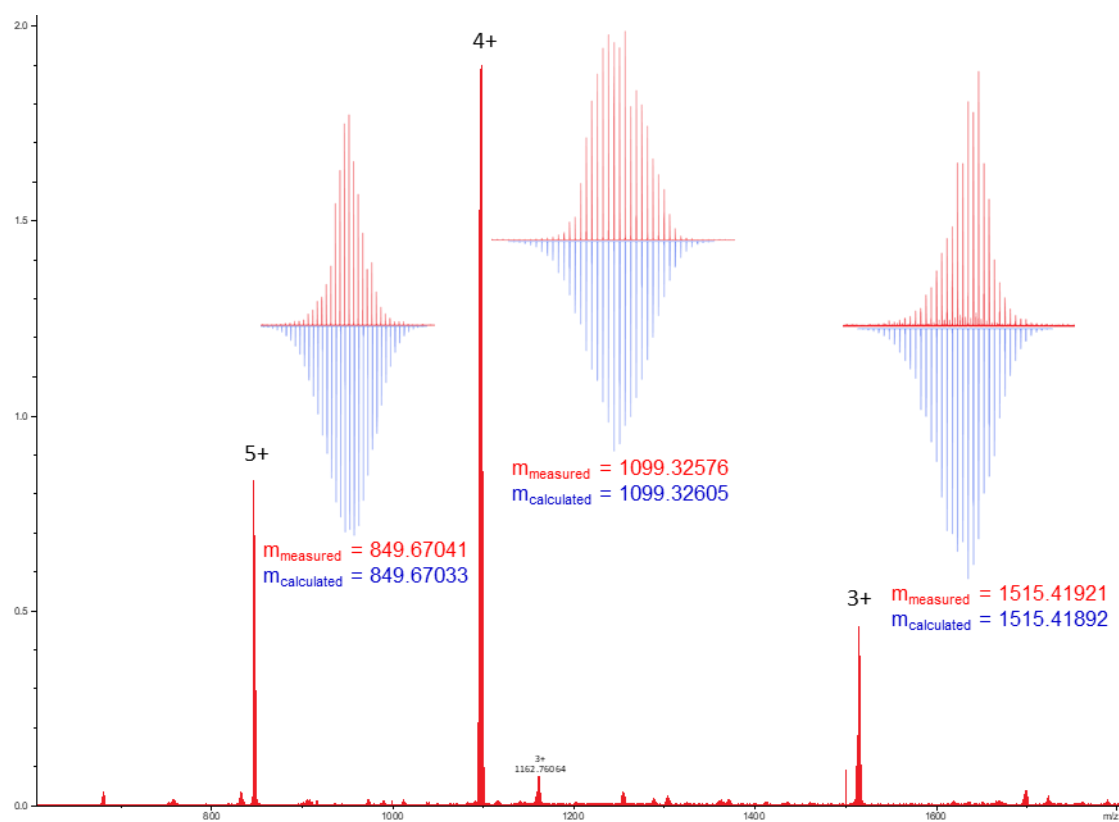
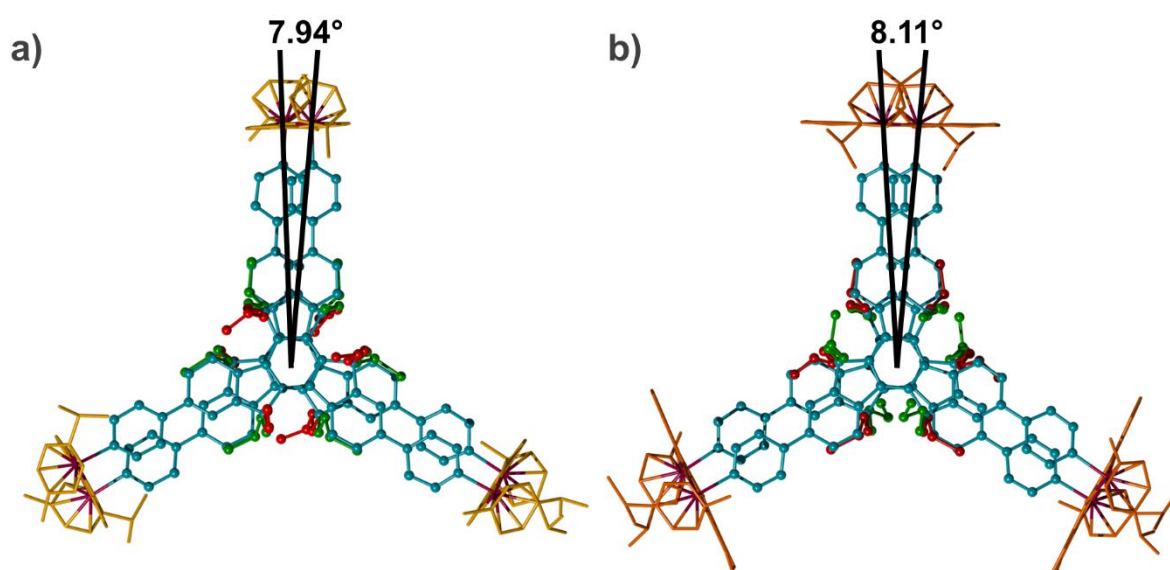


Figure S16. ESI-FTICR HRMS spectrum of **TruxNaph** in MeOH at $C = 10^{-4}$ M.**Figure S17.** ESI-FTICR HRMS spectrum of **TruxTetra** in MeOH at $C = 10^{-4}$ M.**Figure S18.** Representation of Bailar twist angles in **TruxNaph** and **TruxTetra**.