

Palladium-Catalyzed Arylations Towards 3,6-Diaryl-1,3a,6a-triazapentalenes and Evaluation of Their Fluorescence Properties

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1D NMR spectra

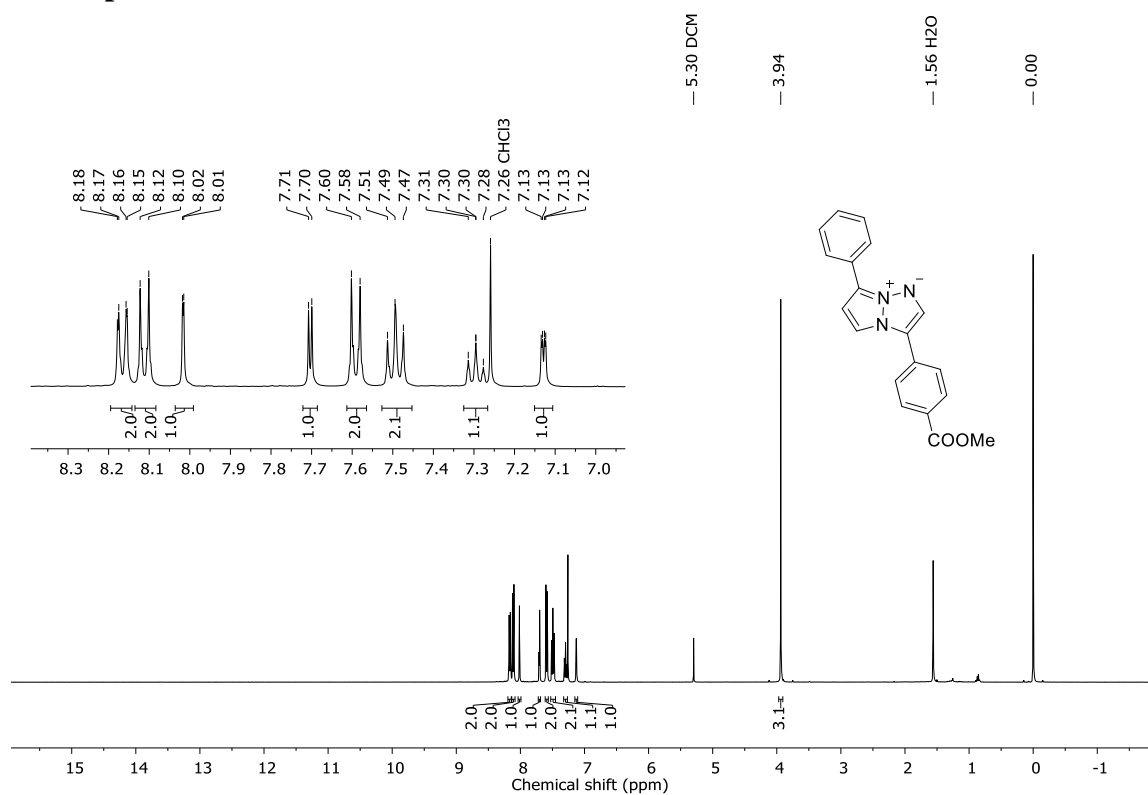


Figure S1. **TAP4a**, ¹H, 400 MHz, CDCl₃

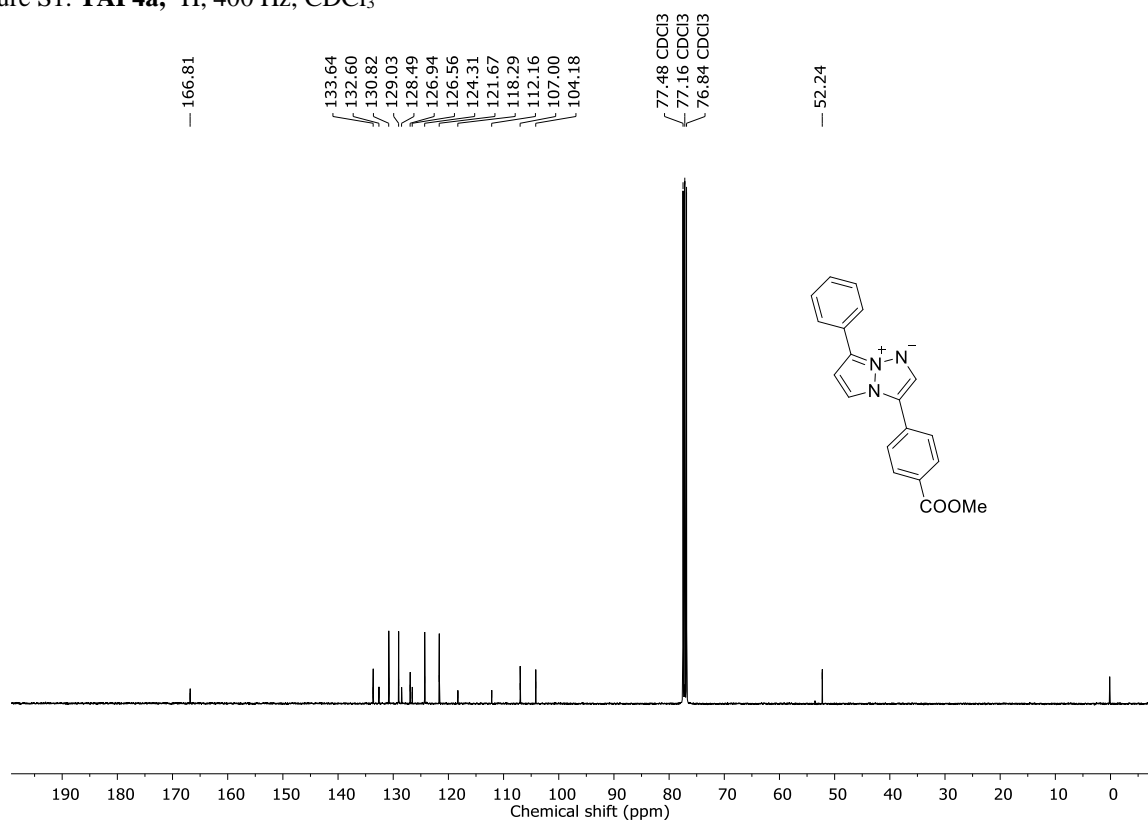


Figure S2. **TAP4a**, ¹³C{¹H}, 101 MHz, CDCl₃

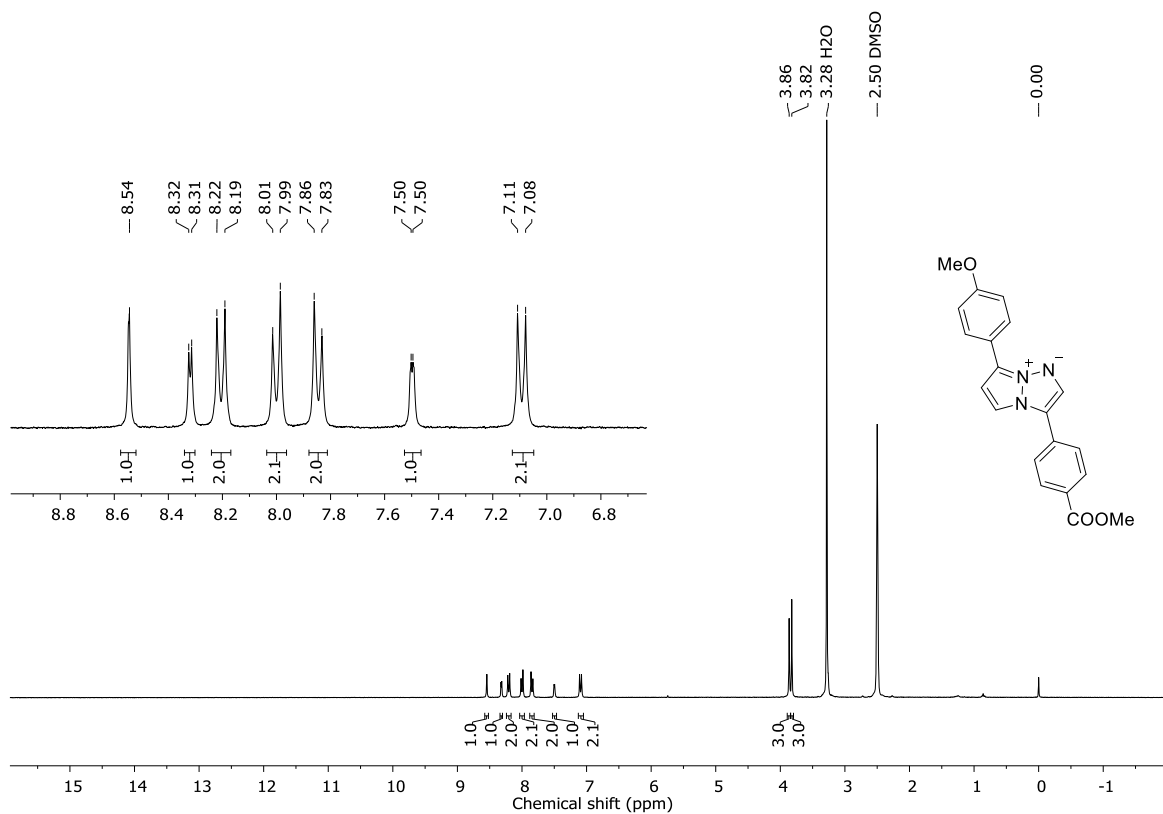


Figure S3. TAP4b, ^1H , 300 Hz, $\text{DMSO}-d_6$

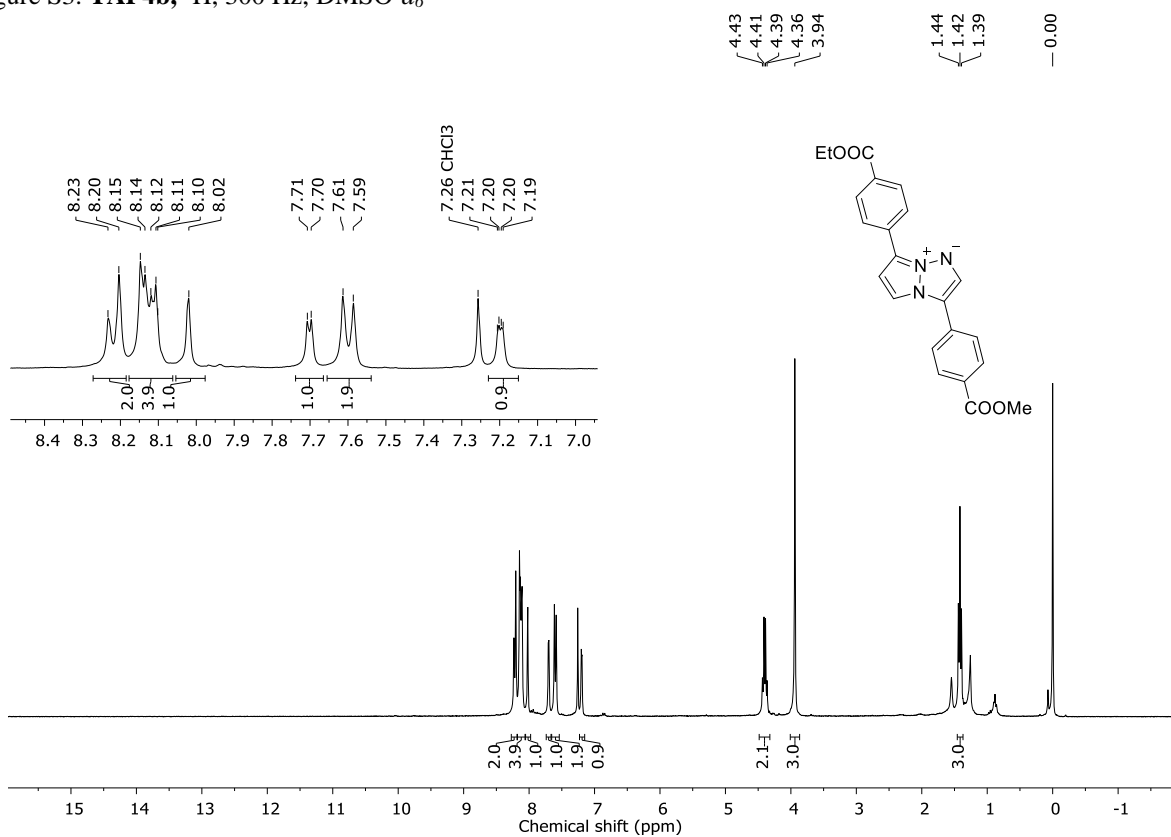


Figure S4. TAP4c, ^1H , 300 MHz, CDCl_3

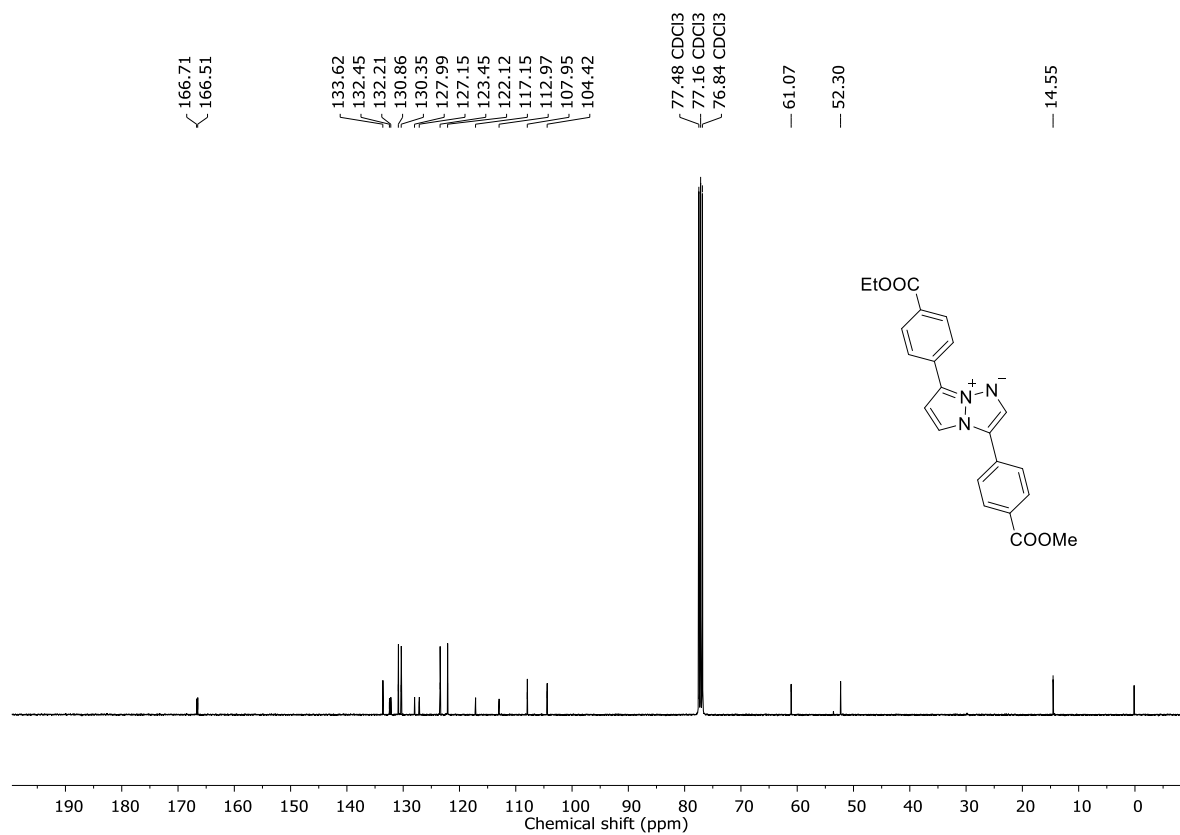


Figure S5. TAP4c, $^{13}\text{C}\{^1\text{H}\}$, 101 MHz, CDCl₃

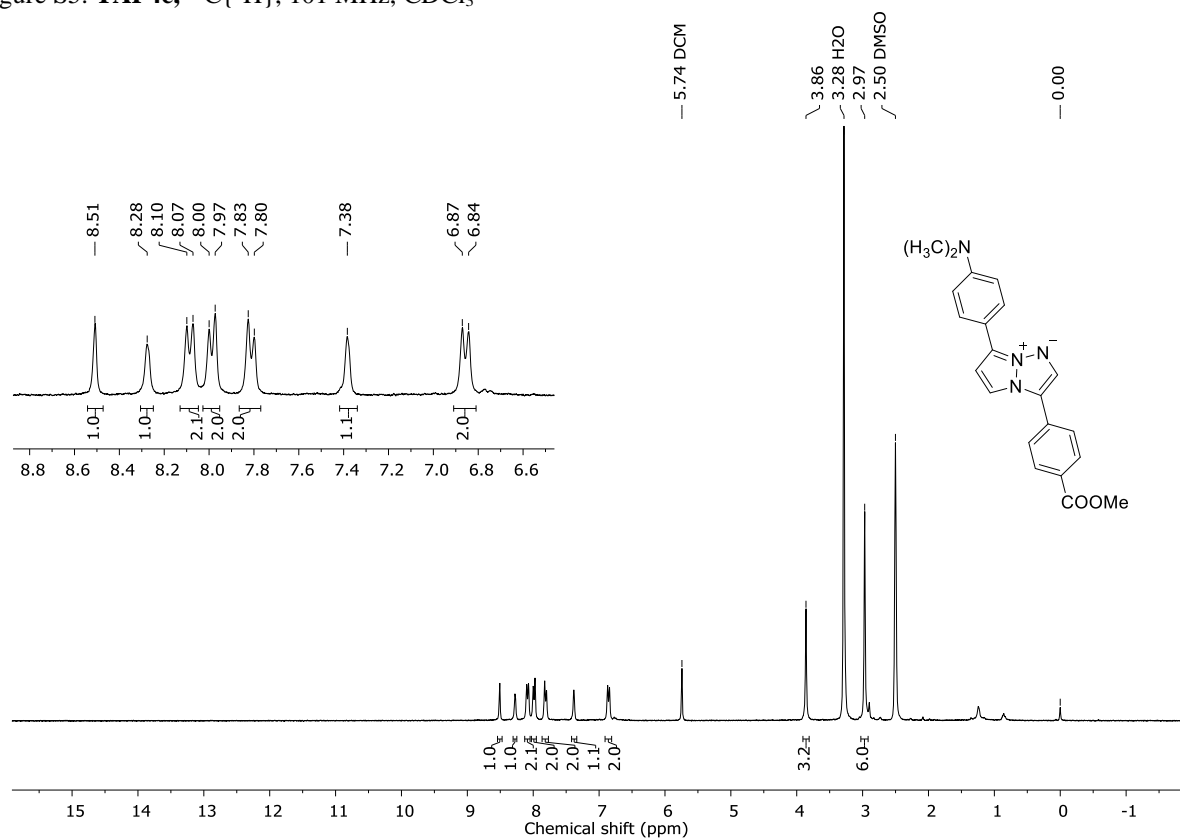


Figure S6. TAP4d, ^1H , 300 MHz, DMSO-*d*₆

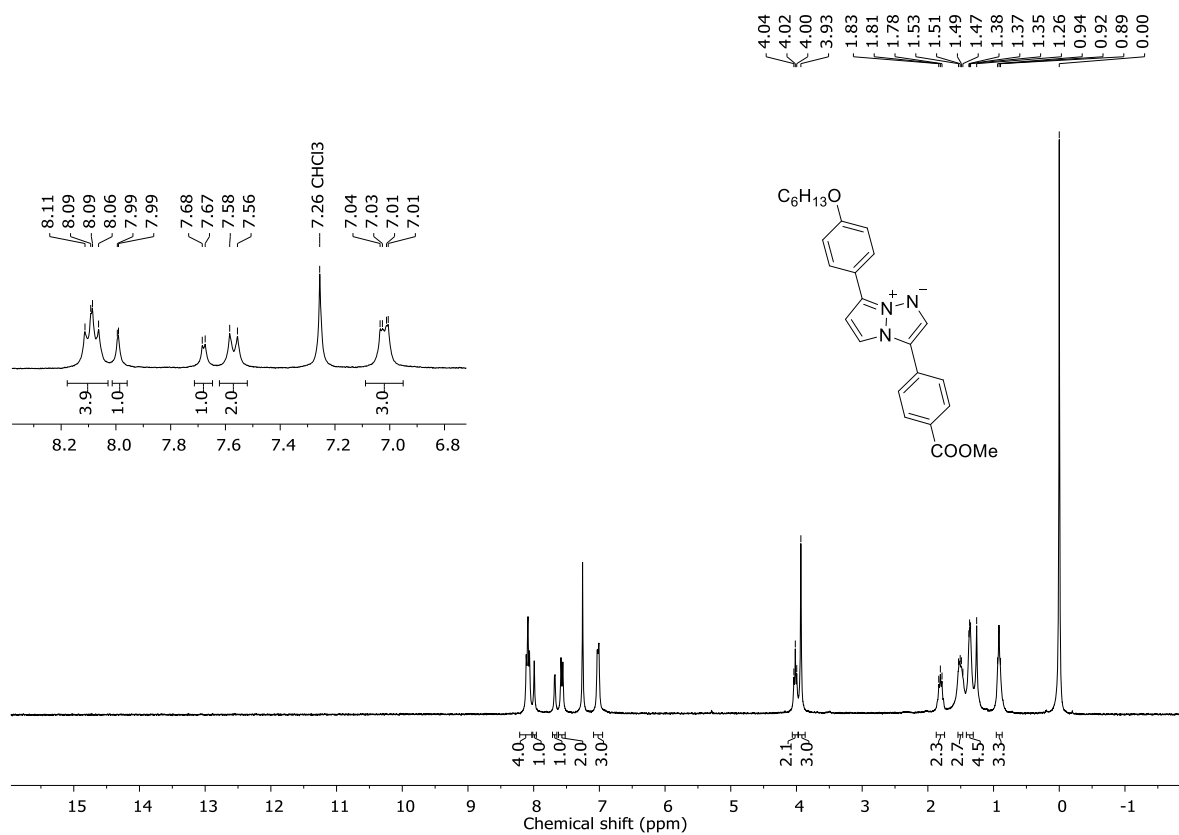


Figure S7. TAP4e, ¹H, 300 MHz, CDCl₃

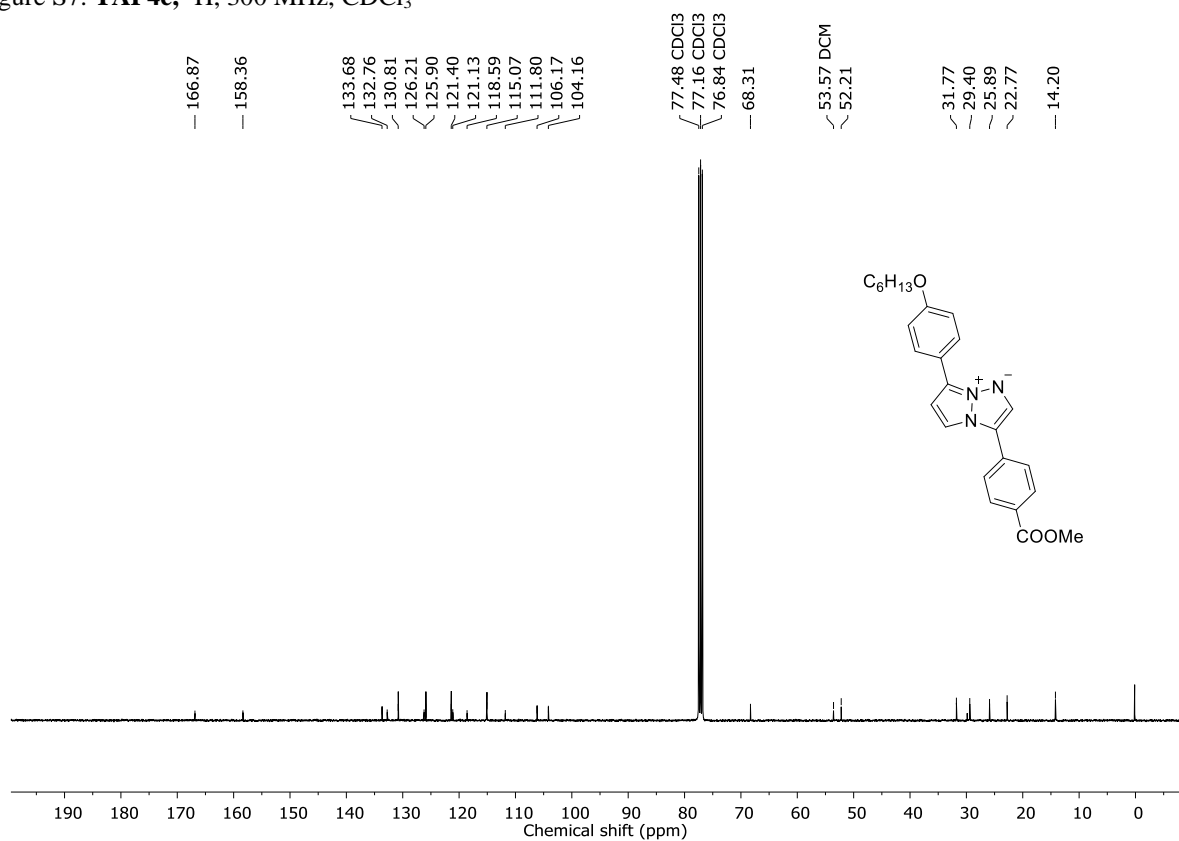


Figure S8. TAP4e, ¹³C{¹H}, 101 MHz, CDCl₃

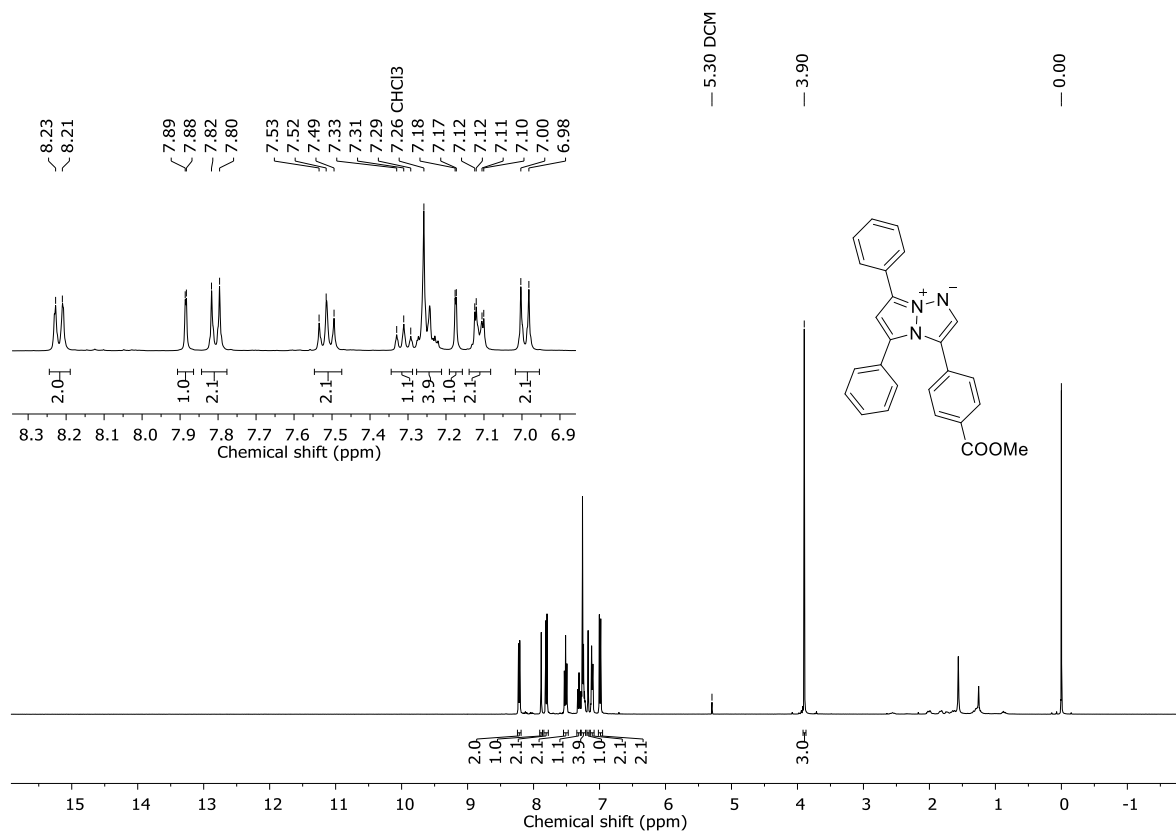


Figure S9. **TAP5a**, ¹H, 400 MHz, CDCl₃

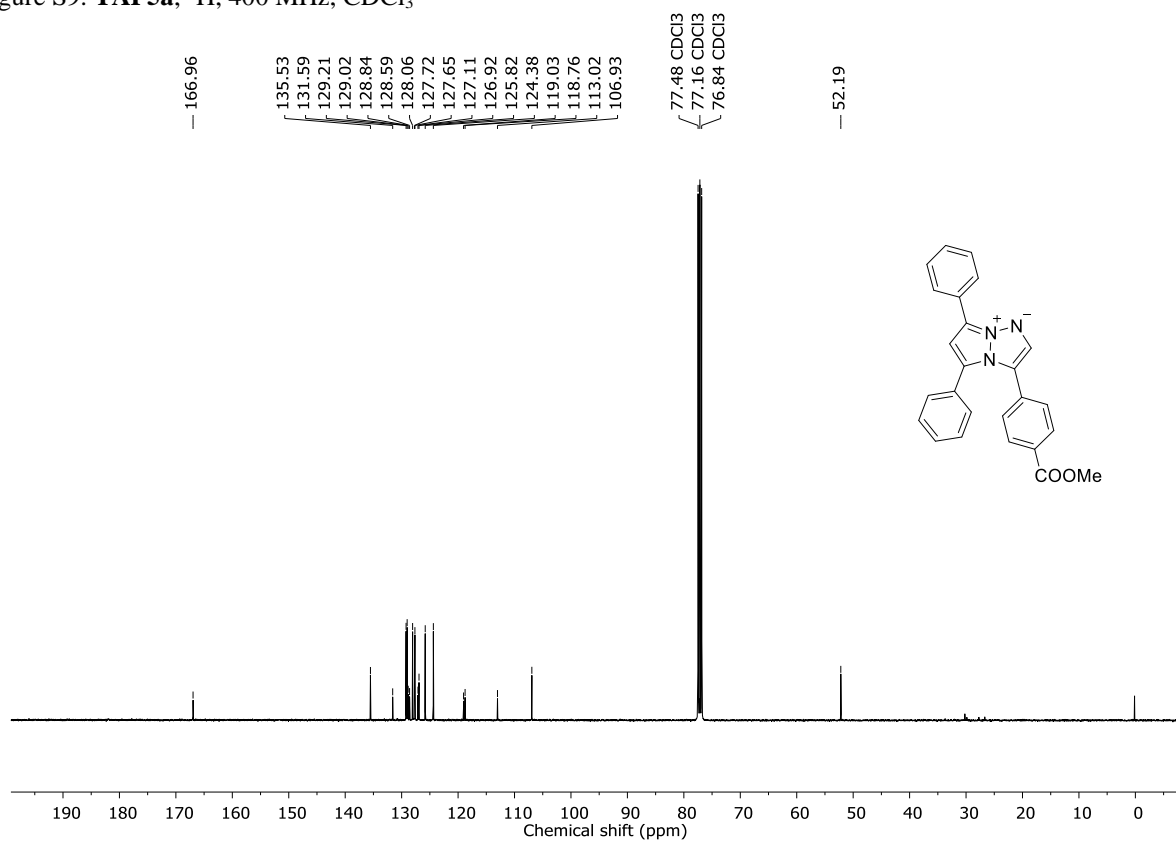
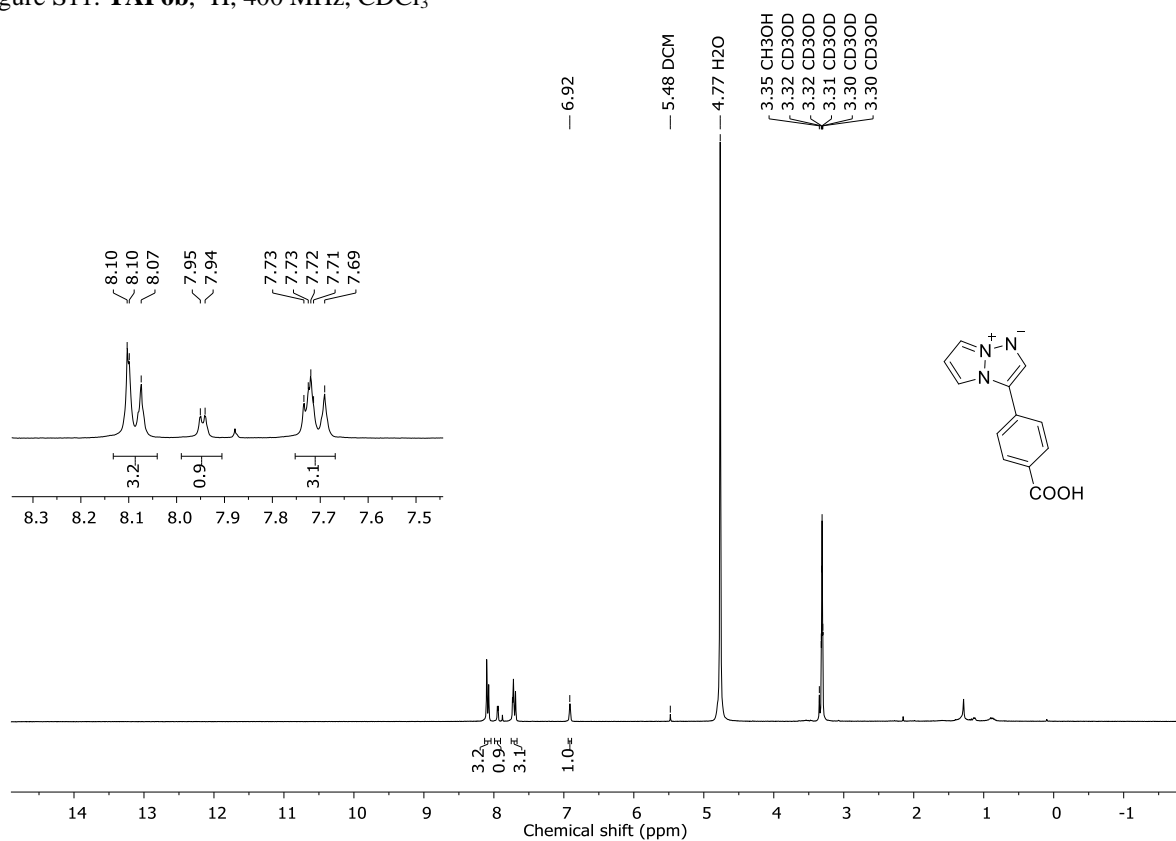
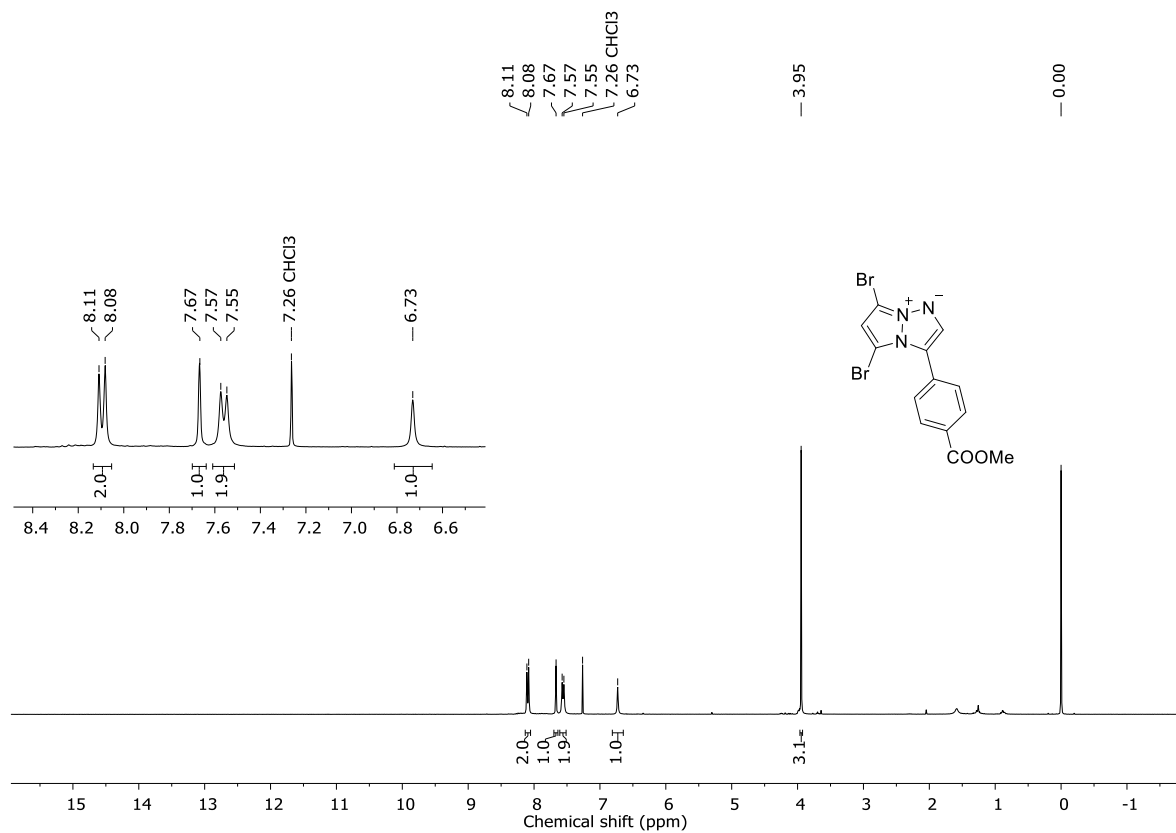


Figure S10. **TAP5a**, ¹³C{¹H}, 101 MHz, CDCl₃



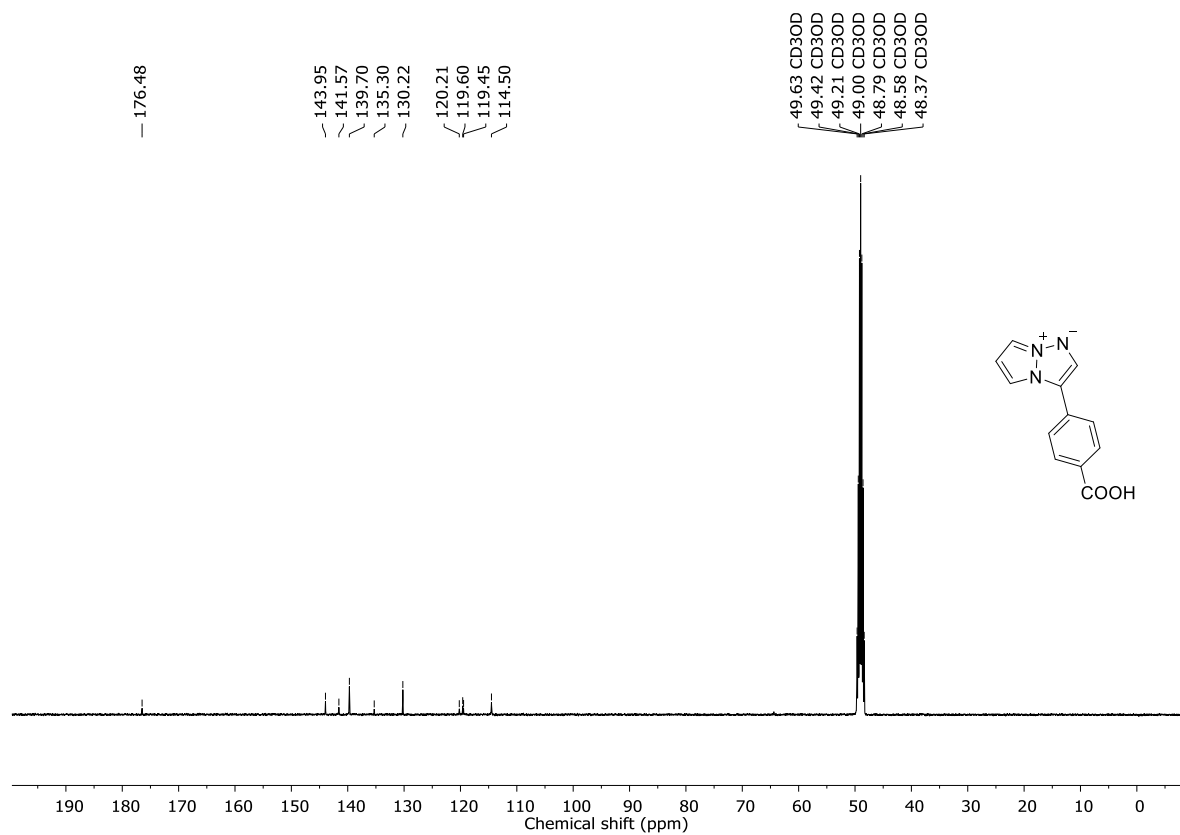


Figure S13. **TAP7**, $^{13}\text{C}\{^1\text{H}\}$, 101 MHz, CD_3OD

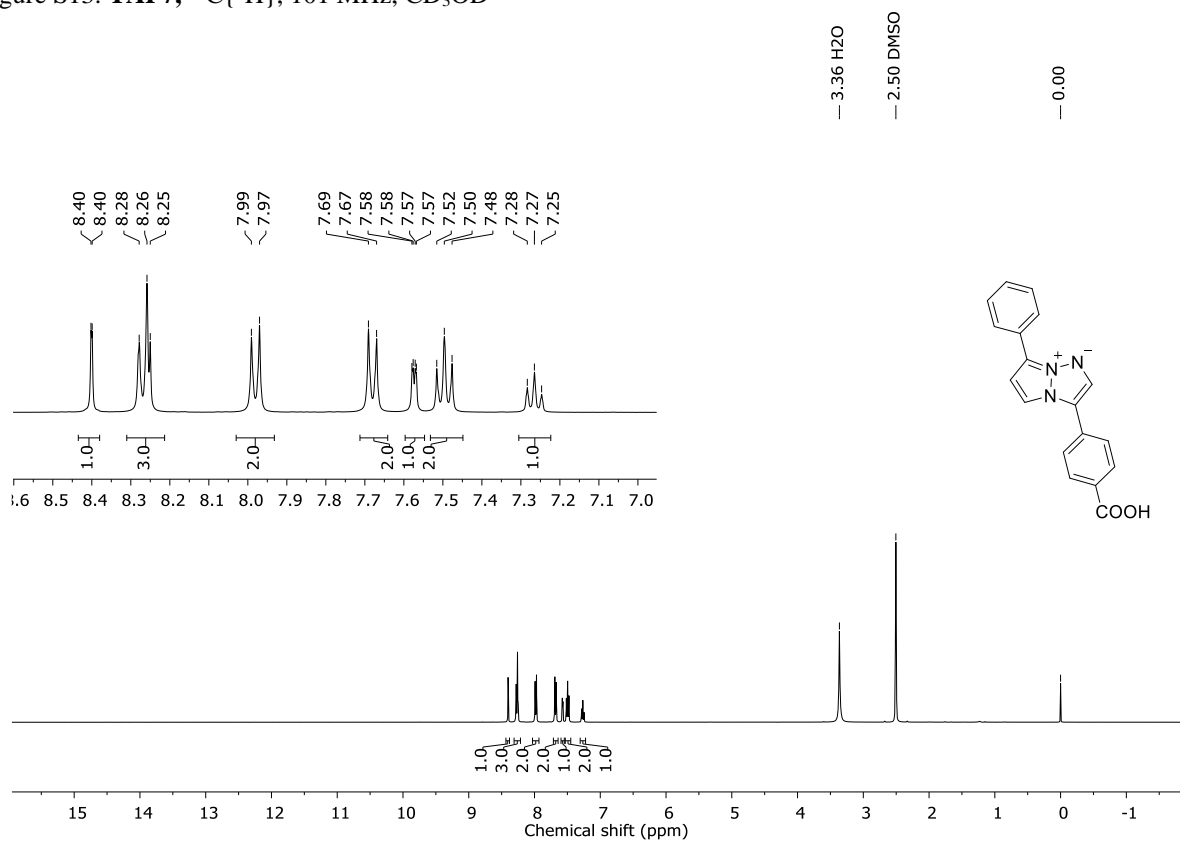


Figure S14. **TAP8**, ^1H , 400 MHz, $\text{DMSO}-d_6$

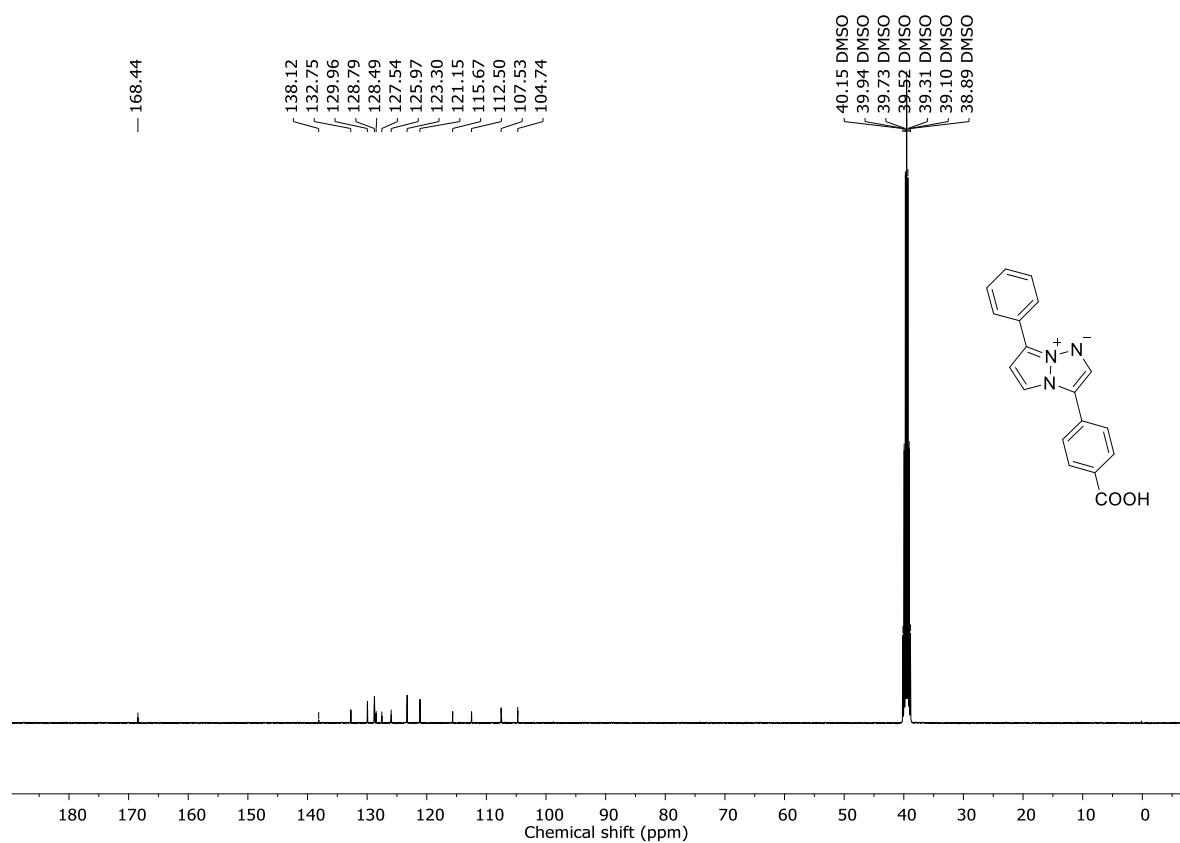


Figure S15. **TAP8**, ¹³C{¹H}, 101 MHz, DMSO-*d*₆

2D NMR spectra

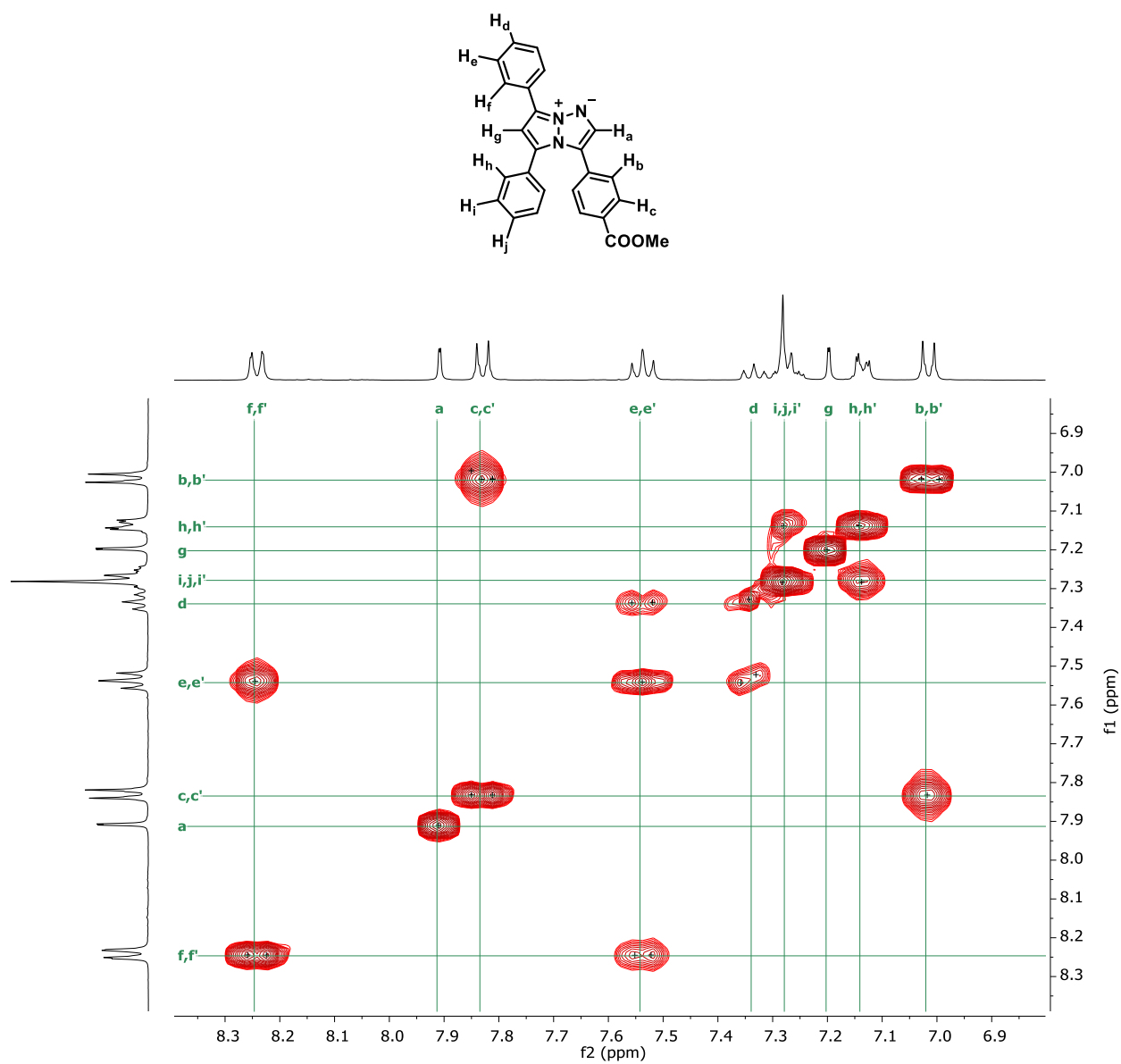


Figure S16. Structure and ^1H - ^1H COSY NMR spectrum (400 MHz, CDCl_3) of **TAP5a**.

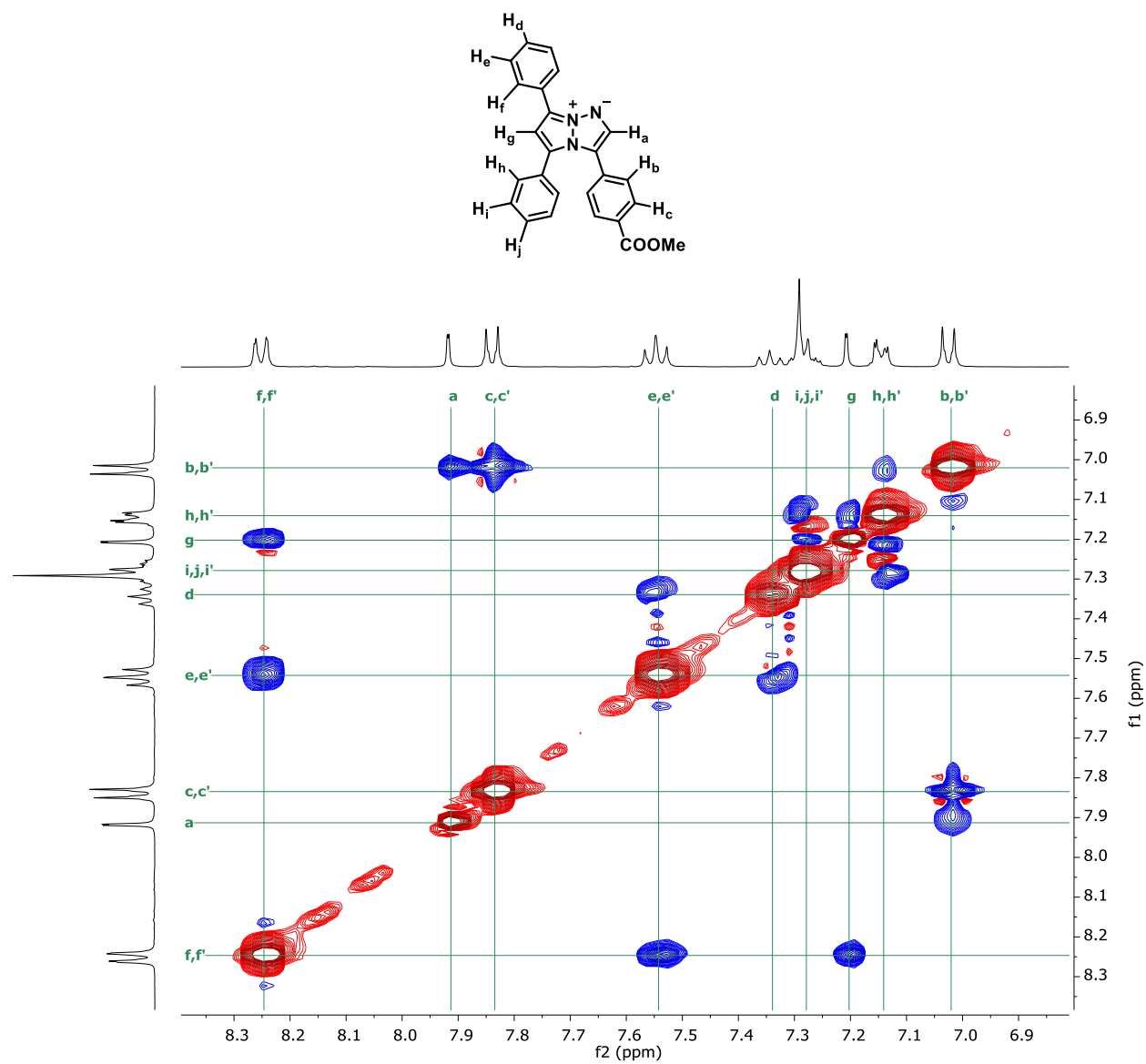


Figure S17. Structure and ^1H - ^1H NOESY NMR spectrum (400 MHz, CDCl_3) of **TAP5a**.

Crystal structure of TAP4a

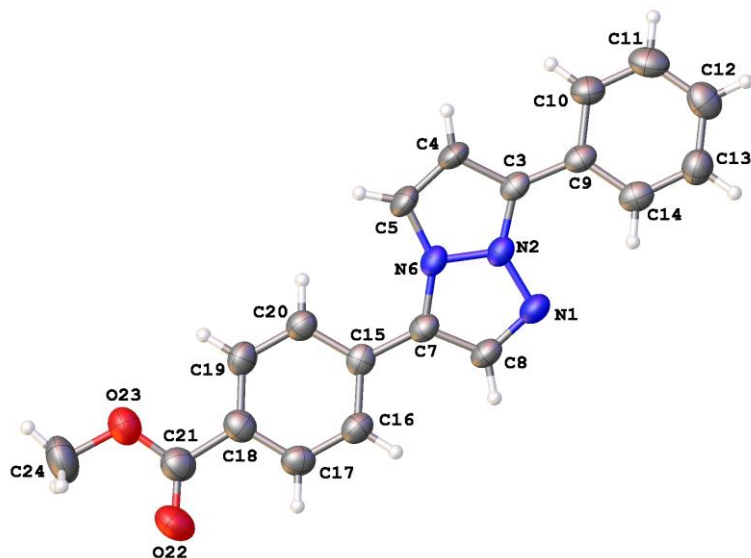


Figure S18. Crystal structure of **TAP4a**. Thermal ellipsoids are drawn at the 50% probability level.