

Supporting Information

Governing the DNA-binding mode of styryl dyes by the length of their alkyl substituents – From intercalation to major groove binding

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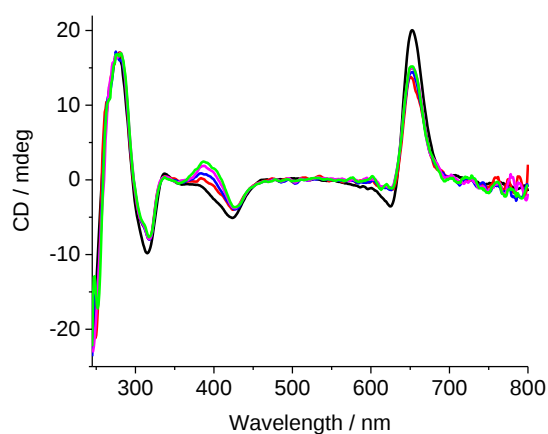
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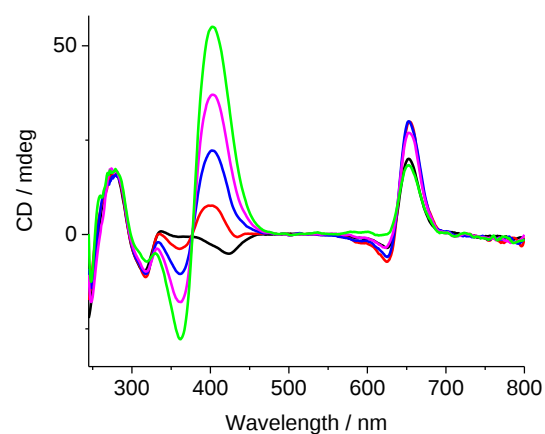
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1. DNA-binding experiments with methyl green (MG)

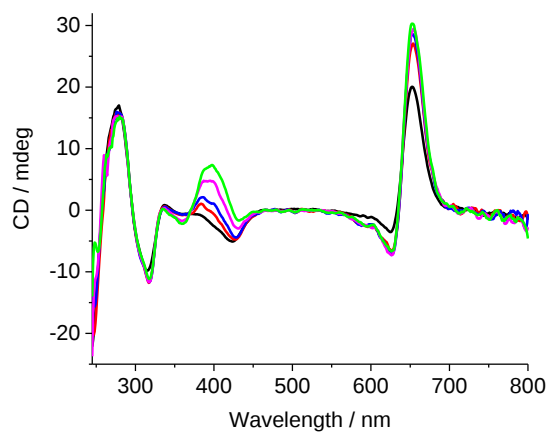
3a



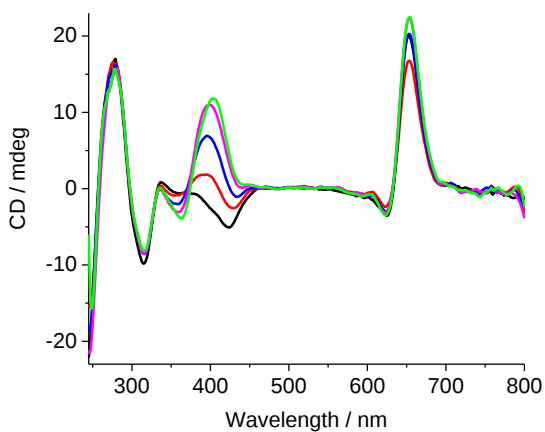
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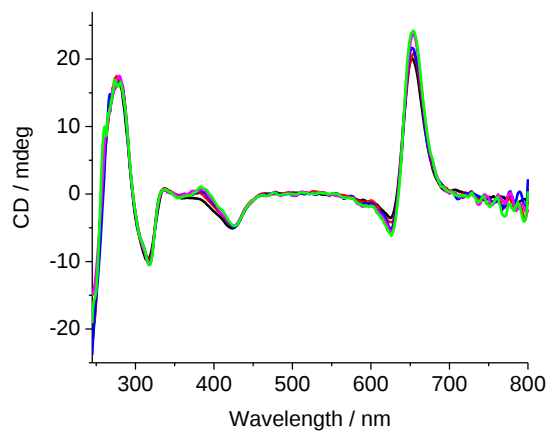
3b



4b



3c



4c

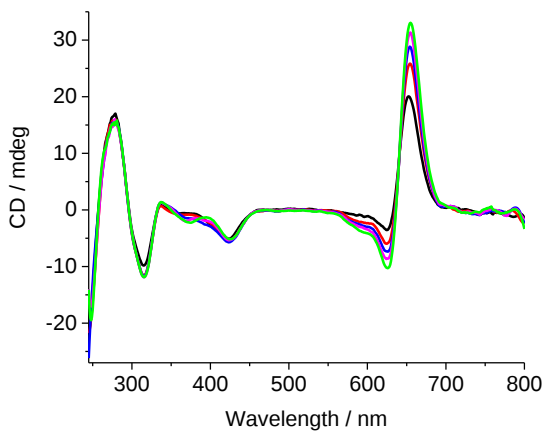


Figure S1. CD spectra of mono- and bis-styryl dyes **3a–3c** and **4a–4c** in the presence of major groove binder methyl green and ct DNA ($c_{\text{DNA}} = 50 \mu\text{M}$). For methyl green, the ligand-to-DNA ratio (LDR) is 0.45 for all samples. The LDR values for the dyes: 0 (black); 0.15 (red); 0.30 (blue); 0.45 (magenta); 0.60 (green). In all cases: BPE buffer with 3% (v/v) DMSO, 20 °C.

2. NMR data

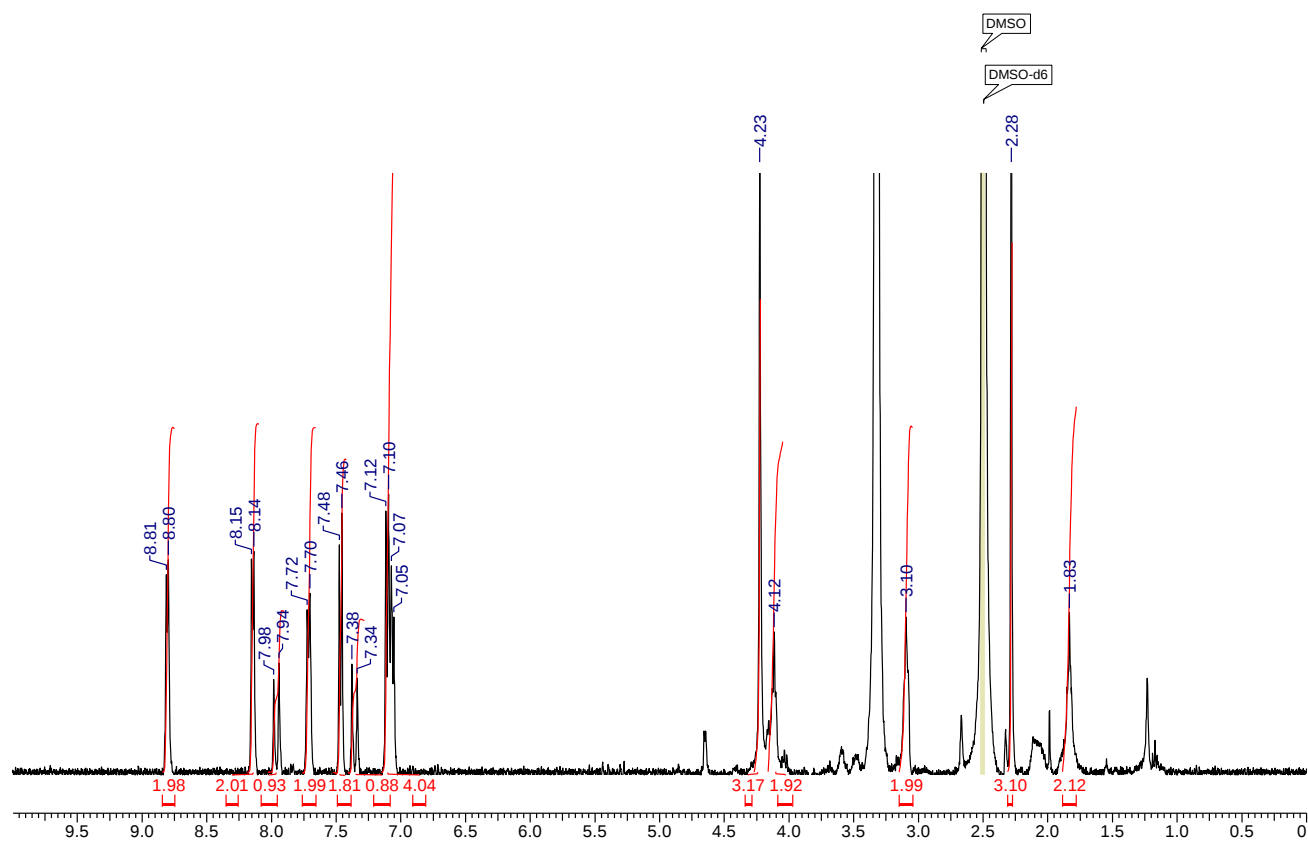


Figure S2. ¹H NMR spectrum of **3a** in DMSO-*d*₆.

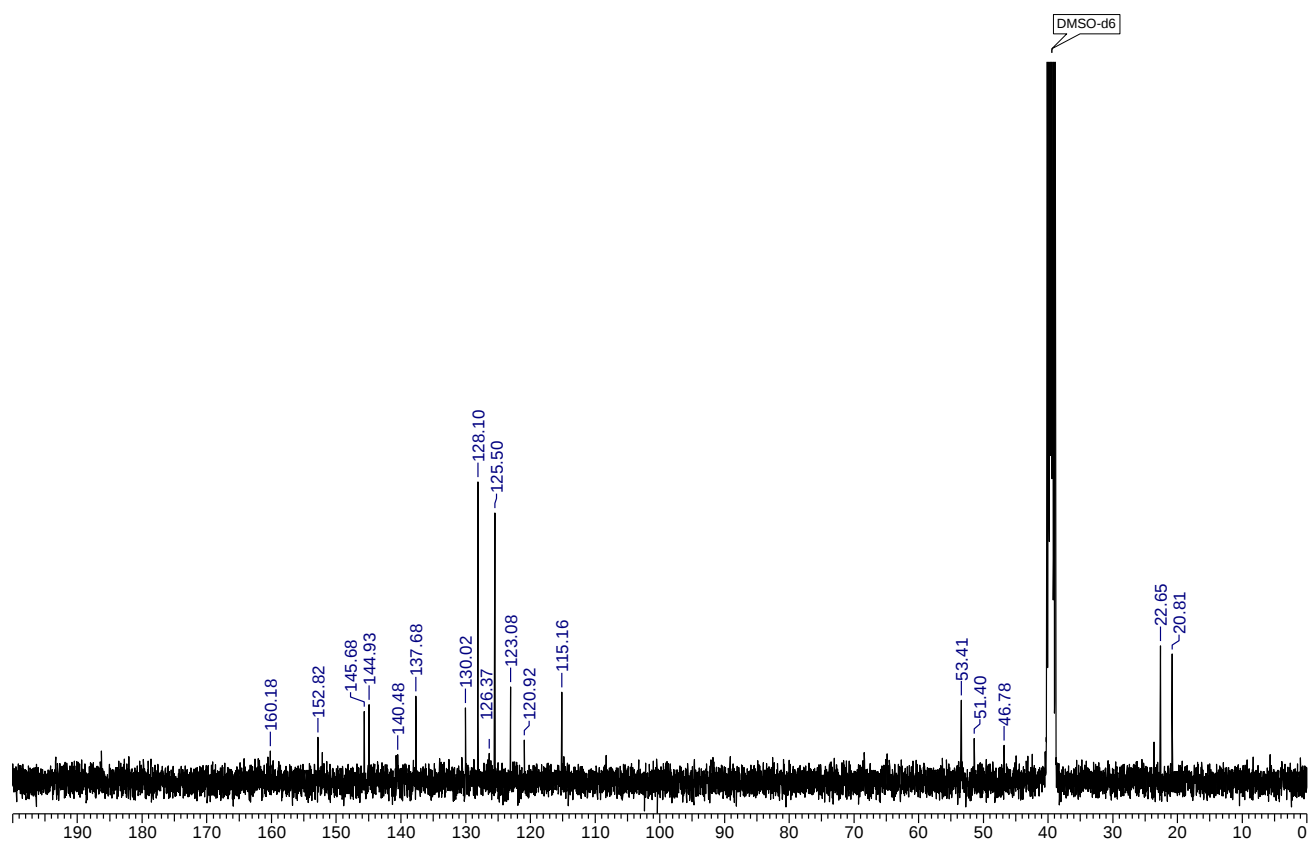


Figure S3. ¹³C NMR spectrum of **3a** in DMSO-*d*₆.

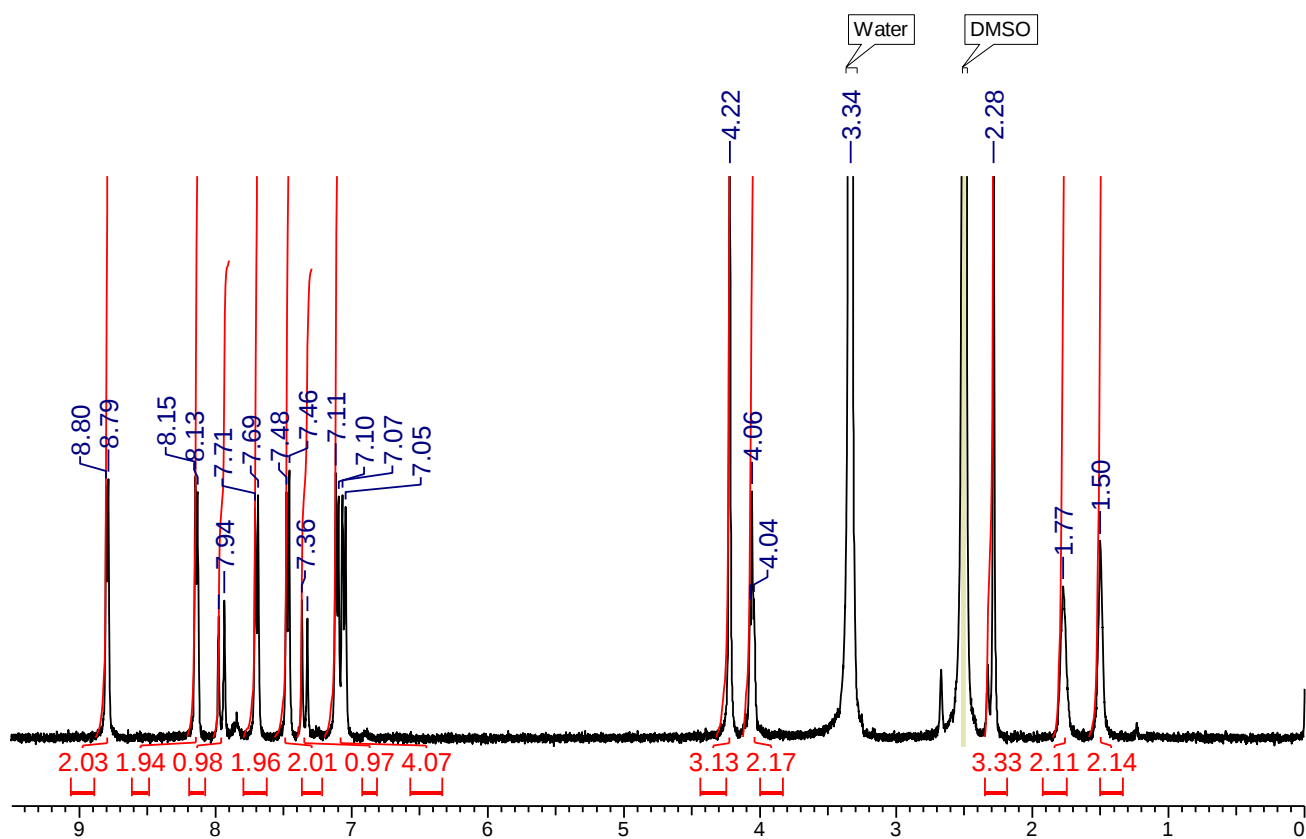


Figure S4. ¹H NMR spectrum of **3b** in DMSO-*d*₆.

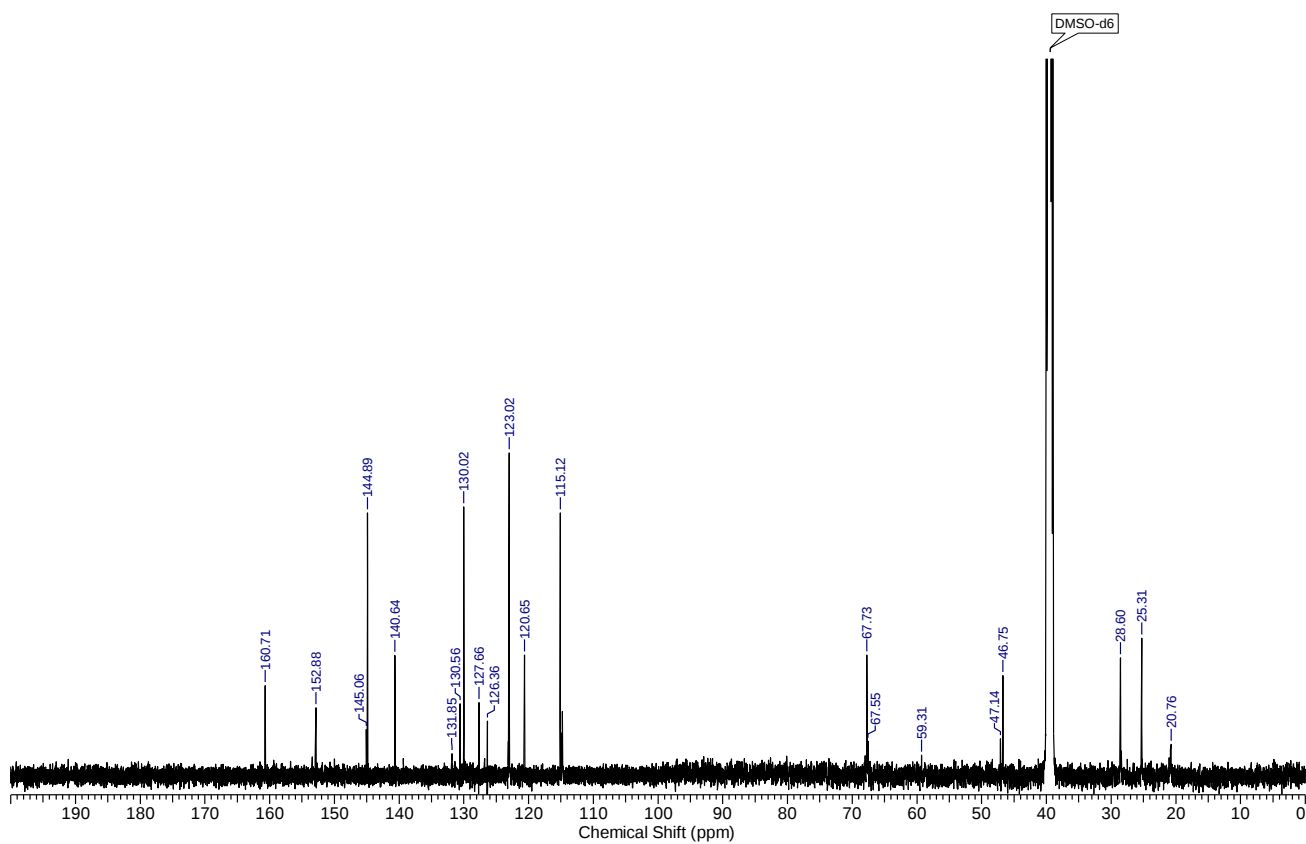


Figure S5. ¹³C NMR spectrum of **3b** in DMSO-*d*₆.

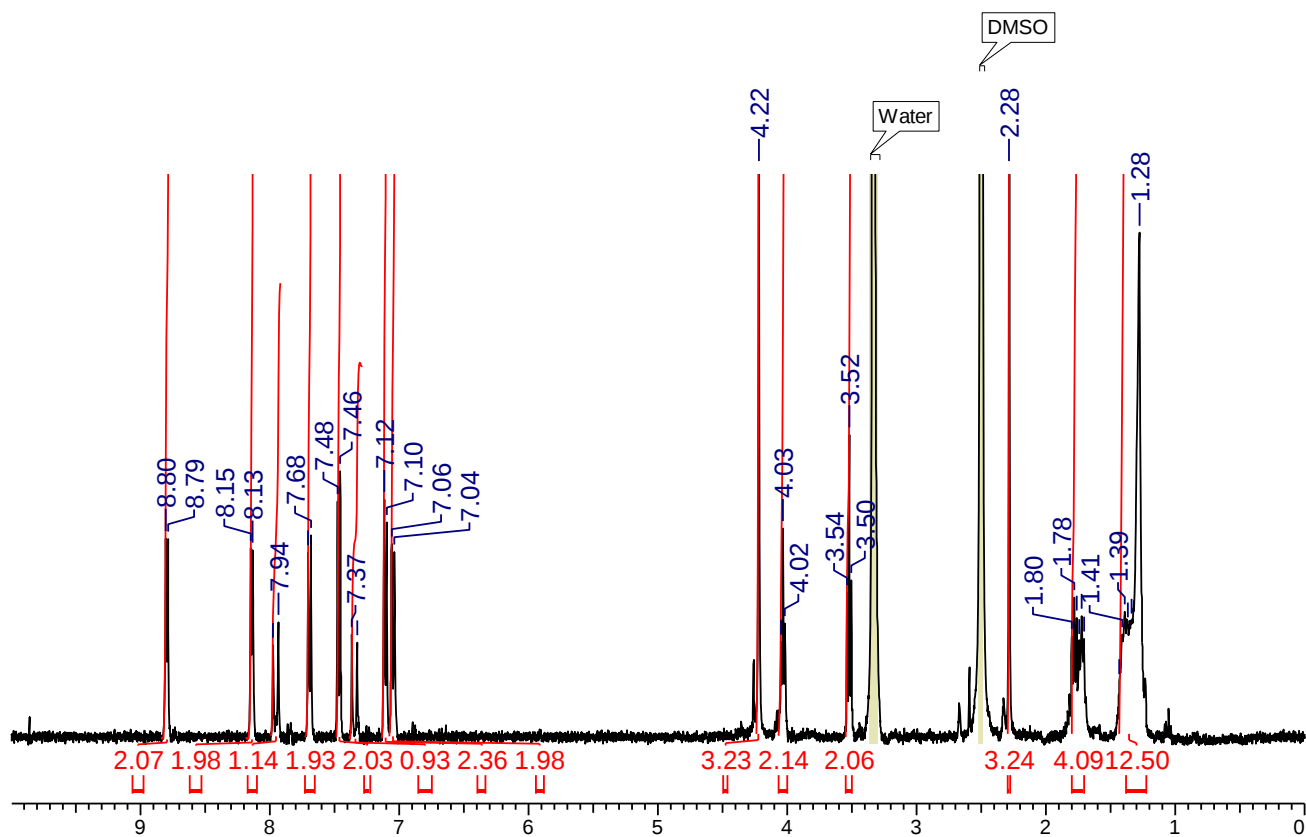


Figure S6. ¹H NMR spectrum of 3c in DMSO-*d*₆.

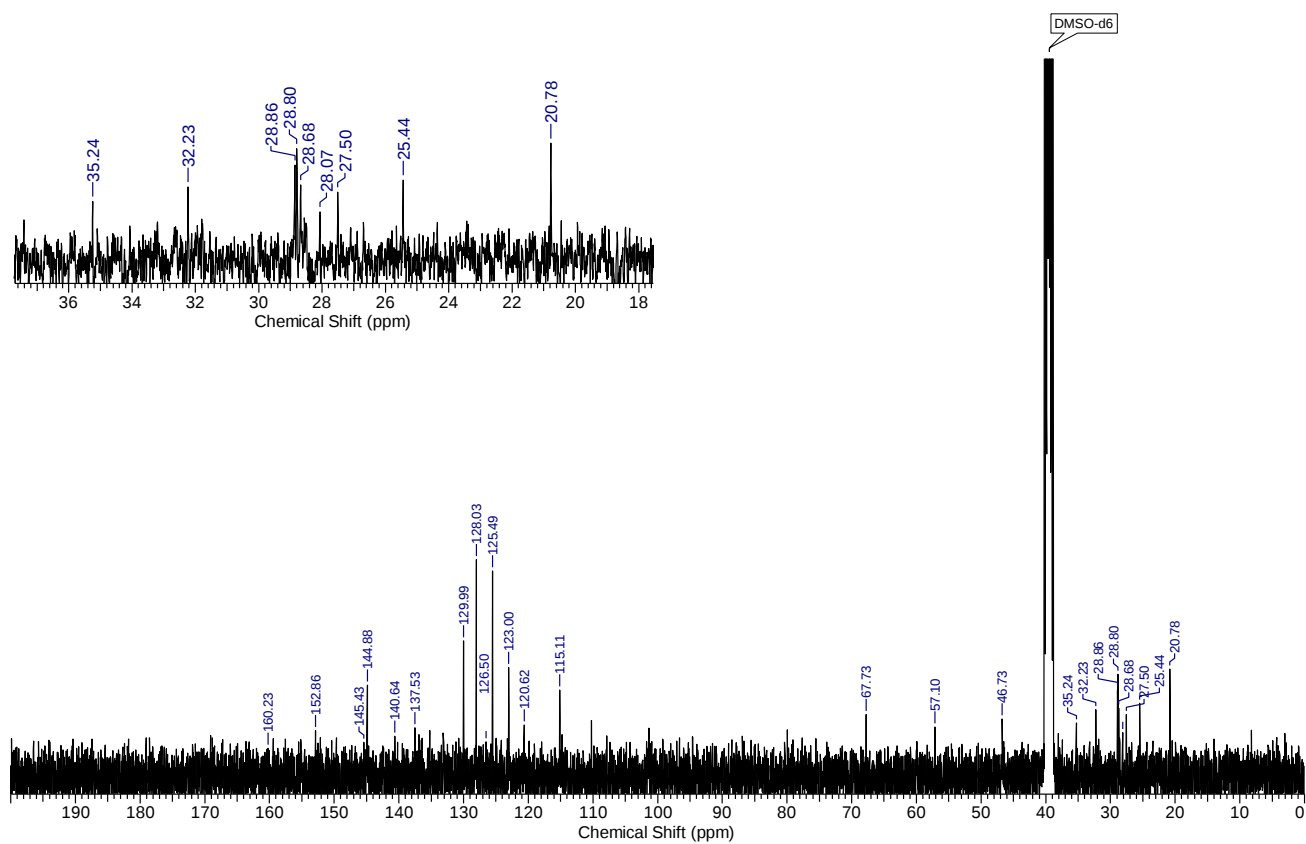


Figure S7. ¹³C NMR spectrum of 3c in DMSO-*d*₆.

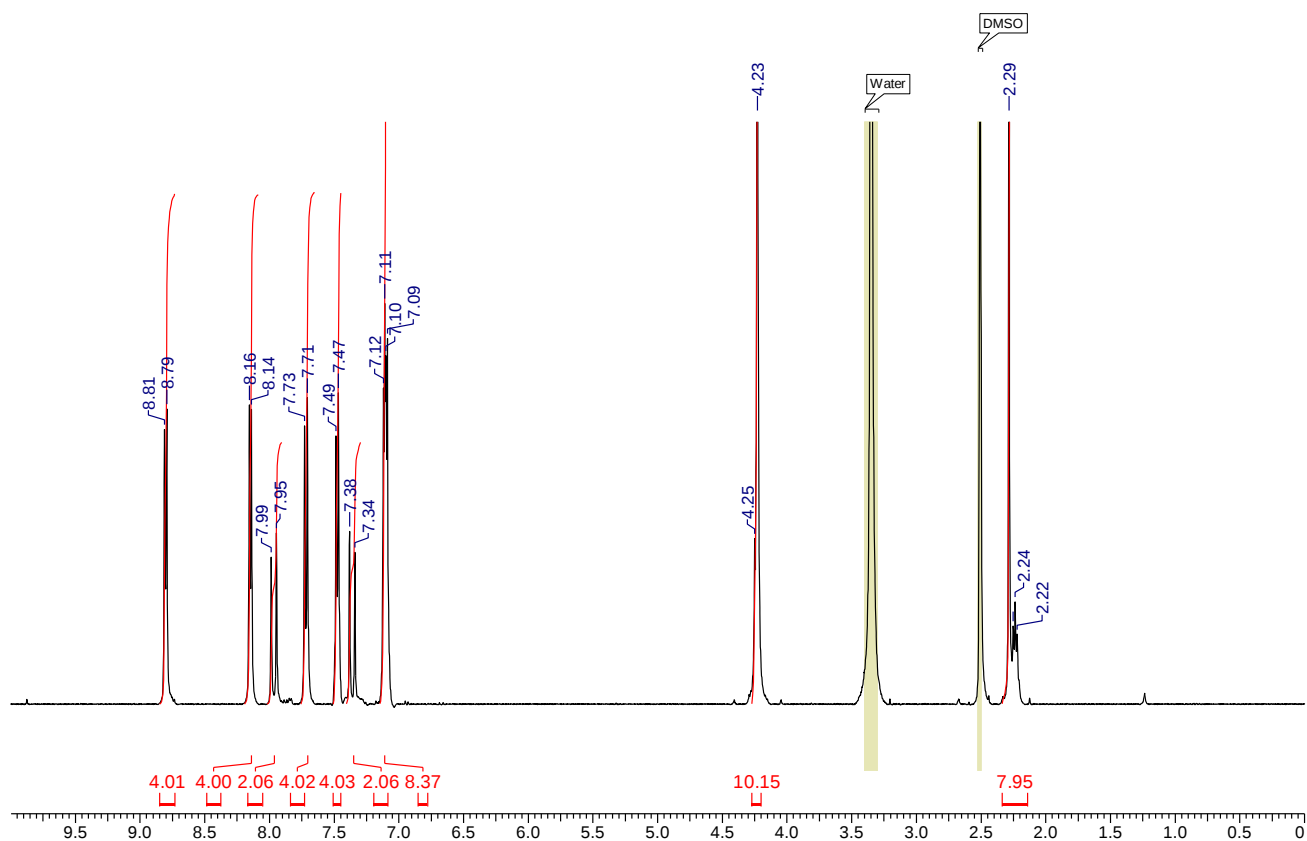


Figure S8. ¹H NMR spectrum of **4a** in DMSO-*d*₆.

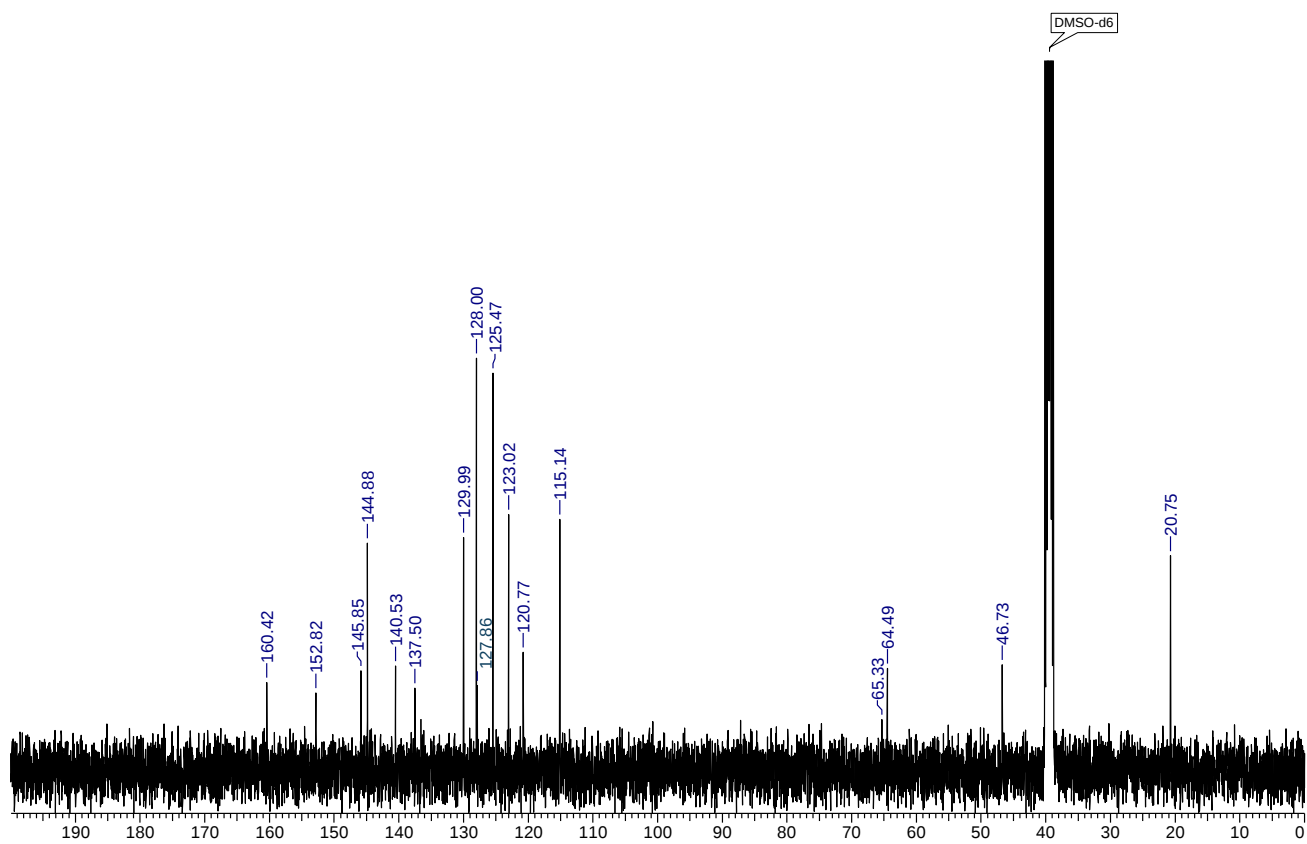


Figure S9. ¹³C NMR spectrum of **4a** in DMSO-*d*₆.

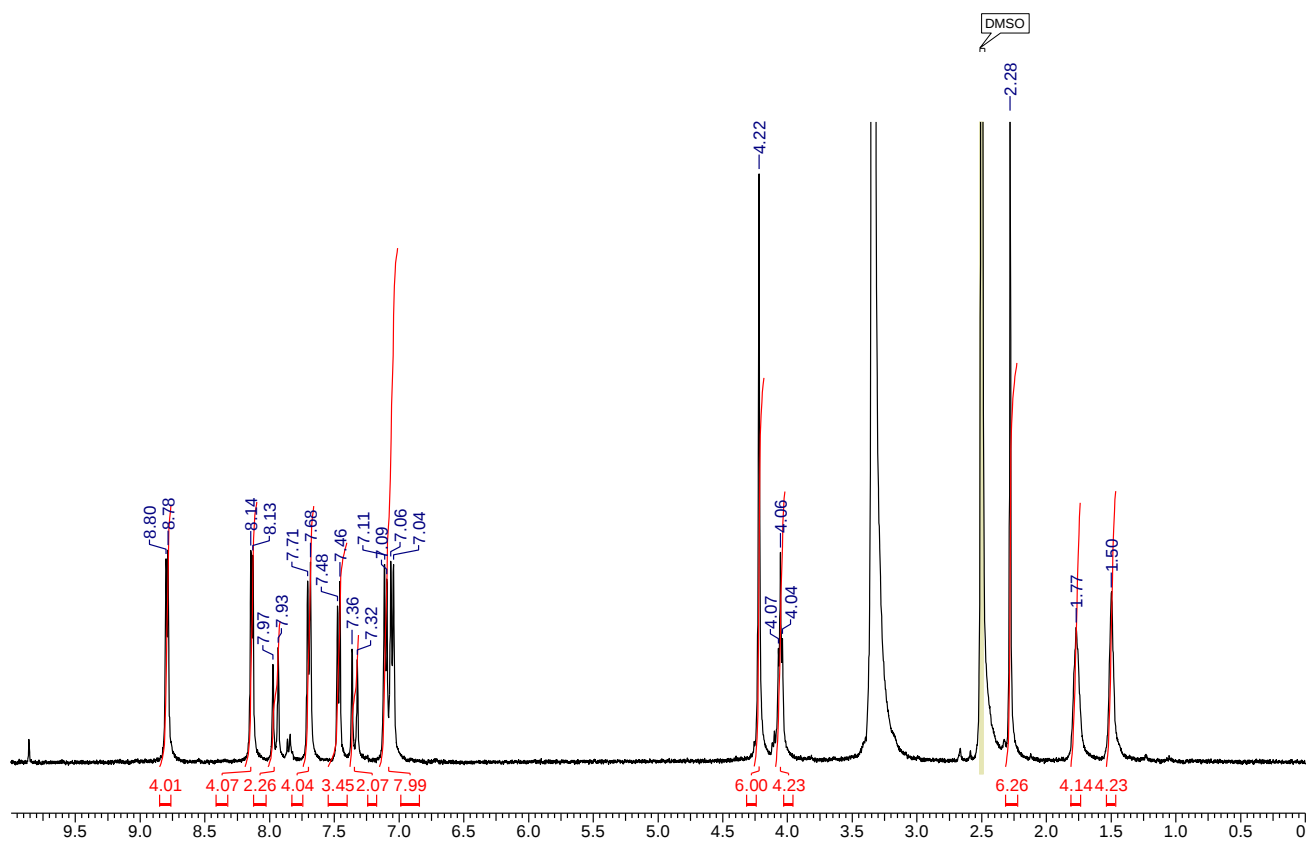


Figure S10. ¹H NMR spectrum of **4b** in DMSO-*d*₆.

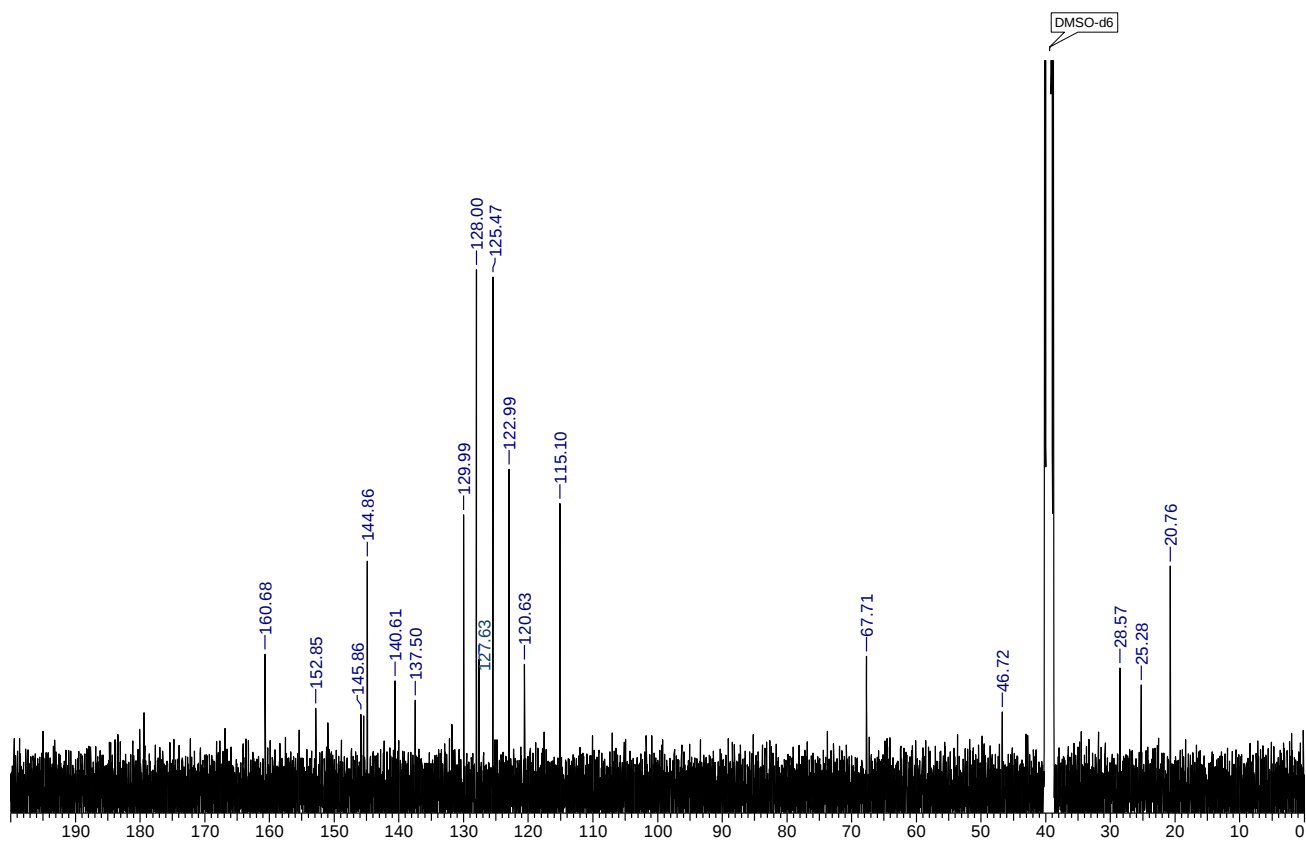


Figure S11. ¹³C NMR spectrum of **4b** in DMSO-*d*₆.

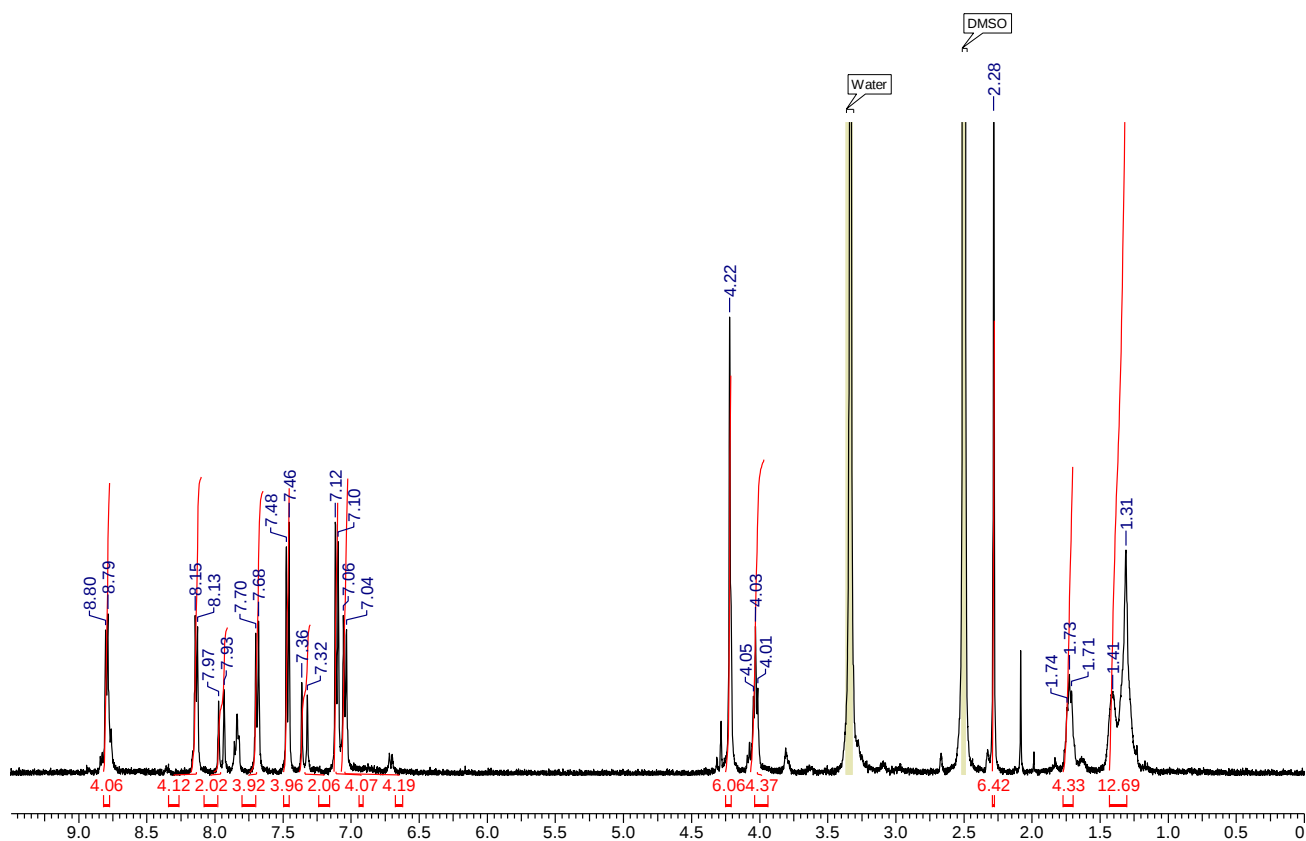


Figure S12. ¹H NMR spectrum of **4c** in DMSO-*d*₆.

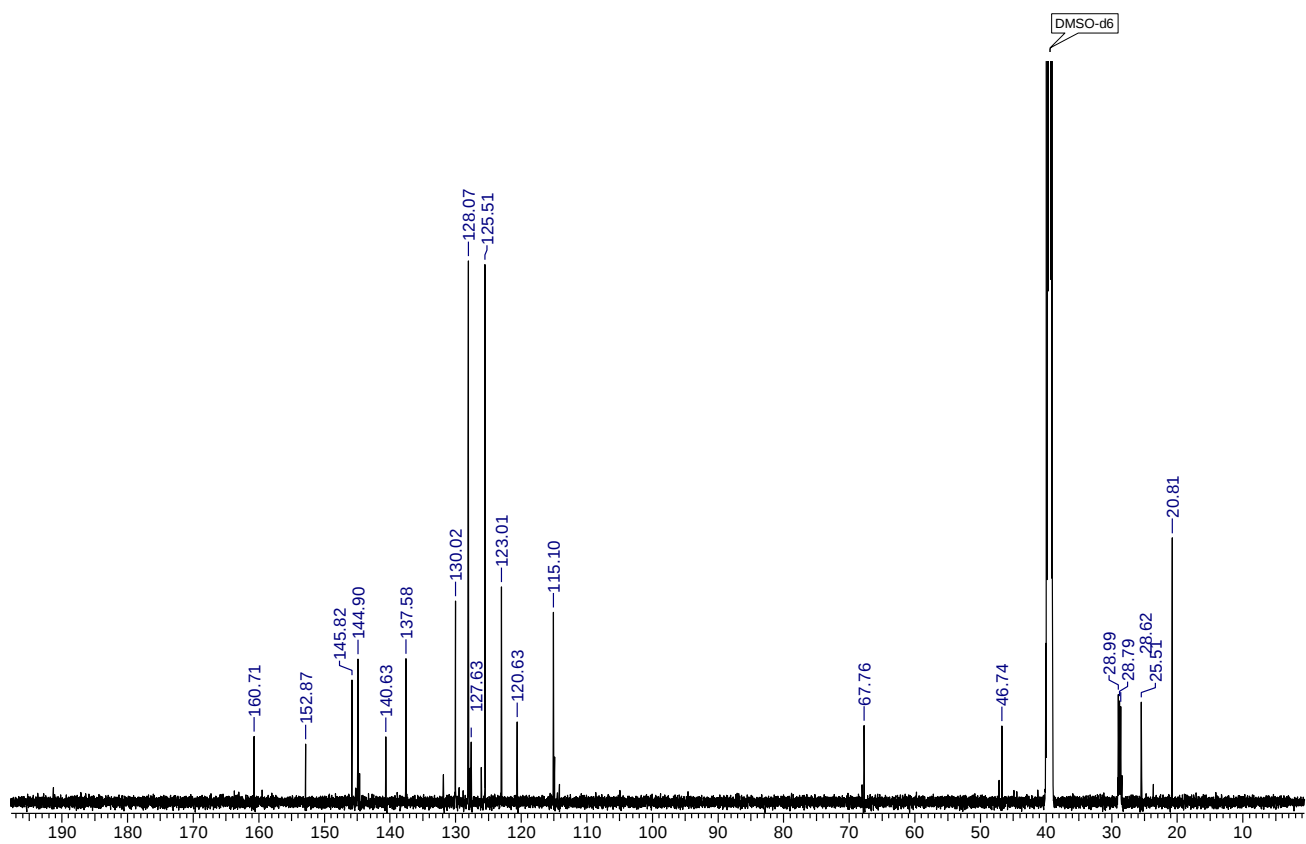


Figure S13. ¹³C NMR spectrum of **4c** in DMSO-*d*₆.