

Supplementary Information

Chiral Bistacrine Analogues: Synthesis, Cholinesterase Inhibitory Activity and a Molecular Modeling Approach

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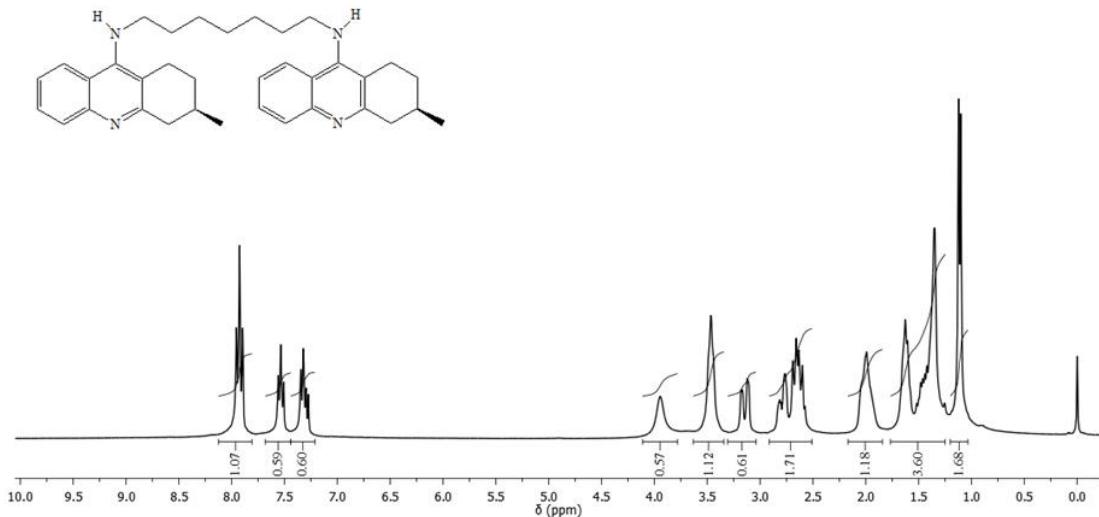


Figure S1. ¹H NMR spectrum (300 MHz, CDCl₃) of homodimer (R)-3a.

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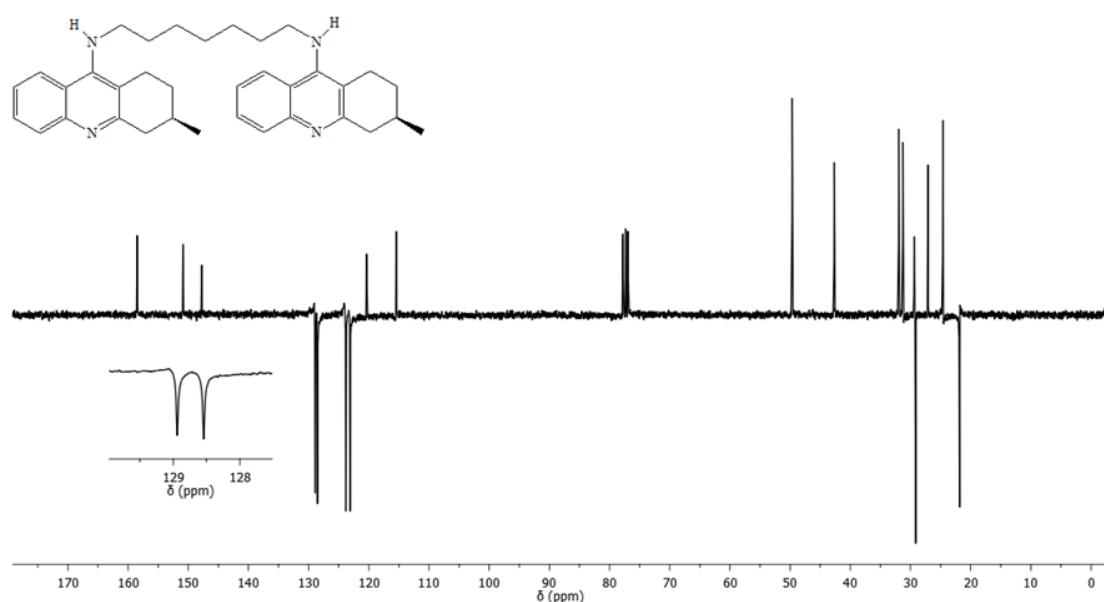


Figure S2. ^{13}C NMR (APT) spectrum (75 MHz, CDCl_3) of homodimer (*R*)-**3a**.

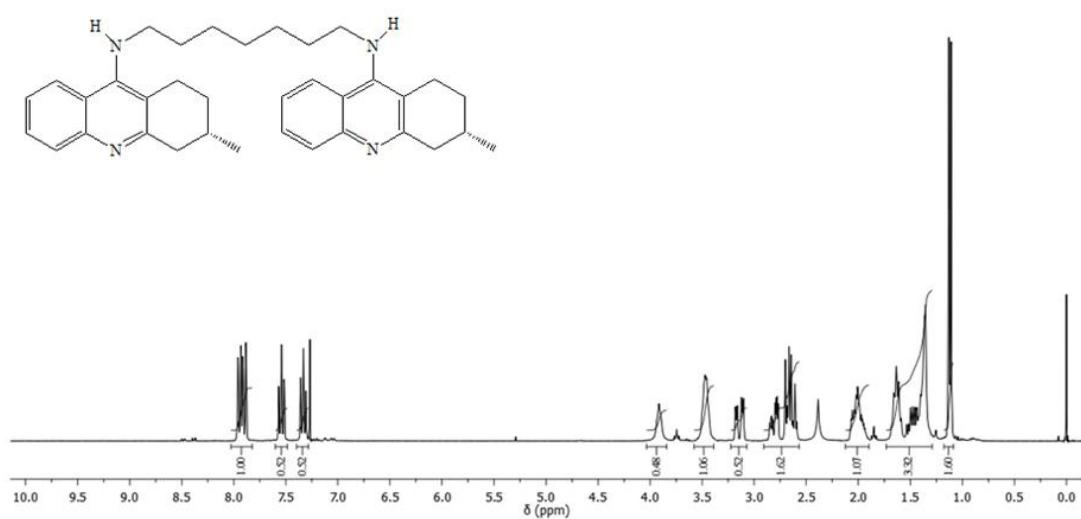


Figure S3. ^1H NMR spectrum (300 MHz, CDCl_3) of homodimer (*S*)-**3a**.

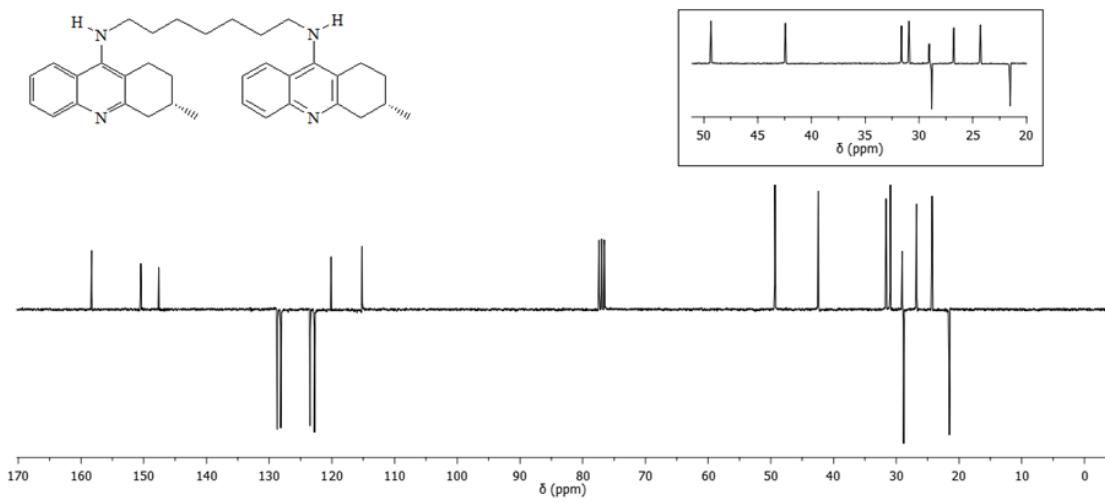


Figure S4. ^{13}C NMR (APT) spectrum (75 MHz, CDCl_3) of homodimer (*S*)-3a.

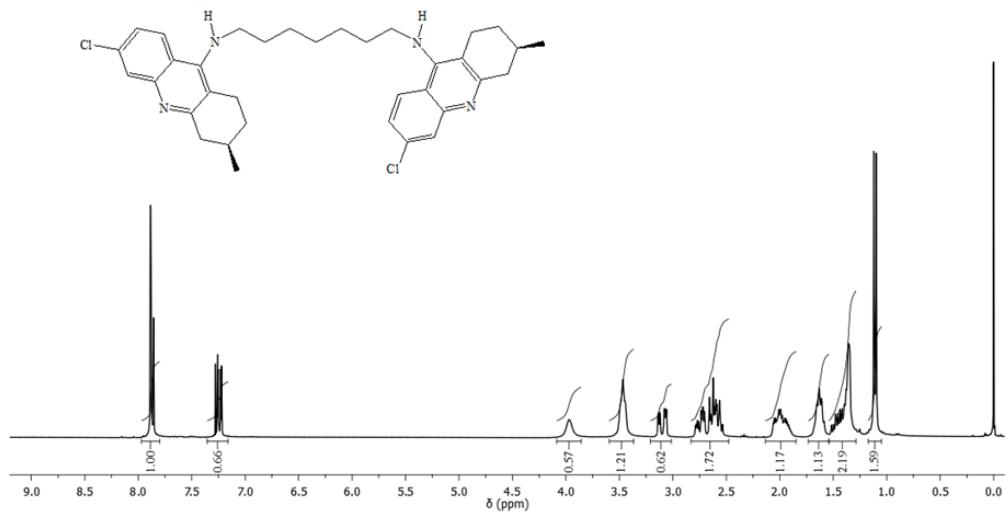


Figure S5. ^1H NMR spectrum (300 MHz, CDCl_3) of homodimer (*R*)-3b.

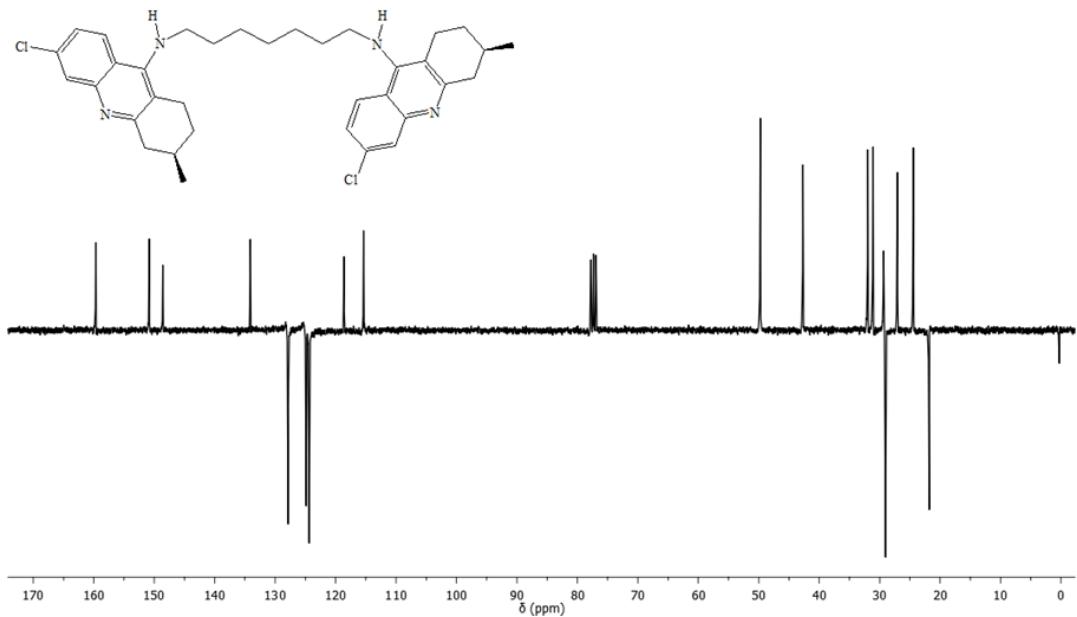


Figure S6. ^{13}C NMR (APT) spectrum (75 MHz, CDCl_3) of homodimer (R)-3b.

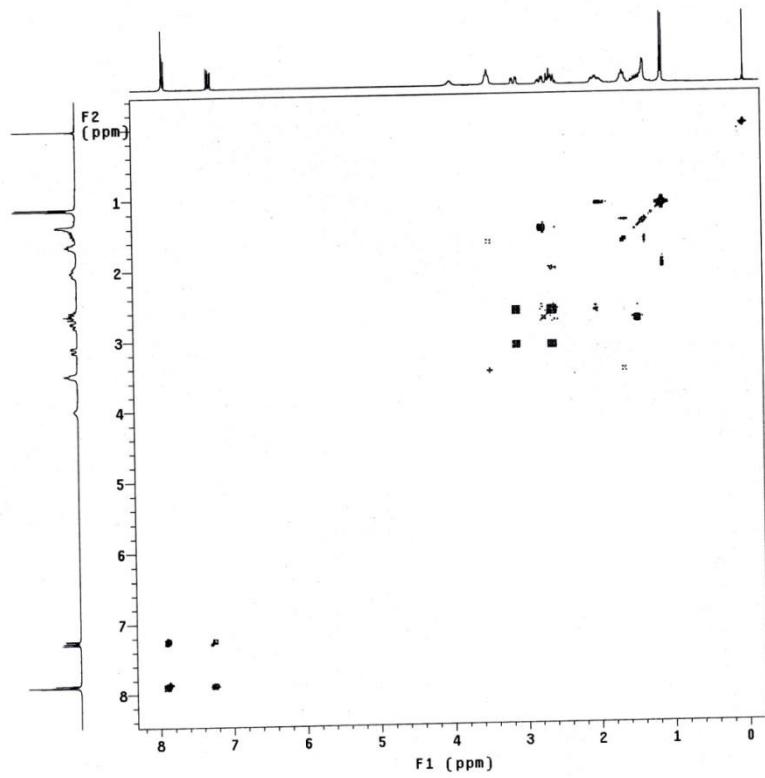


Figure S7. 2D COSY NMR of homodimer (R)-3b.

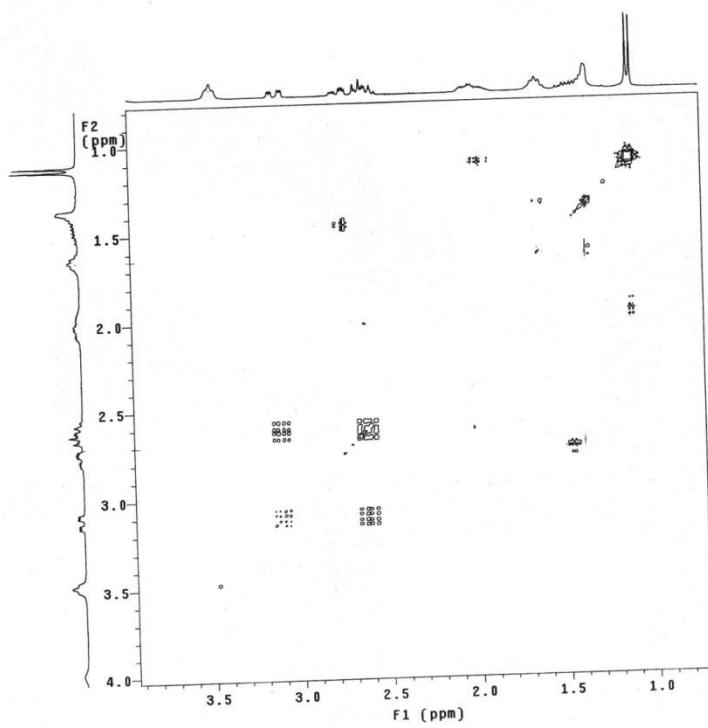


Figure S8. Expansion (about 1.0 to 4.0 ppm) of 2D COSY NMR of homodimer (*R*)-3b.

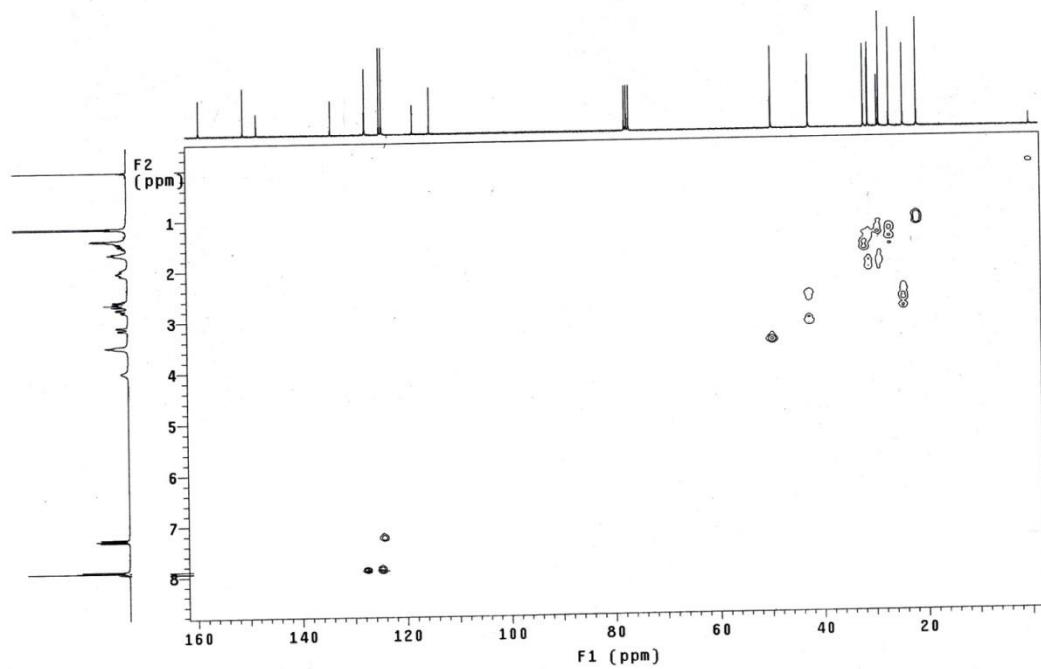


Figure S9. 2D HMQC NMR of homodimer (*R*)-3b.

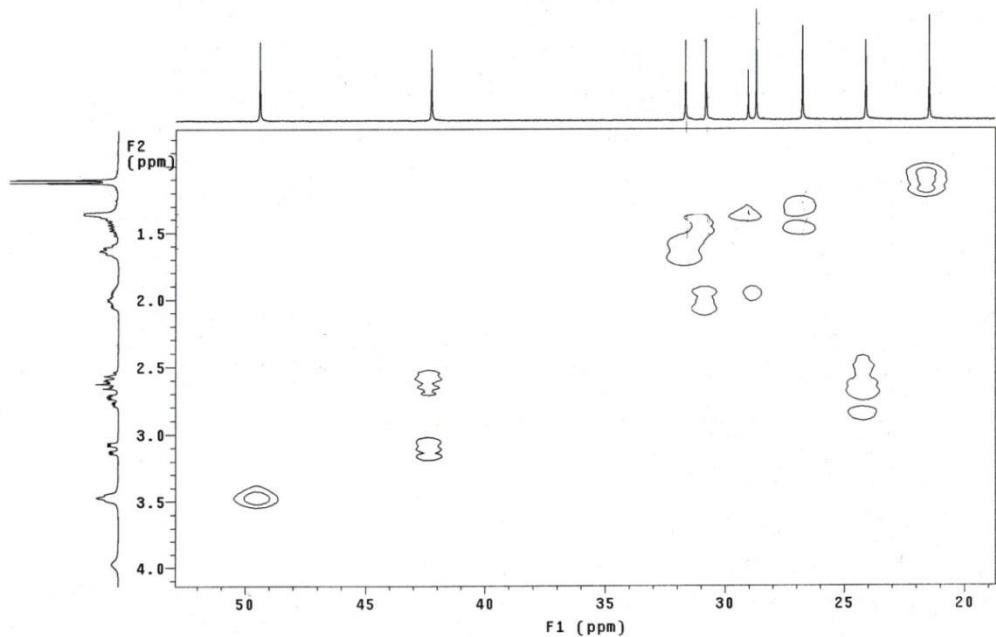


Figure S10. Expansion (about 1.0 to 4.0 ppm of ^1H and 20.0 to 50.0 ppm of ^{13}C) of 2D HMQC NMR of homodimer (*R*)-3b.

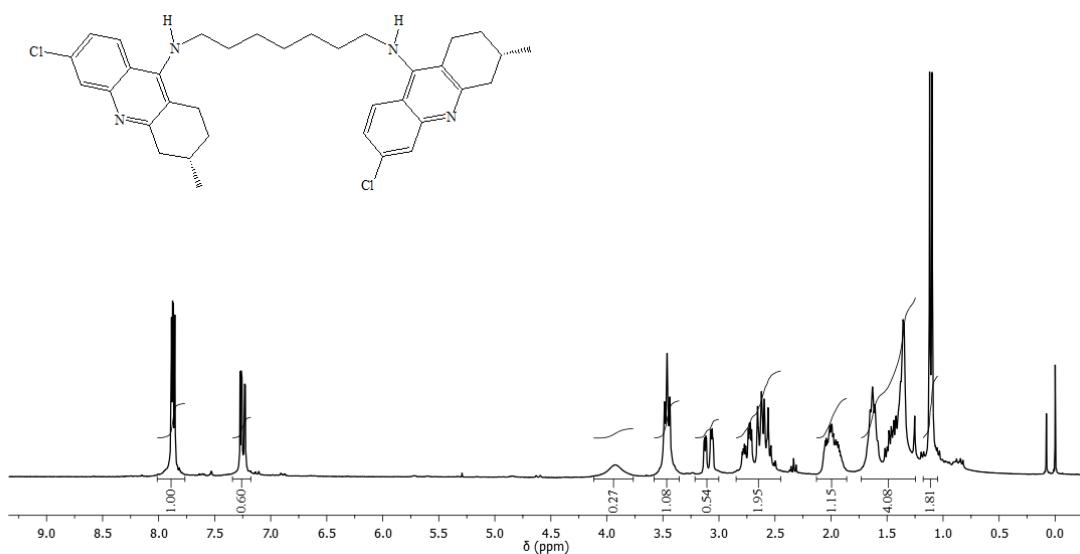


Figure S11. ^1H NMR spectrum (300 MHz, CDCl_3) of homodimer (*S*)-3b.

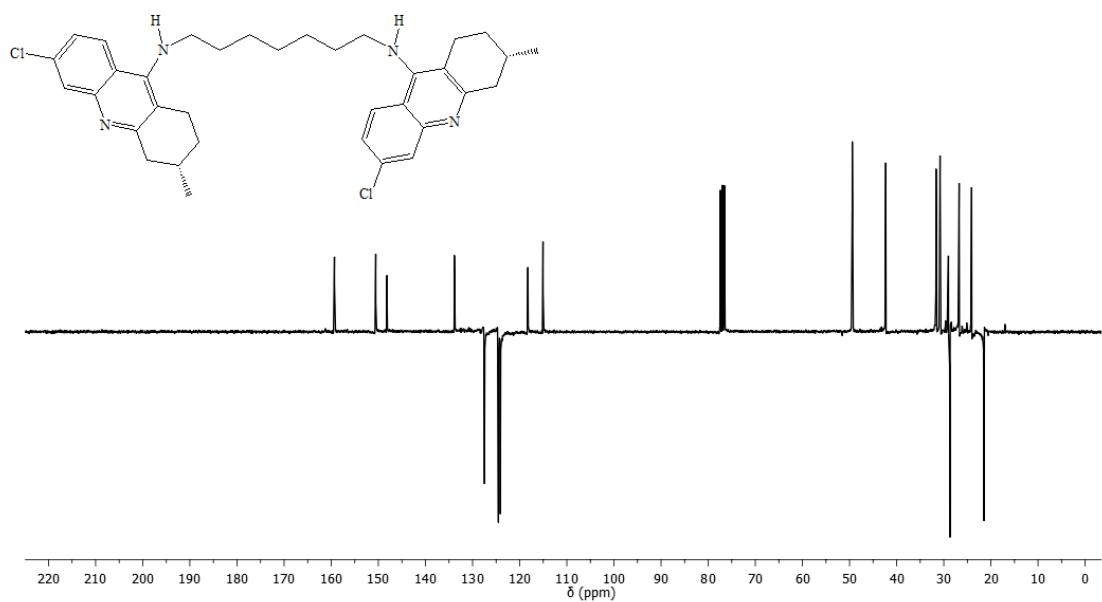


Figure S12. ^{13}C NMR (APT) spectrum (75 MHz, CDCl_3) of homodimer (*S*)-3b.

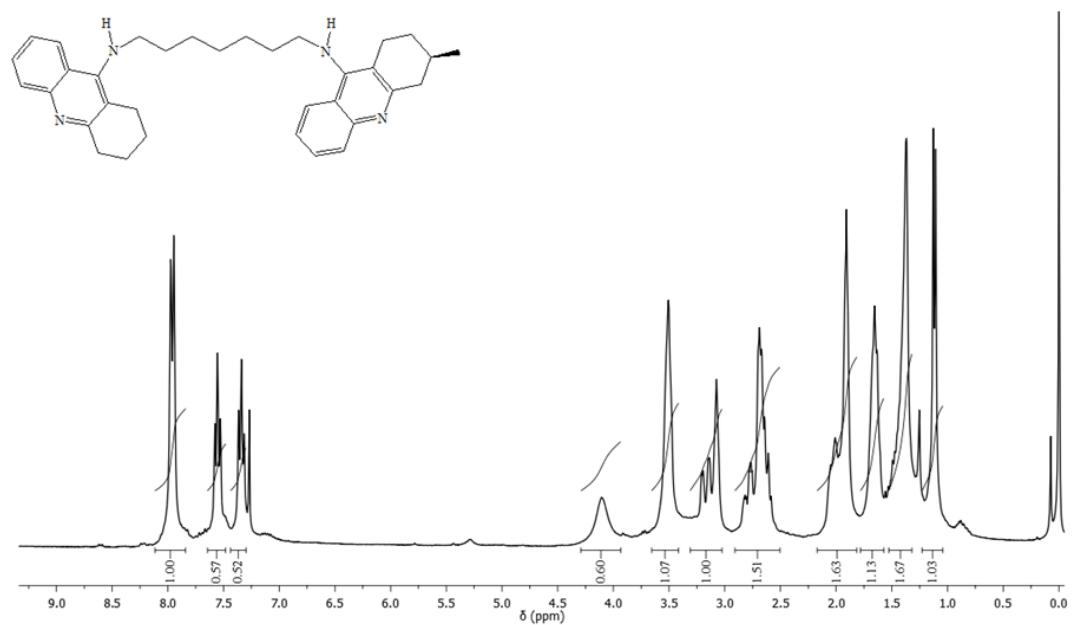


Figure S13. ^1H NMR spectrum (300 MHz, CDCl_3) of heterodimer (*R*)-3c.

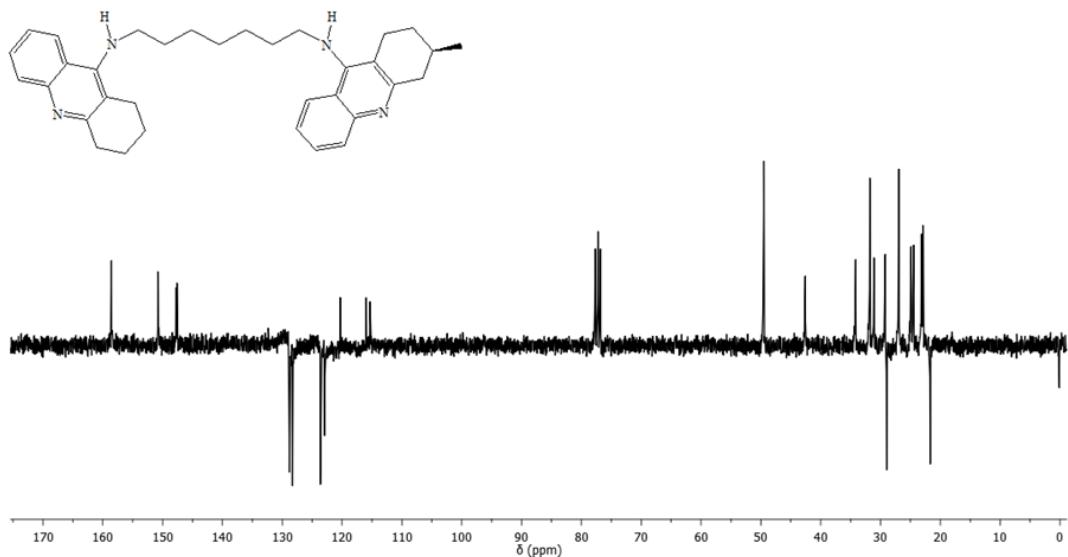


Figure S14. ^{13}C NMR (APT) spectrum (75 MHz, CDCl_3) of heterodimer (R)-3c.

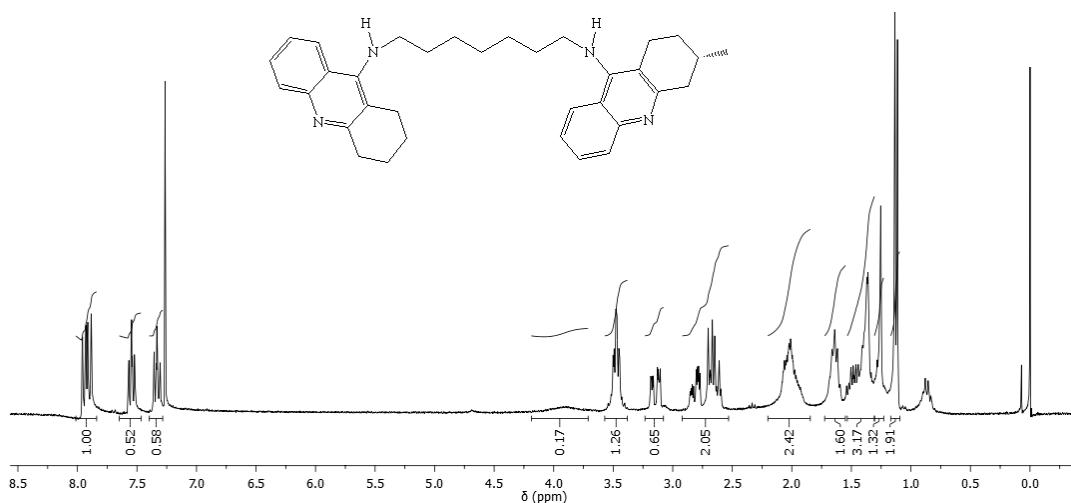


Figure S15. ^1H NMR spectrum (300 MHz, CDCl_3) of heterodimer (S)-3c.

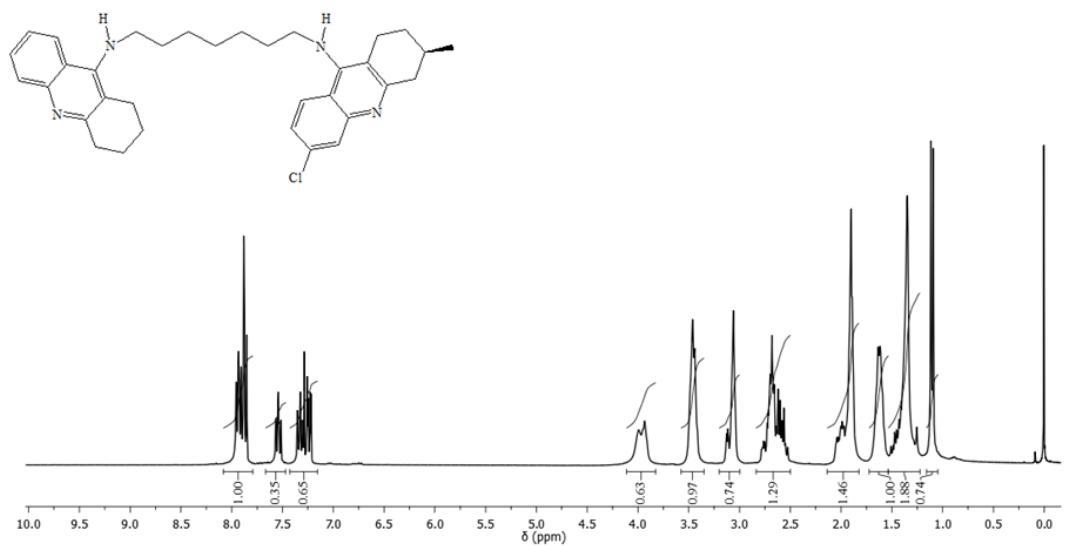


Figure S16. ^1H NMR spectrum (300 MHz, CDCl_3) of heterodimer (*R*)-3d.

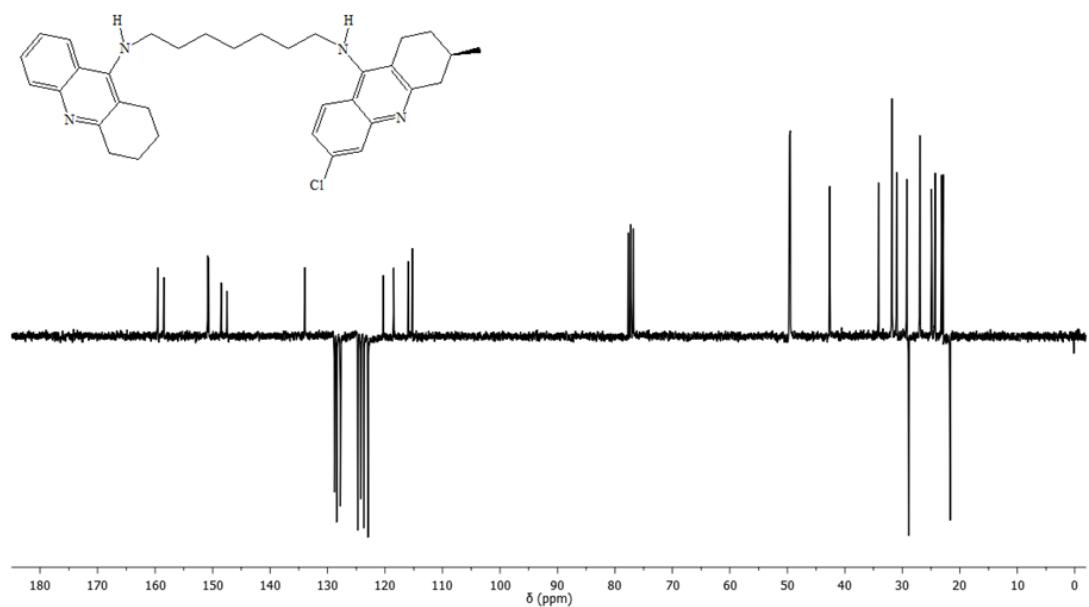


Figure S17. ^{13}C NMR (APT) spectrum (75 MHz, CDCl_3) of heterodimer (*R*)-3d.

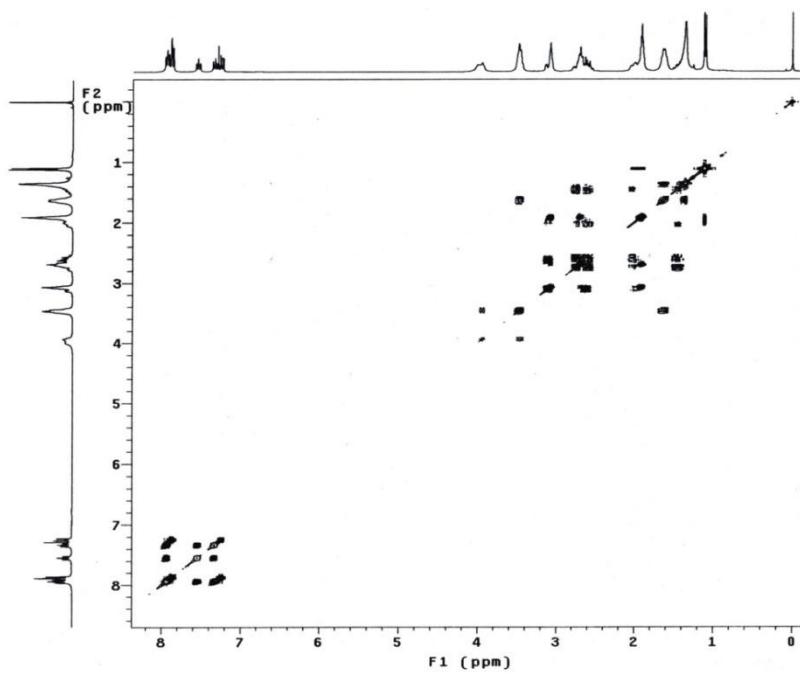


Figure S18. 2D COSY NMR of heterodimer (*R*)-3d.

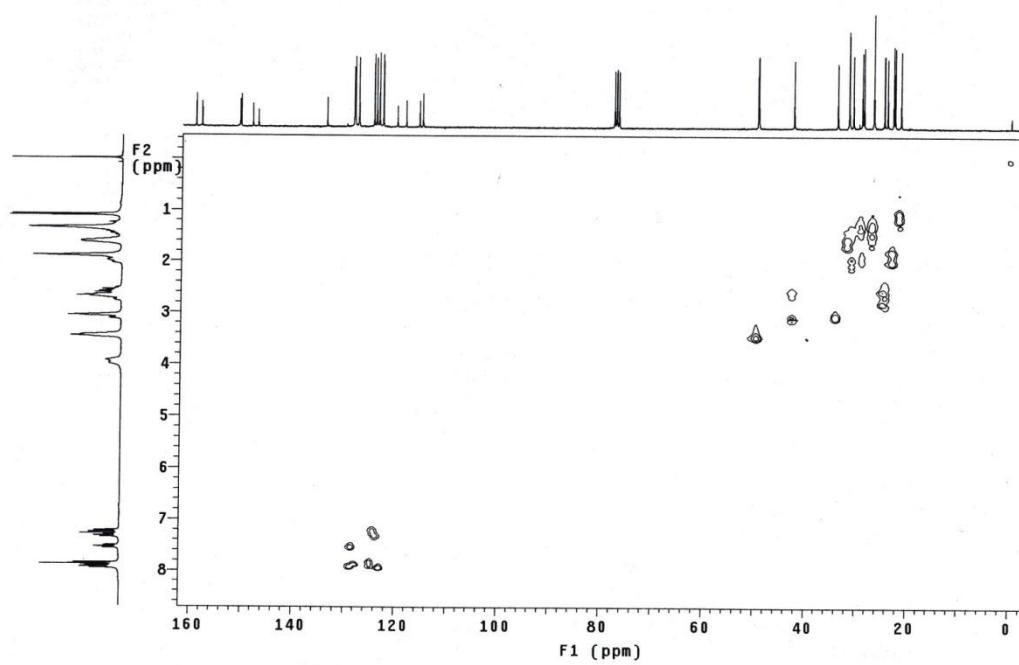


Figure S19. 2D HMQC NMR of heterodimer (*R*)-3d.

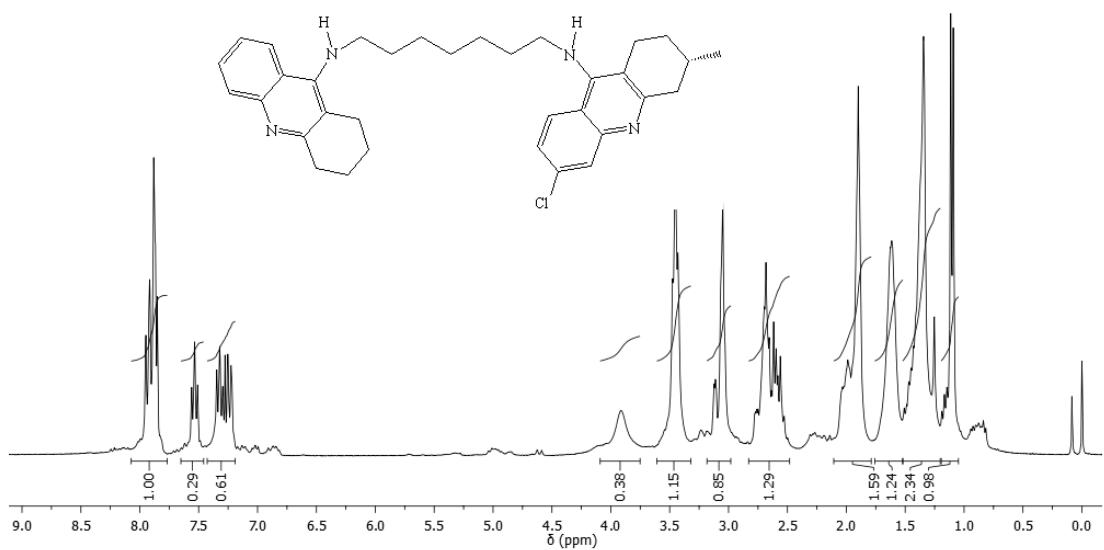


Figure S20. ^1H NMR spectrum (300 MHz, CDCl_3) of heterodimer (S)-3d.

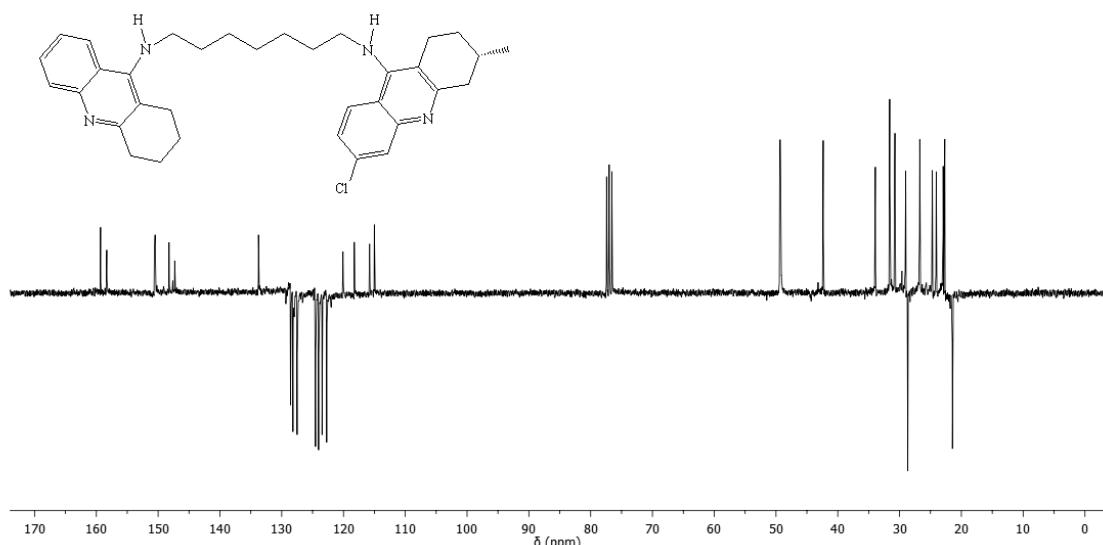


Figure S21. ^{13}C NMR (APT) spectrum (75 MHz, CDCl_3) of heterodimer (S)-3d.

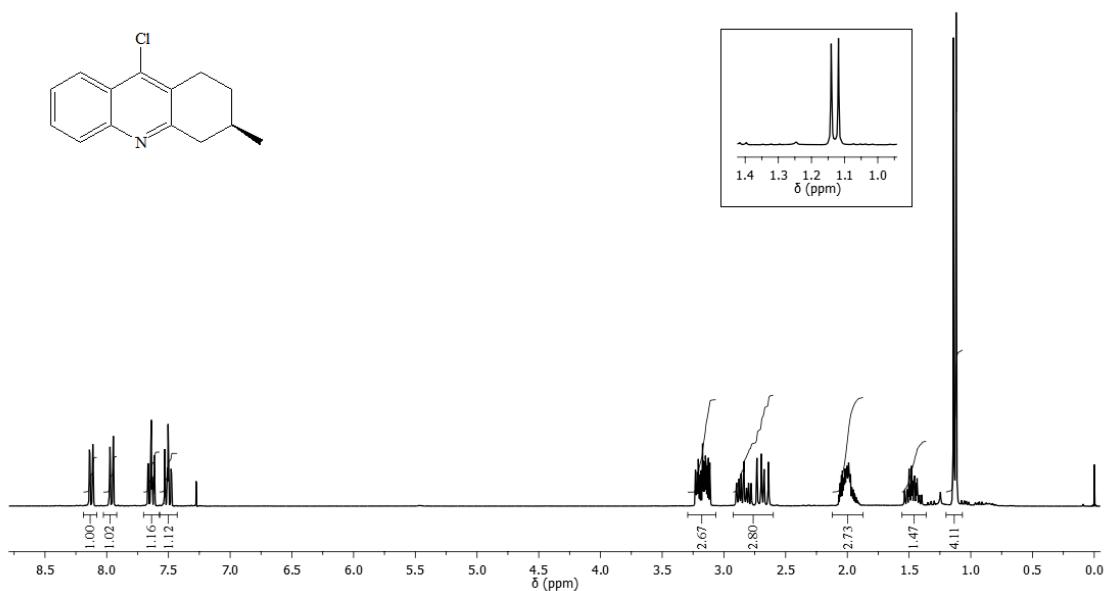


Figure S22. ^1H NMR spectrum (300 MHz, CDCl_3) of compound (R)-6b.

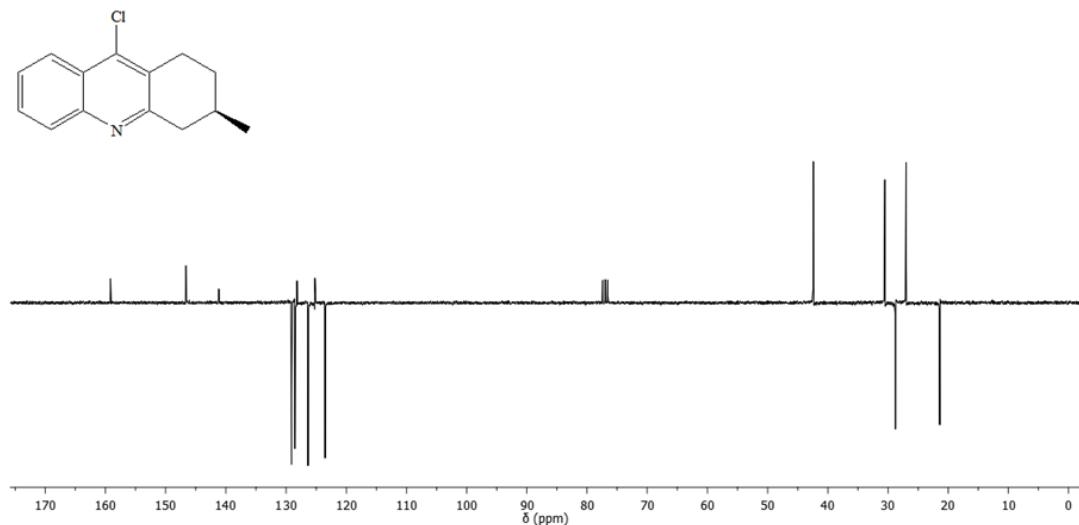


Figure S23. ^{13}C NMR (APT) spectrum (75 MHz, CDCl_3) of compound (R)-6b.

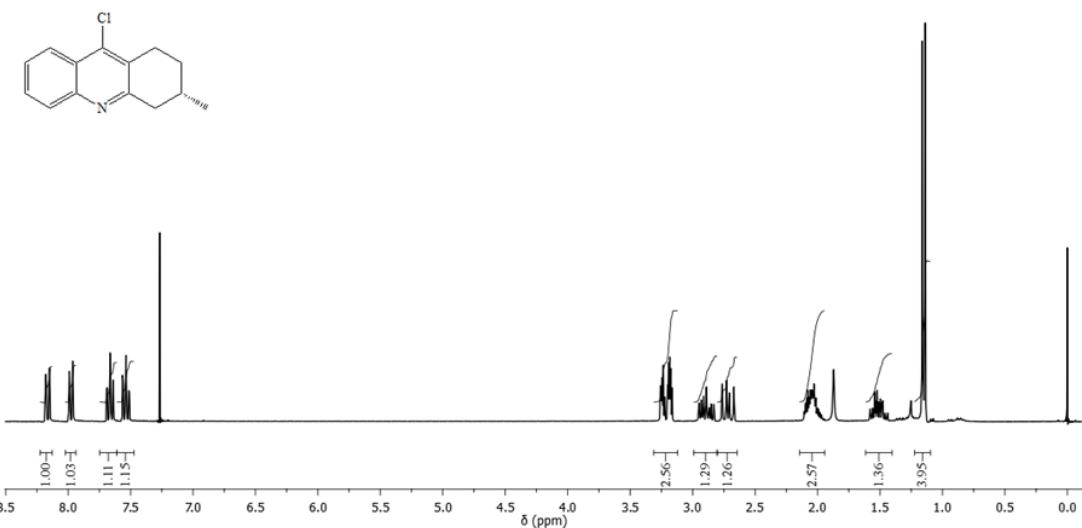


Figure S24. ¹H NMR spectrum (300 MHz, CDCl₃) of compound (S)-6b.

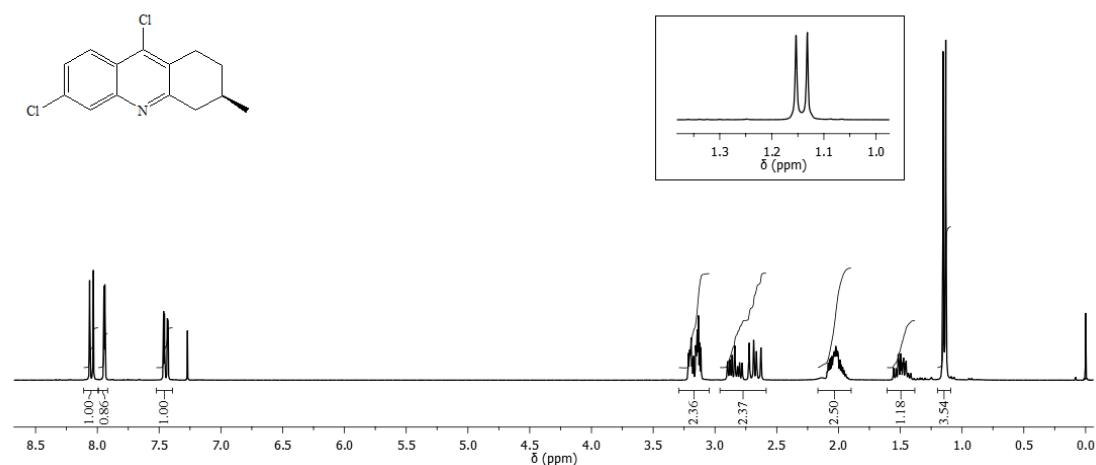


Figure S25. ¹H NMR spectrum (300 MHz, CDCl₃) of compound (R)-6c.

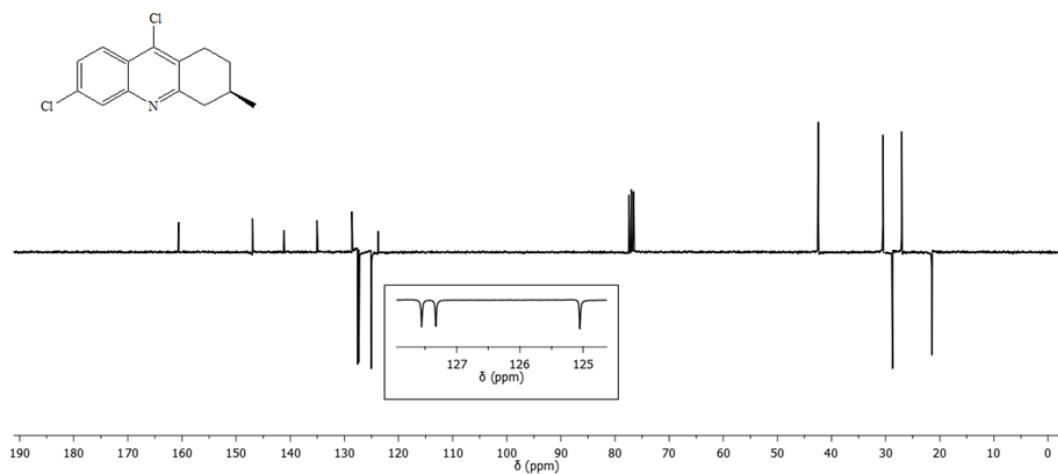


Figure S26. ¹³C NMR (APT) spectrum (75 MHz, CDCl₃) of compound (R)-6c.

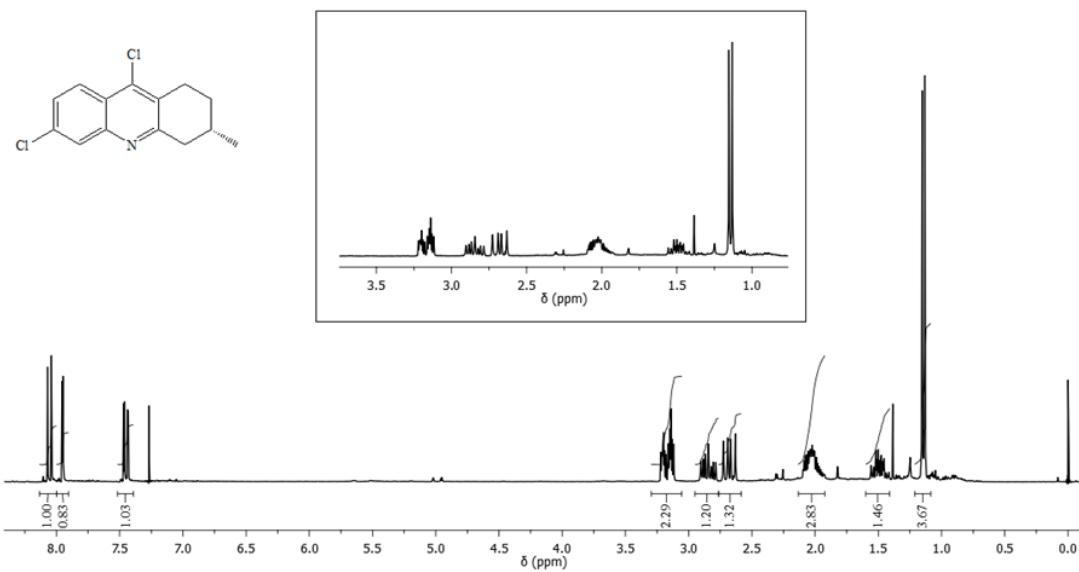


Figure S27. ^1H NMR spectrum (300 MHz, CDCl_3) of compound (*S*)-6c.

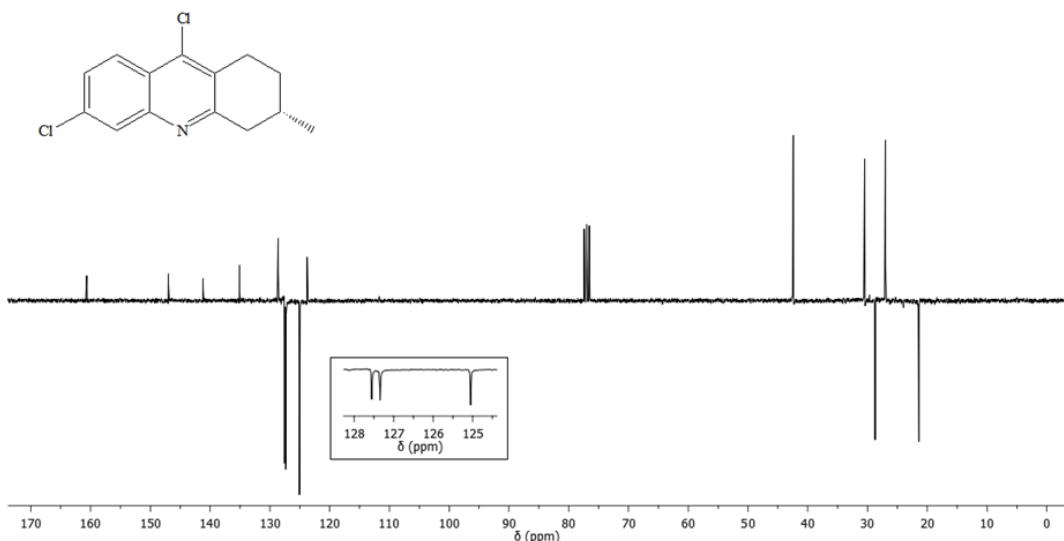


Figure S28. ^{13}C NMR (APT) spectrum (75 MHz, CDCl_3) of compound (*S*)-6c.