Supporting Information

Marine AChE inhibitors isolated from *Geodia baretti*: Natural compounds and their synthetic analogs

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Contents

Figure S19. ^{13}C-NMR spectrum of **8c** in methanol-d_4.

Figure S20. ^{1}H-NMR spectrum of **9a** in methanol-d_4.

Figure S21. ^{13}C-NMR spectrum of **9a** in methanol-d_4.

Figure S22. ^{1}H-NMR spectrum of **9b** in methanol-d_4.

Figure S23. ^{13}C-NMR spectrum of **9b** in methanol-d_4.

Figure S24. ^{1}H-NMR spectrum of **9c** in acetone-d_6.

Figure S25. ^{13}C-NMR spectrum of **9c** in methanol-d_4.

Figure S26. ^{1}H-NMR spectrum of **9d** in methanol-d_4.

Figure S27. ^{13}C-NMR spectrum of **9d** in methanol-d_4.

Figure S1. High-resolution MS spectrum of **1.**

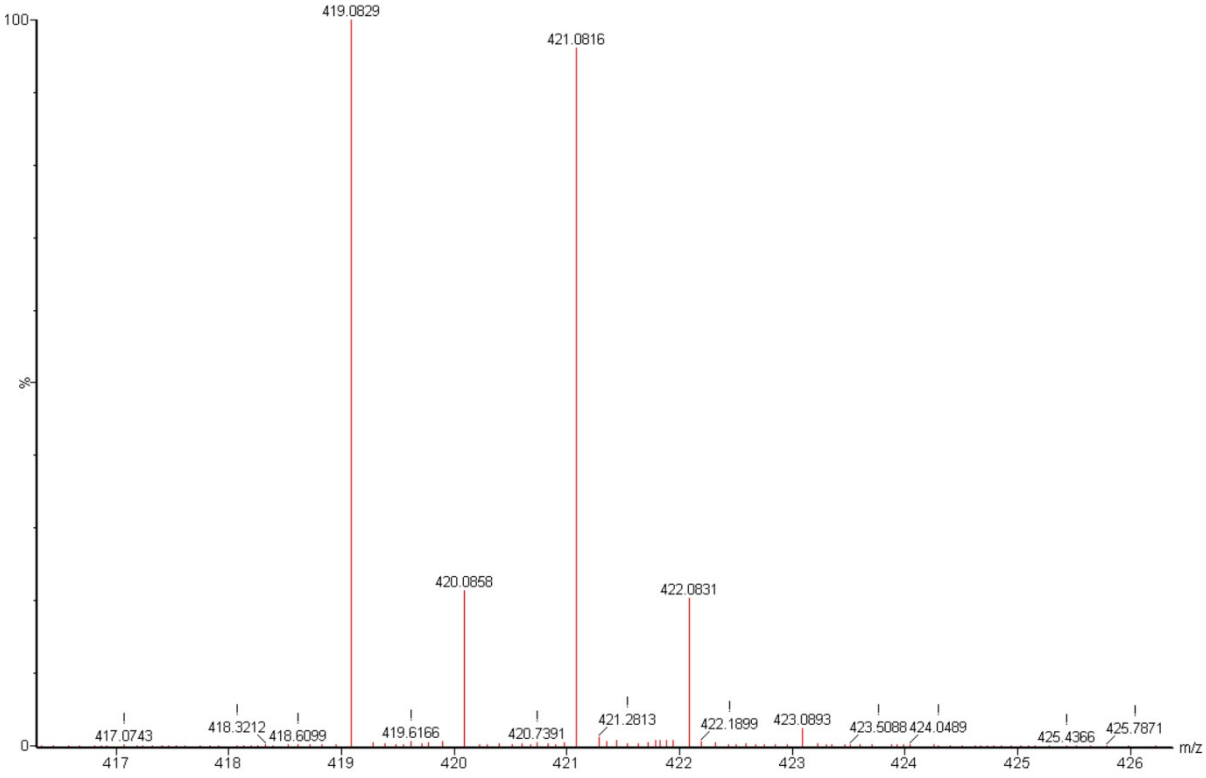


Figure S2. High-resolution MS spectrum of **2**.

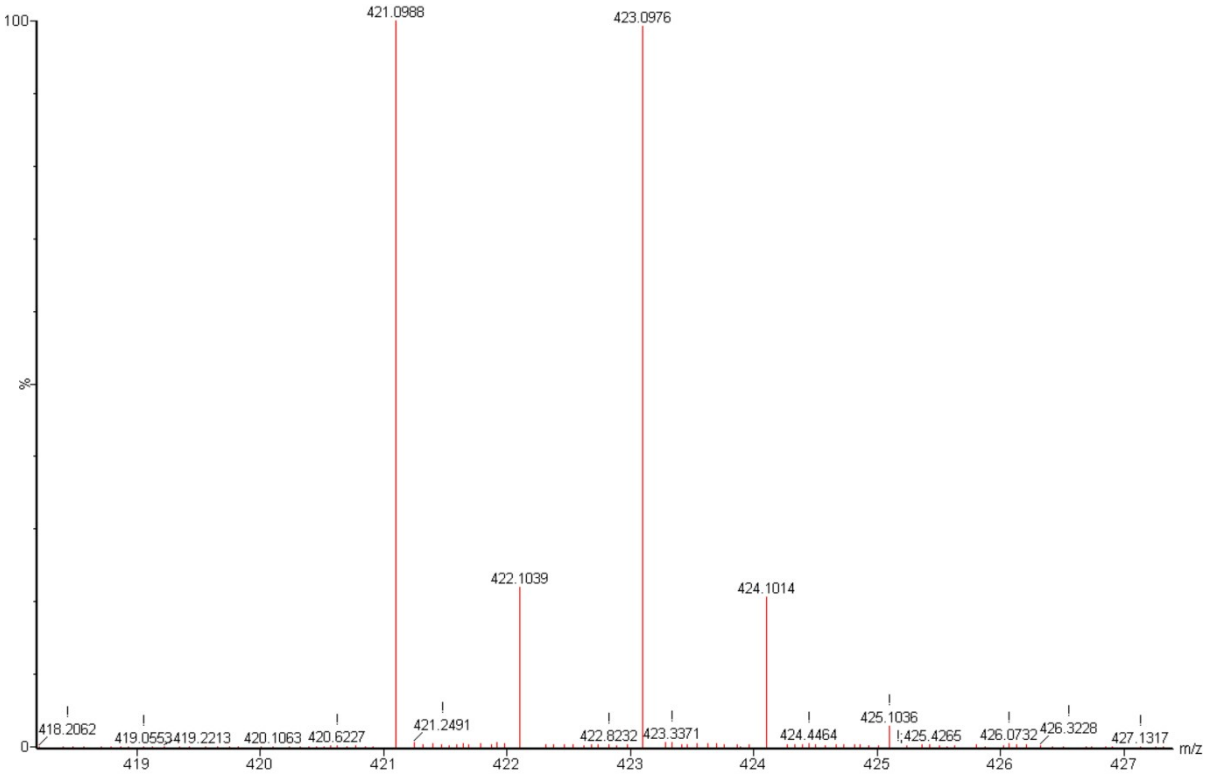


Figure S3. High-resolution MS spectrum of **3**.

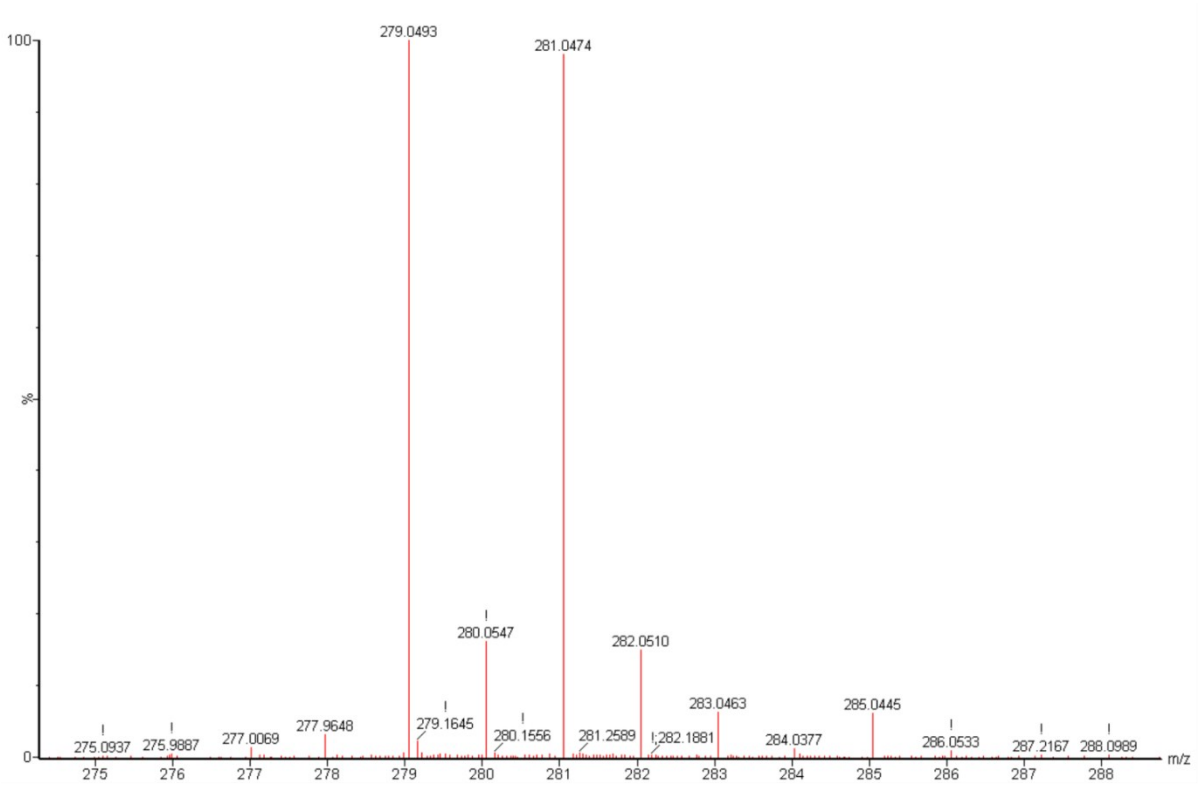


Figure S4. High-resolution MS spectrum of **4**.

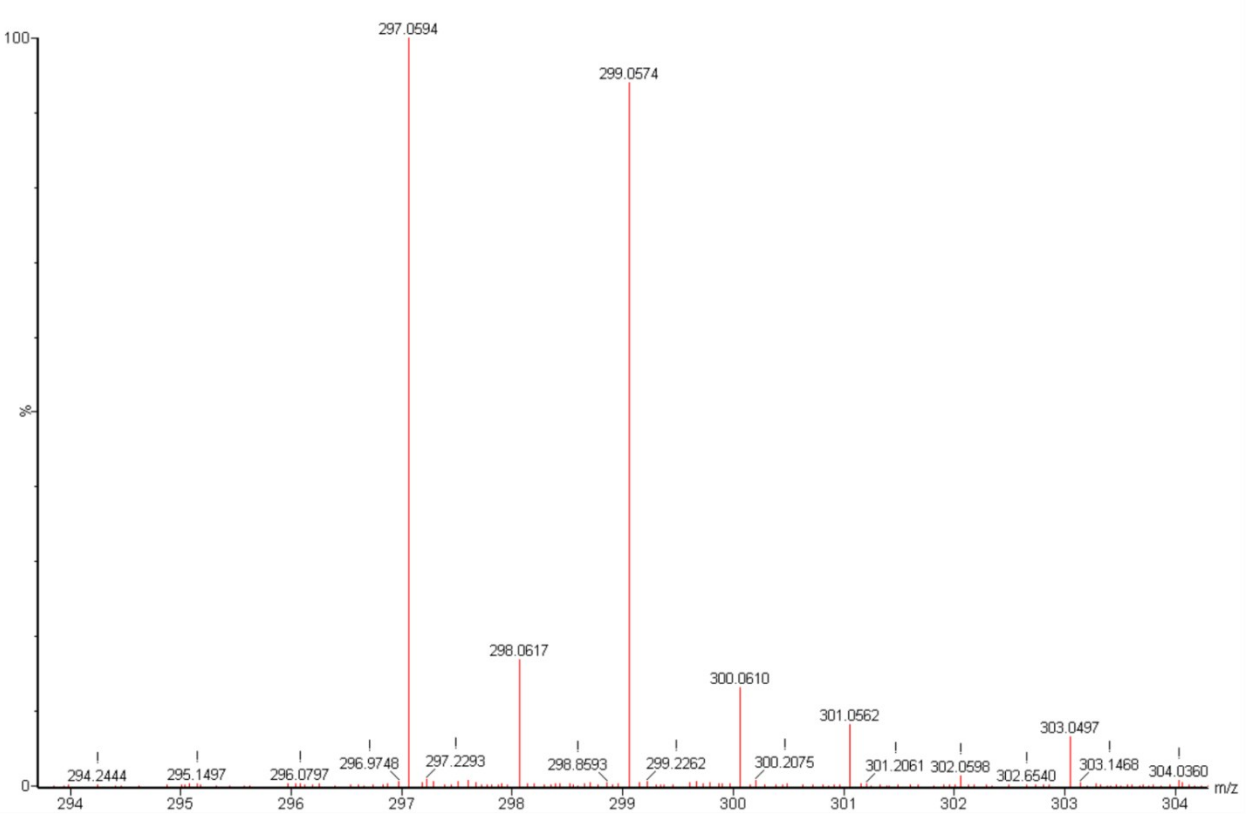
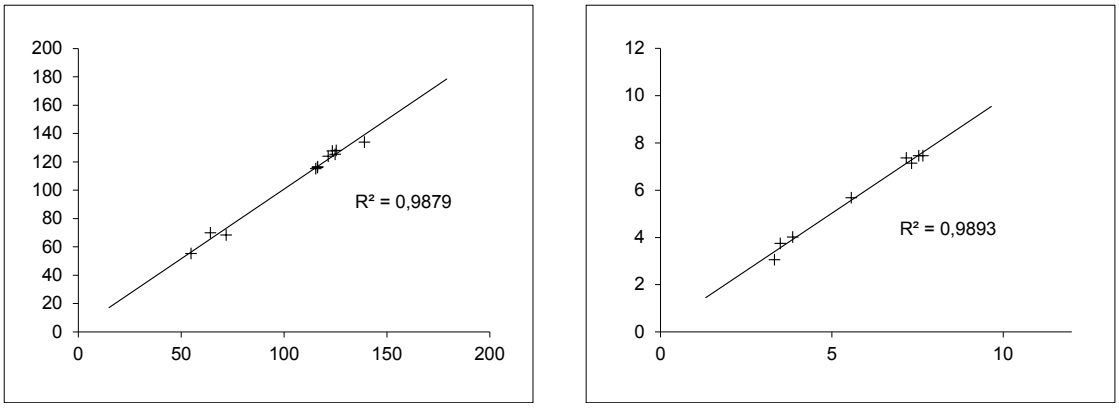


Table S1 Experimental parameters for acquired NMR spectra in methanol-d_4 and methanol-d_3 at 25 ºC

Experiment	Pulse sequence	Parameters
1D ^{1}H	Proton	sw: 16 ppm, complex points: 24k, nt: 64, d1: 10s
	wet1D	sw: 16 ppm, complex points: 24k, nt: 64, d1: 1.5s, wet suppression @ 22ms pulse width (wet)
	dpfgsewater	sw: 20 ppm, complex points: 36k, nt: 64, d1: 1s, water flipback
^{1}H,^{1}H-DQFCOSY	gDQCOSY	sw: 16 ppm, complex points: 4000x200, nt: 8, d1: 1s, wet, homospoils, gradient selected
^{1}H,^{1}H-ROESY	ROESYAD	sw: 14 ppm, complex points: 2000x128, nt: 8, d1: 1s, mix: 300ms @ 8188 Hz, wet, homospoils, adiabatic
^{1}H,^{13}C-HSQC	gc2hsqcse	sw: 16x220 ppm, complex points: 2000x200, nt: 32, $^1J_{CH}$: 146 Hz, ME, BIP, wet, homospoils, gradient selected
^{1}H,^{13}C-HMBC	gc2hmbc	sw: 16x240 ppm, complex points: 1440x256, nt: 32, $^nJ_{CH}$: 8 and 3 Hz, dual $^1J_{CH}$ suppression: 165 and 130 Hz, BIP, wet, homospoils, gradient selected

Figure S5. Correlation plots between neural network based predicted chemical shifts and experimental chemical shifts for ^{13}C, mean error: 2.3 ppm, and ^{1}H, mean error: 0.18 ppm.



^{13}C ^{1}H

Figure S6. ^{1}H-NMR spectrum of **4** in methanol-d_4.

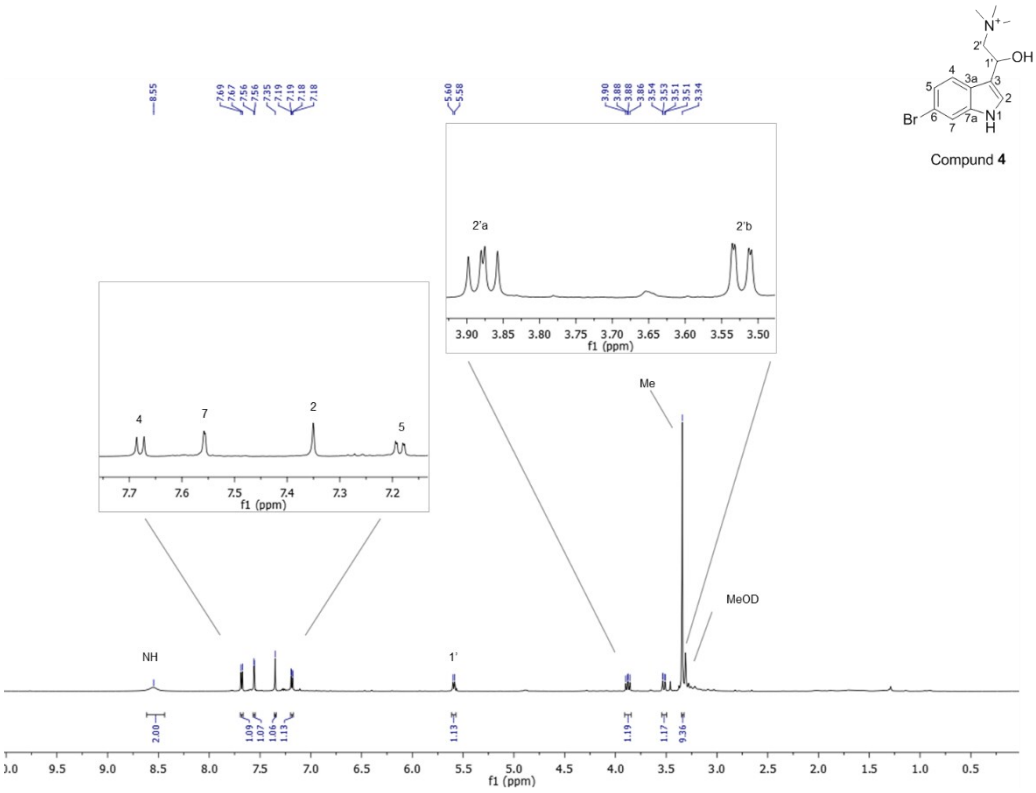


Figure S7. ^{13}C-NMR spectrum of **4** in methanol-d_4.

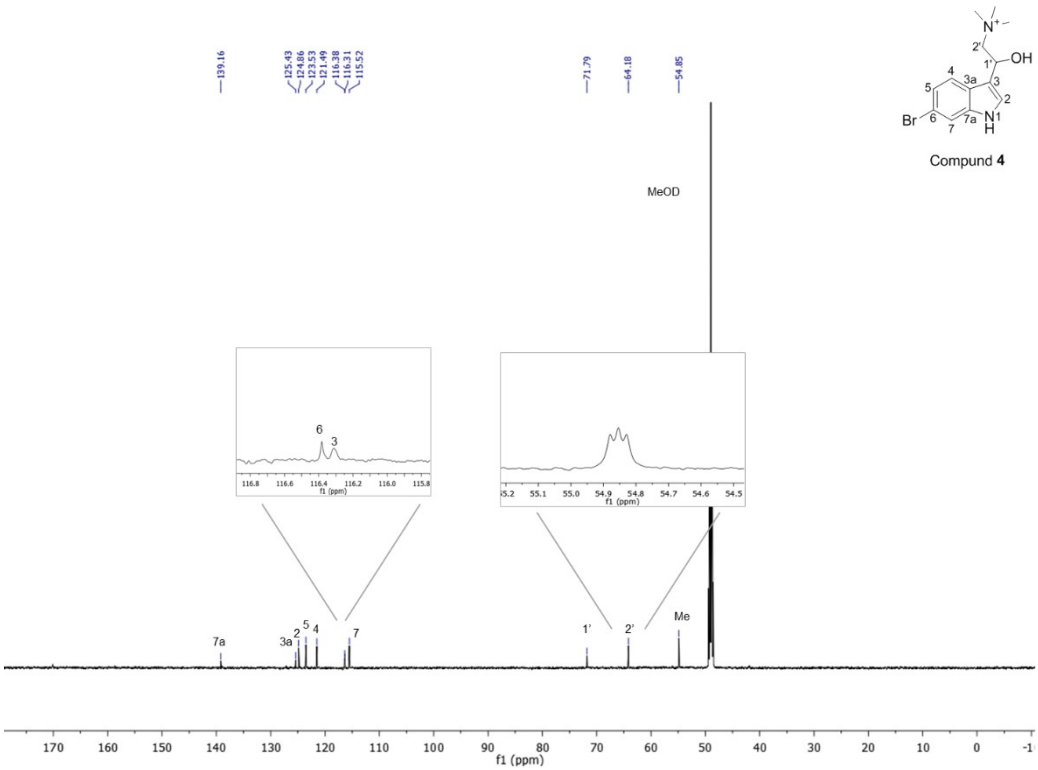


Figure S8. ^{1}H-^{1}H COSY spectrum of **4** in methanol-d_4.

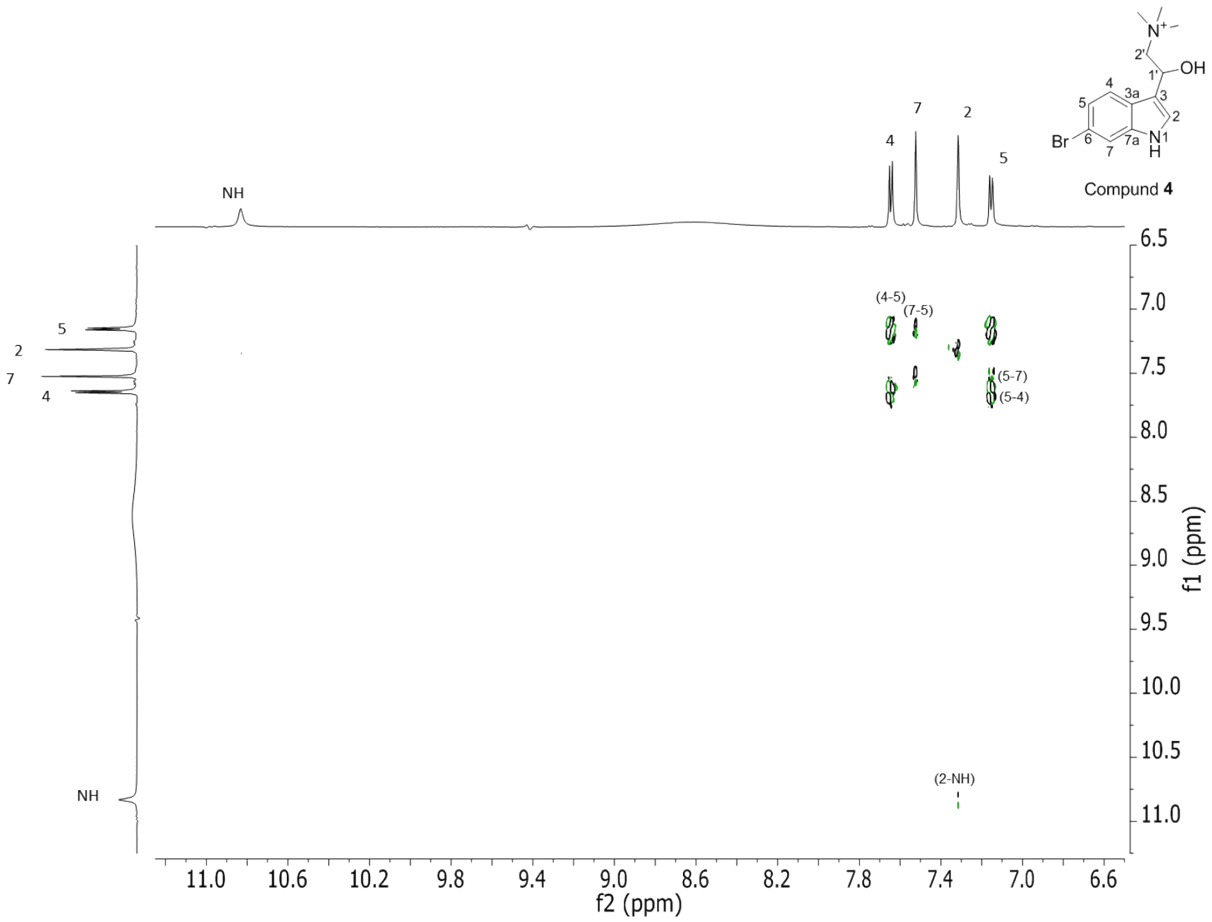


Figure S9. ^{1}H-^{1}H COSY spectrum of **4** in methanol-d_4.

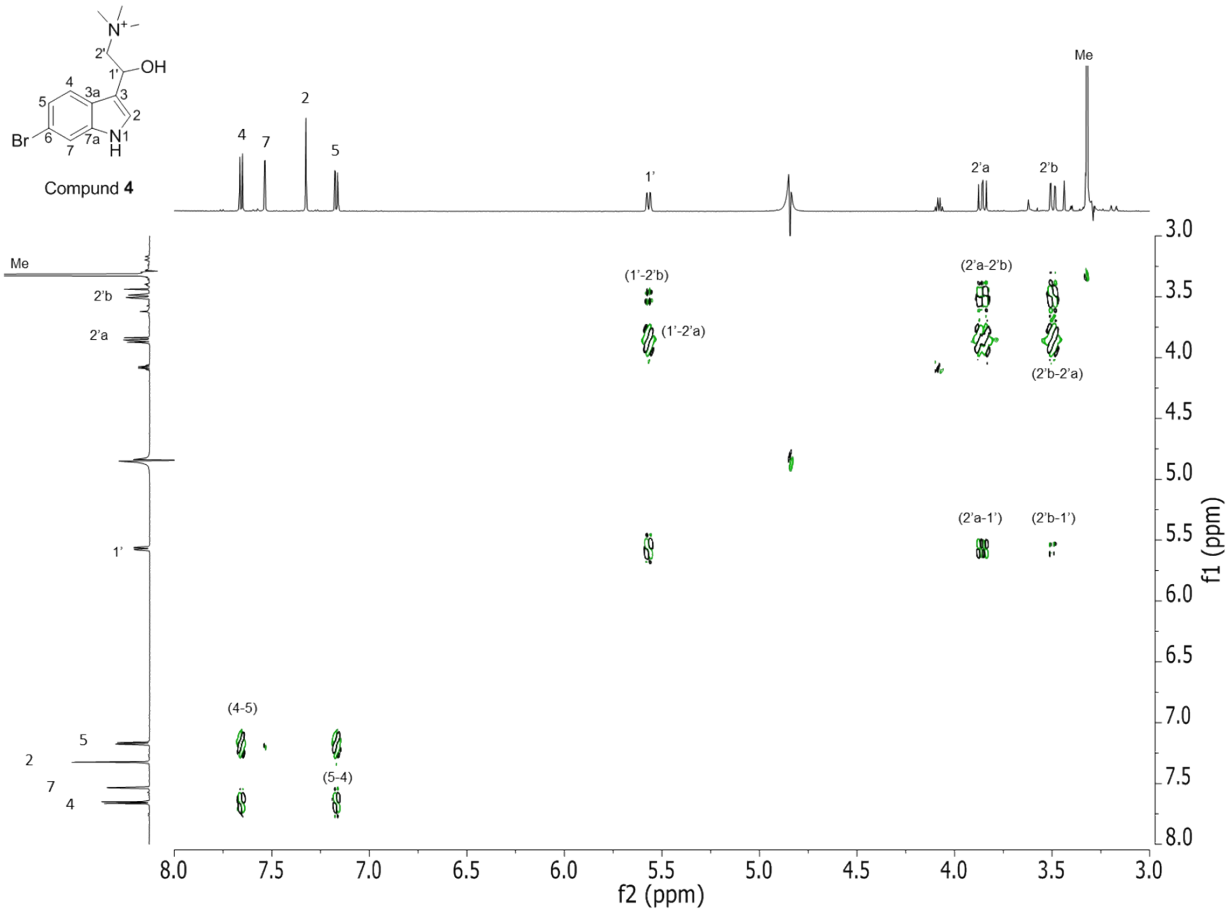


Figure S10. ROSEY spectrum of **4** in methanol-d_4.

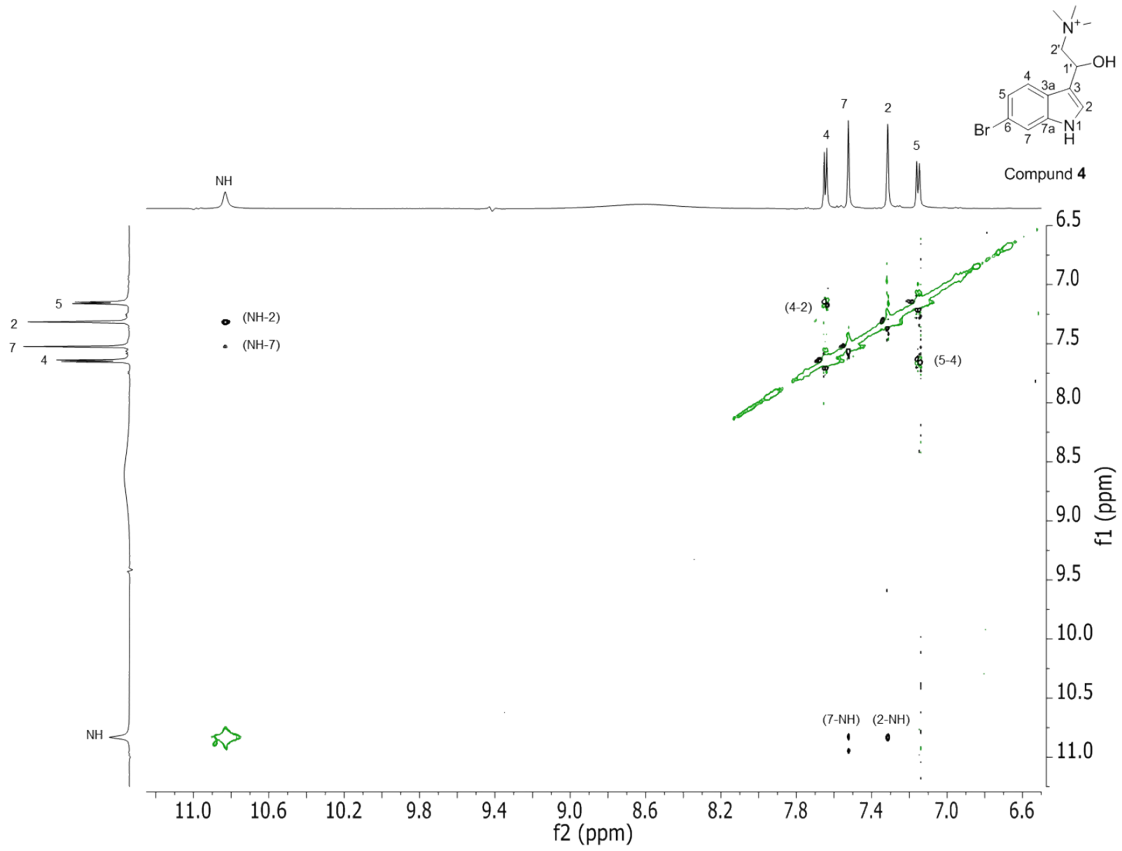


Figure S11. ROSEY spectrum of **4** in methanol-d_4.

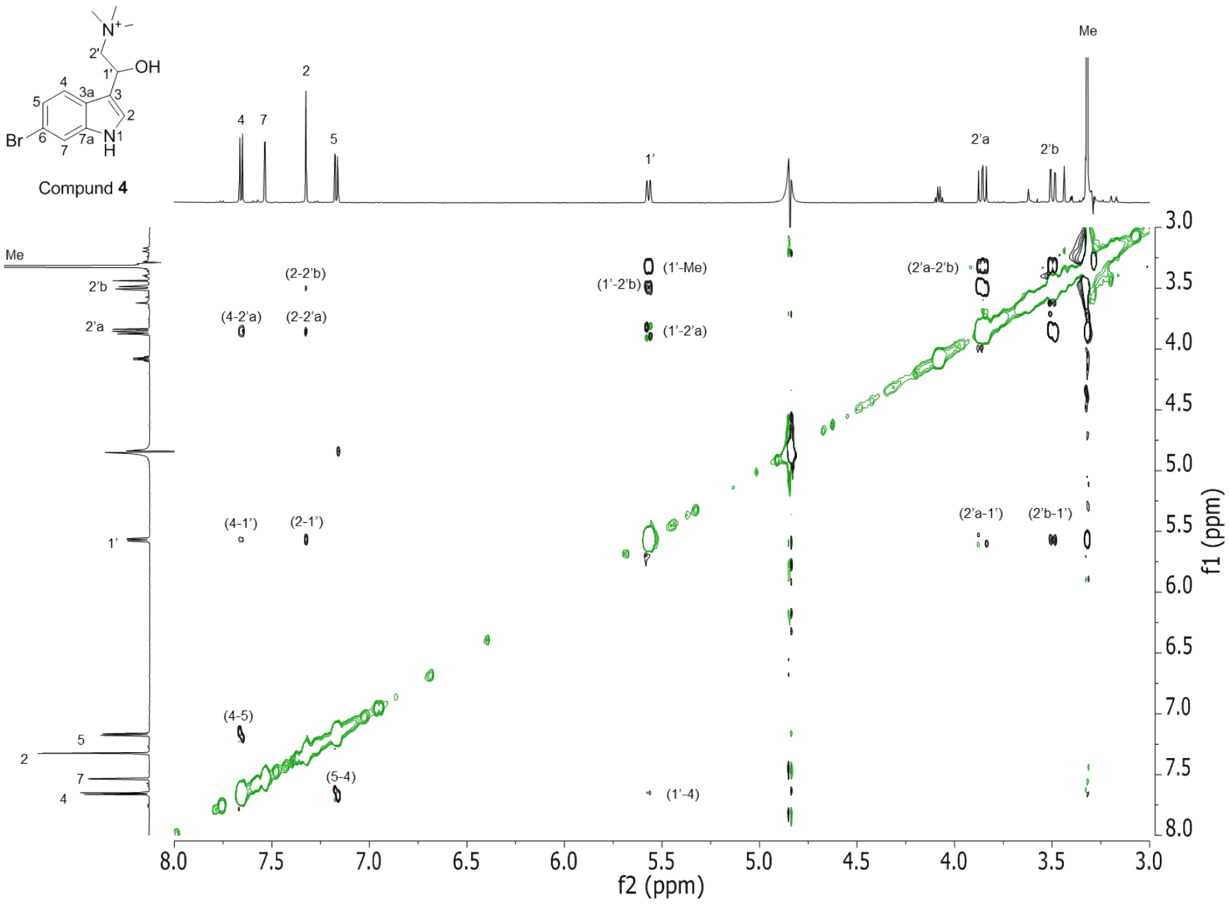


Figure S12. gHSQC spectrum of **4** in methanol-d_4.

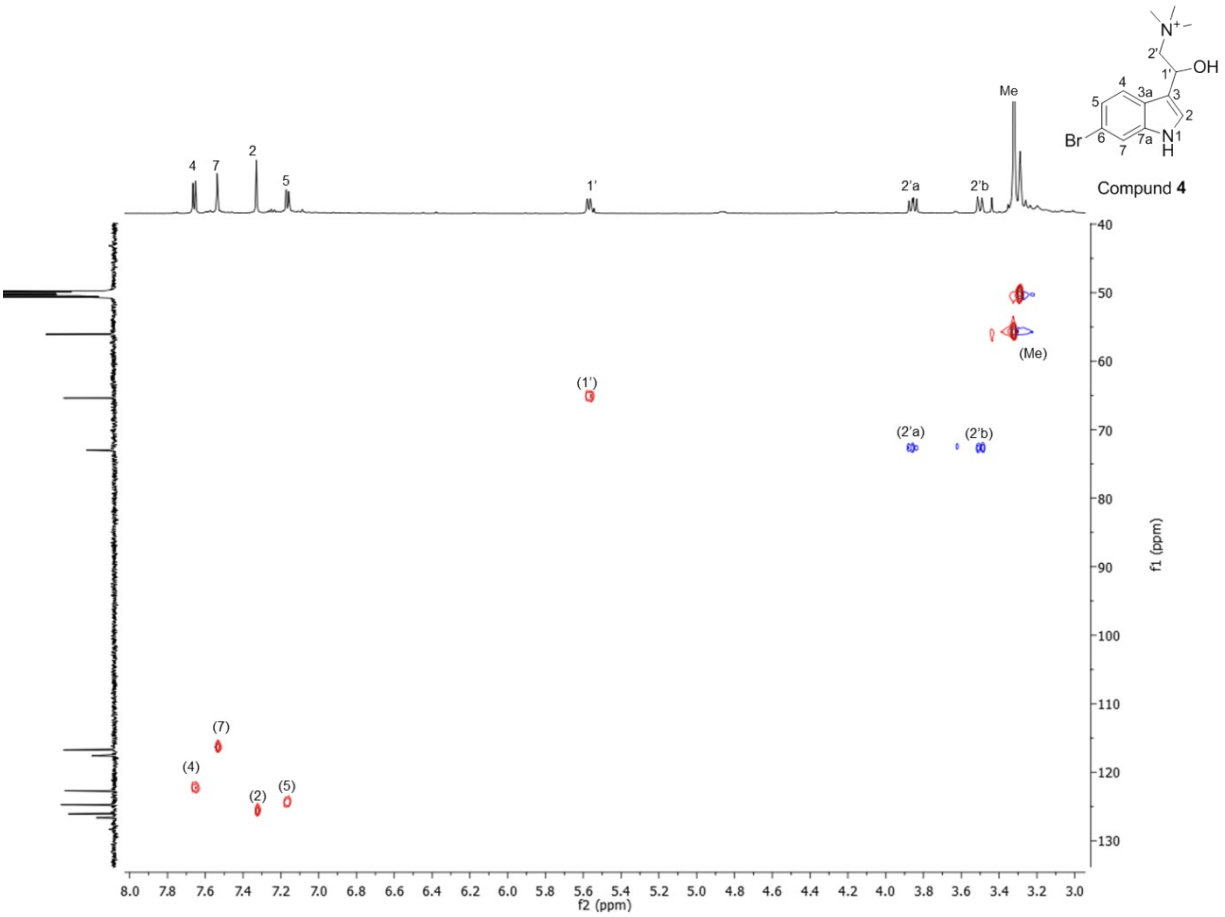


Figure S13. gHMBC spectrum of **4** in methanol-d_4.

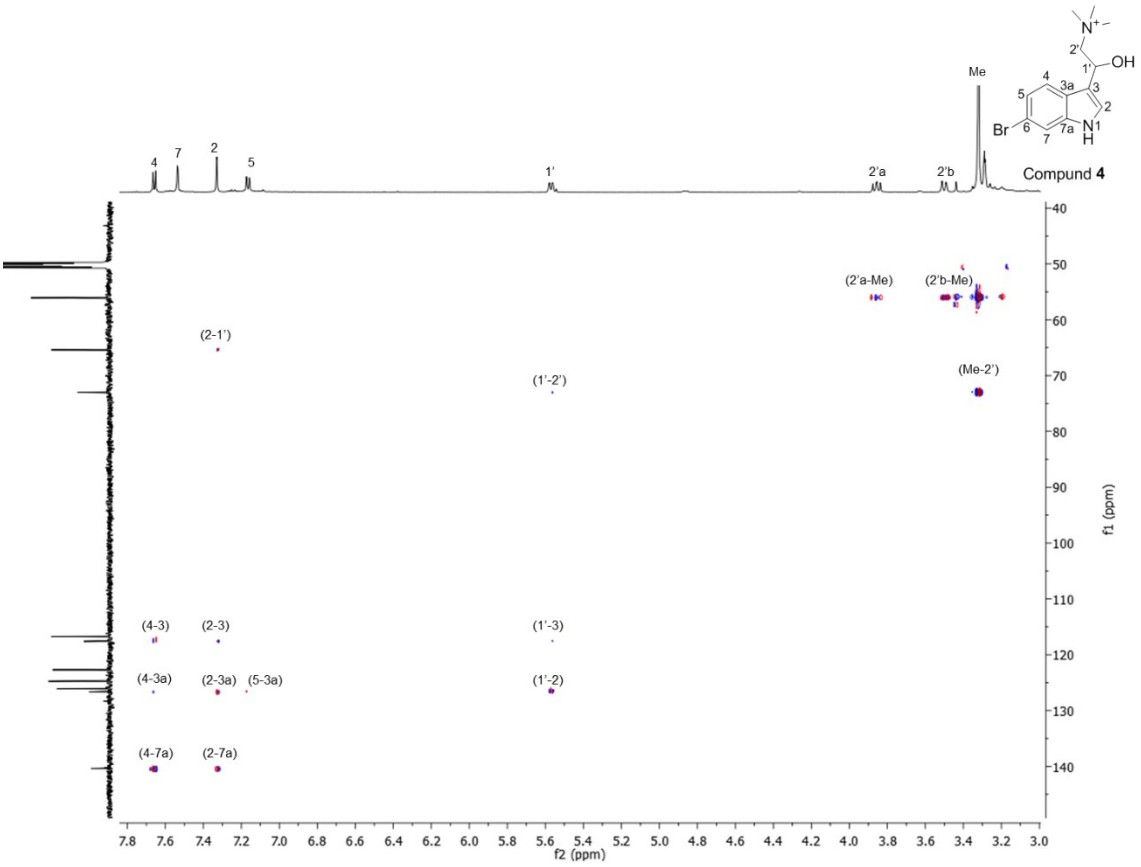


Figure S14. ^{1}H-NMR spectrum of **6a** in methanol-d_4.

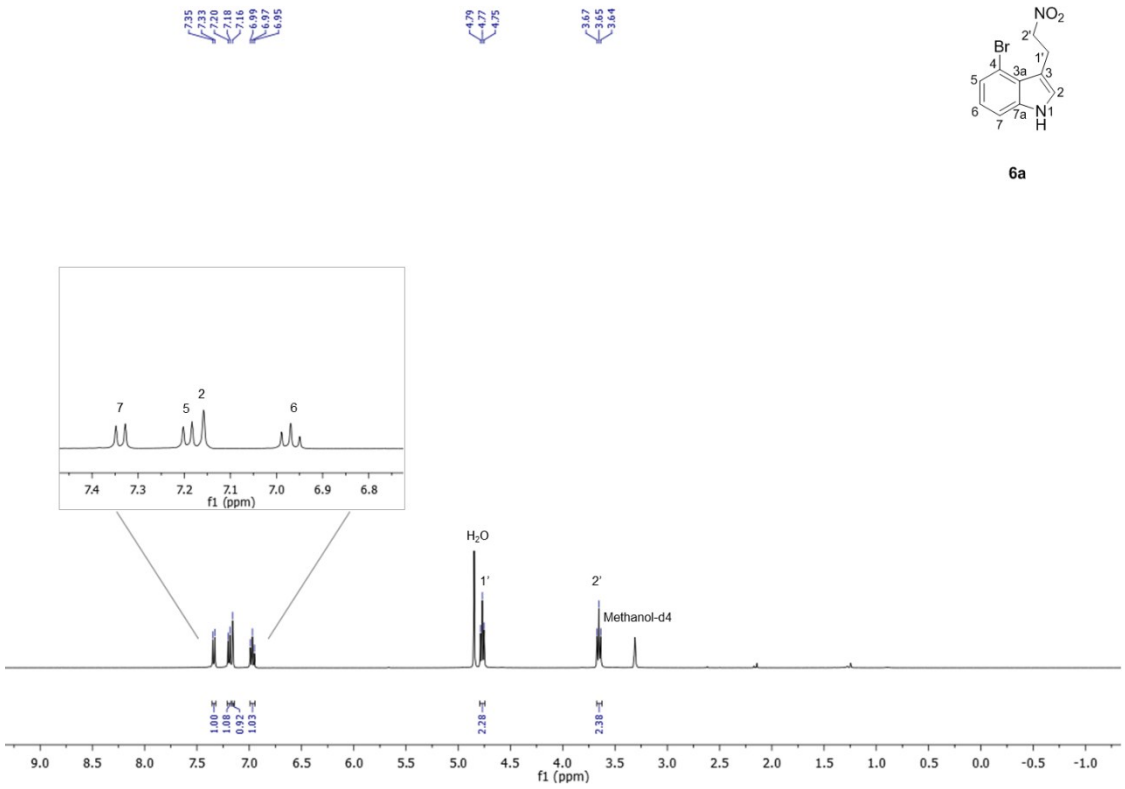


Figure S15. ^{13}C-NMR spectrum of **6a** in acetone-d_6.

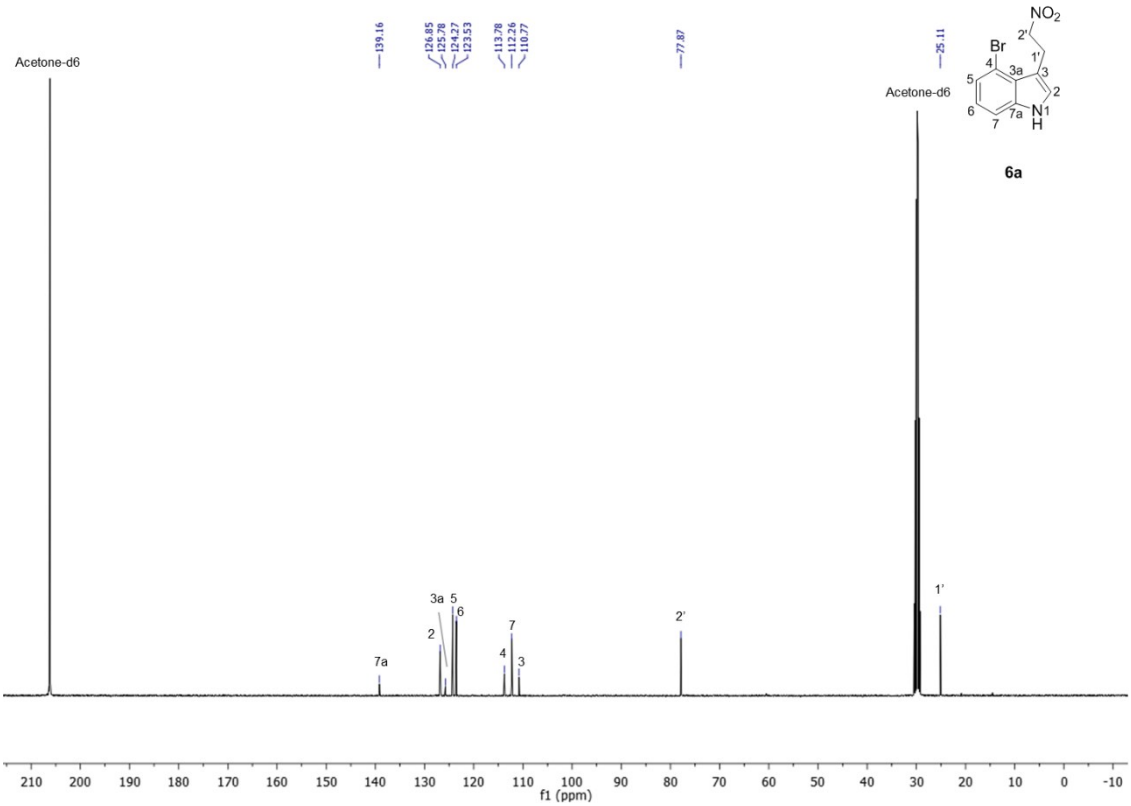


Figure S16. ^{1}H-NMR spectrum of **6d** in methanol-d_4.

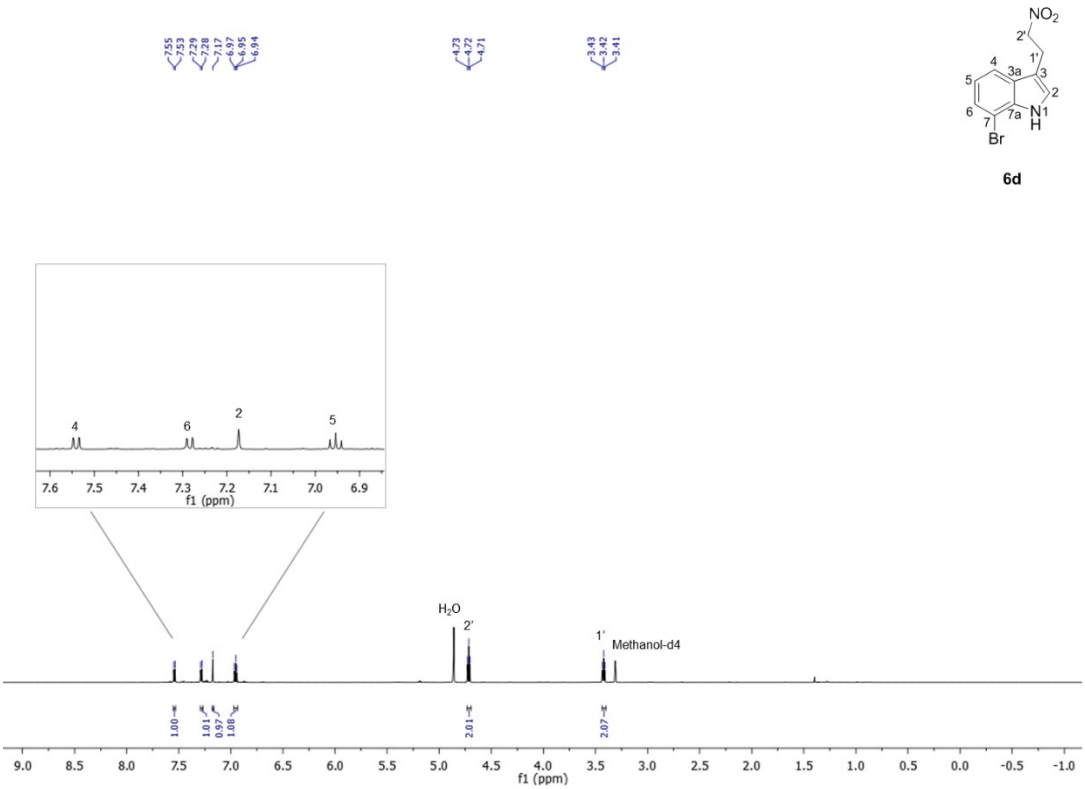


Figure S17. ^{13}C-NMR spectrum of **6d** in methanol-d_4.

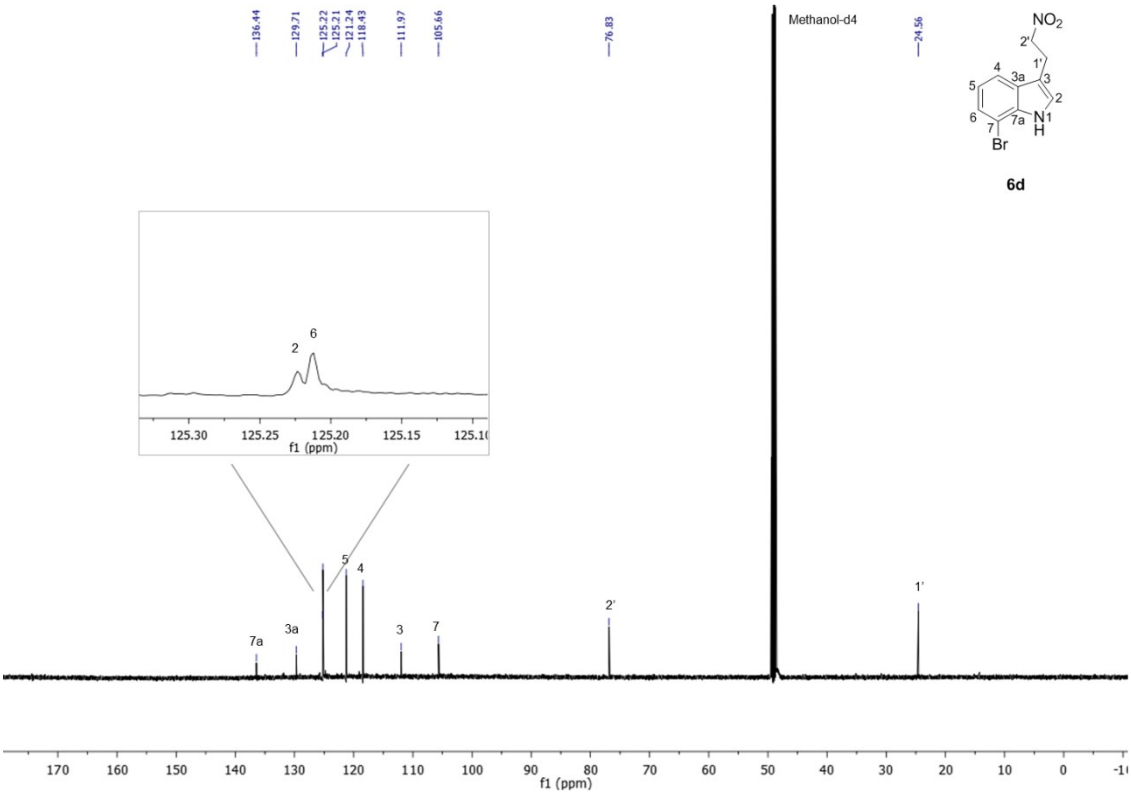


Figure S18. ^{1}H-NMR spectrum of **8c** in methanol-d_4.

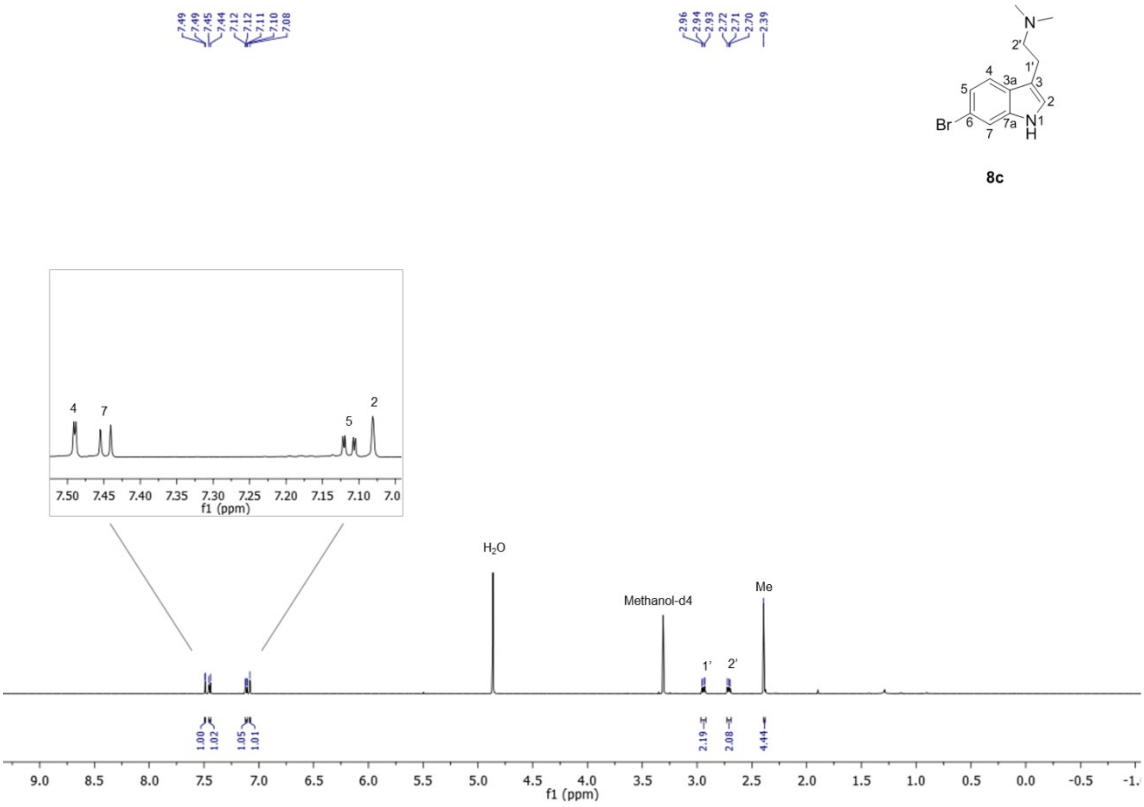


Figure S19. ^{13}C-NMR spectrum of **8c** in methanol-d_4.

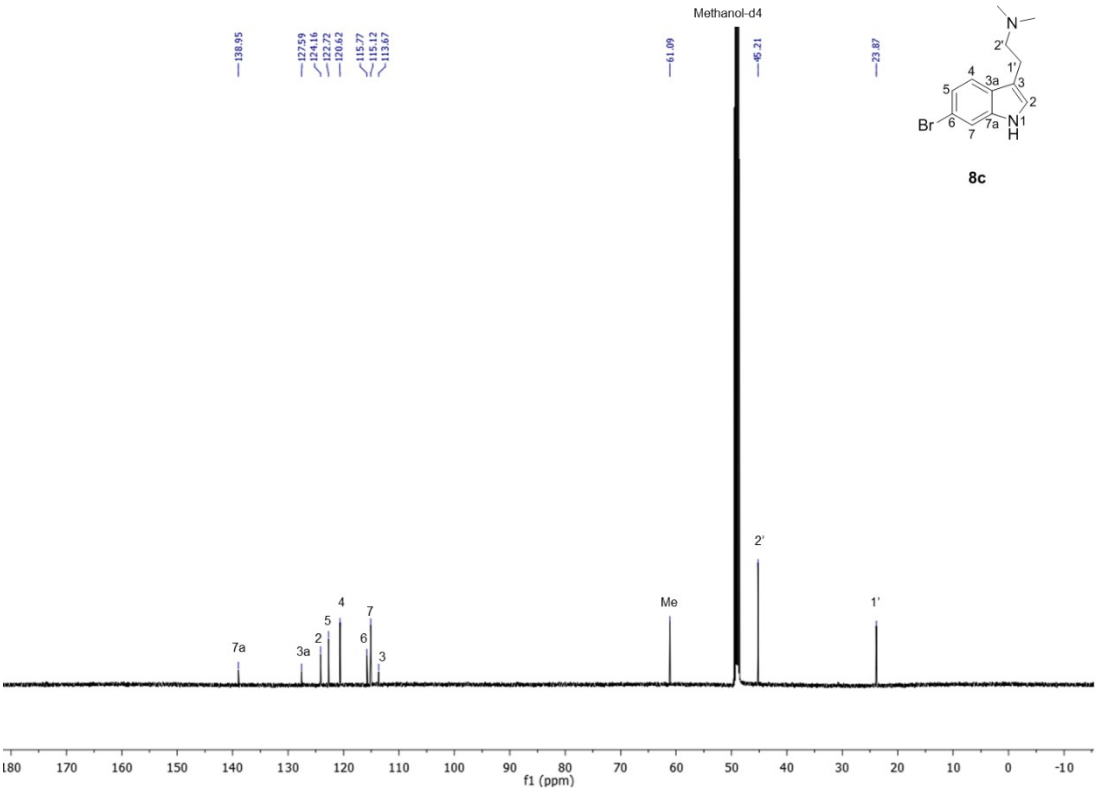


Figure S20. ^{1}H-NMR spectrum of **9a** in methanol-d_4.

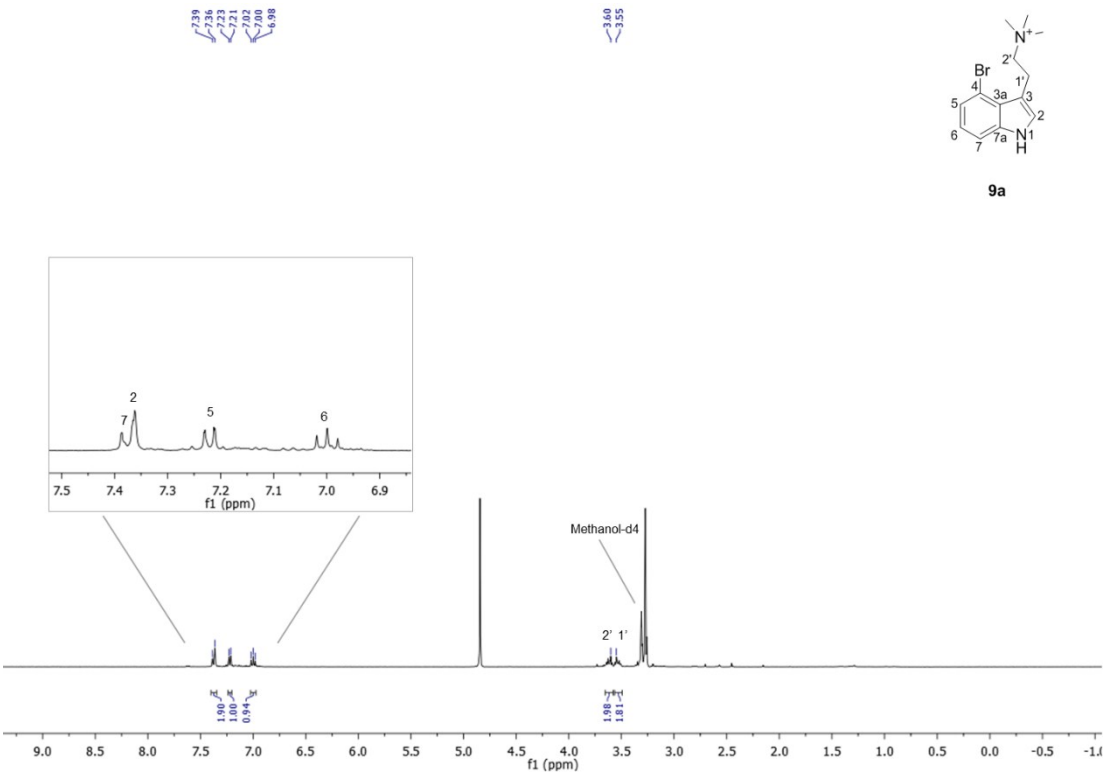


Figure S21. ^{13}C-NMR spectrum of **9a** in methanol-d_4.

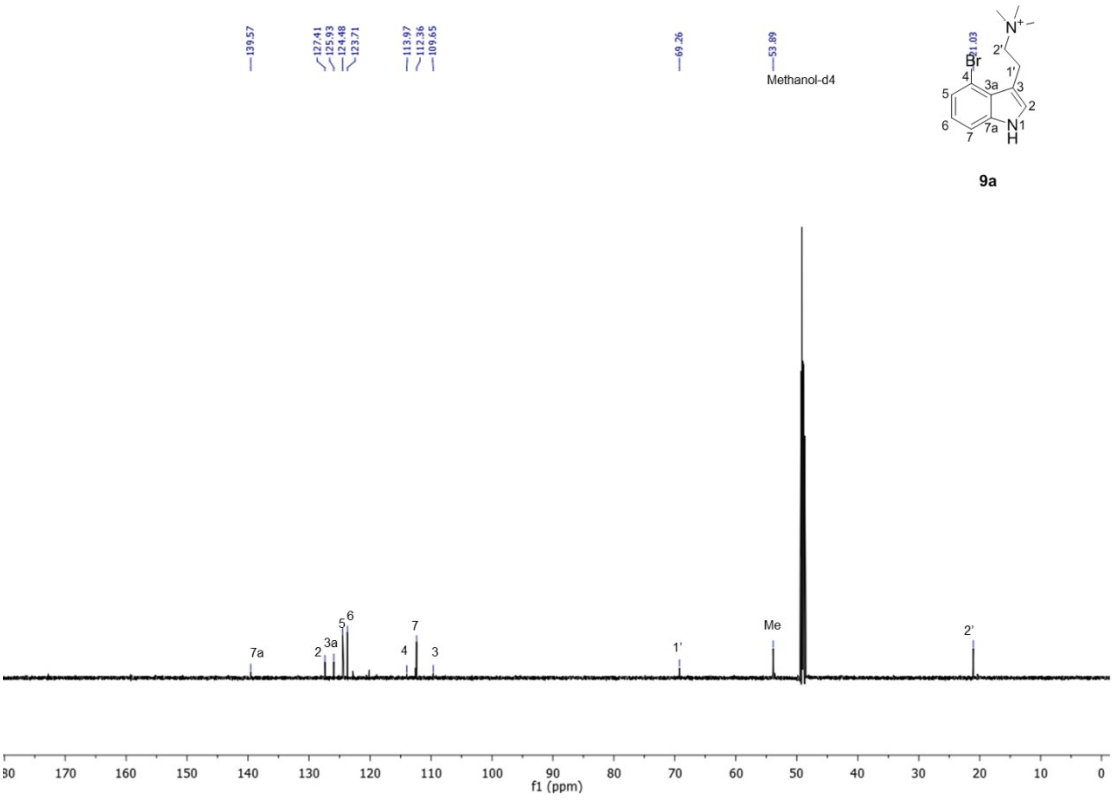


Figure S22. ^{1}H-NMR spectrum of **9b** in methanol-d_4. The 1’ and Me-peak overlaps.

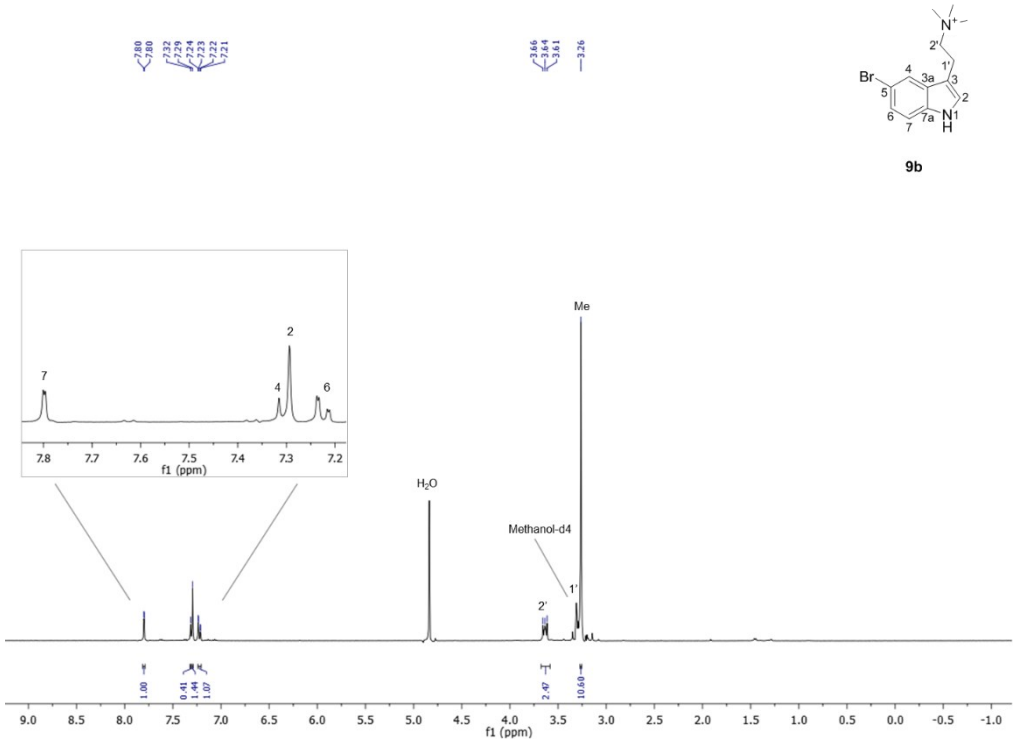


Figure S23. ^{13}C-NMR spectrum of **9b** in methanol-d_4.

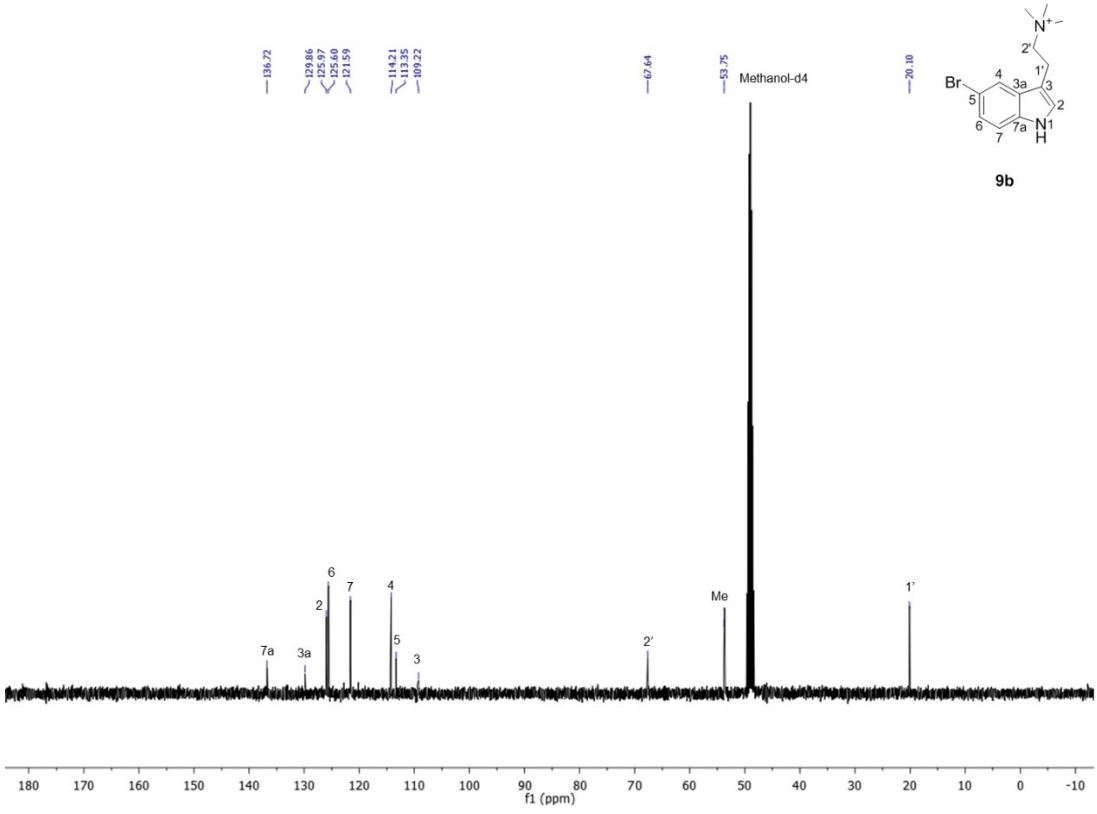


Figure S24. ^{1}H-NMR spectrum of **9c** in acetone-d_6.

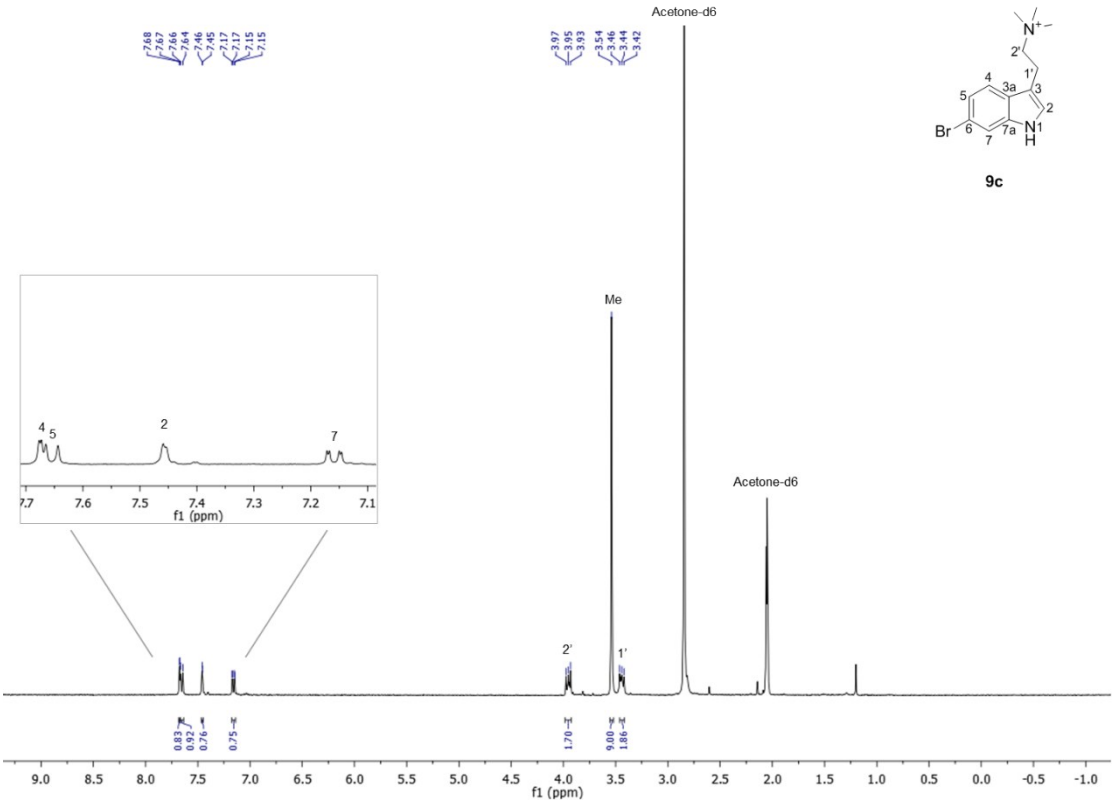


Figure S25. ^{13}C-NMR spectrum of **9c** in methanol-d_4.

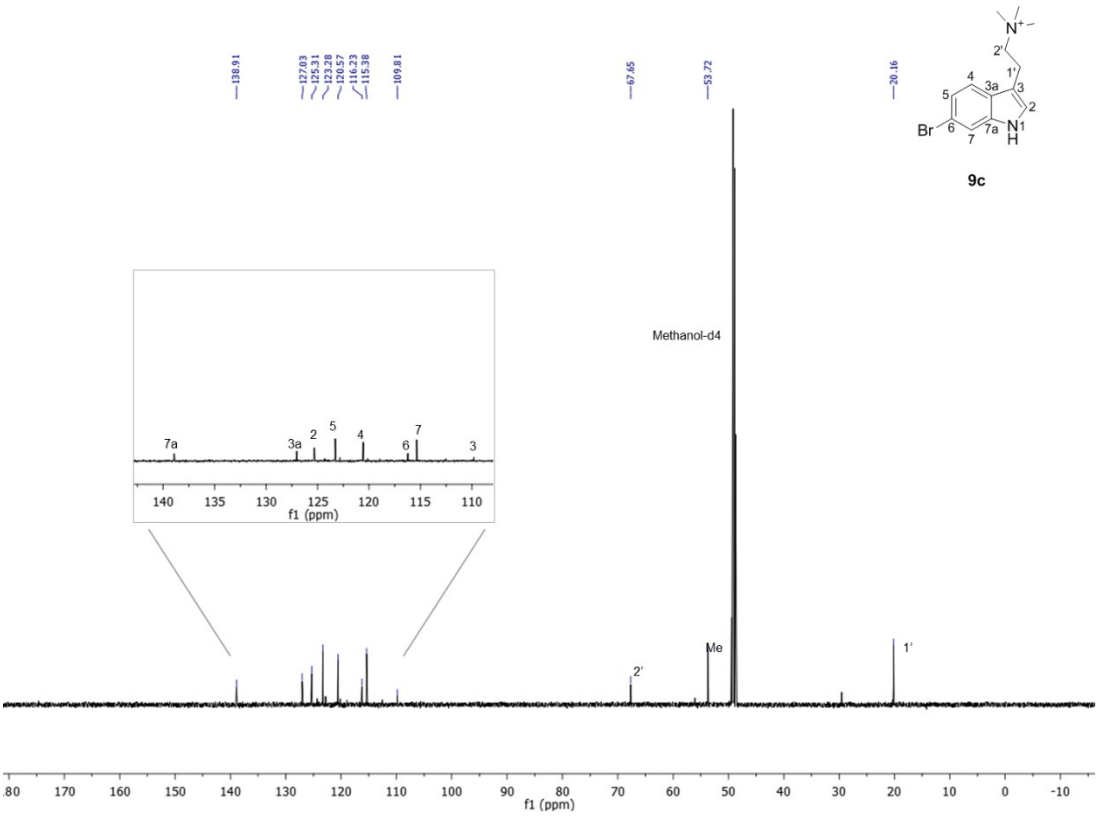


Figure S26. ^{1}H-NMR spectrum of **9d** in methanol-d_4. The singlet of 2 appears in the middle of the 6 doublet. The peaks of 1’ and 2’ are overlapping.

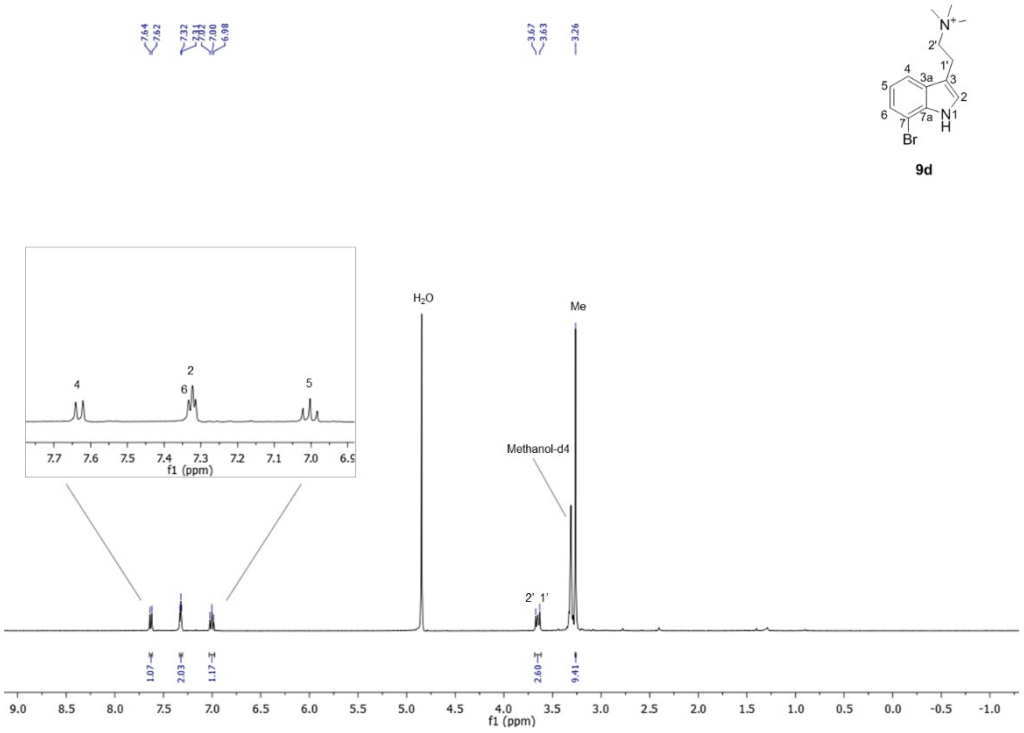


Figure S27. ^{13}C-NMR spectrum of **9d** in methanol-d_4.