

Supplementary Materials

Synthesis of Novel Planar-Chiral Charge-Compensated *nido*-Carborane-Based Amino Acid

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Table of Content

NMR Spectra	S-2
HPLC Data	S-18
HRMS Data	S-19

NMR Spectra

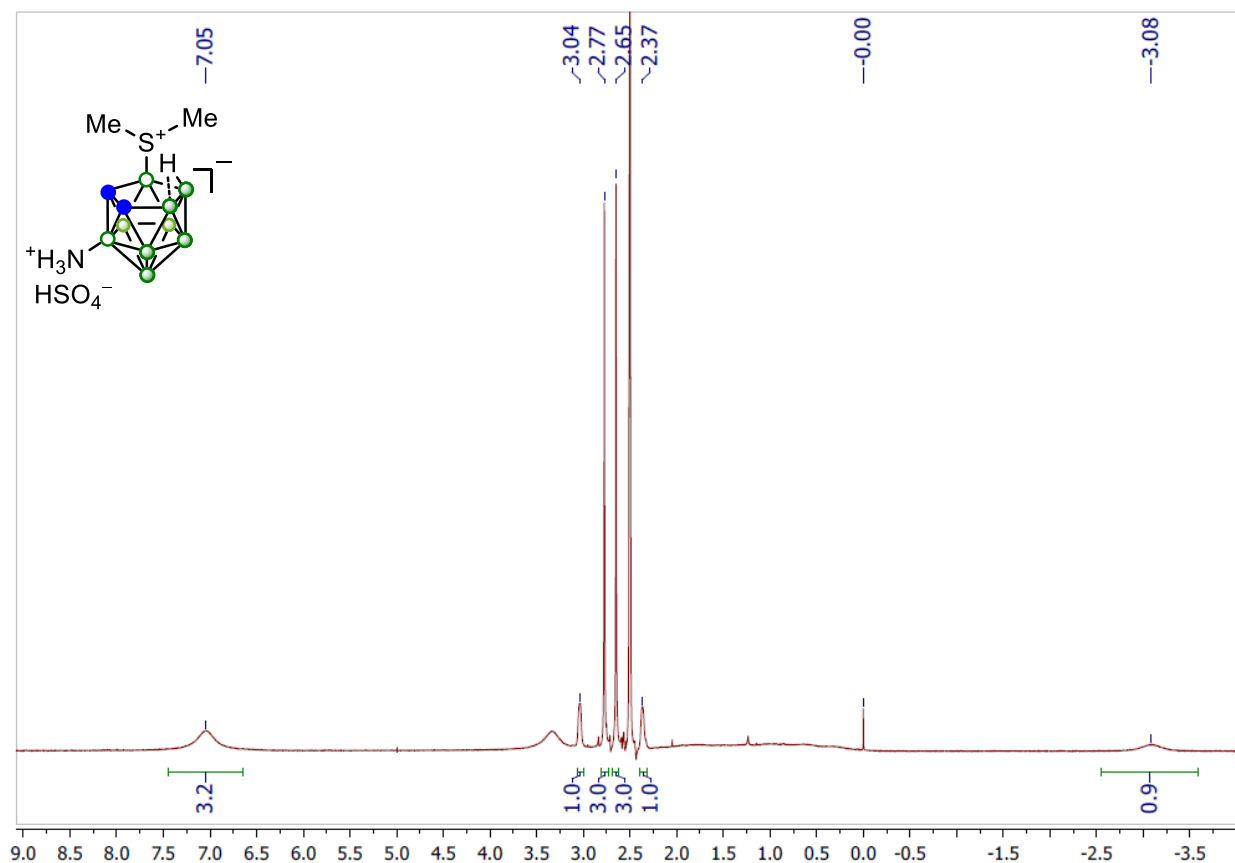


Figure S1. ¹H NMR spectrum of compound **2'** (DMSO-*d*₆, 400 MHz)

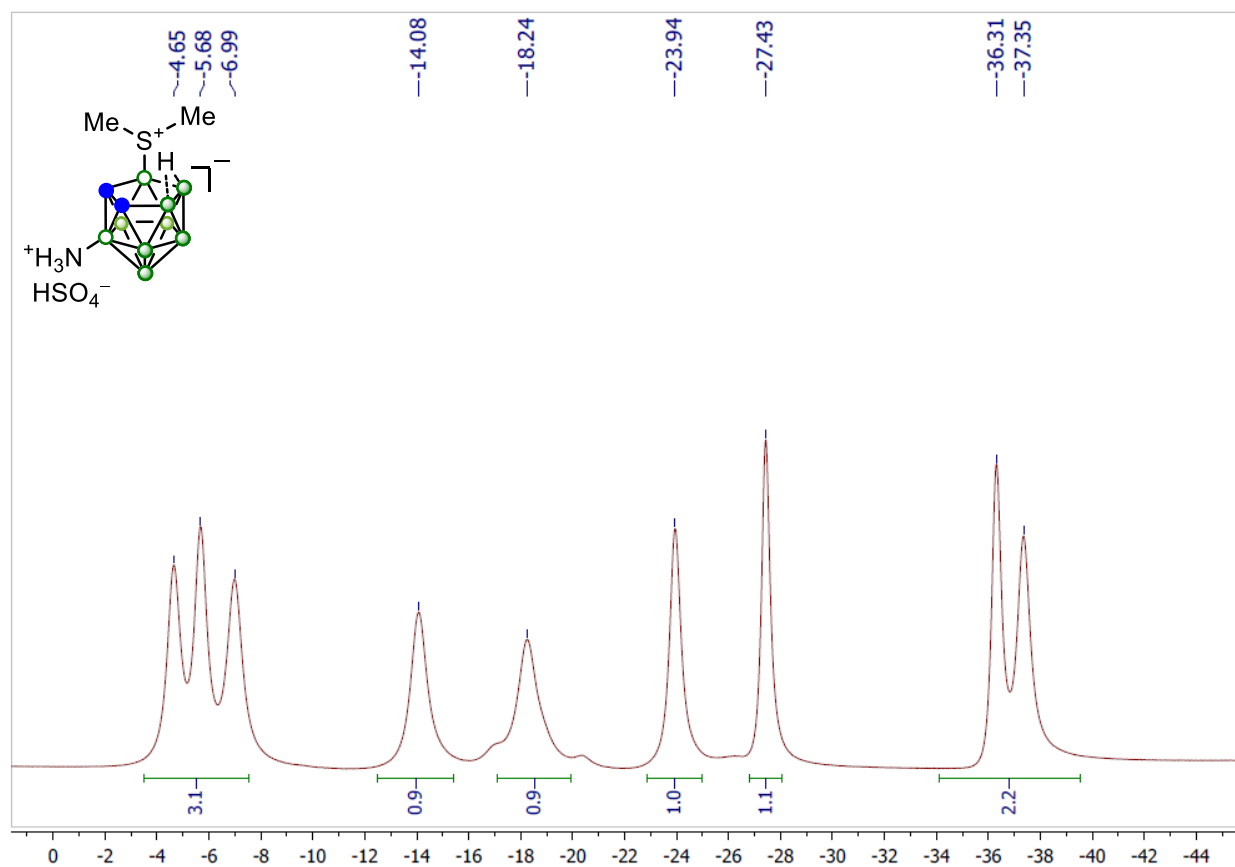


Figure S2. ¹¹B{¹H} NMR spectrum of compound **2'** (DMSO-*d*₆, 193 MHz)

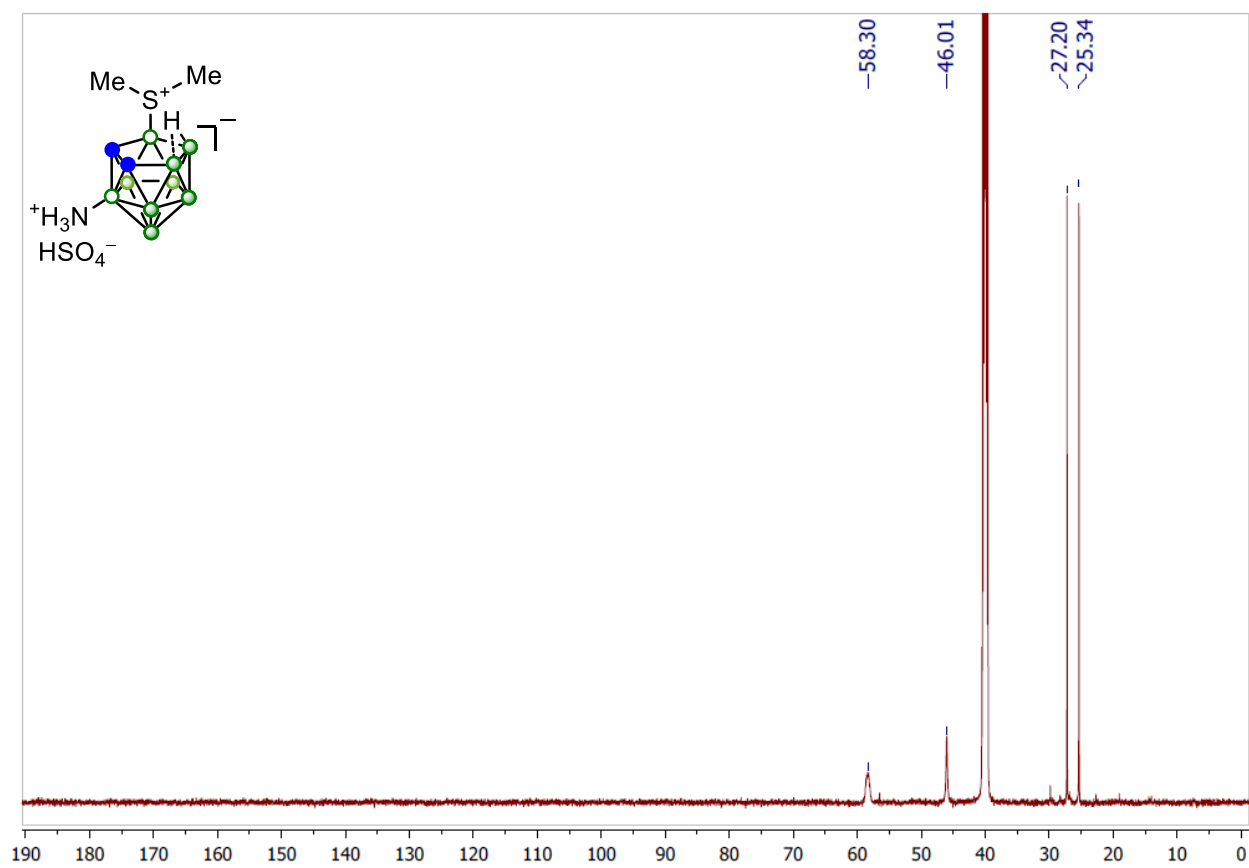


Figure S3. ^{13}C NMR spectrum of compound **2'** (DMSO- d_6 , 151 MHz)

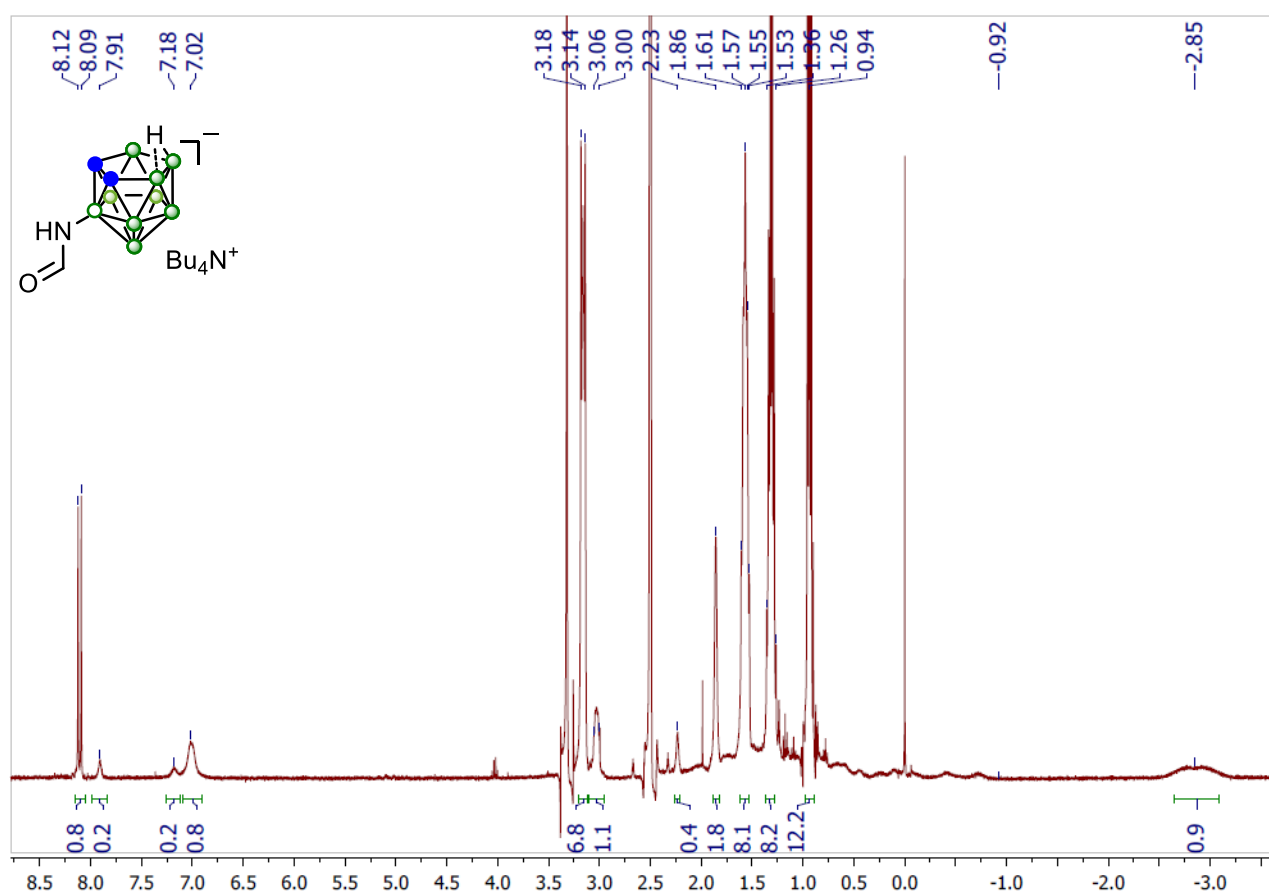


Figure S4. ^1H NMR spectrum of compound **5a** (DMSO- d_6 , 400 MHz)

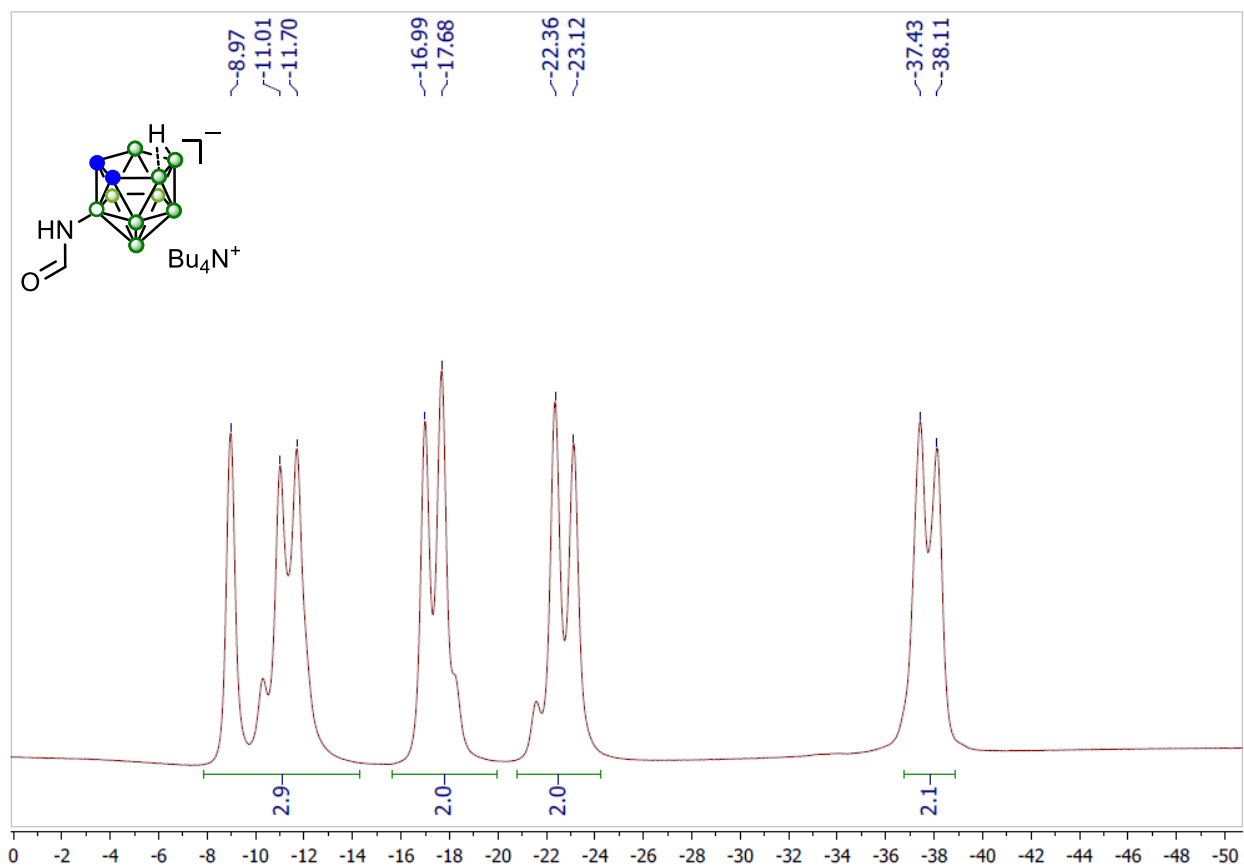


Figure S5. ^{11}B NMR spectrum of compound **5a** (DMSO- d_6 , 193 MHz)

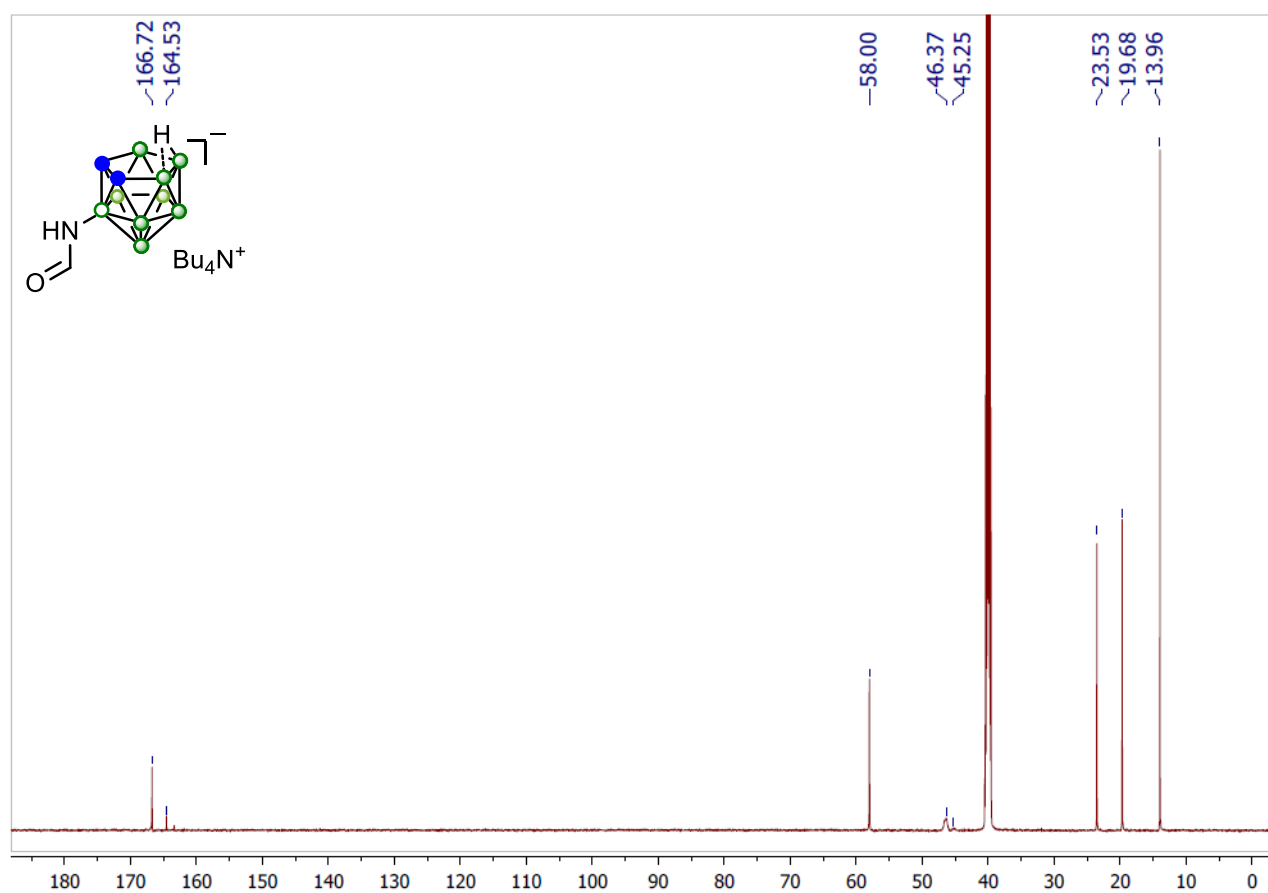


Figure S6. ^{13}C NMR spectrum of compound **5a** (DMSO- d_6 , 151 MHz)

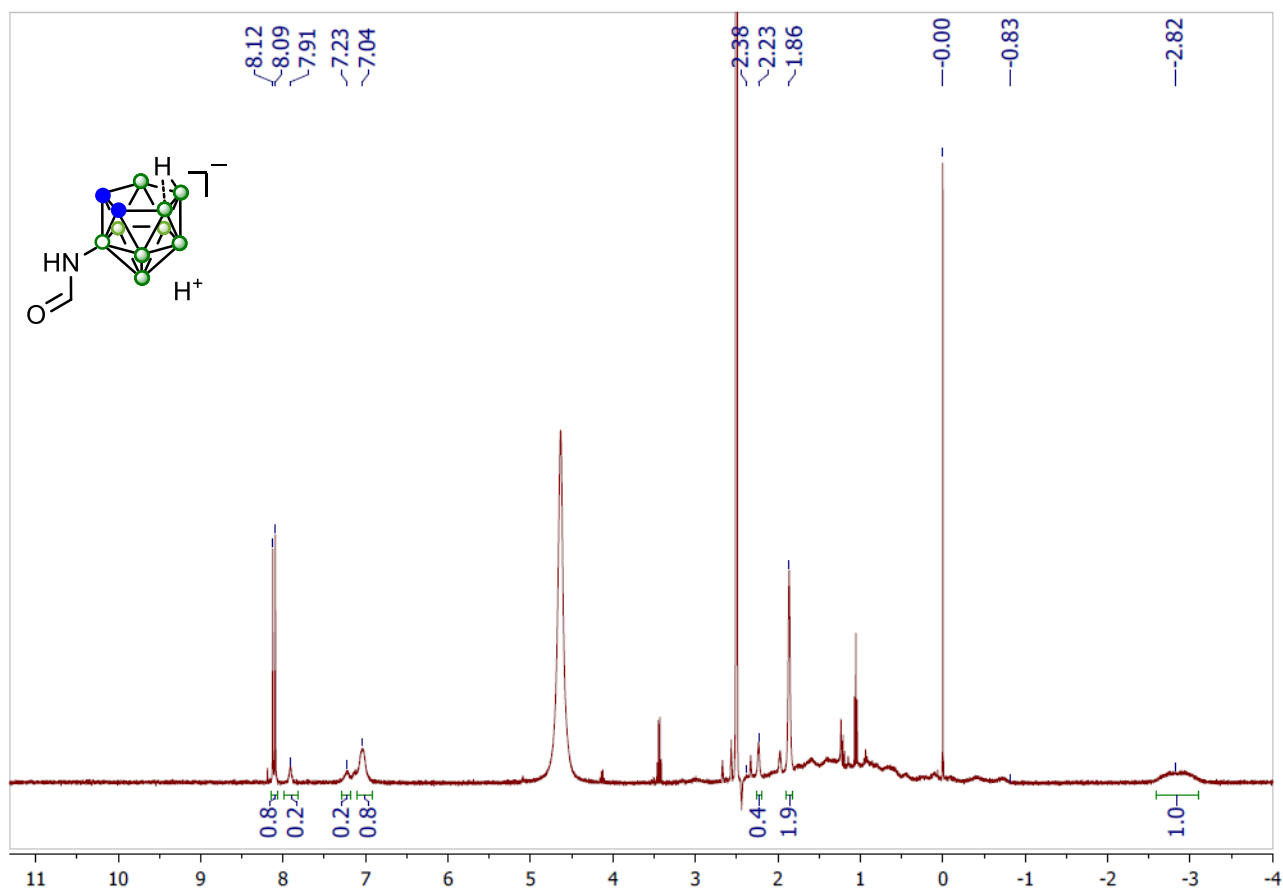


Figure S7. ^1H NMR spectrum of compound **5b** ($\text{DMSO-}d_6$, 400 MHz)

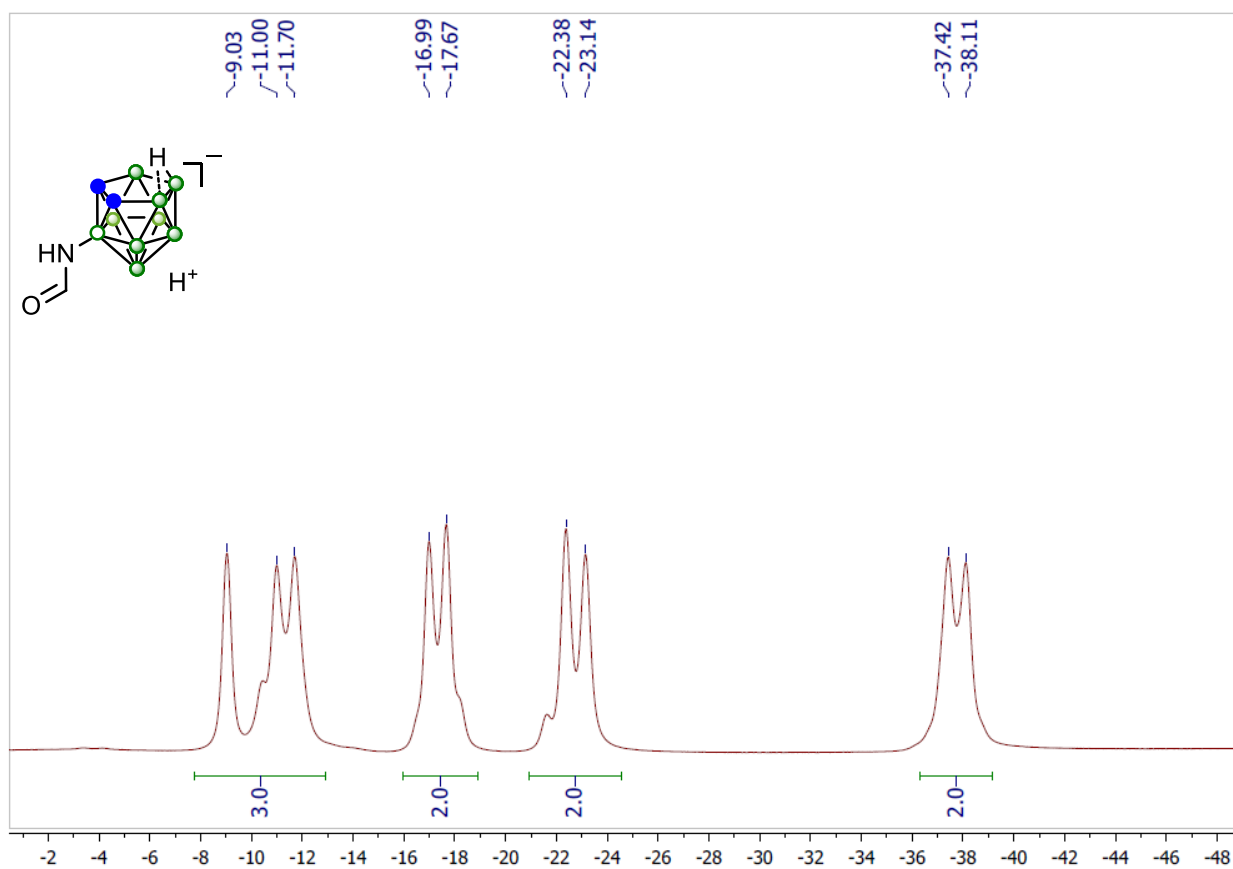


Figure S8. ^{11}B NMR spectrum of compound **5b** ($\text{DMSO-}d_6$, 193 MHz)

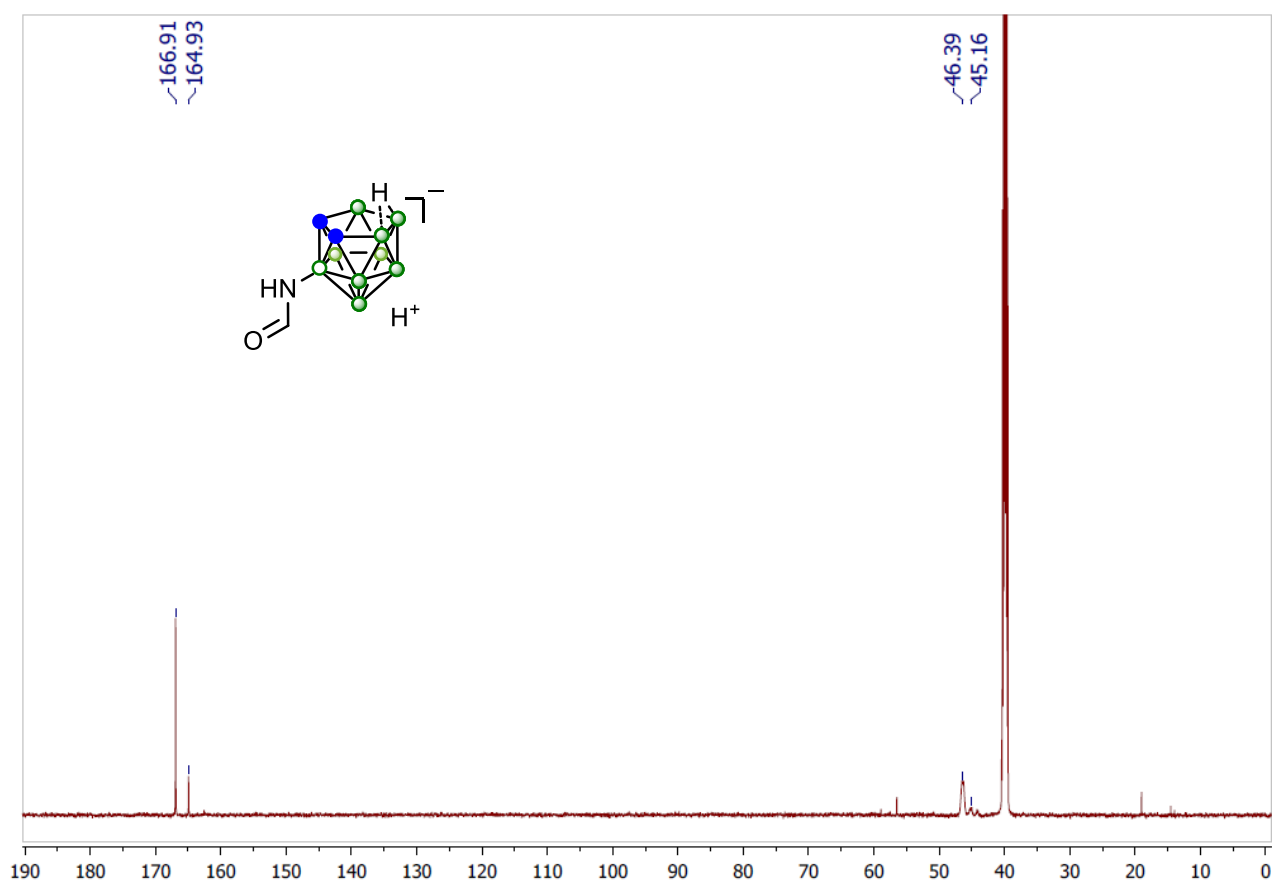


Figure S9. ¹³C NMR spectrum of compound **5b** (DMSO-*d*₆, 151 MHz)

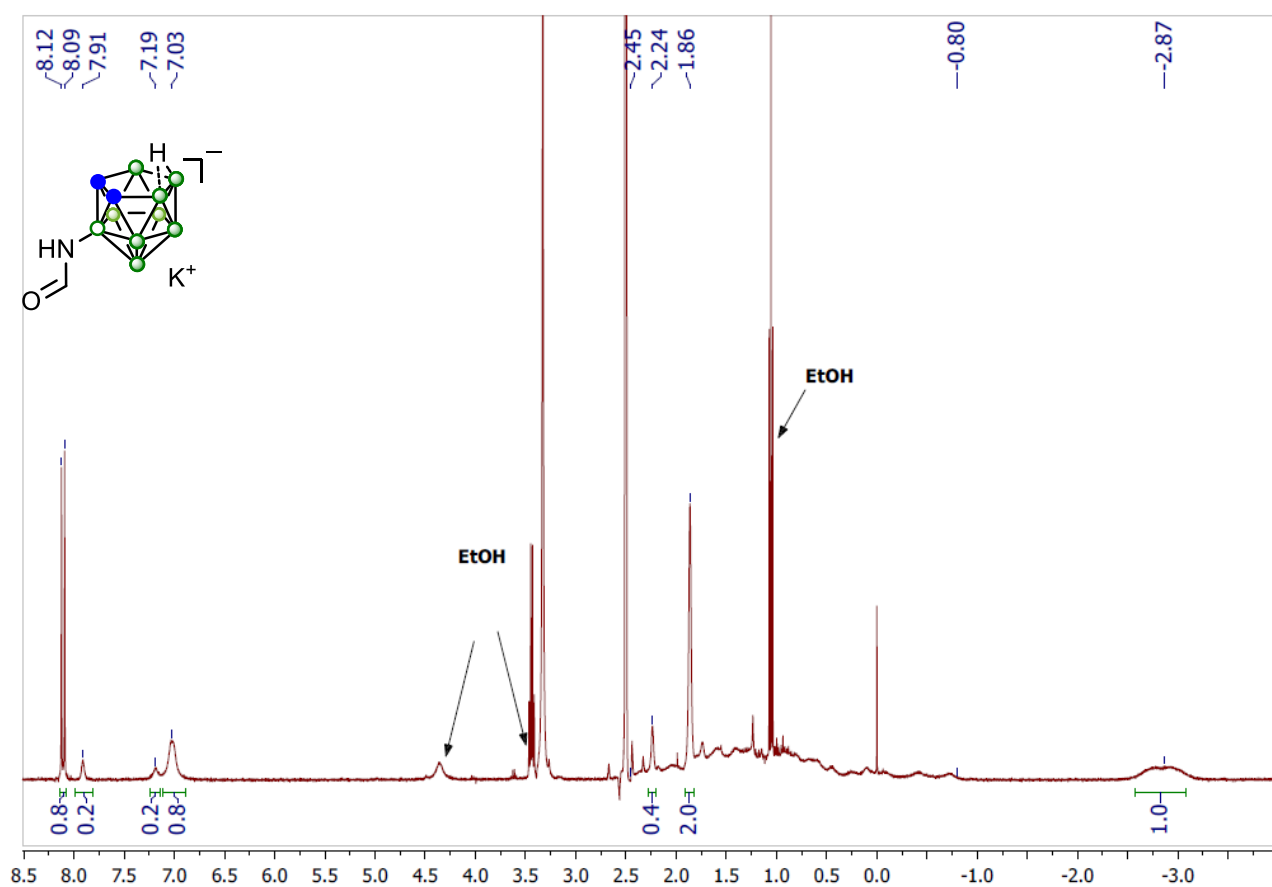


Figure S10. ¹H NMR spectrum of compound **5c** (DMSO-*d*₆, 400 MHz)

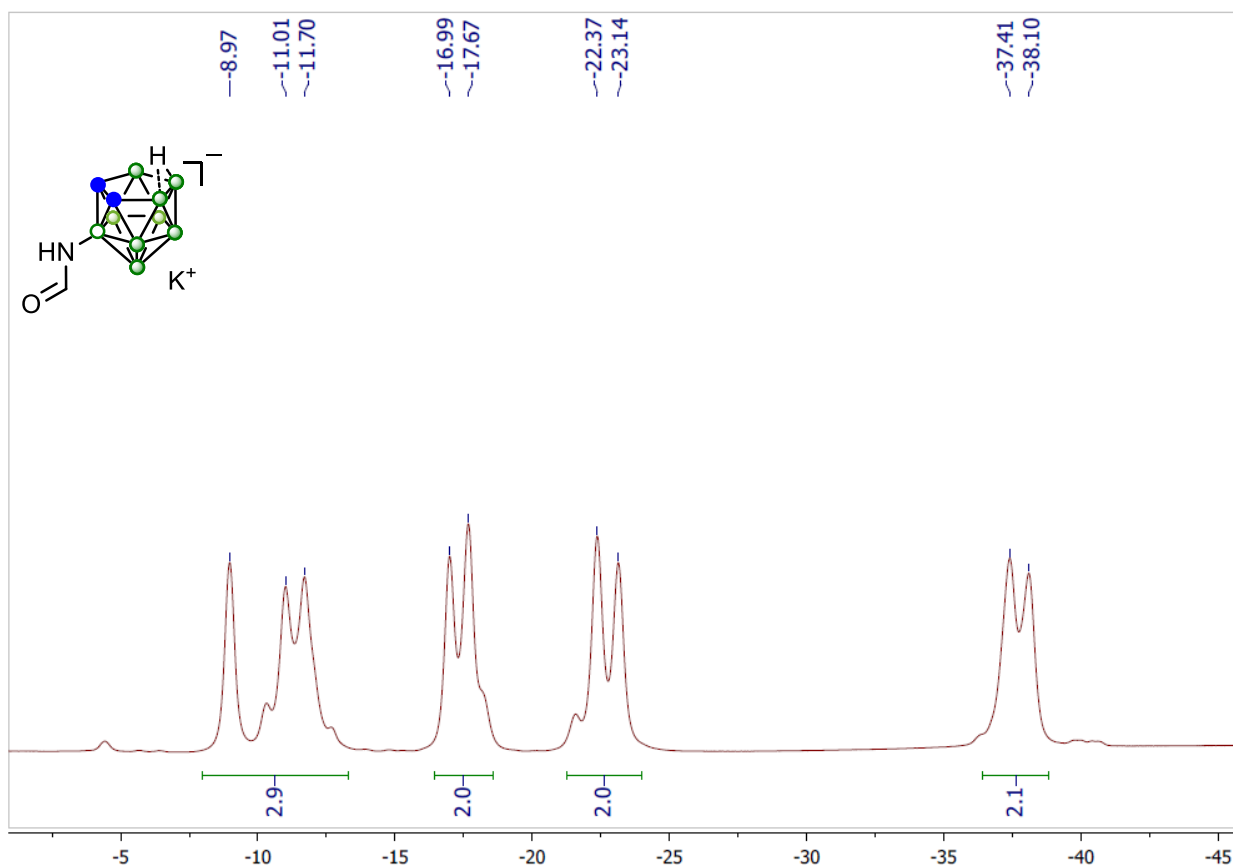


Figure S11. ¹¹B NMR spectrum of compound **5c** (DMSO-*d*₆, 193 MHz)

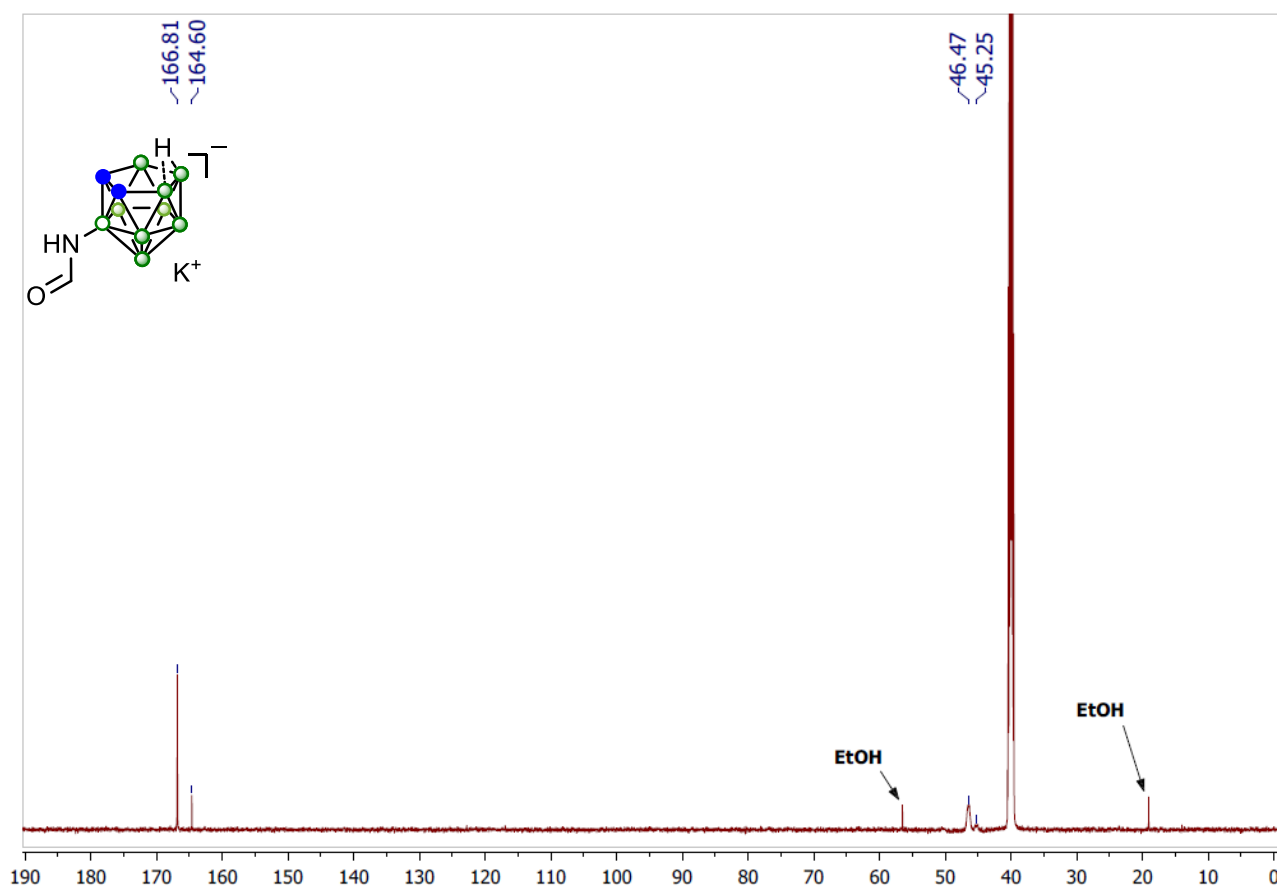


Figure S12. ¹³C NMR spectrum of compound **5c** (DMSO-*d*₆, 151 MHz)

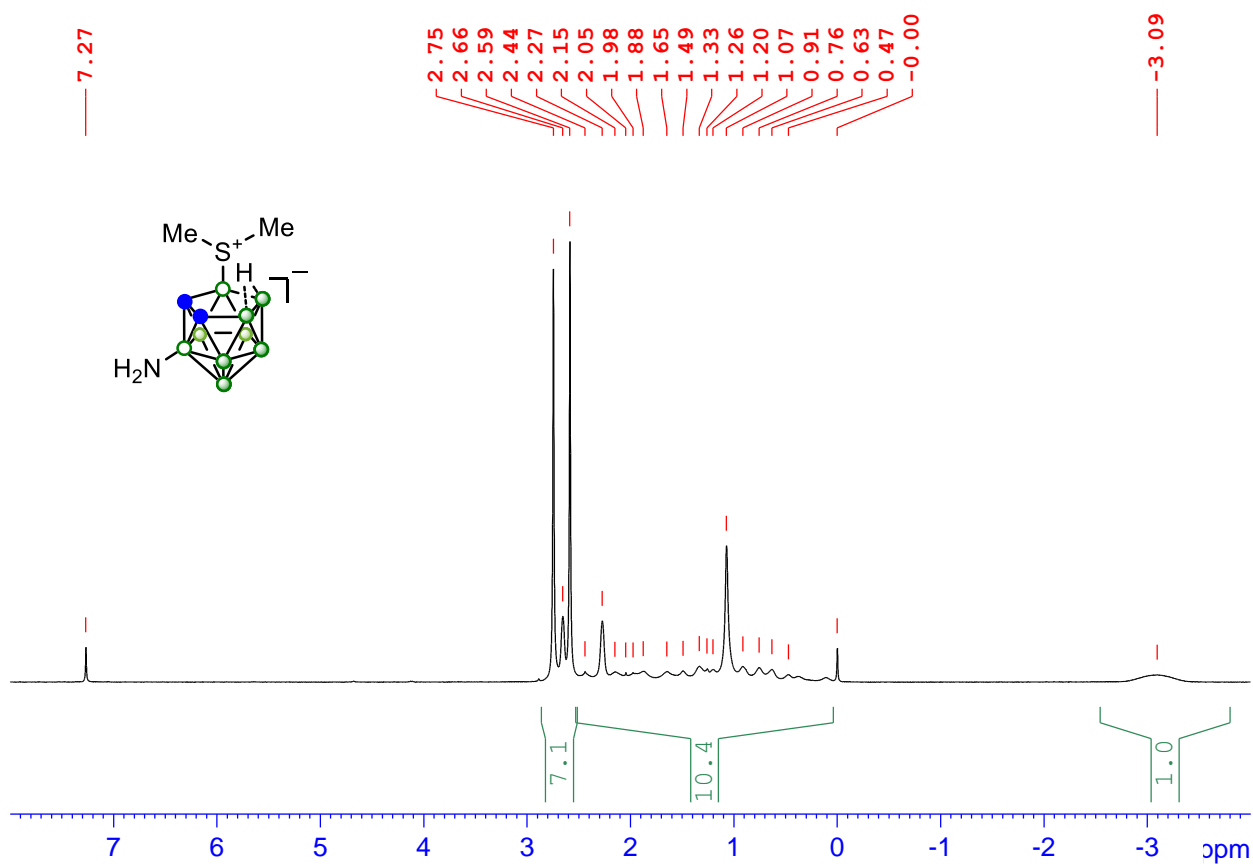


Figure S13. ^1H NMR spectrum of compound **2** (CDCl₃, 500 MHz)

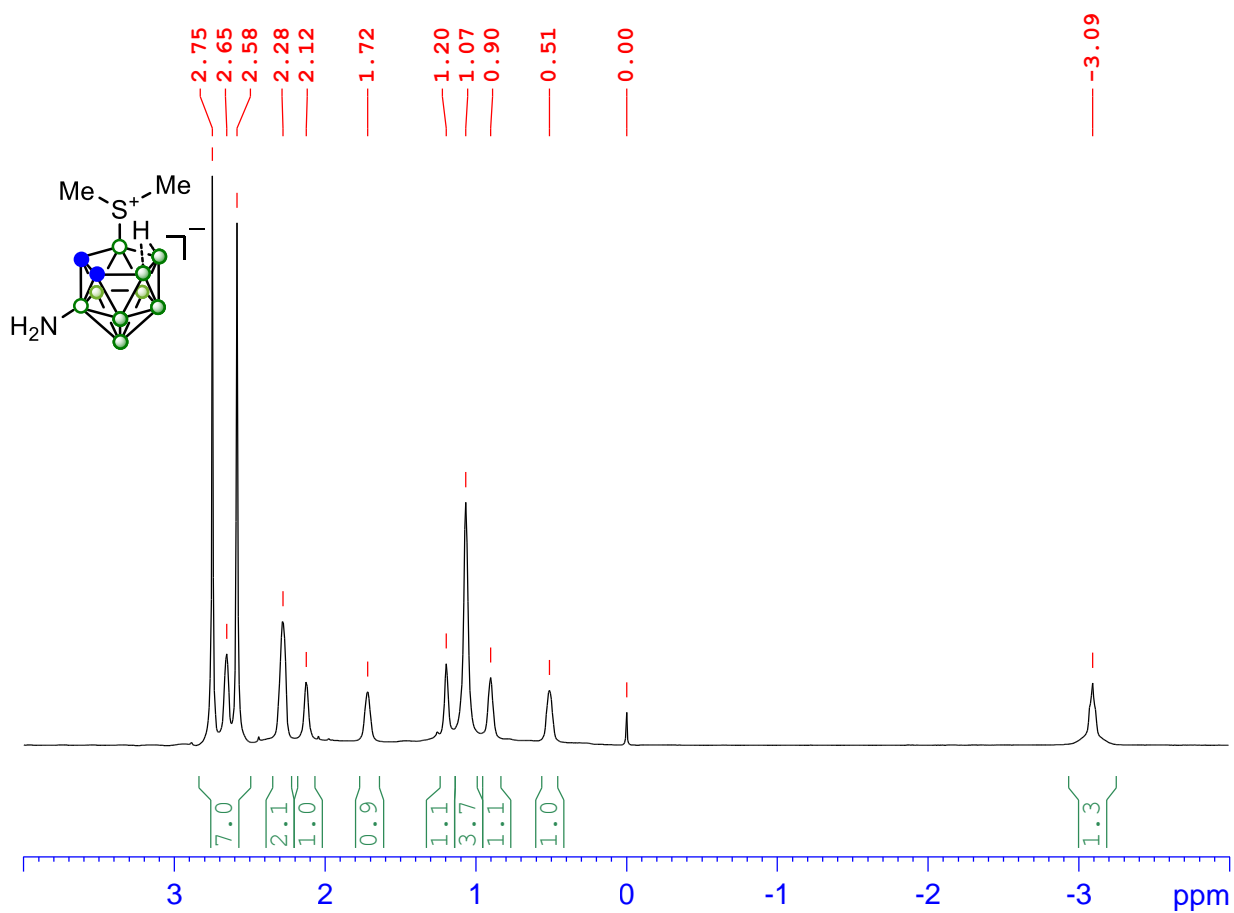


Figure S14. $^1\text{H}\{^{11}\text{B}\}$ NMR spectrum of compound **2** (CDCl₃, 500 MHz)

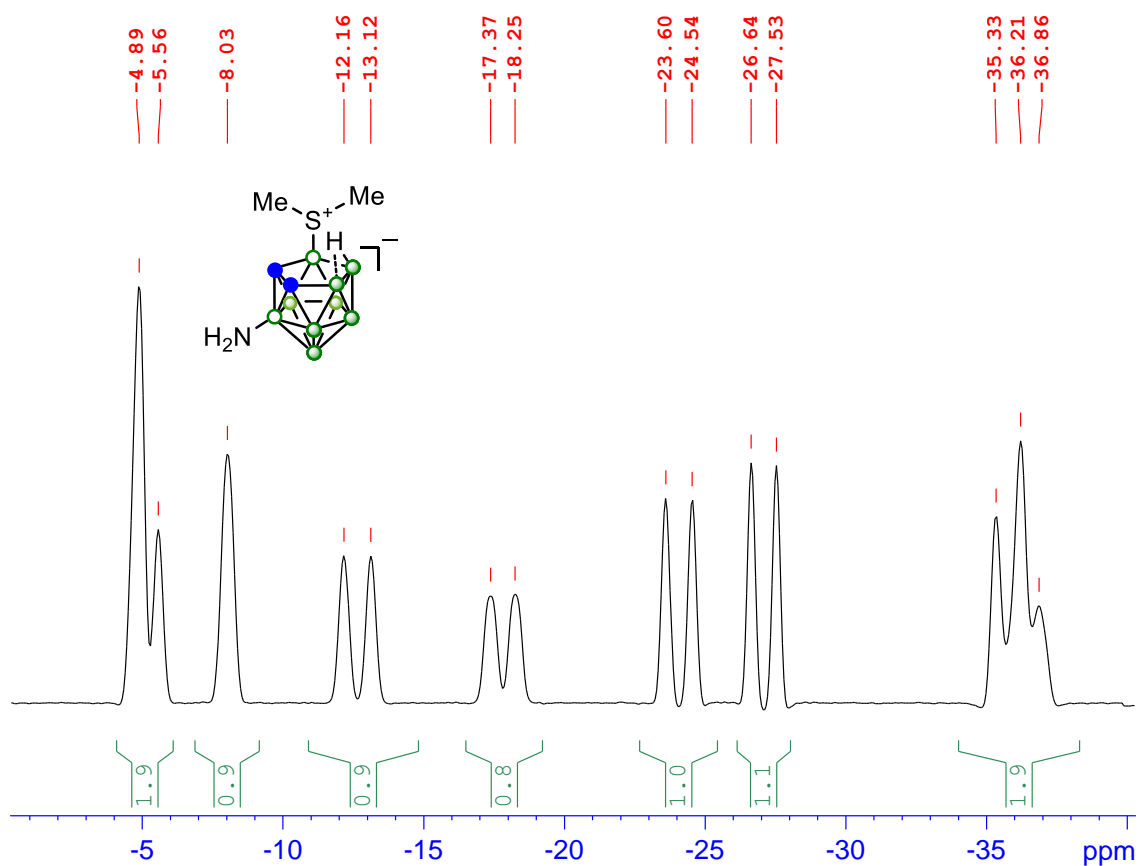


Figure S15. ¹¹B NMR spectrum of compound **2** (CDCl₃, 160 MHz)

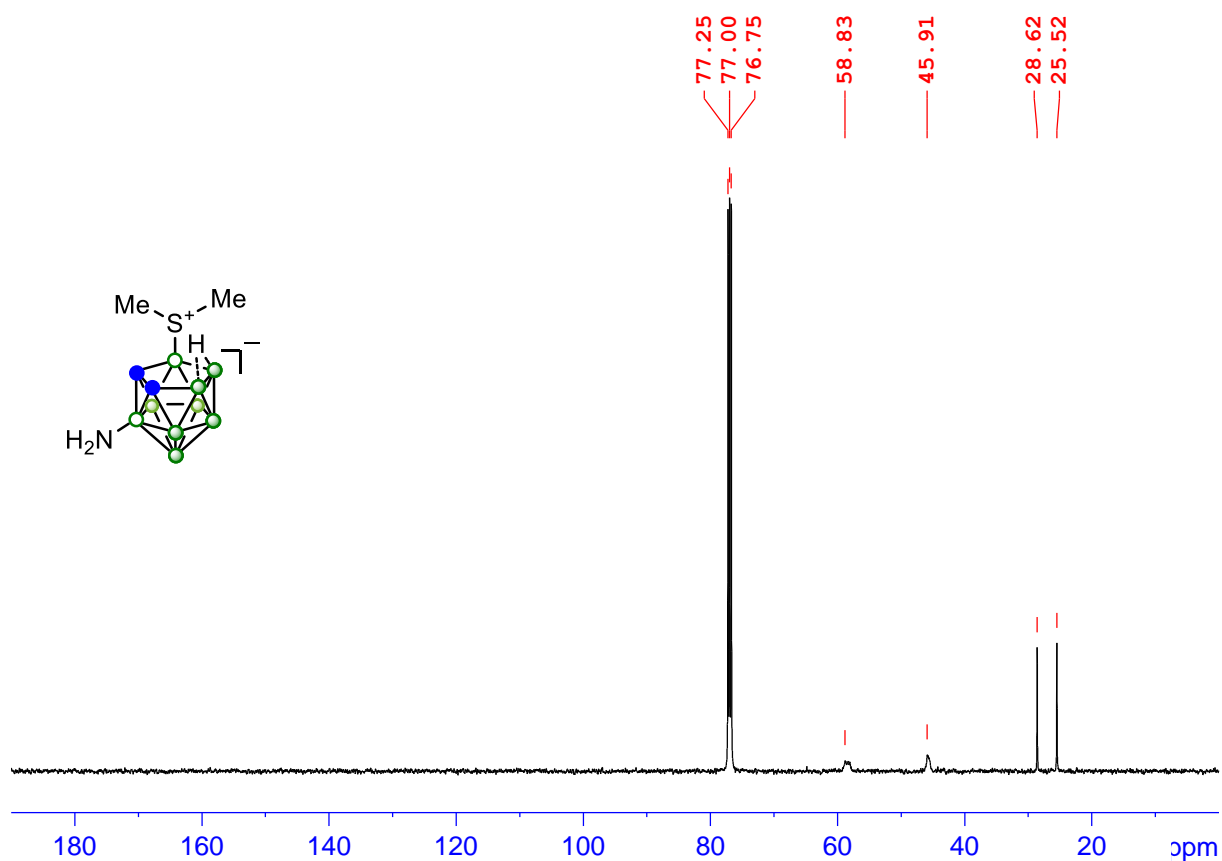


Figure S16. ¹³C NMR spectrum of compound **2** (CDCl₃, 126 MHz)

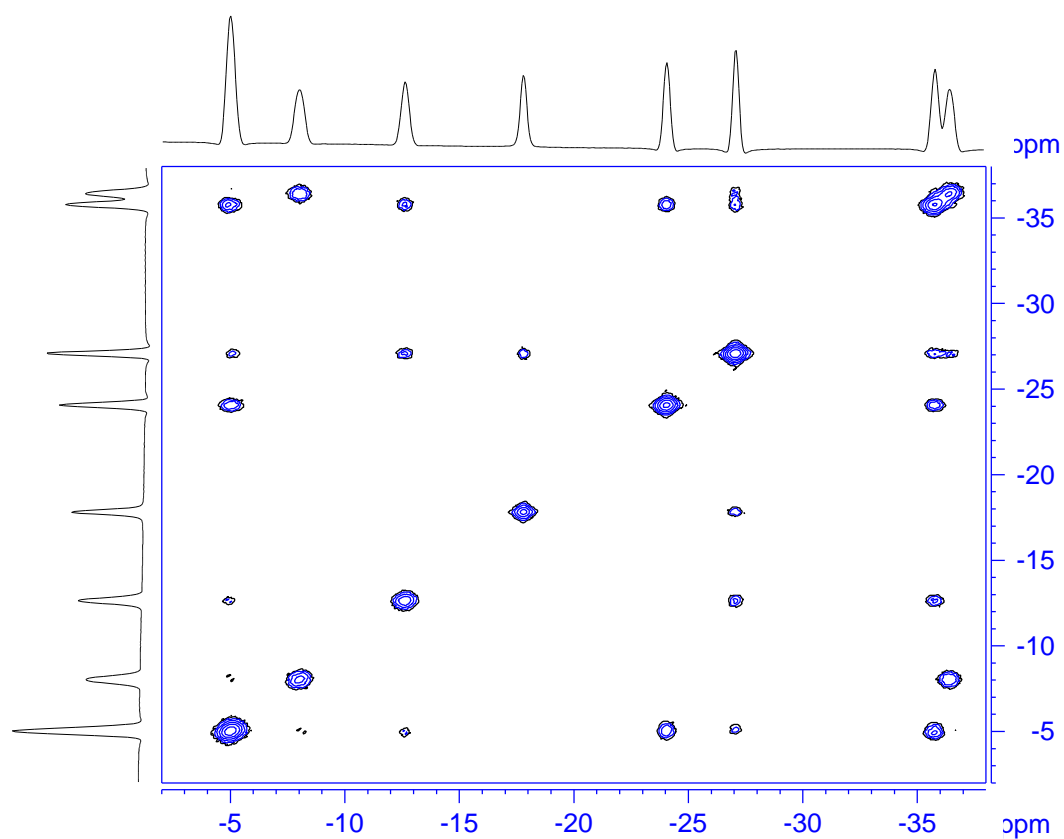


Figure S17. 2D ^{11}B - ^{11}B COSY spectrum of compound **2** (CDCl_3 , 160 MHz)

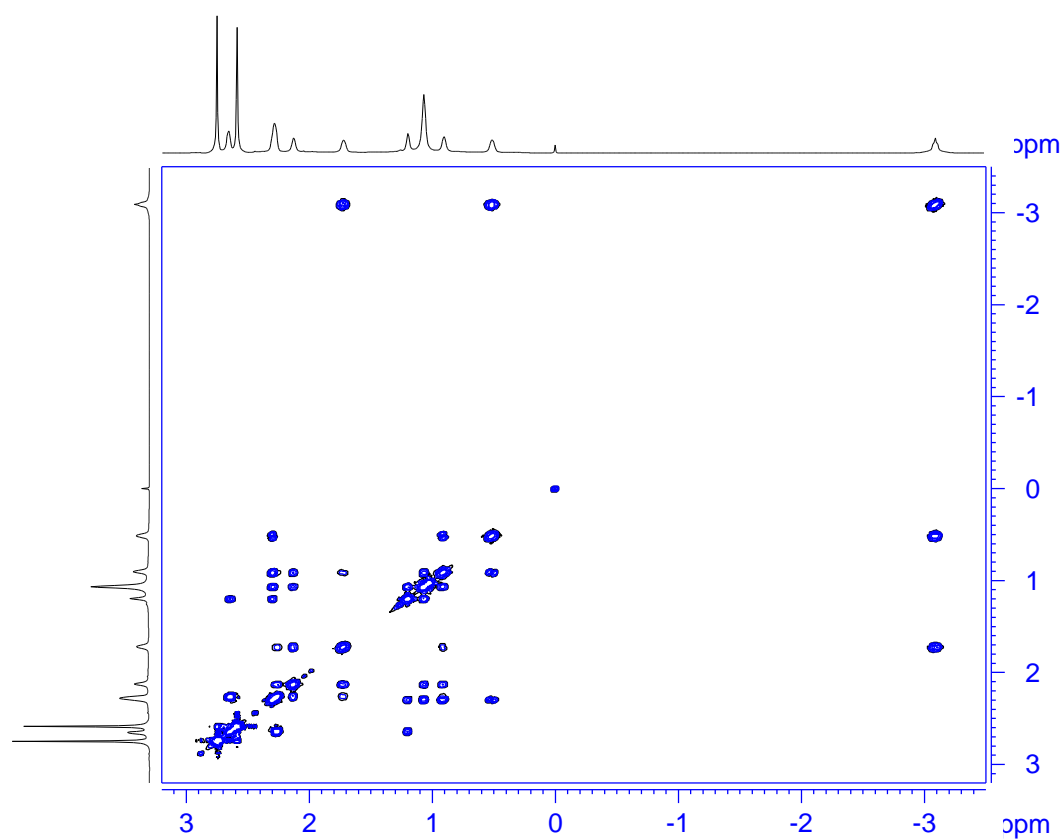


Figure S18. 2D ^1H - $^1\text{H}\{^{11}\text{B}\}$ COSY spectrum of compound **2** (CDCl_3 , 500 MHz)

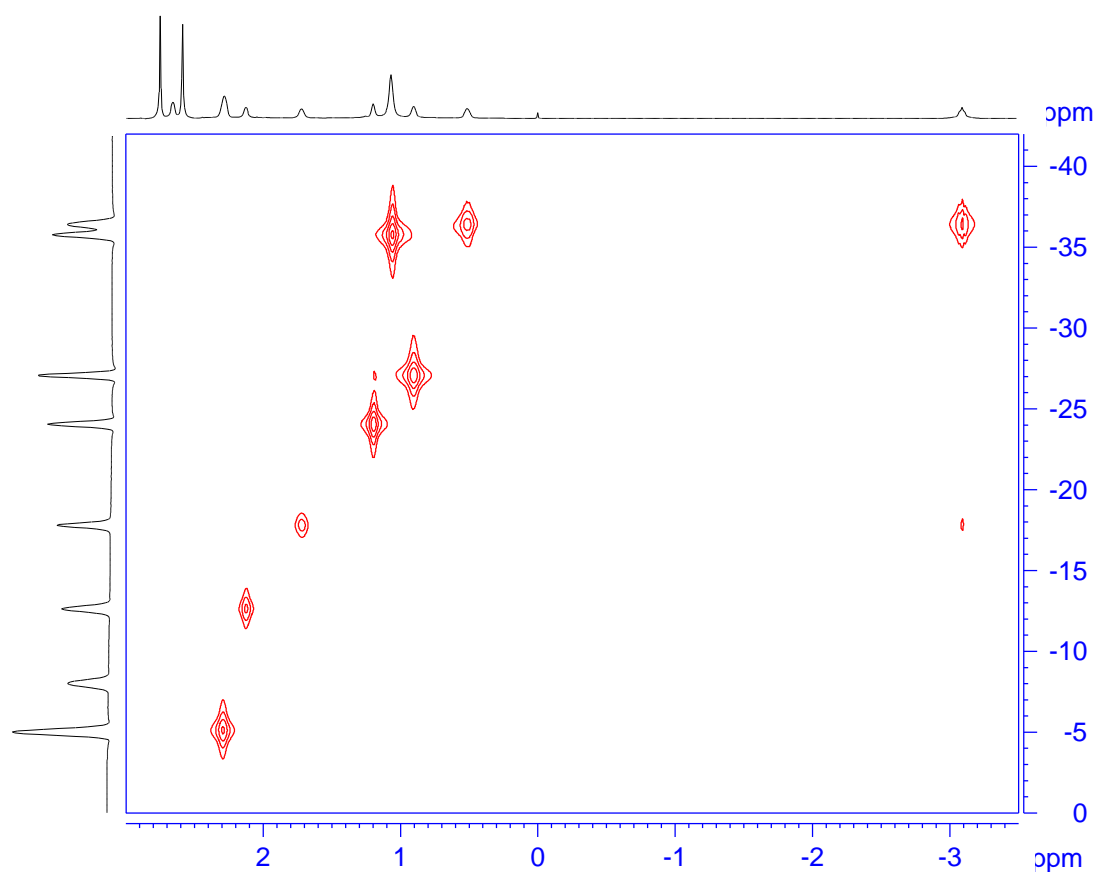


Figure S19. 2D $^1\text{H}\{^{11}\text{B}\}\text{-}^{11}\text{B}$ HMQC spectrum of compound **2** (CDCl_3 , 500 MHz)

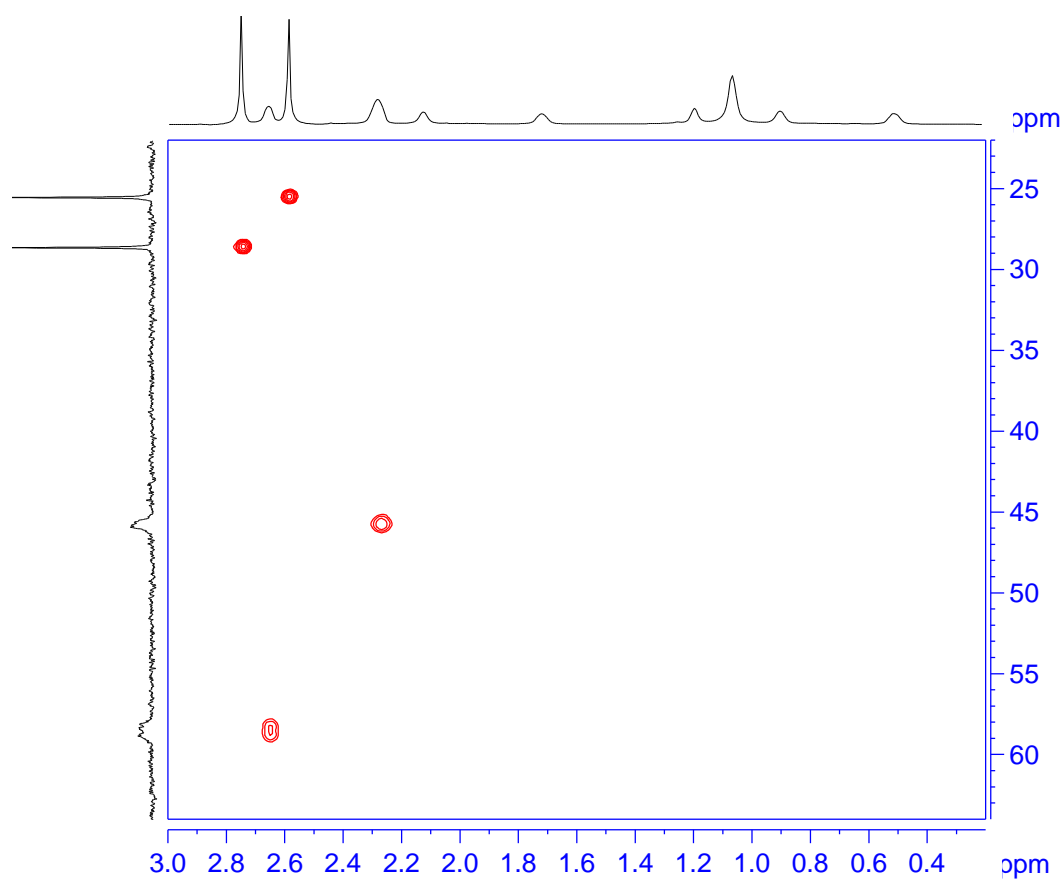


Figure S20. 2D $^1\text{H}\text{-}^{13}\text{C}$ HSQC spectrum of compound **2** (CDCl_3 , 500 MHz)

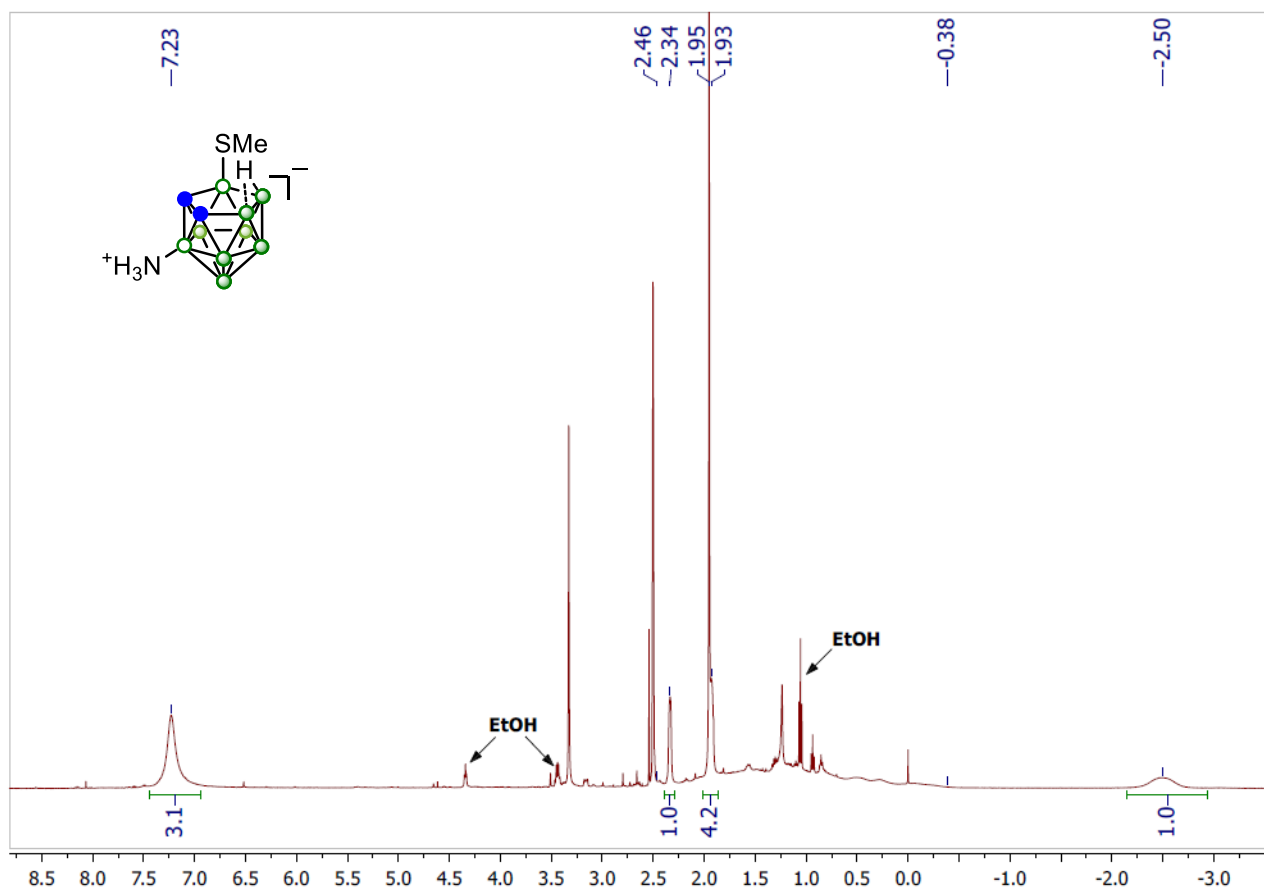


Figure S21. ¹H NMR spectrum of compound **6** (DMSO-*d*₆, 500 MHz)

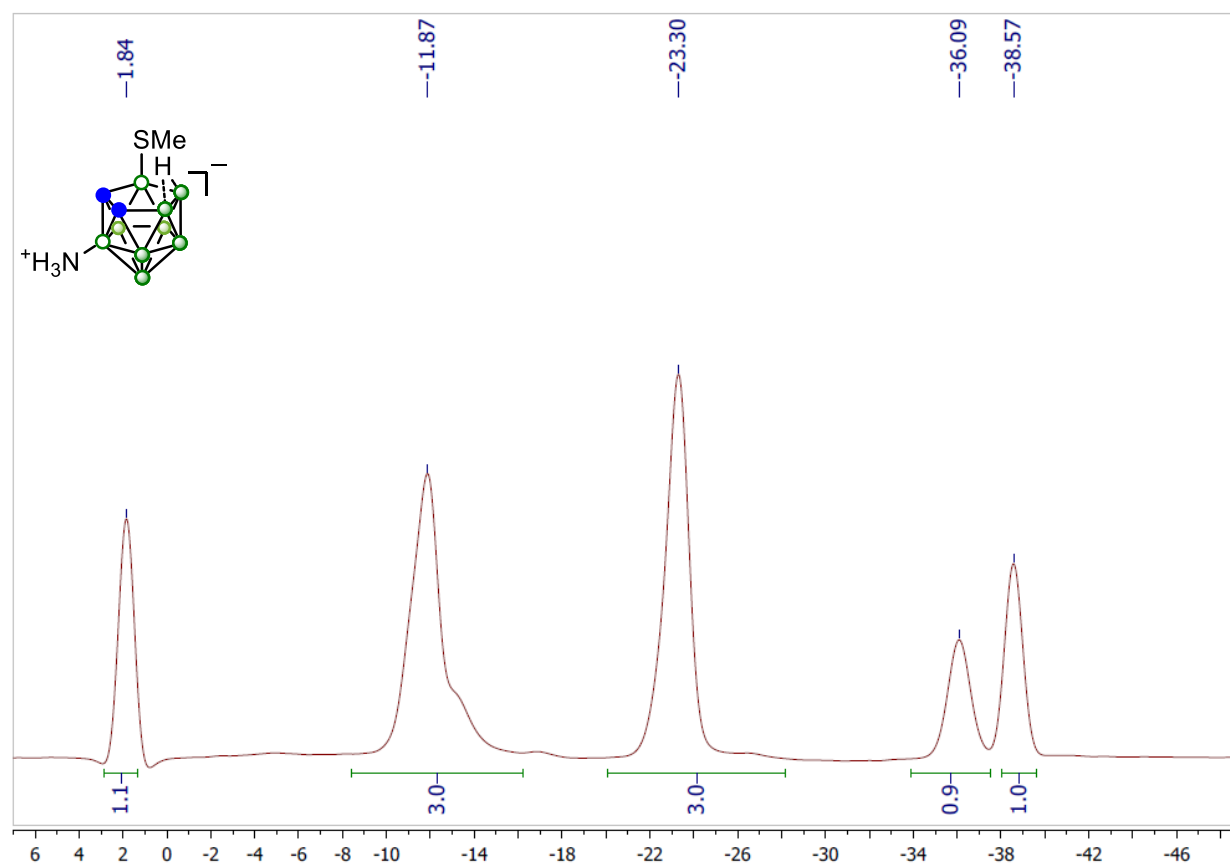


Figure S22. ¹¹B{¹H} NMR spectrum of compound **6** (DMSO-*d*₆, 128 MHz)

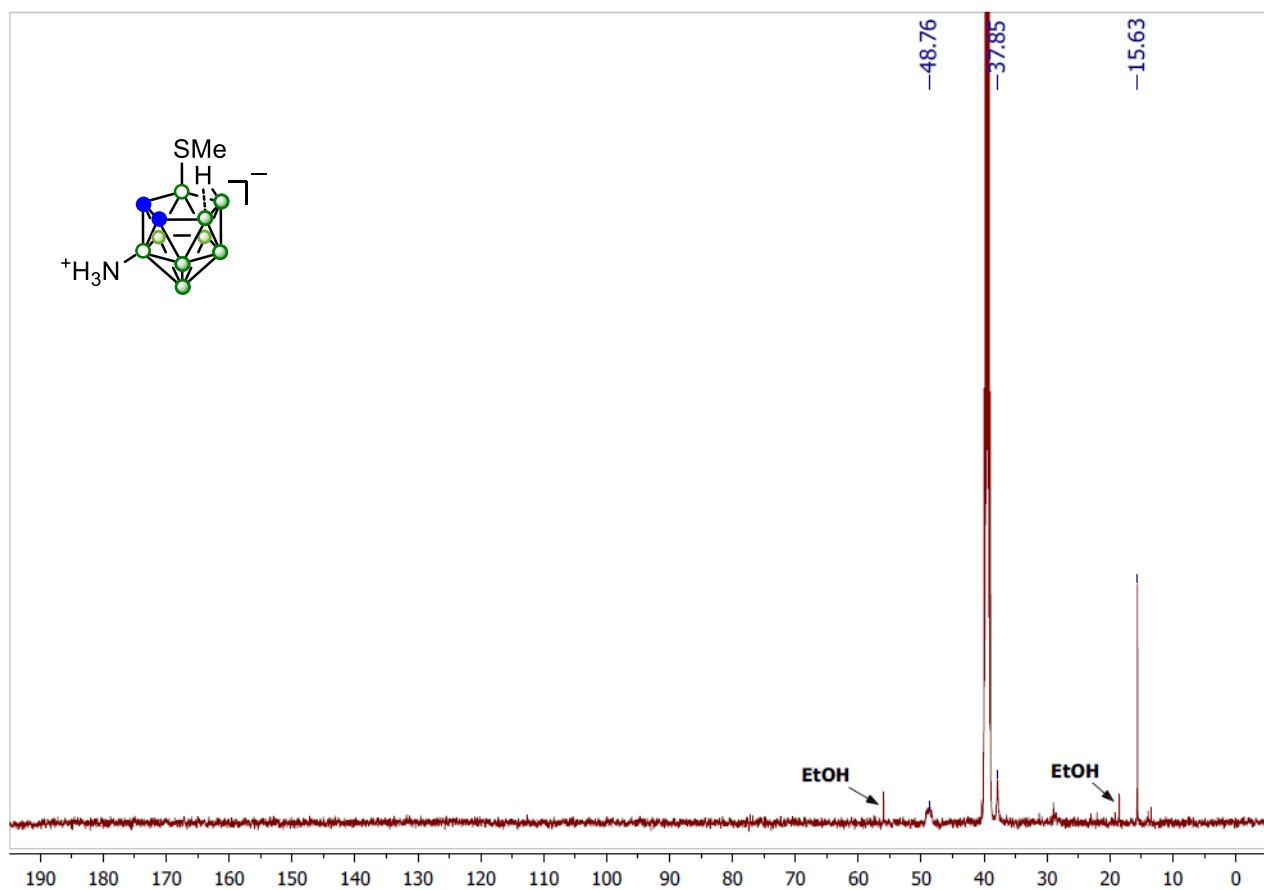


Figure S23. ^{13}C NMR spectrum of compound 6 (DMSO- d_6 , 126 MHz)

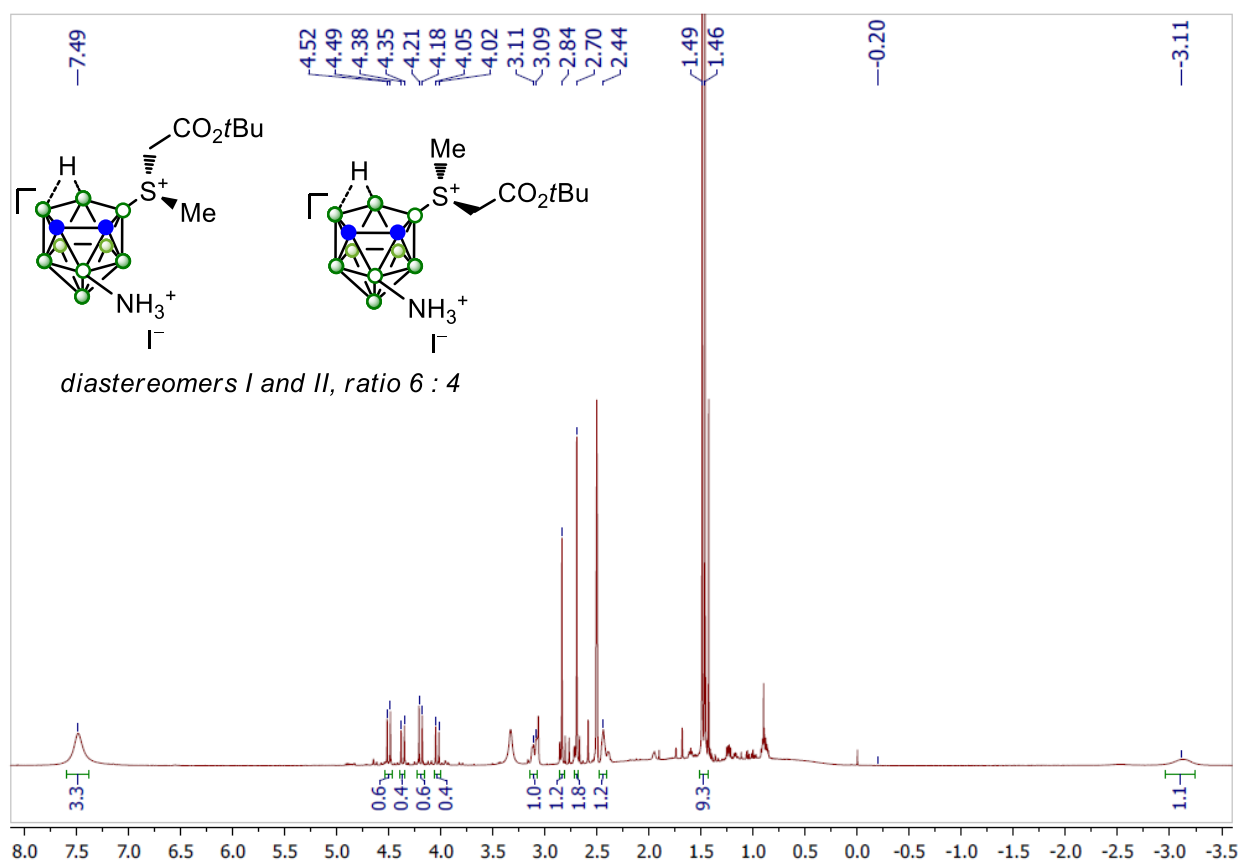


Figure S24. ^1H NMR spectrum of compound 7 (DMSO- d_6 , 500 MHz)

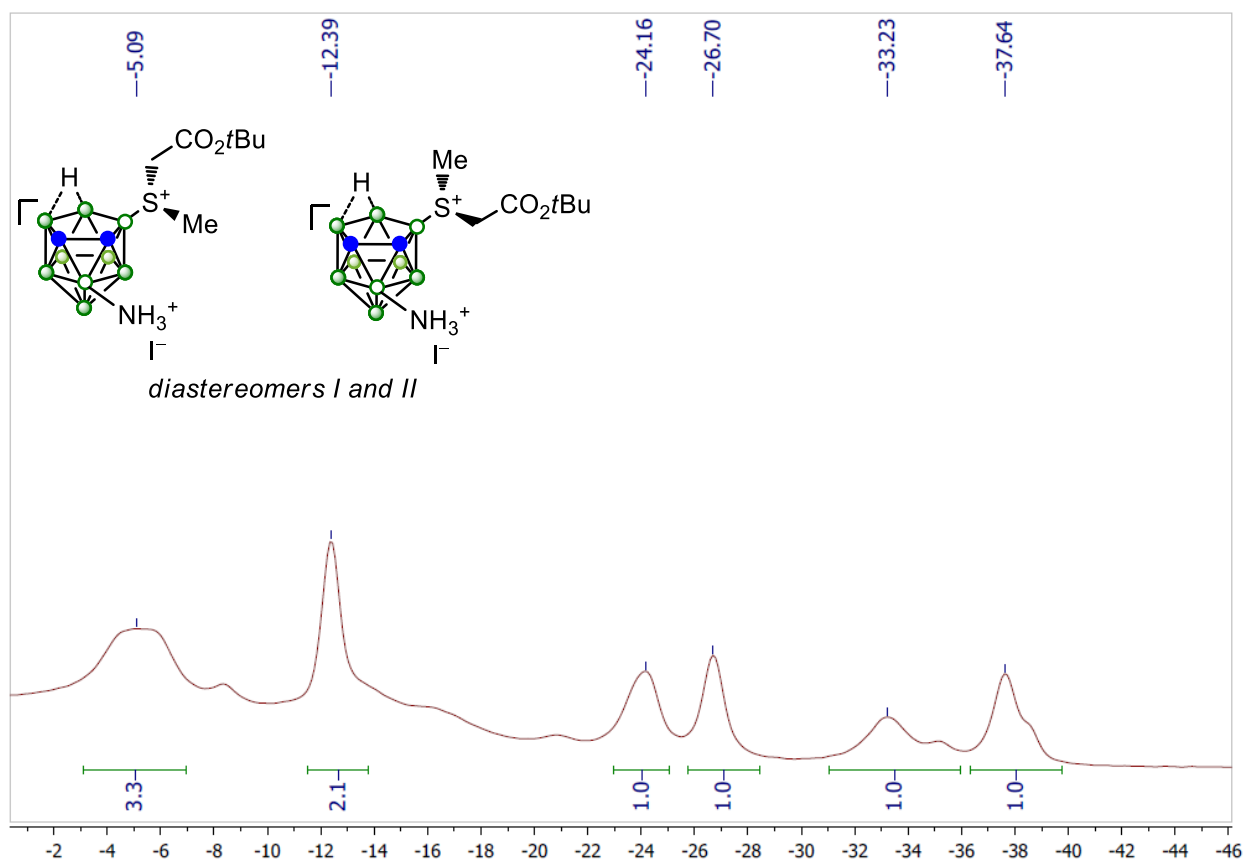


Figure S25. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **7** (DMSO- d_6 , 160 MHz)

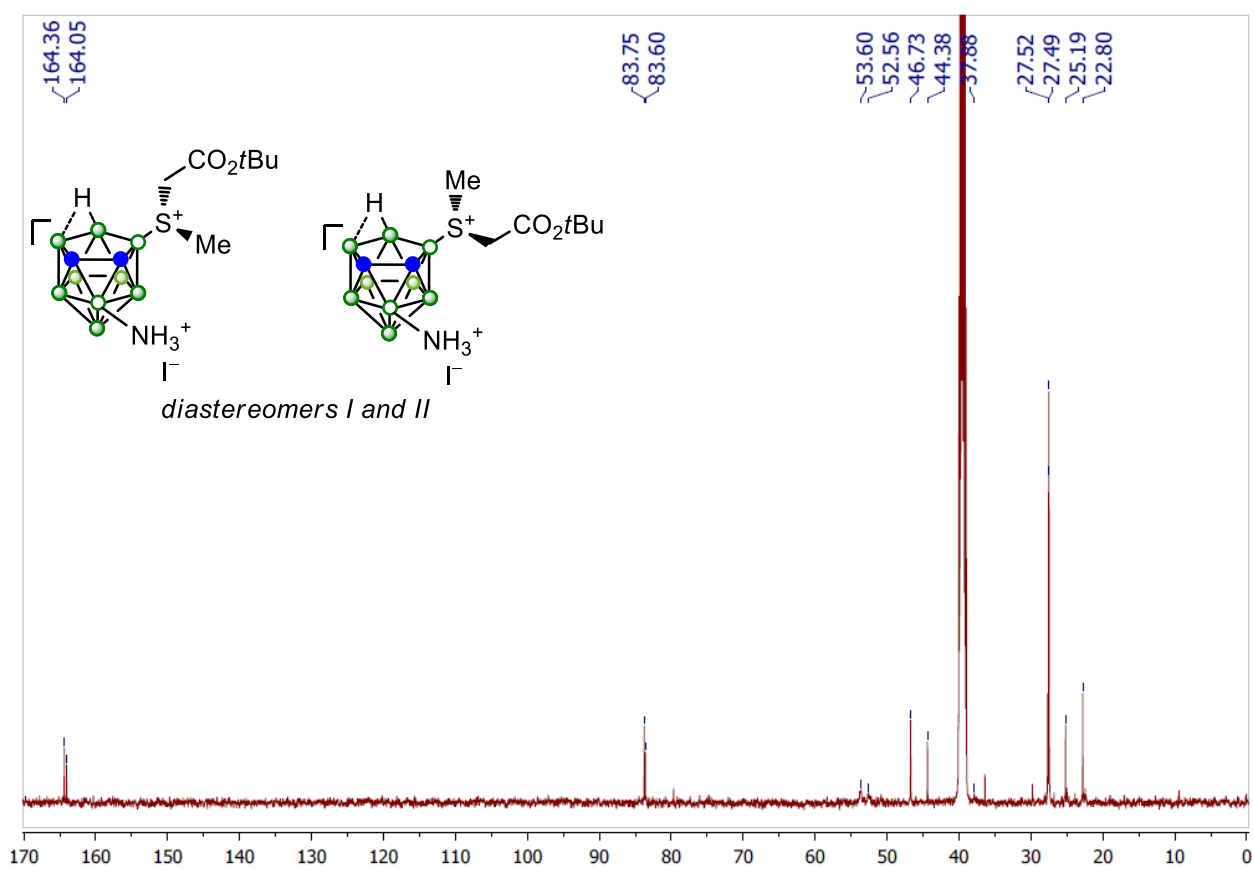


Figure S26. ^{13}C NMR spectrum of compound **7** (DMSO- d_6 , 126 MHz)

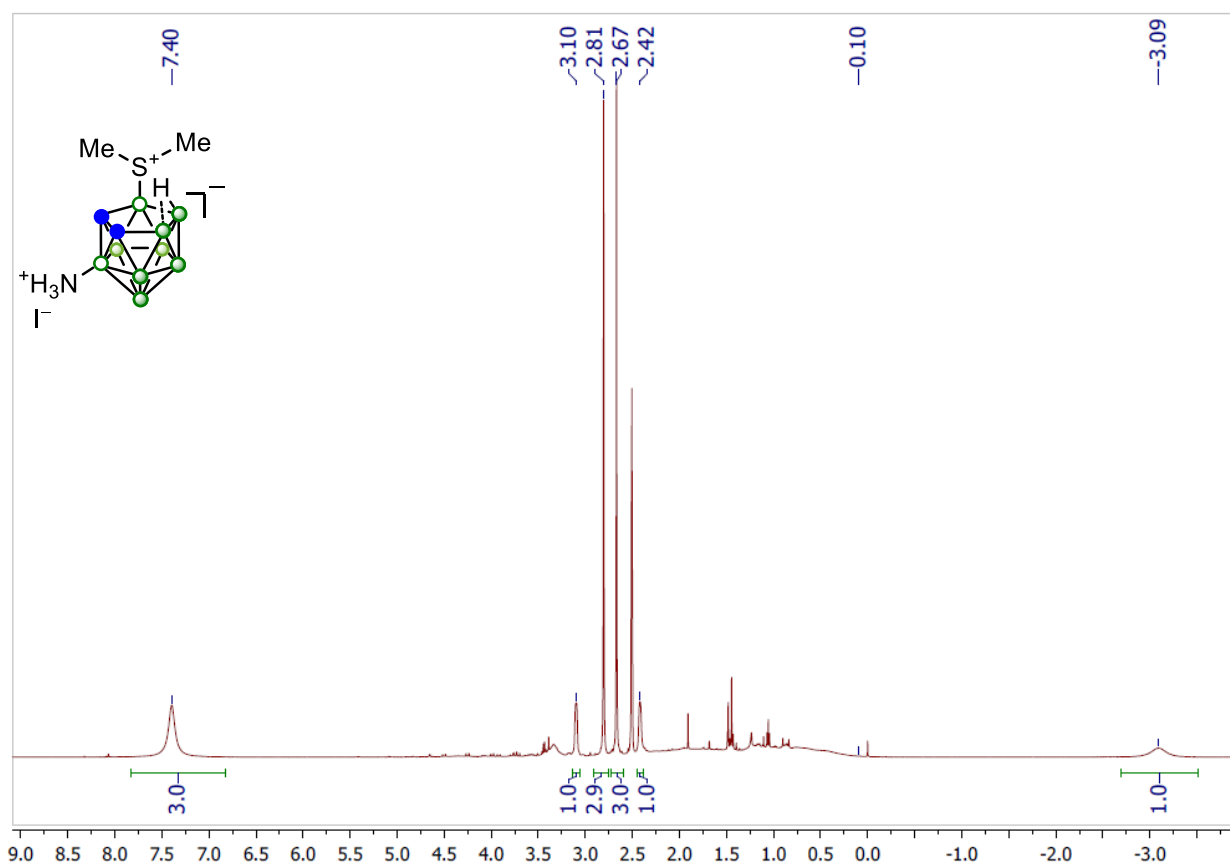


Figure S27. ¹H NMR spectrum of compound **2''** (DMSO-*d*₆, 500 MHz)

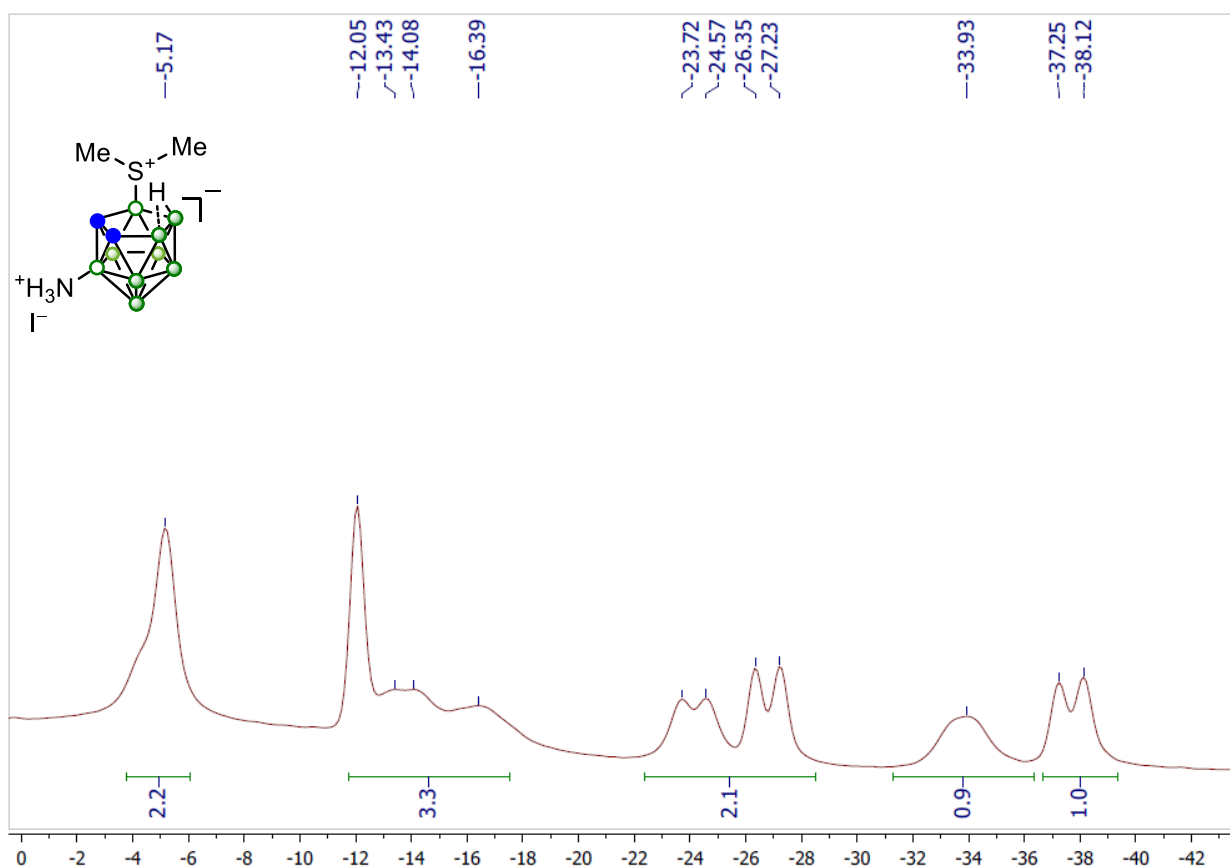


Figure S28. ¹¹B NMR spectrum of compound **2''** (DMSO-*d*₆, 160 MHz)

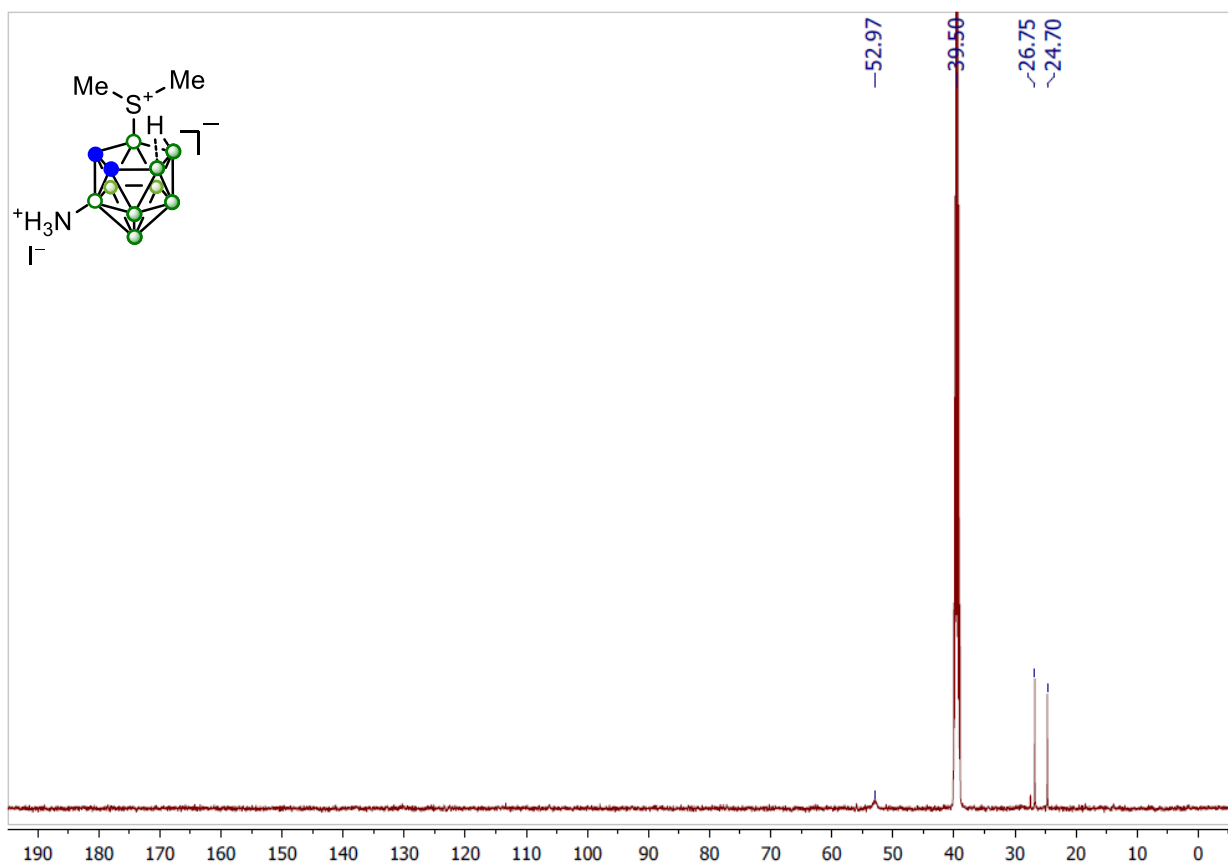


Figure S29. ^{13}C NMR spectrum of compound **2''** (DMSO- d_6 , 126 MHz)

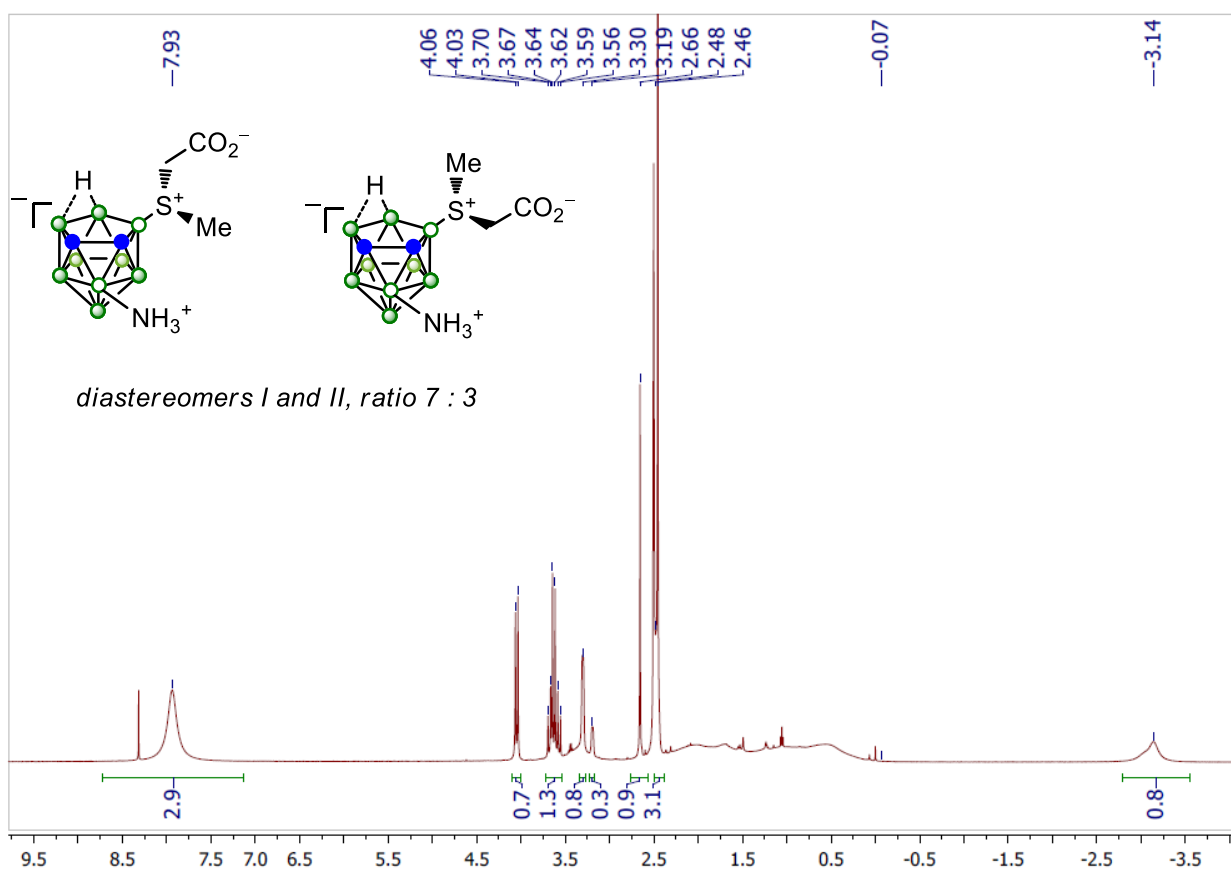


Figure S30. ^1H NMR spectrum of compound **1** (DMSO- d_6 , 500 MHz)

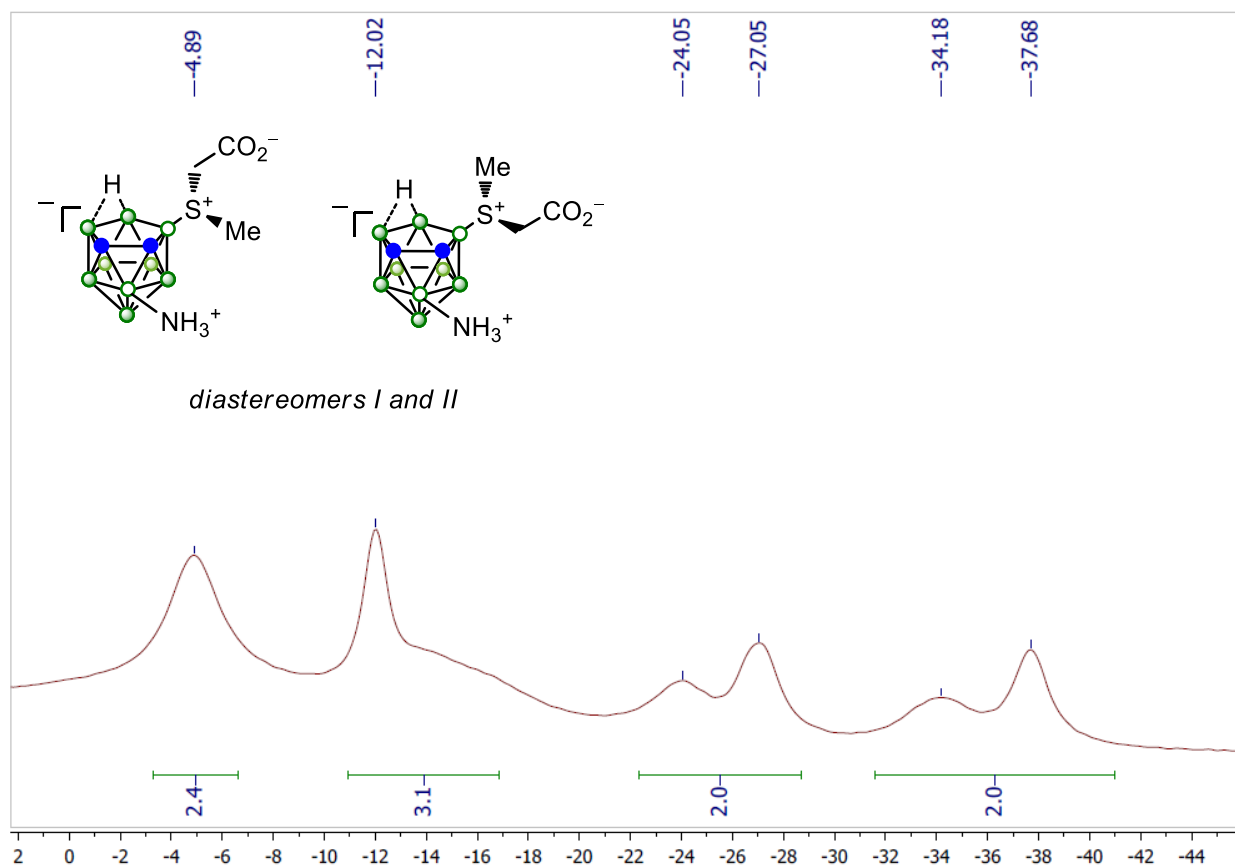


Figure S31. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **1** ($\text{DMSO-}d_6$, 160 MHz)

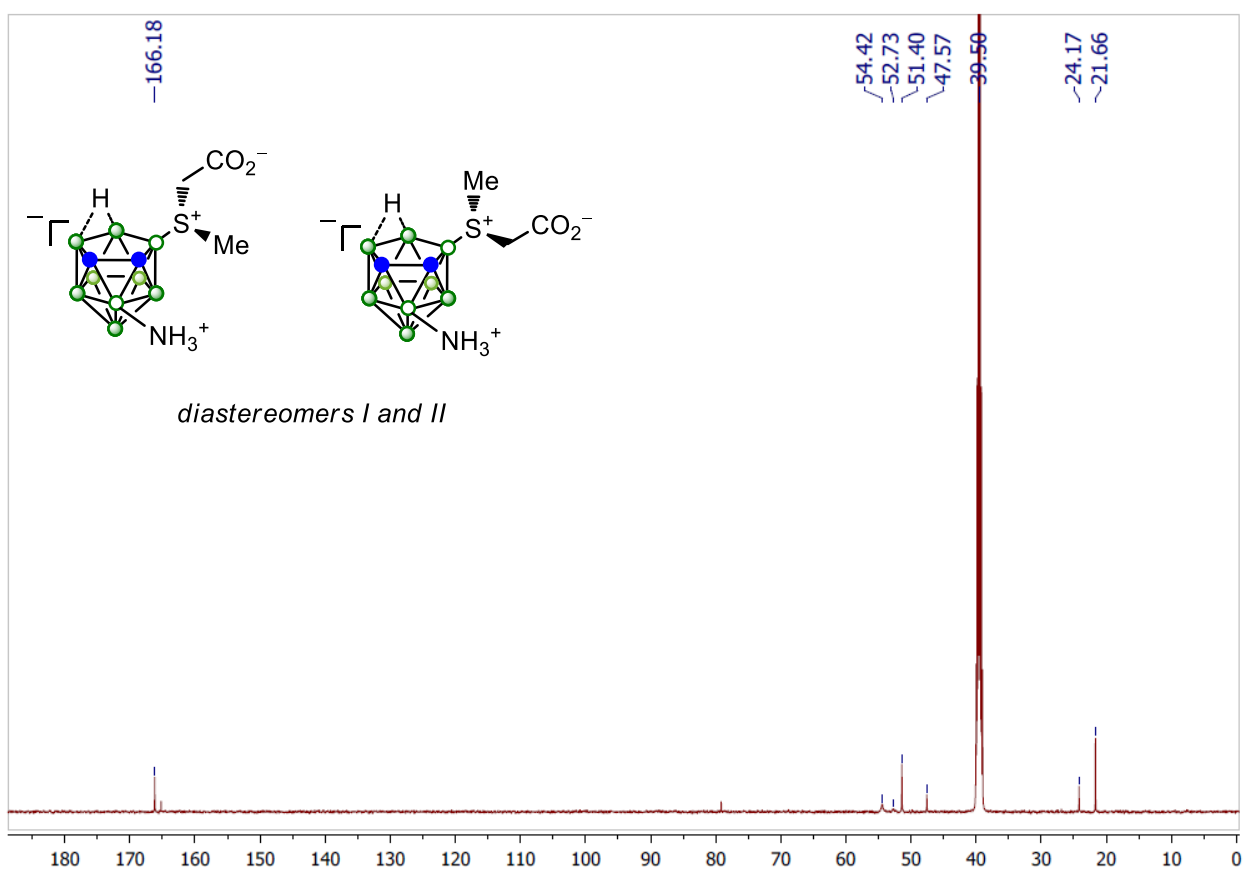
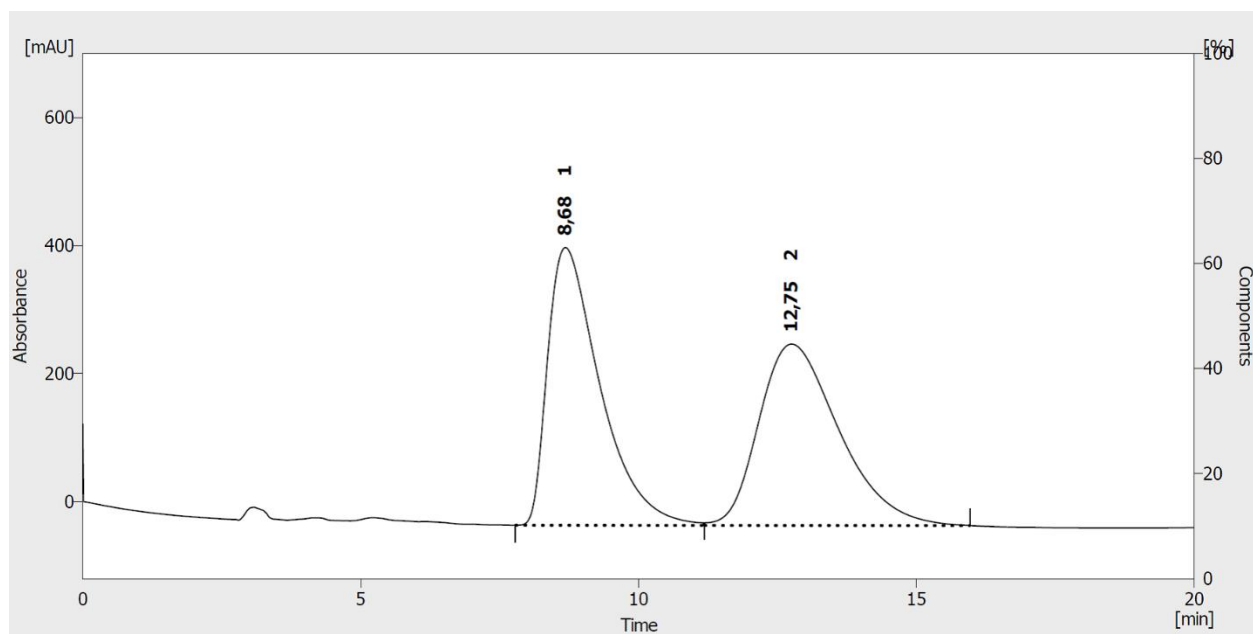


Figure S32. ^{13}C NMR spectrum of compound **1** ($\text{DMSO-}d_6$, 126 MHz)

HPLC Data



	Reten. Time [min]	Area [mAU.s]	Height [mAU]	Area [%]	Height [%]	W05 [min]
1	8,683	28440,888	433,772	50,1	60,5	1,00
2	12,750	28357,276	283,246	49,9	39,5	1,55
	Total	56798,163	717,018	100,0	100,0	

Figure S33. Chromatogram of compound **6** (Chiralpak AS-H, *n*-hexane-*i*PrOH 5:1, 1.0 mL/min, 220 nm)

HRMS Data

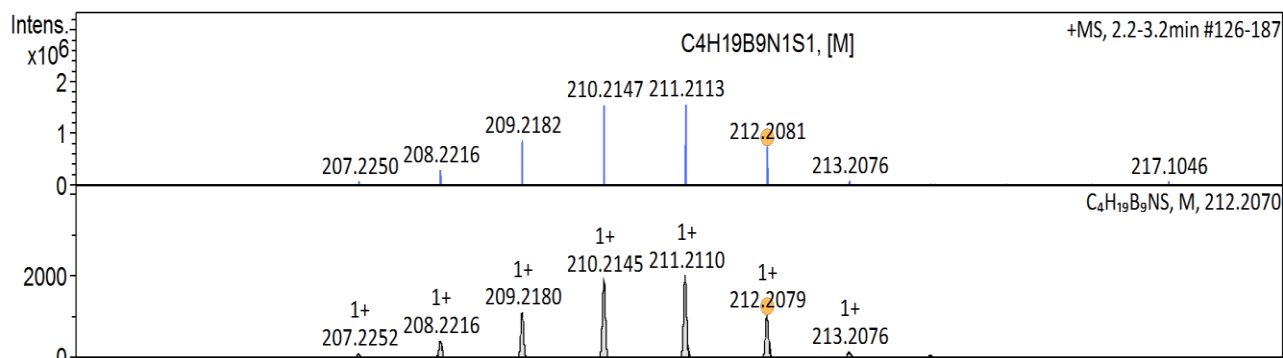


Figure S34. Experimental and simulated peak distribution in high-resolution mass spectrum of compound **2'**

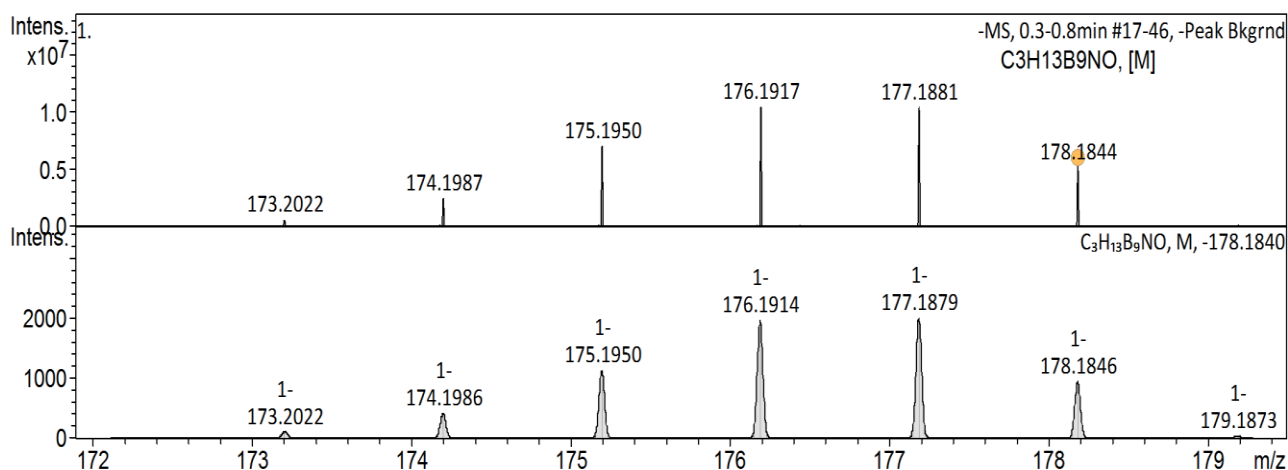


Figure S35. Experimental and simulated peak distribution in high-resolution mass spectrum of compound **5a**

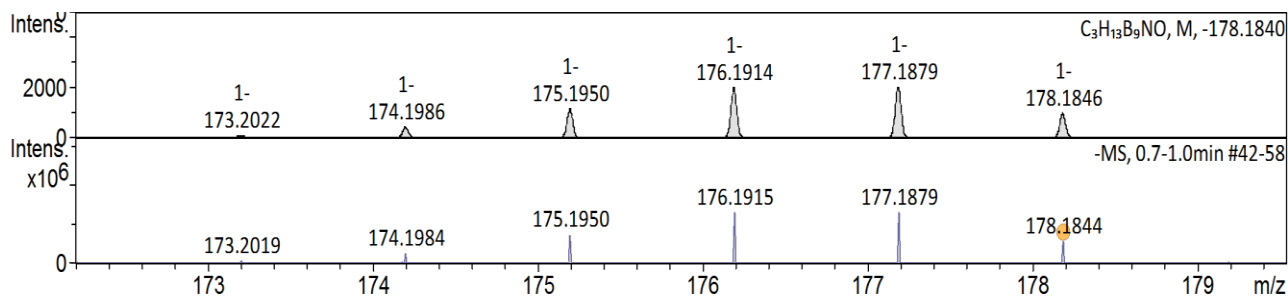


Figure S36. Experimental and simulated peak distribution in high-resolution mass spectrum of compound **5b**

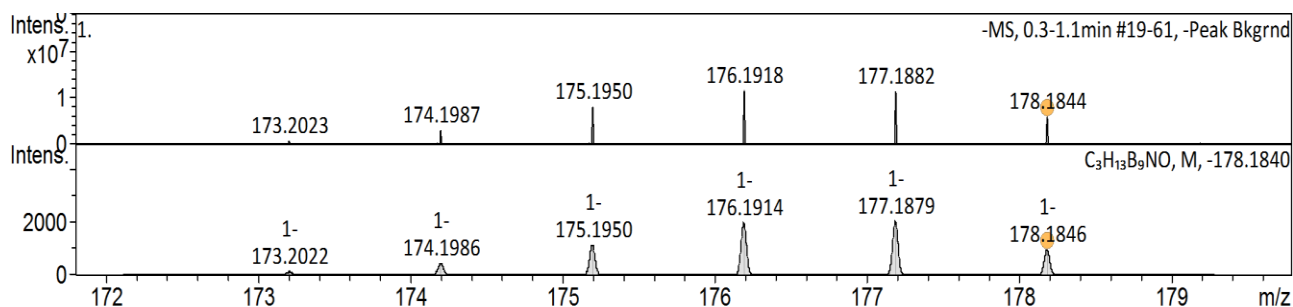


Figure S37. Experimental and simulated peak distribution in high-resolution mass spectrum of compound **5c**

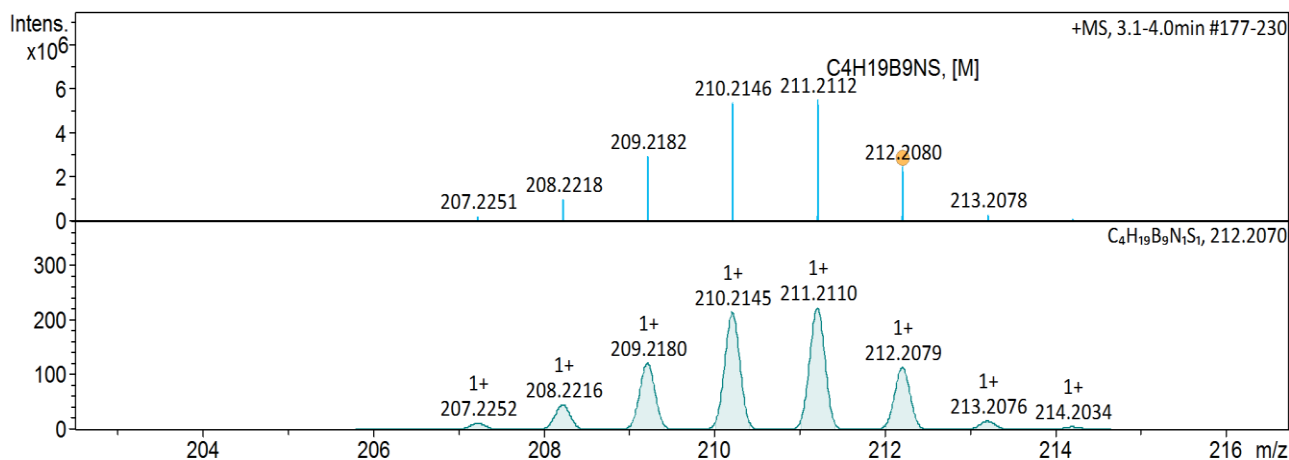


Figure S38. Experimental and simulated peak distribution in high-resolution mass spectrum of compound **2**

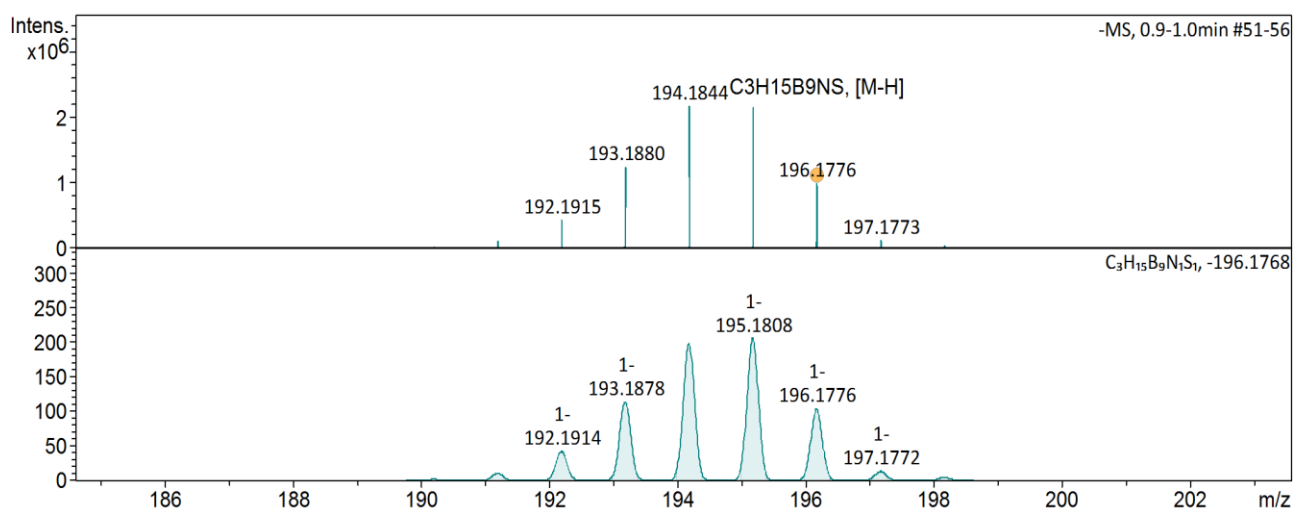


Figure S39. Experimental and simulated peak distribution in high-resolution mass spectrum of compound **6**

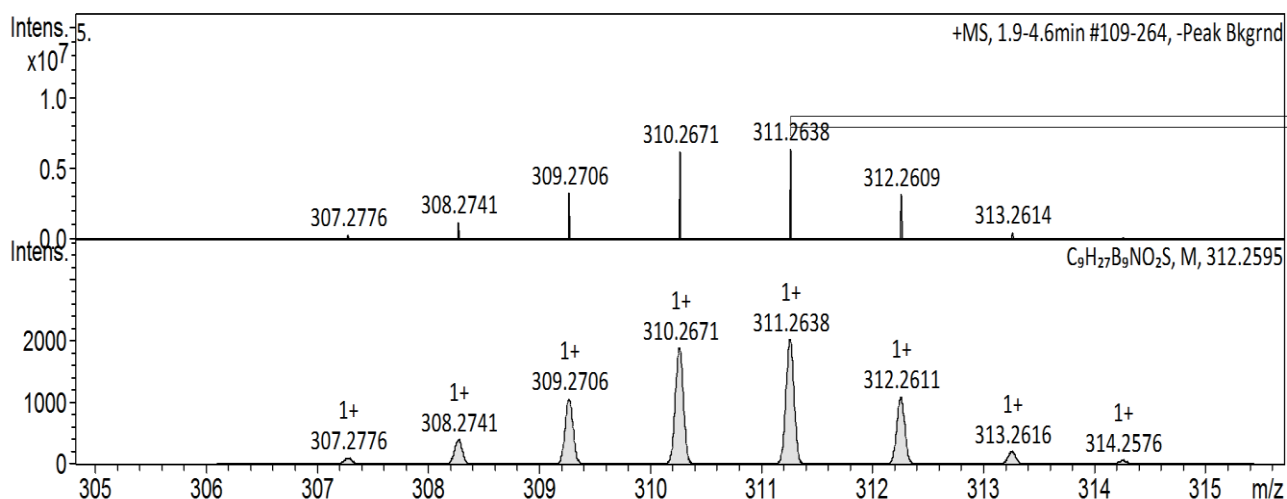


Figure S40. Experimental and simulated peak distribution in high-resolution mass spectrum of compound **7**

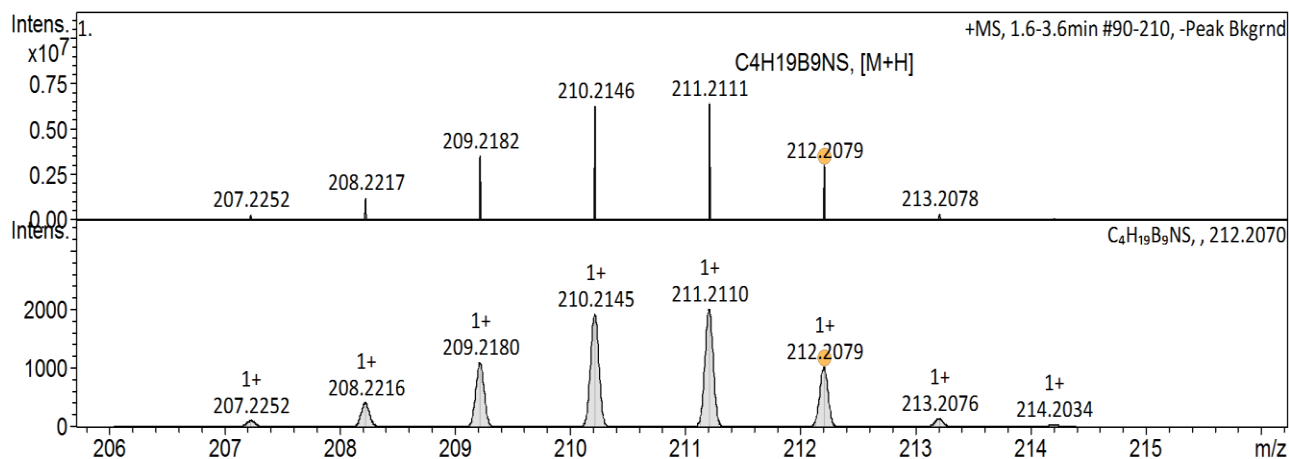


Figure S41. Experimental and simulated peak distribution in high-resolution mass spectrum of compound **2''**

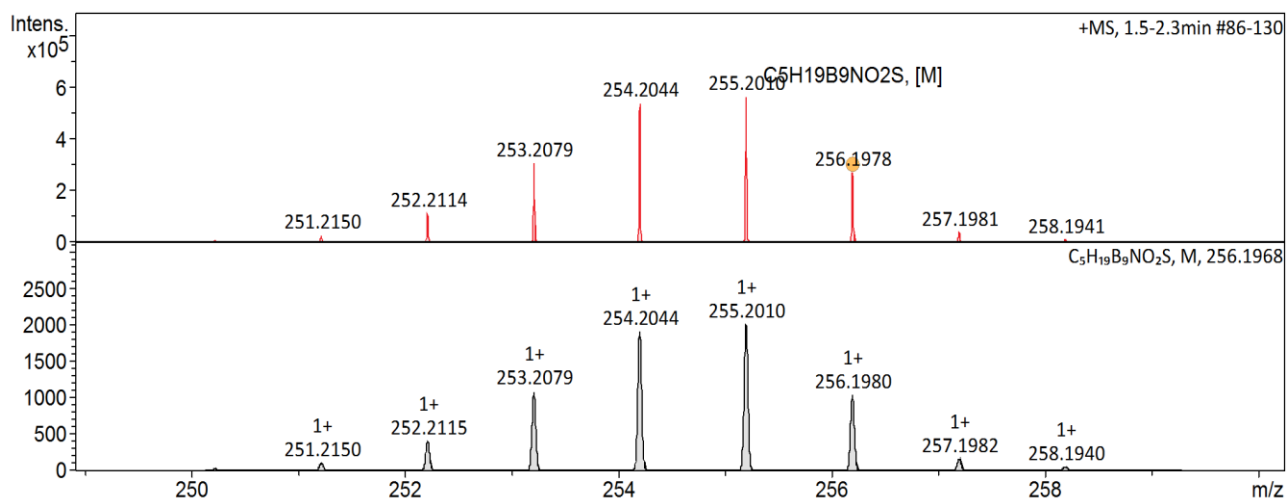


Figure S42. Experimental and simulated peak distribution in high-resolution mass spectrum of compound **1**

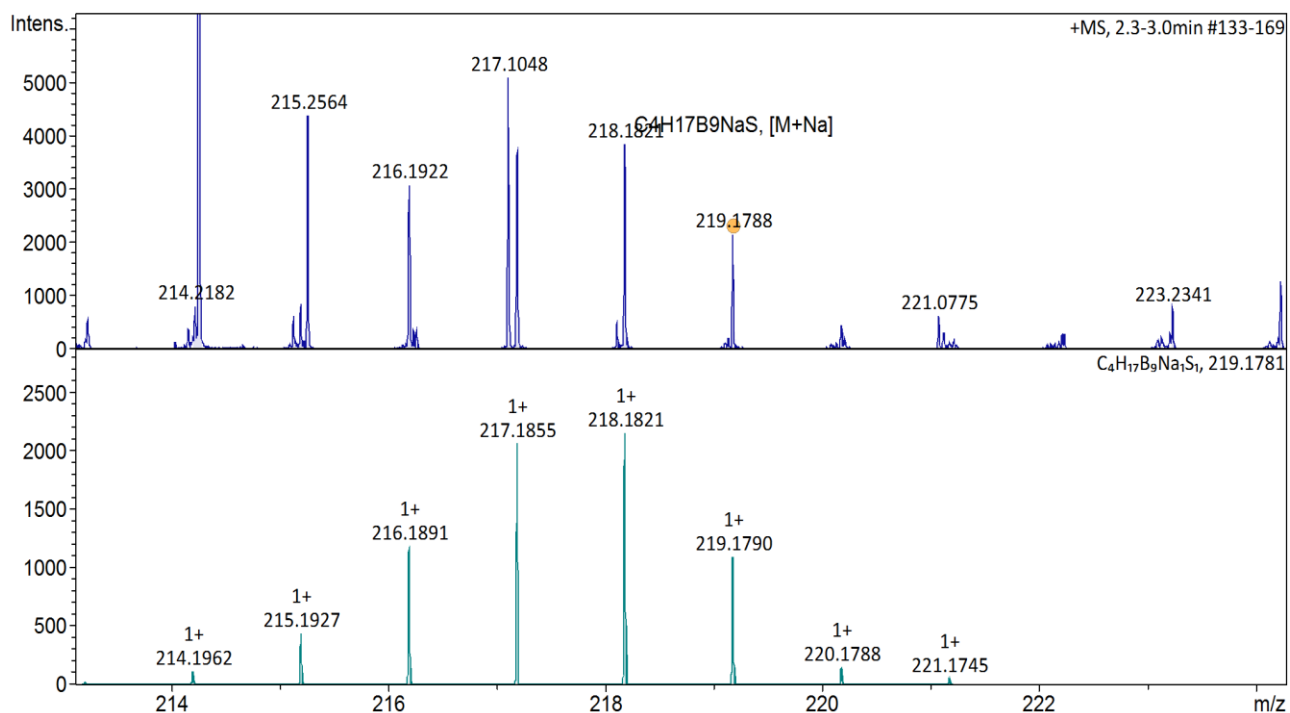


Figure S43. Experimental and simulated peak distribution in high-resolution mass spectrum of compound **9**