

Supplementary Information

For

Supramolecular amphiphiles based on pillar[5]arene and meroterpenoids: synthesis, self-association and interaction with floxuridine

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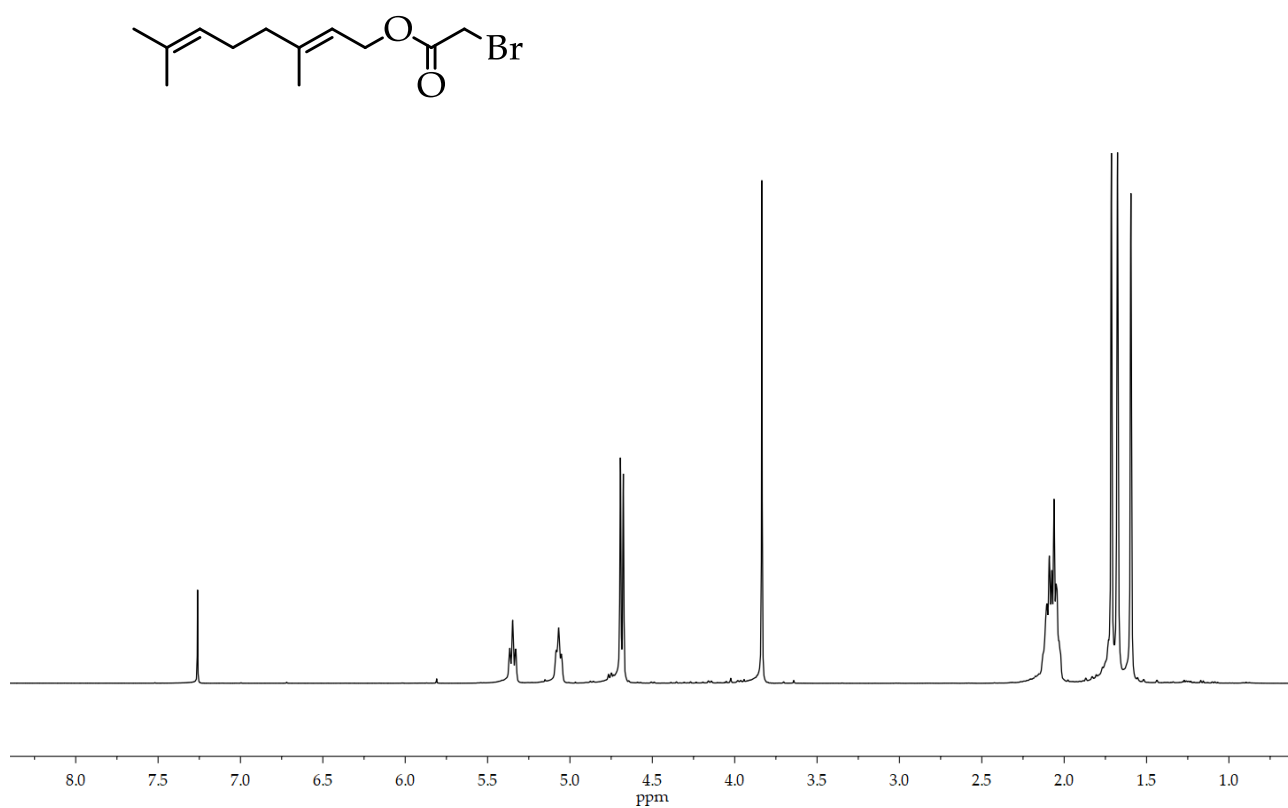


Figure S1. ¹H NMR spectrum of the compound **2a**, CDCl₃, 298 K, 400 MHz.

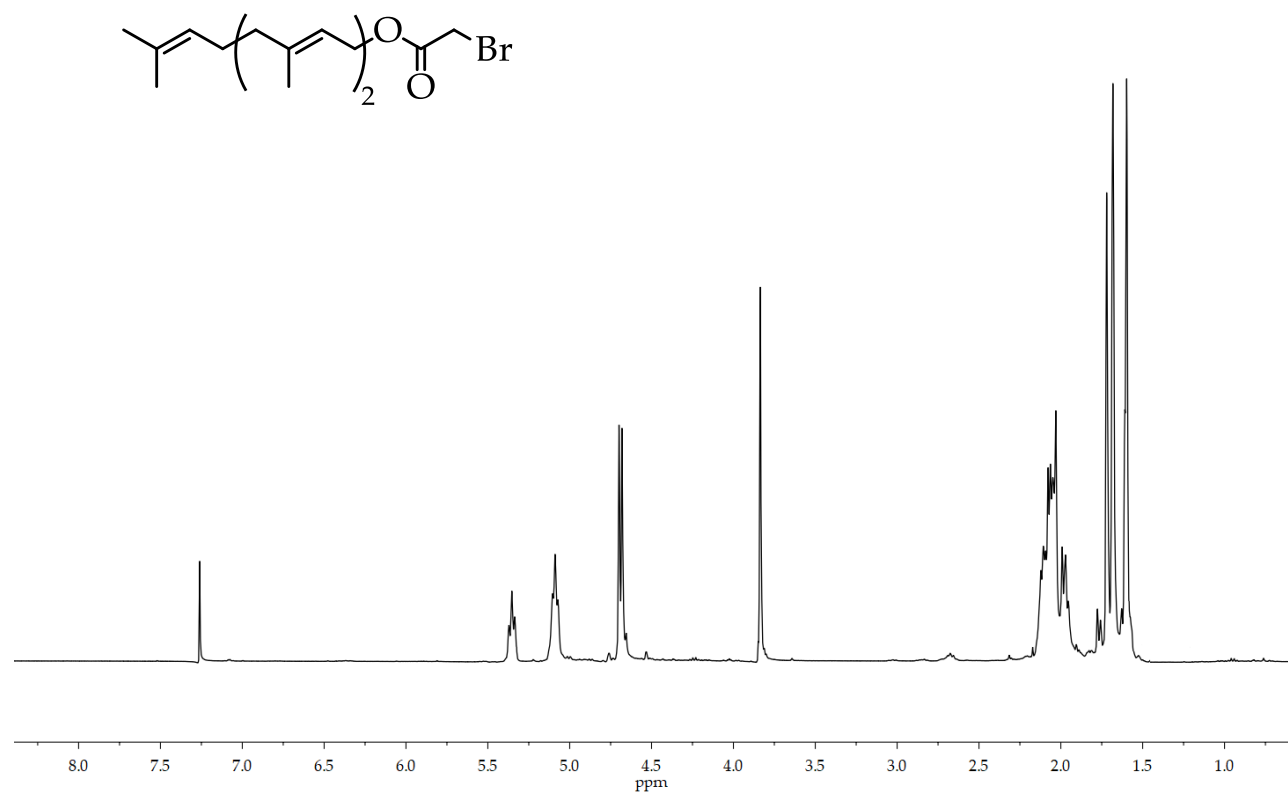


Figure S2. ¹H NMR spectrum of the compound **2b**, CDCl₃, 298 K, 400 MHz.

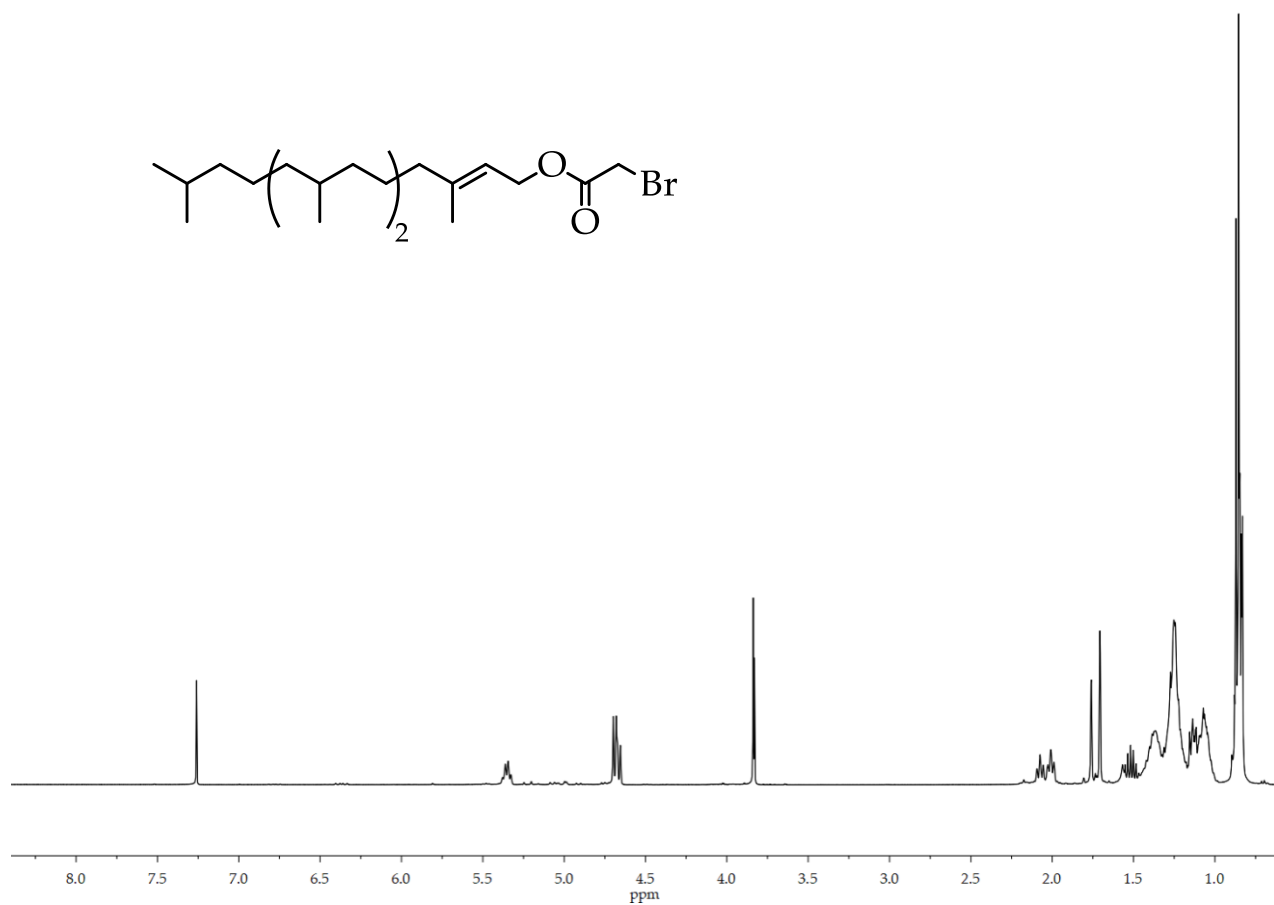


Figure S3. ¹H NMR spectrum of the compound **2c**, CDCl₃, 298 K, 400 MHz.

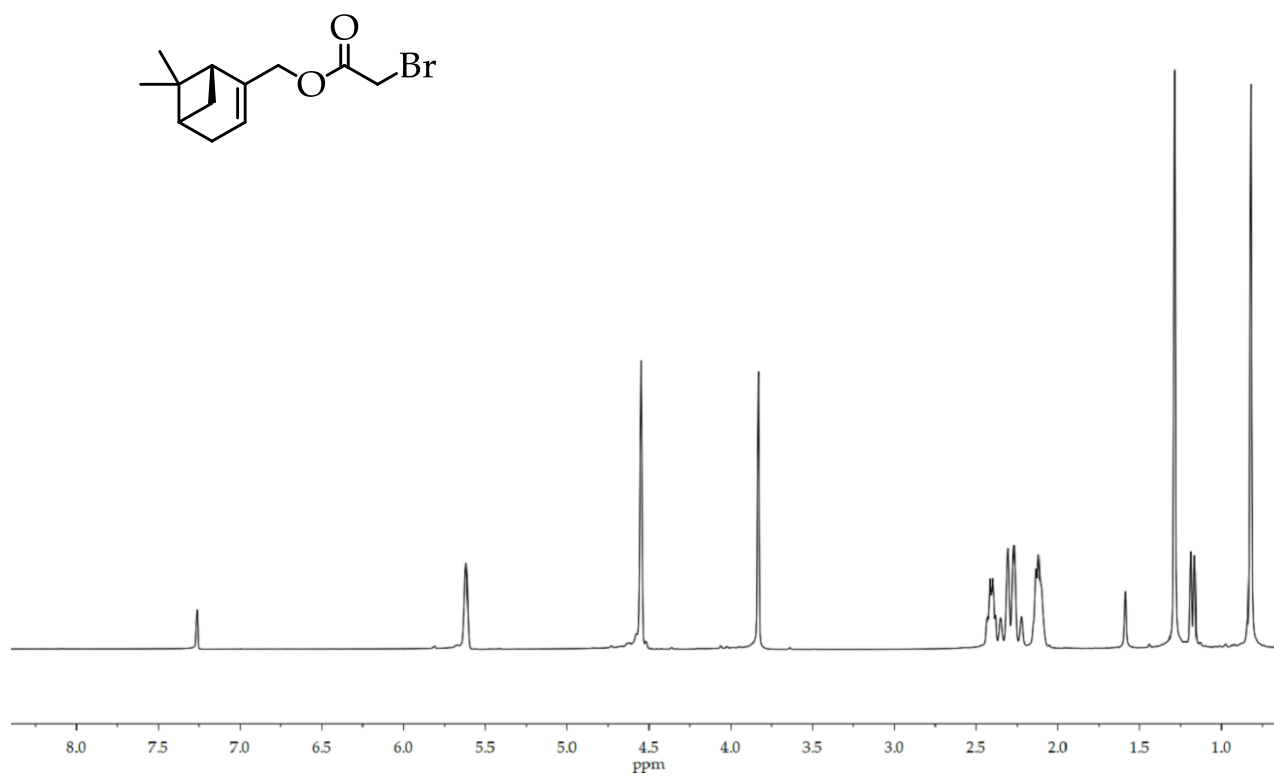


Figure S4. ¹H NMR spectrum of the compound **2d**, CDCl₃, 298 K, 400 MHz.

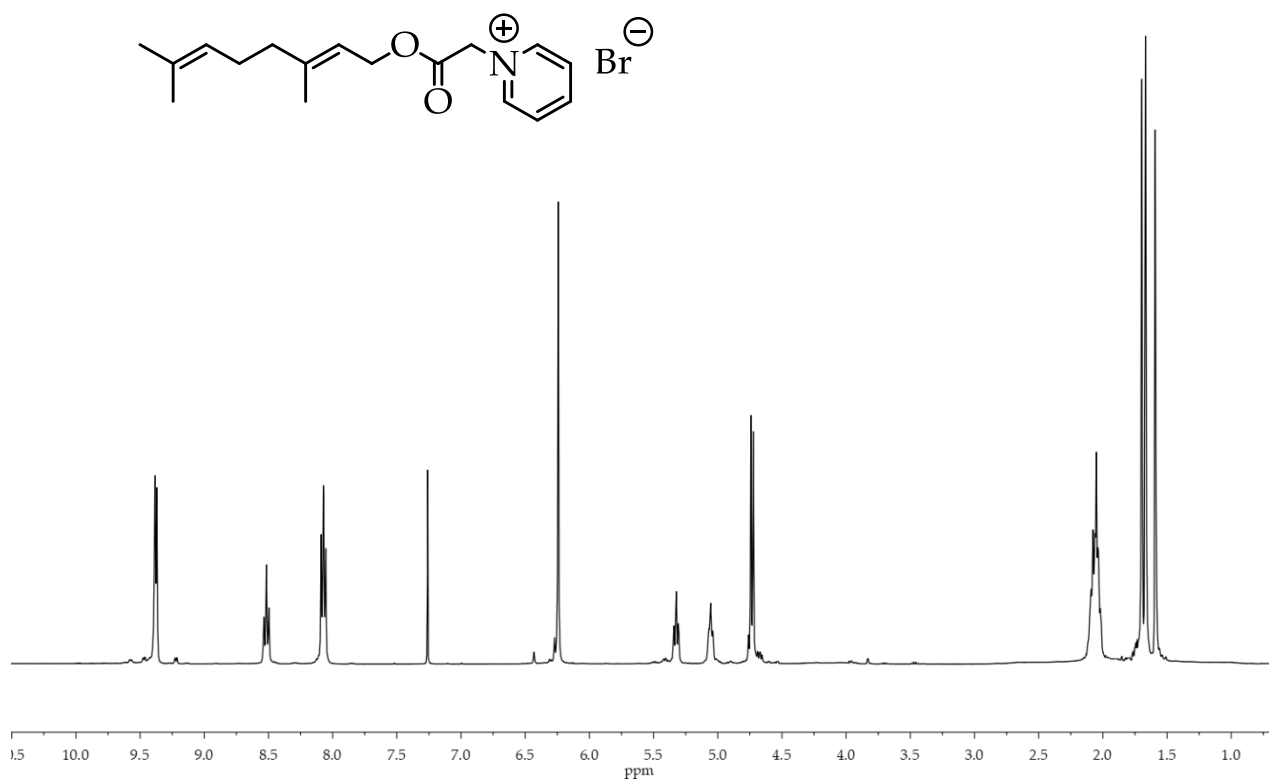


Figure S5. ¹H NMR spectrum of the compound **3a**, CDCl₃, 298 K, 400 MHz.

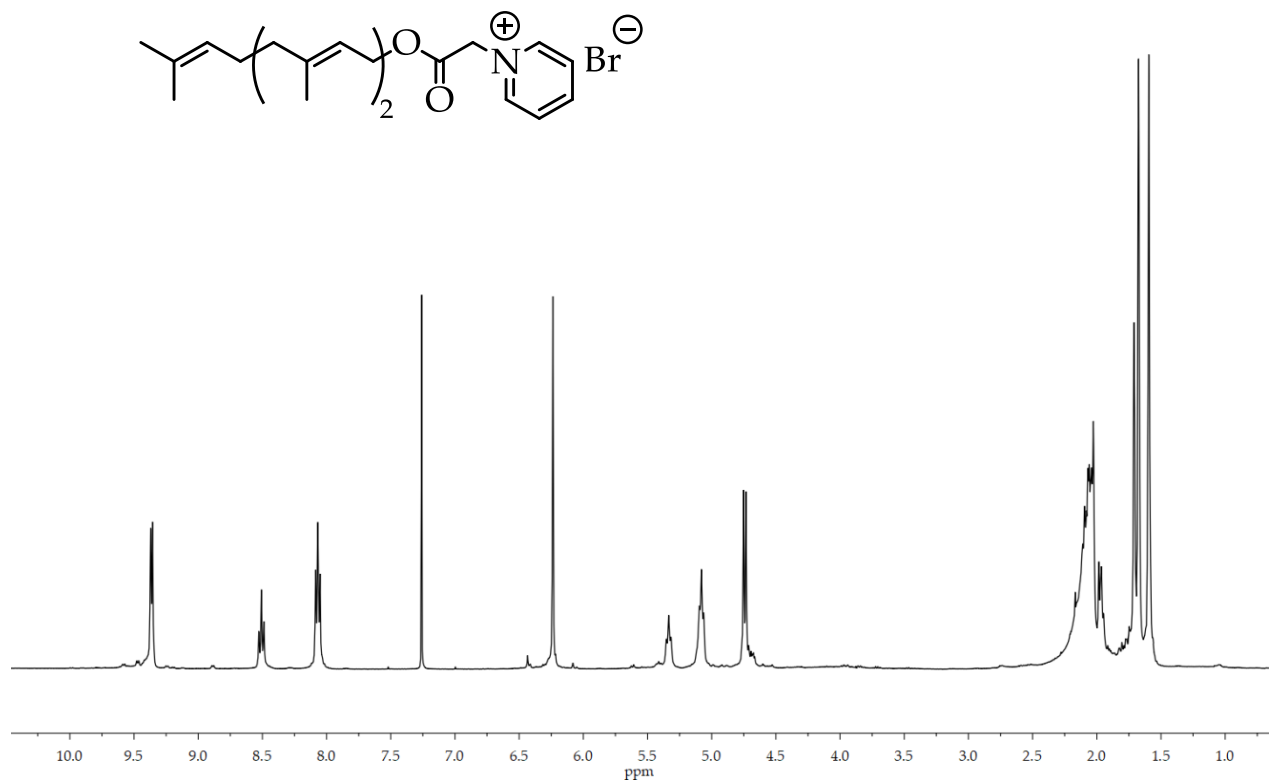


Figure S6. ¹H NMR spectrum of the compound **3b**, CDCl₃, 298 K, 400 MHz.

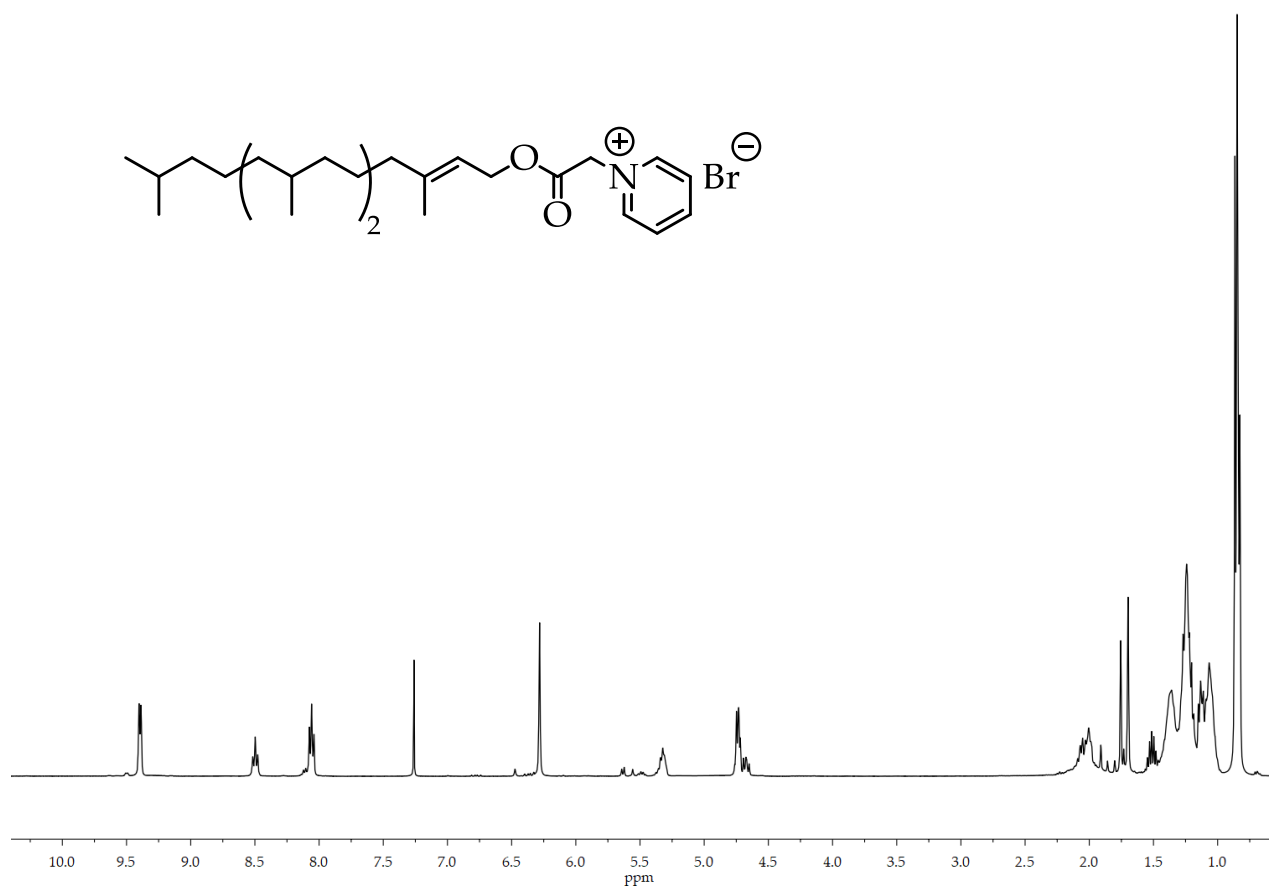


Figure S7. ^1H NMR spectrum of the compound **3c**, CDCl_3 , 298 K, 400 MHz.

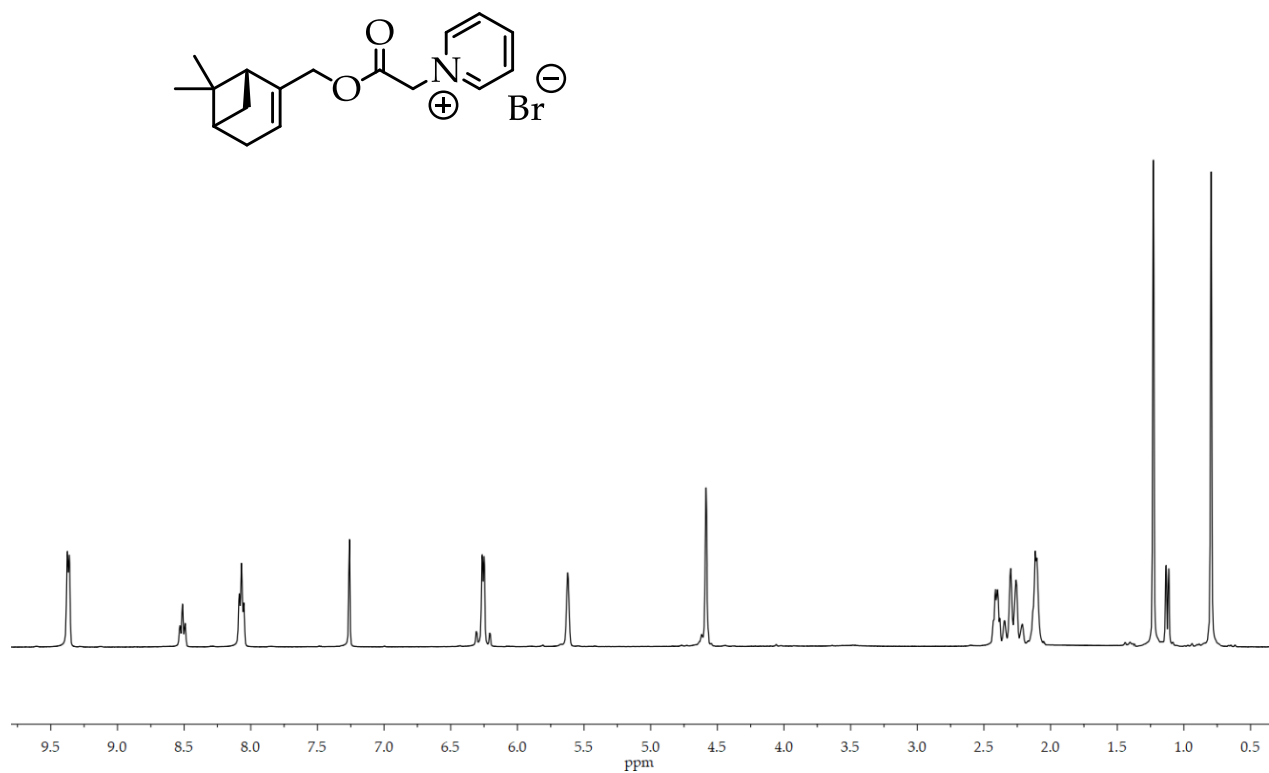


Figure S8. ^1H NMR spectrum of the compound **3d**, CDCl_3 , 298 K, 400 MHz.

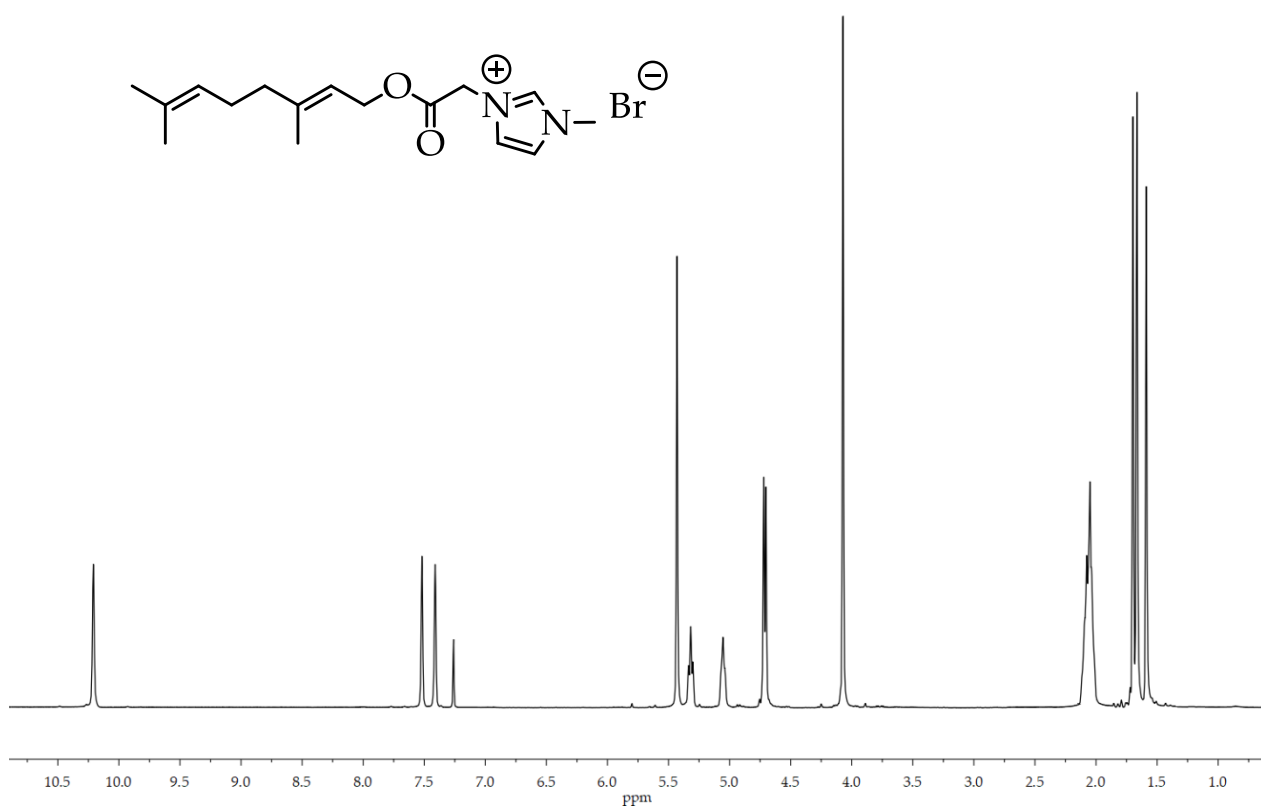


Figure S9. ¹H NMR spectrum of the compound **4a**, CDCl₃, 298 K, 400 MHz.



Figure S10. ¹H NMR spectrum of the compound **4b**, CDCl₃, 298 K, 400 MHz.

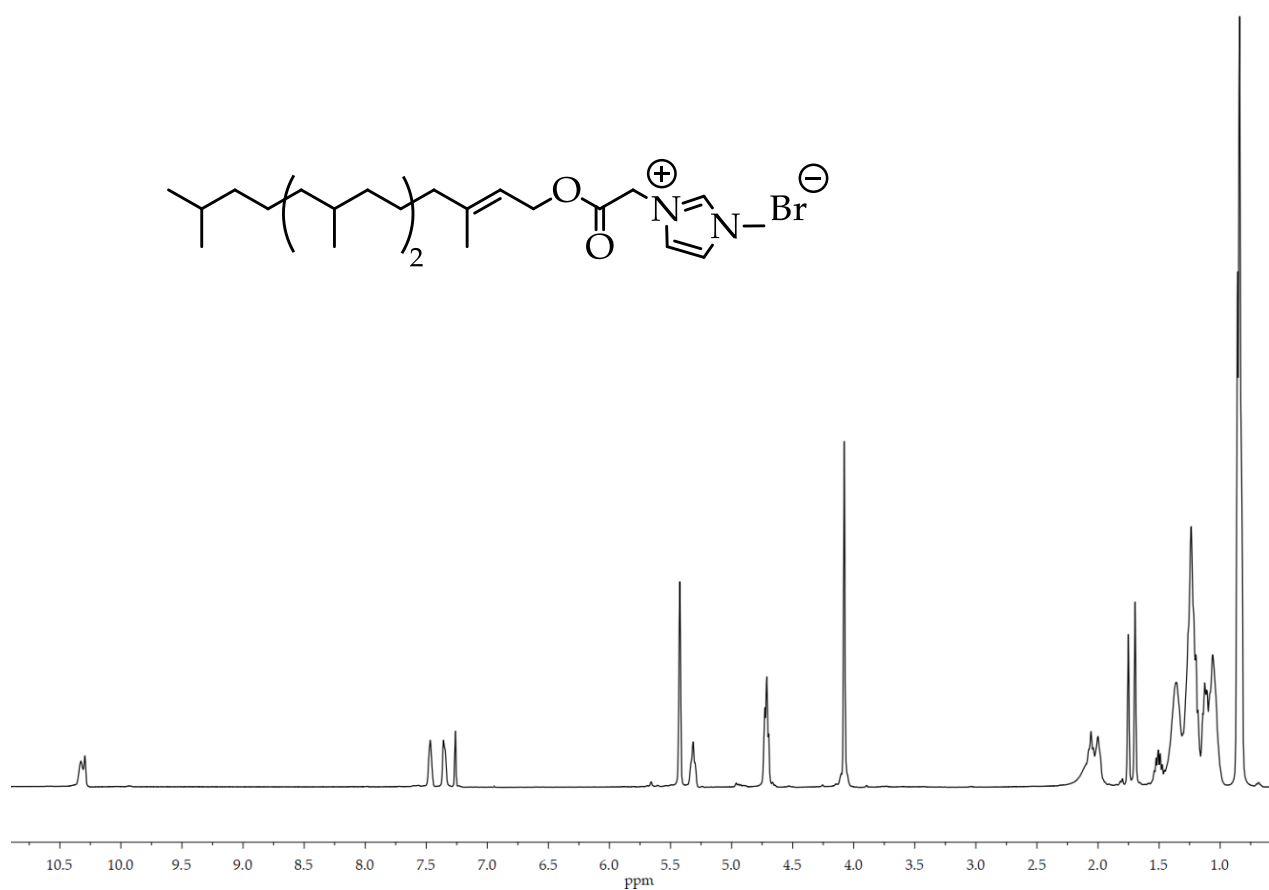


Figure S11. ^1H NMR spectrum of the compound **4c**, CDCl_3 , 298 K, 400 MHz.

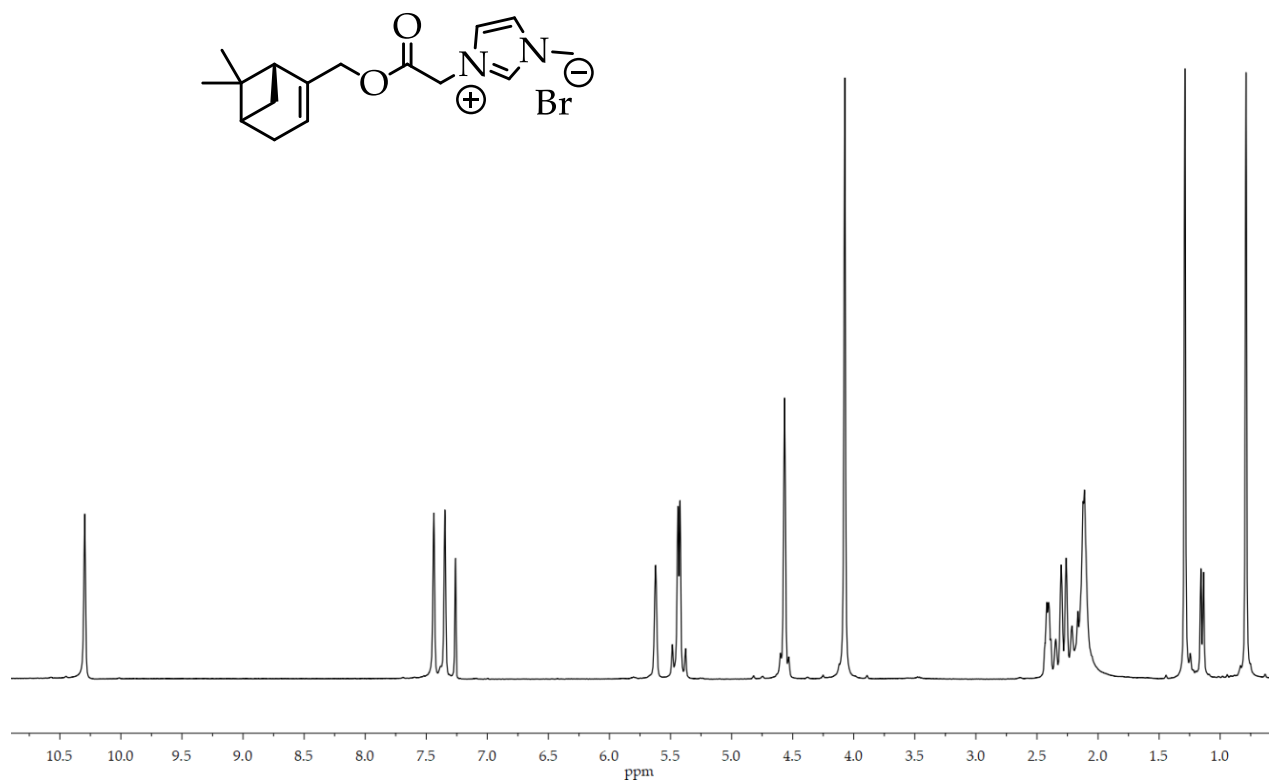


Figure S12. ^1H NMR spectrum of the compound **4d**, CDCl_3 , 298 K, 400 MHz.

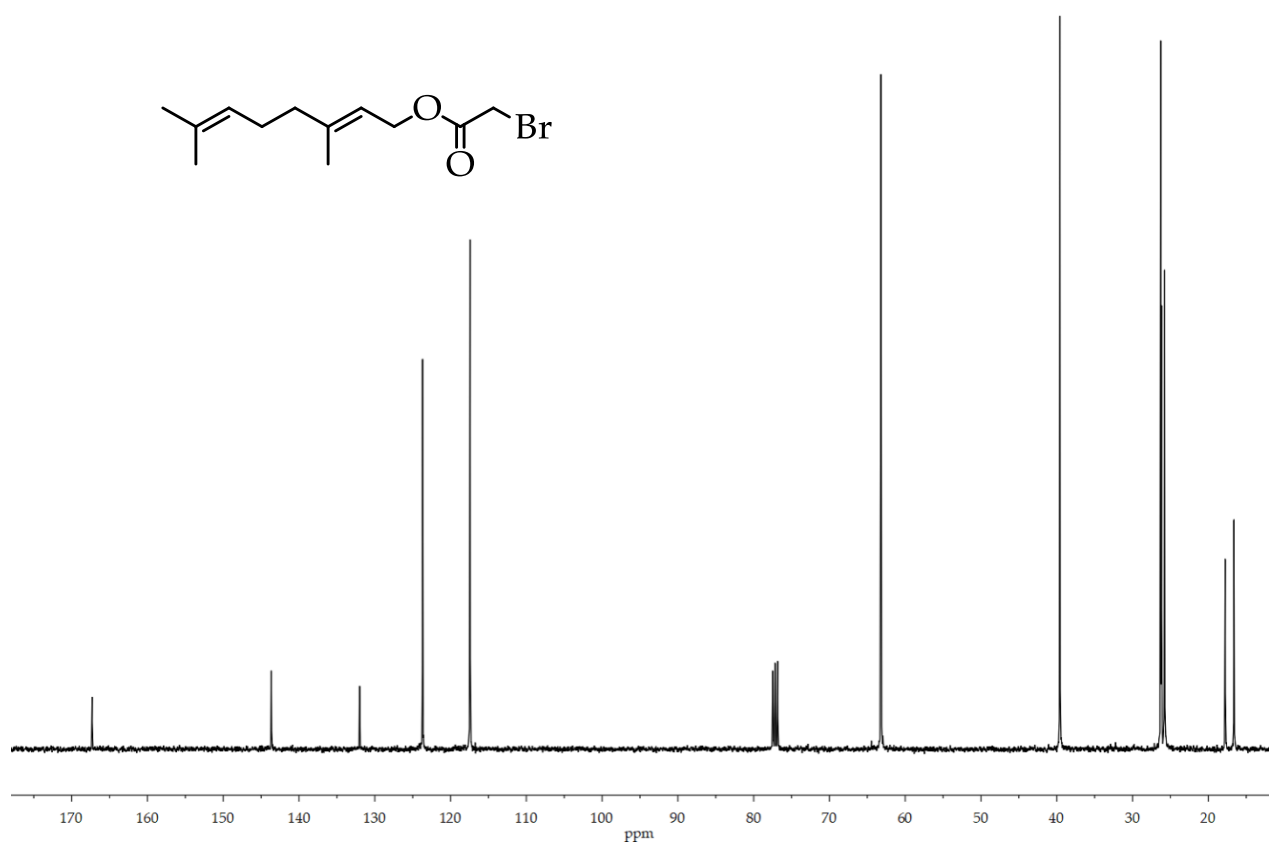


Figure S13. ¹³C NMR spectrum of the compound **2a**, CDCl₃, 298 K, 100 MHz.

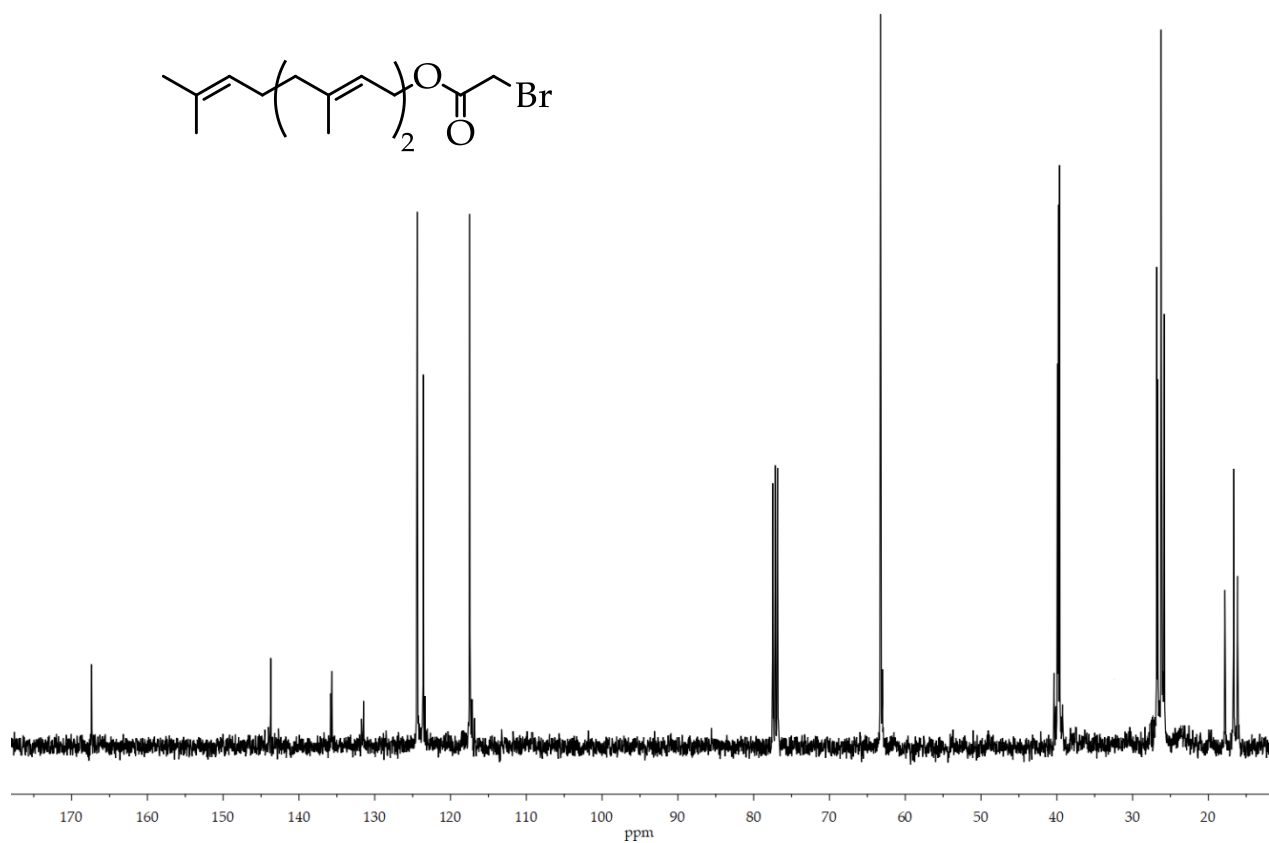


Figure S14. ¹³C NMR spectrum of the compound **2b**, CDCl₃, 298 K, 100 MHz.

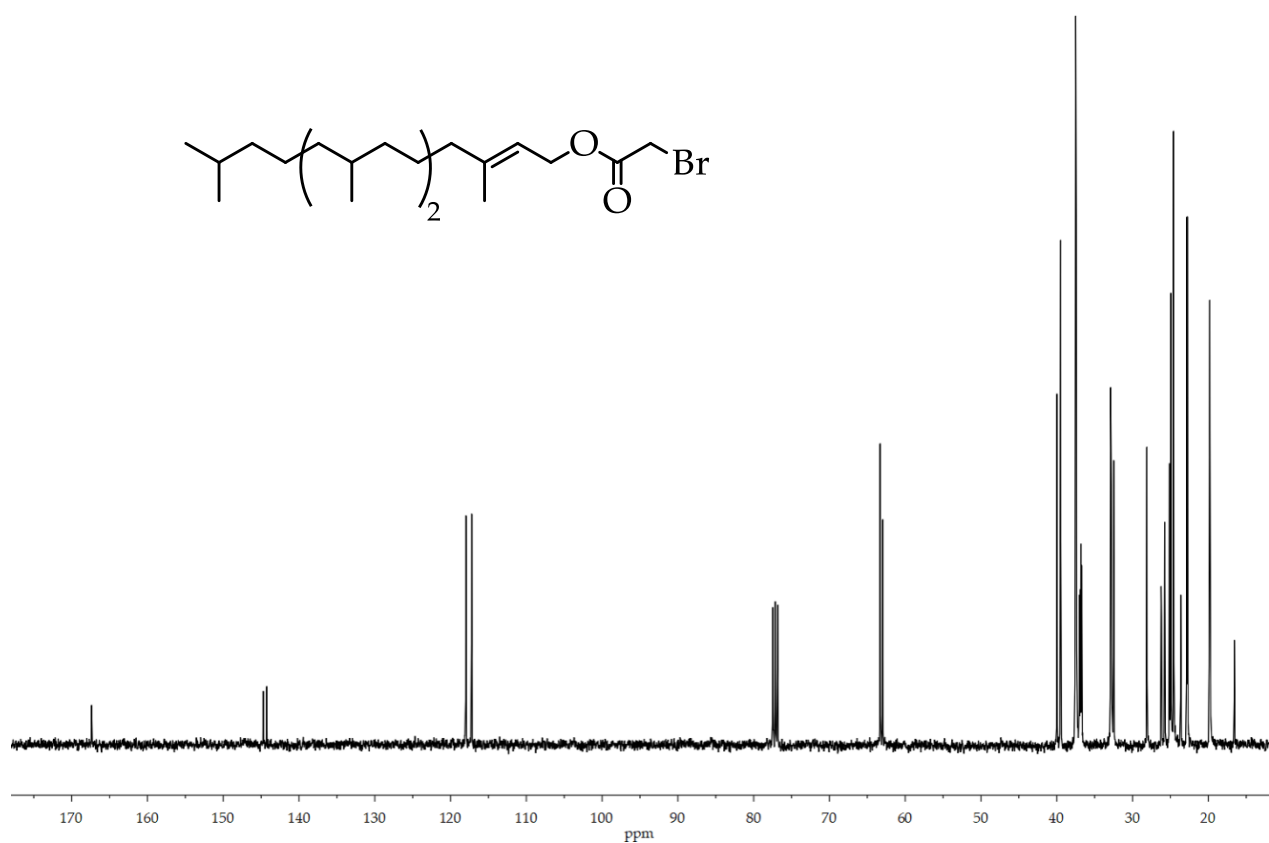


Figure S15. ¹³C NMR spectrum of the compound **2c**, CDCl₃, 298 K, 100 MHz.

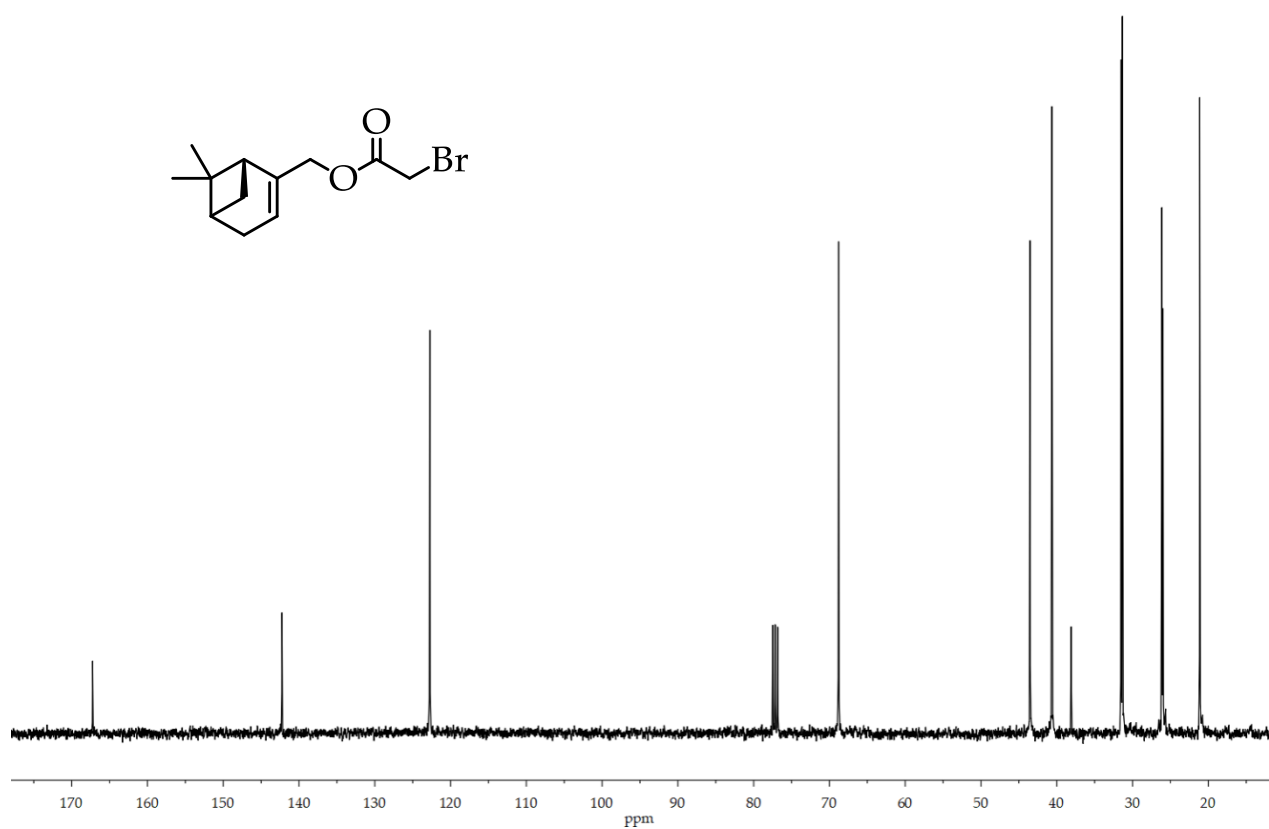


Figure S16. ¹³C NMR spectrum of the compound **2d**, CDCl₃, 298 K, 100 MHz.

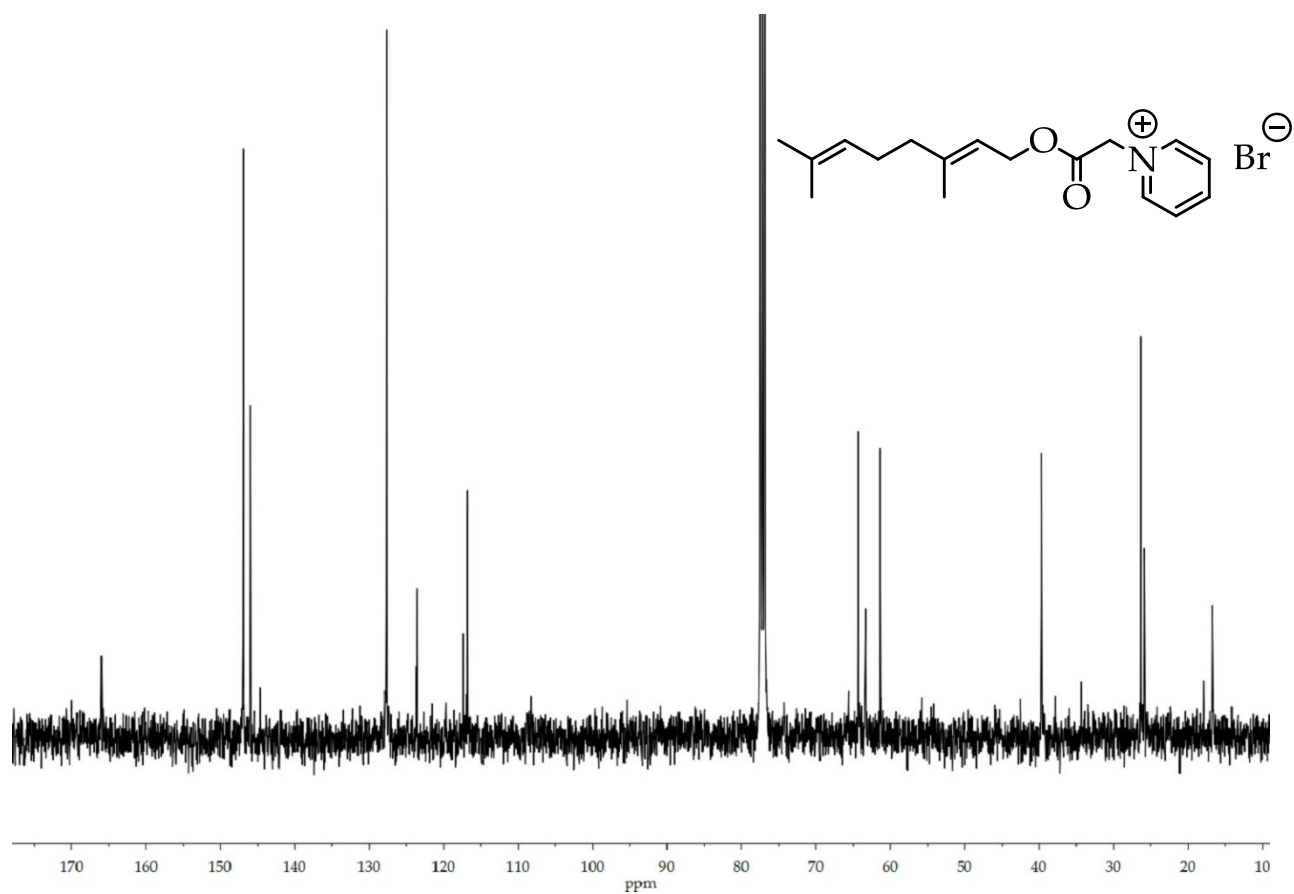


Figure S17. ¹³C NMR spectrum of the compound **3a**, CDCl₃, 298 K, 100 MHz.

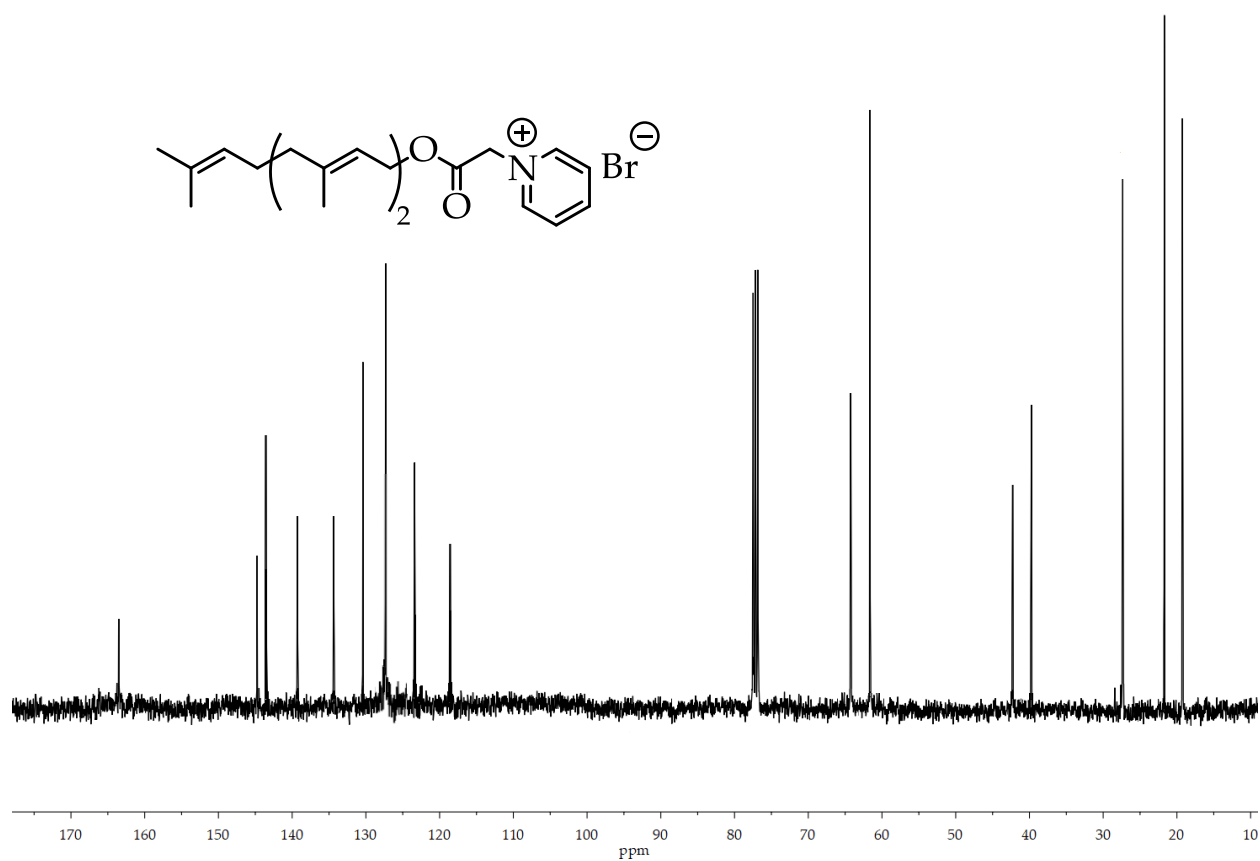


Figure S18. ¹³C NMR spectrum of the compound **3b**, CDCl₃, 298 K, 100 MHz.

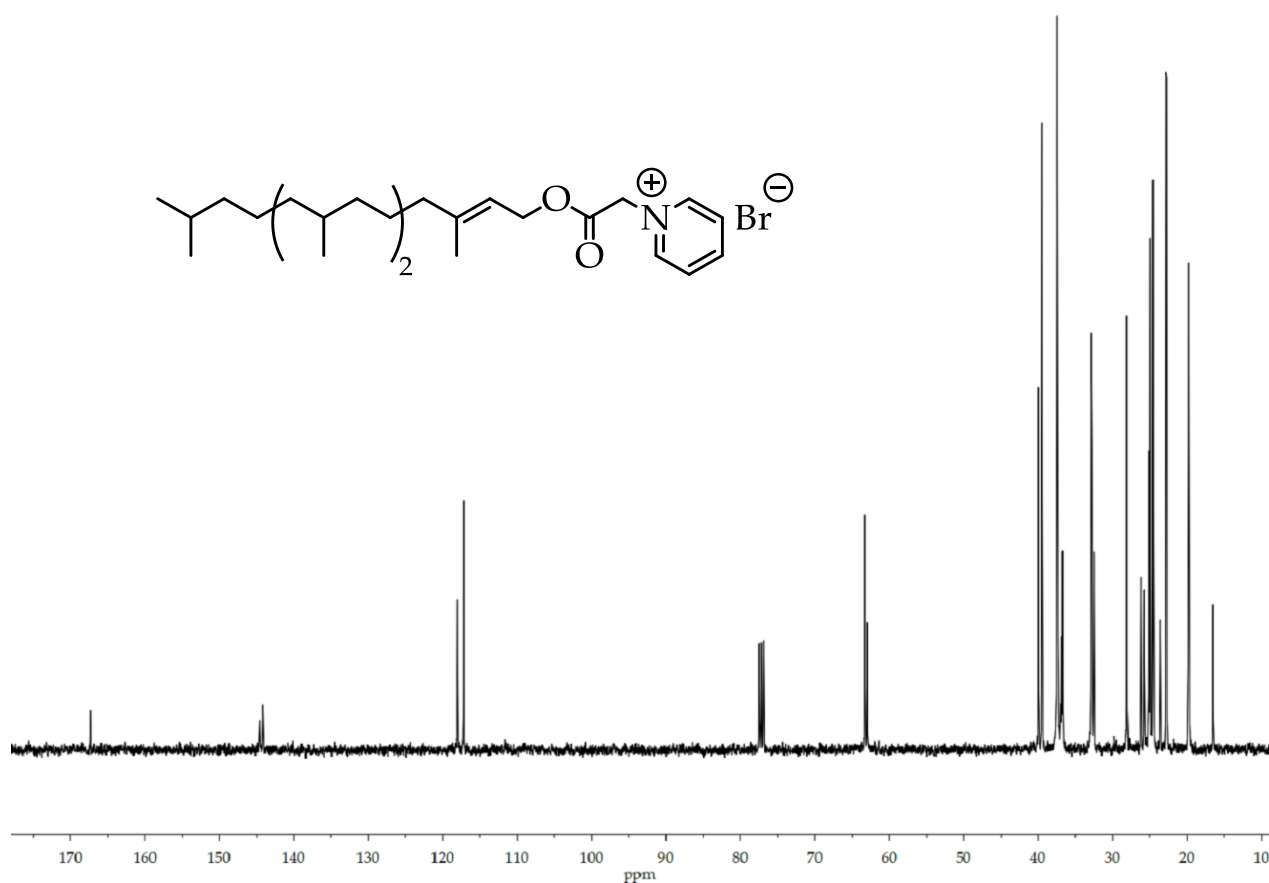


Figure S19. ¹³C NMR spectrum of the compound **3c**, CDCl₃, 298 K, 100 MHz.

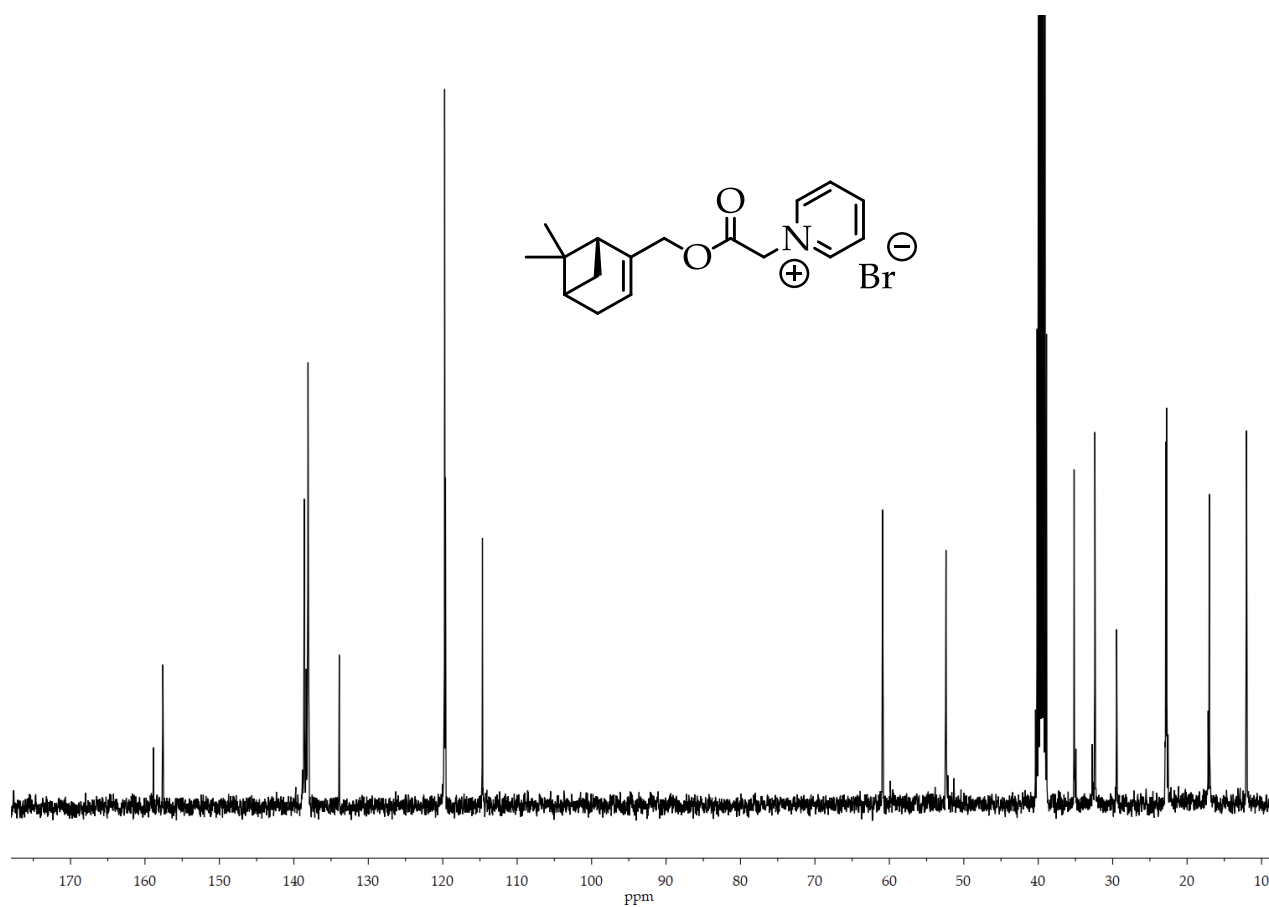


Figure S20. ¹³C NMR spectrum of the compound **3d**, DMSO-d₆, 298 K, 100 MHz.

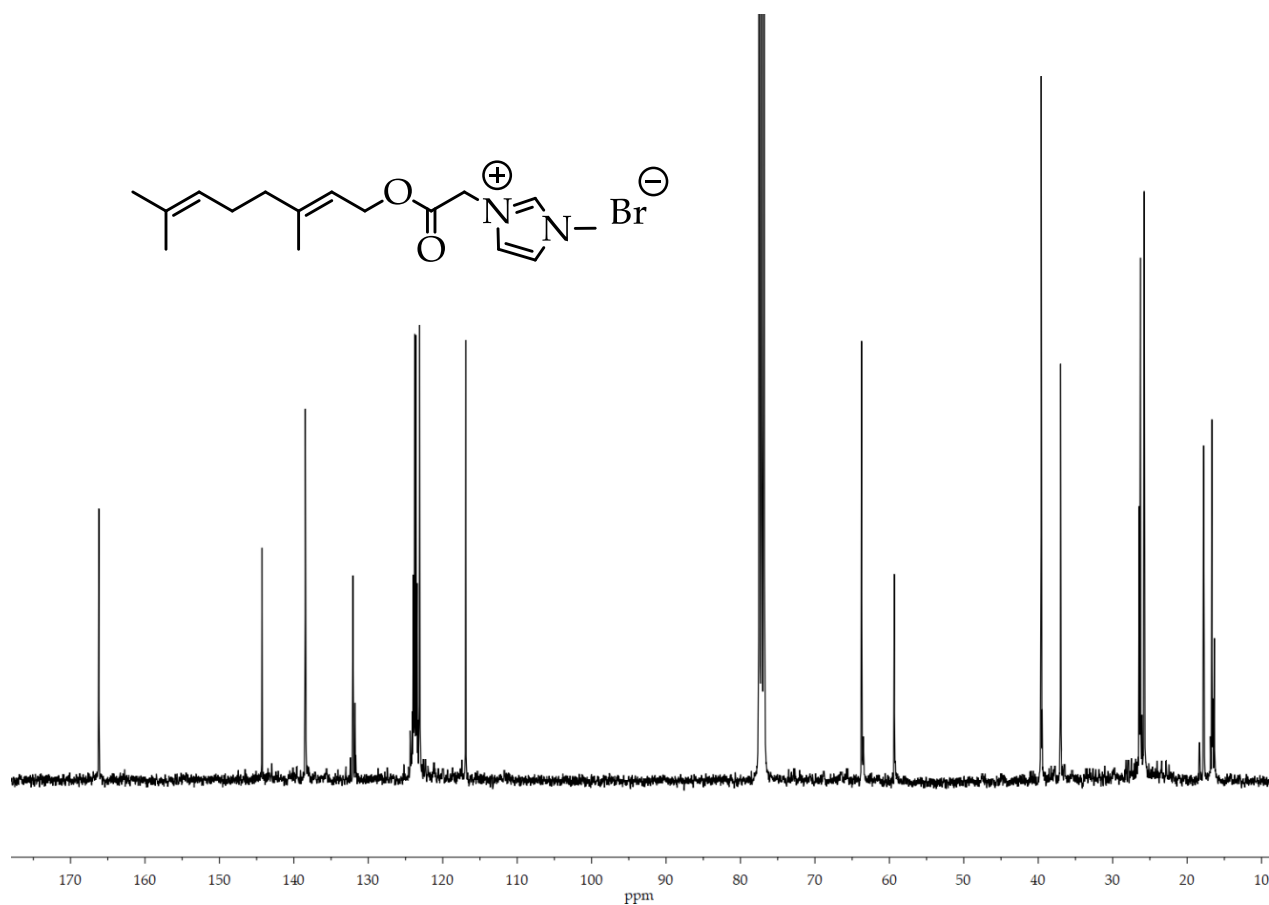


Figure S21. ¹³C NMR spectrum of the compound **4a**, CDCl₃, 298 K, 100 MHz.

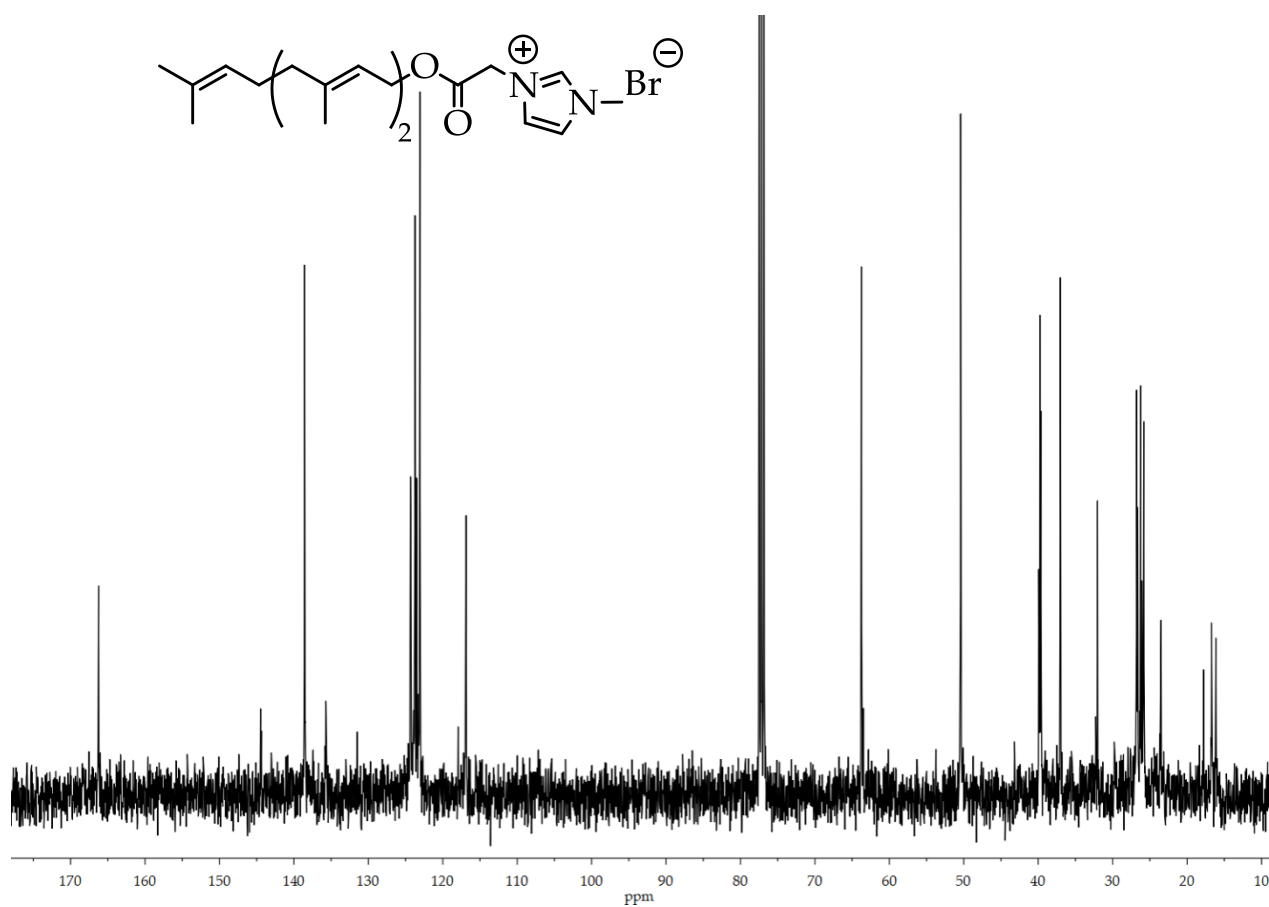


Figure S22. ¹³C NMR spectrum of the compound **4b**, CDCl₃, 298 K, 100 MHz.

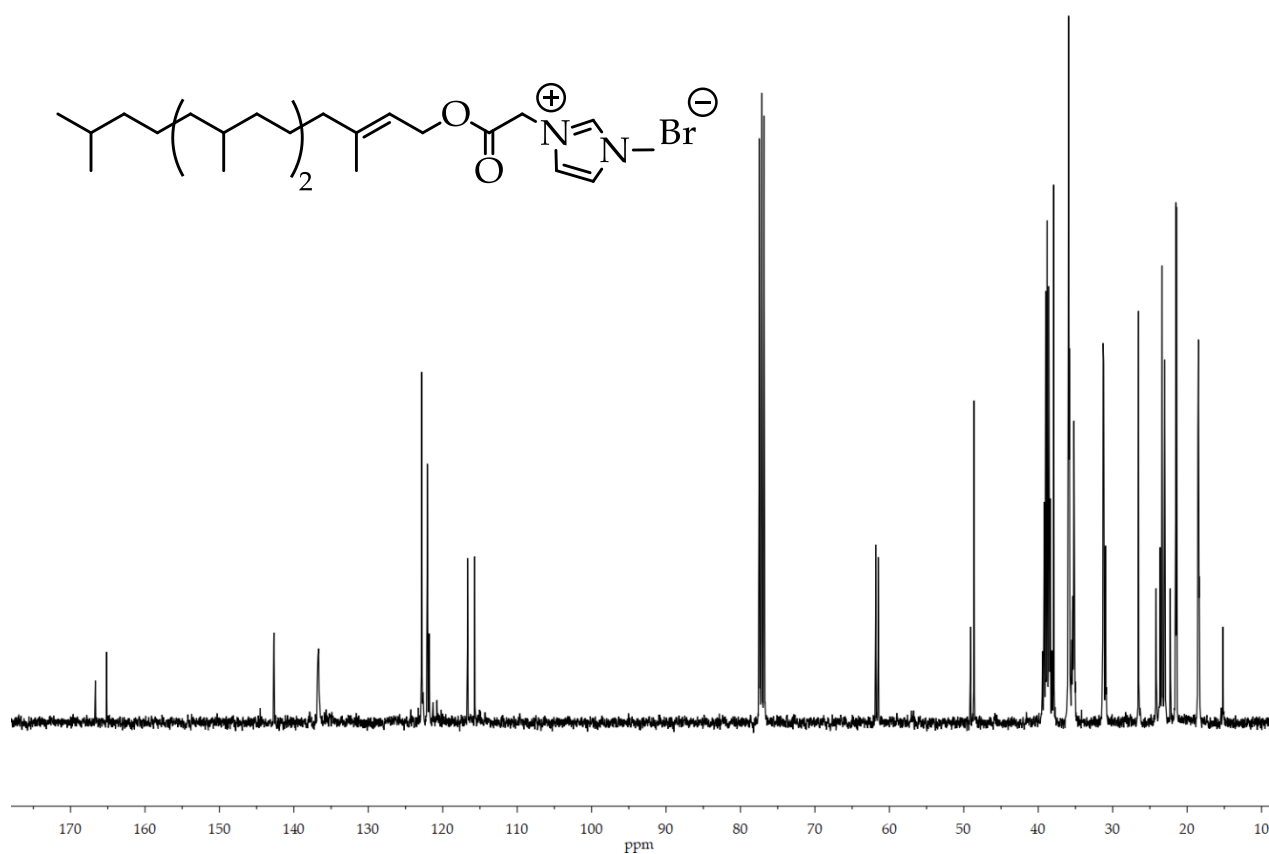


Figure S23. ¹³C NMR spectrum of the compound **4c**, CDCl₃, 298 K, 100 MHz.

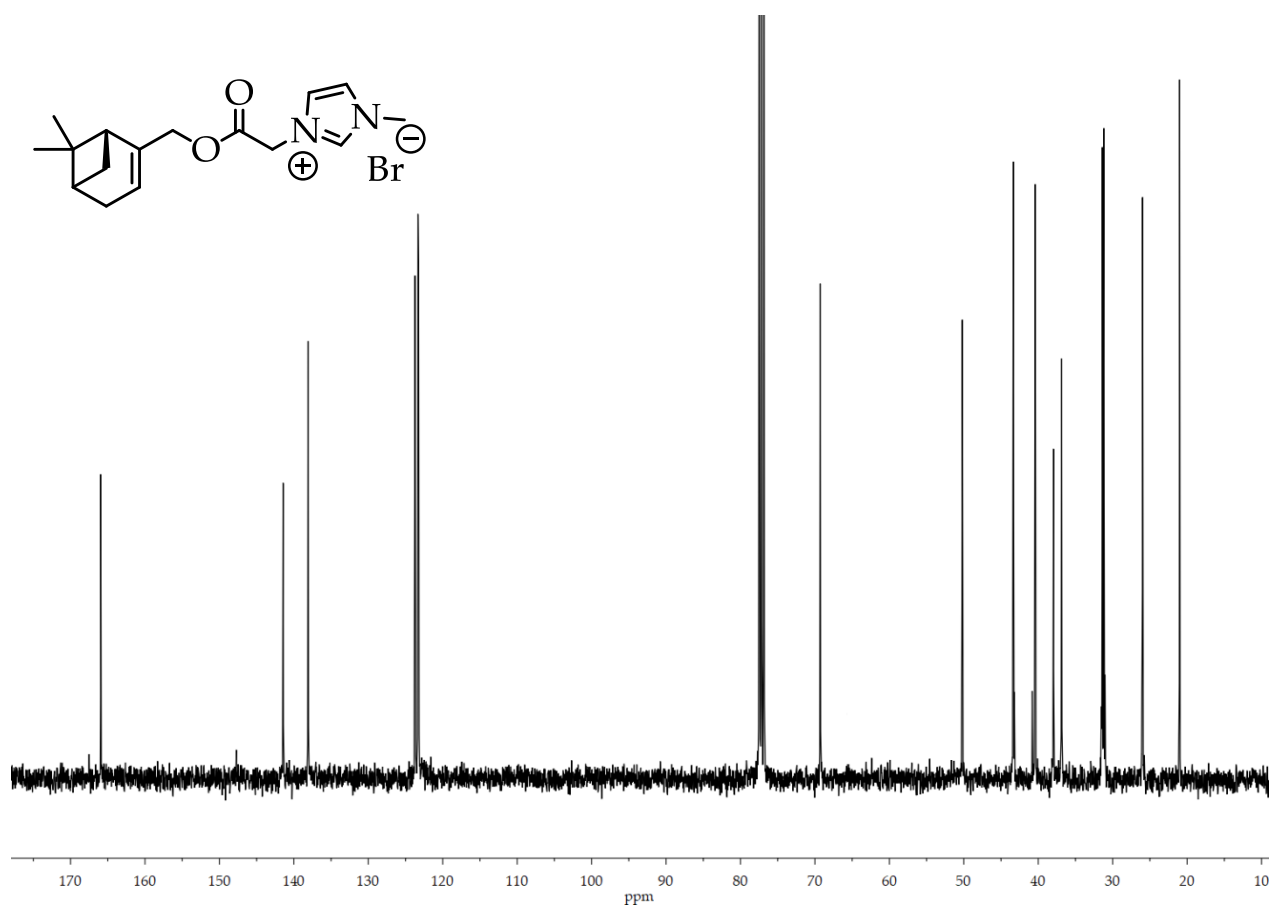


Figure S24. ¹³C NMR spectrum of the compound **4d**, CDCl₃, 298 K, 100 MHz.

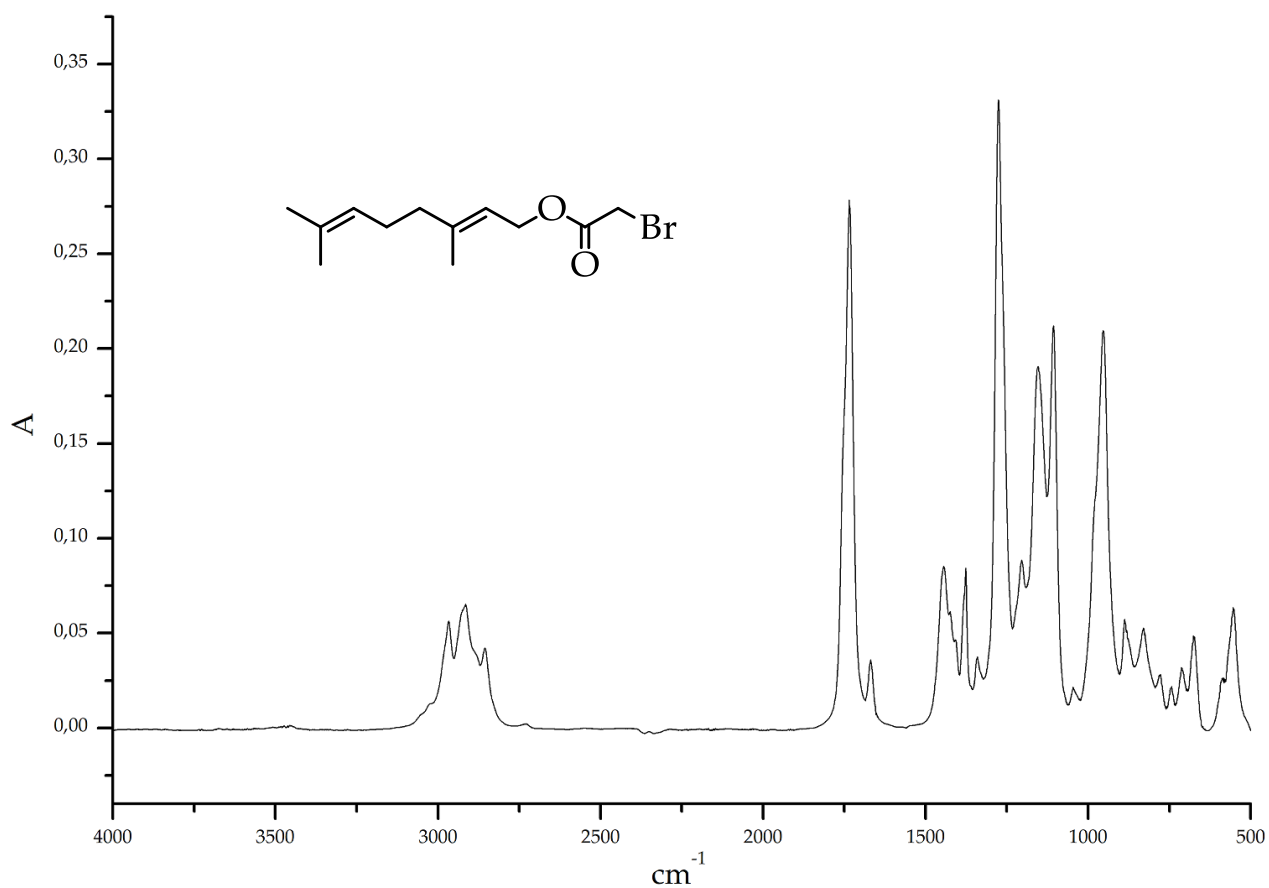


Figure S25. FT-IR spectrum of the compound **2a**.

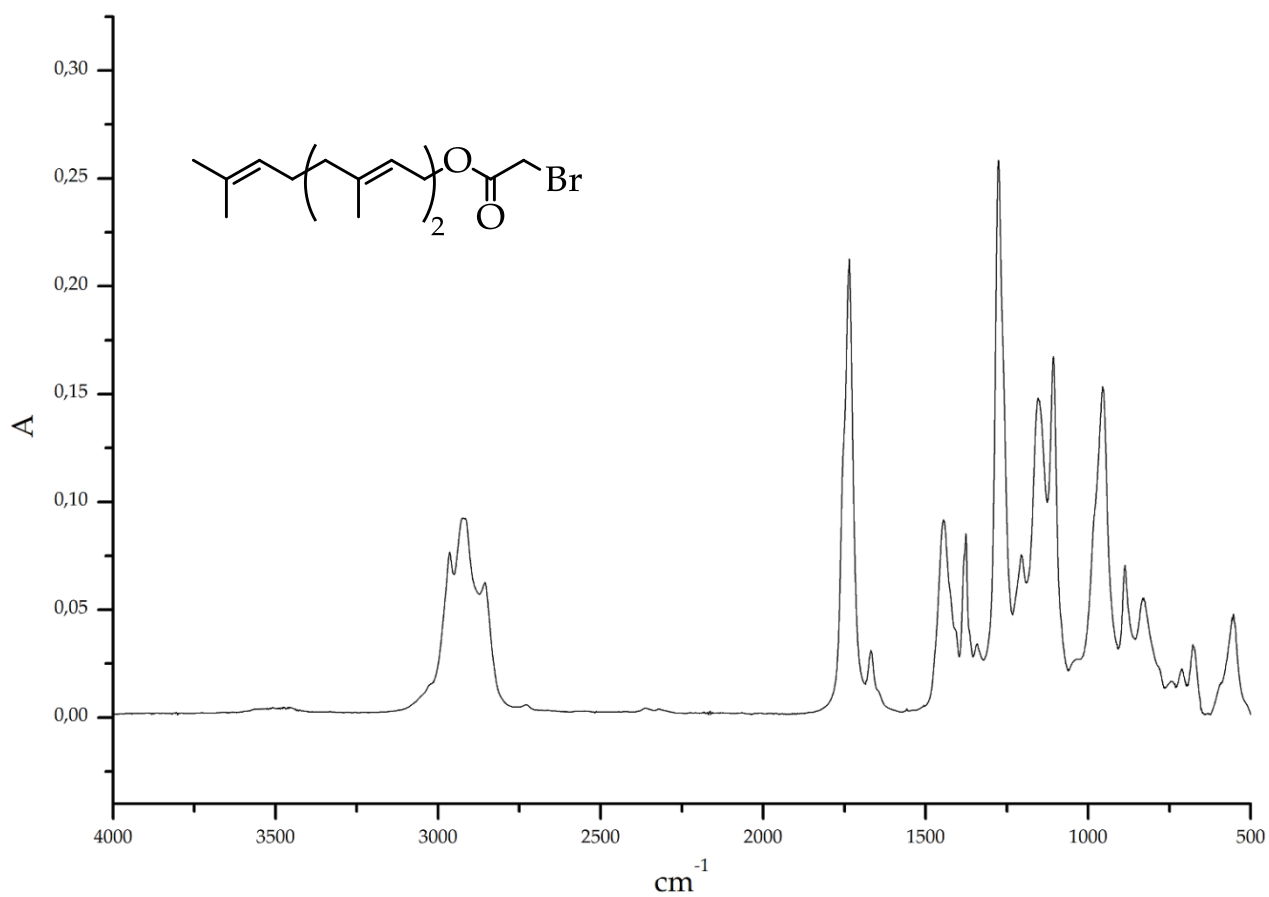


Figure S26. FT-IR spectrum of the compound **2b**.

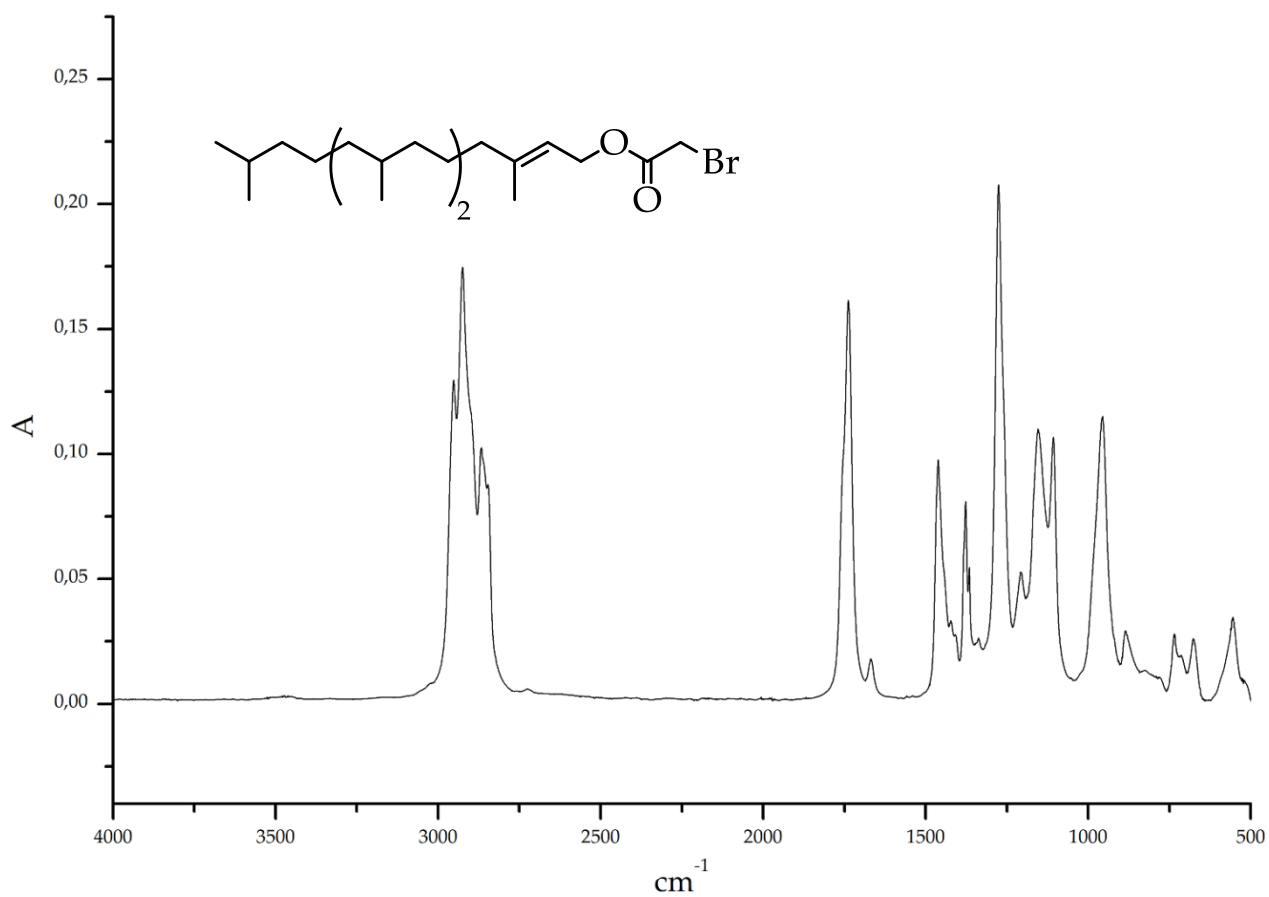


Figure S27. FT-IR spectrum of the compound **2c**.

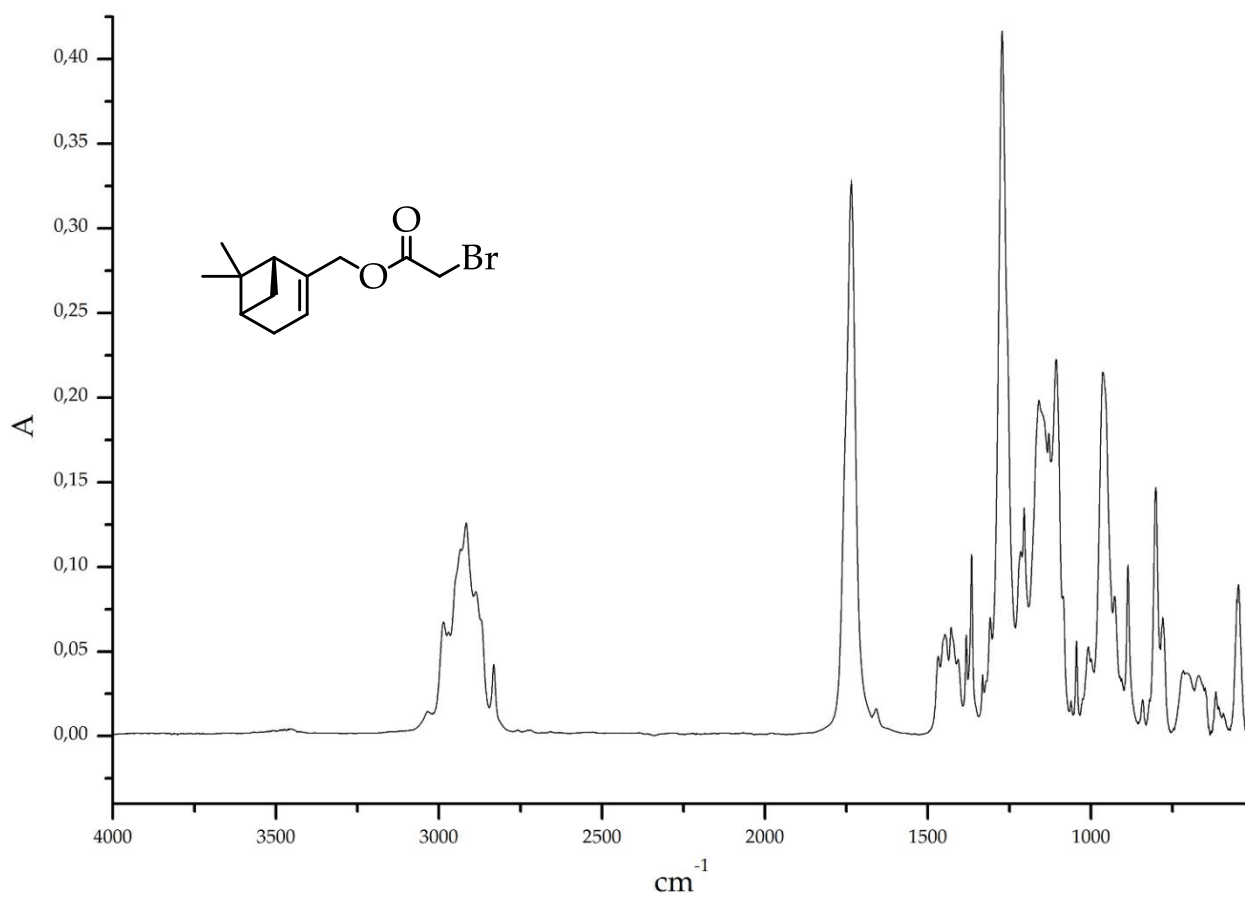


Figure S28. FT-IR spectrum of the compound **2d**.

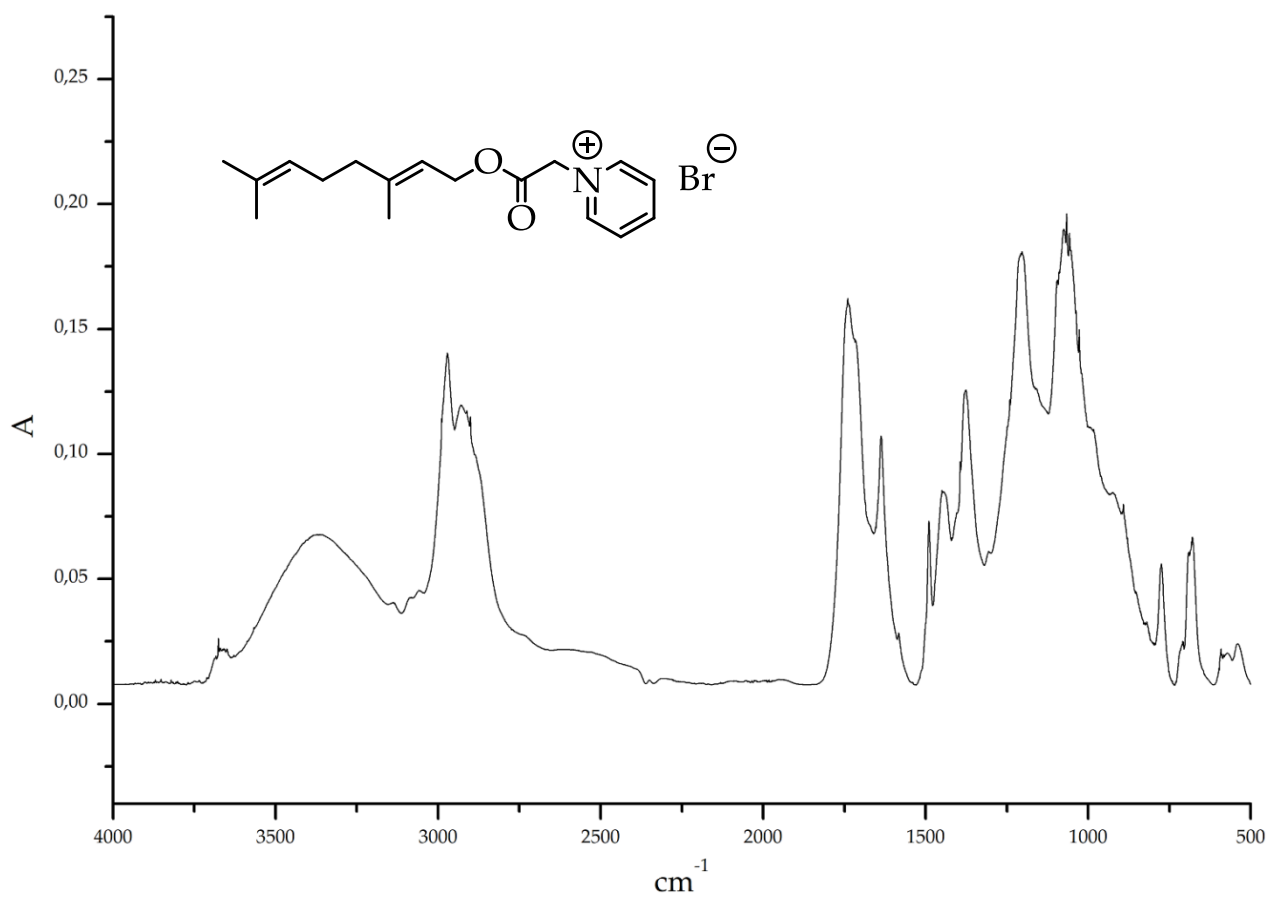


Figure S29. FT-IR spectrum of the compound **3a**.

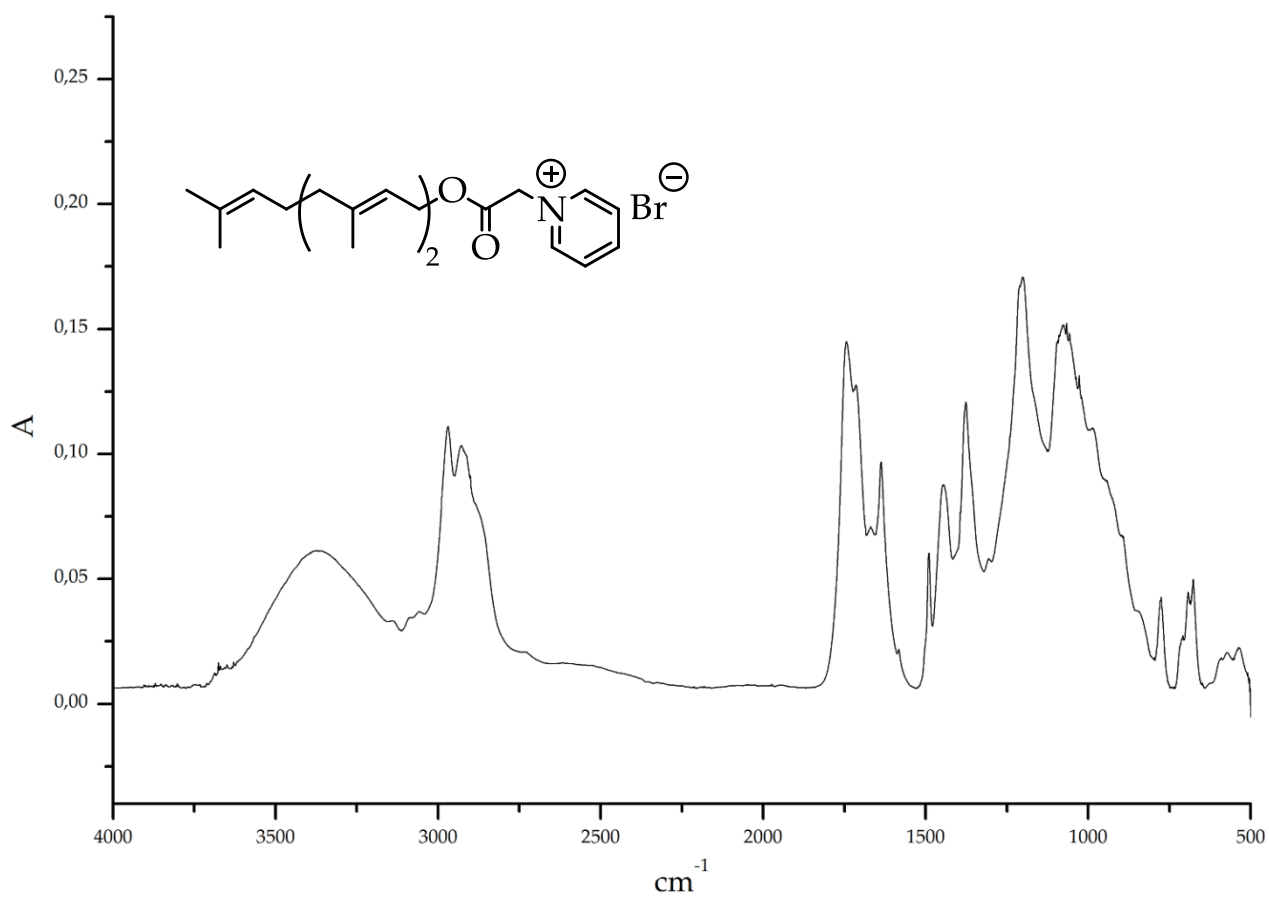


Figure S30. FT-IR spectrum of the compound **3b**.

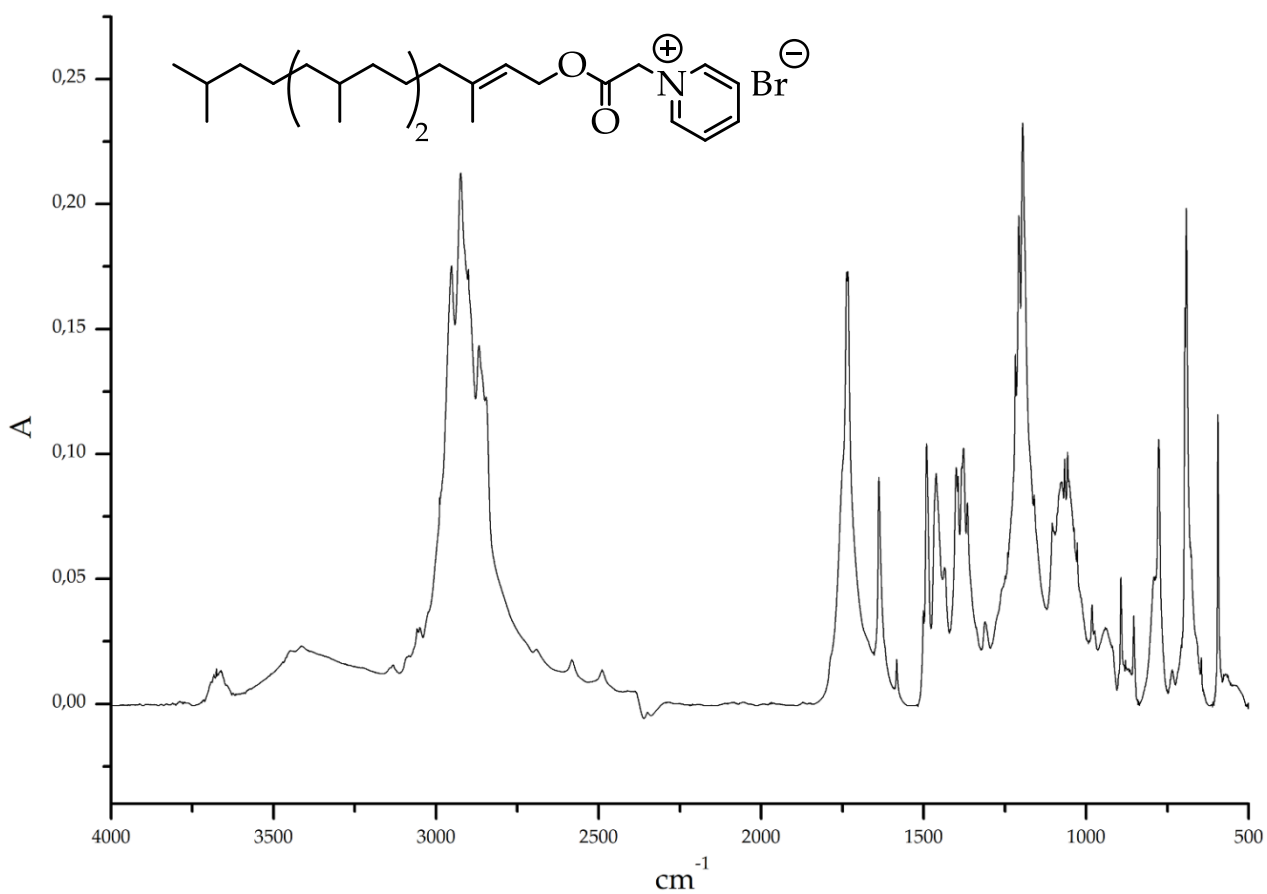


Figure S31. FT-IR spectrum of the compound **3c**.

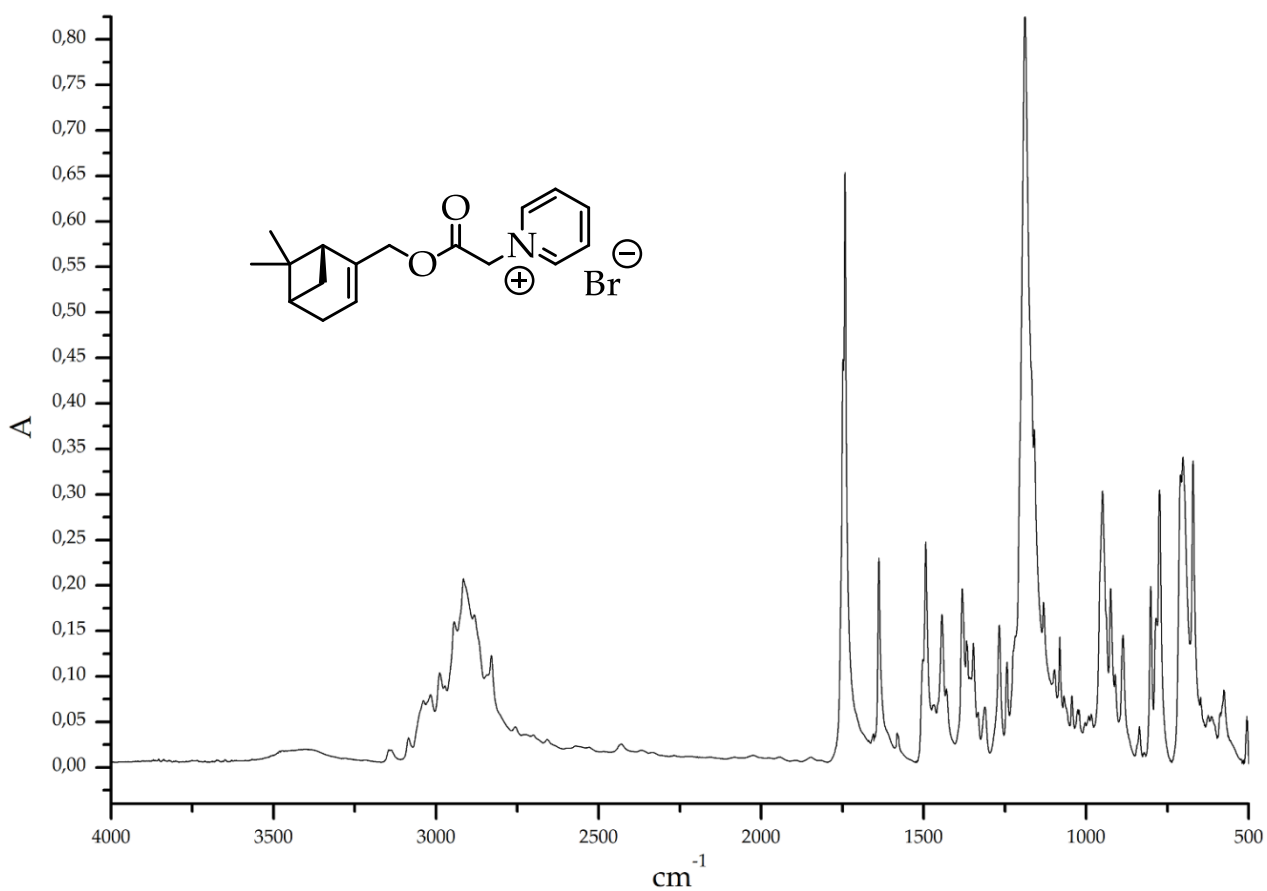


Figure S32. FT-IR spectrum of the compound **3d**.

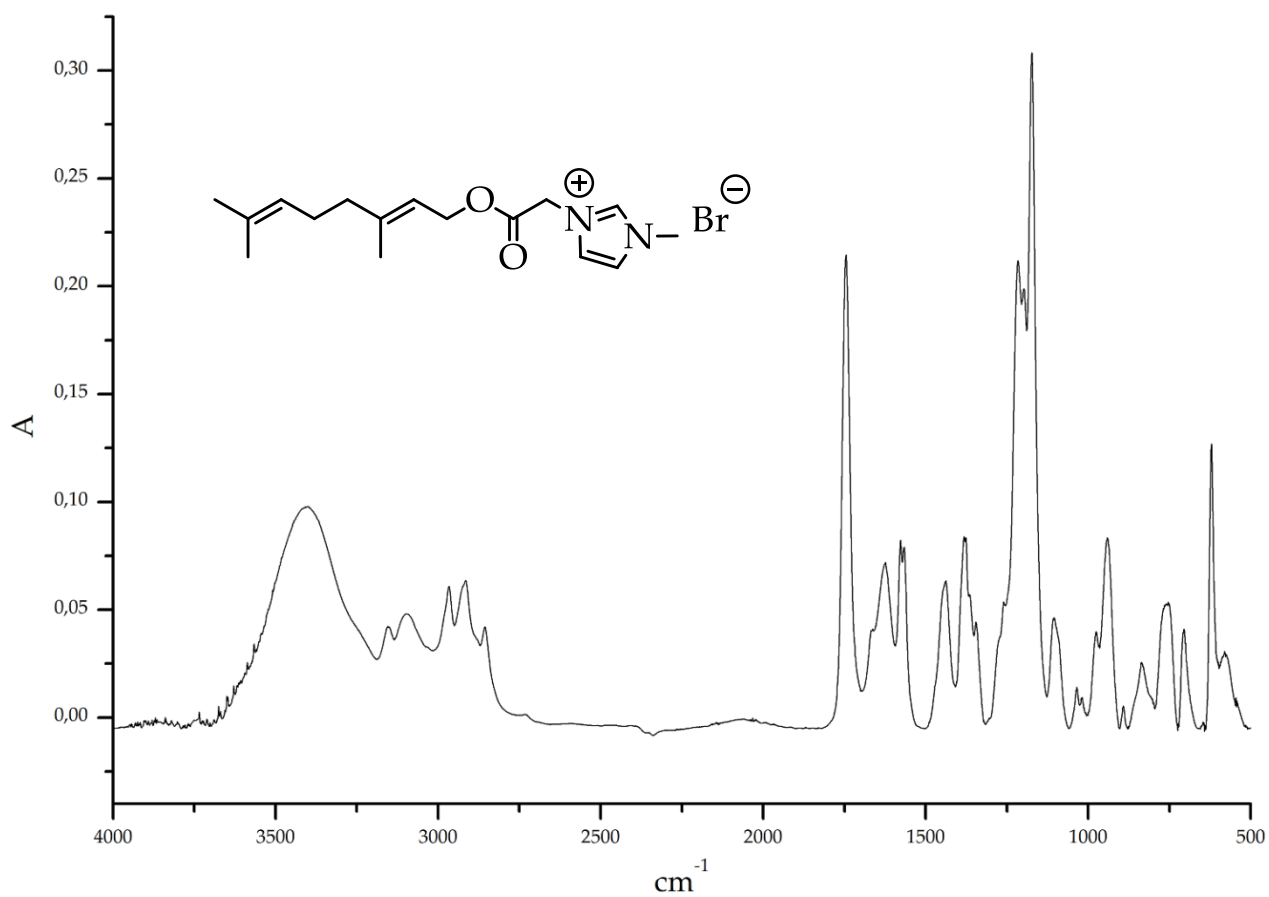


Figure S33. FT-IR spectrum of the compound **4a**.

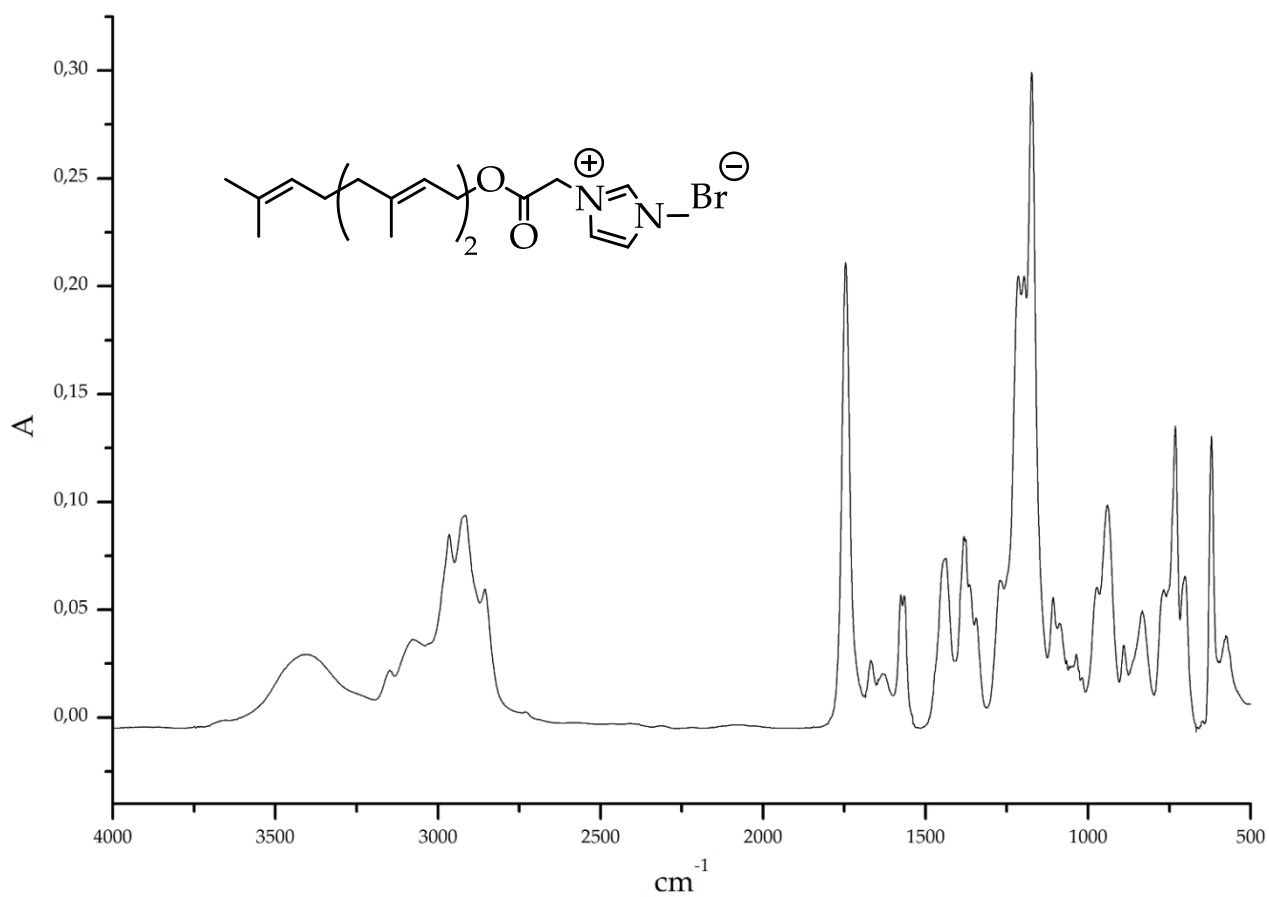


Figure S34. FT-IR spectrum of the compound **4b**.

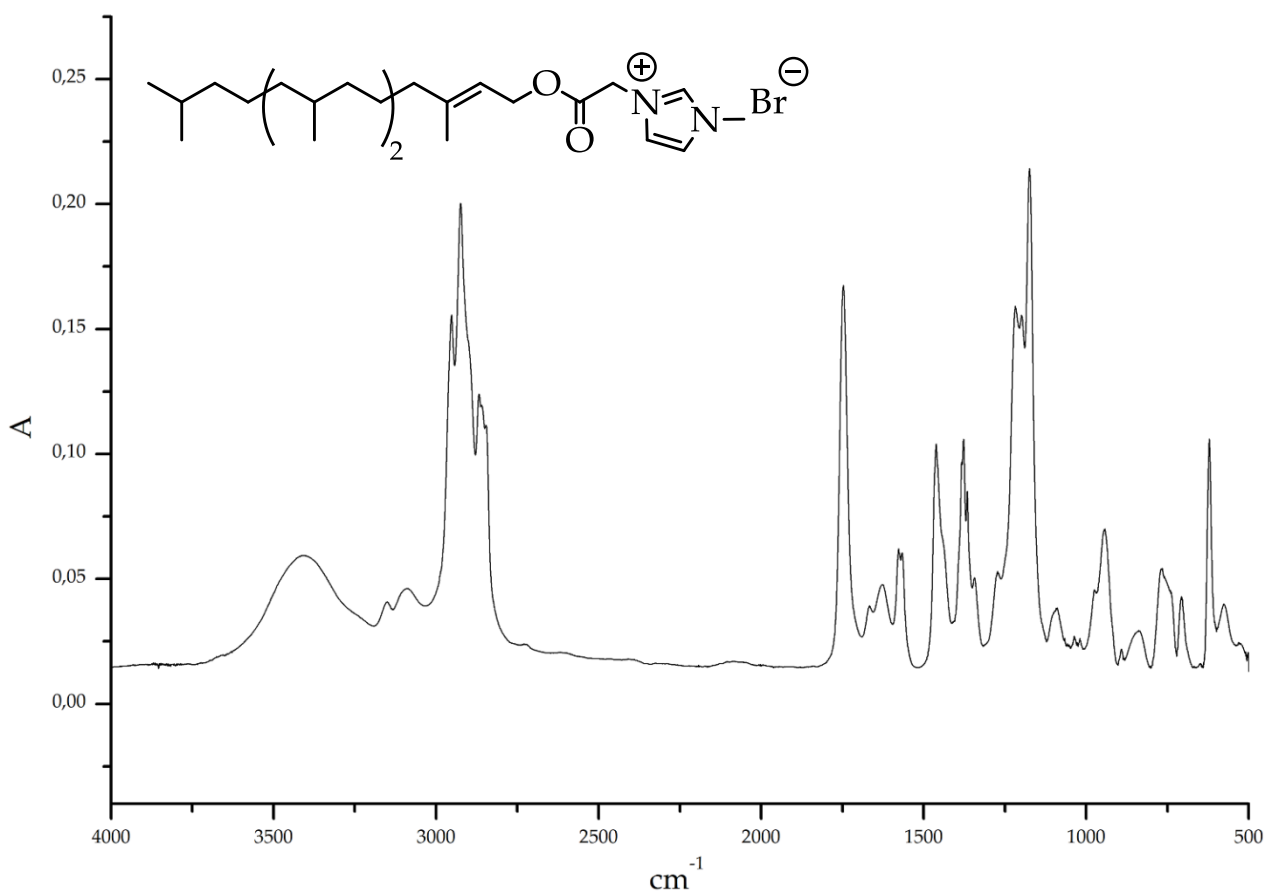


Figure S35. FT-IR spectrum of the compound **4c**.

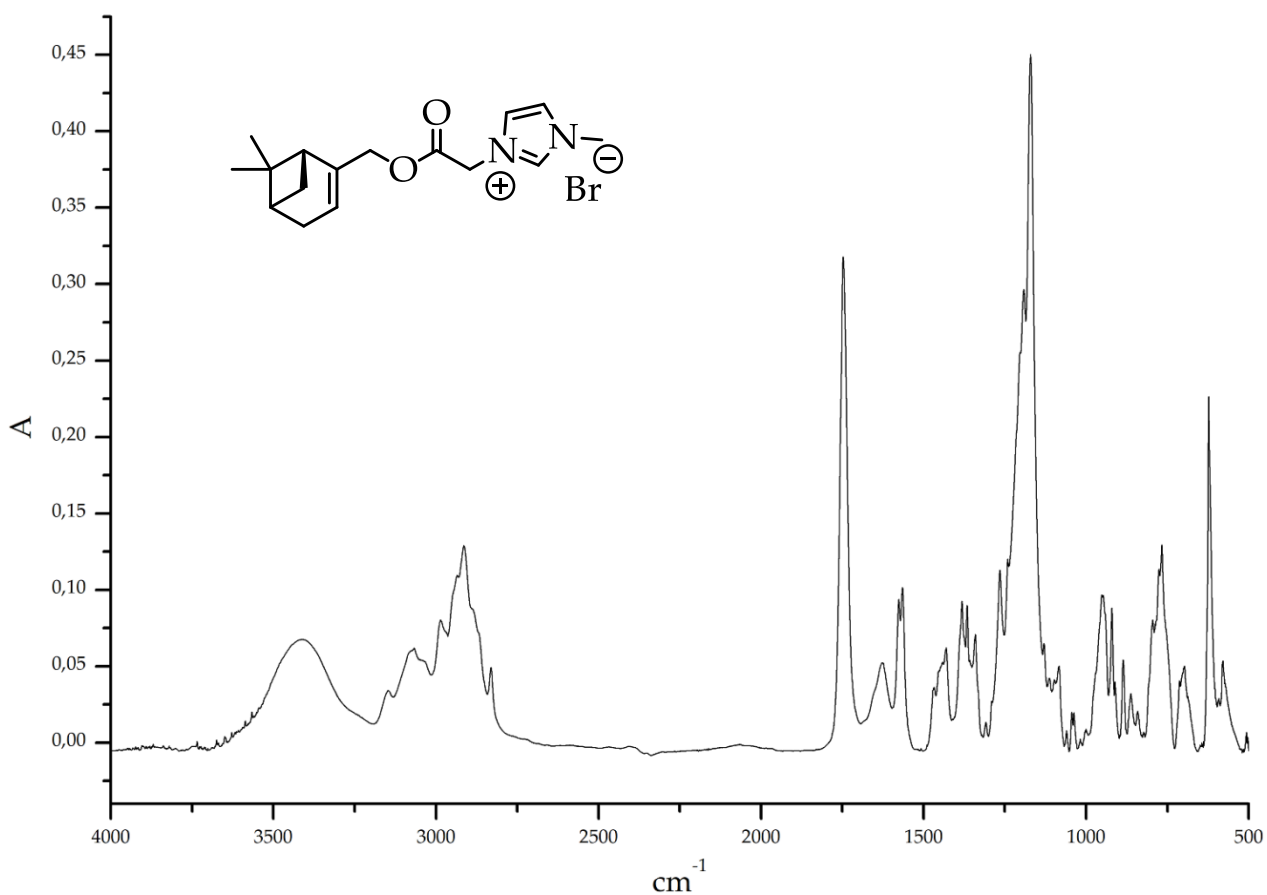


Figure S36. FT-IR spectrum of the compound **4d**.

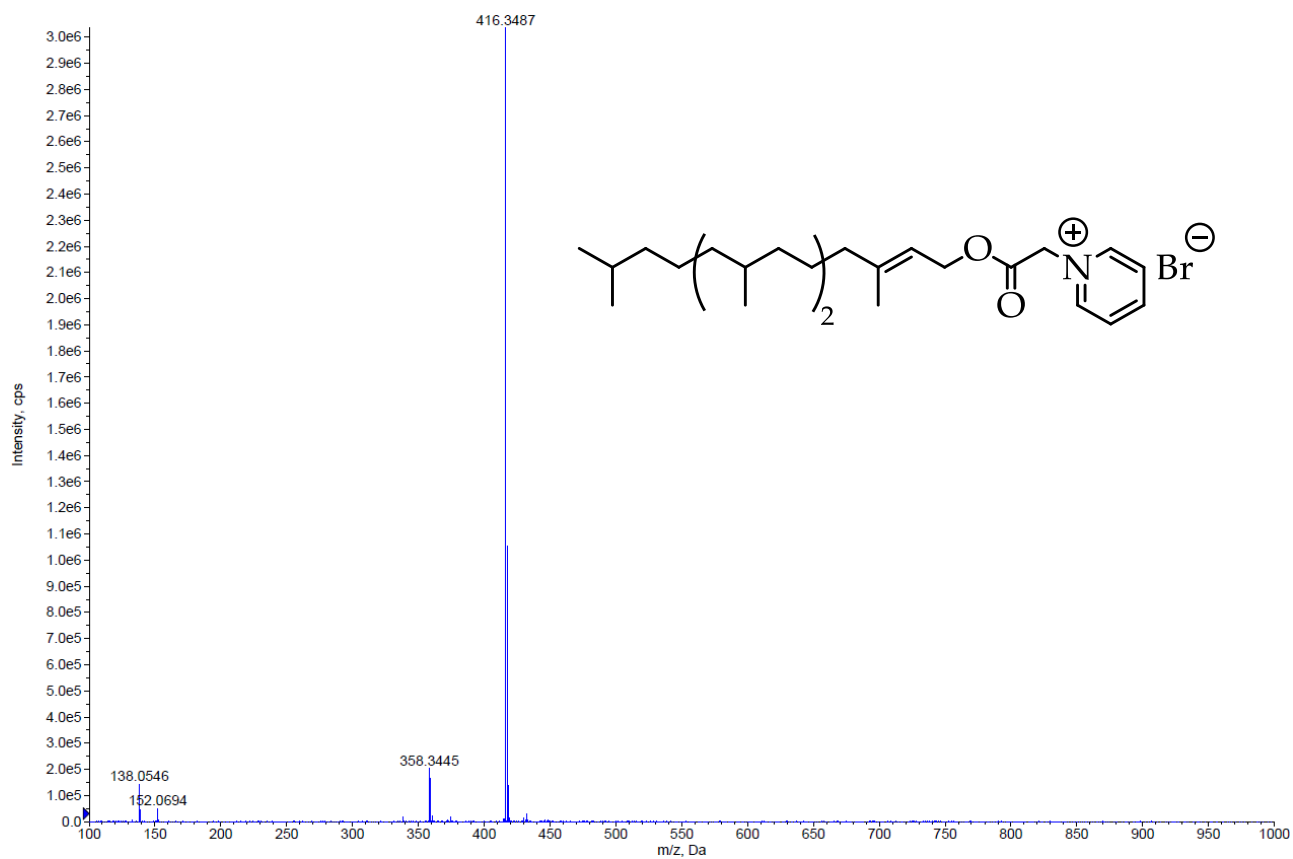


Figure S37. HRMS spectrum of the compound 3c.

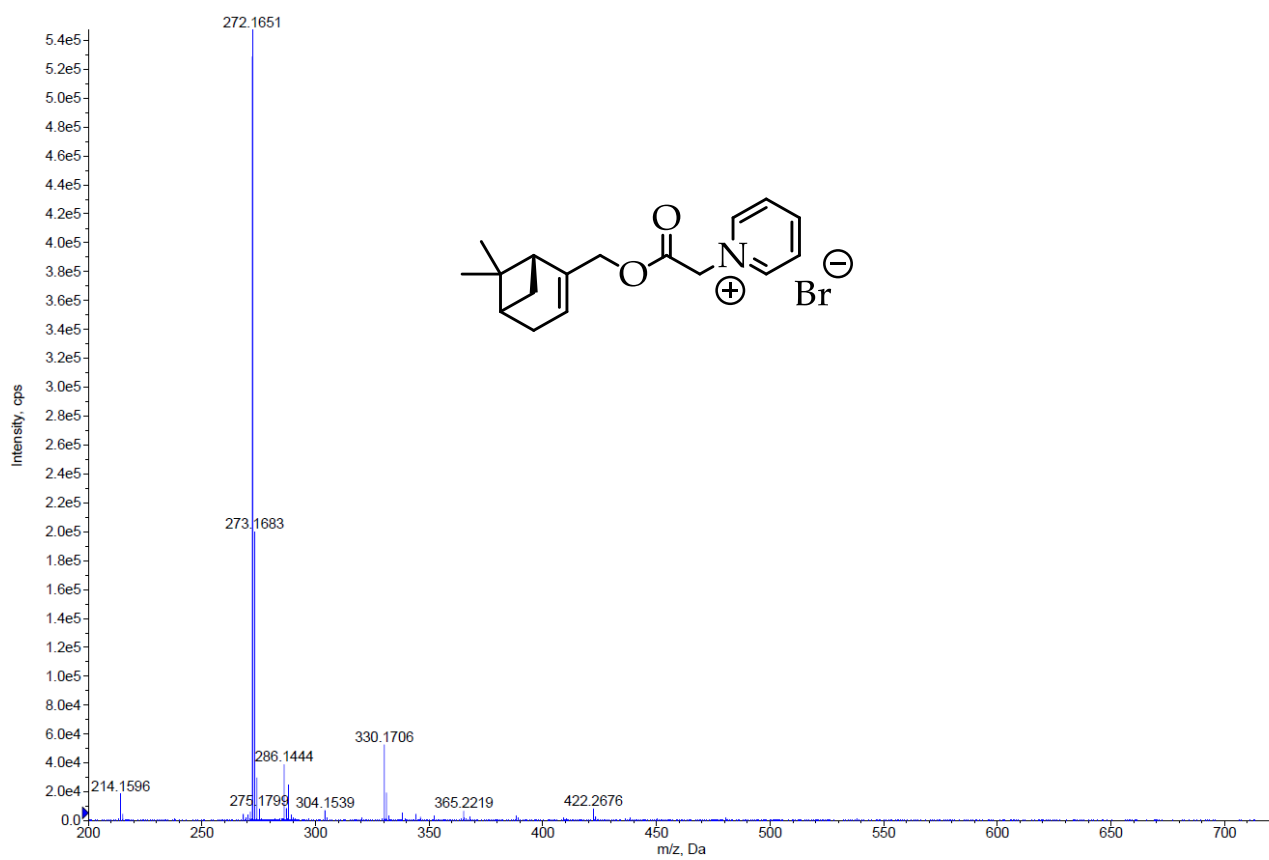


Figure S38. HRMS spectrum of the compound 3d.

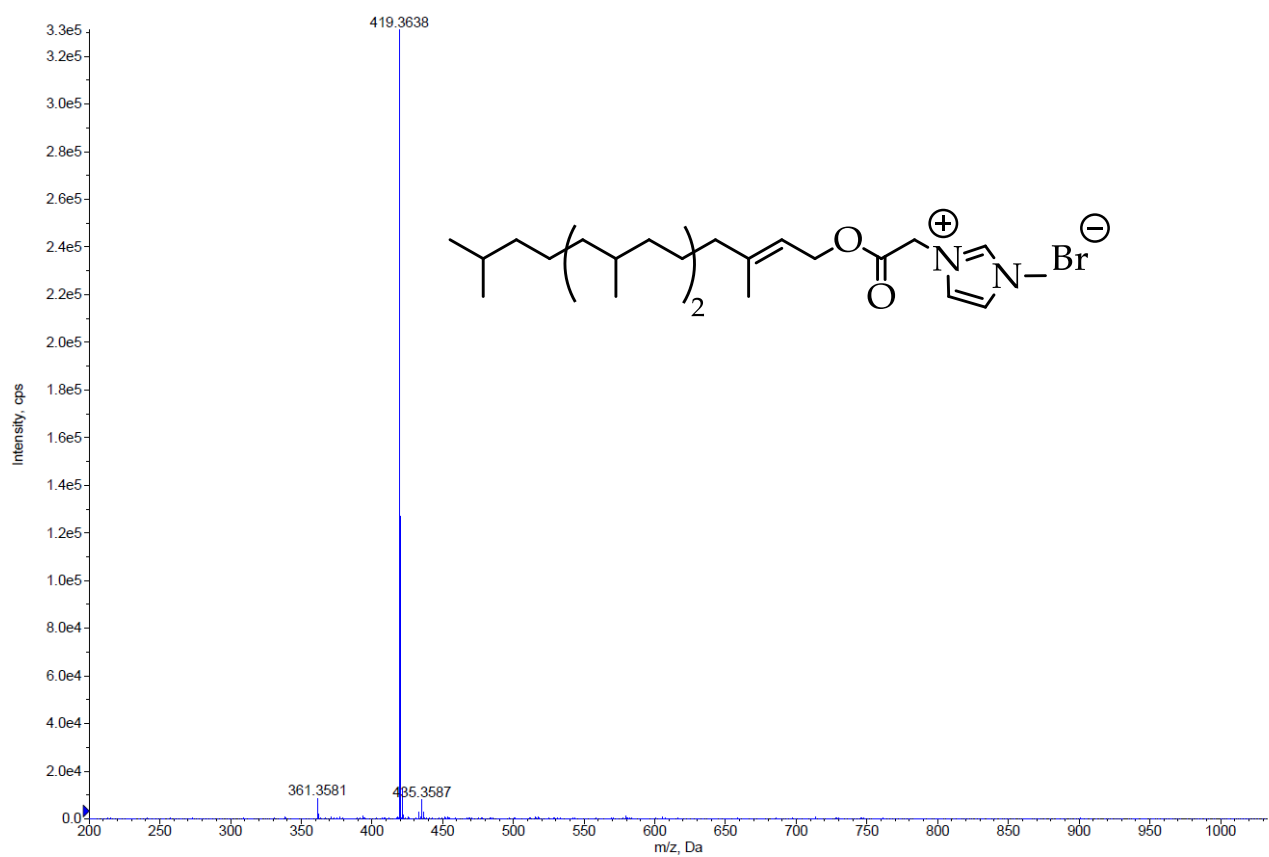


Figure S39. HRMS spectrum of the compound **4c**.

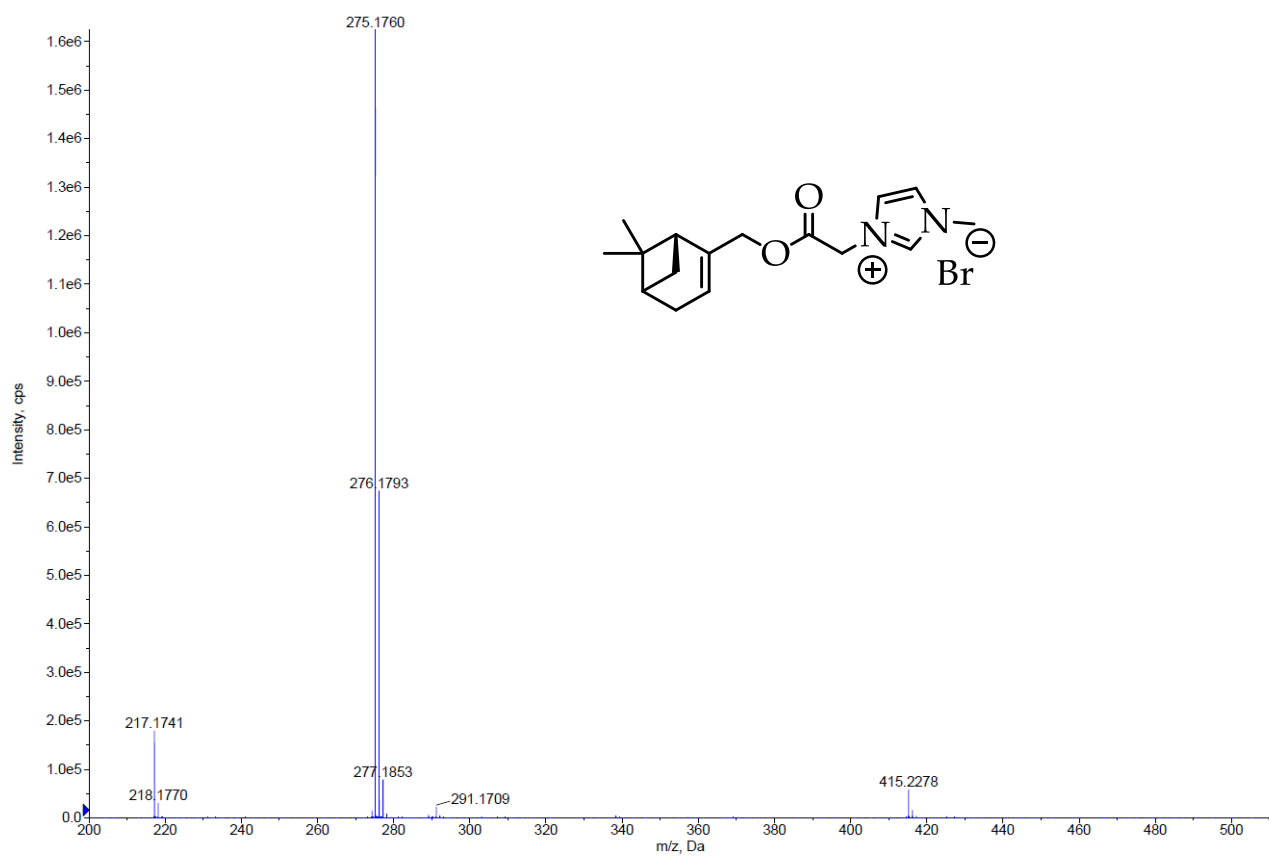


Figure S40. HRMS spectrum of the compound **4d**.

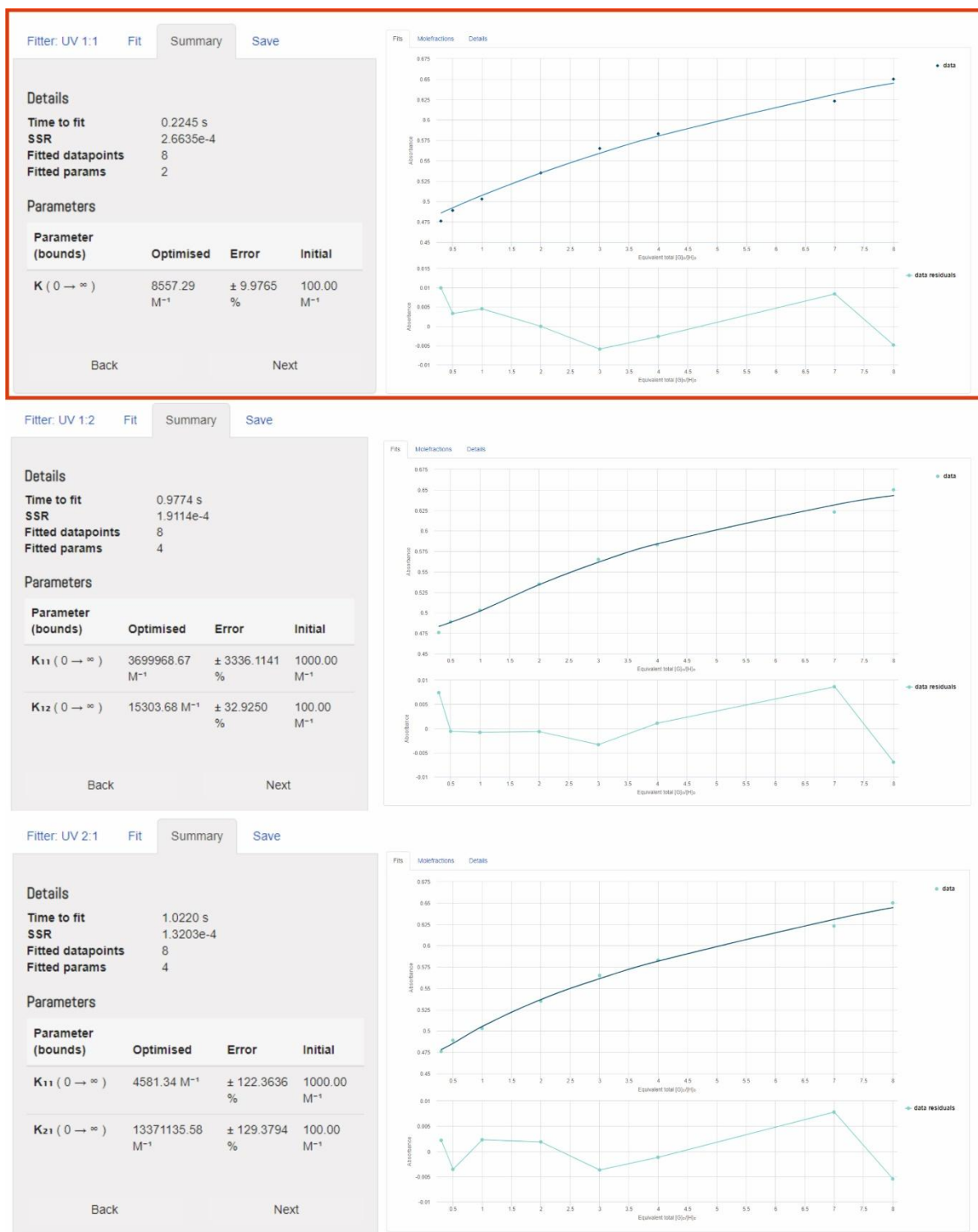


Figure S41. Bindfit (Fit data to 1:1, 1:2 and 2:1 Host-Guest equilibria) Screenshots taken from the summary window of the website supramolecular.org. This screenshots shows the raw data for UV-vis titration of **5** with **3a**.

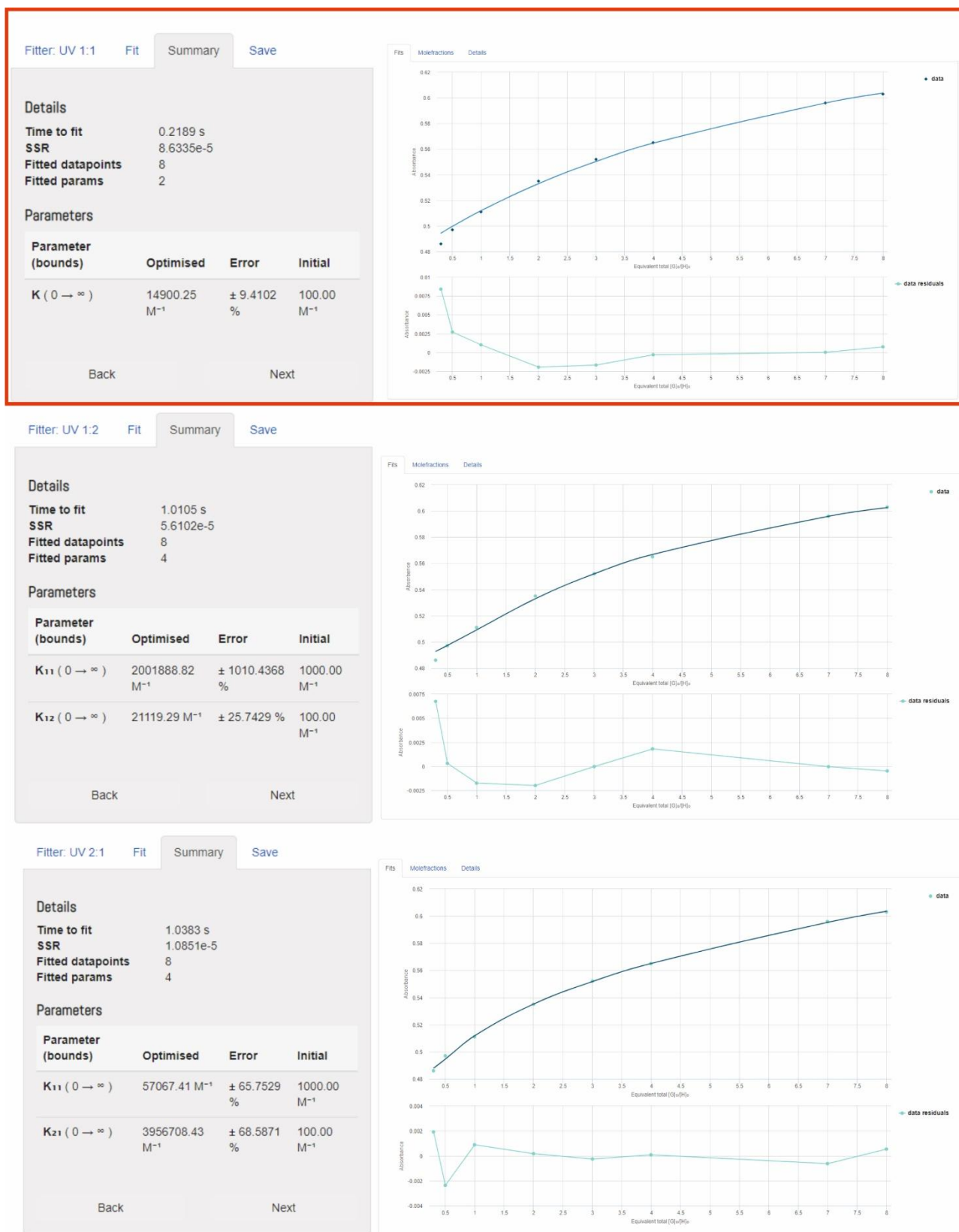


Figure S42. Bindfit (Fit data to 1:1, 1:2 and 2:1 Host-Guest equilibria) Screenshots taken from the summary window of the website supramolecular.org. This screenshots shows the raw data for UV-vis titration of **5** with **3b**.

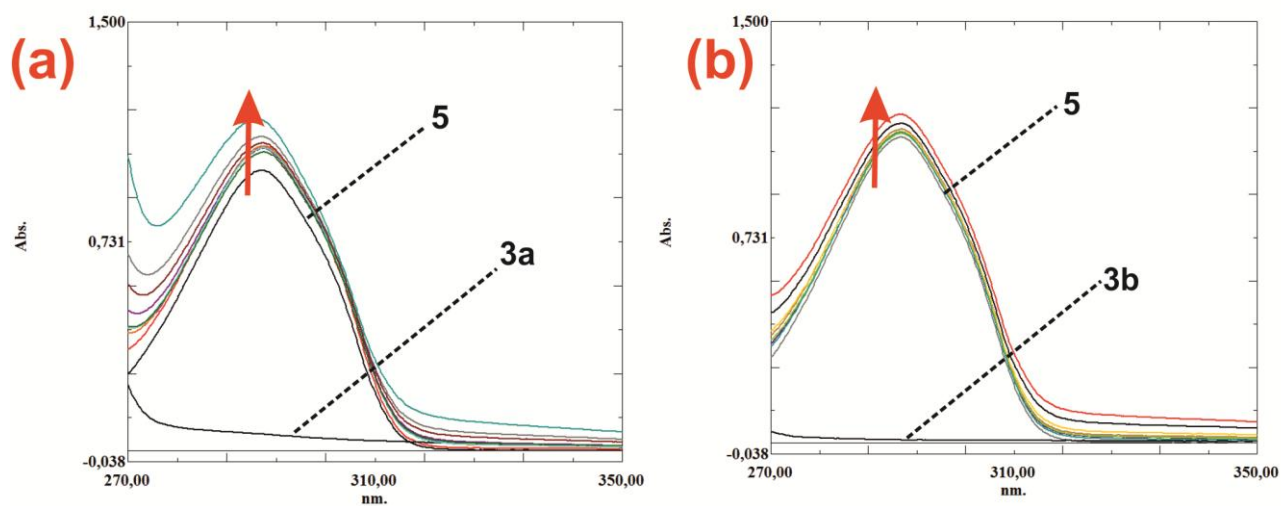


Figure S43. UV-vis titration spectra for the system: (a) pillar[5]arene **5** (1 × 10⁻⁵ M)/ **3a** (C = 3.33 × 10⁻⁶ – 5 × 10⁻⁵ M) in buffer (pH=7.4); (b) pillar[5]arene **5** (1 × 10⁻⁵ M)/ **3b** (C = 3.33 × 10⁻⁶ – 5 × 10⁻⁵ M) in buffer (pH=7.4).