Supplementary Information

For

Towards potential antifungal agents: synthesis, supramolecular self-assembly and in vitro activity of azole mono-, sesqui- and diterpenoids

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Content

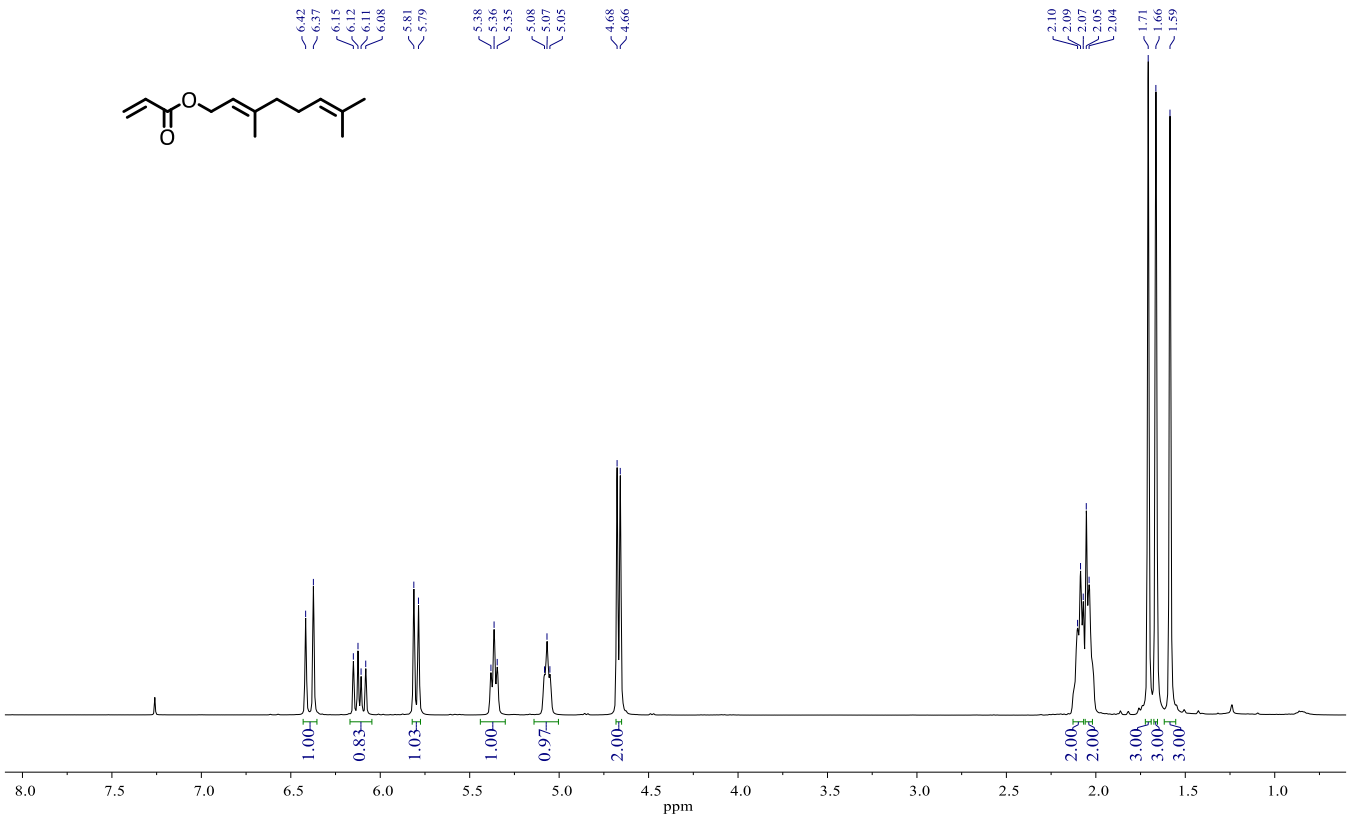


Figure S01. ^{1}H NMR spectrum of the compound **2a**, $CDCl_3$, 298 K, 400 MHz.

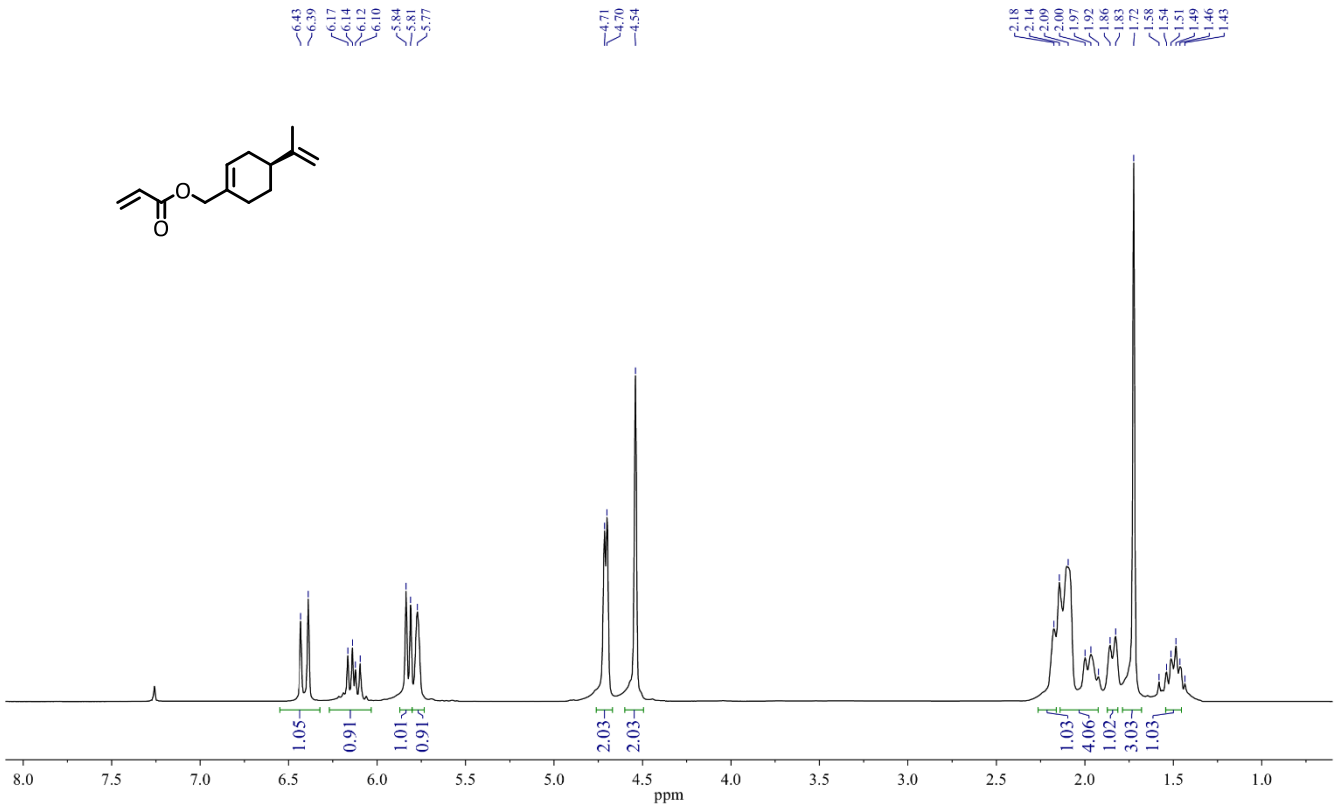


Figure S02. ^{1}H NMR spectrum of the compound **2b**, $CDCl_3$, 298 K, 400 MHz.

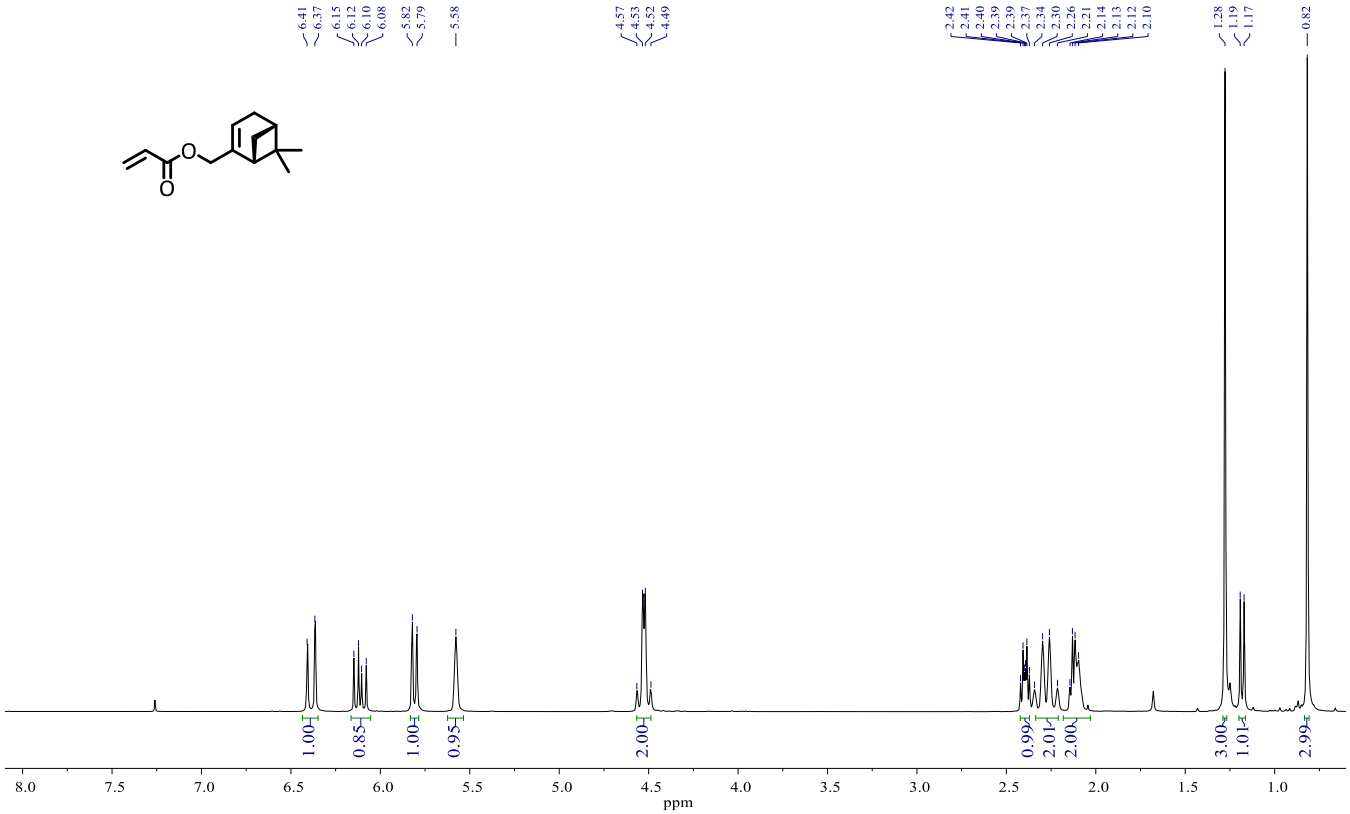


Figure S03. ^{1}H NMR spectrum of the compound **2c**, $CDCl_3$, 298 K, 400 MHz.

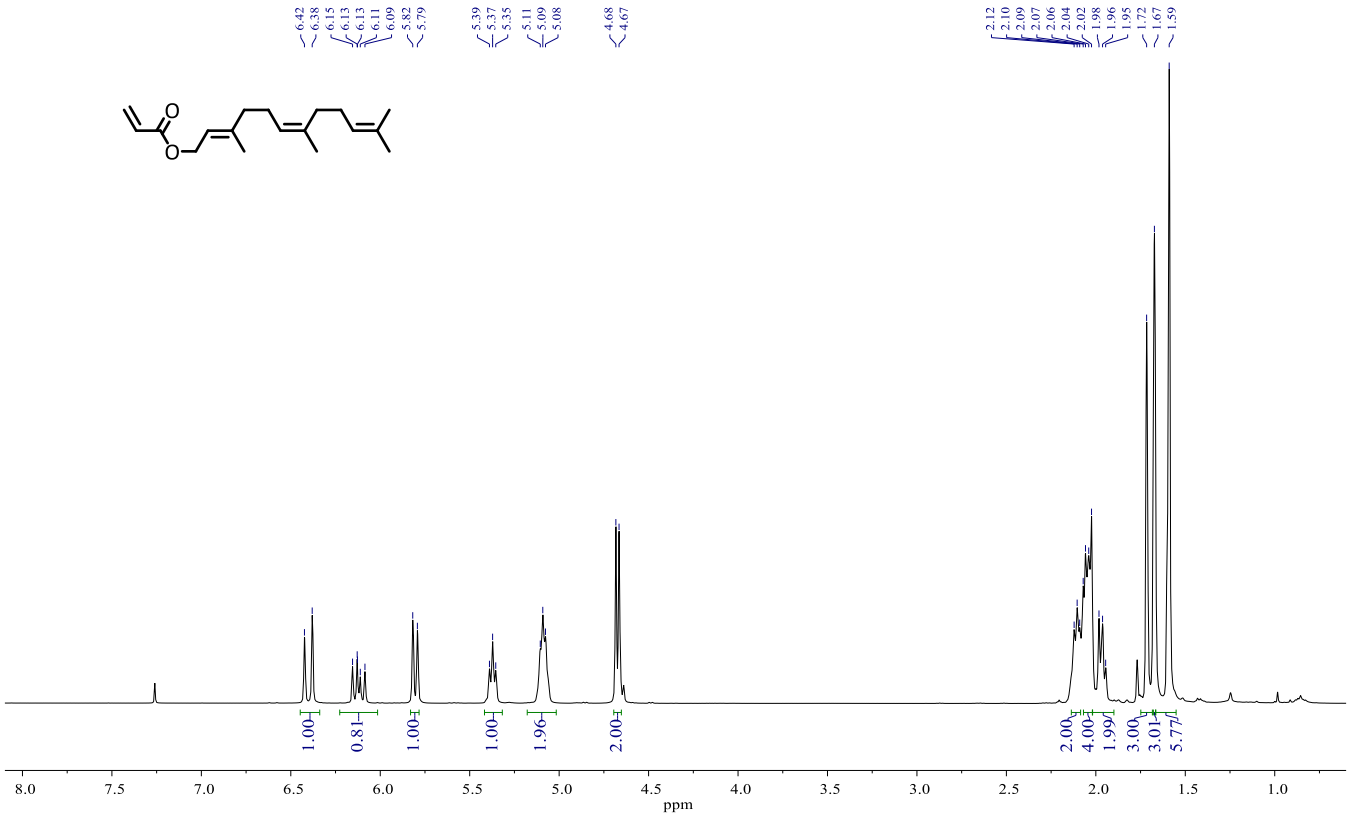


Figure S04. ^{1}H NMR spectrum of the compound **2d**, $CDCl_3$, 298 K, 400 MHz.

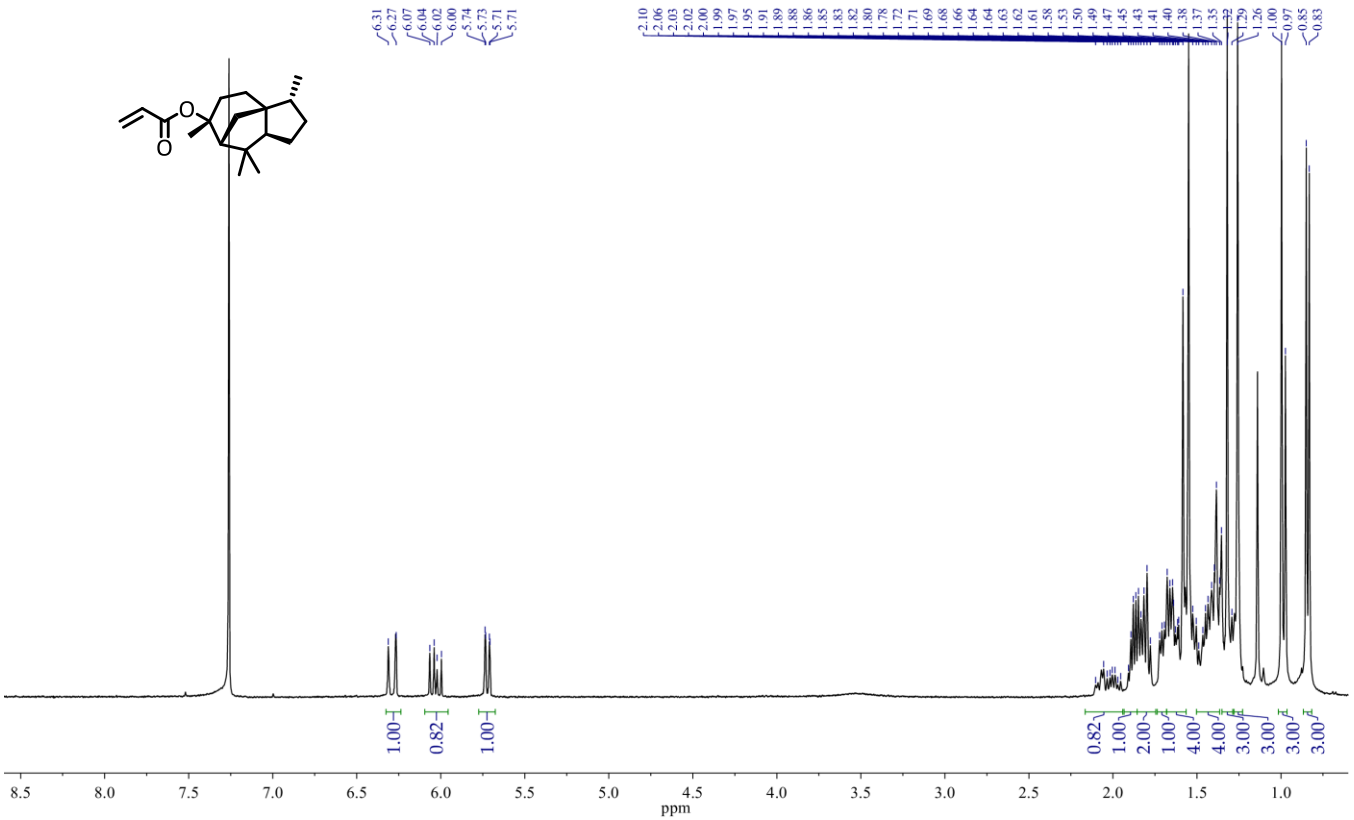


Figure S05. ^{1}H NMR spectrum of the compound **2e**, $CDCl_3$, 298 K, 400 MHz.

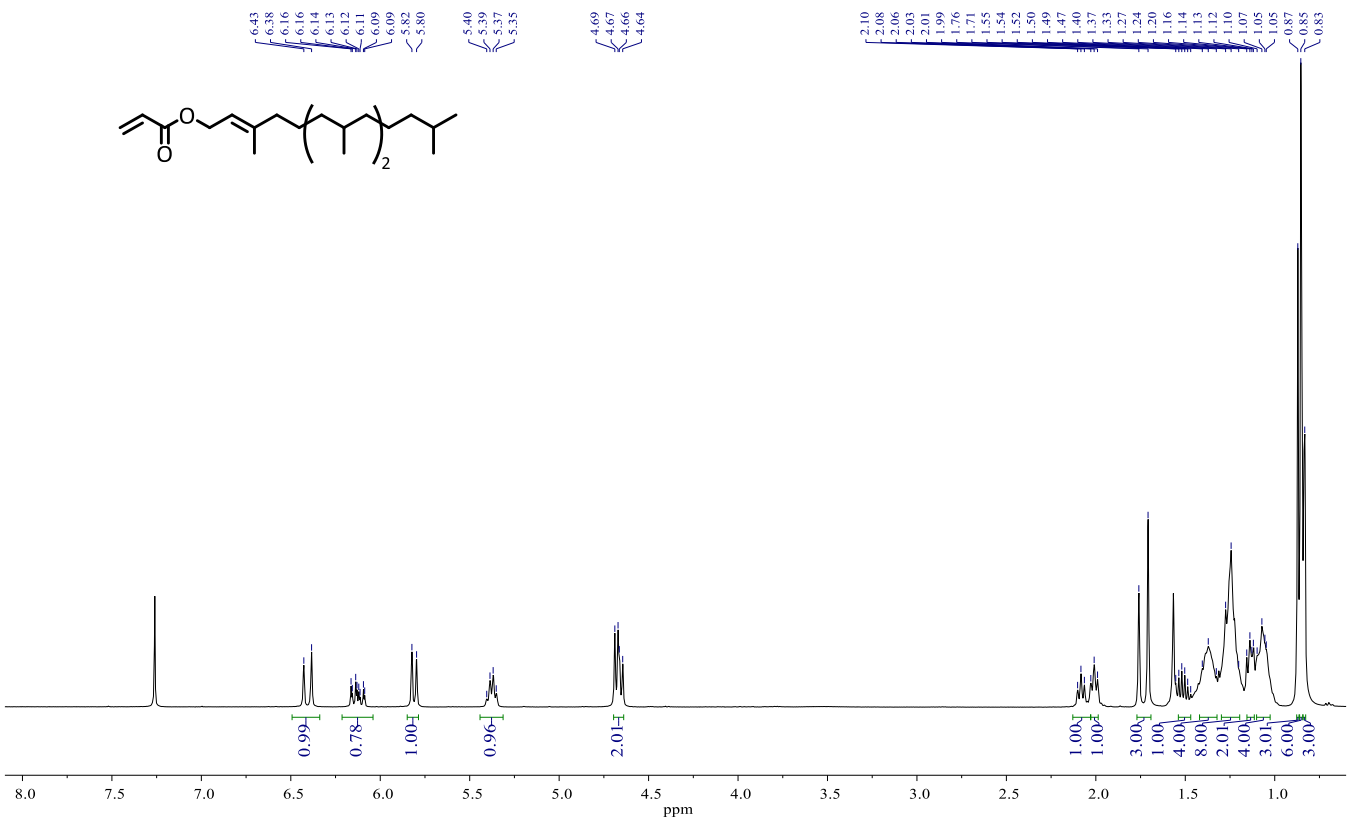


Figure S06. ^{1}H NMR spectrum of the compound **2f**, $CDCl_3$, 298 K, 400 MHz.

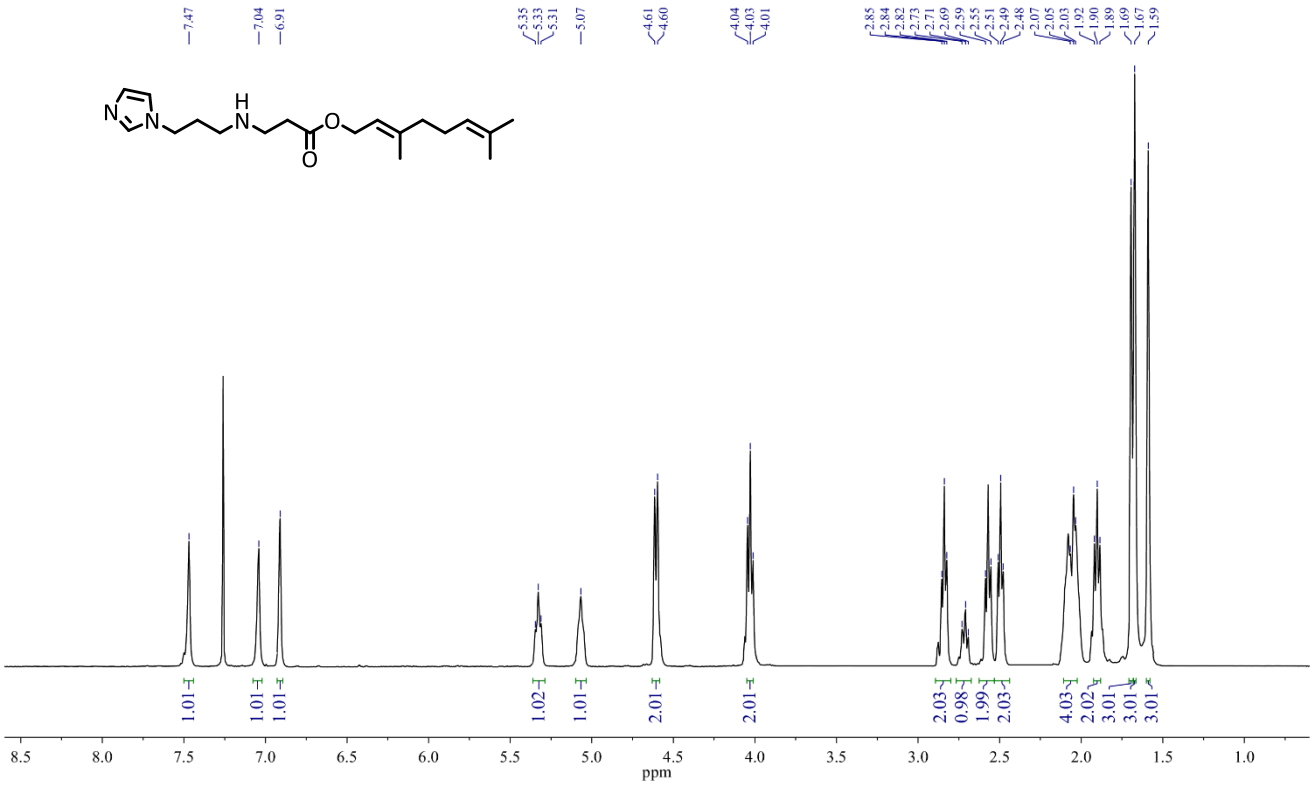


Figure S07. ^{1}H NMR spectrum of the compound **3a**, $CDCl_3$, 298 K, 400 MHz.

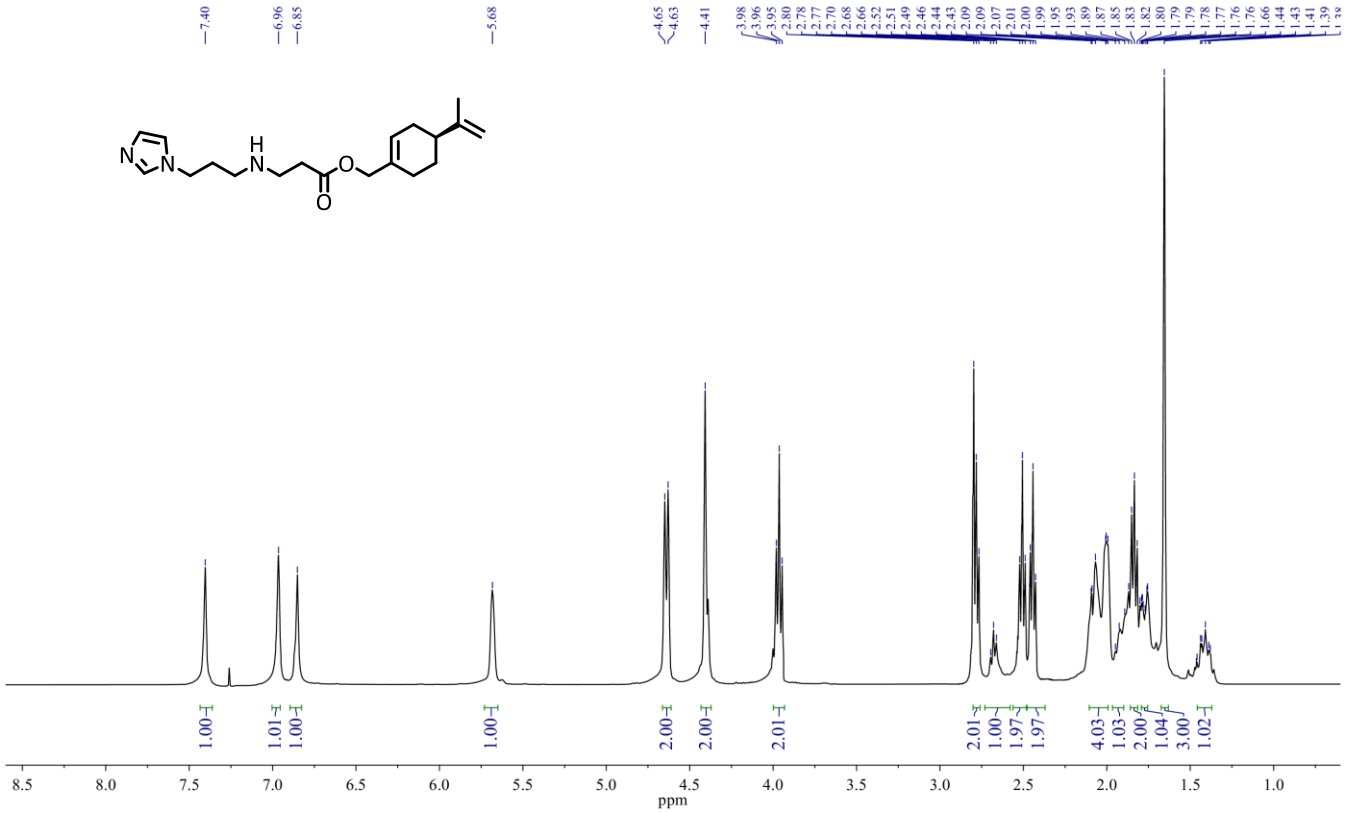


Figure S08. ^{1}H NMR spectrum of the compound **3b**, $CDCl_3$, 298 K, 400 MHz.

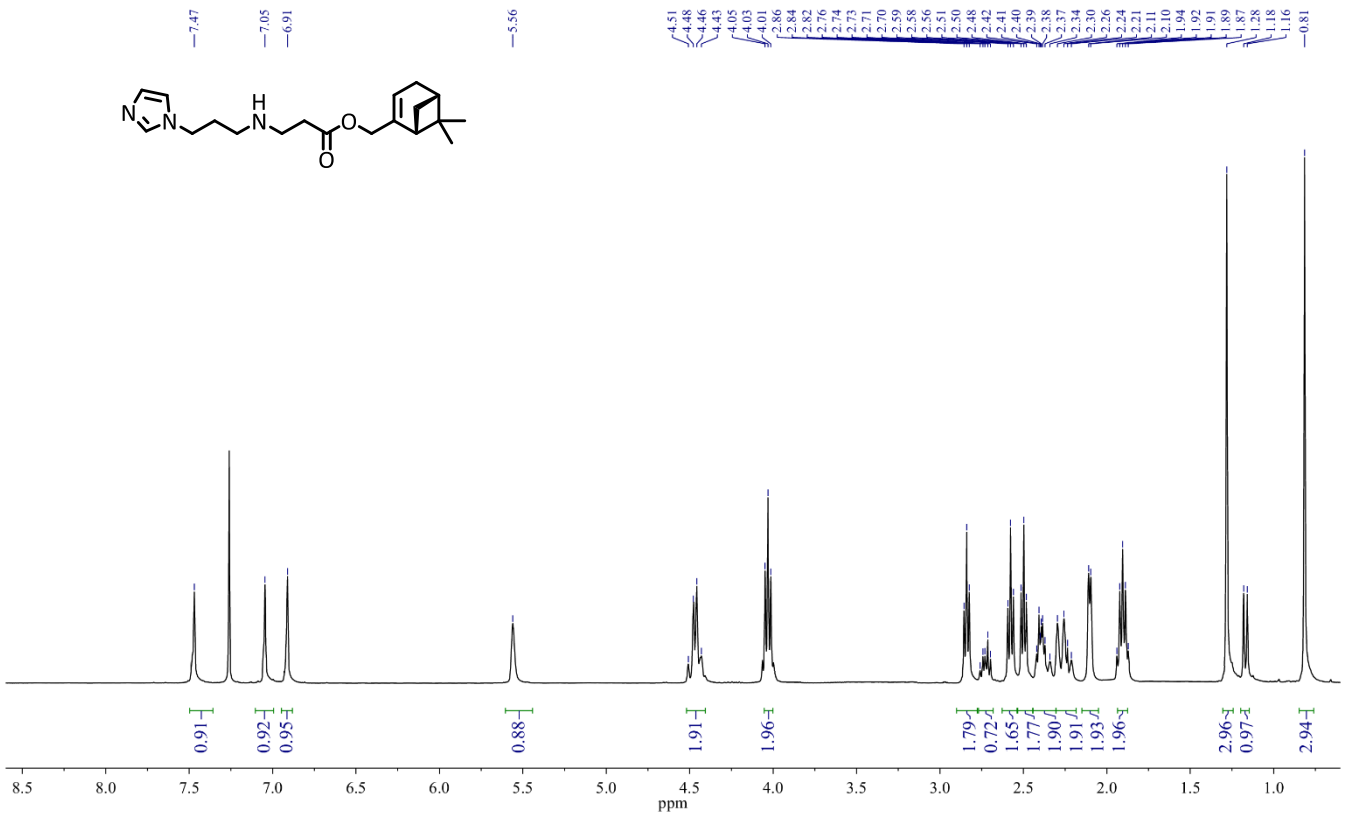


Figure S09. ^{1}H NMR spectrum of the compound **3c**, $CDCl_3$, 298 K, 400 MHz.

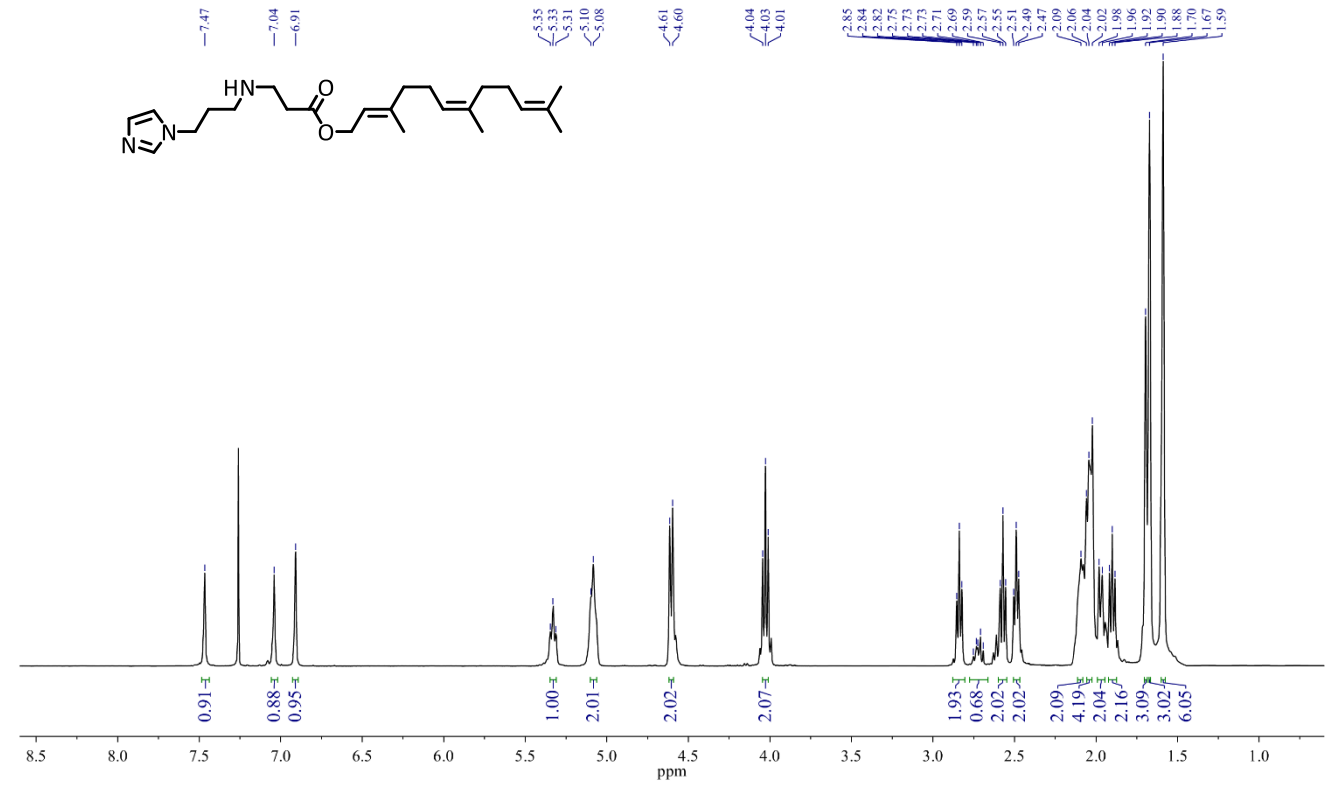


Figure S10. ^{1}H NMR spectrum of the compound **3d**, $CDCl_3$, 298 K, 400 MHz.

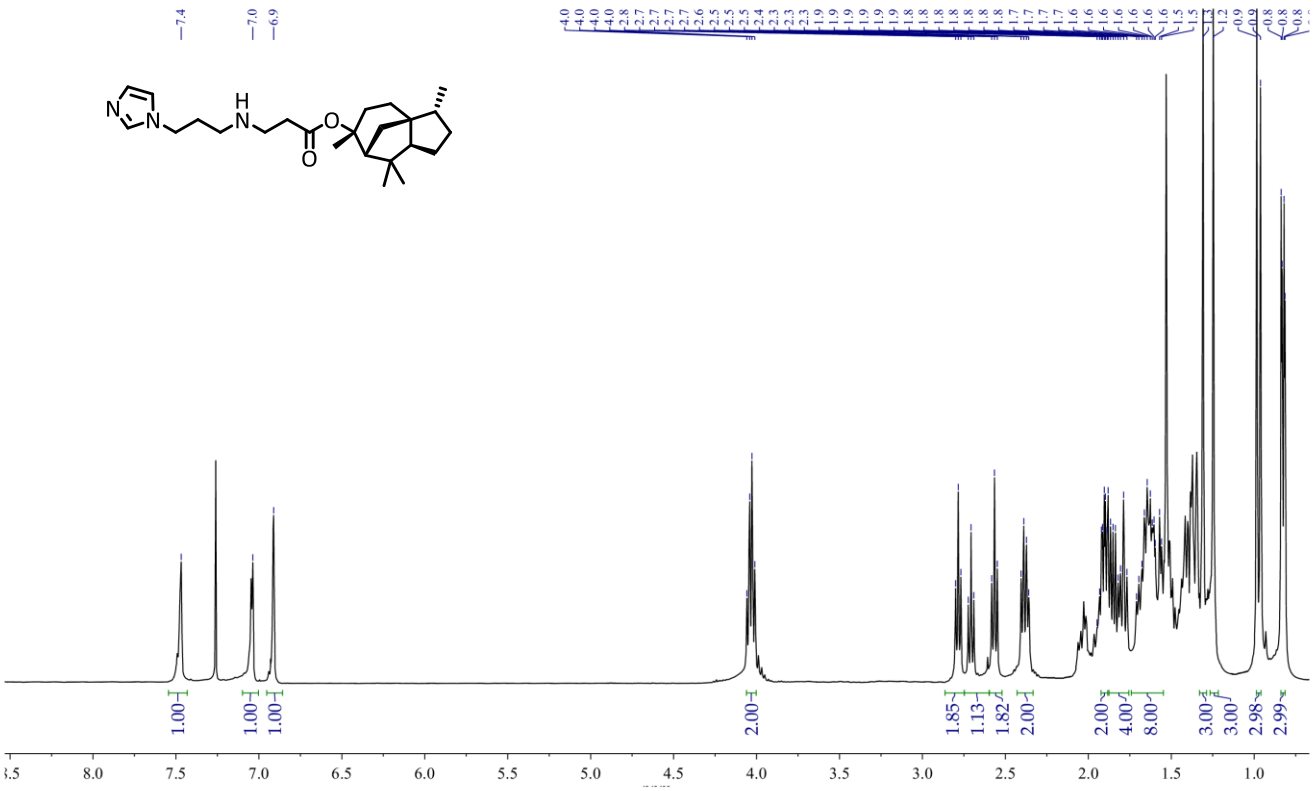


Figure S11. ^{1}H NMR spectrum of the compound **3e**, $CDCl_3$, 298 K, 400 MHz.

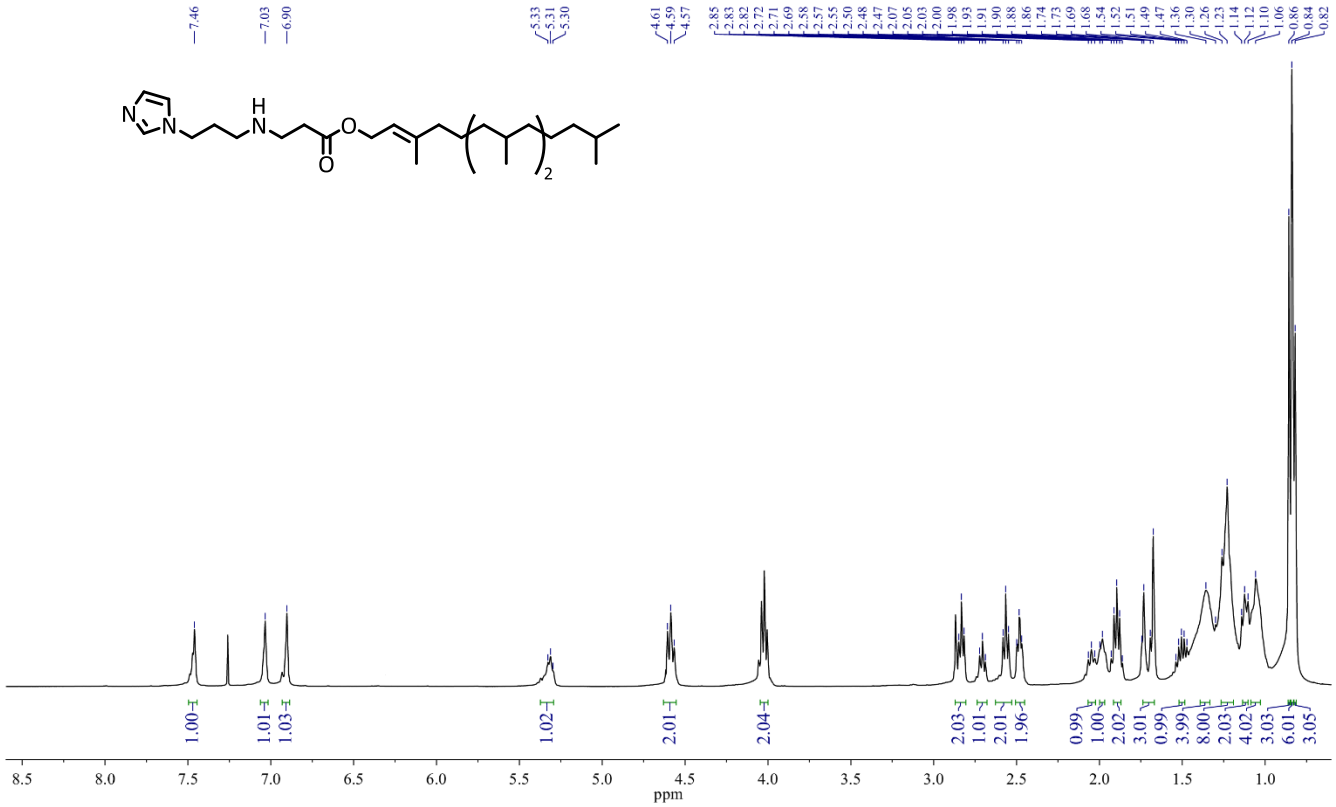


Figure S12. ^{1}H NMR spectrum of the compound **3f**, $CDCl_3$, 298 K, 400 MHz.

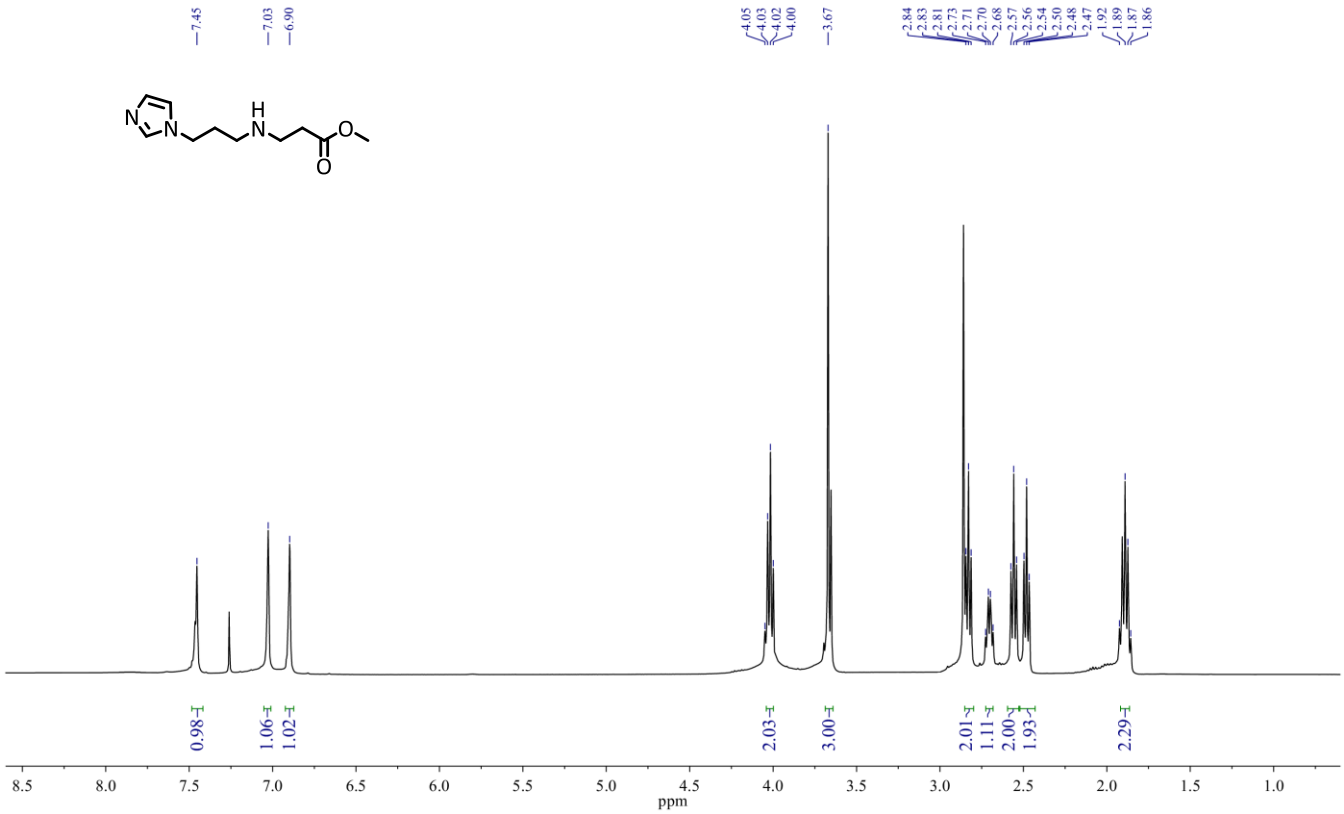


Figure S13. ^{1}H NMR spectrum of the compound **3g**, $CDCl_3$, 298 K, 400 MHz.

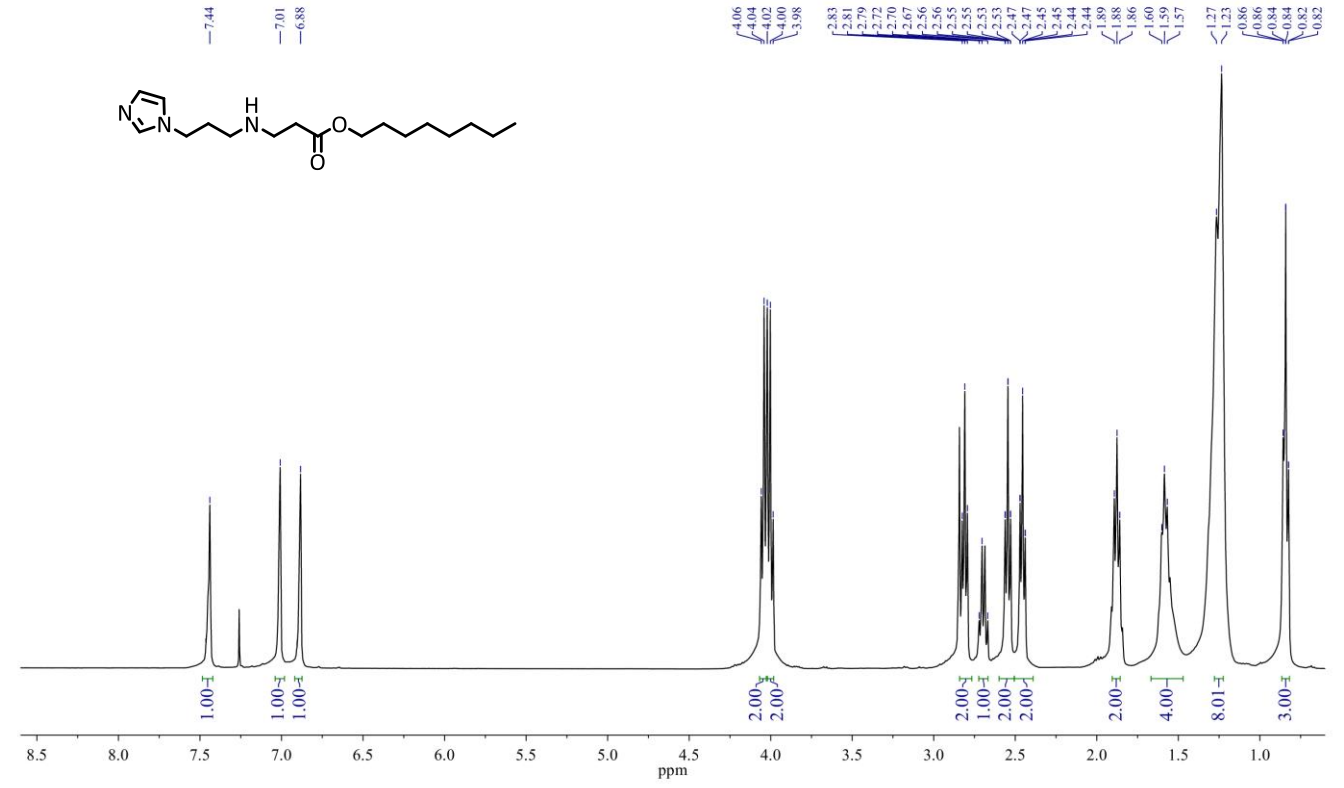


Figure S14. ^{1}H NMR spectrum of the compound **3h**, $CDCl_3$, 298 K, 400 MHz.

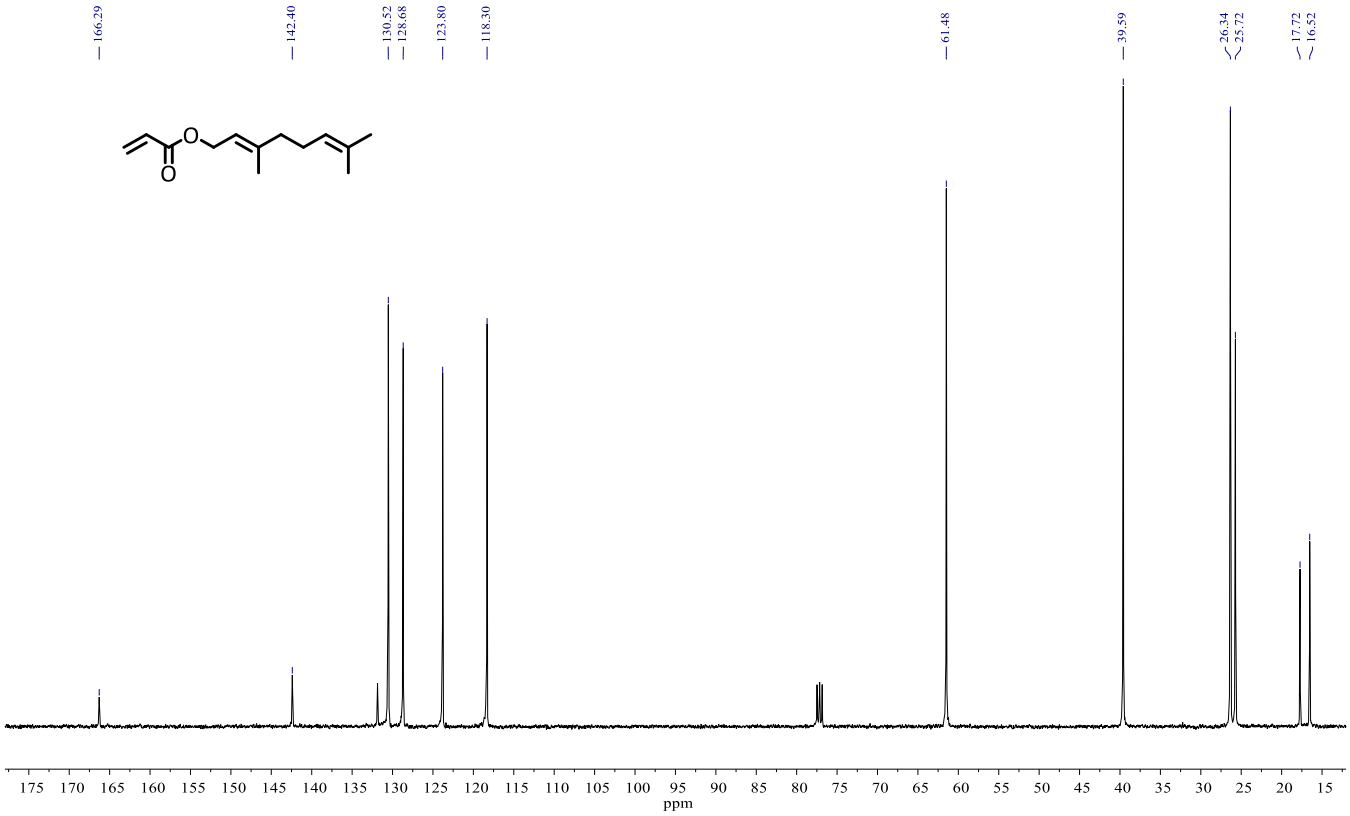


Figure S15. ^{13}C NMR spectrum of the compound **2a**, $CDCl_3$, 298 K, 100 MHz.

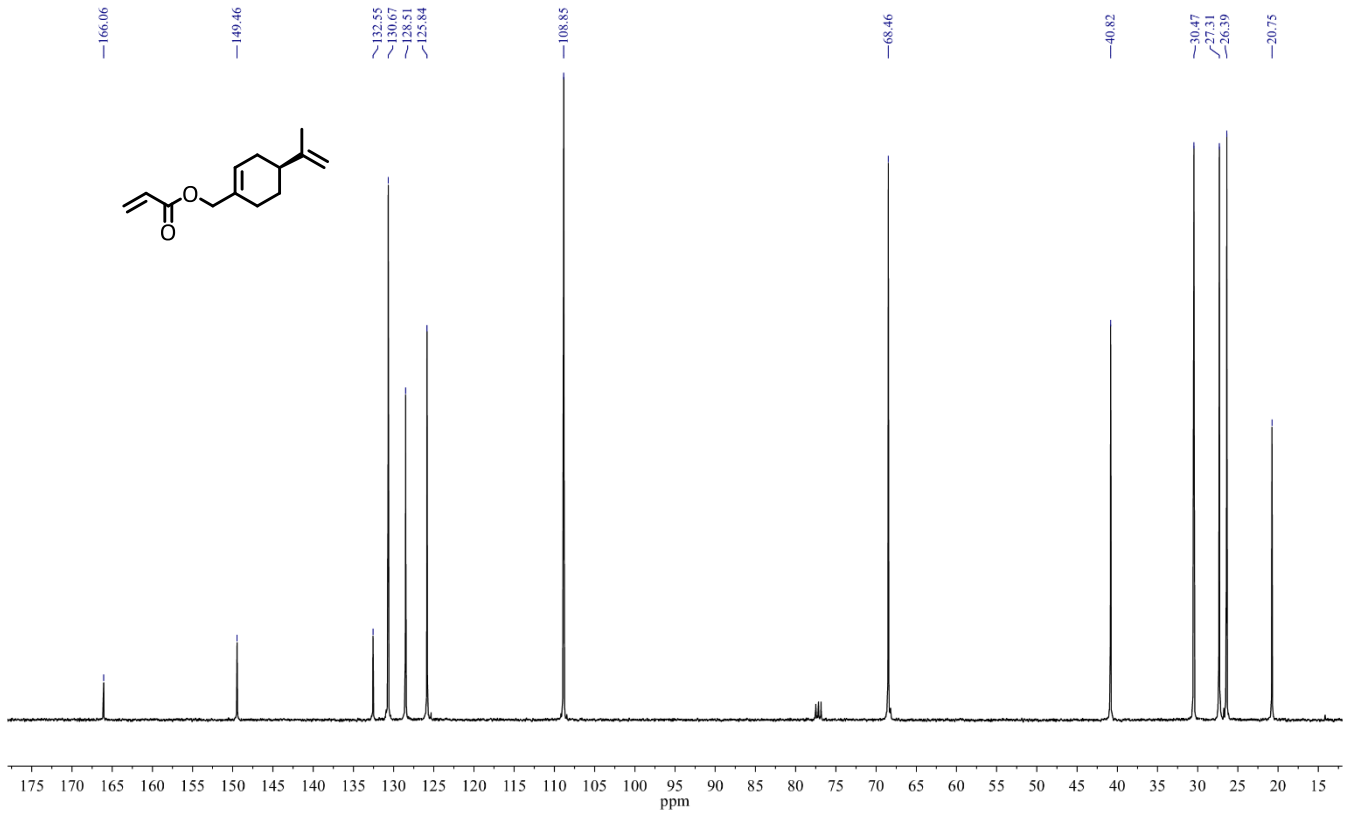


Figure S16. ^{13}C NMR spectrum of the compound **2b**, $CDCl_3$, 298 K, 100 MHz.

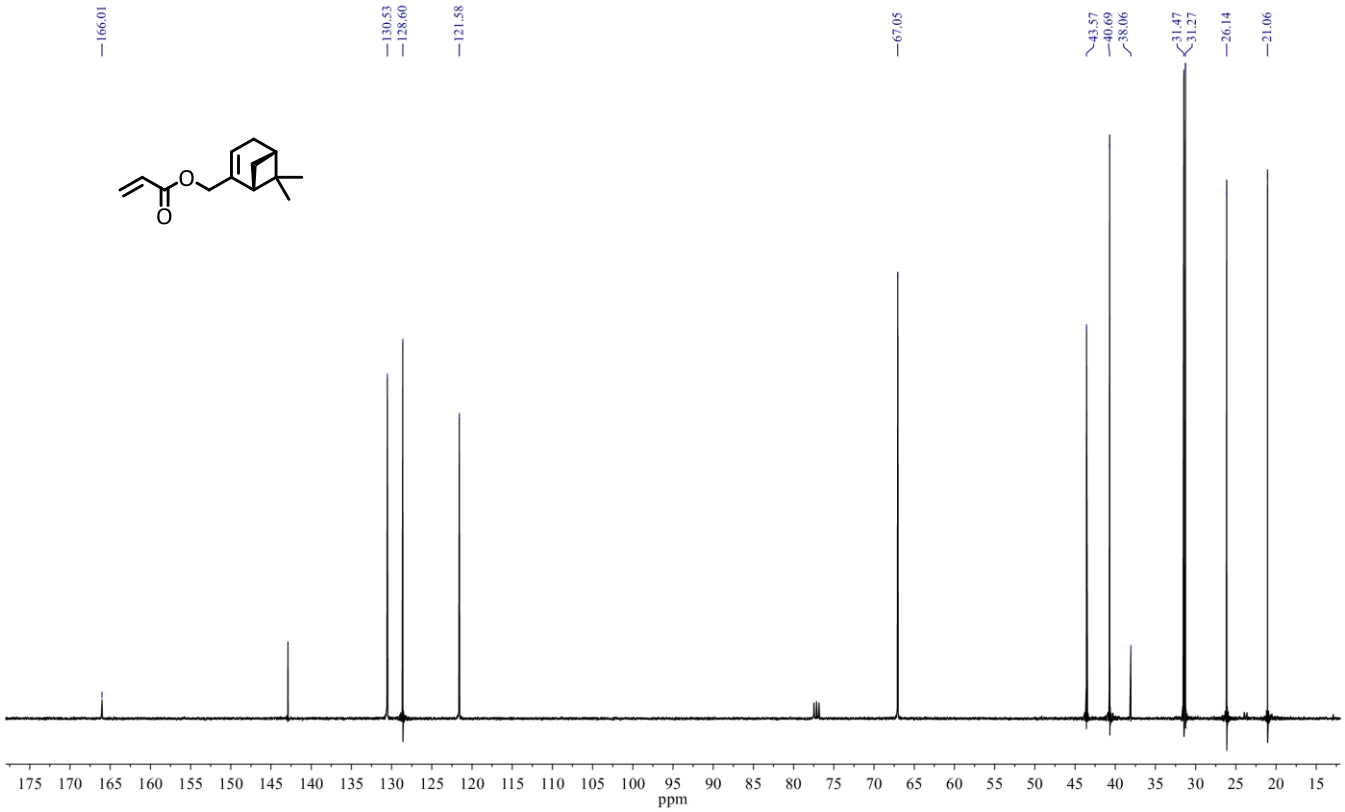


Figure S17. ^{13}C NMR spectrum of the compound **2c**, $CDCl_3$, 298 K, 100 MHz.

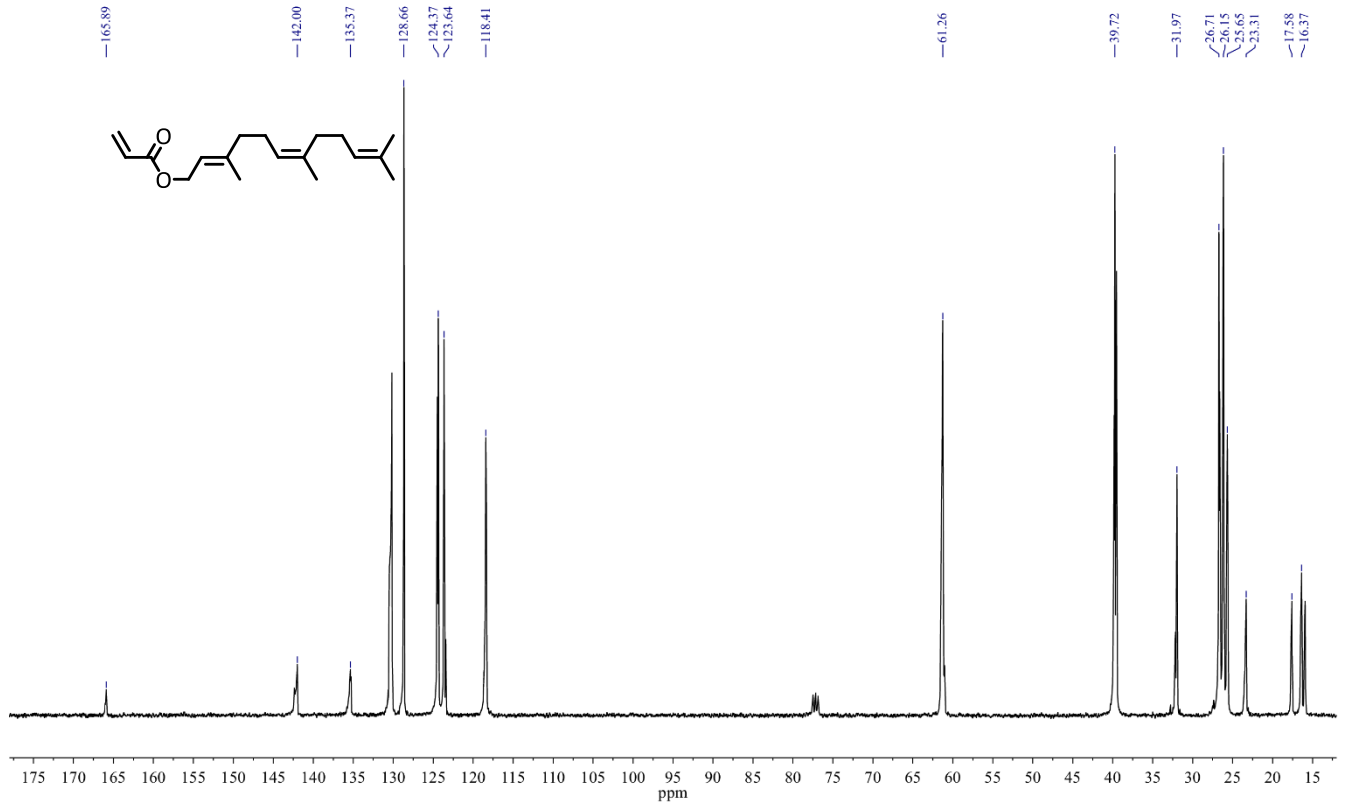


Figure S18. ^{13}C NMR spectrum of the compound **2d**, $CDCl_3$, 298 K, 100 MHz.

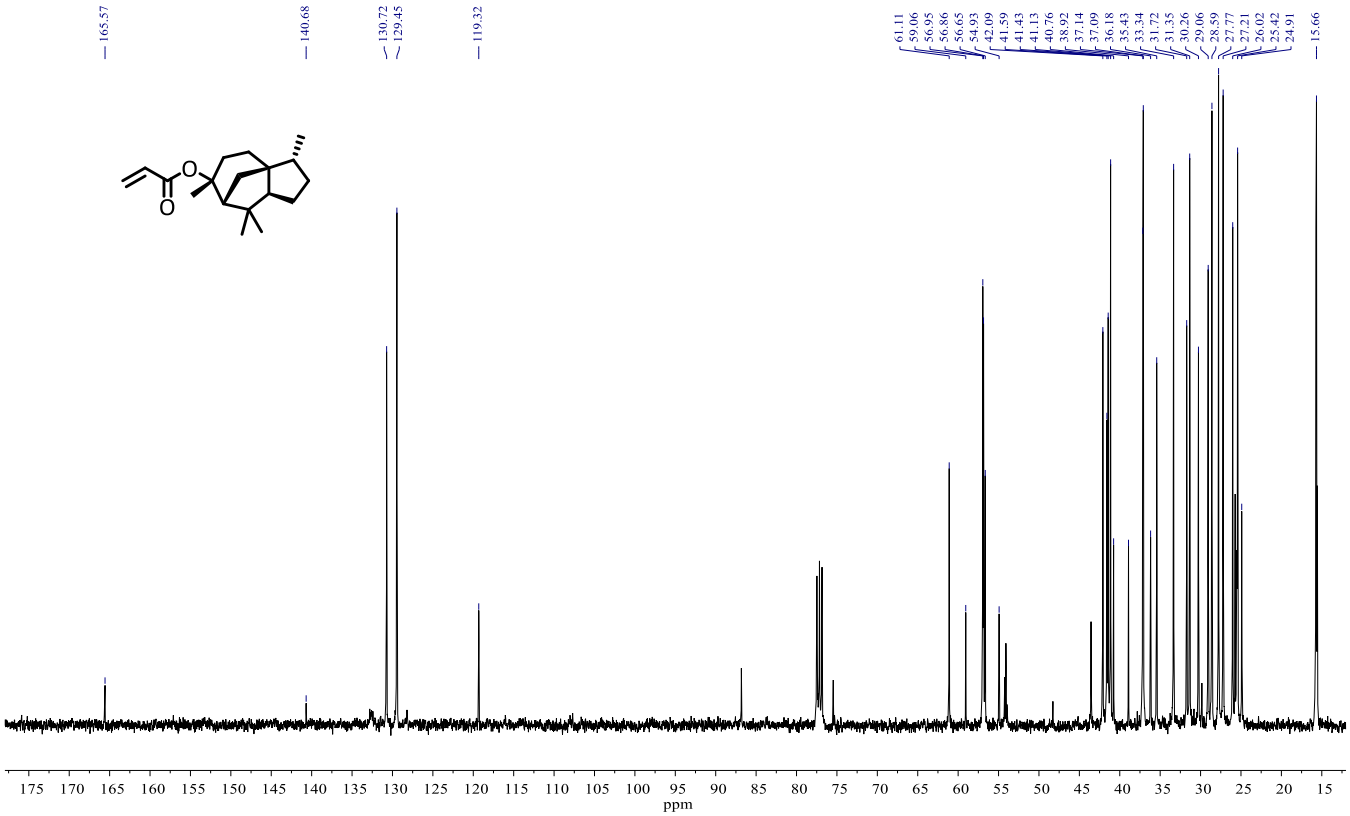


Figure S19. ^{13}C NMR spectrum of the compound **2e**, $CDCl_3$, 298 K, 100 MHz.

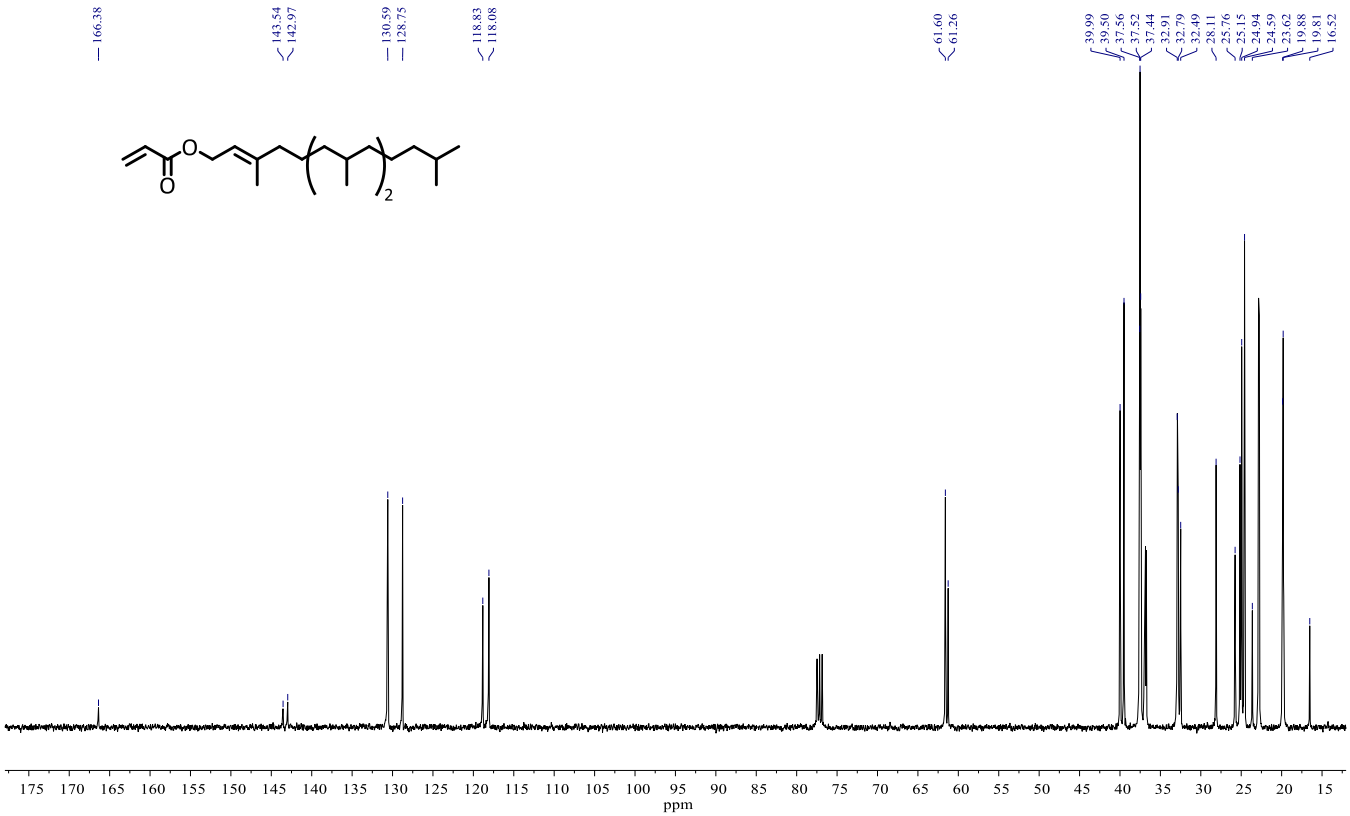


Figure S20. ^{13}C NMR spectrum of the compound **2f**, $CDCl_3$, 298 K, 100 MHz.

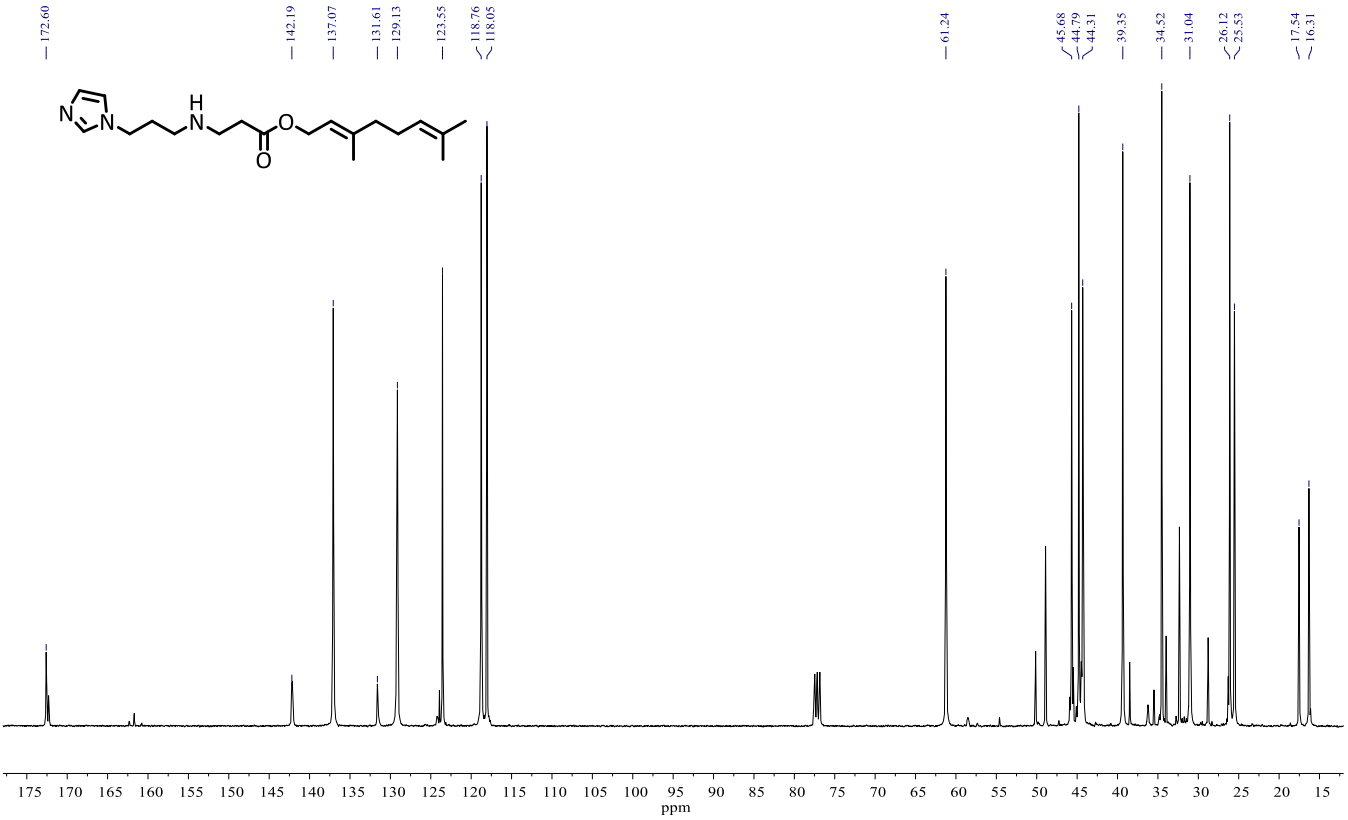


Figure S21. ^{13}C NMR spectrum of the compound **3a**, $CDCl_3$, 298 K, 100 MHz.

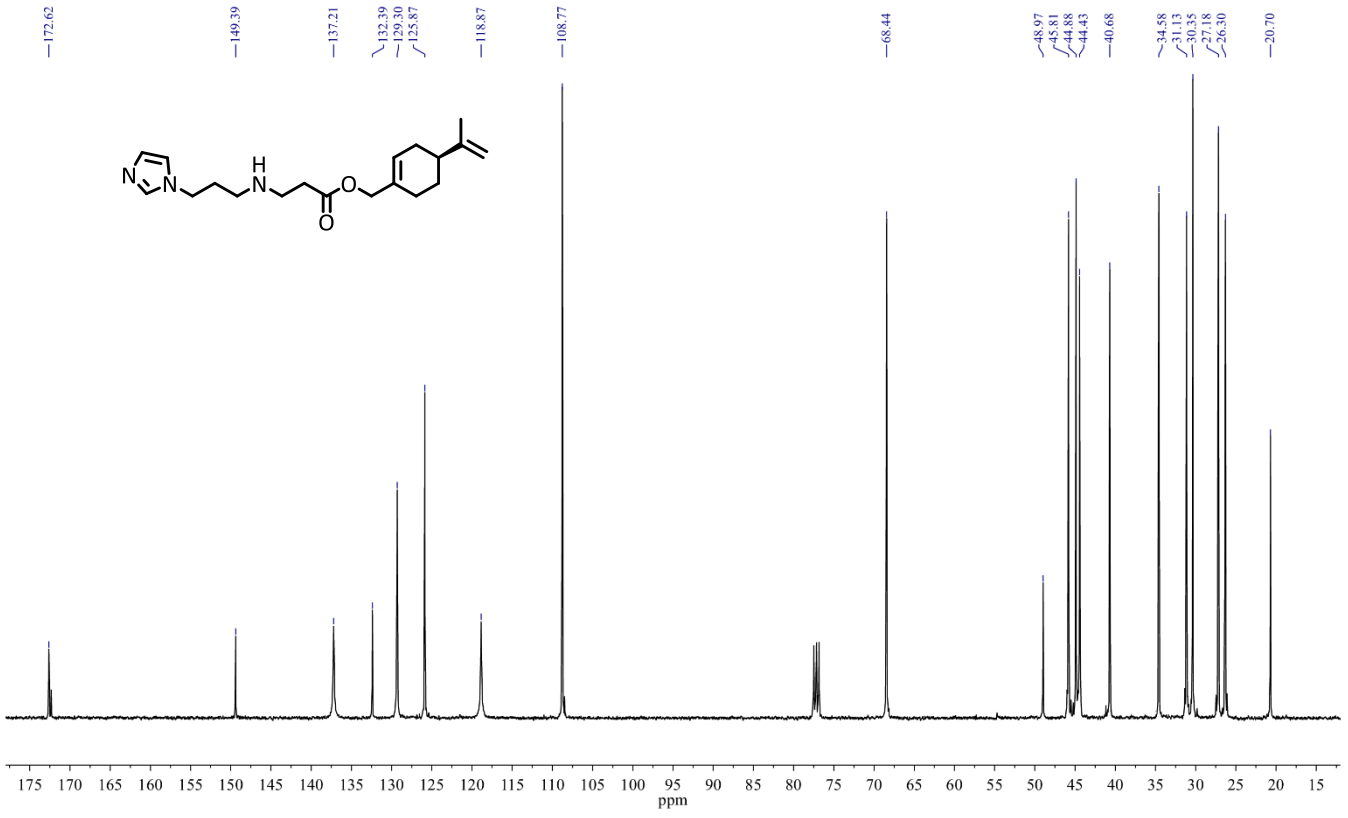


Figure S22. ^{13}C NMR spectrum of the compound **3b**, $CDCl_3$, 298 K, 100 MHz.

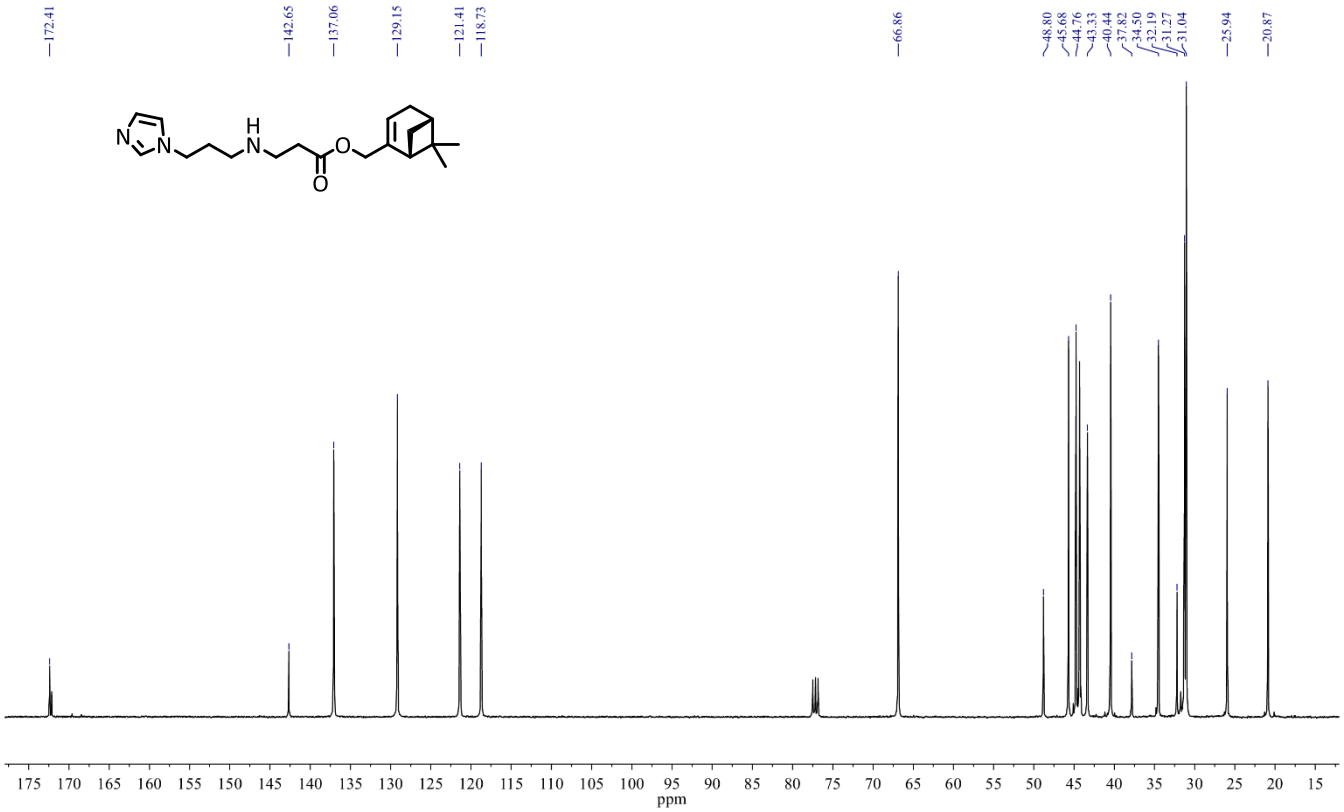


Figure S23. ^{13}C NMR spectrum of the compound **3c**, $CDCl_3$, 298 K, 100 MHz.

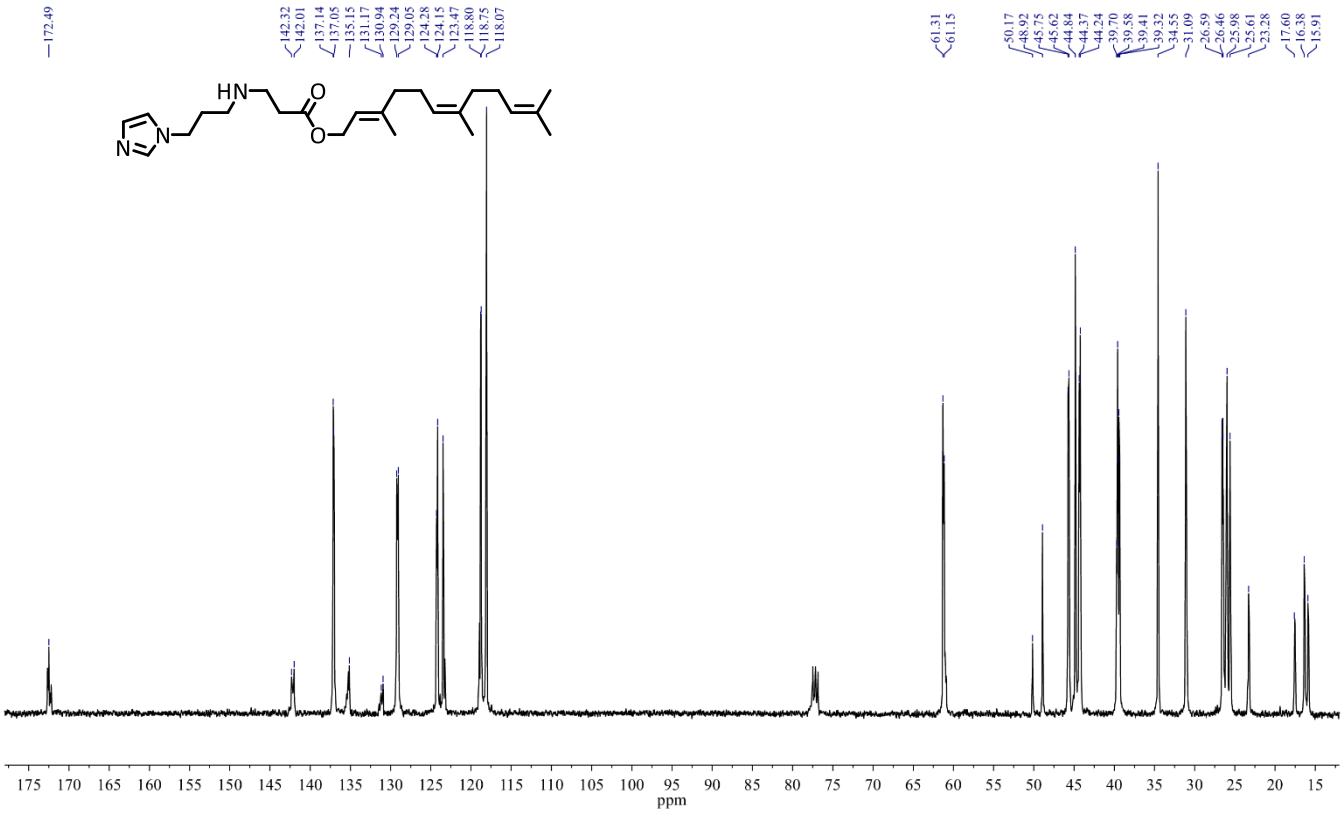


Figure S24. ^{13}C NMR spectrum of the compound **3d**, $CDCl_3$, 298 K, 100 MHz.

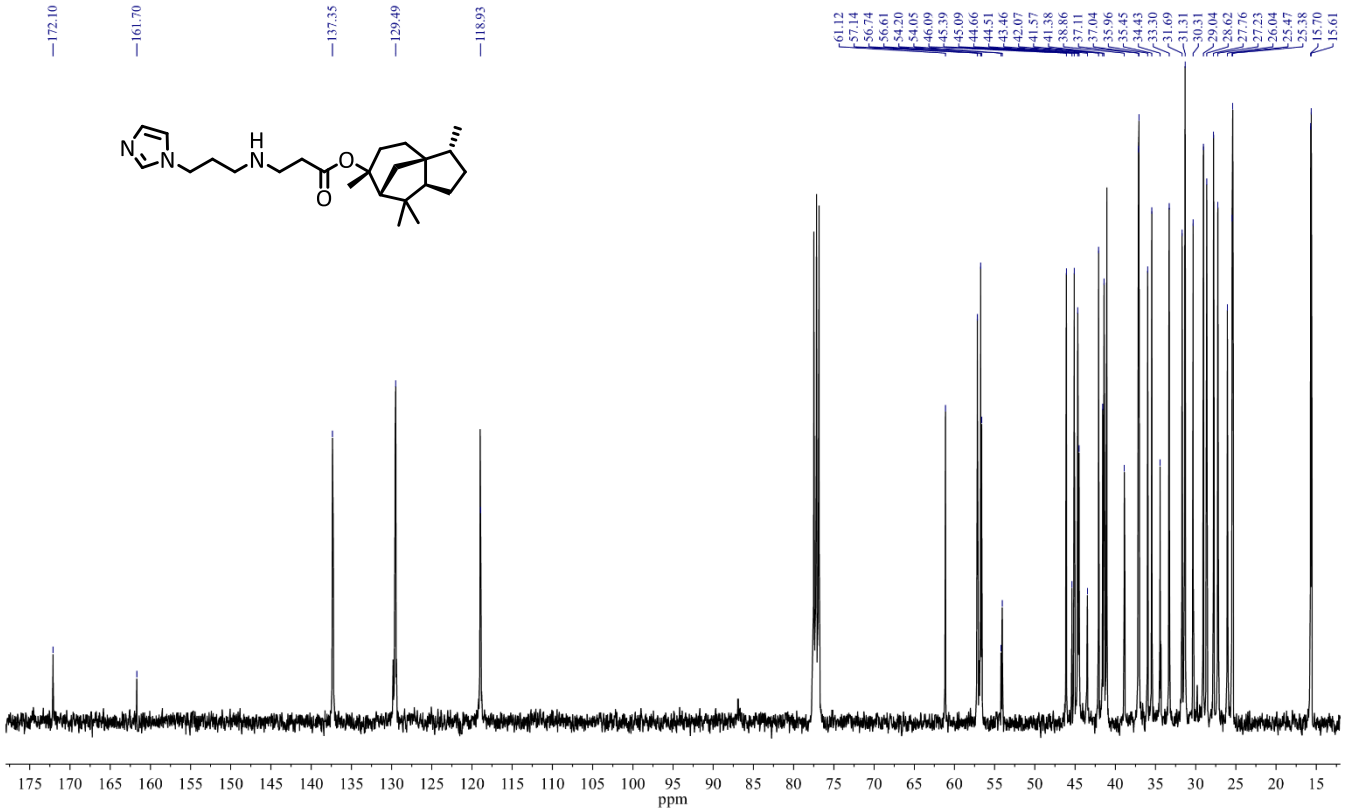


Figure S25. ^{13}C NMR spectrum of the compound **3e**, $CDCl_3$, 298 K, 100 MHz.

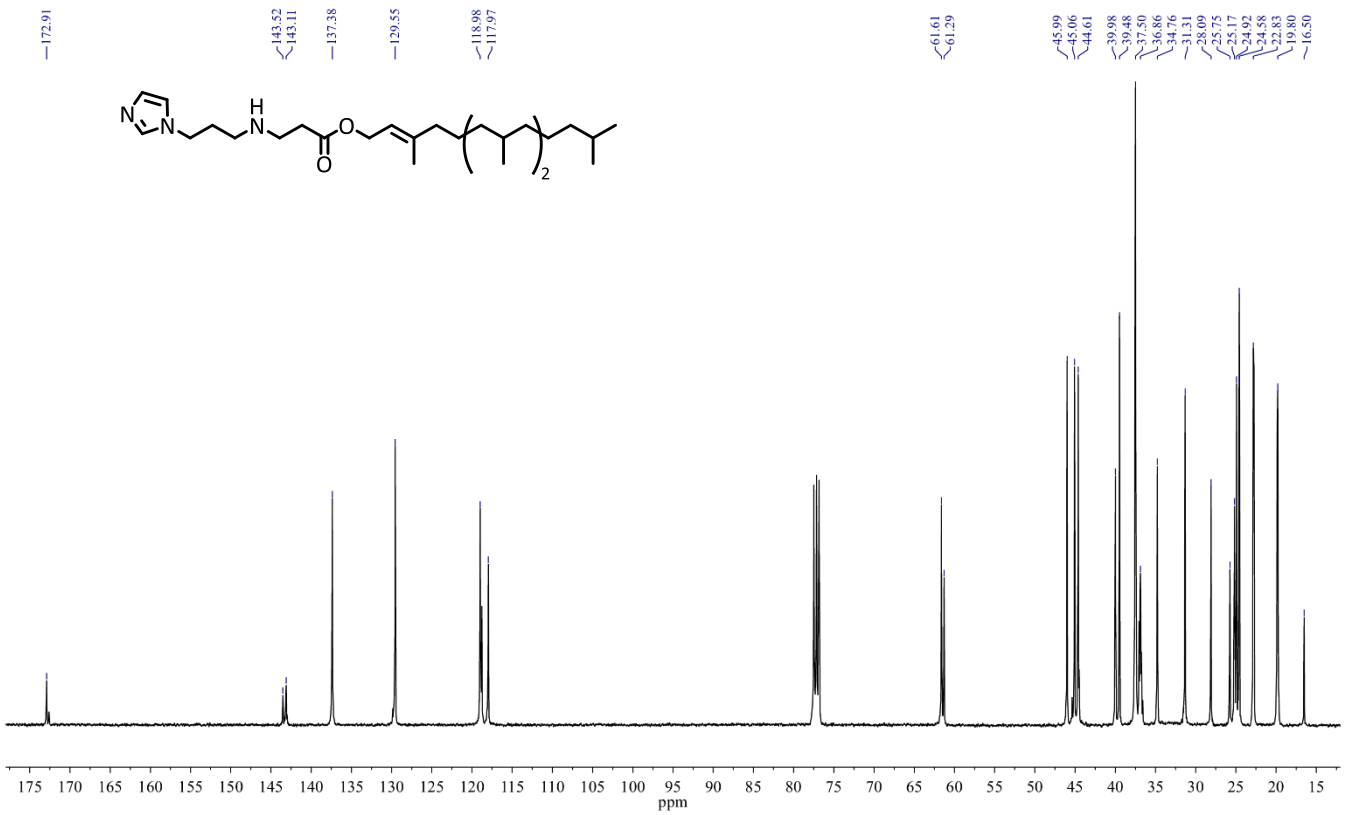


Figure S26. ^{13}C NMR spectrum of the compound **3f**, $CDCl_3$, 298 K, 100 MHz.

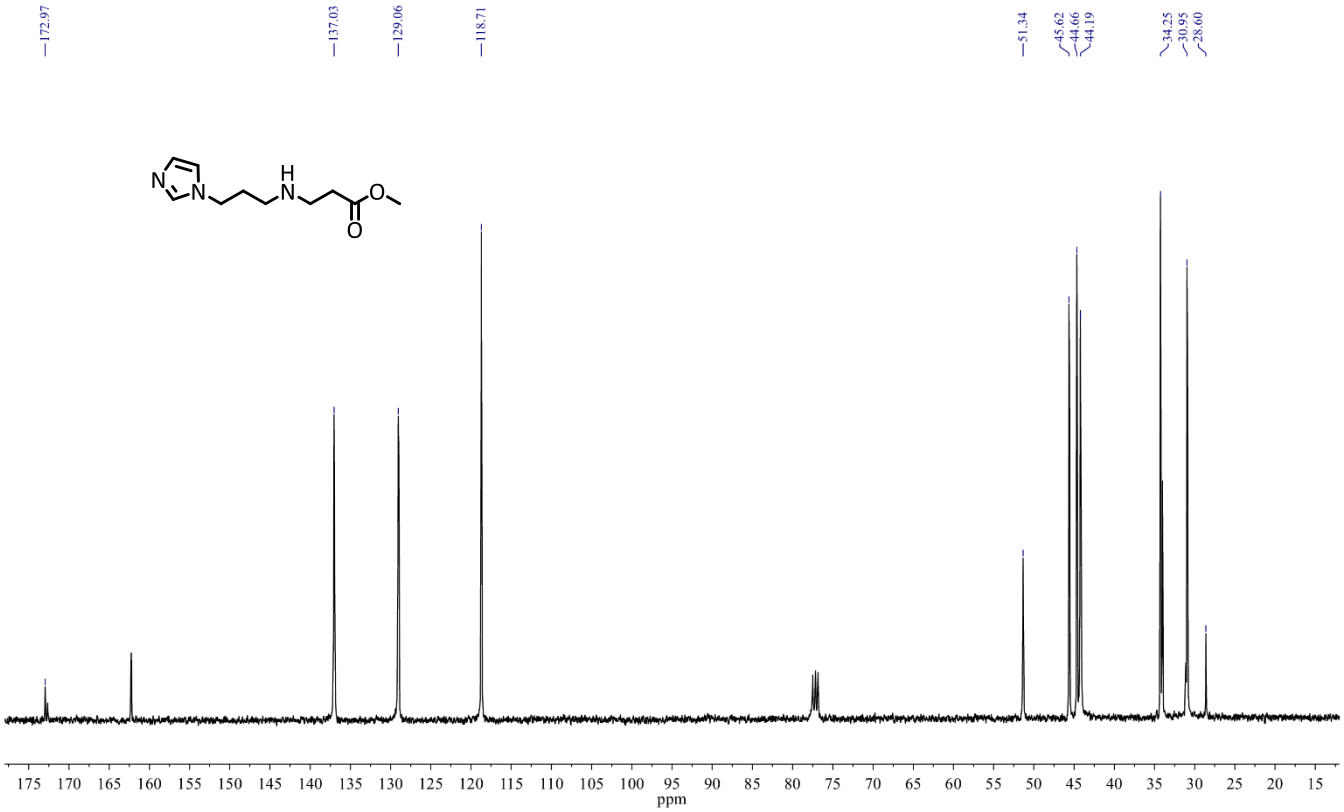


Figure S27. ^{13}C NMR spectrum of the compound **3g**, $CDCl_3$, 298 K, 100 MHz.

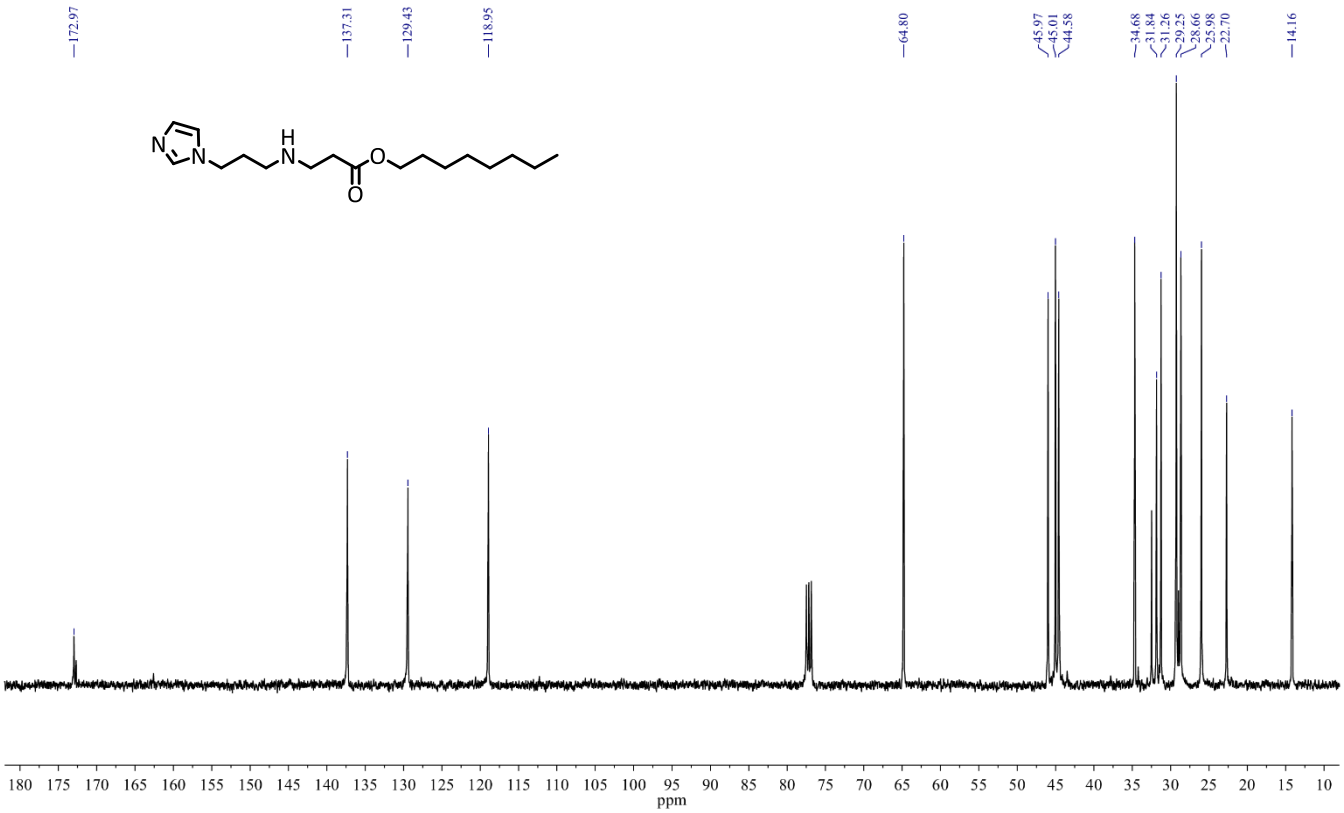


Figure S28. ^{13}C NMR spectrum of the compound **3h**, $CDCl_3$, 298 K, 100 MHz.

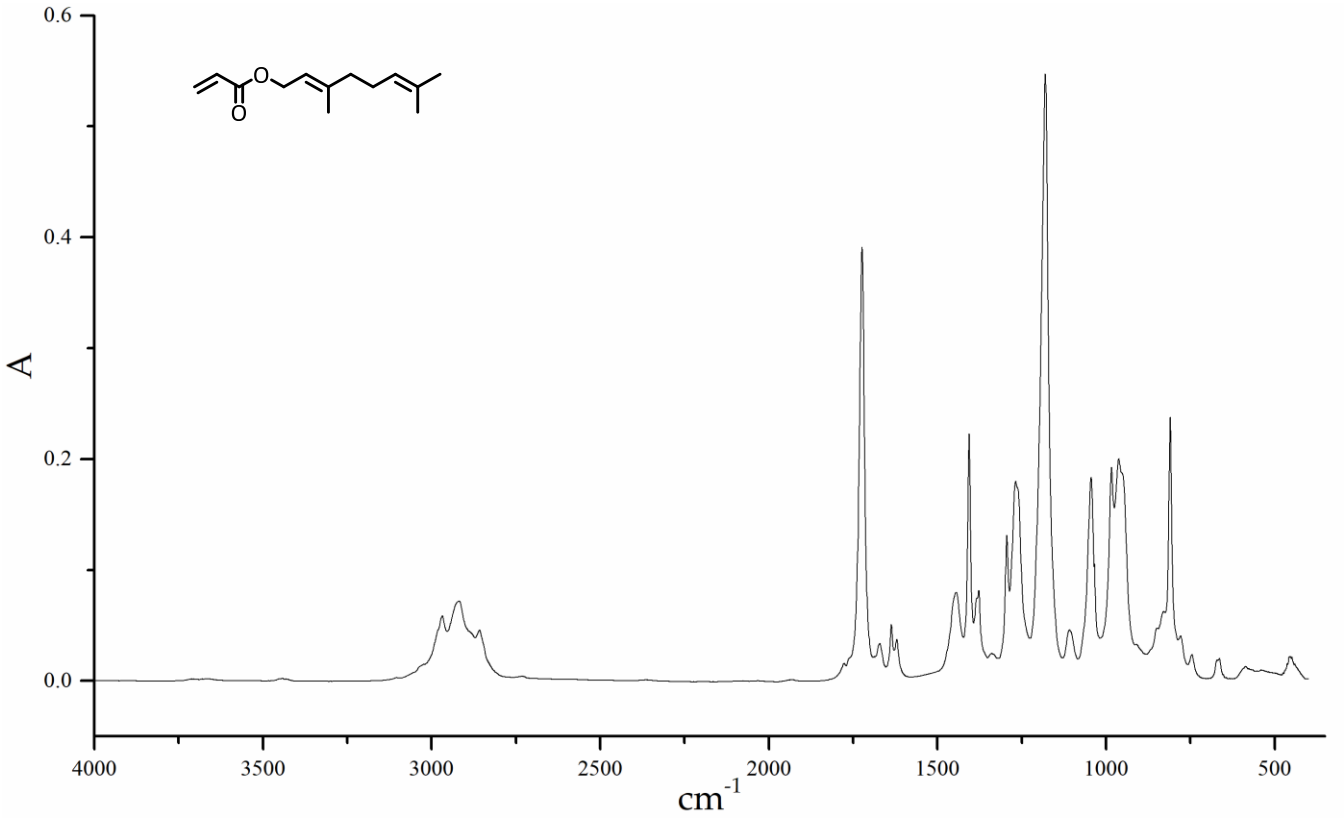


Figure S29. FT-IR spectrum of the compound **2a**.

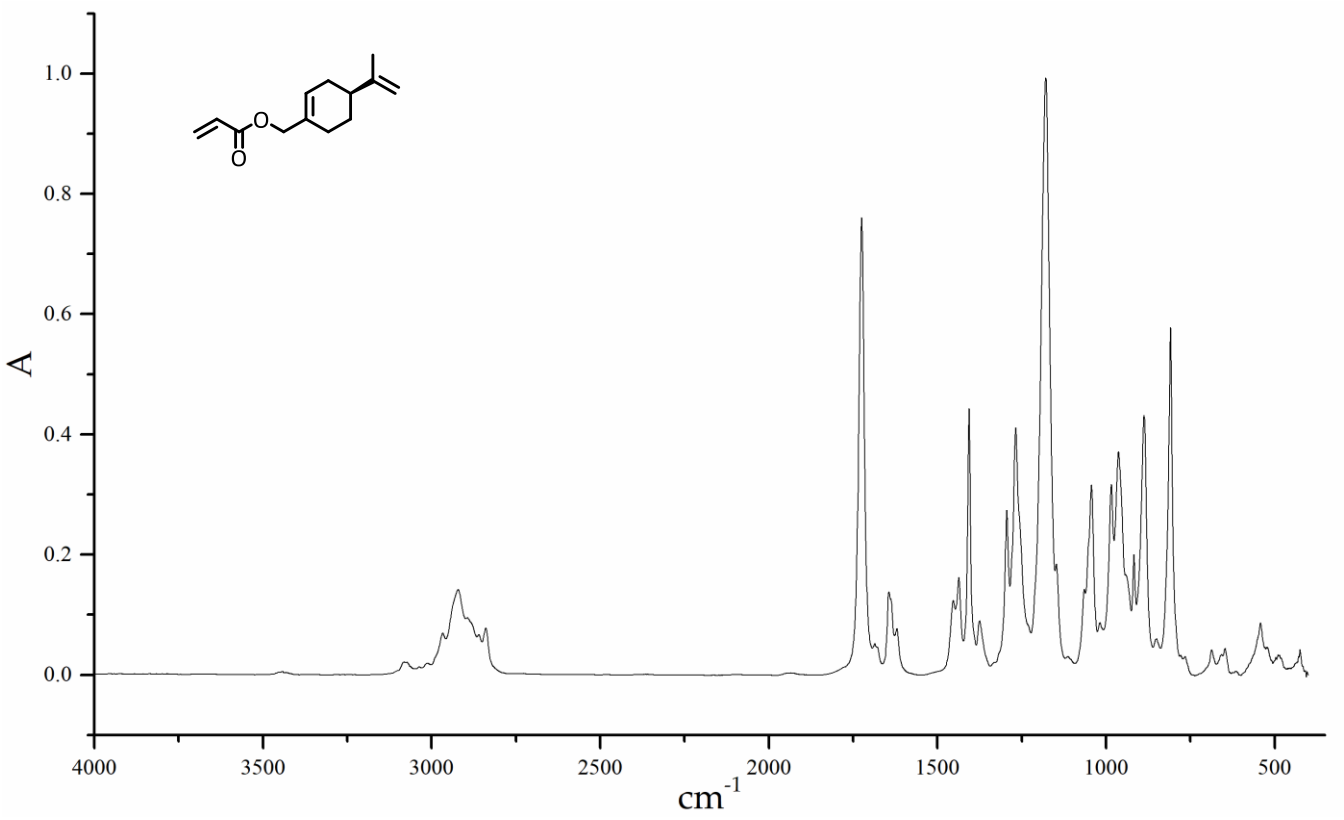


Figure S30. FT-IR spectrum of the compound **2b**.

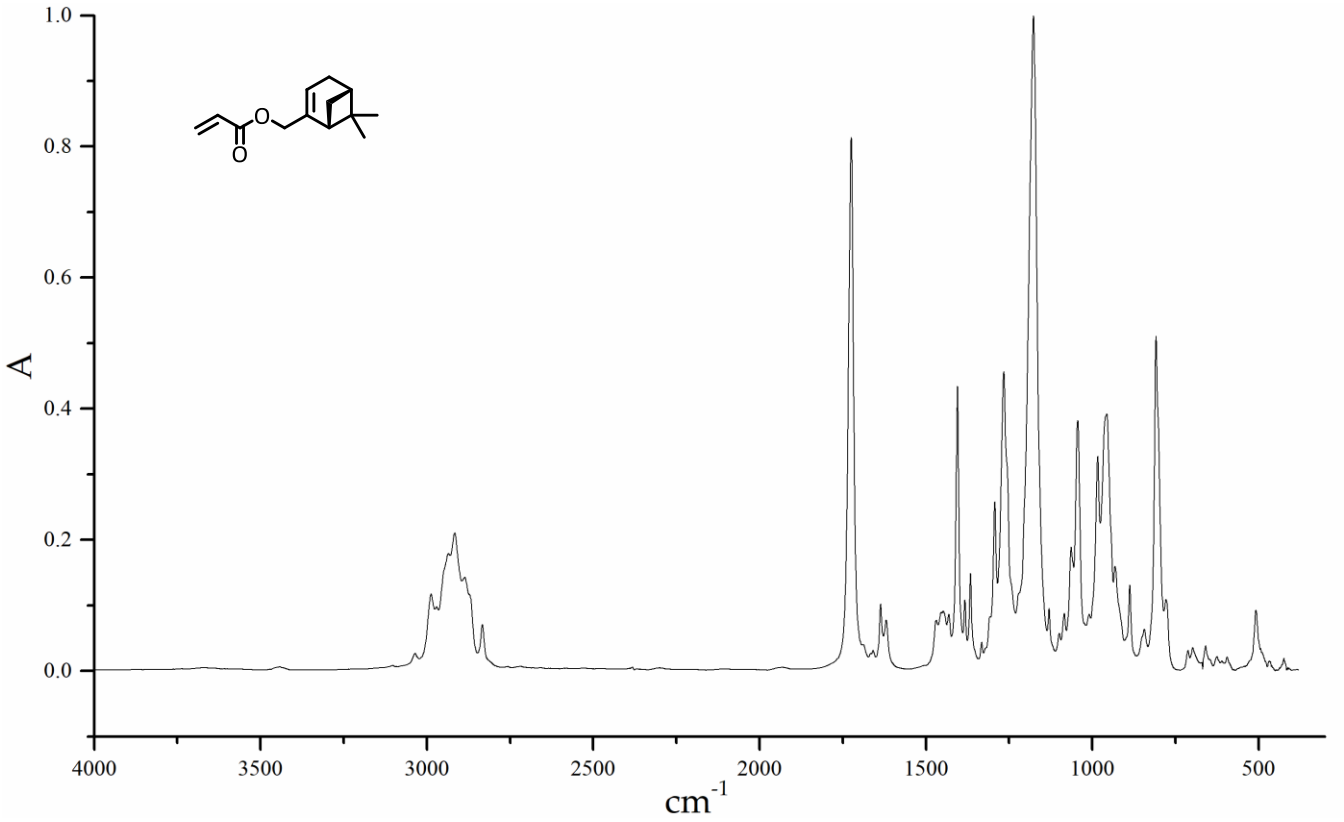


Figure S31. FT-IR spectrum of the compound **2c**.

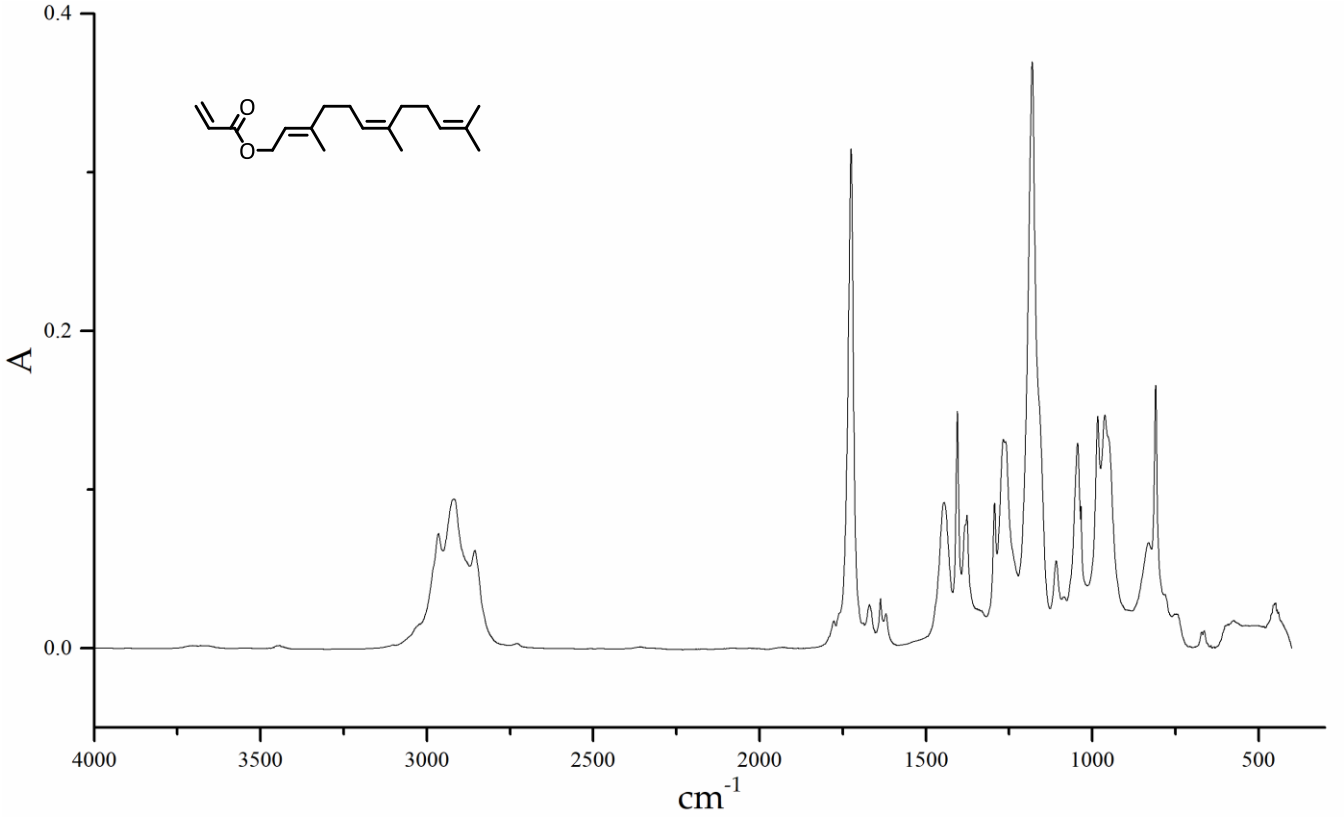


Figure S32. FT-IR spectrum of the compound **2d**.

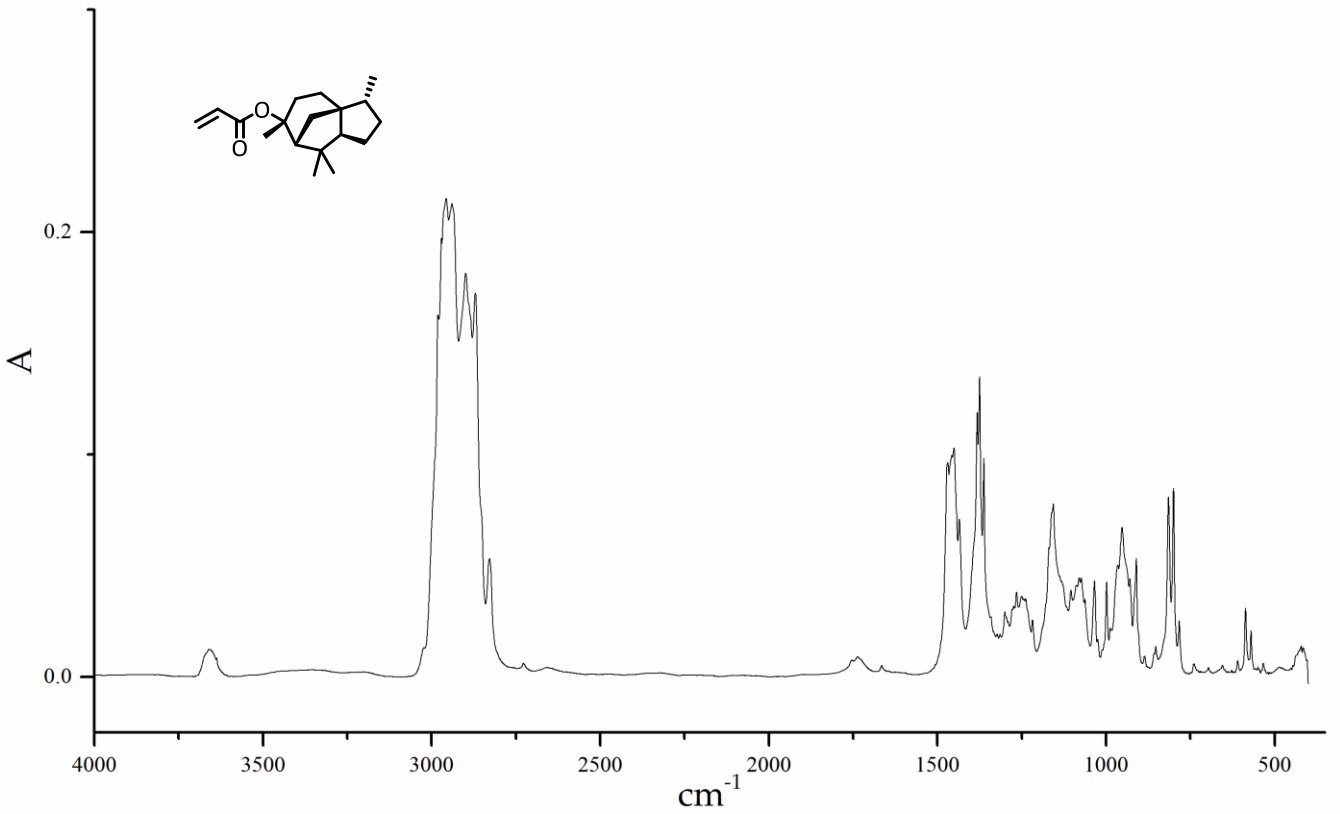


Figure S33. FT-IR spectrum of the compound **2e**.

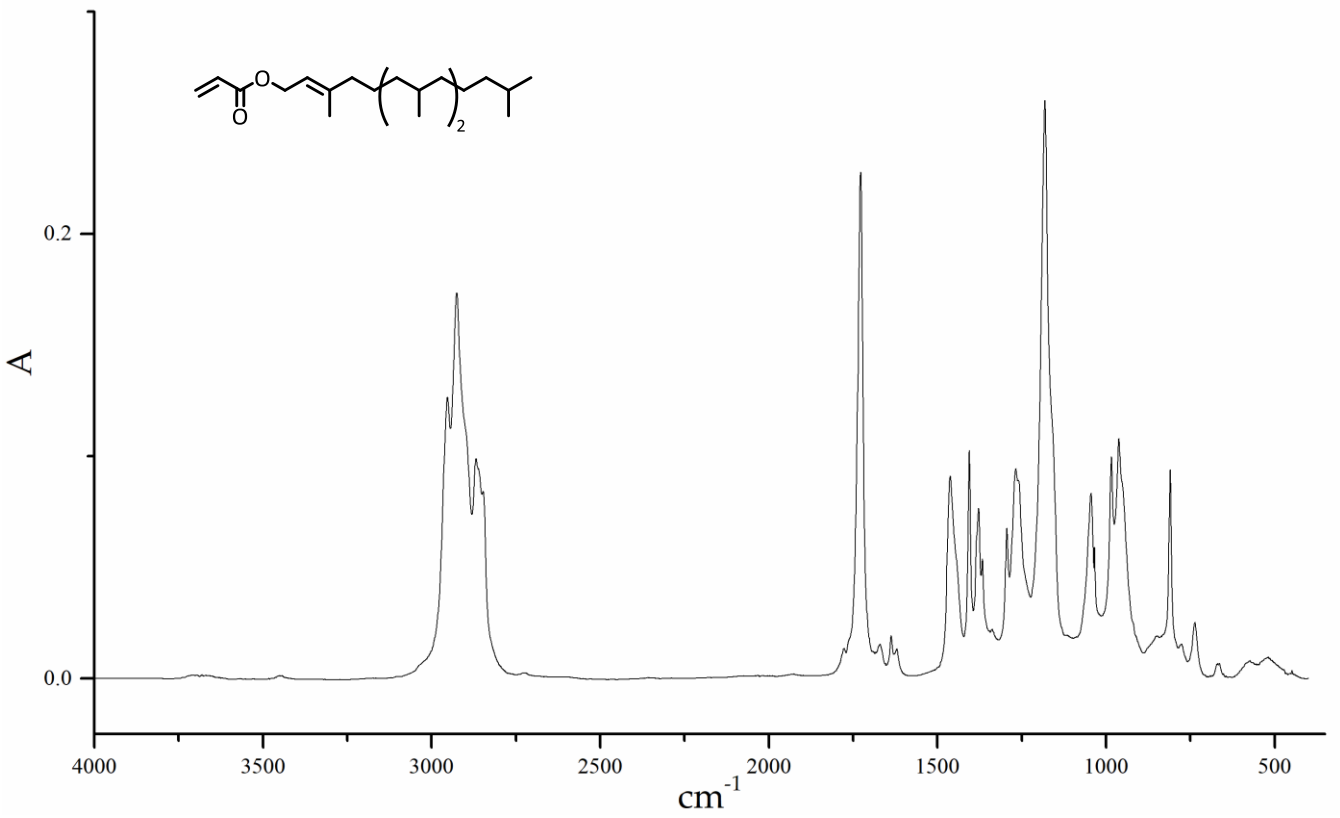


Figure S34. FT-IR spectrum of the compound **2f**.

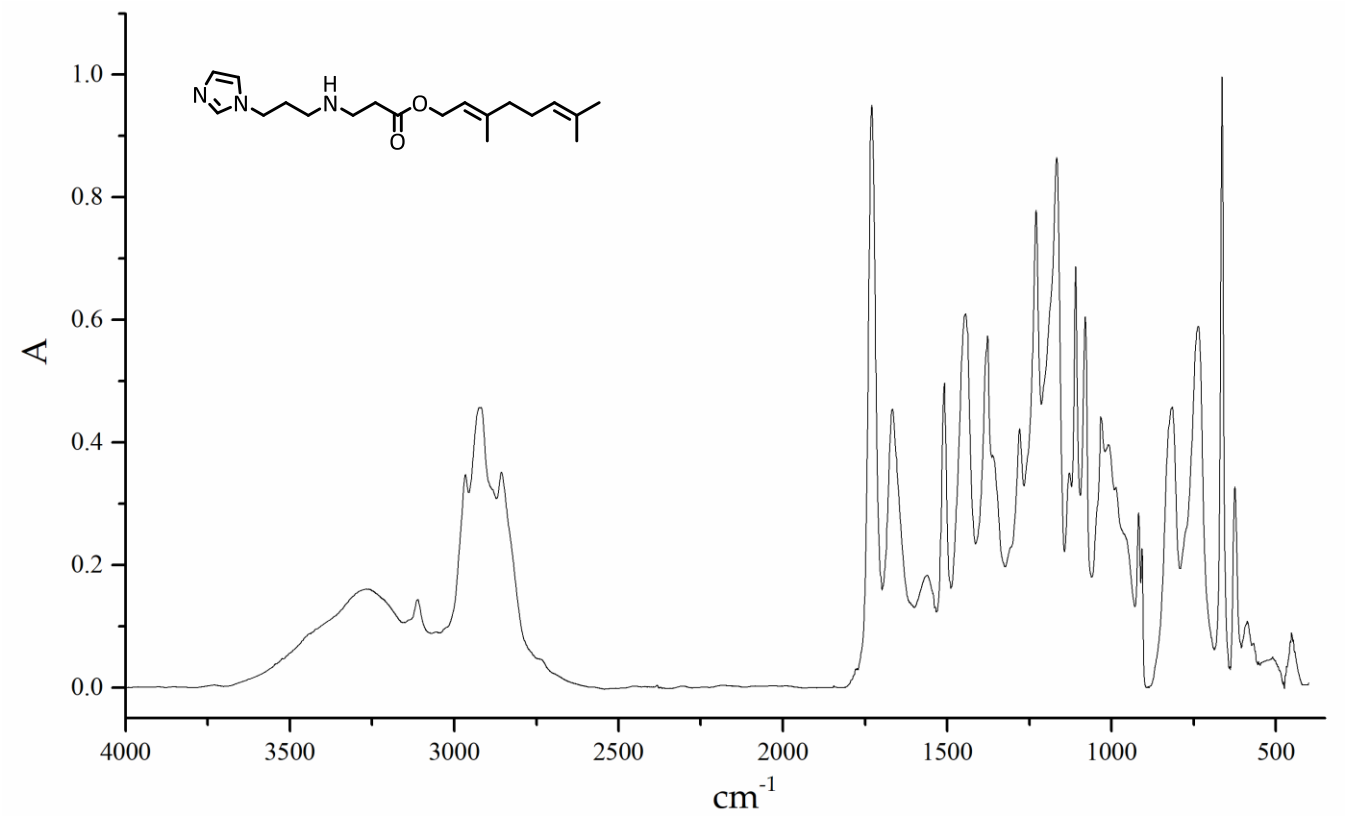


Figure S35. FT-IR spectrum of the compound **3a**.

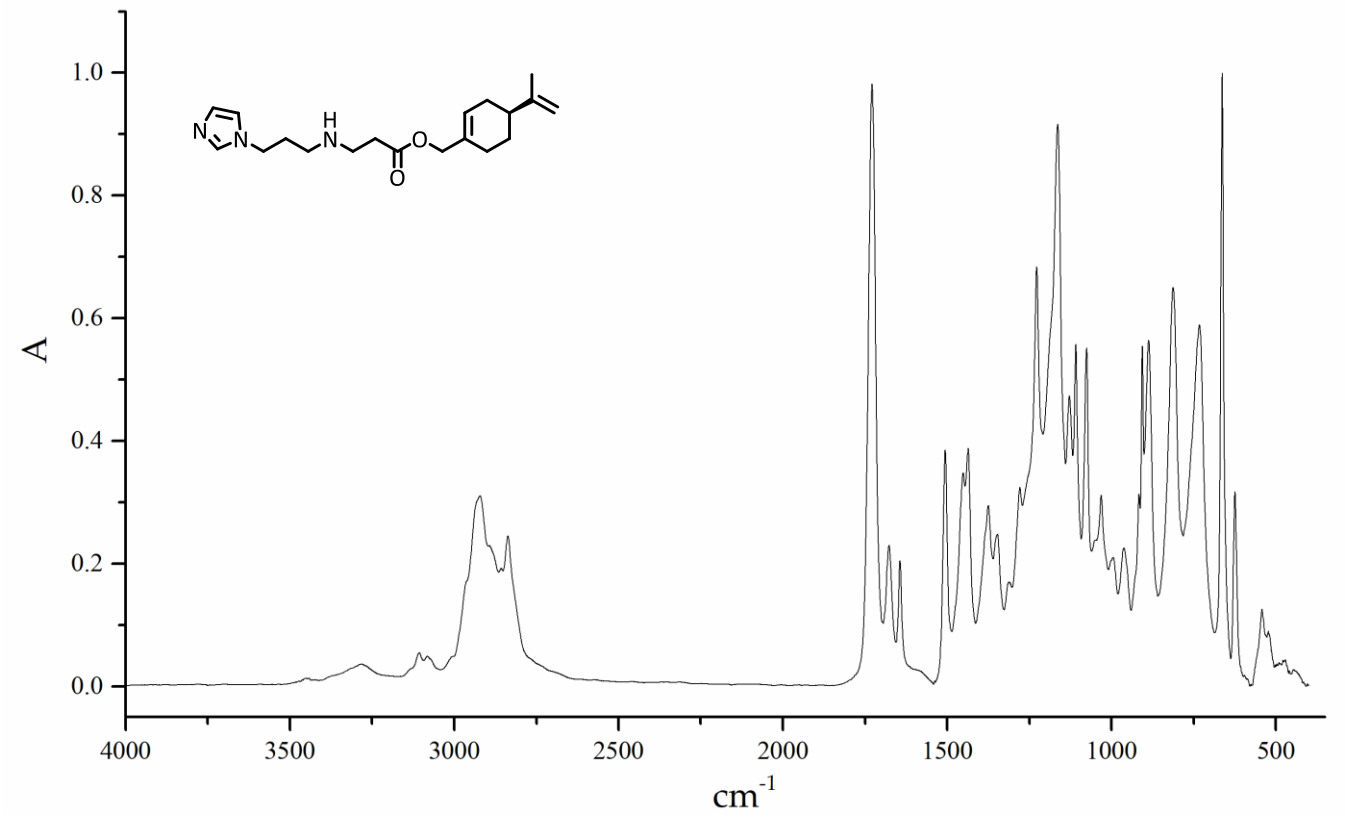


Figure S36. FT-IR spectrum of the compound **3b**.

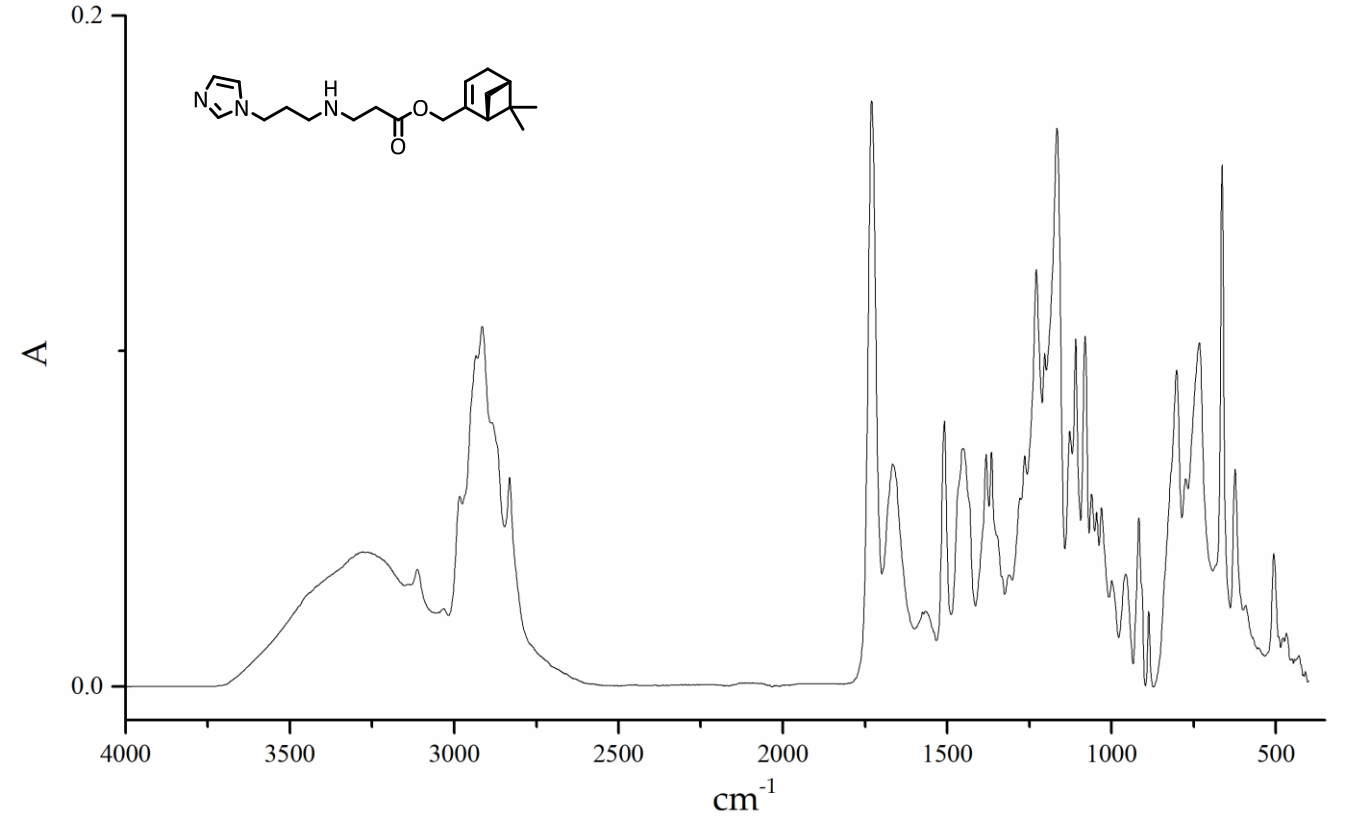


Figure S37. FT-IR spectrum of the compound **3c**.

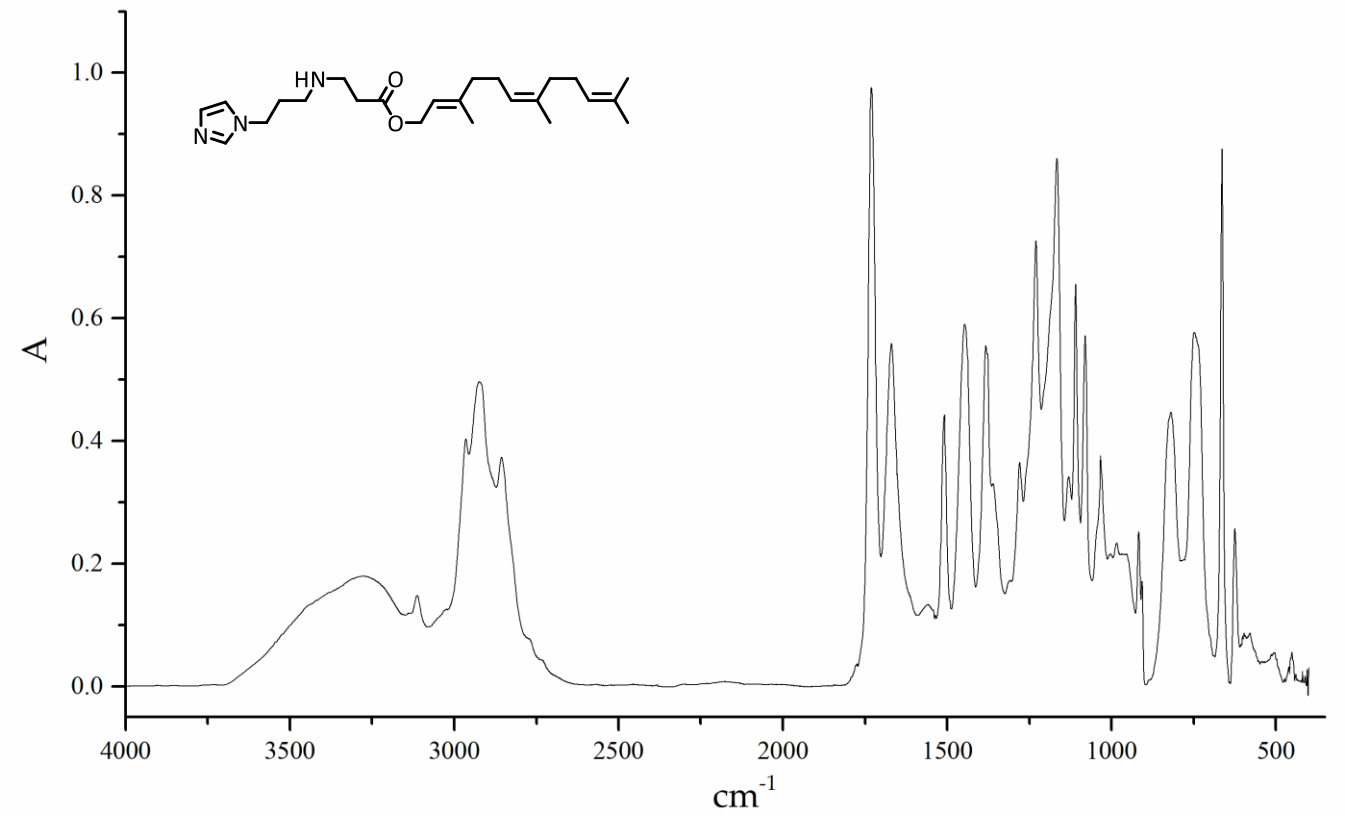


Figure S38. FT-IR spectrum of the compound **3d**.

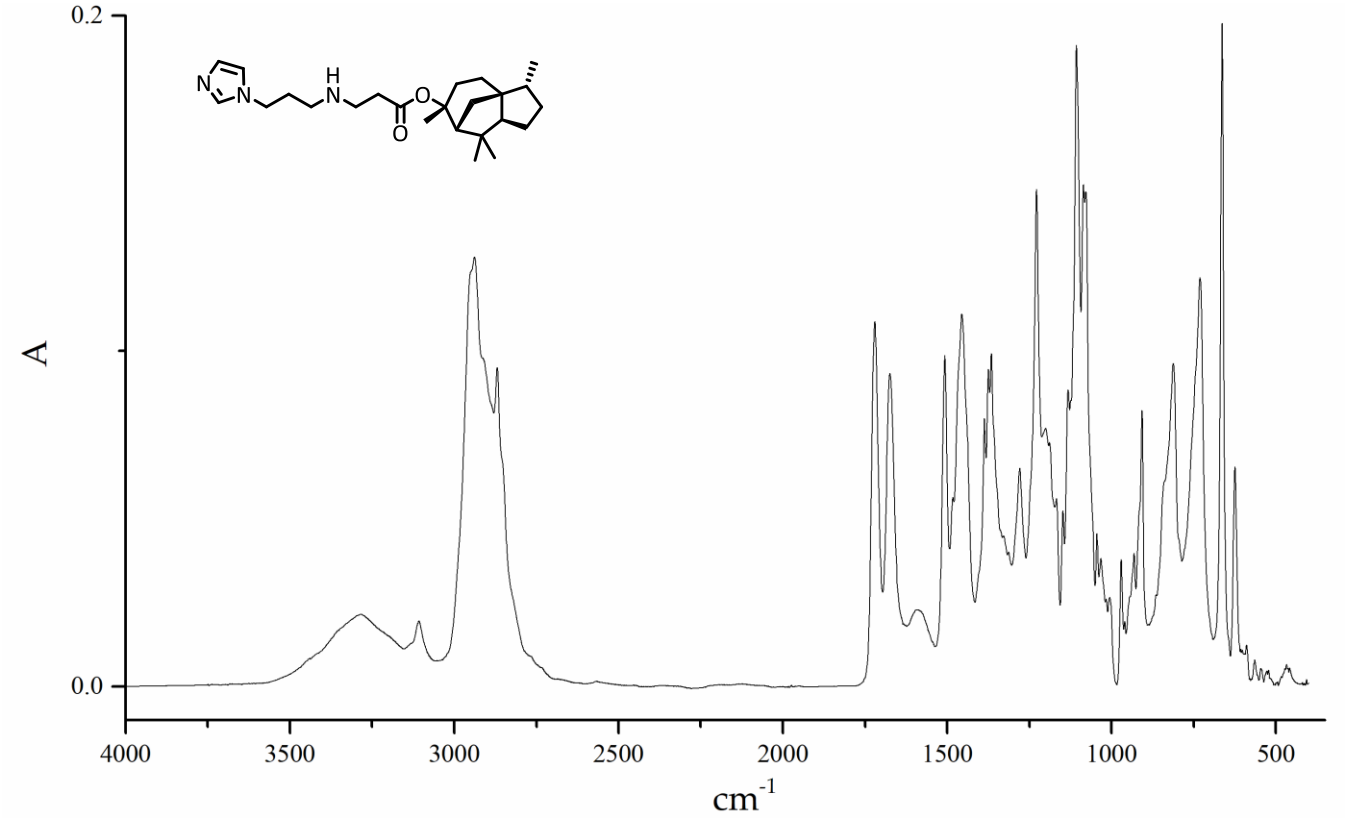


Figure S39. FT-IR spectrum of the compound **3e**.

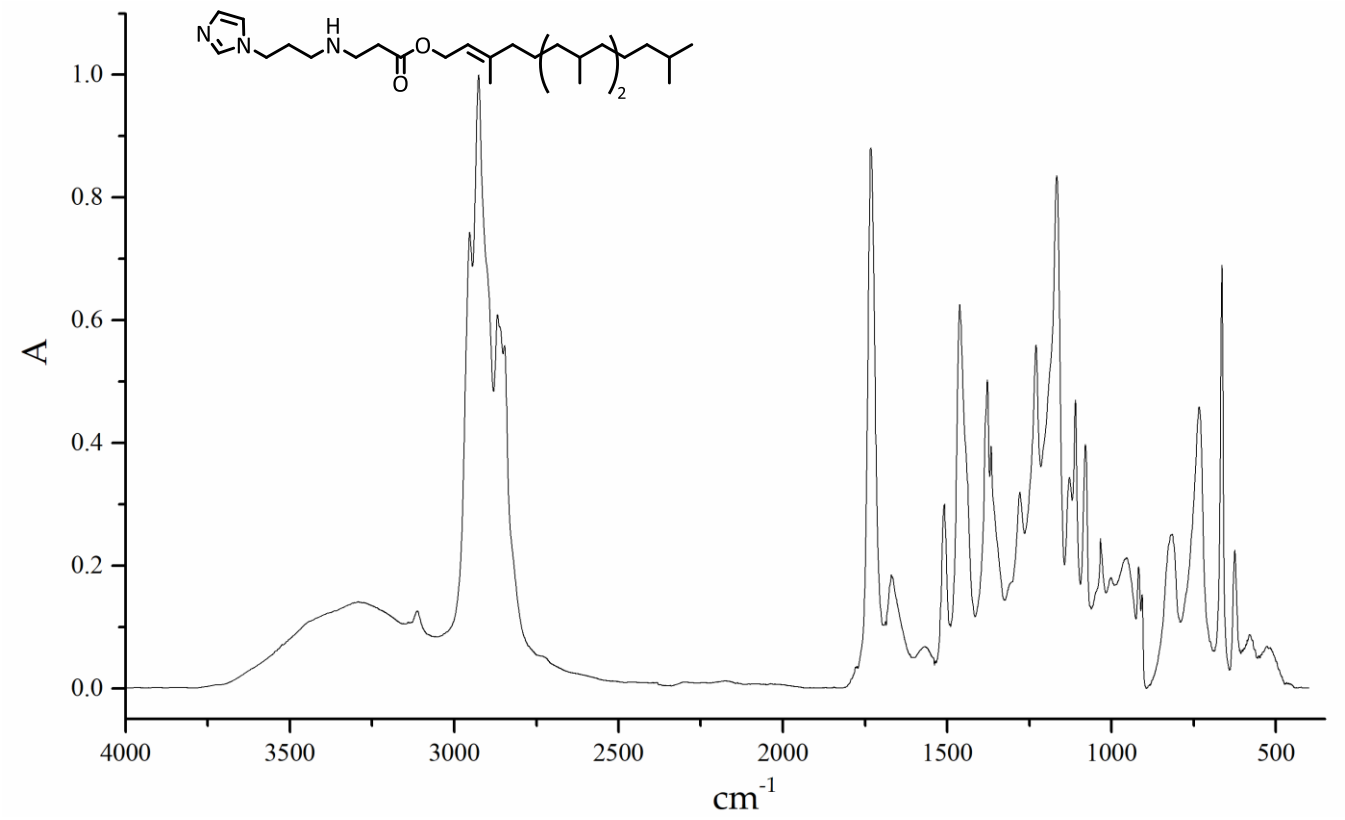


Figure S40. FT-IR spectrum of the compound **3f**.

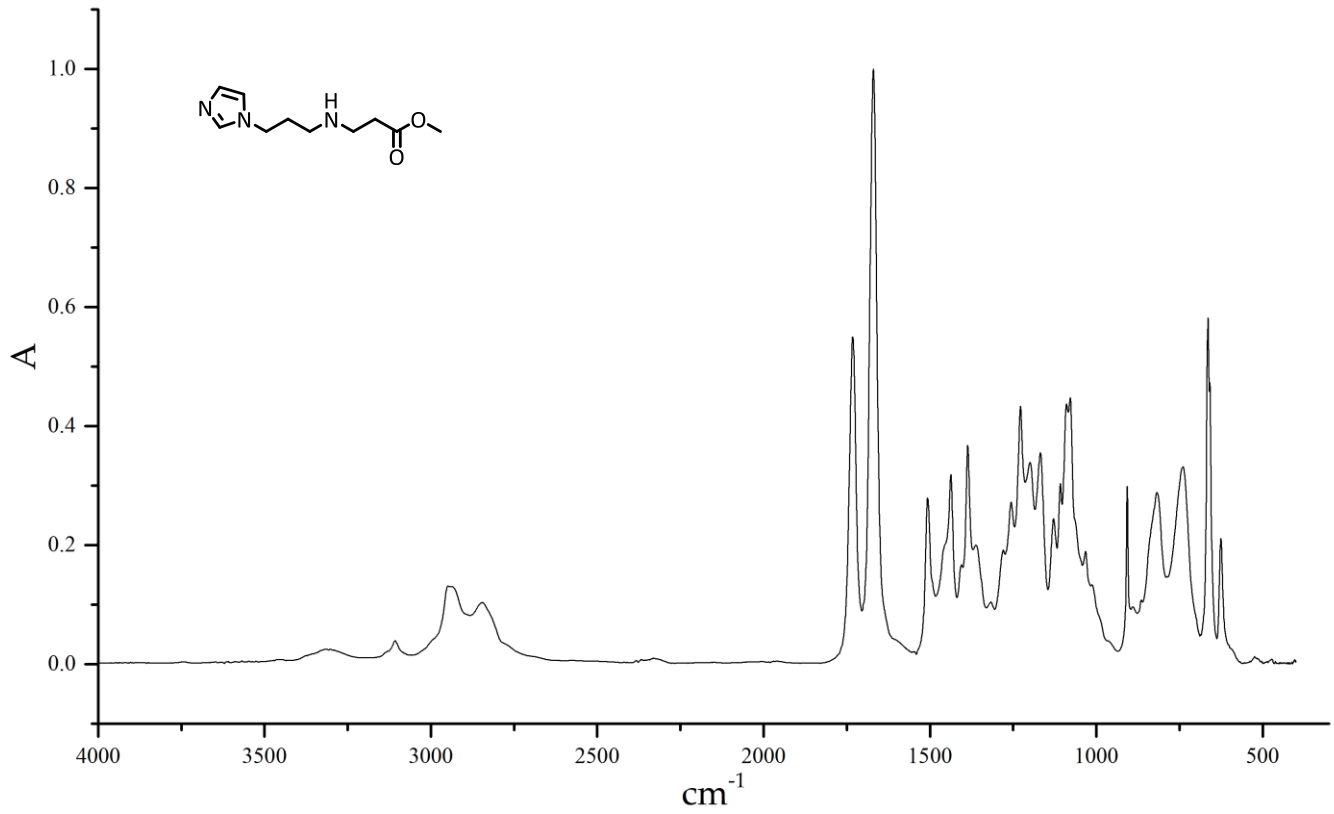


Figure S41. FT-IR spectrum of the compound **3g**.

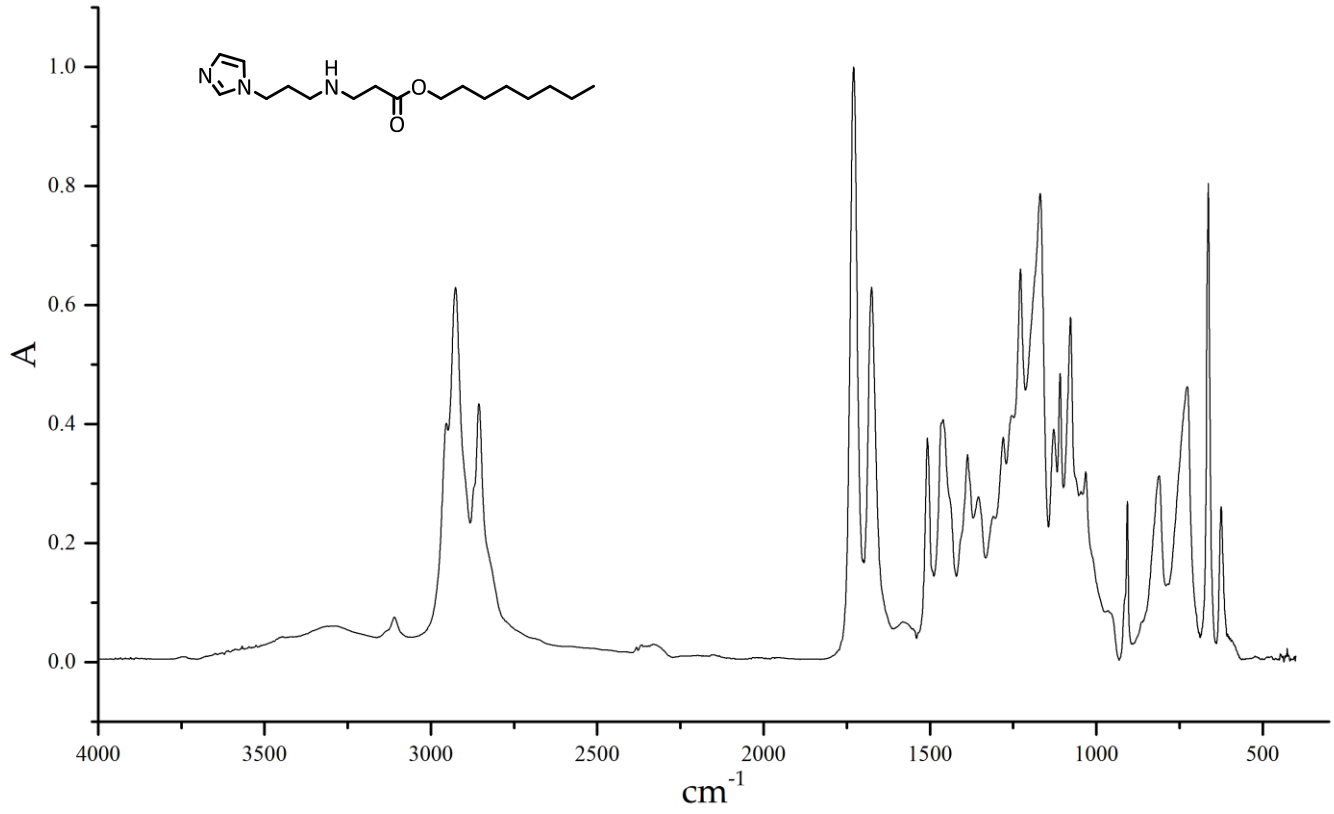


Figure S42. FT-IR spectrum of the compound **3h**.

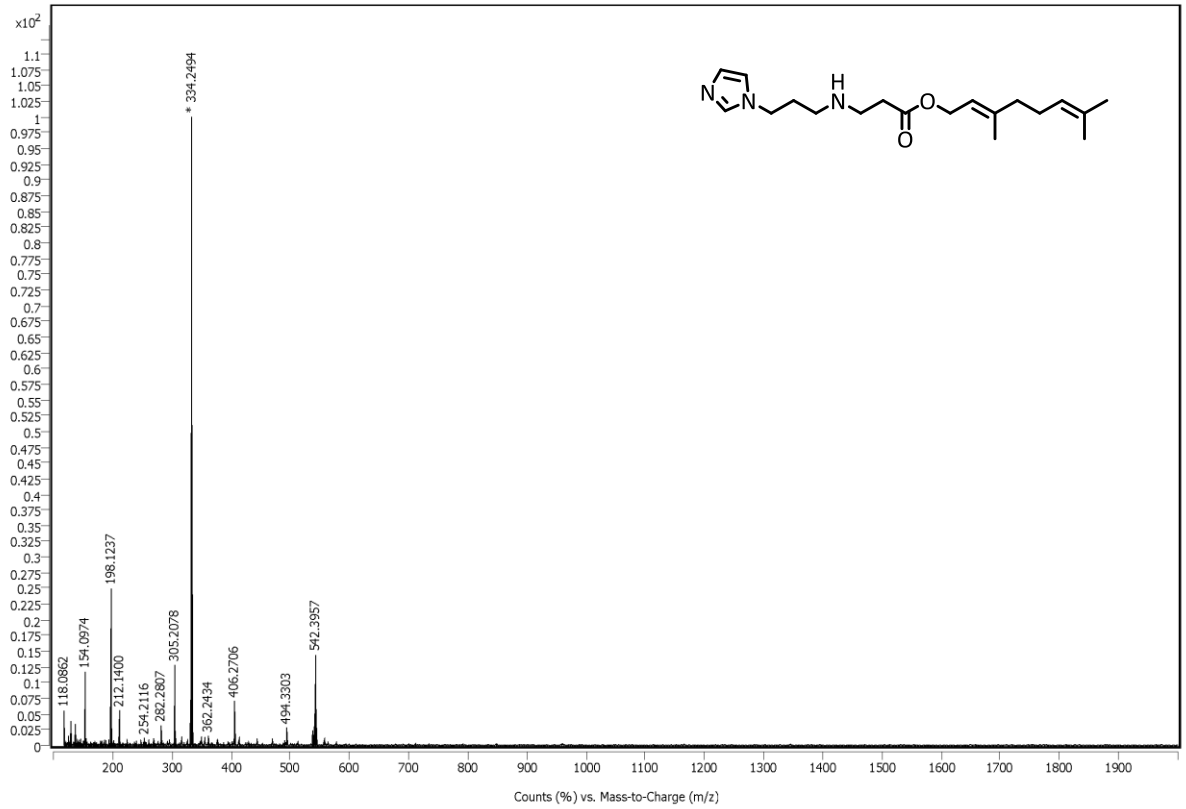


Figure S43. HRMS spectrum of the compound **3a**.

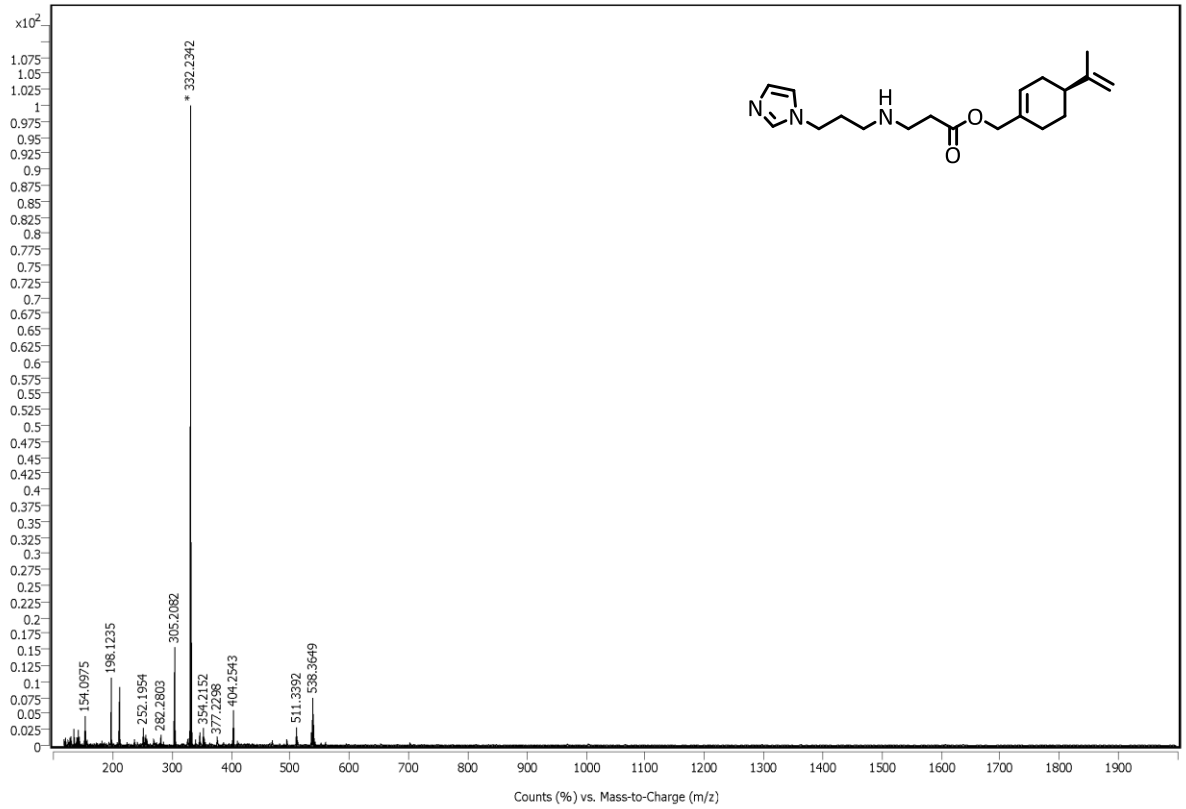


Figure S44. HRMS spectrum of the compound **3b**.

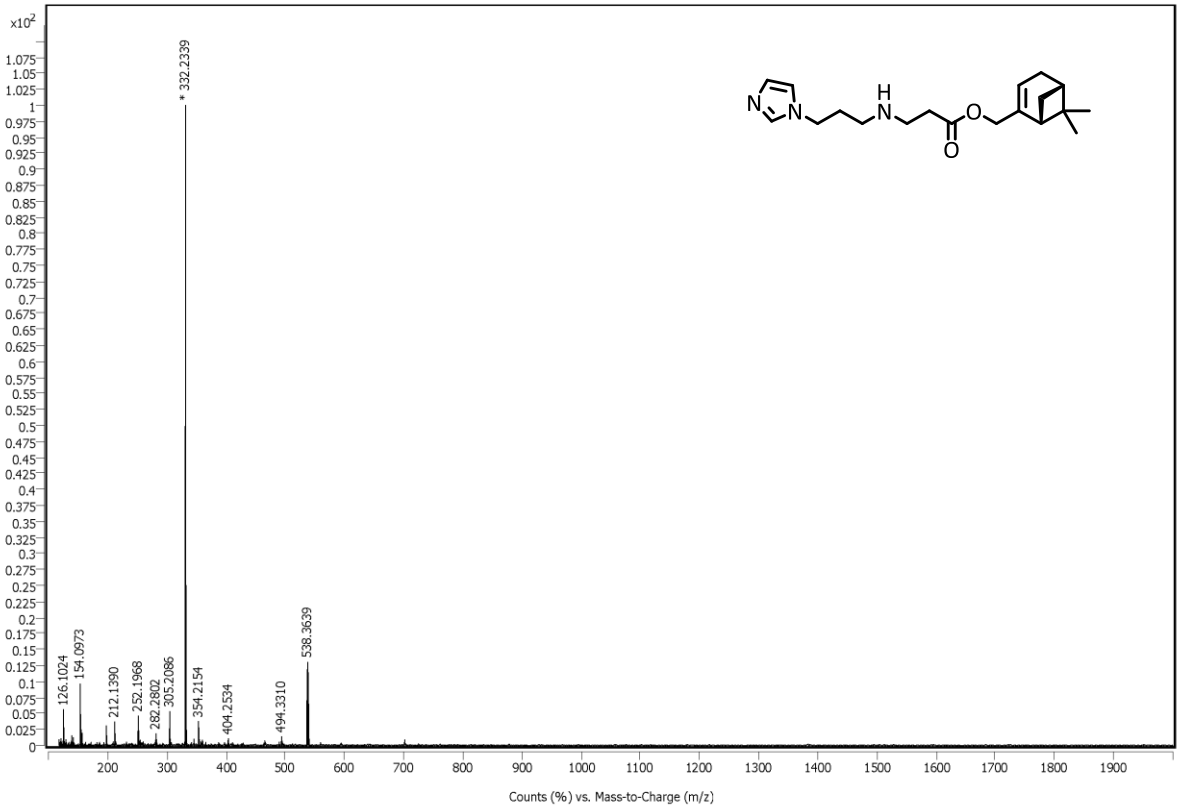


Figure S45. HRMS spectrum of the compound **3c**.

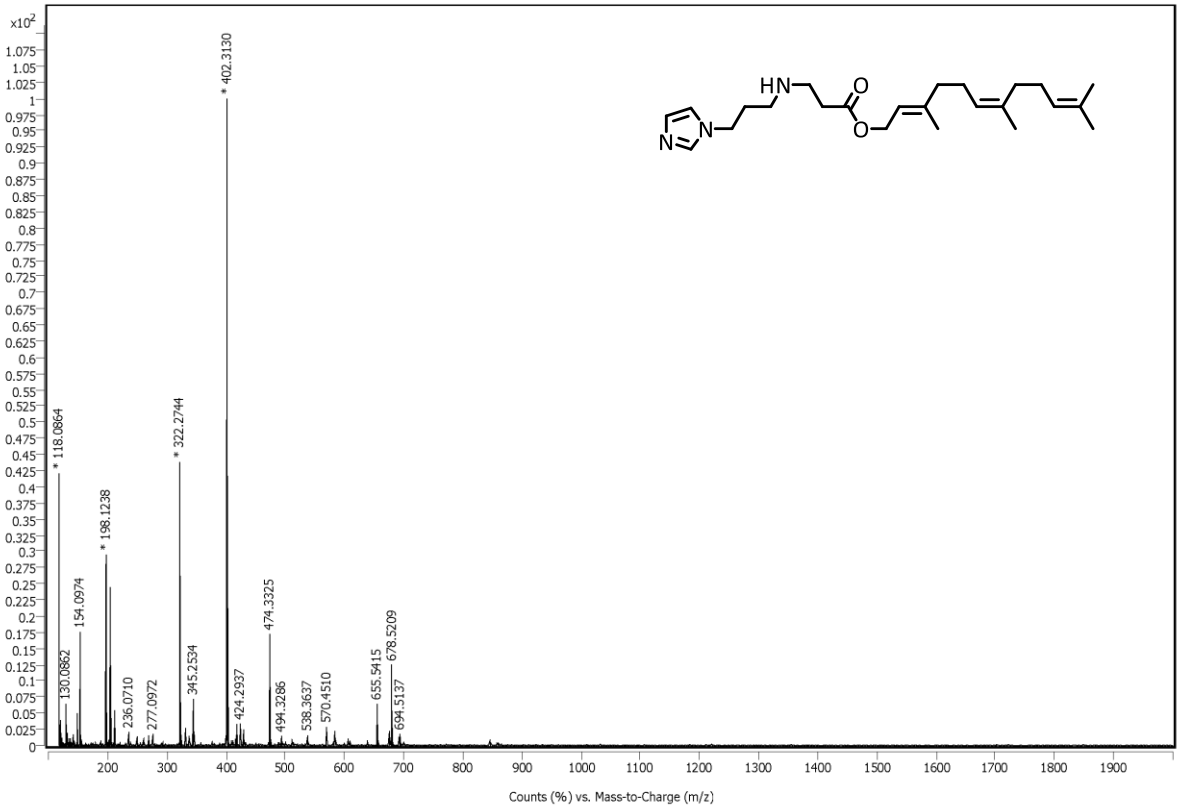


Figure S46. HRMS spectrum of the compound **3d**.

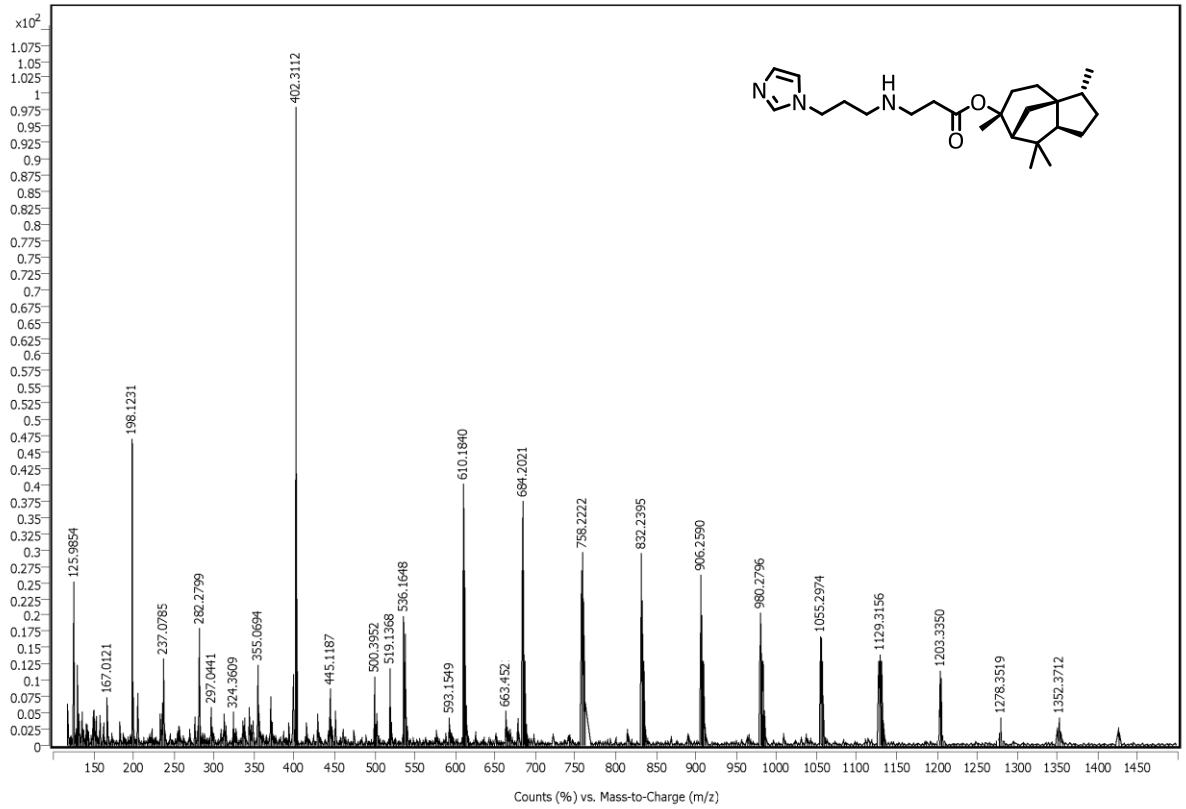


Figure S47. HRMS spectrum of the compound **3e**.

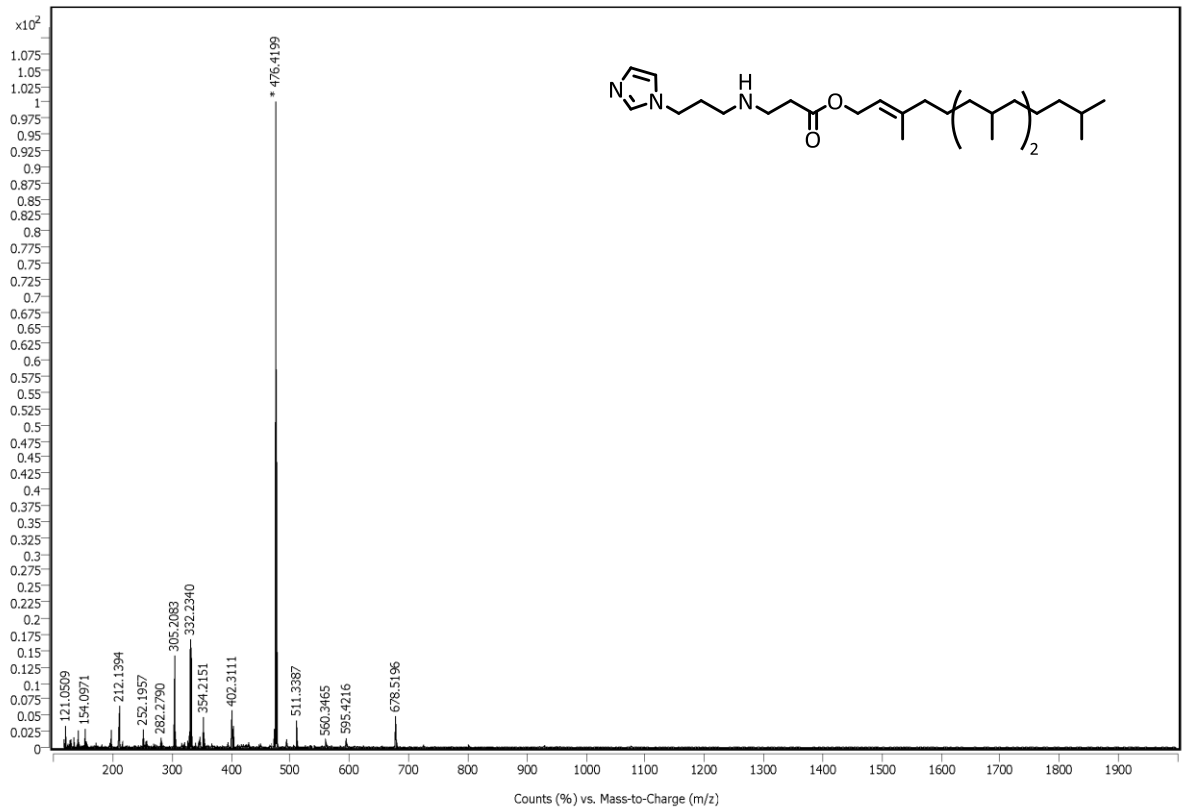


Figure S48. HRMS spectrum of the compound **3f**.

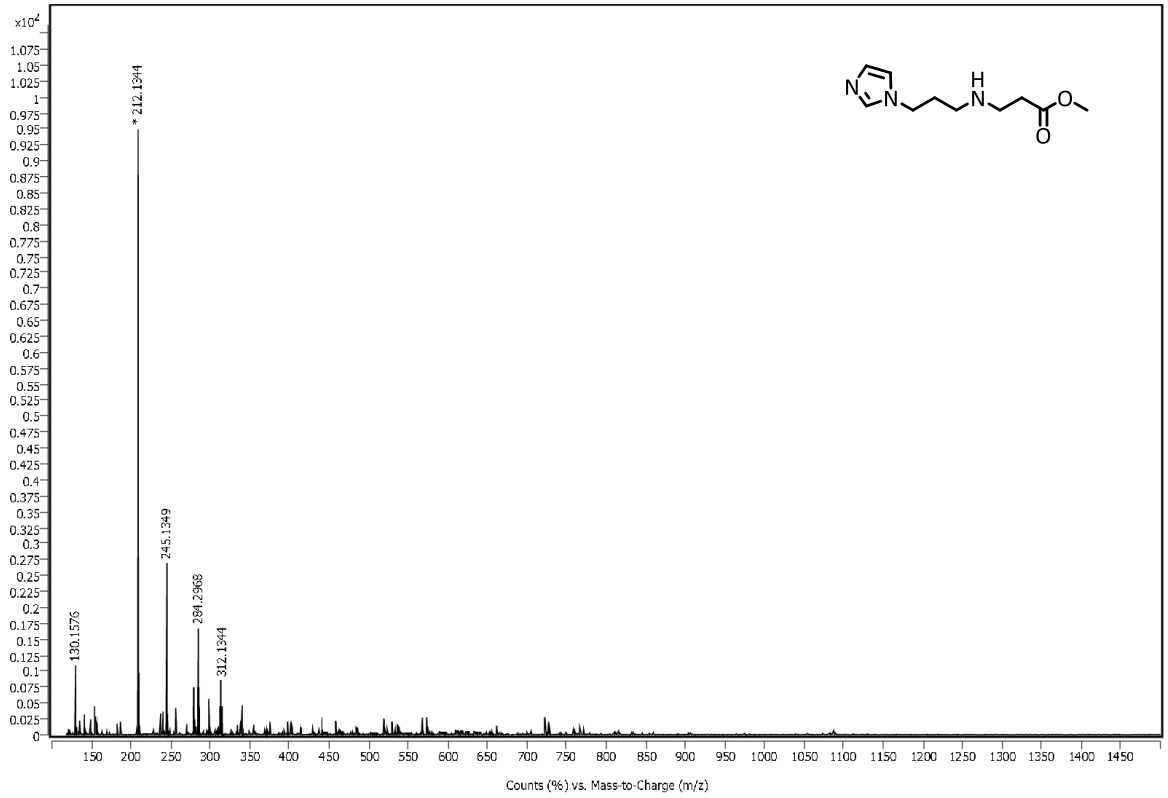


Figure S49. HRMS spectrum of the compound **3e**.

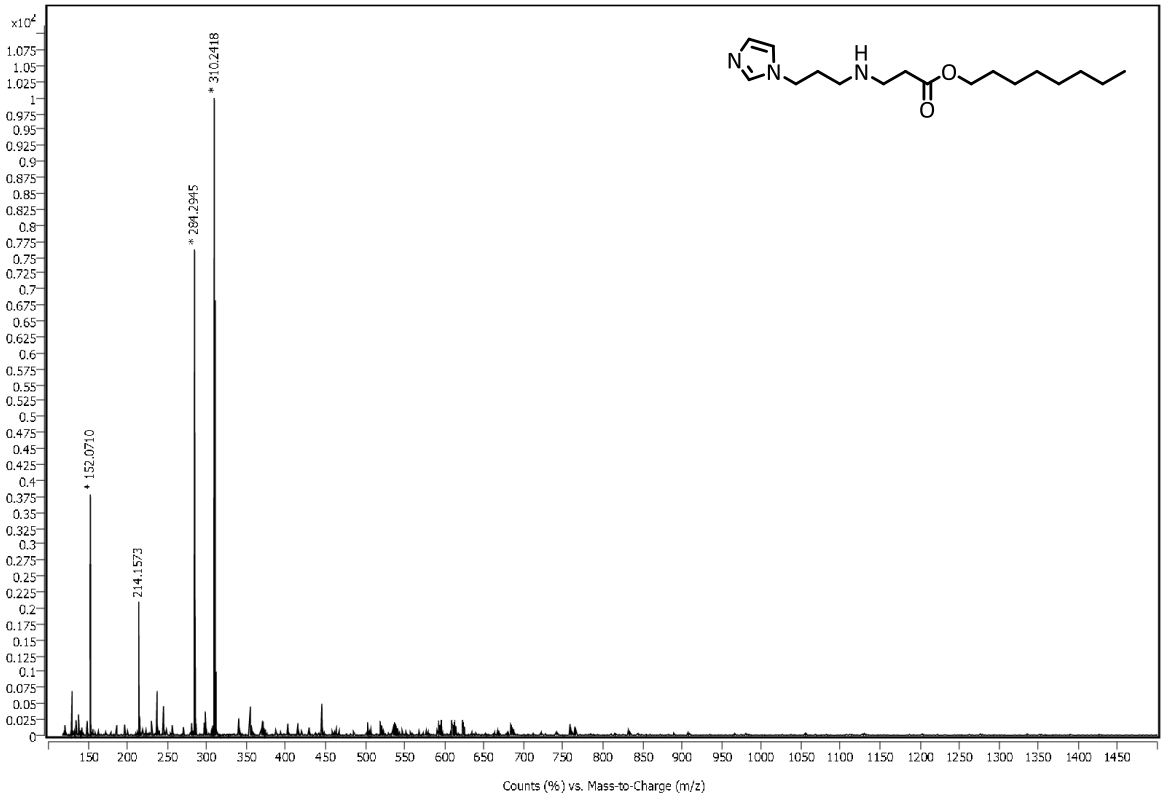
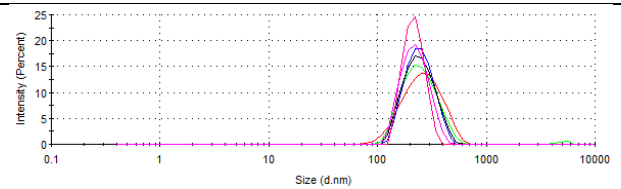
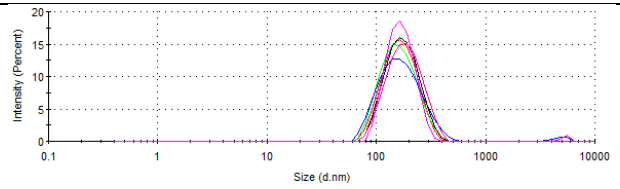
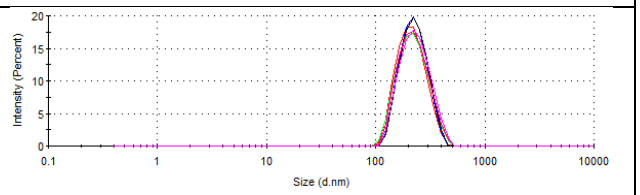
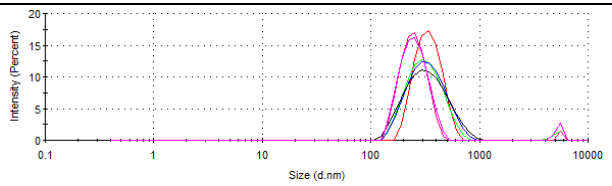
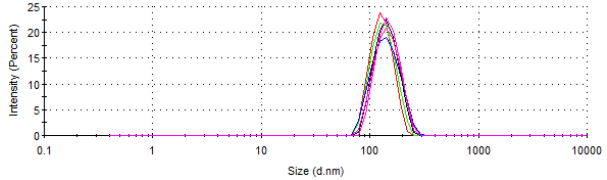
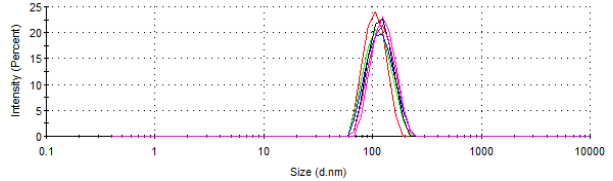
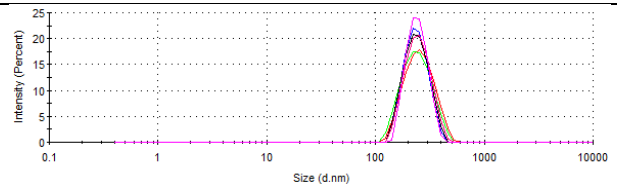
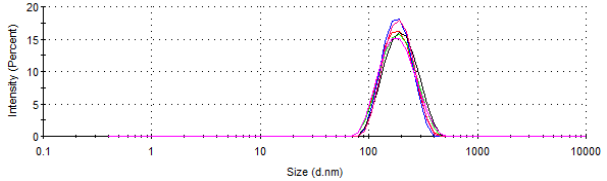
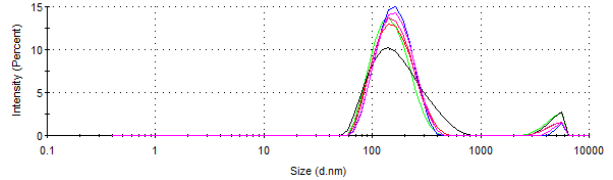
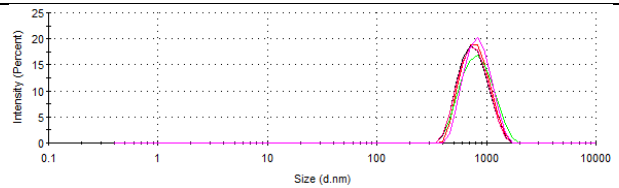
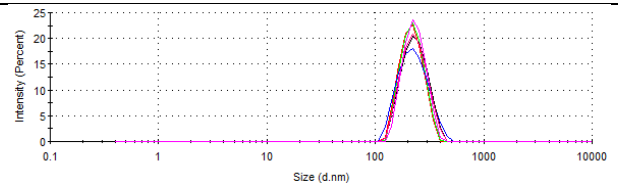
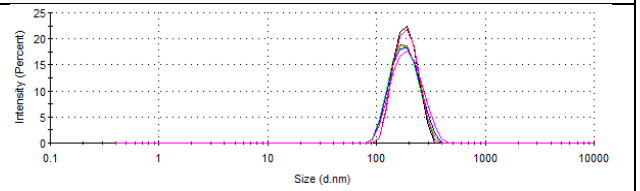
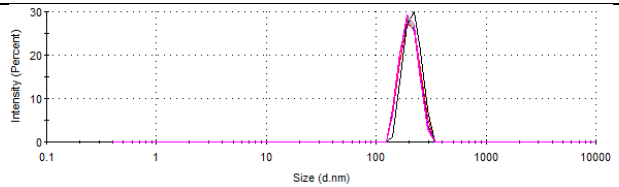
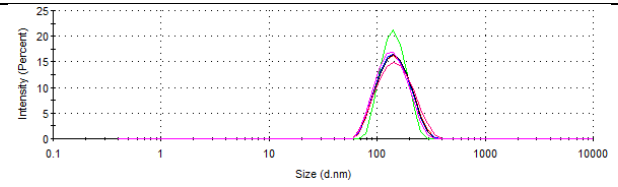
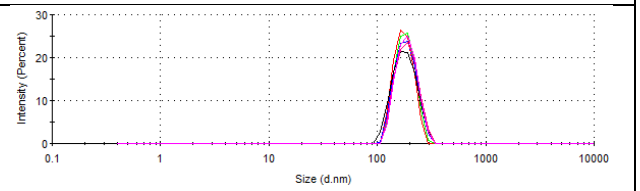
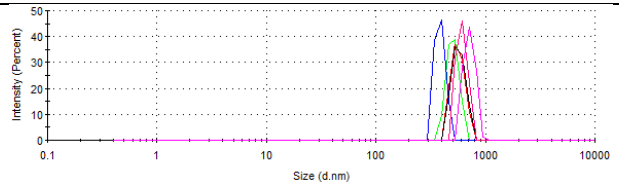
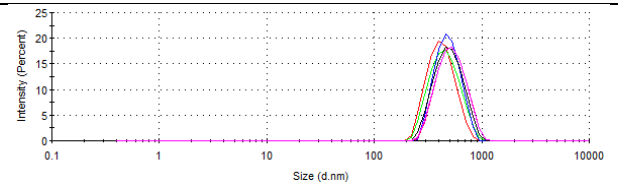
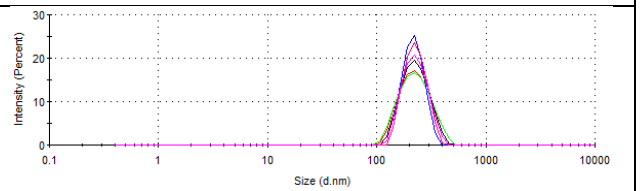


Figure S50. HRMS spectrum of the compound **3h**.

Dynamic light scattering

Conc.	1×10^{-3}	1×10^{-4}	1×10^{-5}
3a			
3b			
3c			
3d			
3e			
3f			

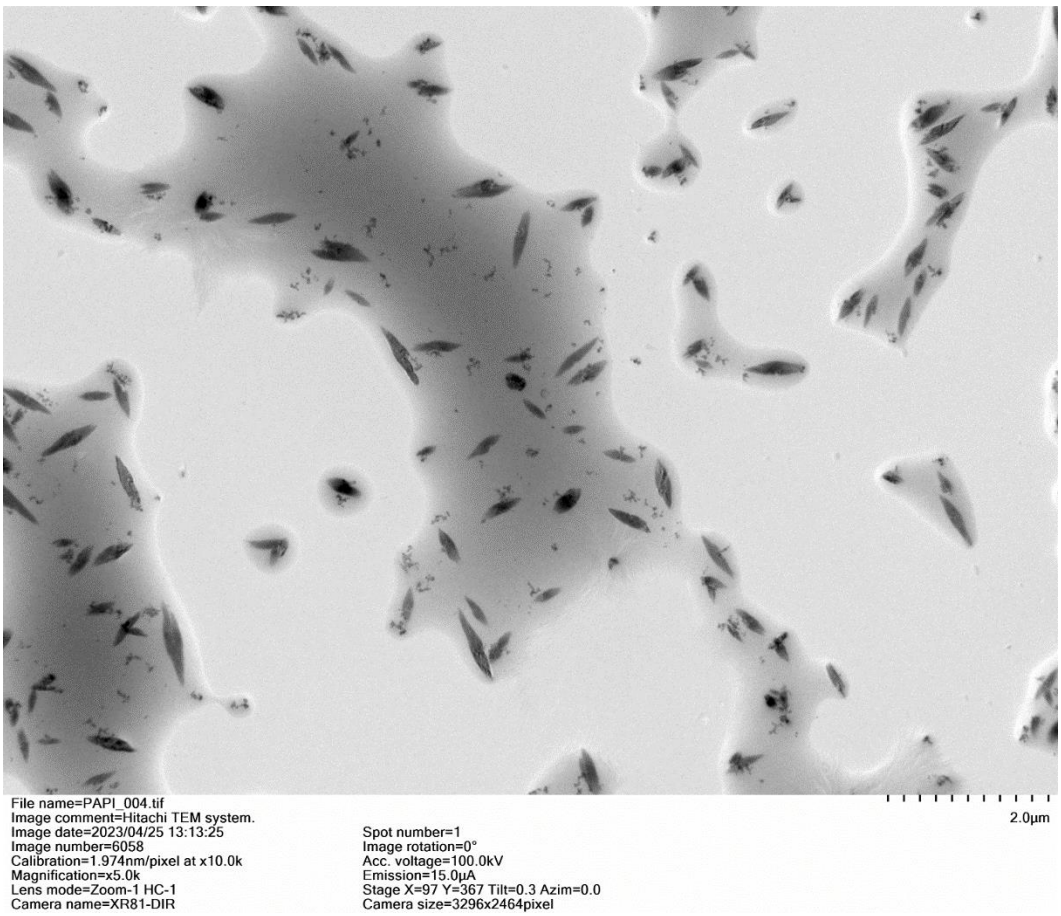


Figure S51. TEM image of associates of the compounds **3f**

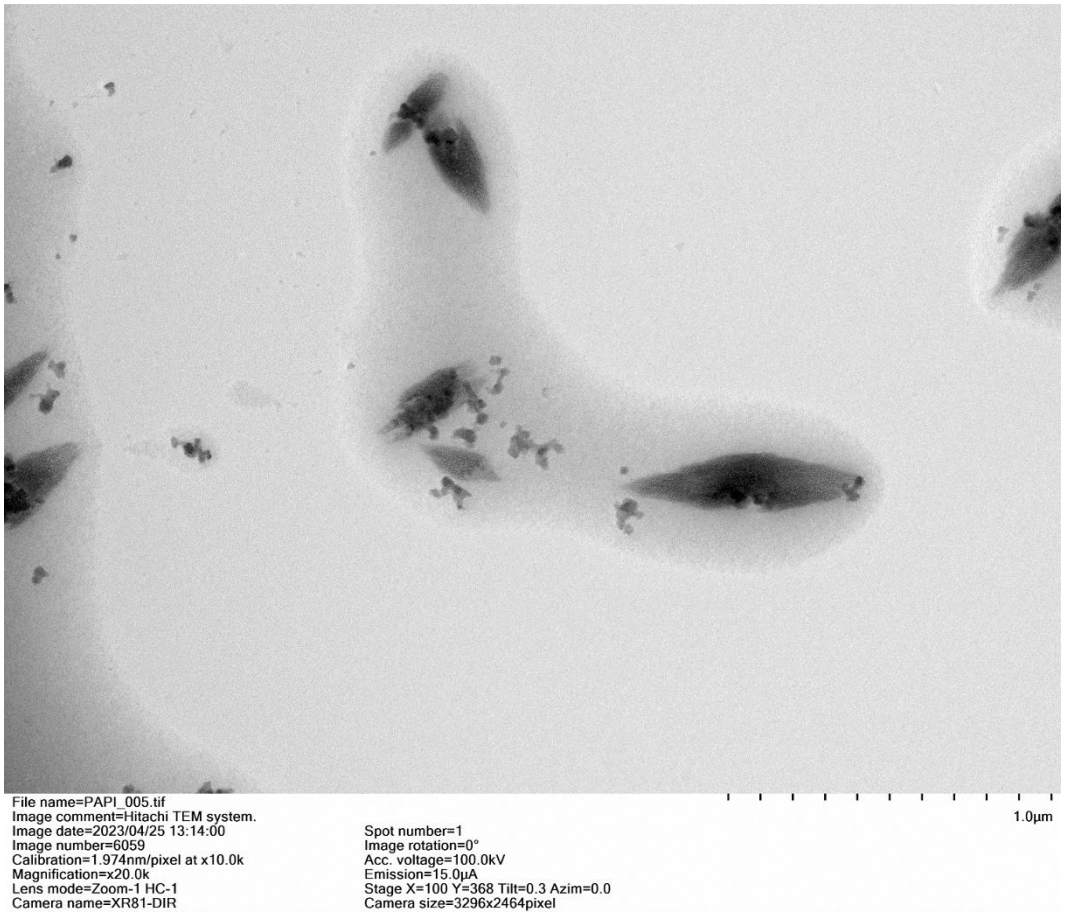
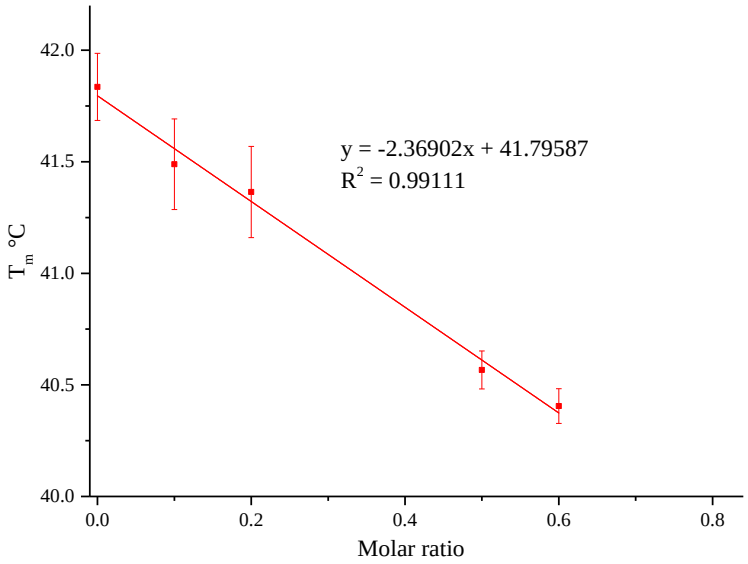


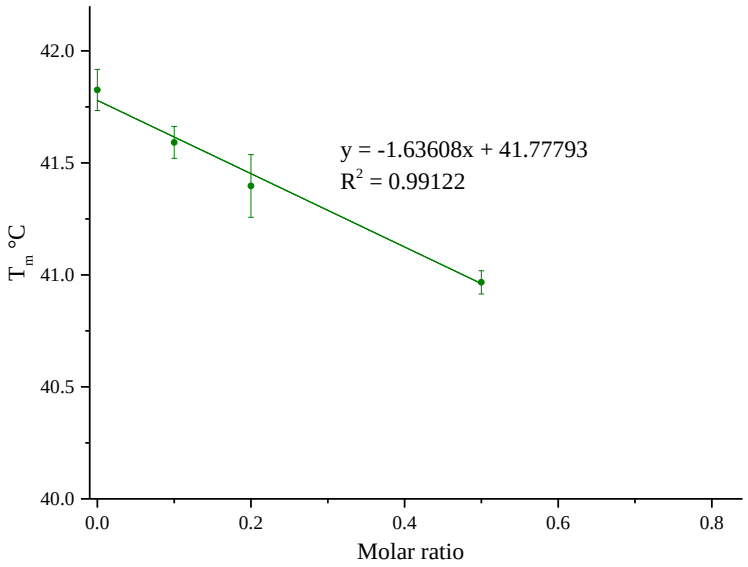
Figure S52. TEM image of associates of the compounds **3f**

Linear equation parameters of T_m against Molar ratio



Compound 3a		
Molar ratio	**T_m**	**T_mEr±**
0	41.83555	0.15025
0.1	41.48899	0.20304
0.2	41.3646	0.20434
0.5	40.56708	0.08498
0.6	40.40513	0.0779

Figure S53. Linear dependence of T_m against Molar ratio for compound **3a**



Compound 3b		
Molar ratio	**T_m**	**T_mEr±**
0	41.82553	0.09189
0.1	41.59147	0.07145
0.2	41.39715	0.14003
0.5	40.96678	0.05187

Figure S54. Linear dependence of T_m against Molar ratio for compound **3b**

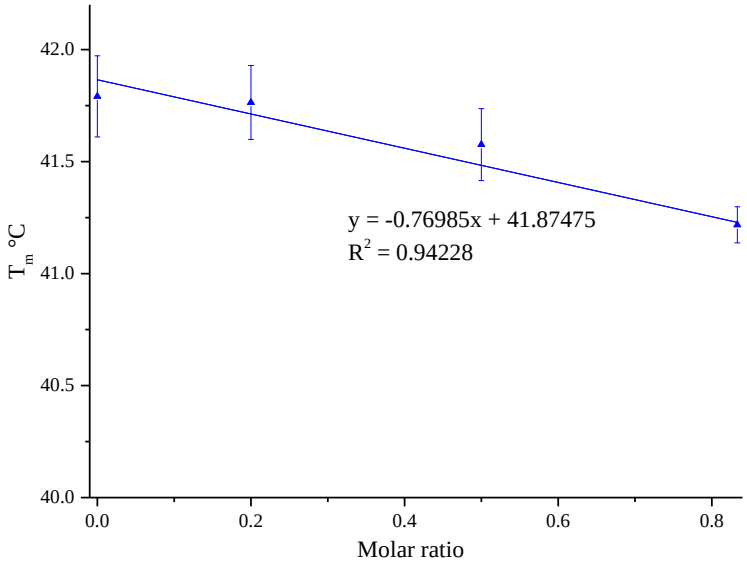


Figure S55. Linear dependence of T_m against Molar ratio for compound **3c**

Compound 3c		
Molar ratio	**T_m**	**T_mEr±**
0	41.7911	0.1811
0.2	41.76406	0.16477
0.5	41.57609	0.16054
0.83333	41.21769	0.08057

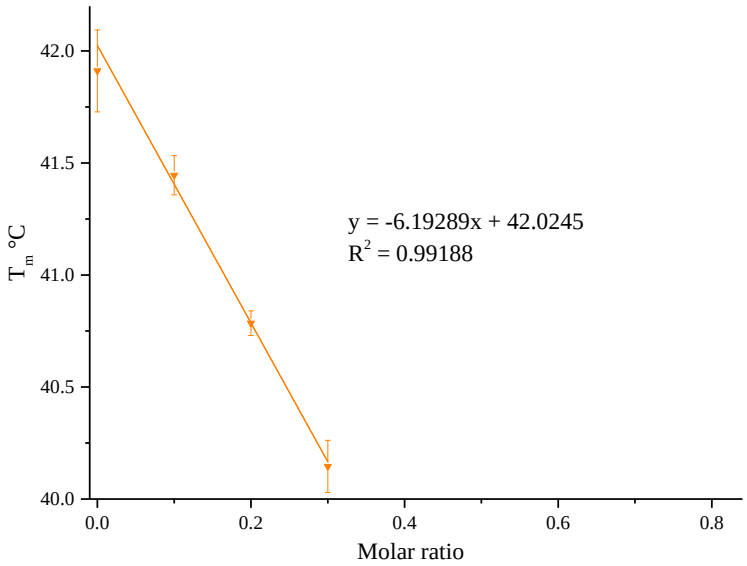
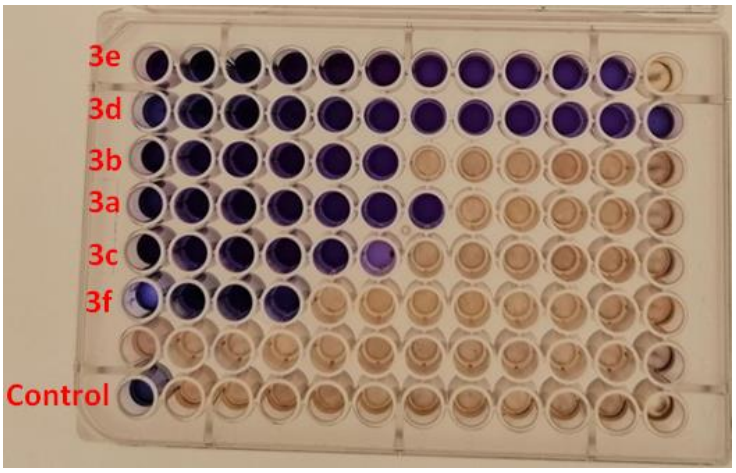


Figure S56. Linear dependence of T_m against Molar ratio for compound **3e**

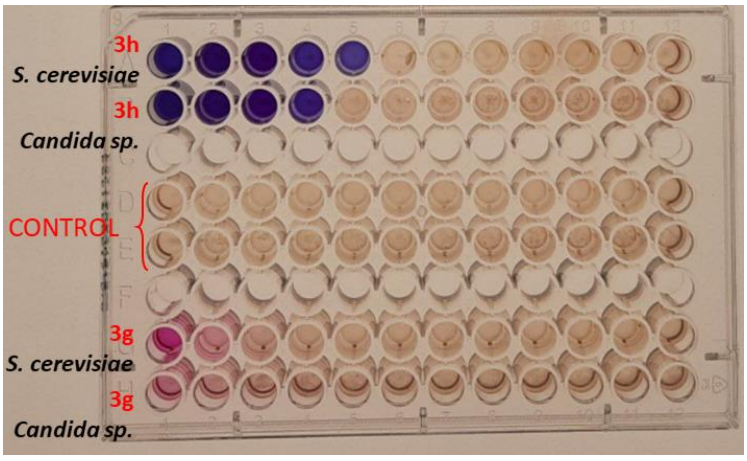
Compound 3e		
Molar ratio	**T_m**	**T_mEr±**
0	41.91109	0.18306
0.1	41.44516	0.08743
0.2	40.78502	0.05515
0.3	40.14568	0.11654

Resazurin assay



Figures S57. The ability of terpenoids (**3e**, **3d**, **3b**, **3a**, **3c**, **3f** respectively) to inhibit the growth of *Saccharomyces cerevisiae*

Figures S58. The ability of terpenoids (**3e**, **3d**, **3b**, **3a**, **3c**, **3f** respectively) to inhibit the growth of *Candida sp.*



Figures S59. The ability of compounds **3g-h** to inhibit the growth of *Saccharomyces cerevisiae* and *Candida sp.*