

Supplementary Information

Synthesis of Pregabalin and its novel lipophilic β -alkyl-substituted analogues from fatty chains

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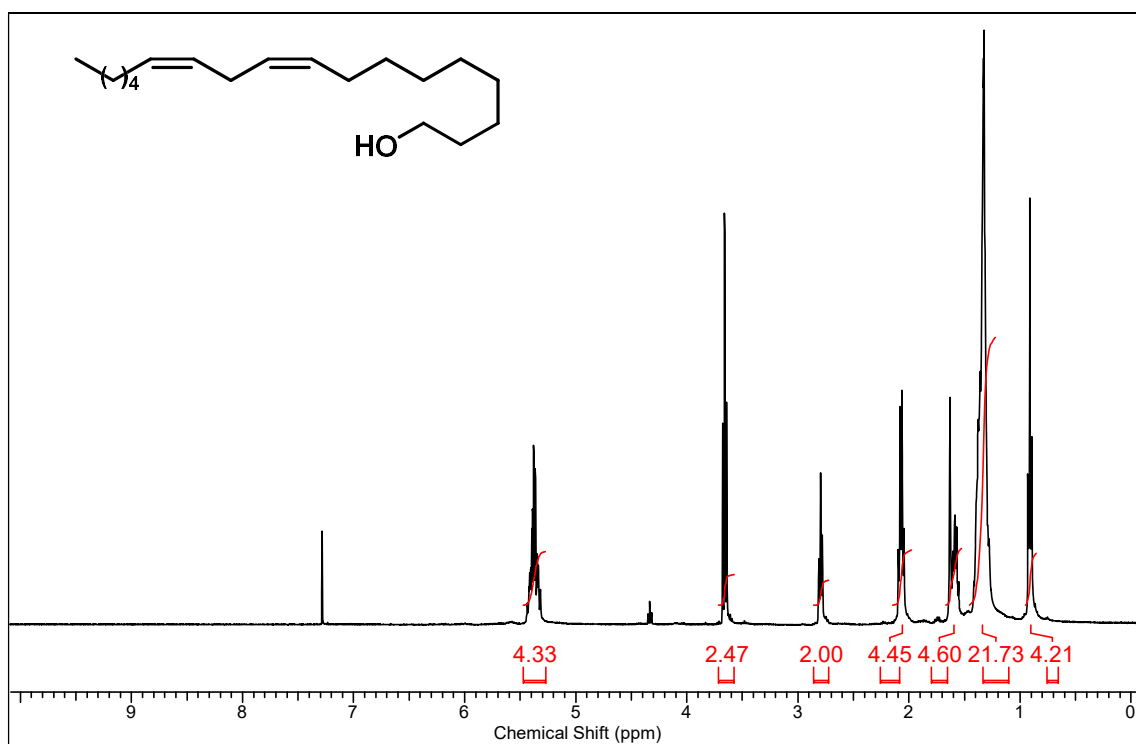


Figure S1. Spectrum of ^1H NMR (300 MHz, CDCl_3) of linoleic alcohol.

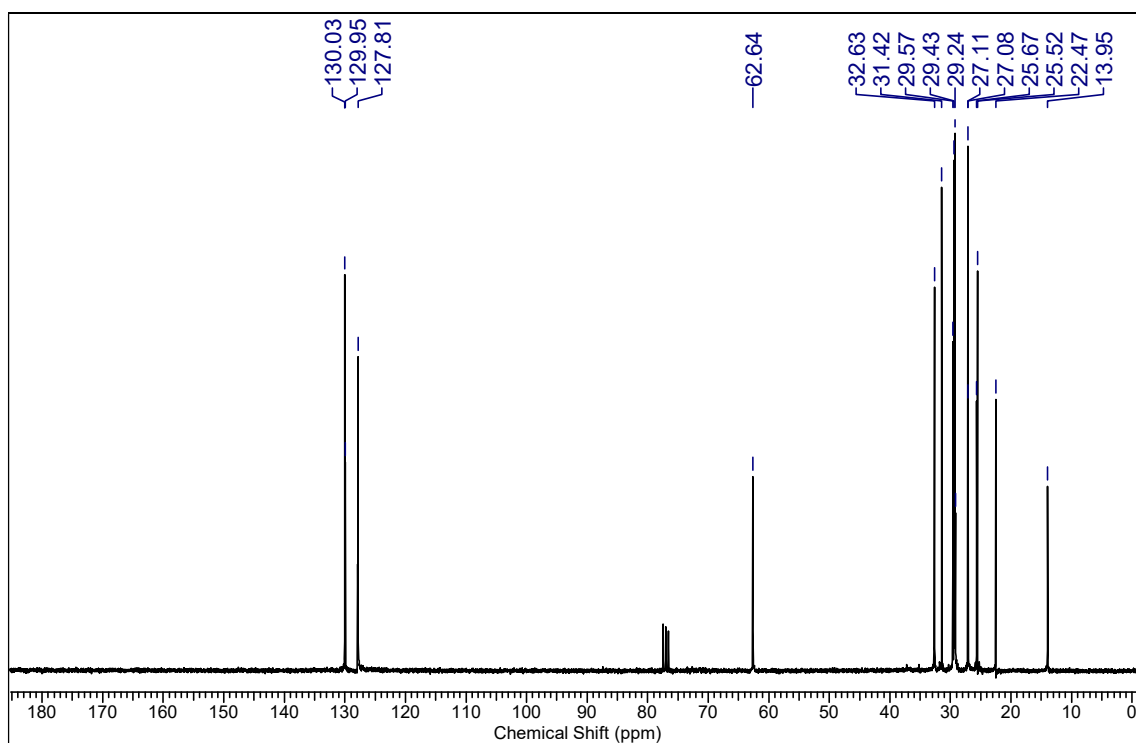


Figure S2. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of linoleic alcohol.

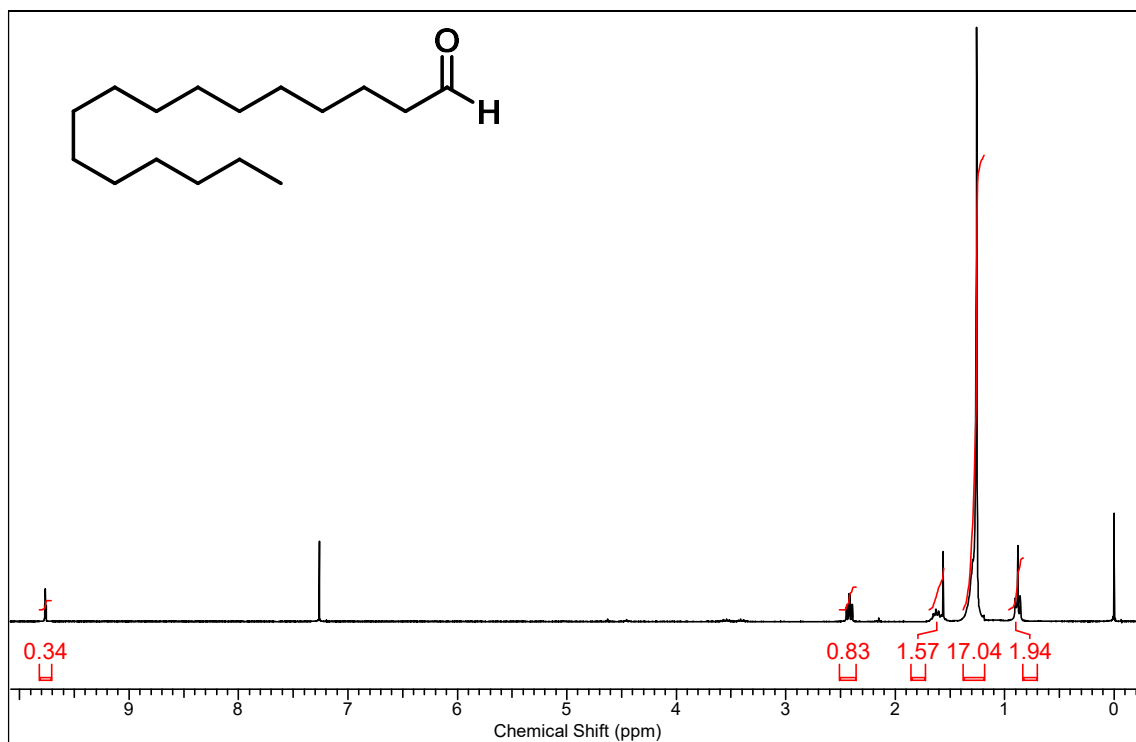


Figure S3. Spectrum of ¹H NMR (300 MHz, CDCl₃) of aldehyde **6f**.

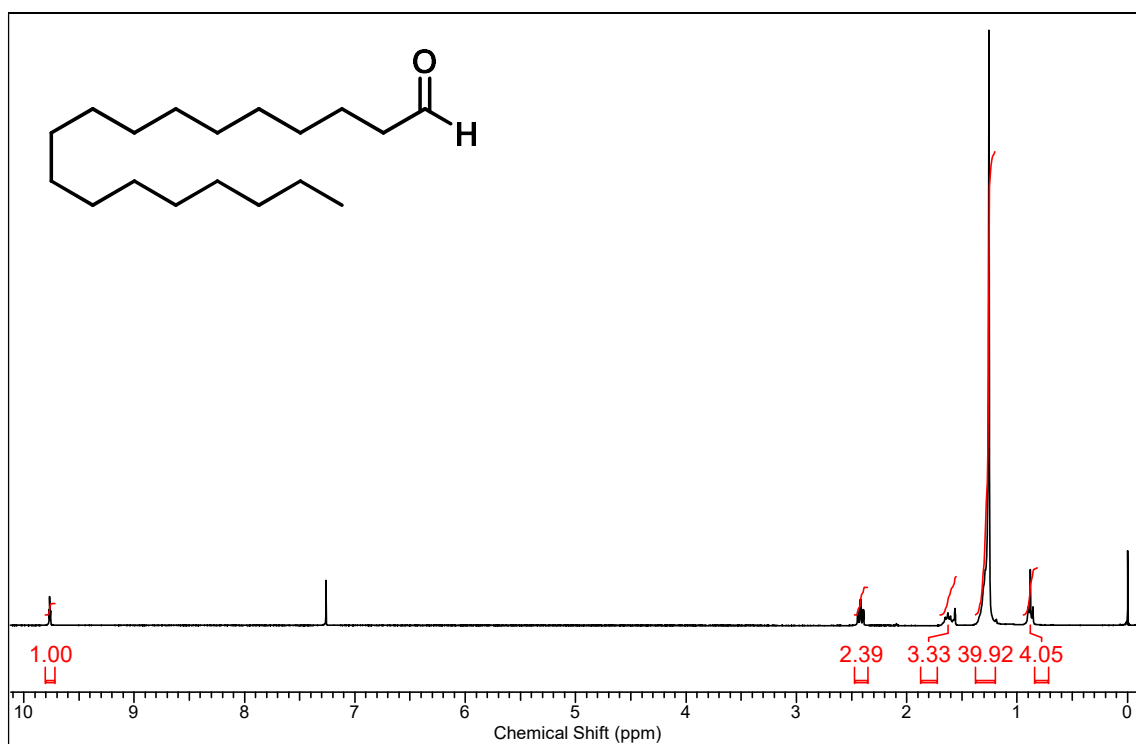


Figure S4. Spectrum of ¹H NMR (300 MHz, CDCl₃) of aldehyde **6g**.

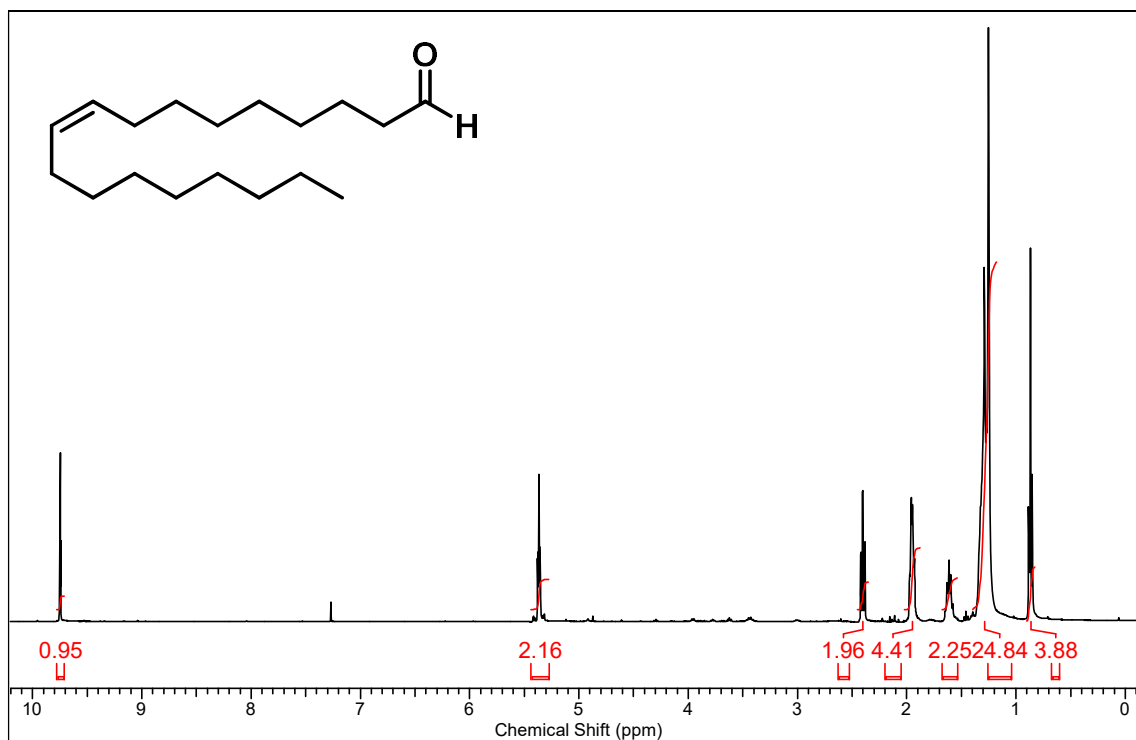


Figure S5. Spectrum of ¹H NMR (300 MHz, CDCl₃) of aldehyde 6h.

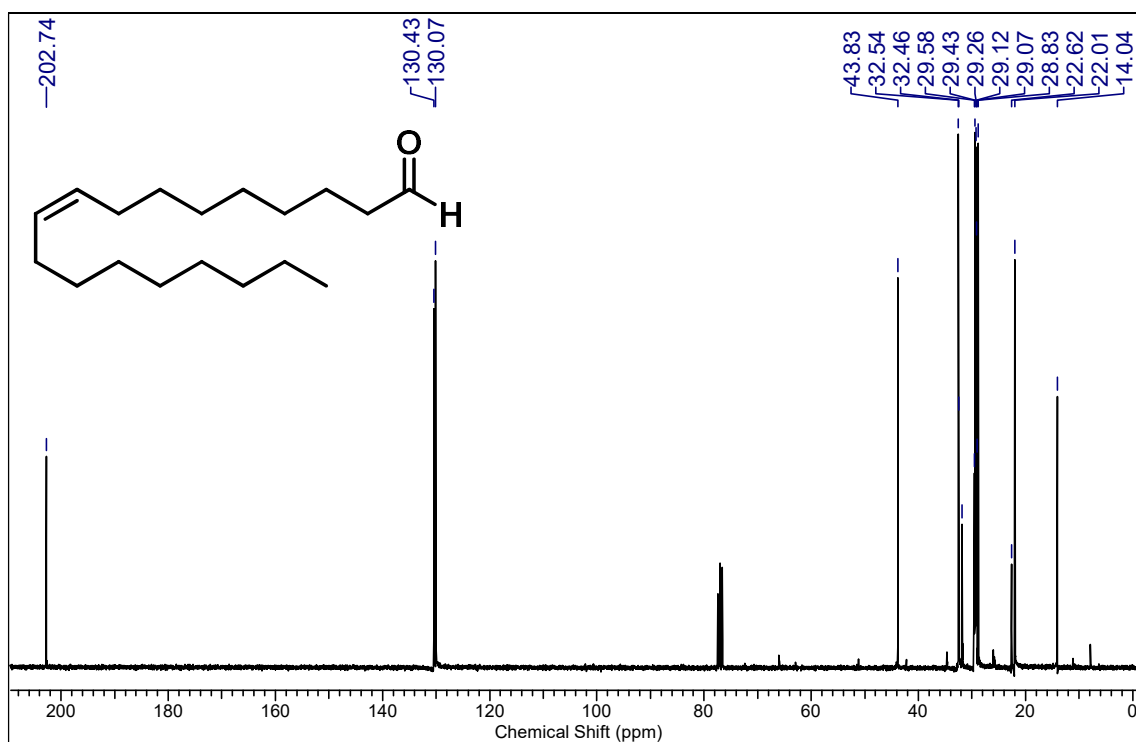


Figure S6. Spectrum of ¹³C NMR (75 MHz, CDCl₃) of aldehyde 6h.

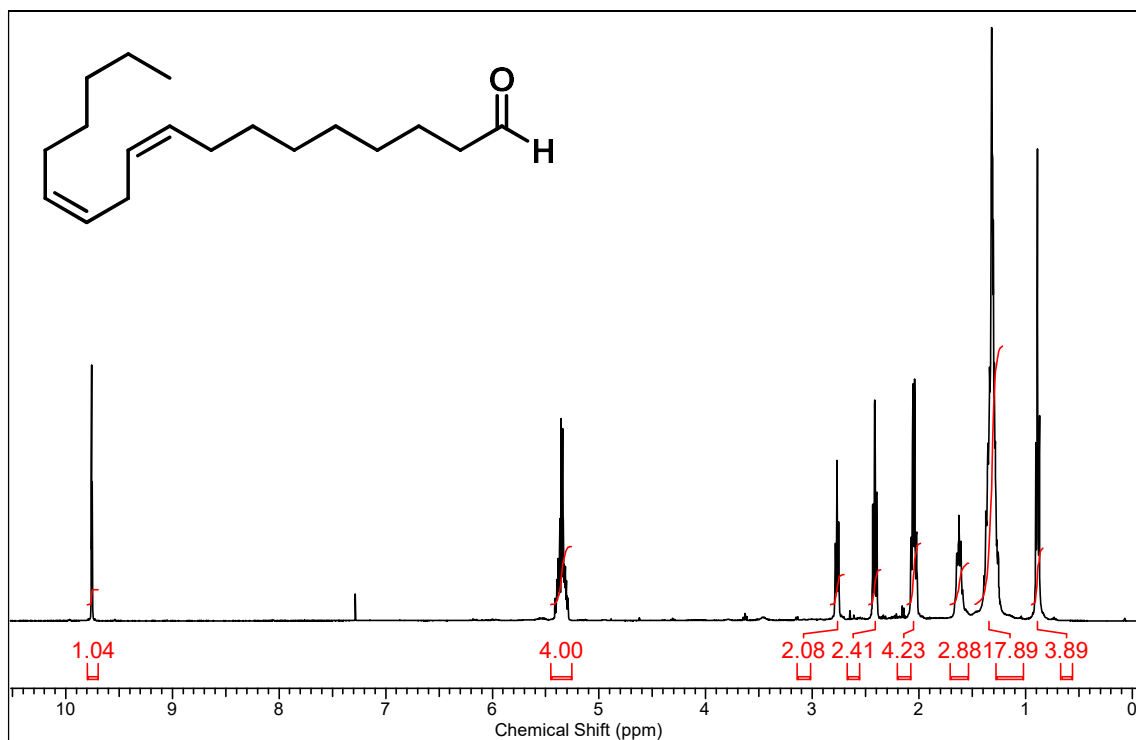


Figure S7. Spectrum of ^1H NMR (300 MHz, CDCl_3) of aldehyde **6i**.

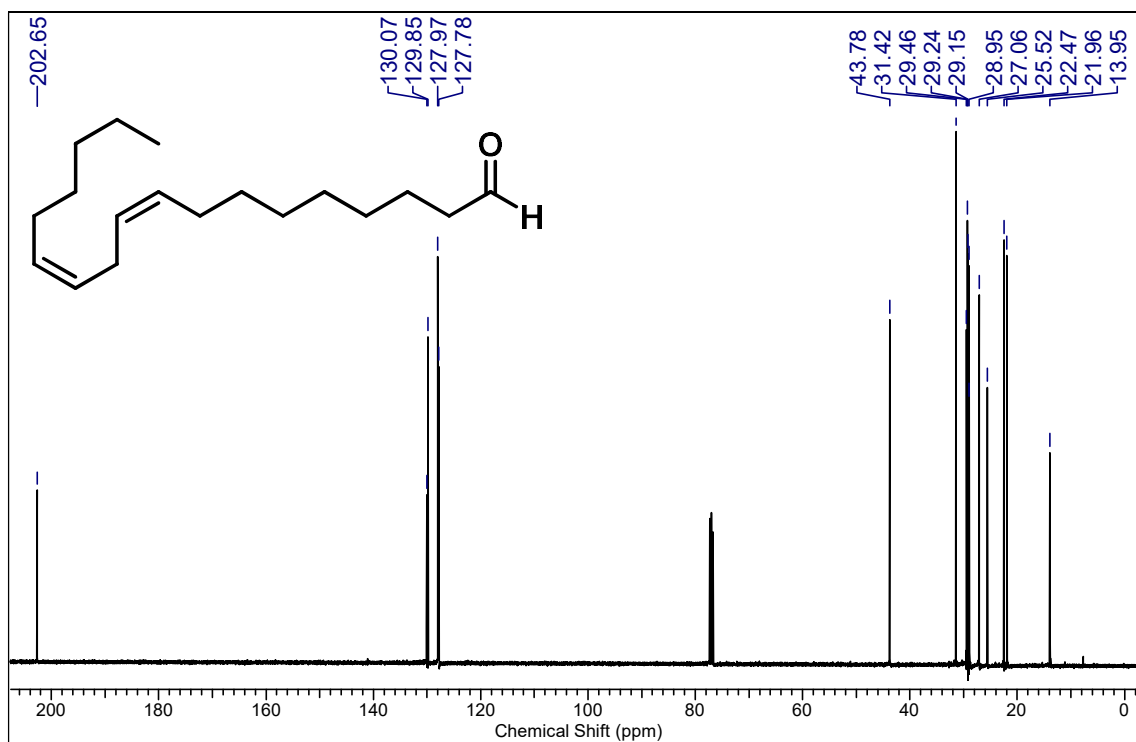


Figure S8. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of aldehyde **6i**.

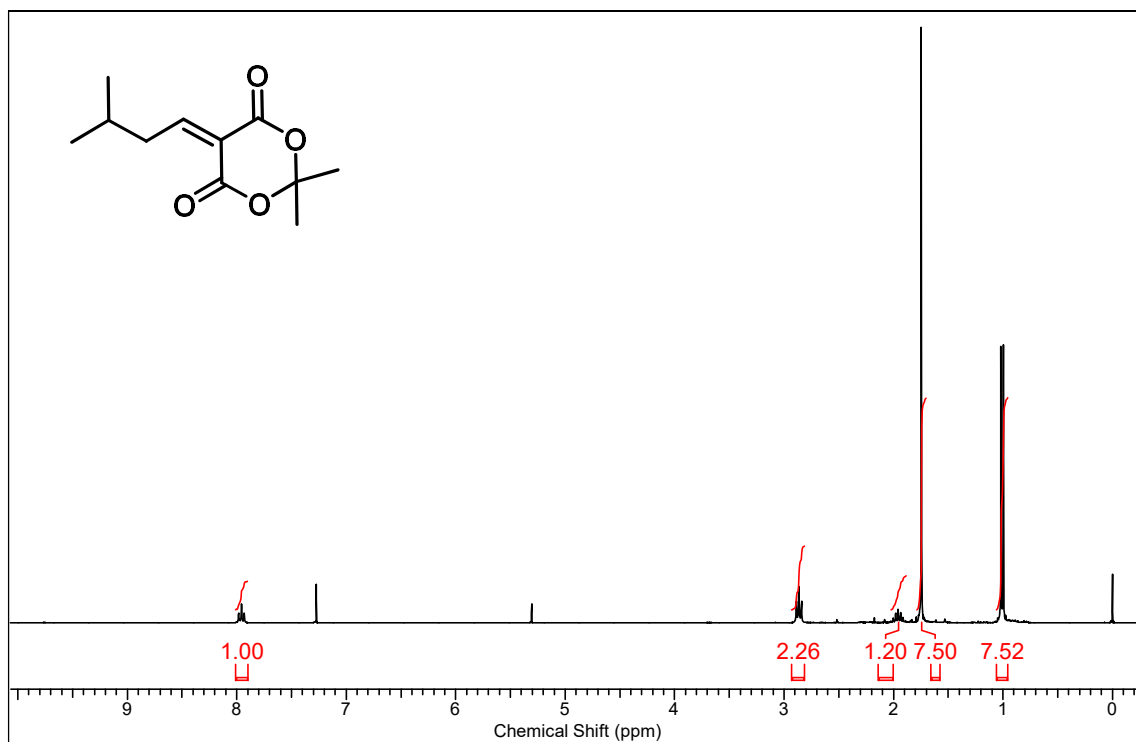


Figure S9. Spectrum of ¹H NMR (300 MHz, CDCl₃) of alkylidene **9a**.

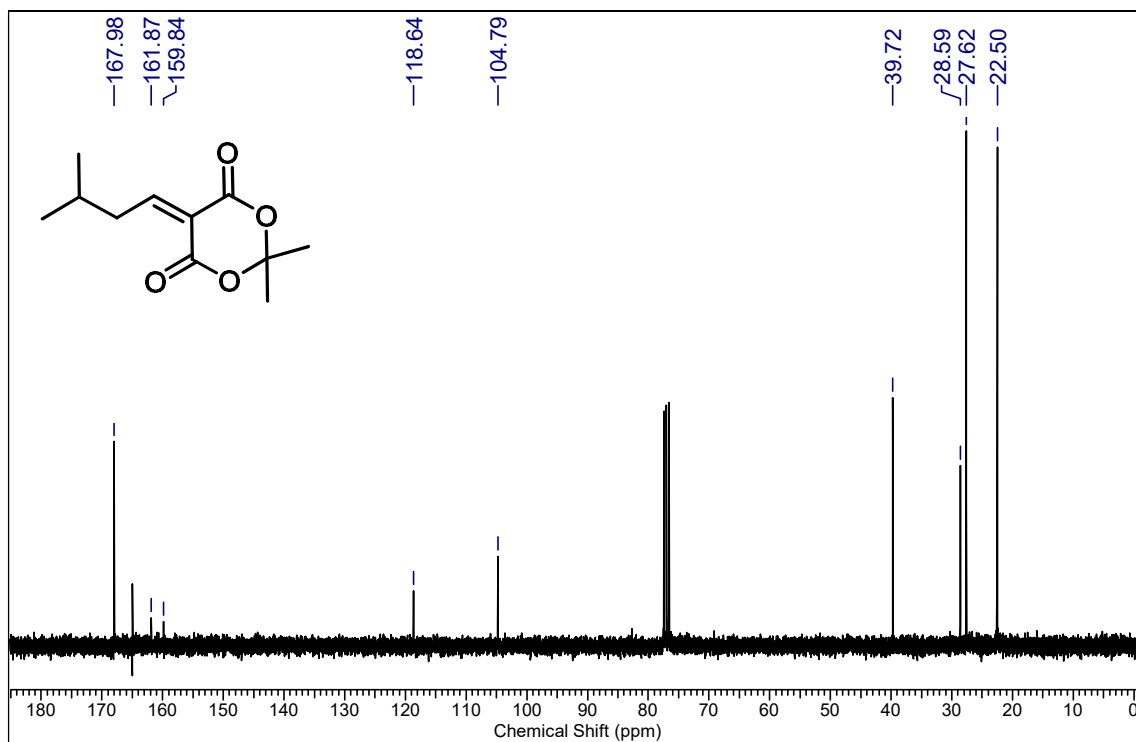


Figure S10. Spectrum of ¹³C NMR (75 MHz, CDCl₃) of alkylidene **9a**.

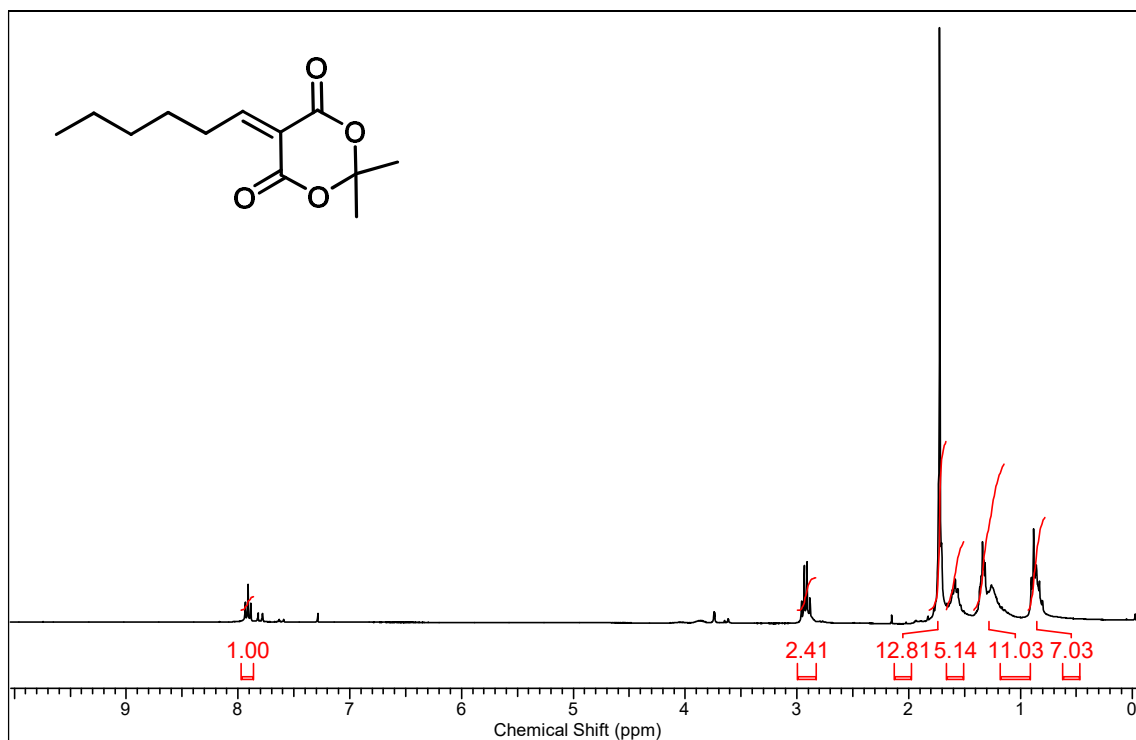


Figure S11. Spectrum of ¹H NMR (300 MHz, CDCl₃) of alkyldiene **9b**.

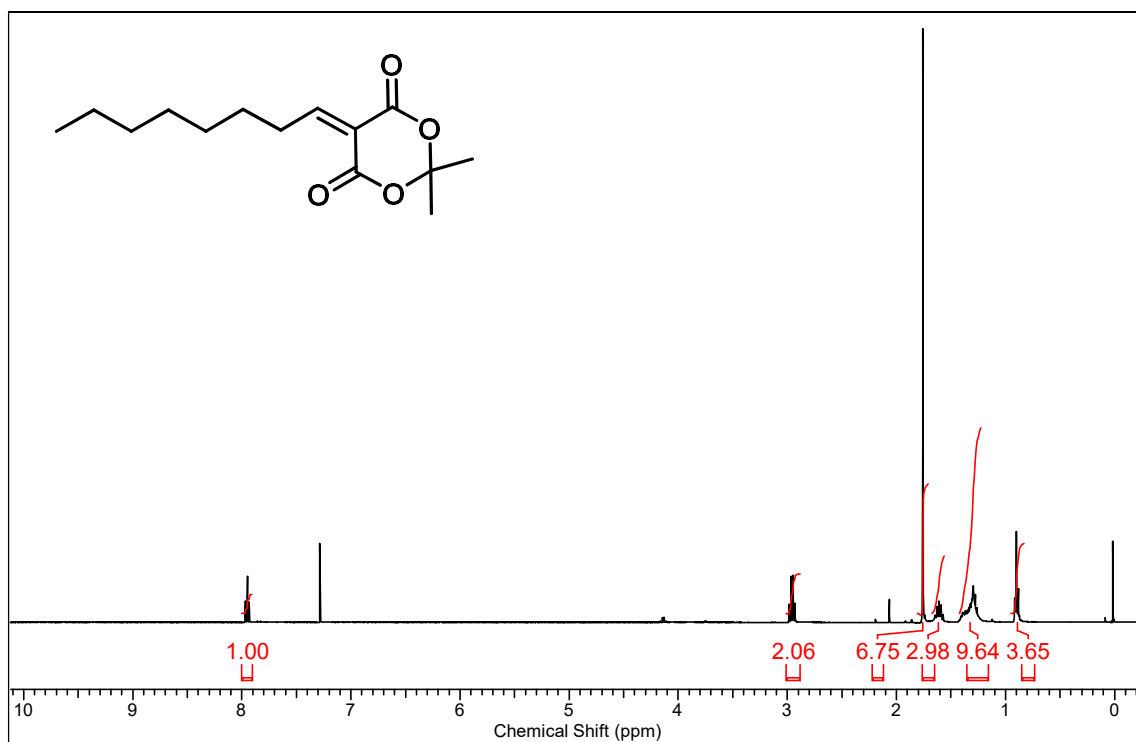


Figure S12. Spectrum of ¹H NMR (300 MHz, CDCl₃) of alkyldiene **9c**.

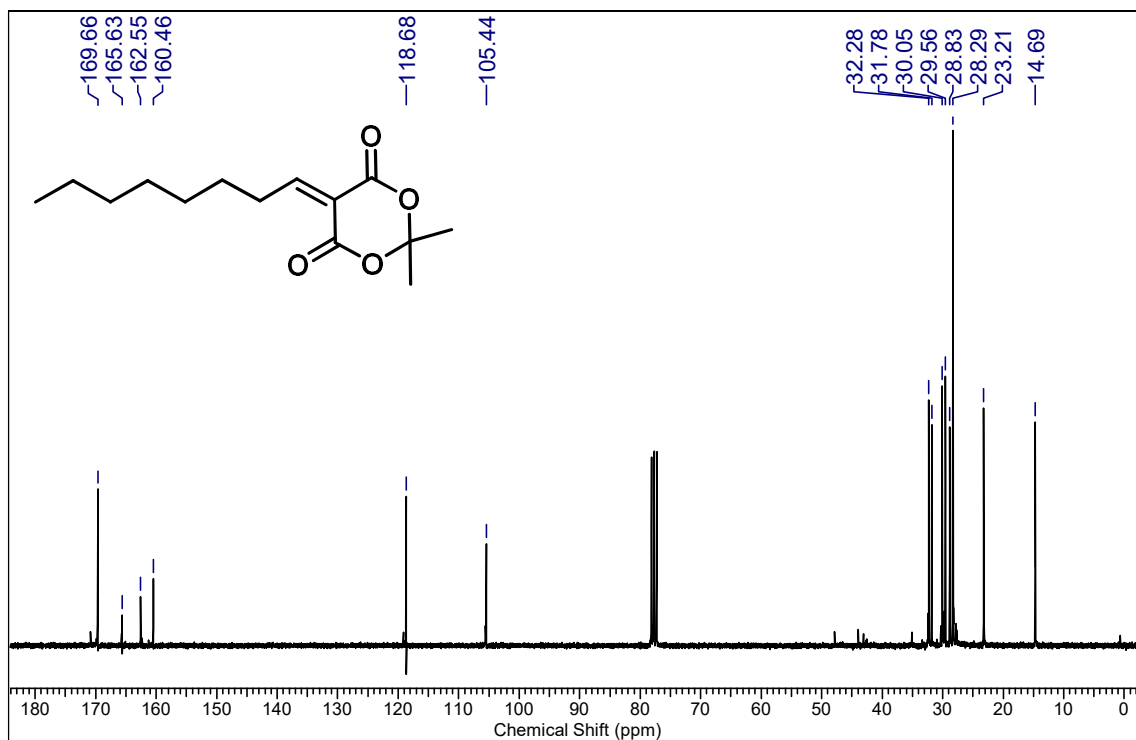


Figure S13. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of alkylidene **9c**.

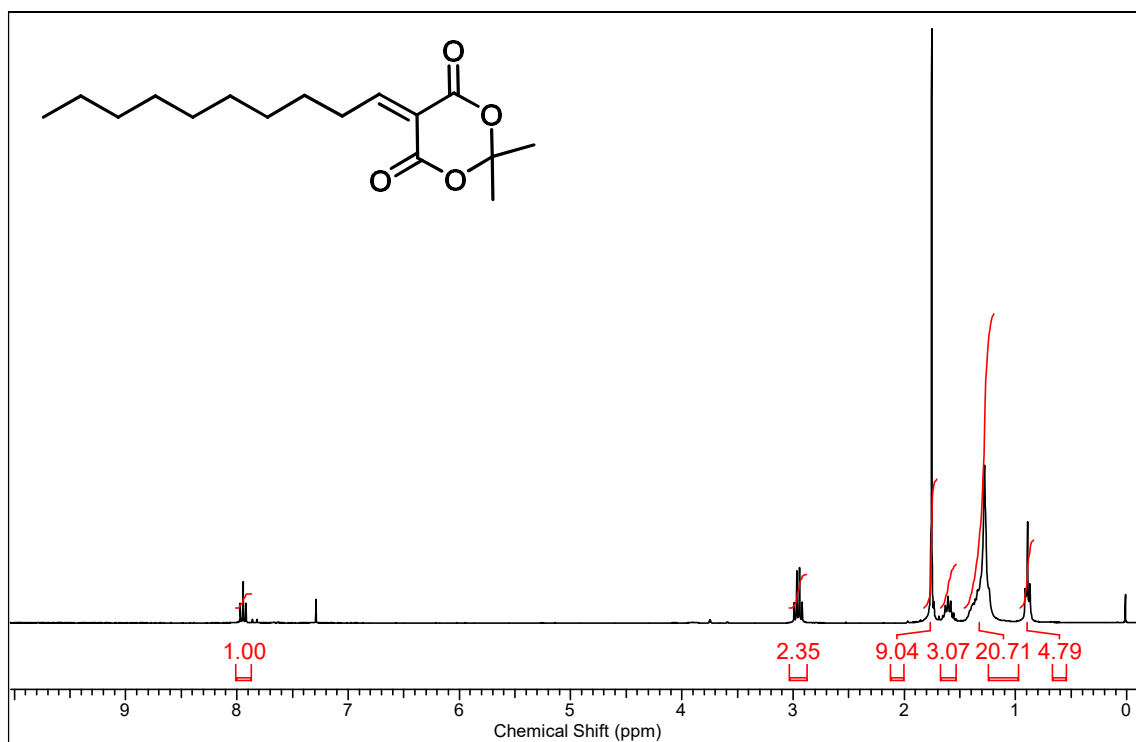


Figure S14. Spectrum of ^1H NMR (300 MHz, CDCl_3) of alkylidene **9d**.

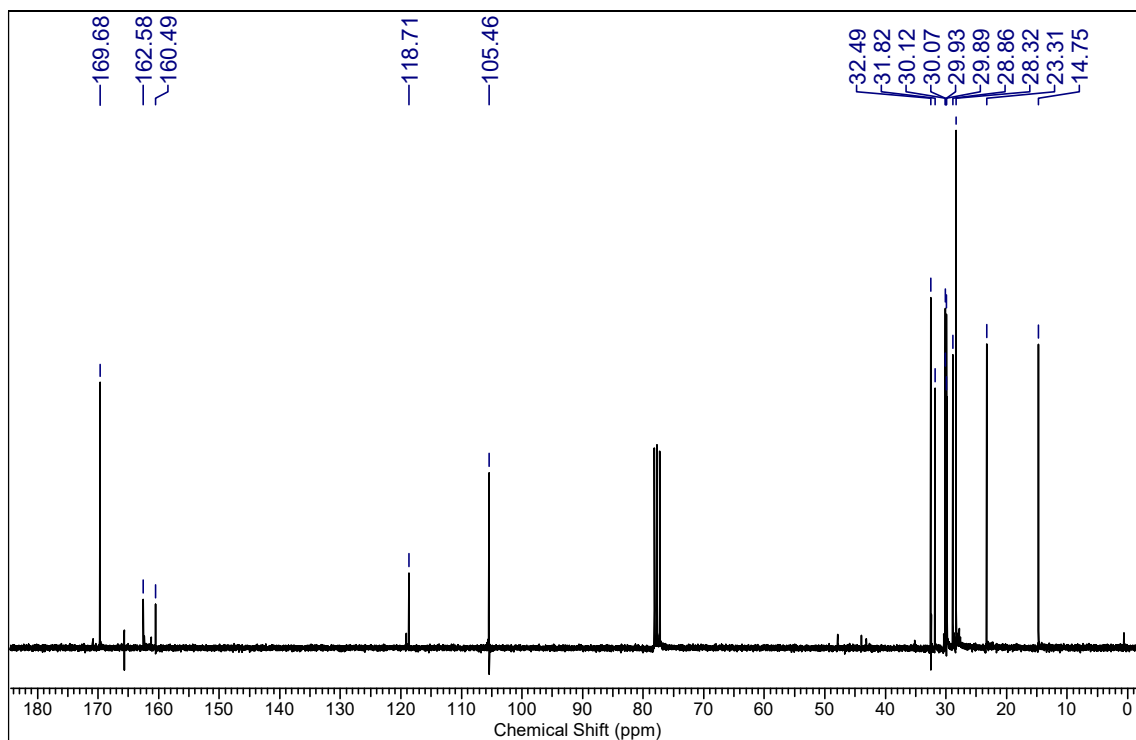


Figure S15. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of alkylidene **9d**.

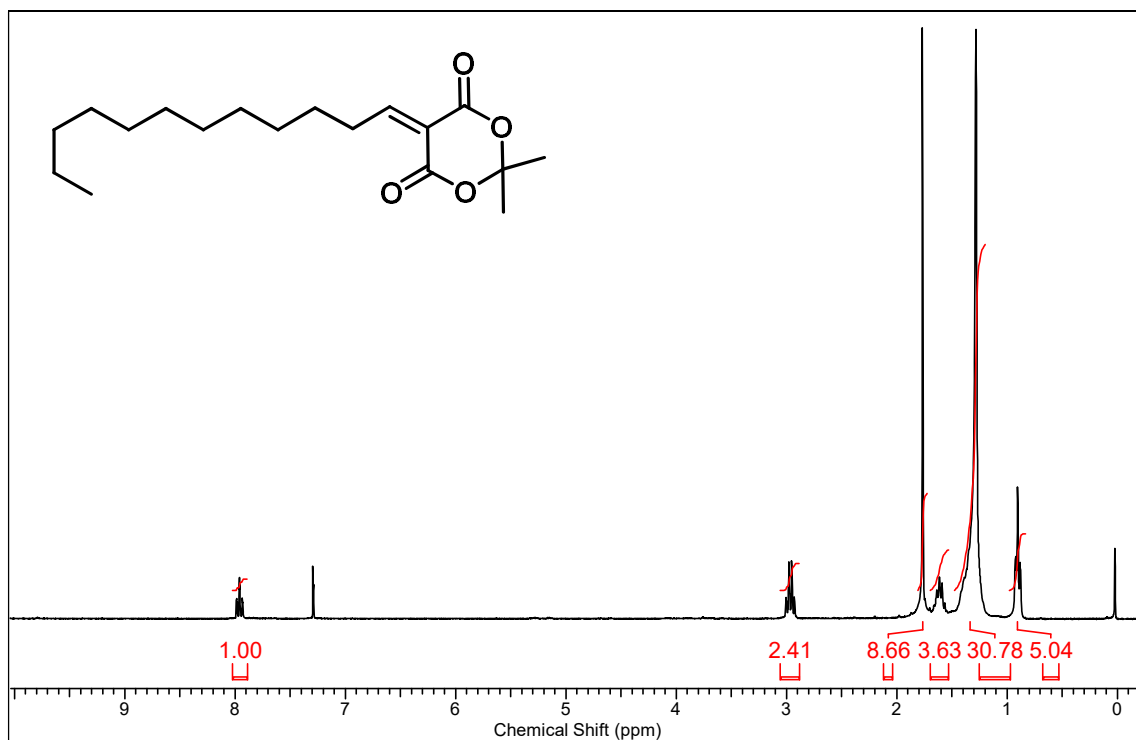


Figure S16. Spectrum of ^1H NMR (300 MHz, CDCl_3) of alkylidene **9e**.

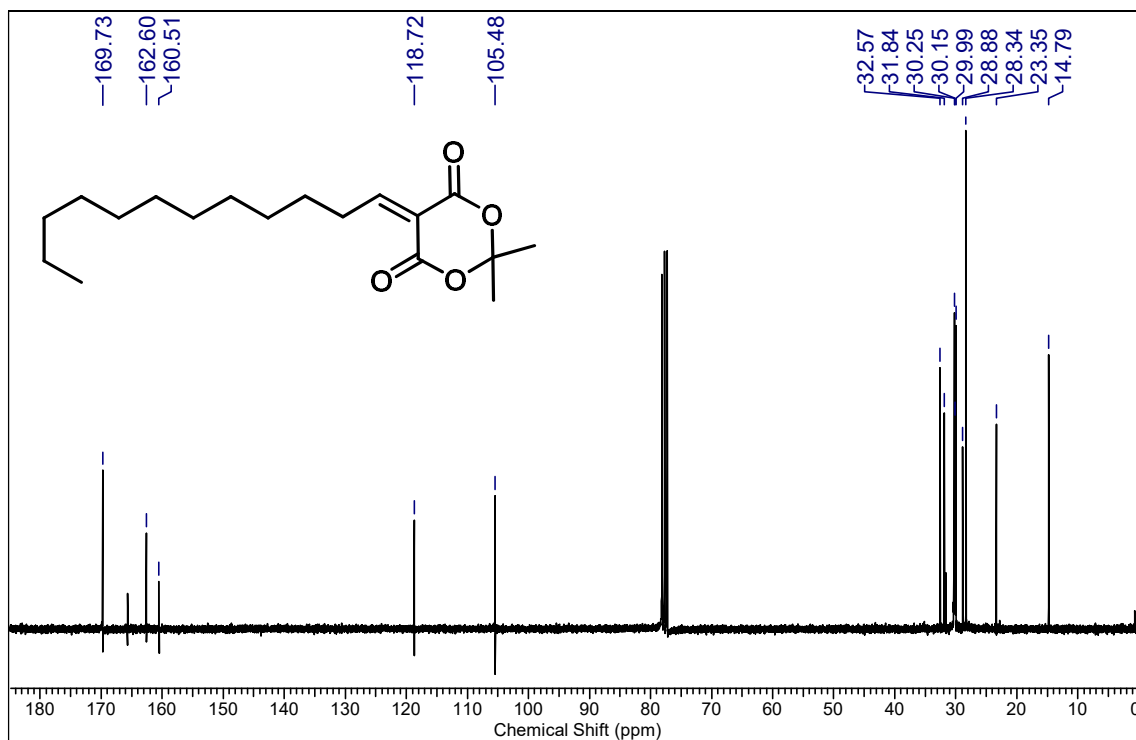


Figure S17. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of alkylidene **9e**.

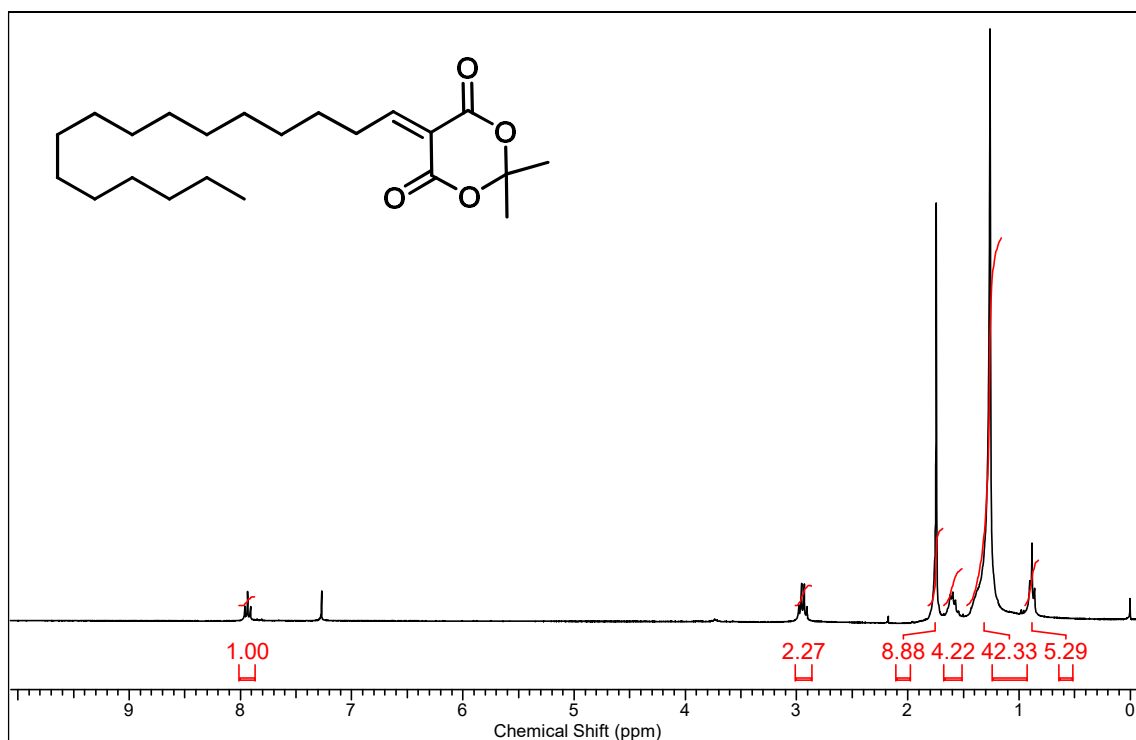


Figure S18. Spectrum of ^1H NMR (300 MHz, CDCl_3) of alkylidene **9f**.

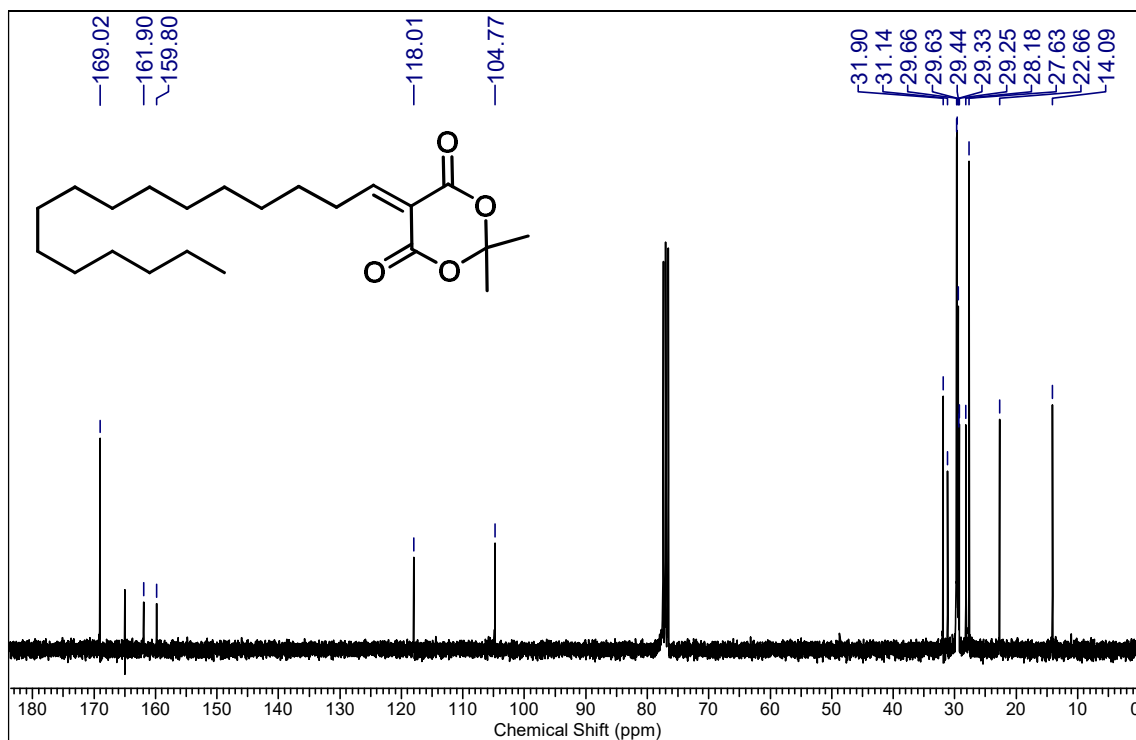


Figure S19. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of alkyldiene **9f**.

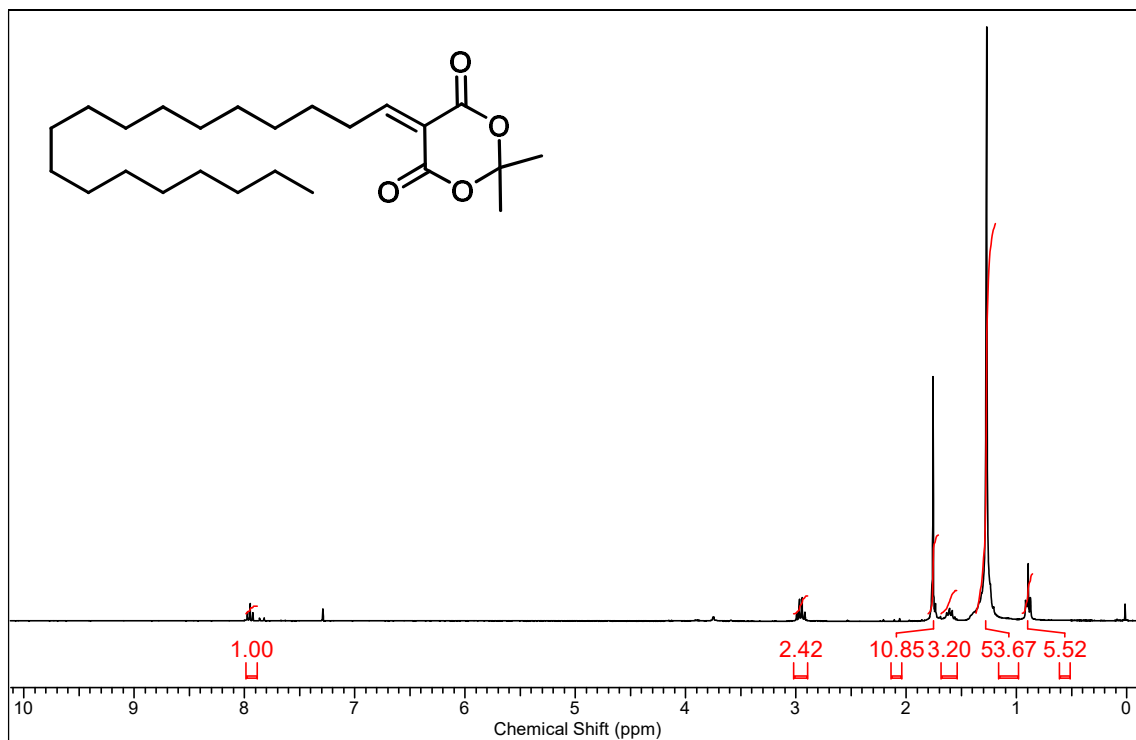


Figure S20. Spectrum of ^1H NMR (300 MHz, CDCl_3) of alkyldiene **9g**.

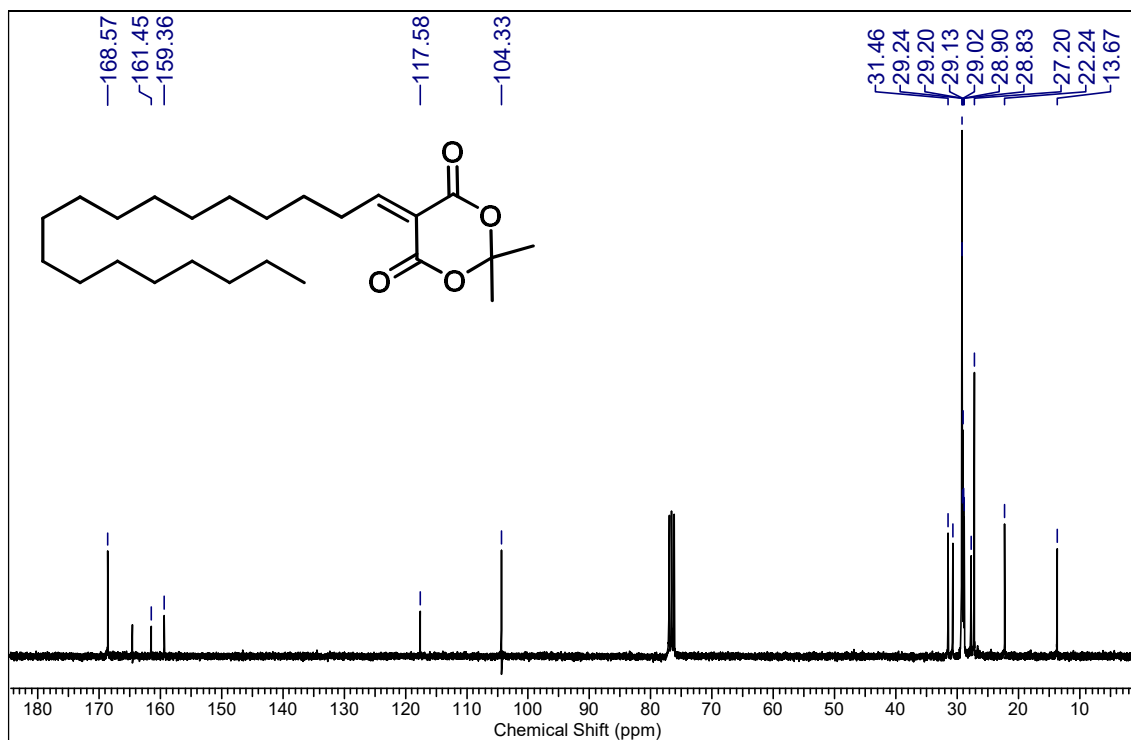


Figure S21. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of alkylidene **9g**.

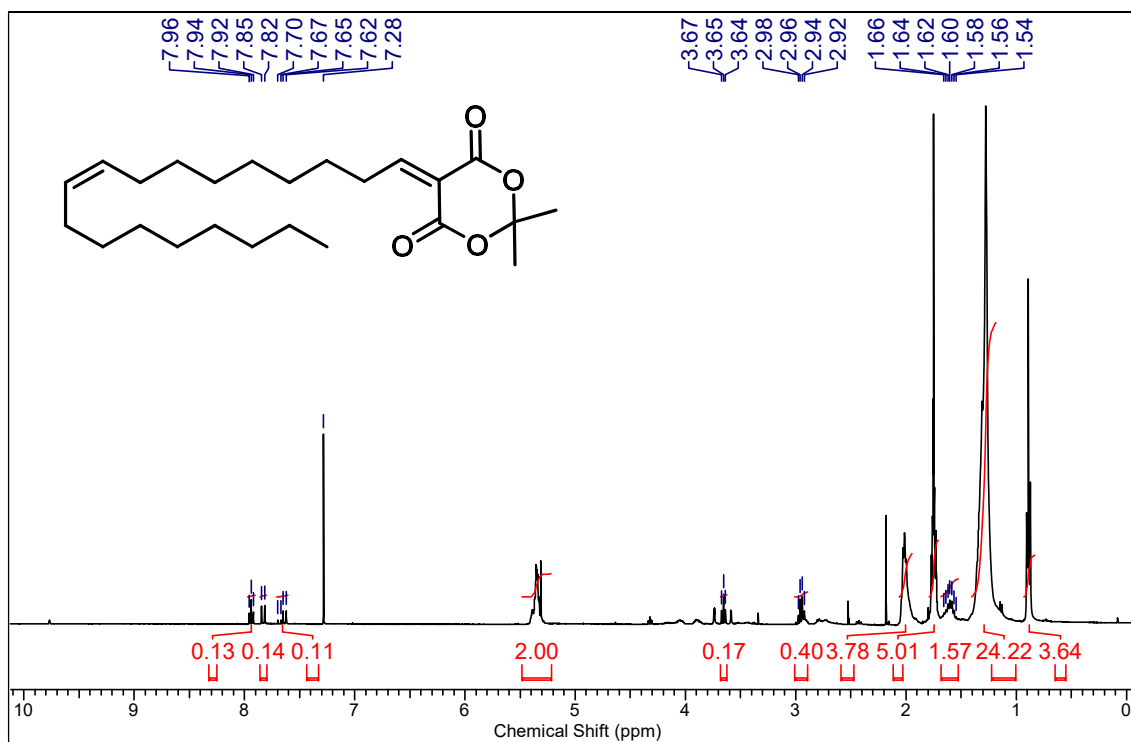


Figure S22. Spectrum of ^1H NMR (300 MHz, CDCl_3) of alkylidene **9h**.

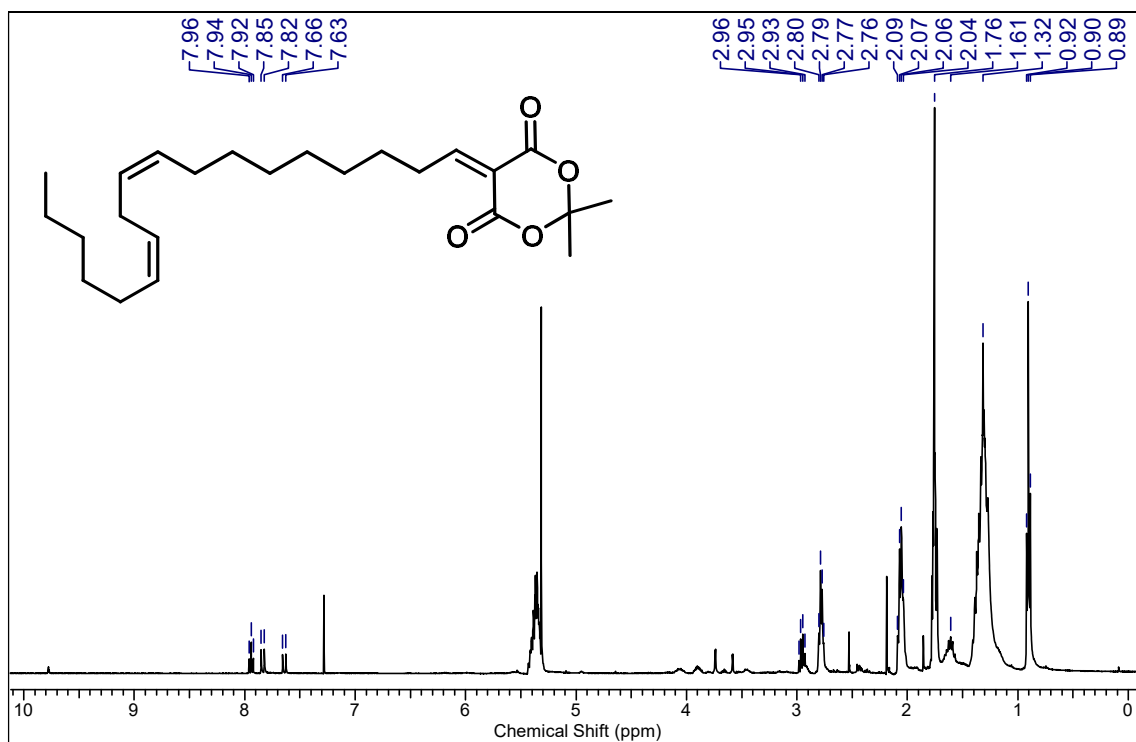


Figure S23. Spectrum of ^1H NMR (300 MHz, CDCl_3) of alkylidene **9i**.

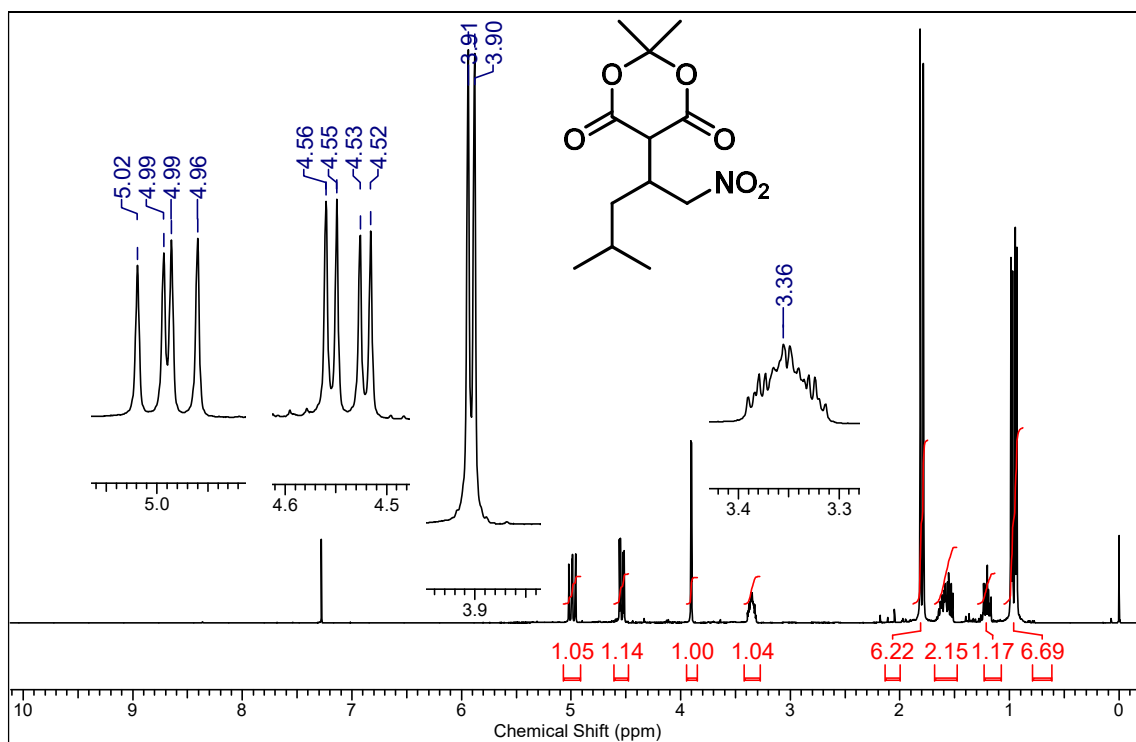


Figure S24. Spectrum of ^1H NMR (300 MHz, CDCl_3) of crude nitro adduct **10a**.

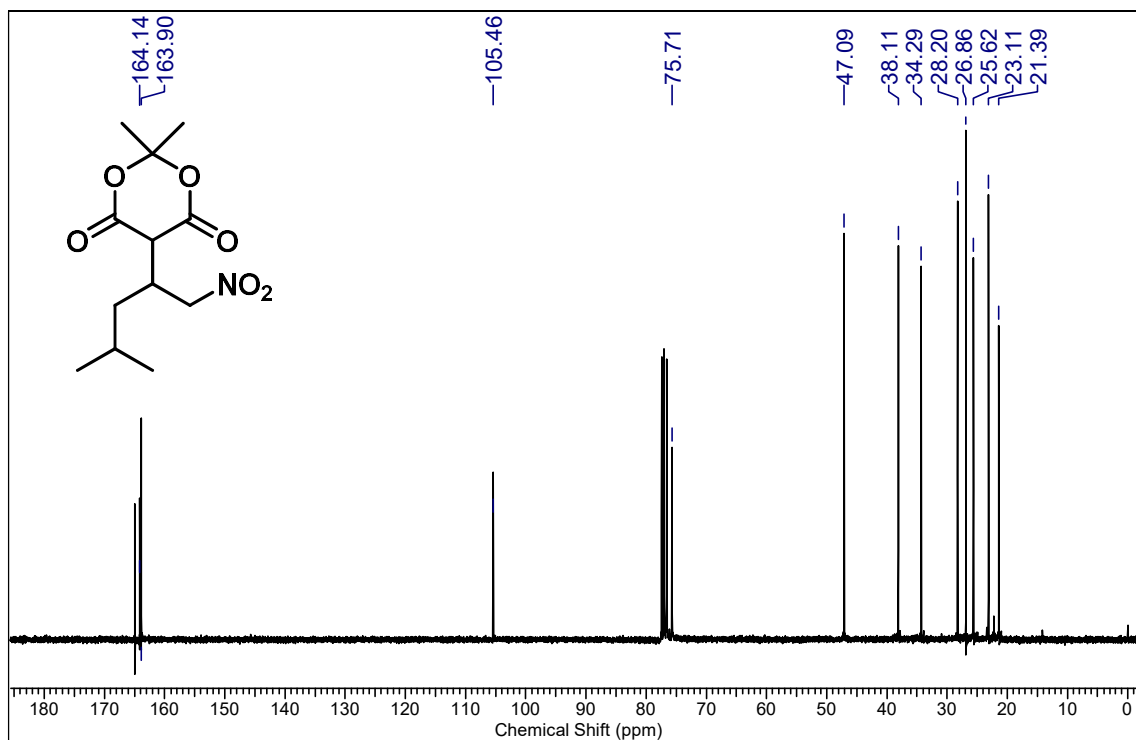


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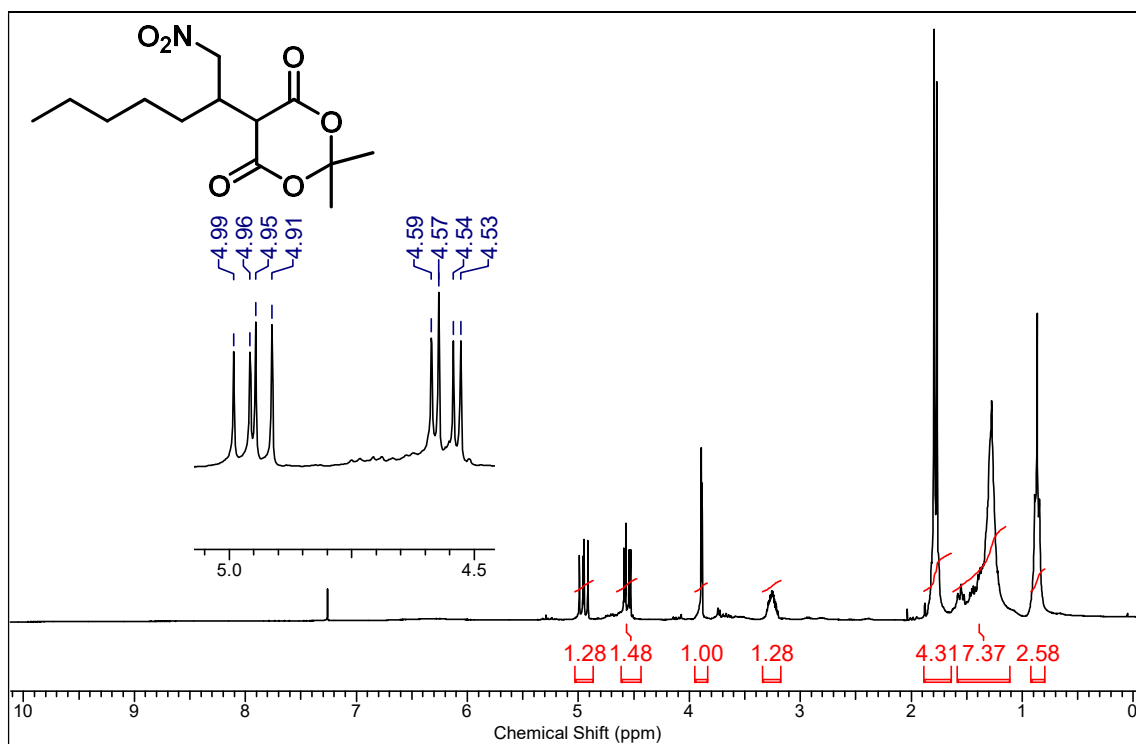


Figure S26. Spectrum of ^1H NMR (300 MHz, CDCl_3) of crude nitro adduct **10b**.

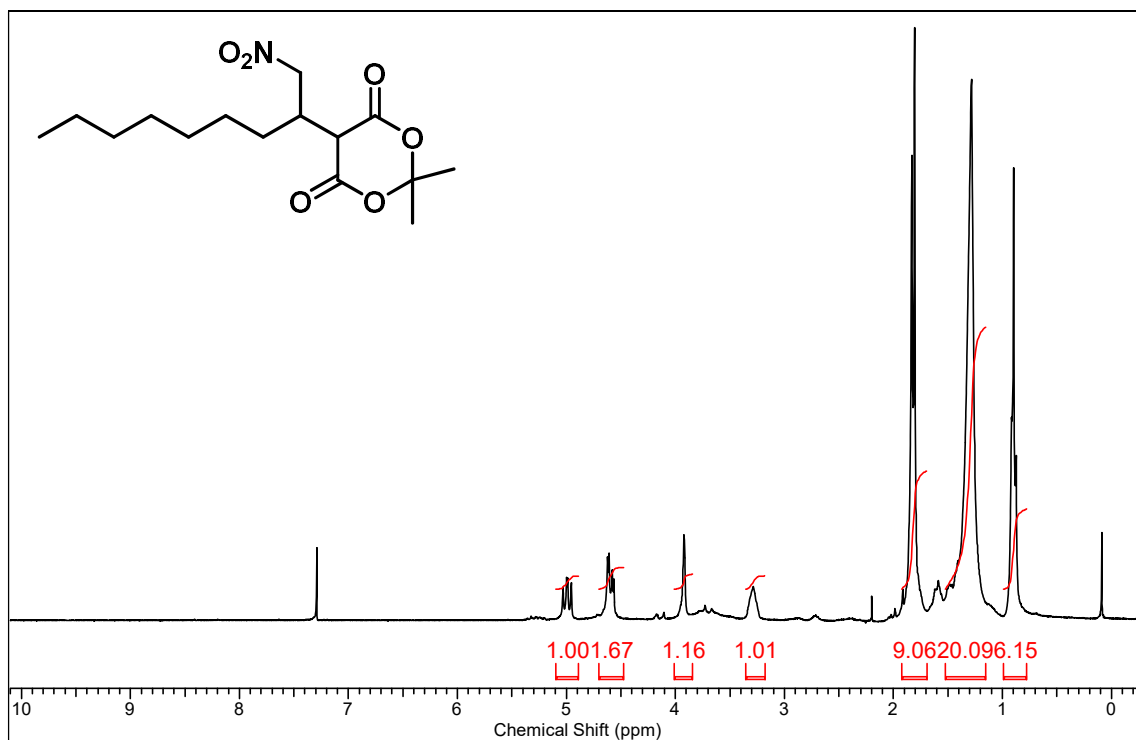


Figure S27. Spectrum of ^1H NMR (300 MHz, CDCl_3) of crude nitro adduct **10c**.

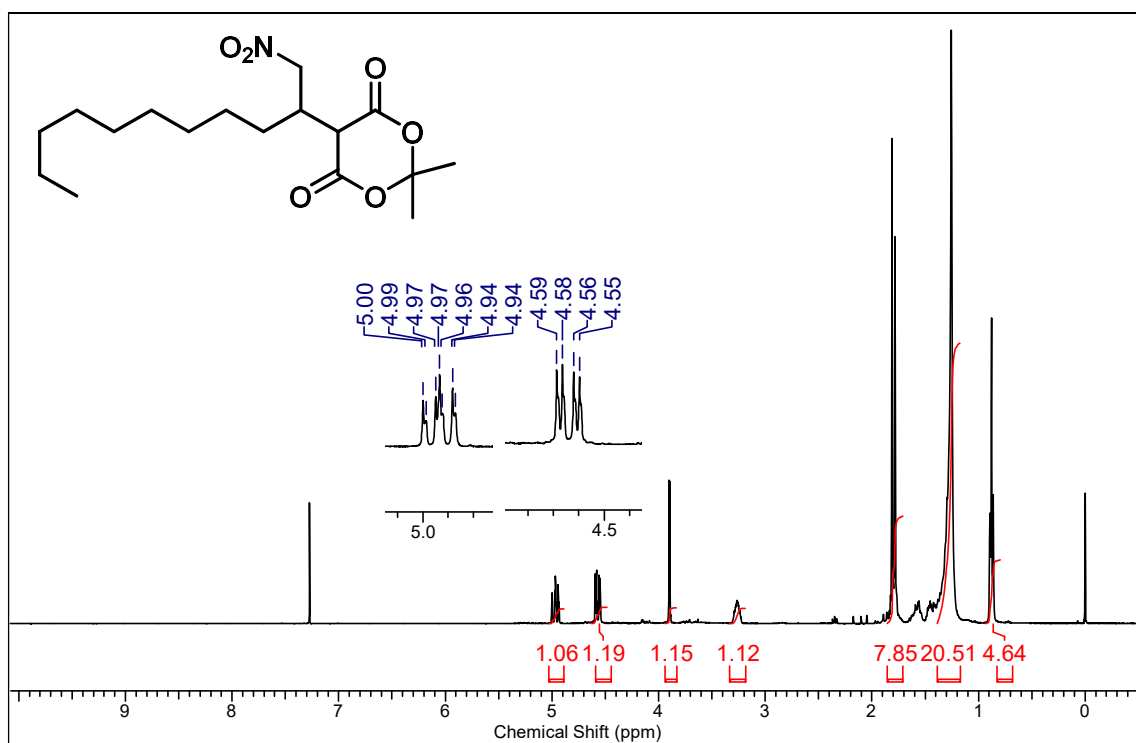


Figure S28. Spectrum of ^1H NMR (300 MHz, CDCl_3) of crude nitro adduct **10d**.

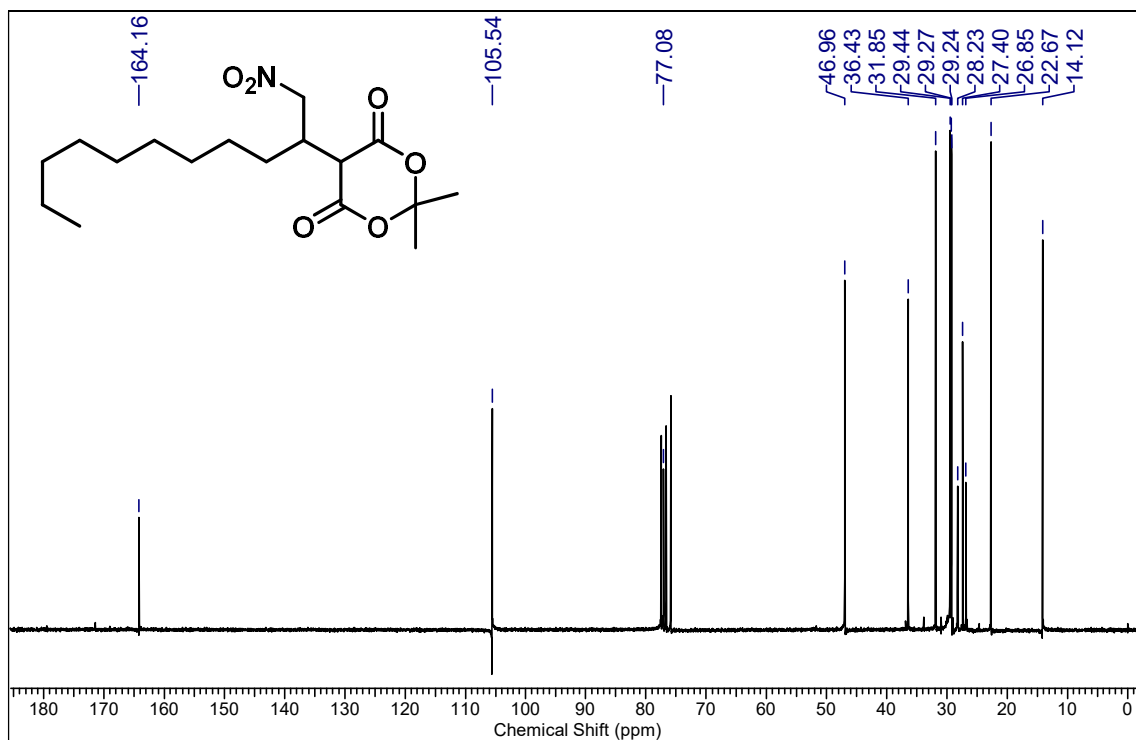


Figure S29. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of crude nitro adduct **10d**.

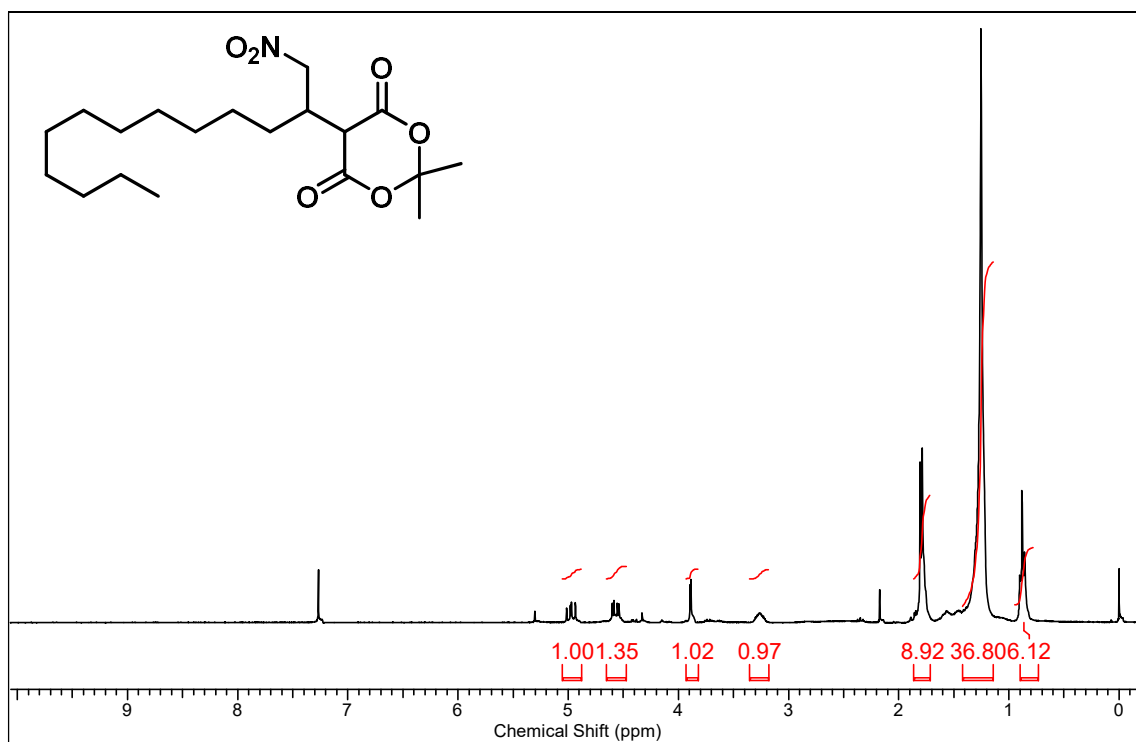


Figure S30. Spectrum of ^1H NMR (300 MHz, CDCl_3) of crude nitro adduct **10e**.

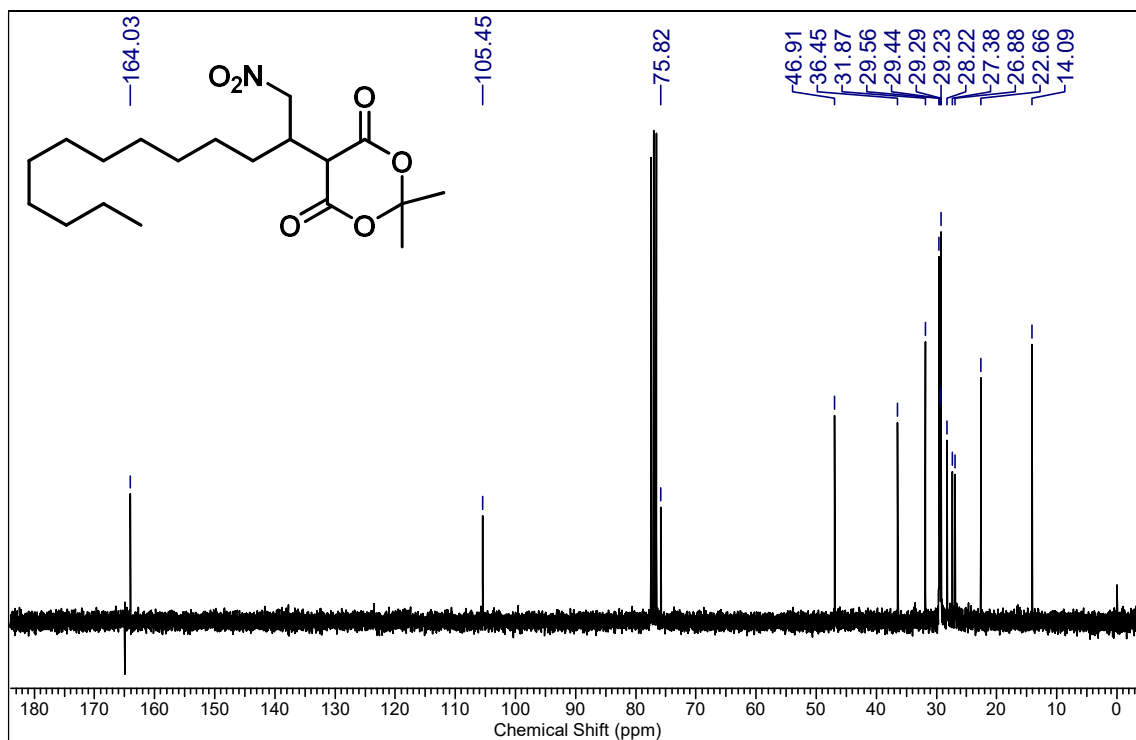


Figure S31. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of crude nitro adduct **10e**.

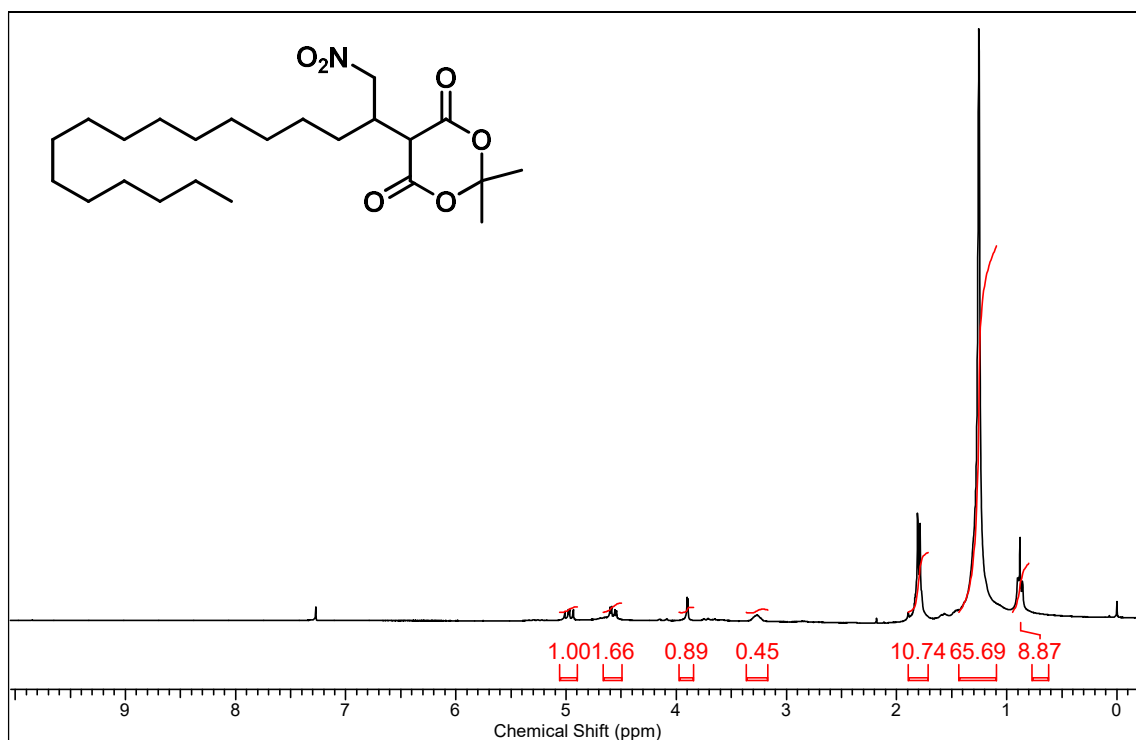


Figure S32. Spectrum of ^1H NMR (300 MHz, CDCl_3) of crude nitro adduct **10f**.

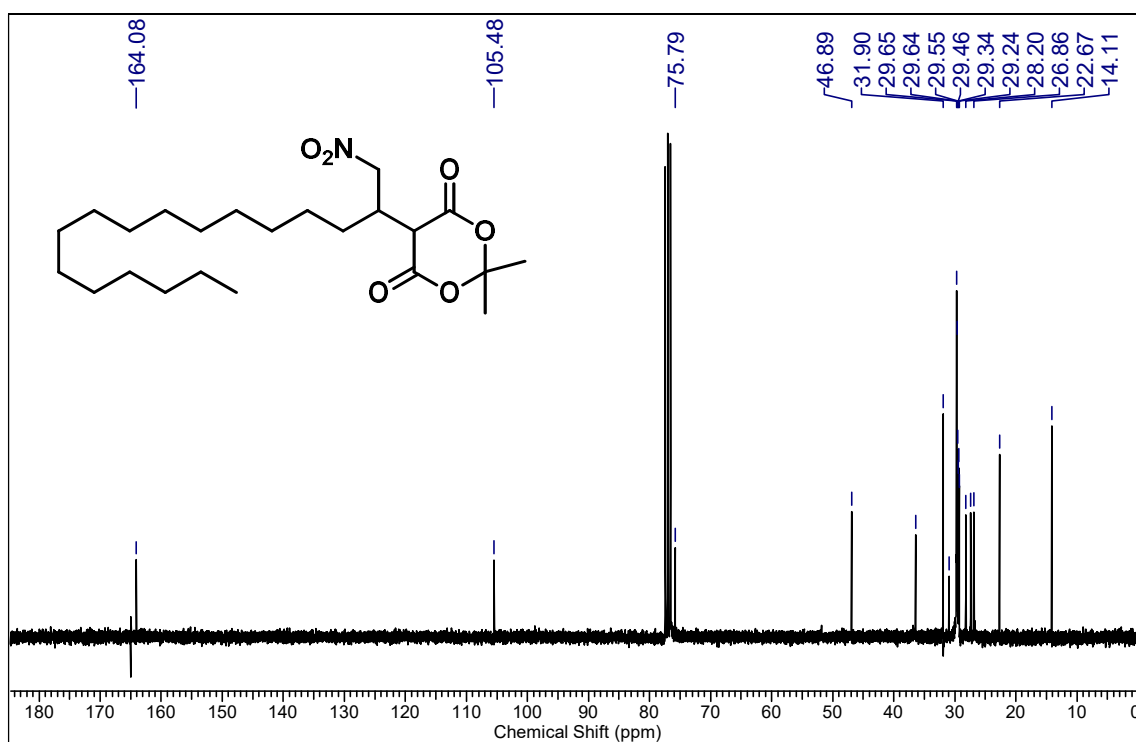


Figure S33. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of crude nitro adduct **10f**.

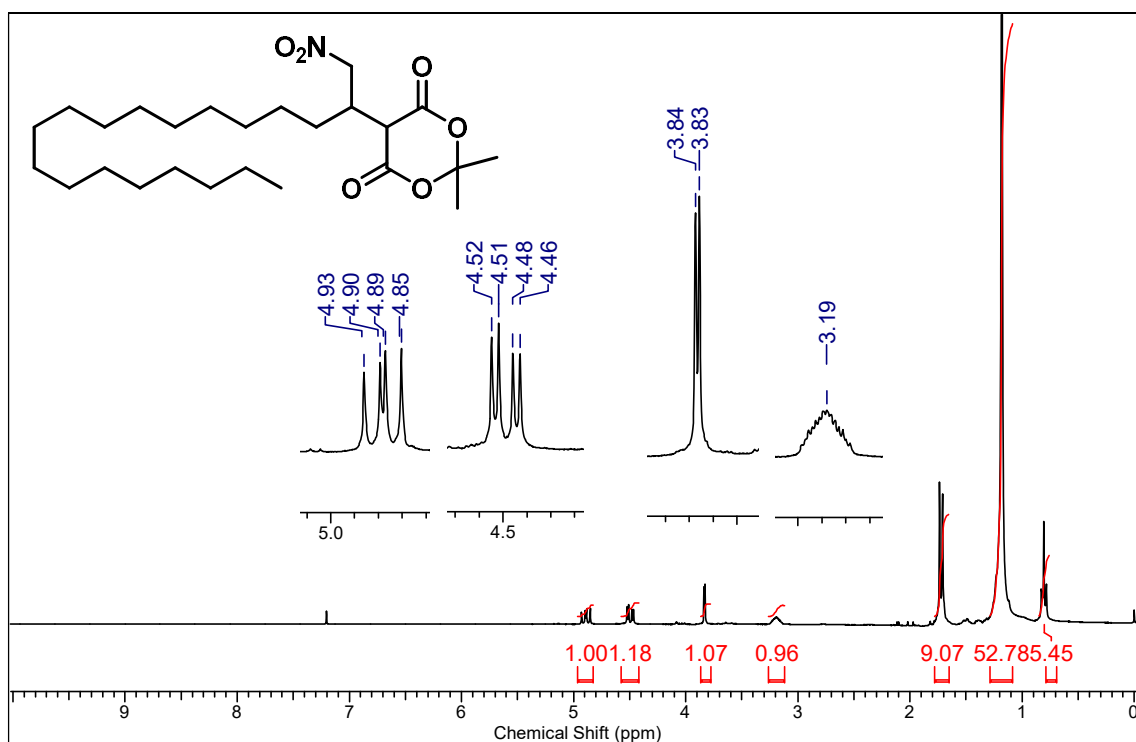


Figure S34. Spectrum of ^1H NMR (300 MHz, CDCl_3) of crude nitro adduct **10g**.

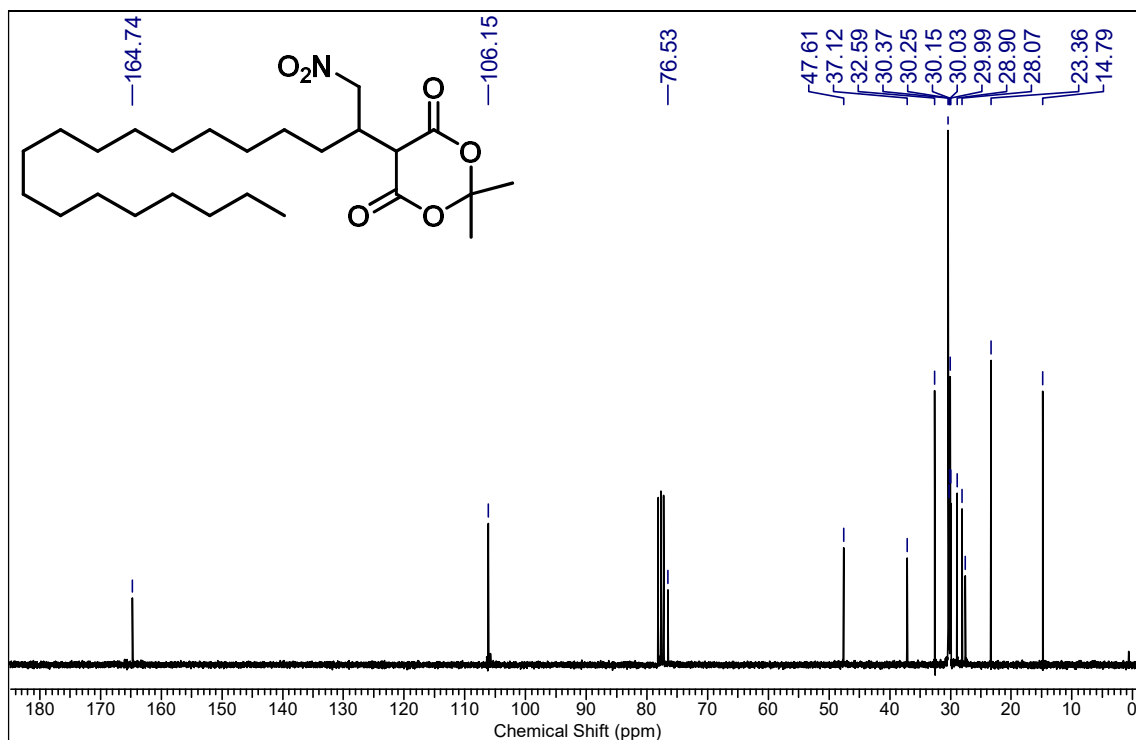


Figure S35. Spectrum of ¹³C NMR (75 MHz, CDCl₃) of crude nitro adduct **10g**.

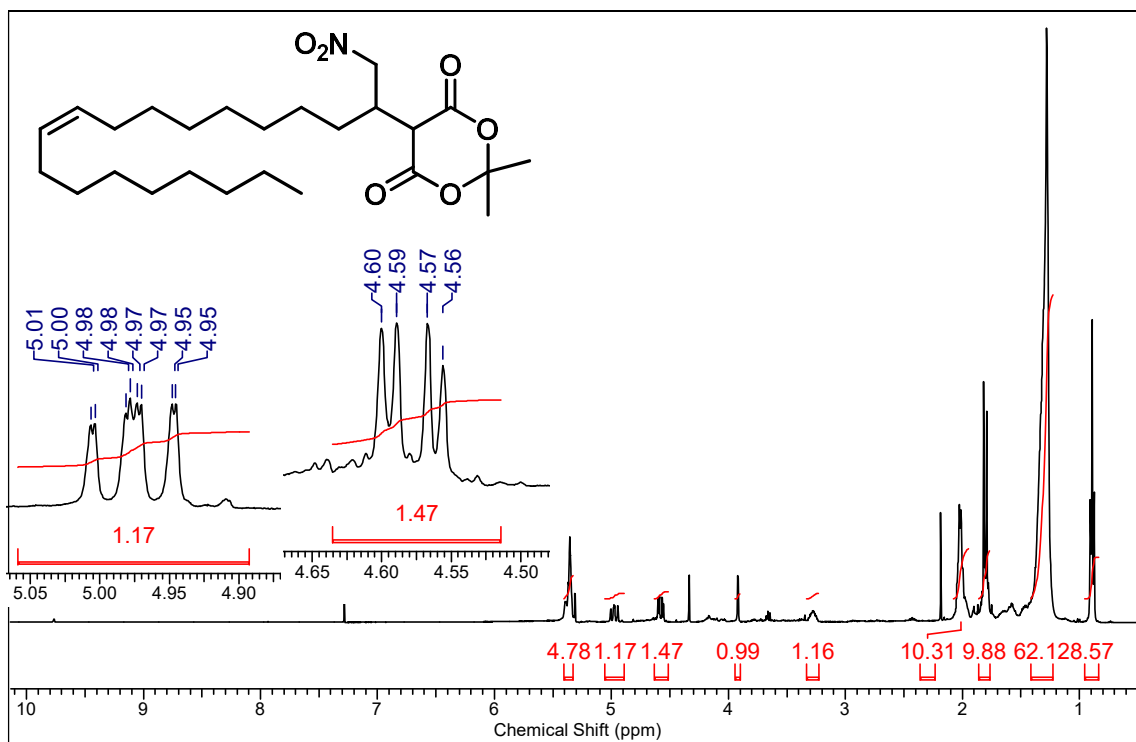


Figure S36. Spectrum of ¹H NMR (300 MHz, CDCl₃) of crude nitro adduct **10h**.

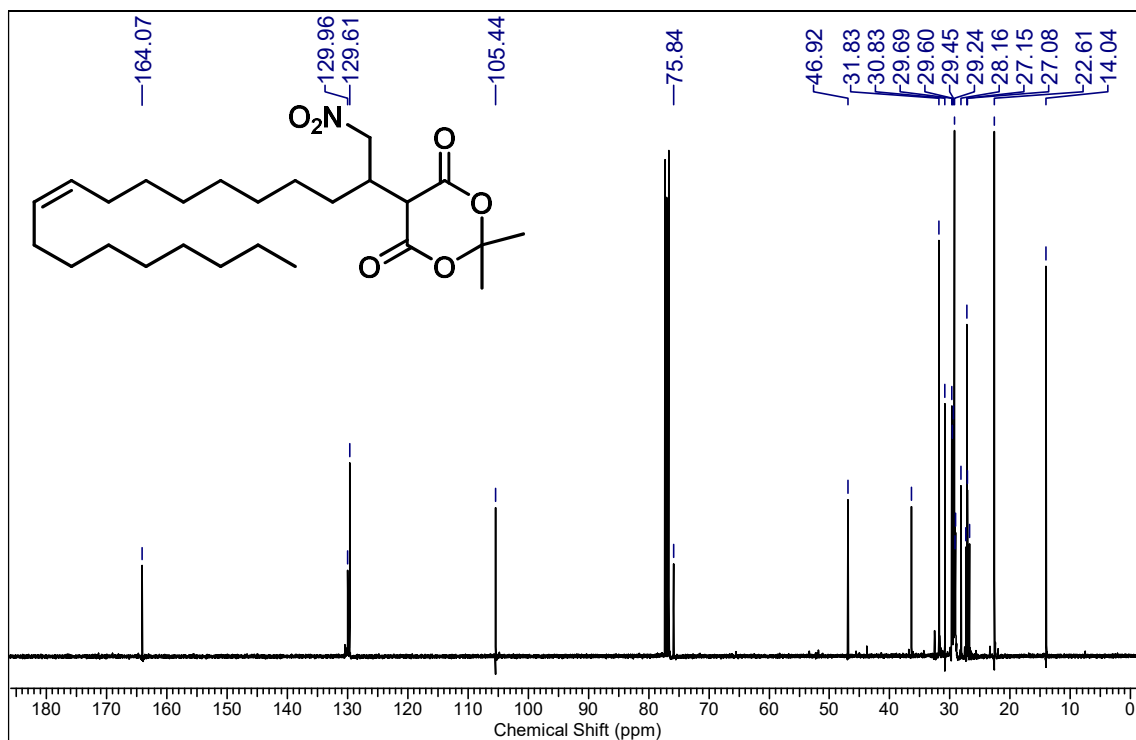


Figure S37. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of crude nitro adduct **10h**.

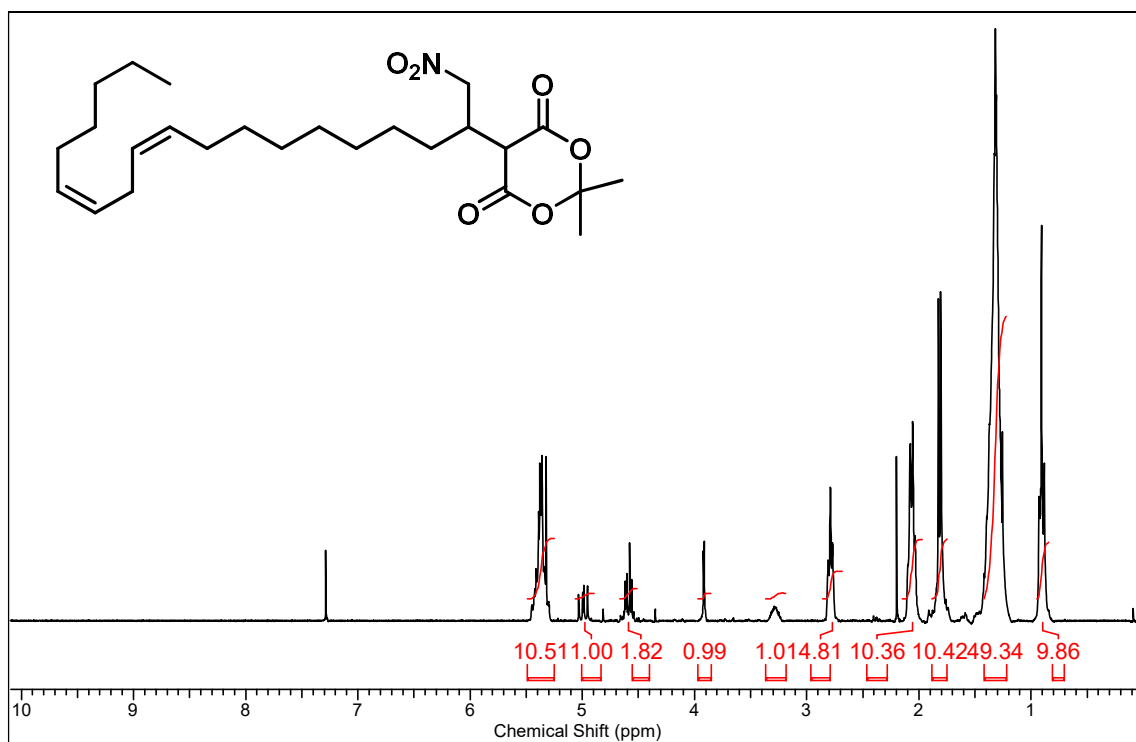


Figure S38. Spectrum of ^1H NMR (300 MHz, CDCl_3) of crude nitro adduct **10i**.

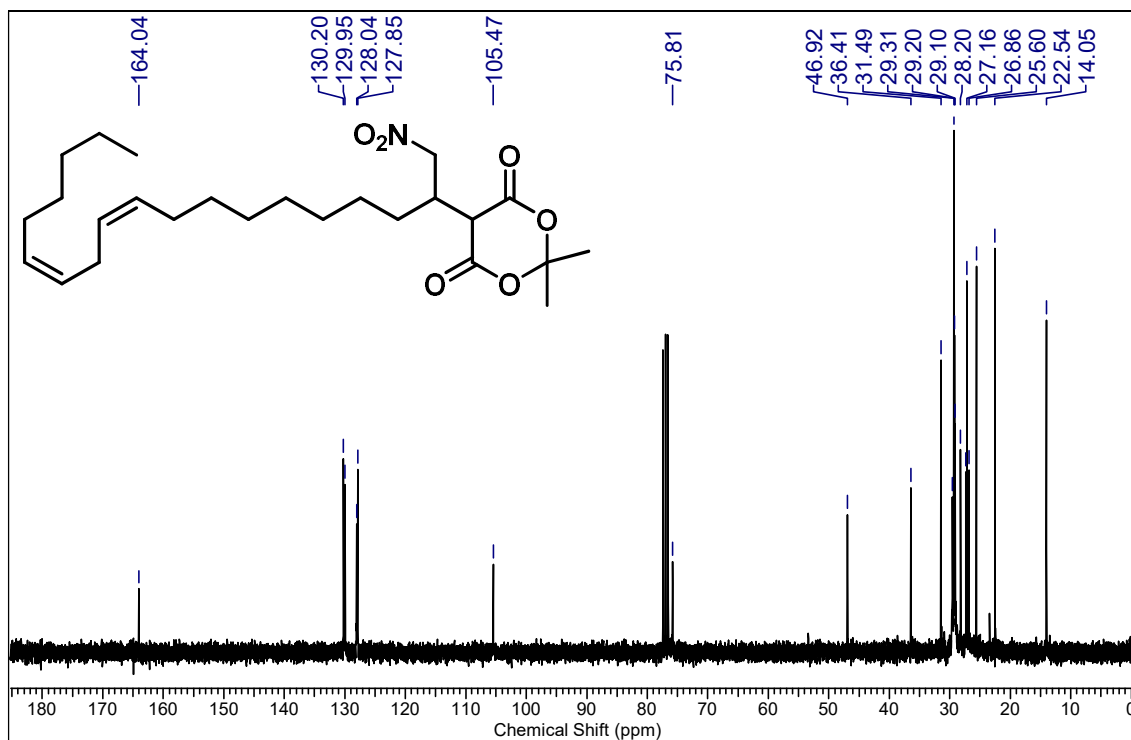


Figure S39. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of crude nitro adduct **10i**.

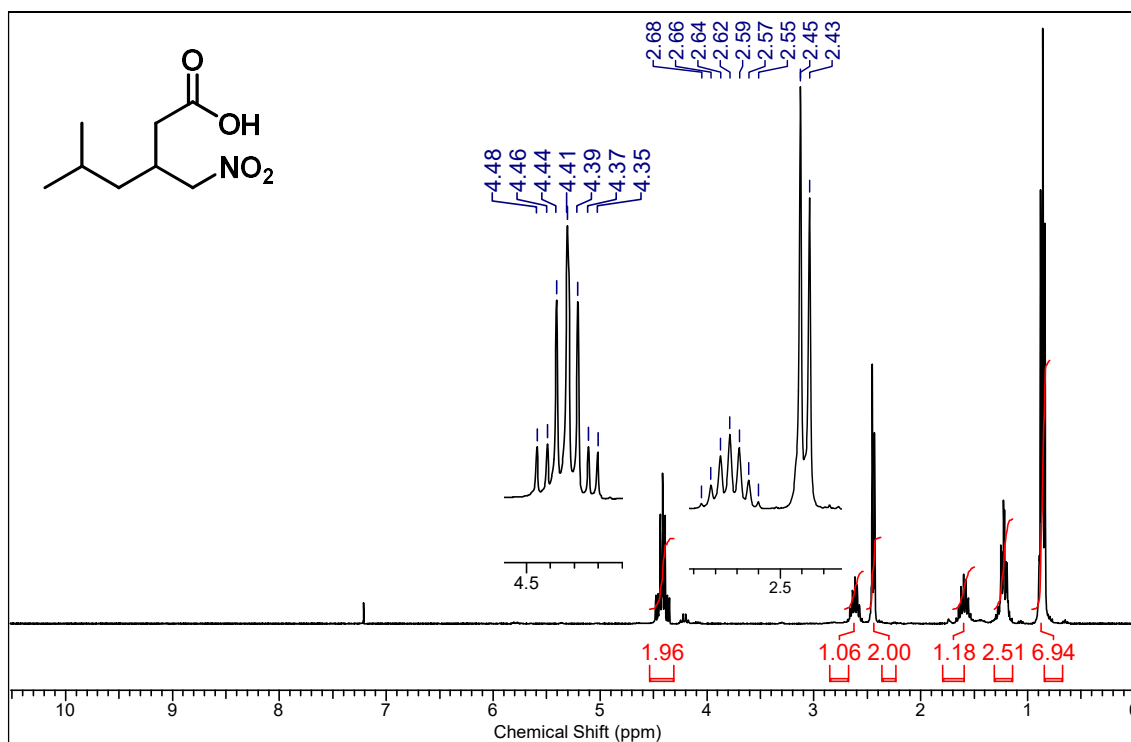


Figure S40. Spectrum of ^1H NMR (300 MHz, CDCl_3) of γ -nitro acid **11a**.

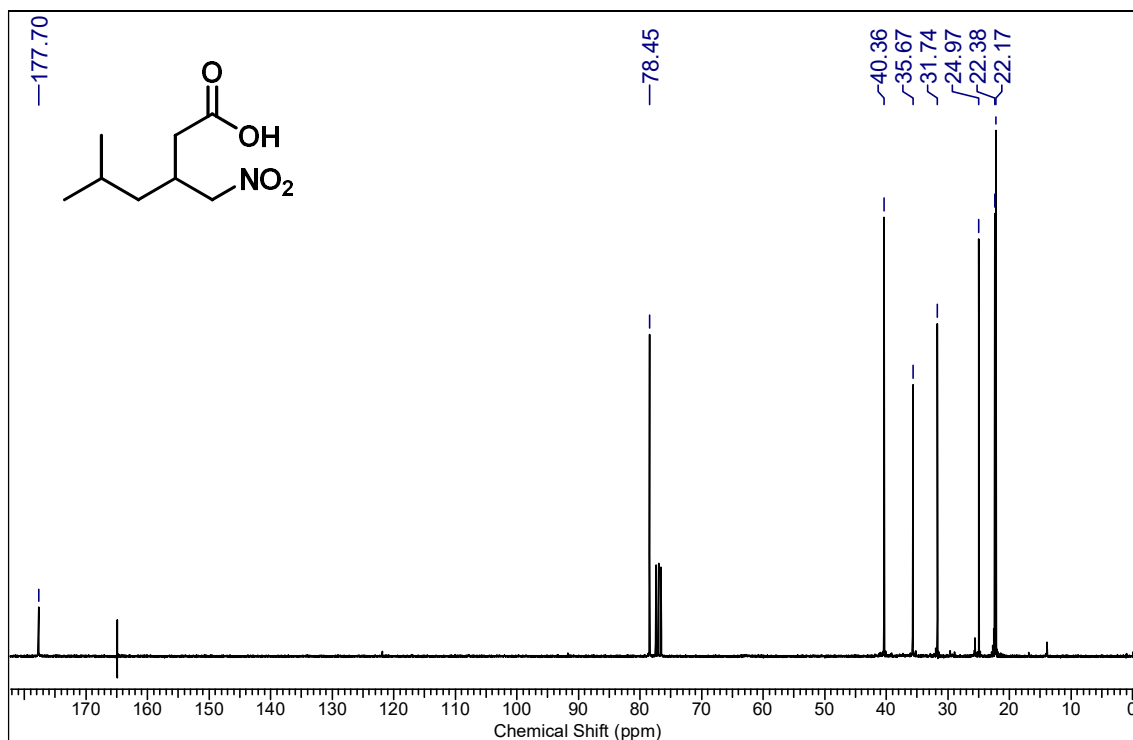


Figure S41. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of γ -nitro acid **11a**.

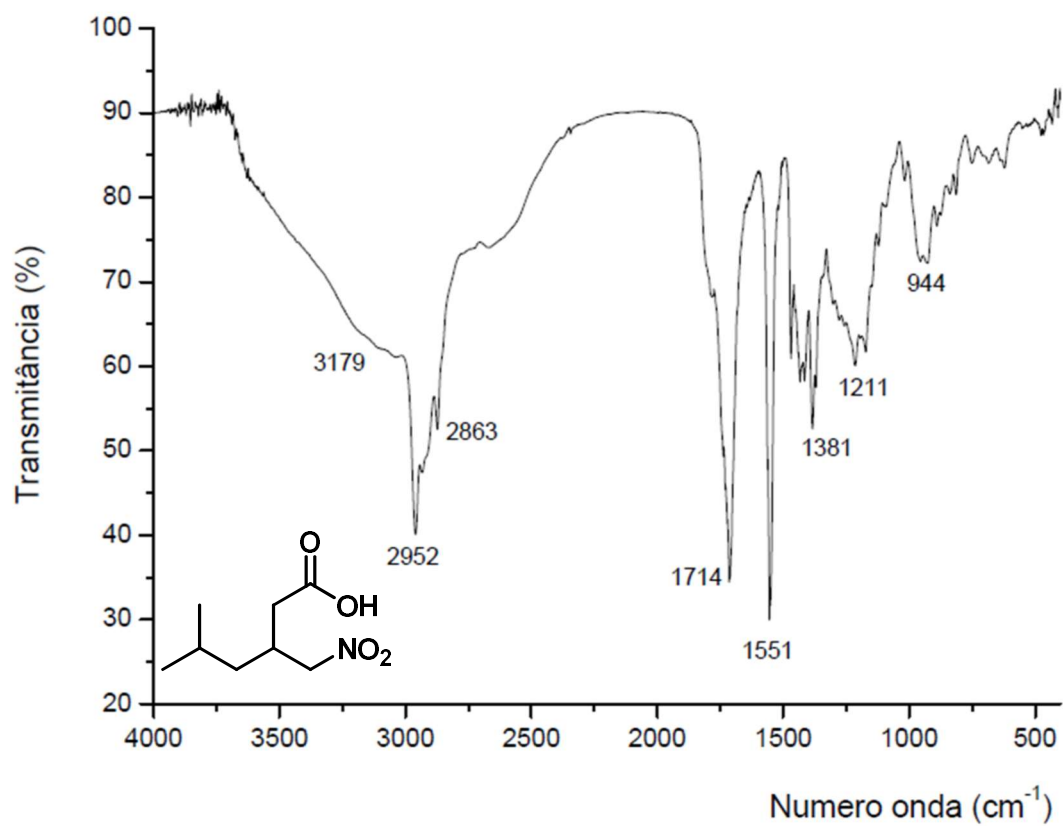


Figure S42. Spectrum of IR (NaCl) of γ -nitro acid **11a**.

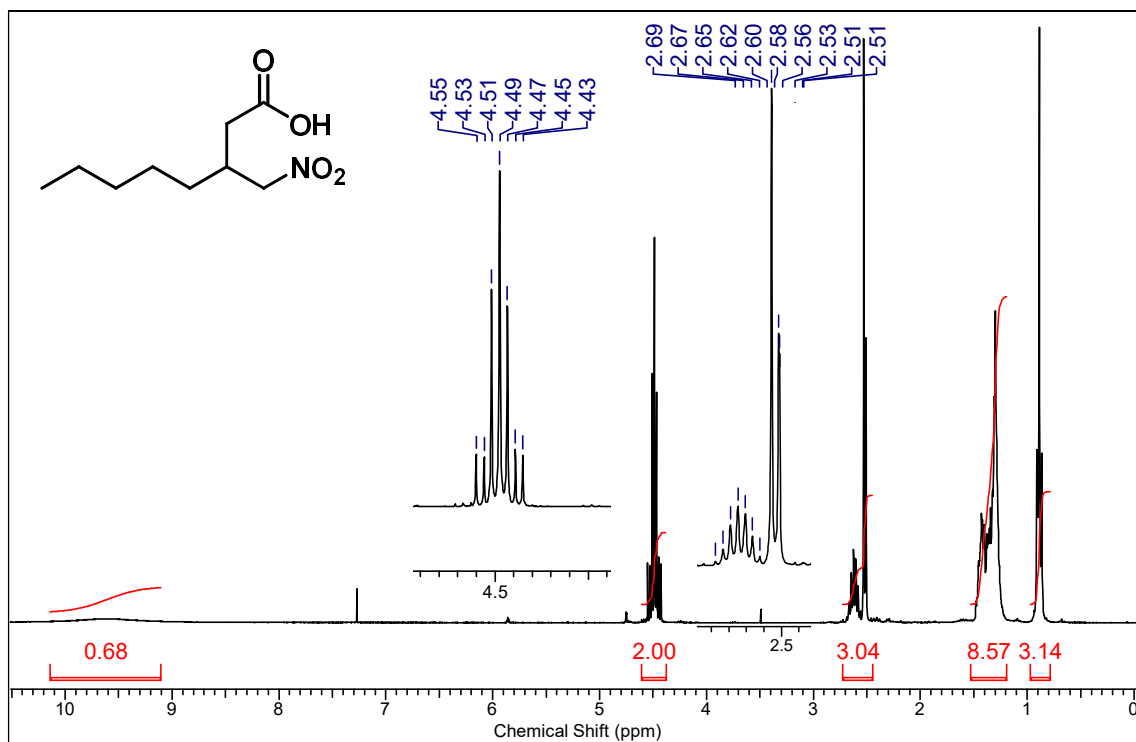


Figure S43. Spectrum of $^1\text{H NMR}$ (300 MHz, CDCl_3) of γ -nitro acid **11b**.

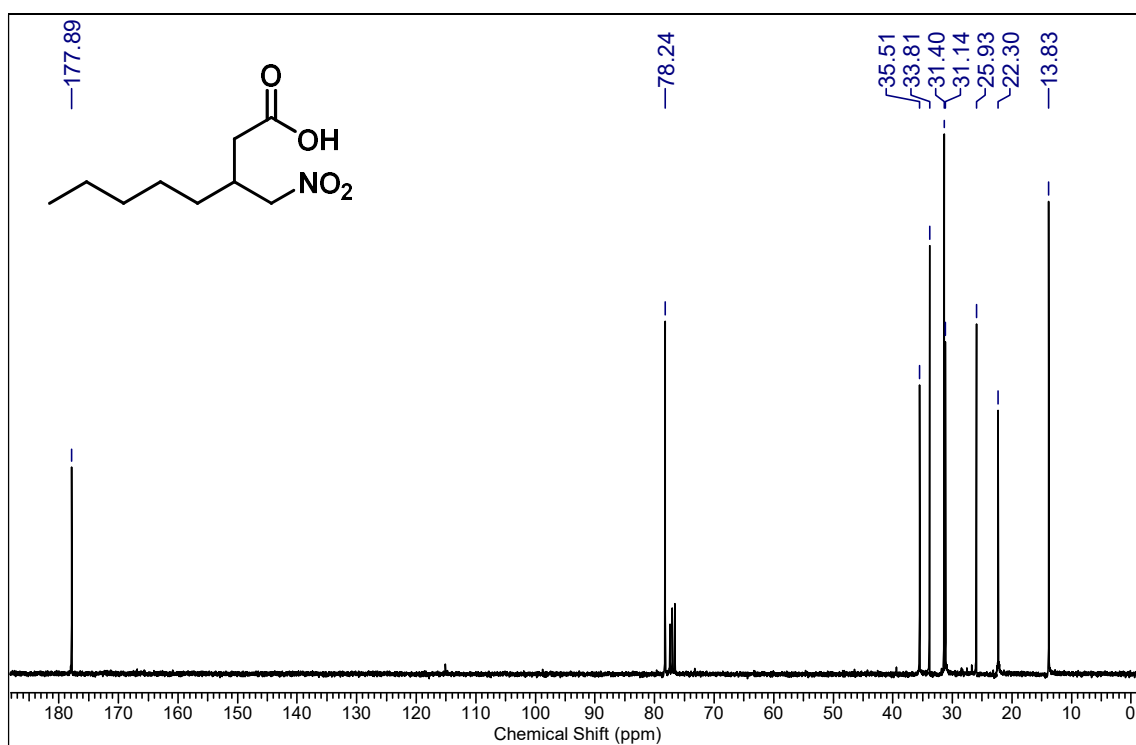


Figure S44. Spectrum of $^{13}\text{C NMR}$ (75 MHz, CDCl_3) of γ -nitro acid **11b**.

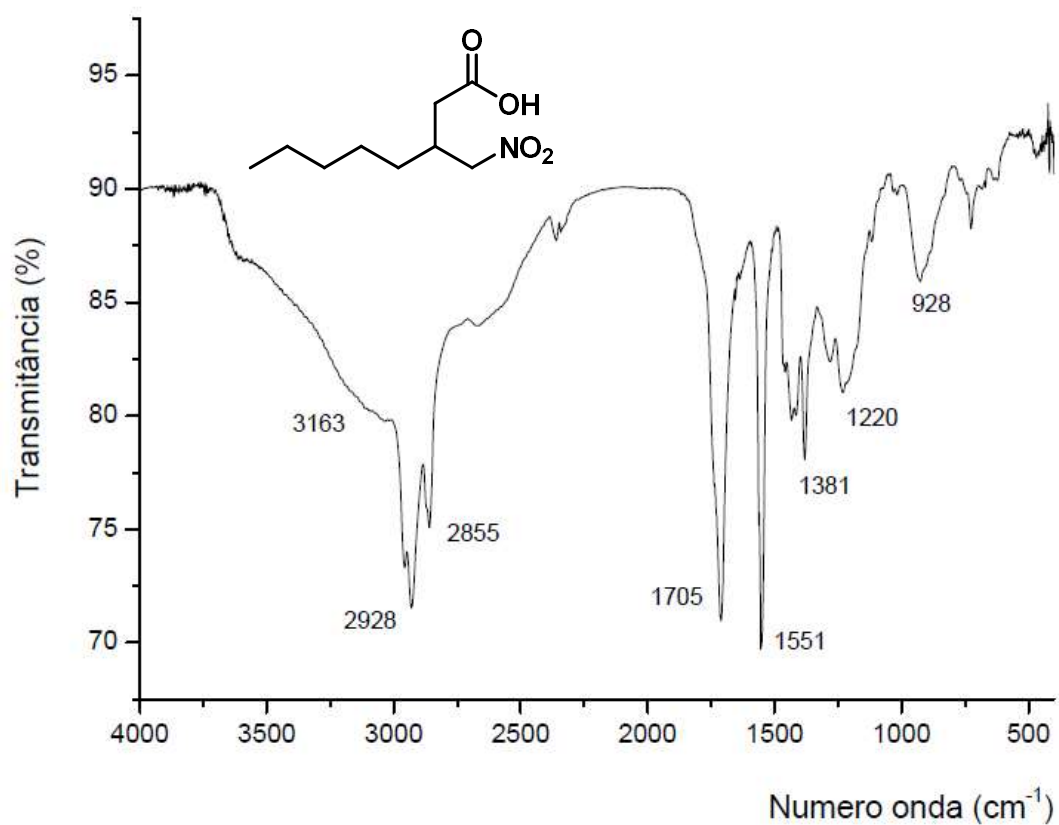


Figure S45. Spectrum of IR (NaCl) of γ -nitro acid **11b**.

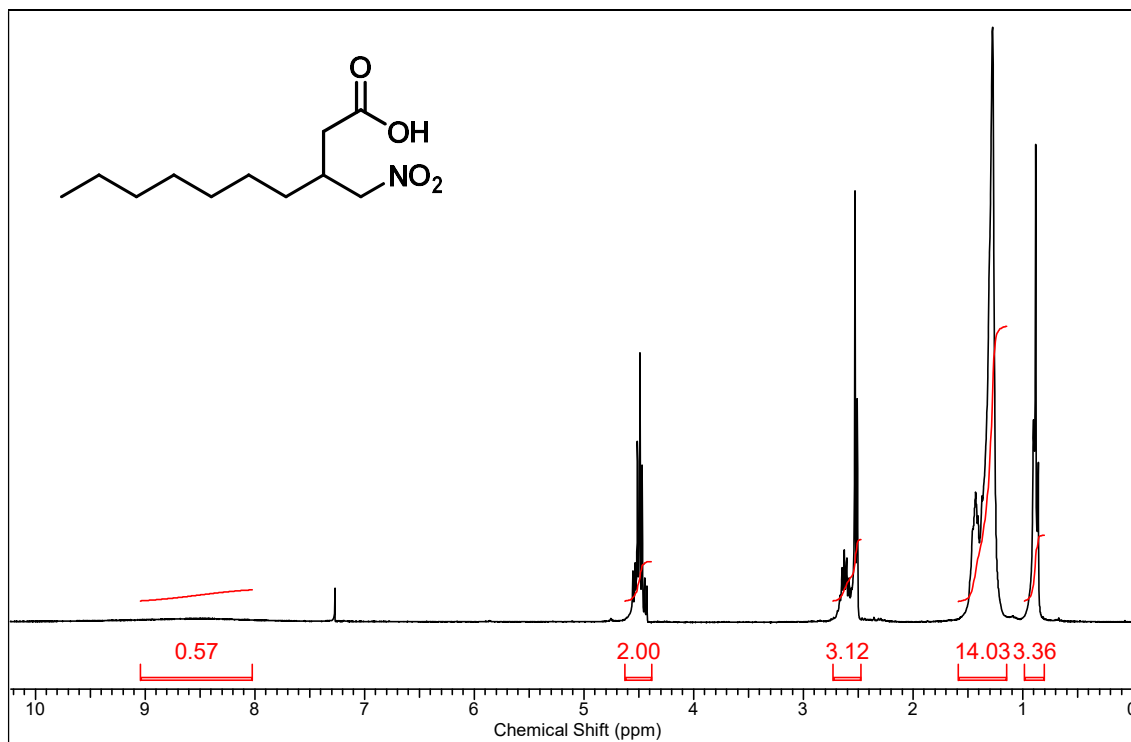


Figure S46. Spectrum of ^1H NMR (300 MHz, CDCl_3) of γ -nitro acid **11c**.

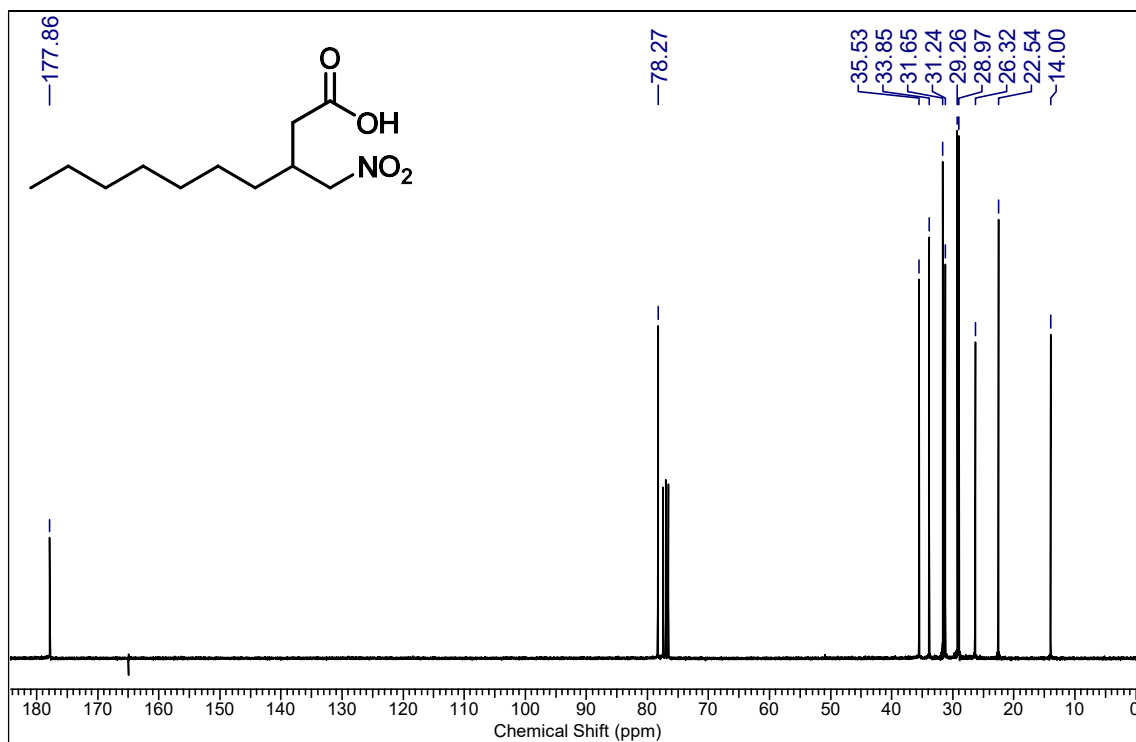


Figure S47. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of γ -nitro acid **11c**.

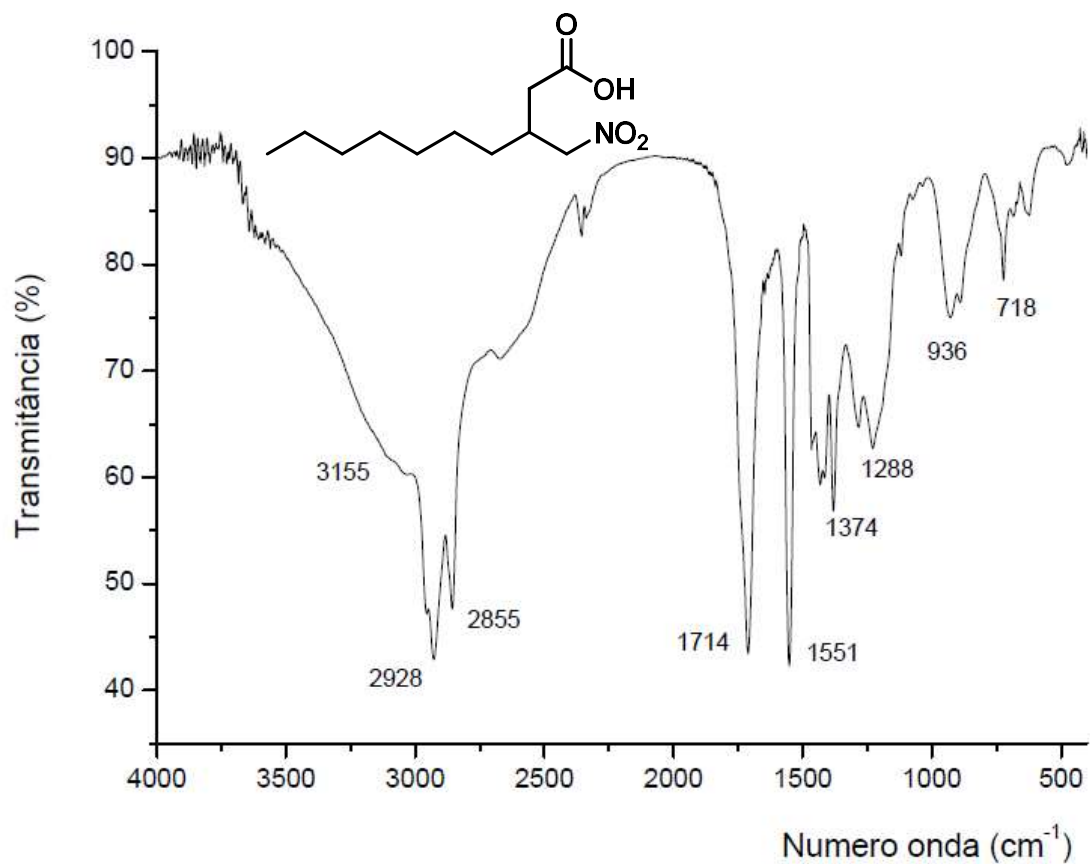


Figure S48. Spectrum of IR (NaCl) of γ -nitro acid **11c**.

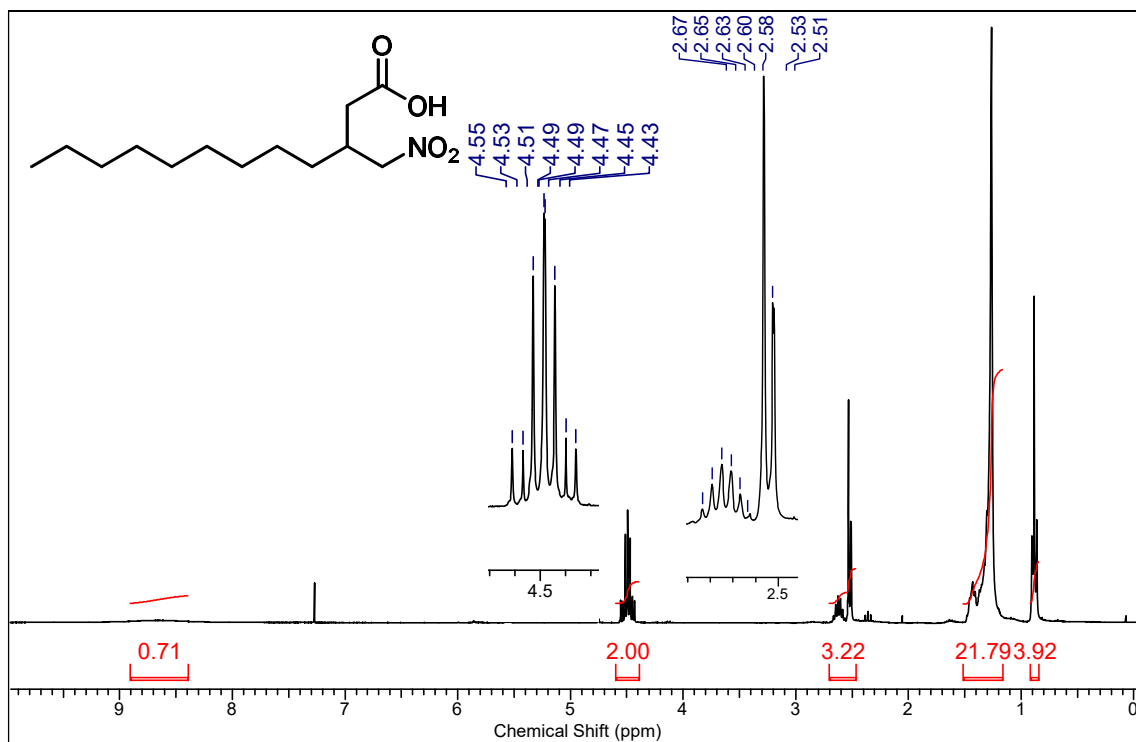


Figure S49. Spectrum of $^1\text{H NMR}$ (300 MHz, CDCl_3) of γ -nitro acid **11d**.

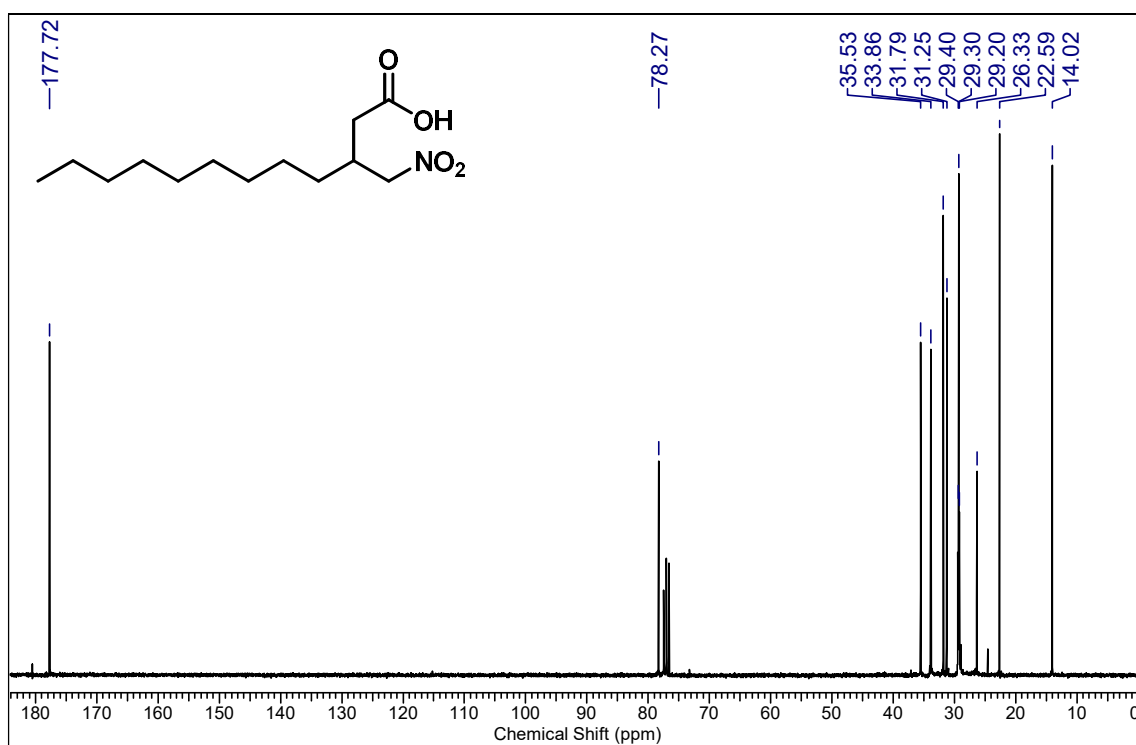


Figure S50. Spectrum of $^{13}\text{C NMR}$ (75 MHz, CDCl_3) of γ -nitro acid **11d**.

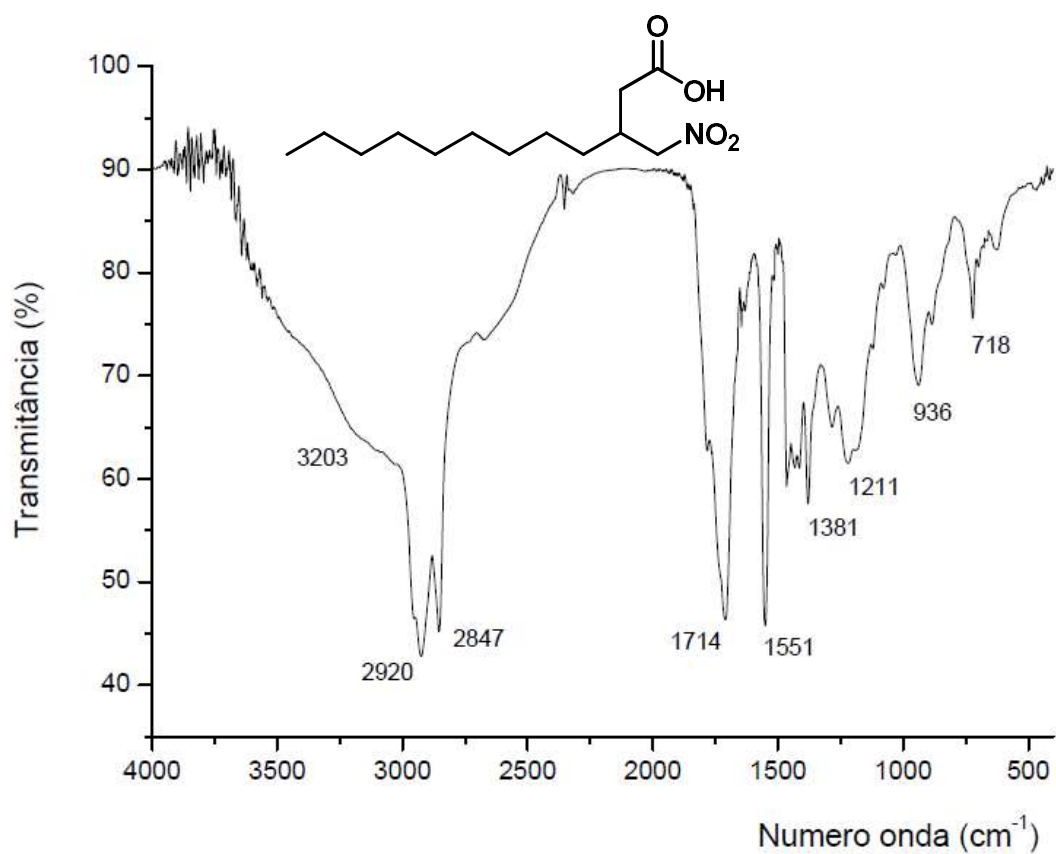


Figure S51. Spectrum of IR (NaCl) of γ -nitro acid **11d**.

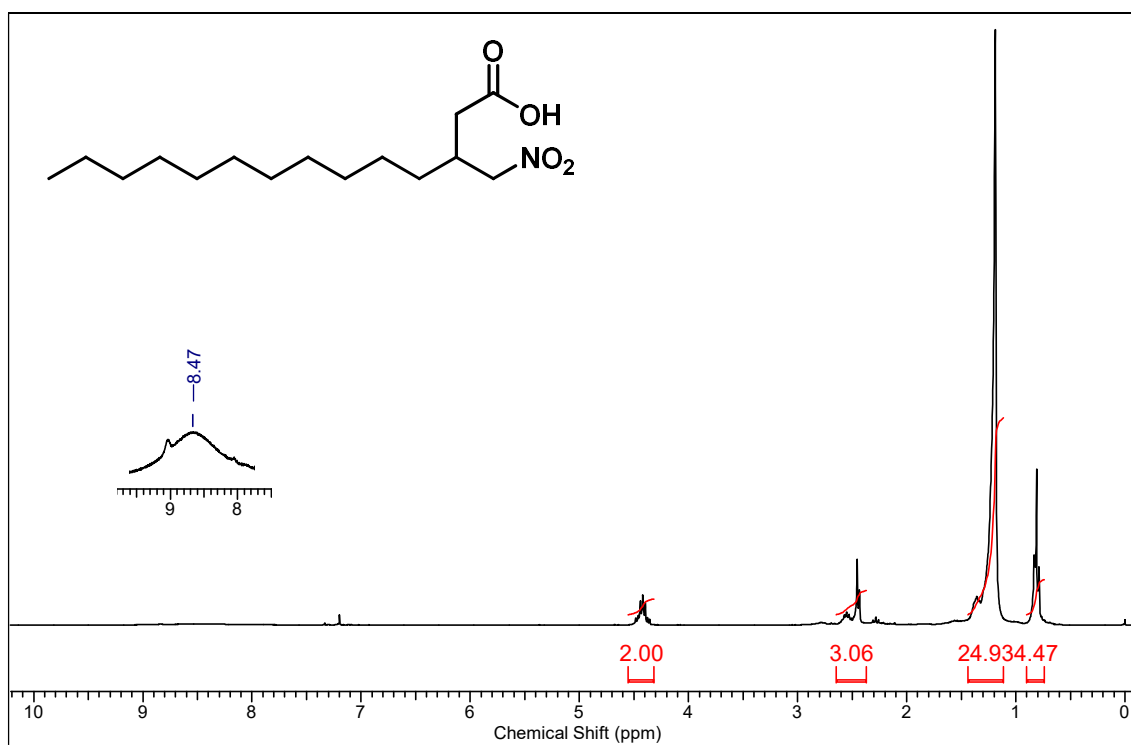


Figure S52. Spectrum of ^1H NMR (300 MHz, CDCl_3) of γ -nitro acid **11e**.

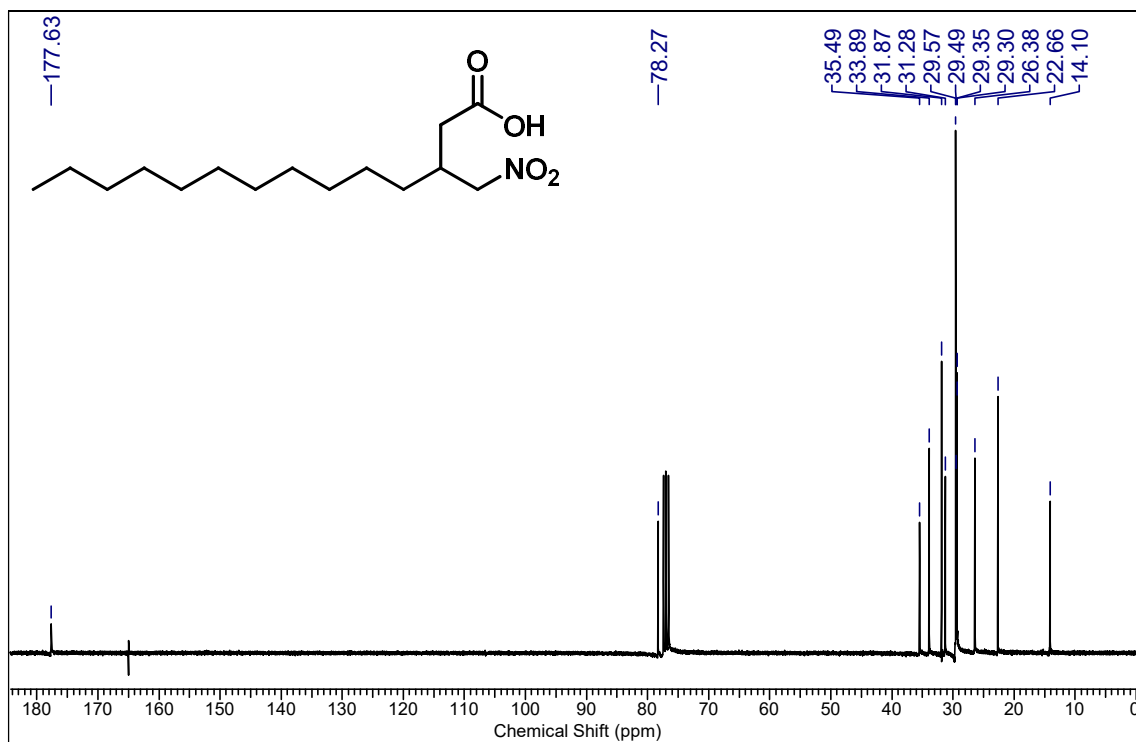


Figure S53. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of γ -nitro acid **11e**.

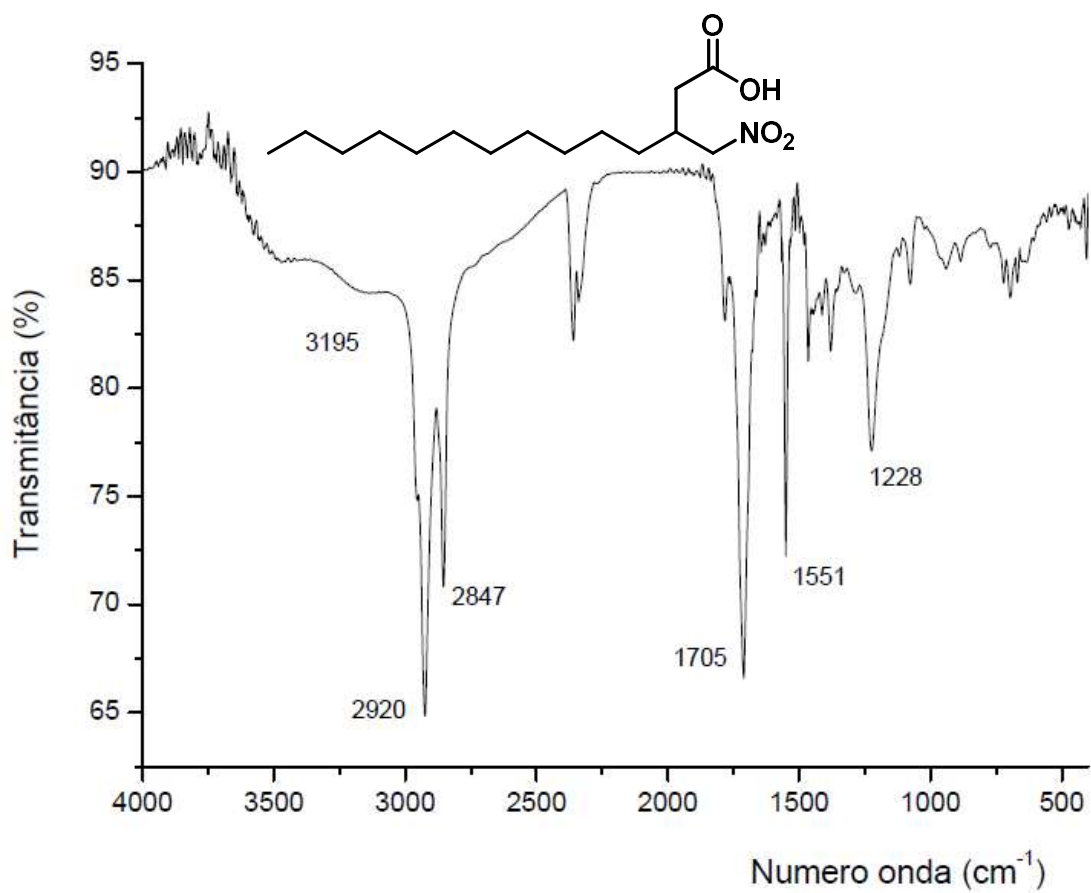


Figure S54. Spectrum of IR (NaCl) of γ -nitro acid **11e**.

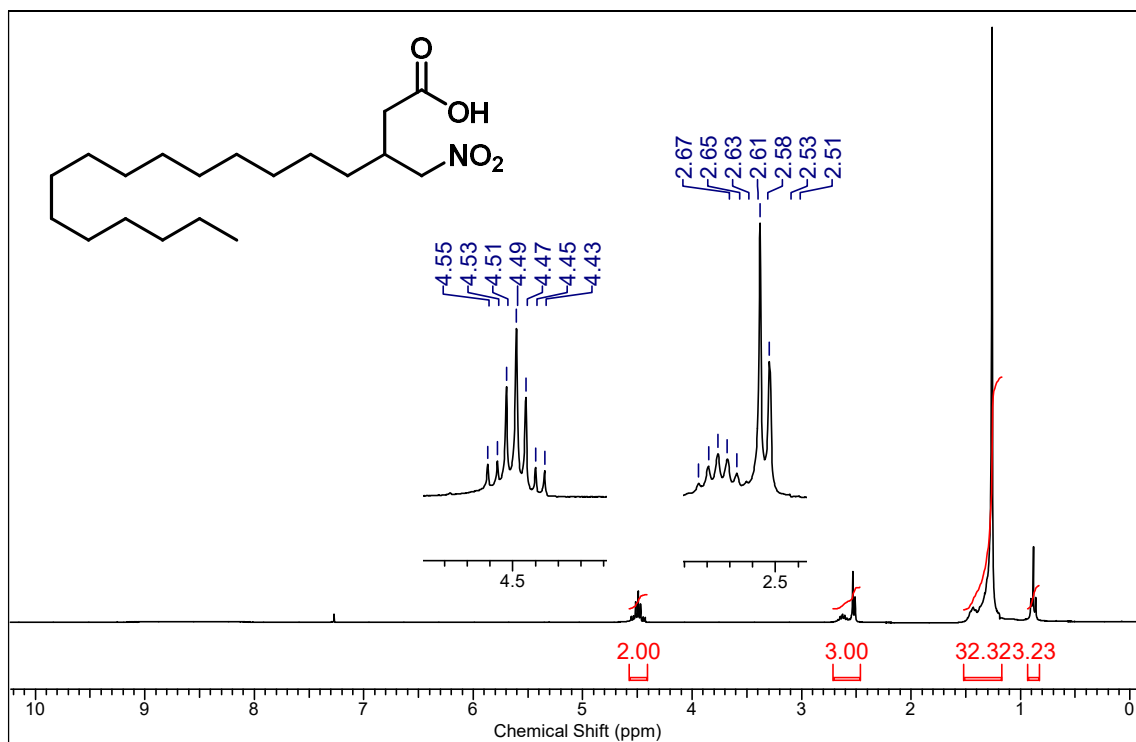


Figure S55. Spectrum of ^1H NMR (300 MHz, CDCl_3) of γ -nitro acid **11f**.

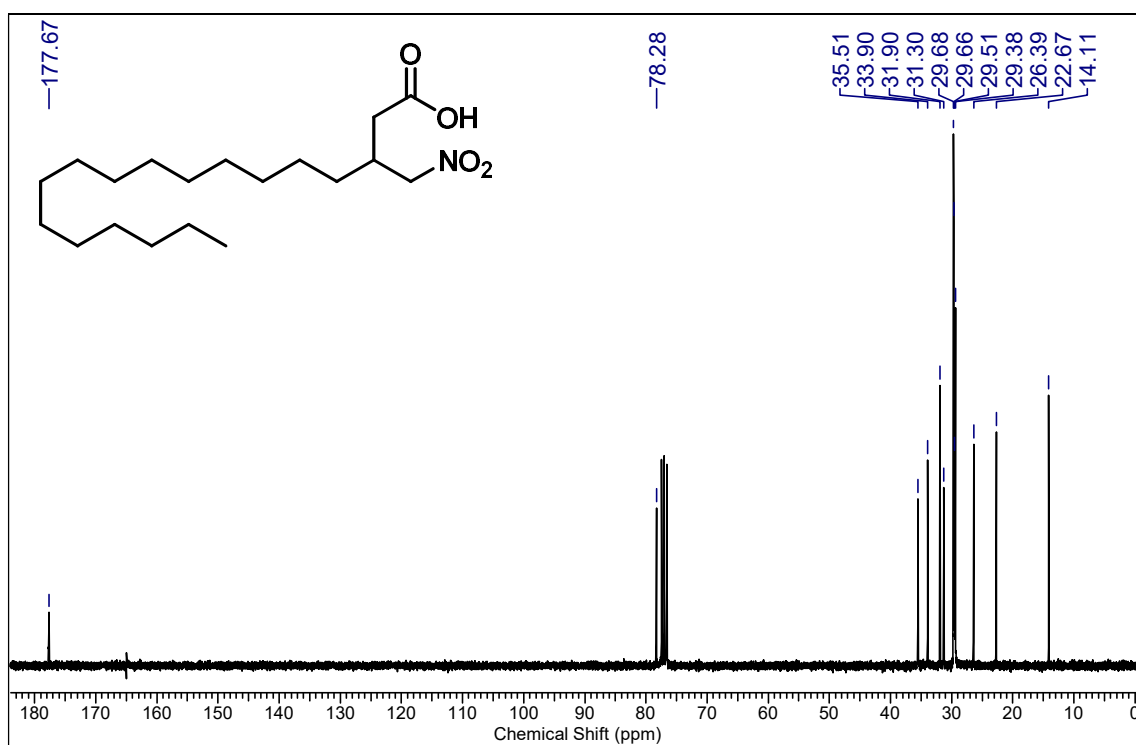


Figure S56. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of γ -nitro acid **11f**.

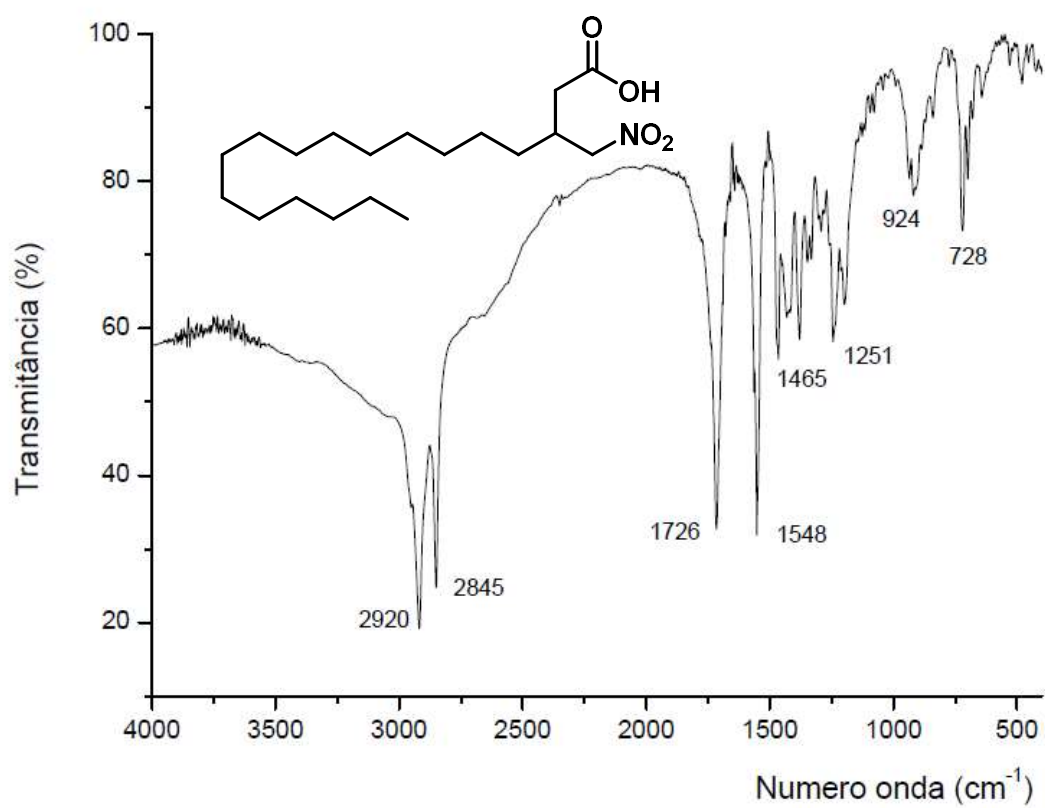


Figure S57. Spectrum of IR (NaCl) of γ -nitro acid **11f**.

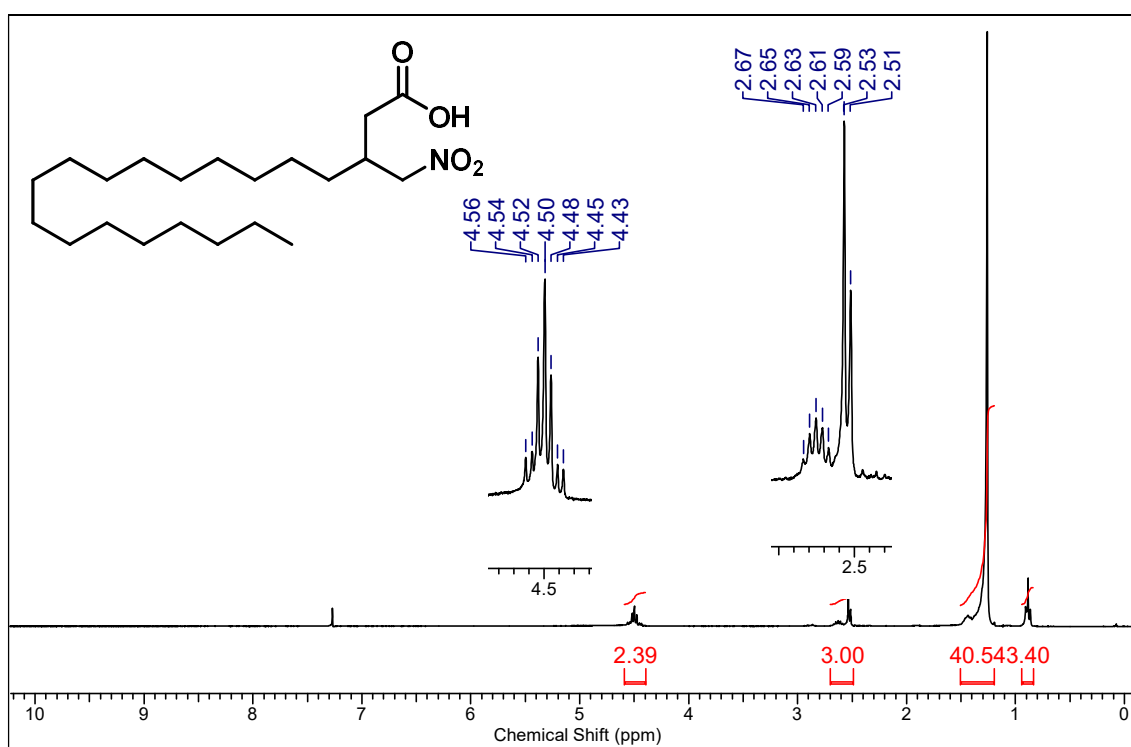


Figure S58. Spectrum of ^1H NMR (300 MHz, CDCl_3) of γ -nitro acid **11g**.

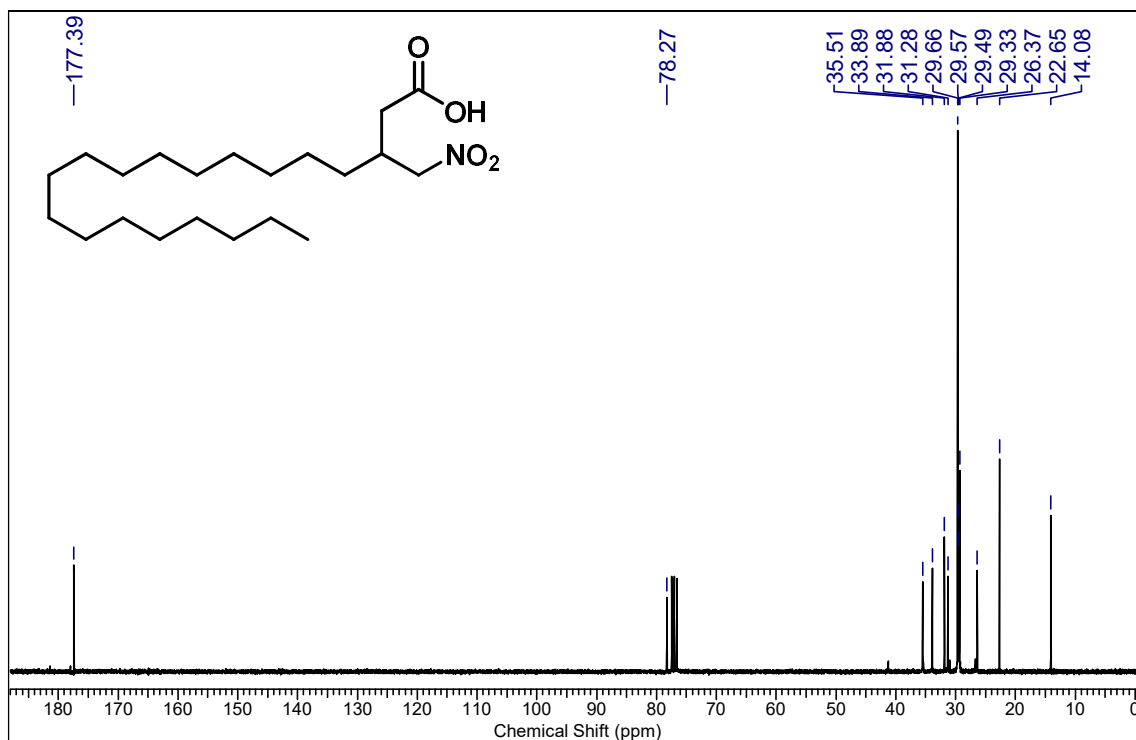


Figure S59. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of γ -nitro acid **11g**.

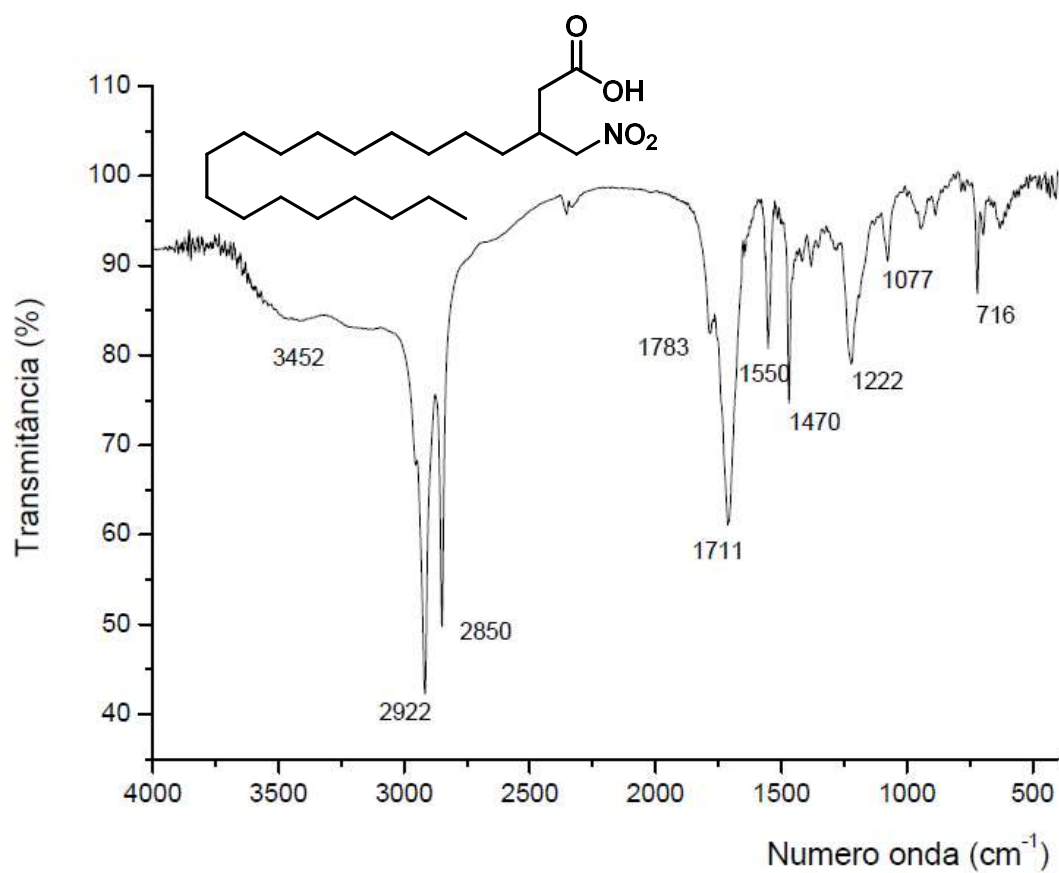


Figure S60. Spectrum of IR (NaCl) of γ -nitro acid **11g**.

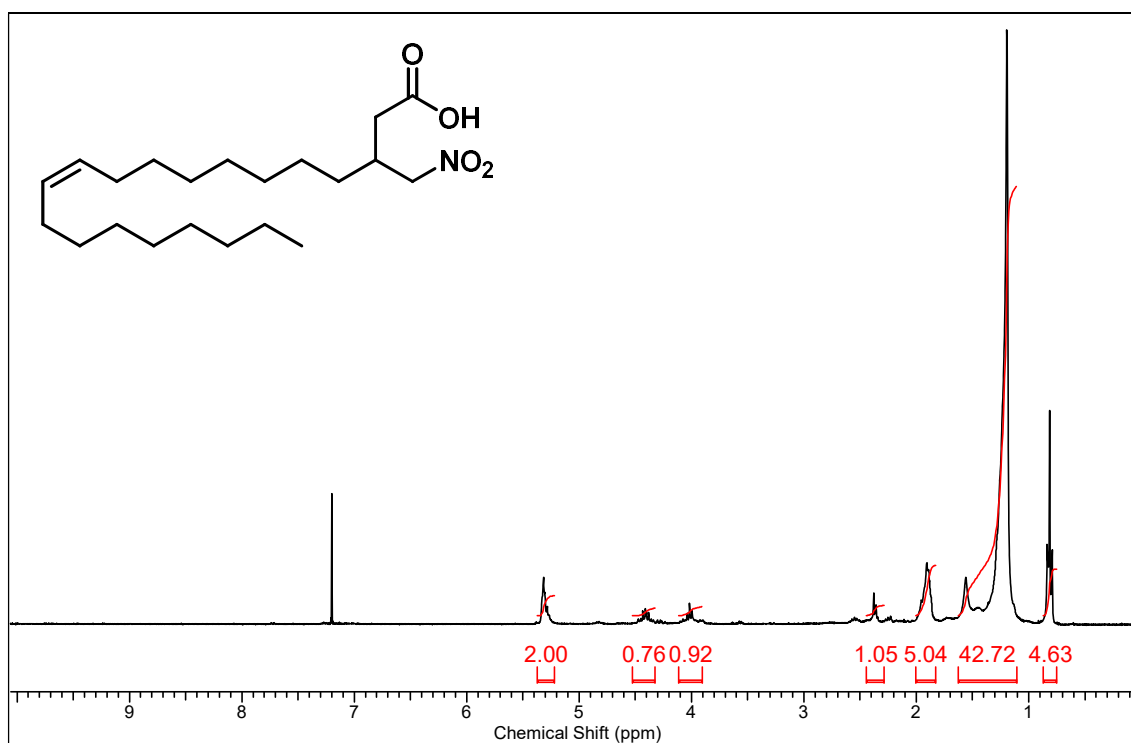


Figure S61. Spectrum of ^1H NMR (300 MHz, CDCl_3) of γ -nitro acid **11h**.

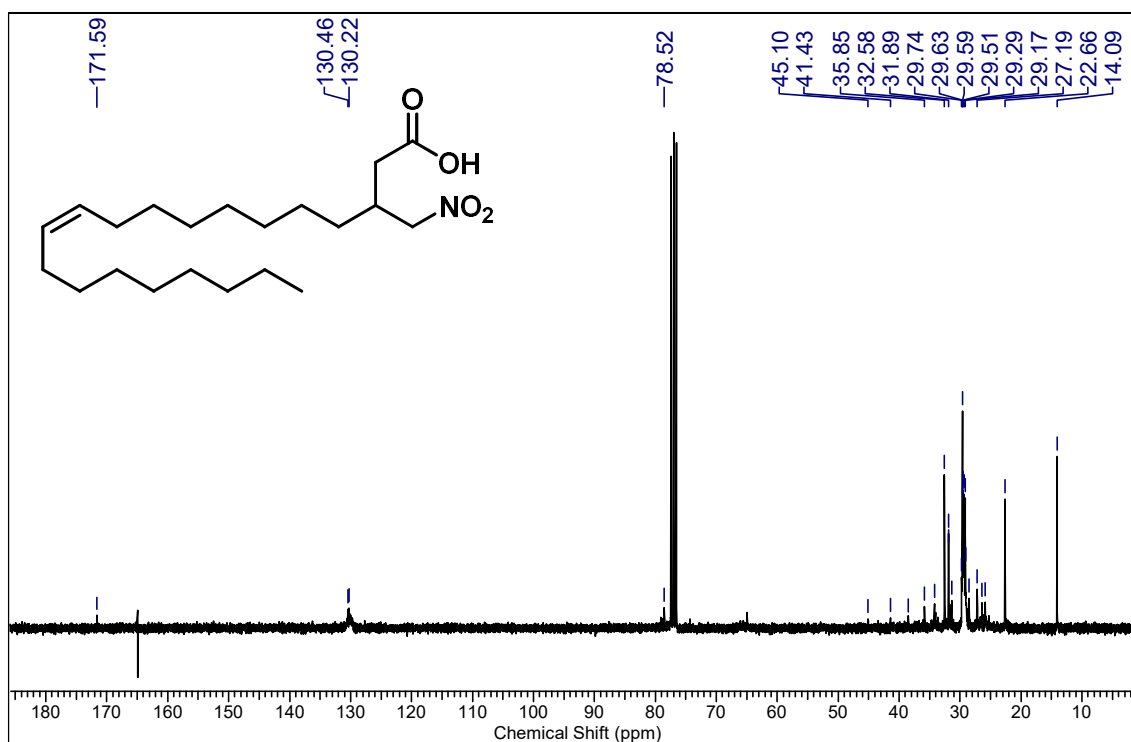


Figure S62. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of γ -nitro acid **11h**.

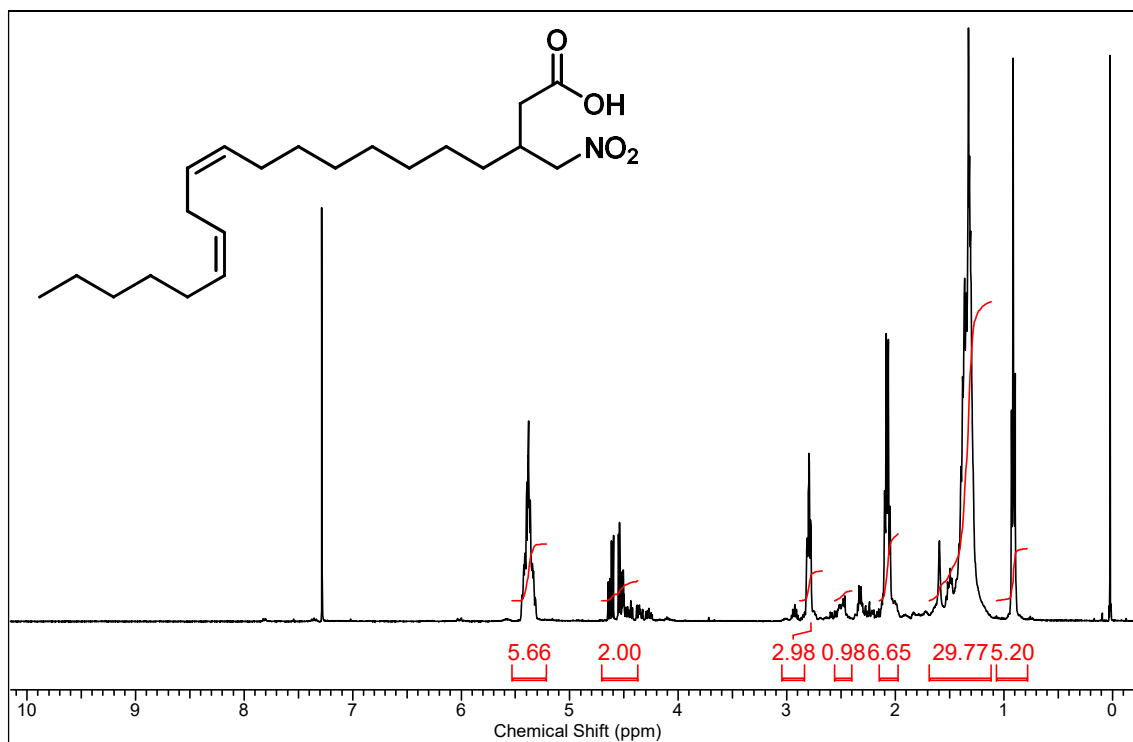


Figure S63. Spectrum of ^1H NMR (300 MHz, CDCl_3) of γ -nitro acid **11i**.

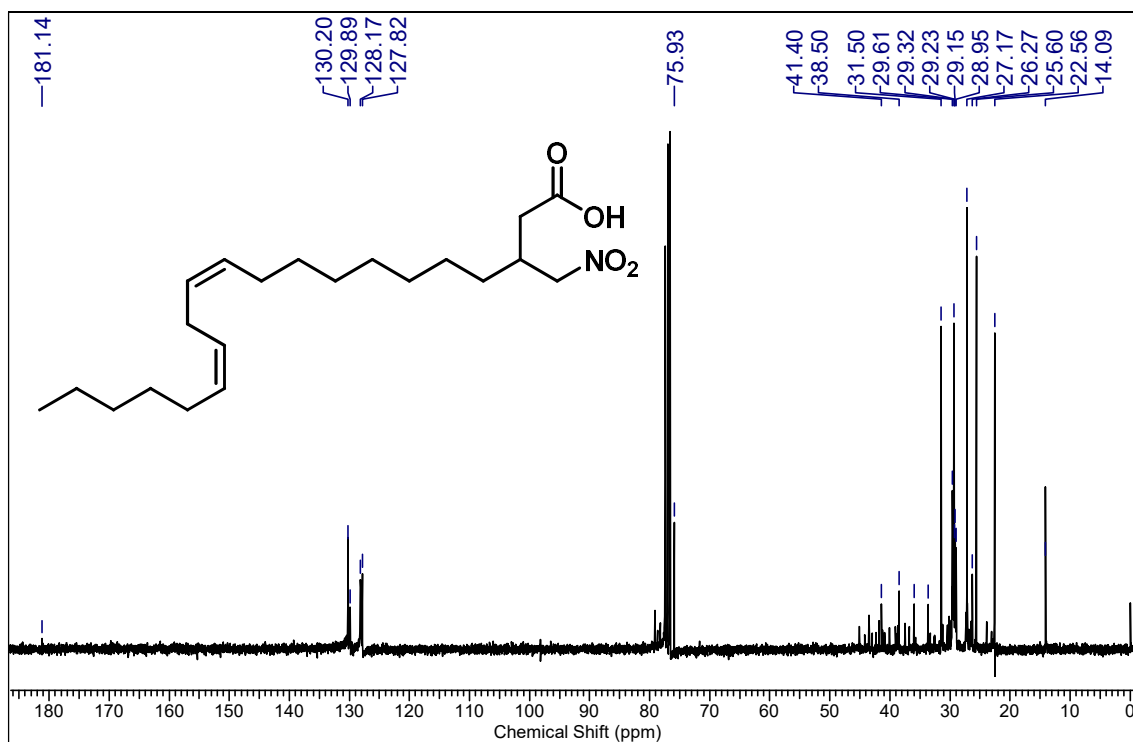


Figure S64. Spectrum of ^{13}C NMR (75 MHz, CDCl_3) of γ -nitro acid **11i**.

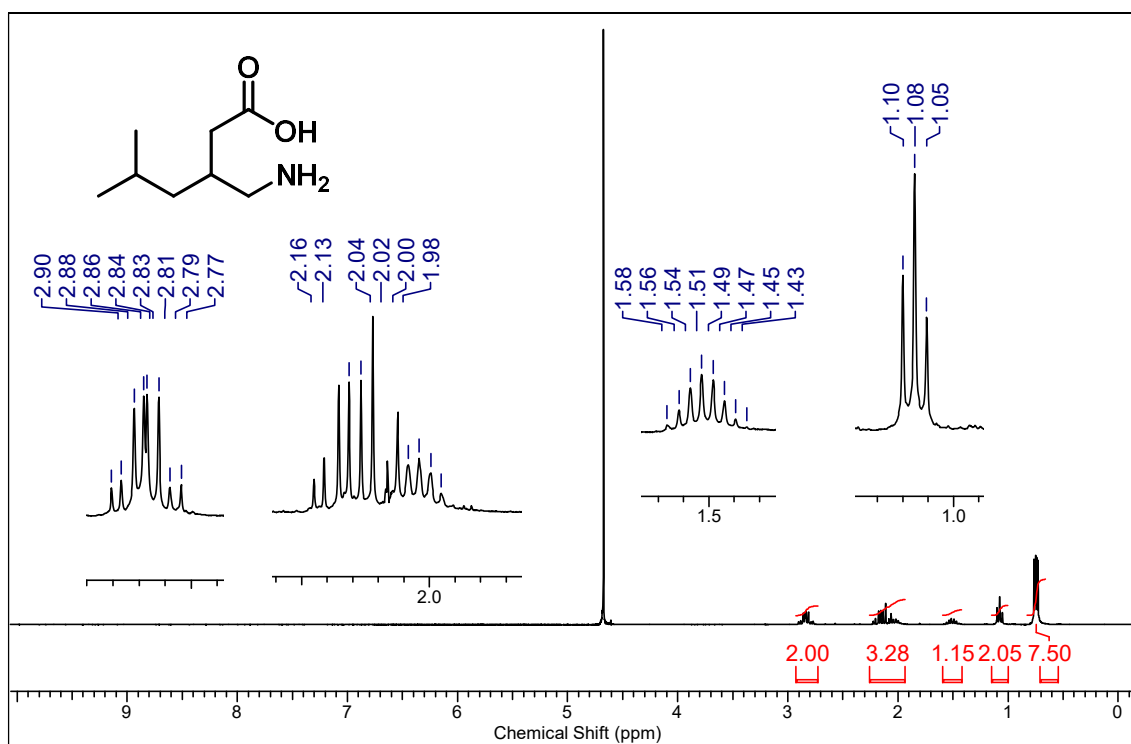


Figure S65. Spectrum of ¹H NMR (300 MHz, D₂O, capillary CDCl₃) of Pregabalin 2a.

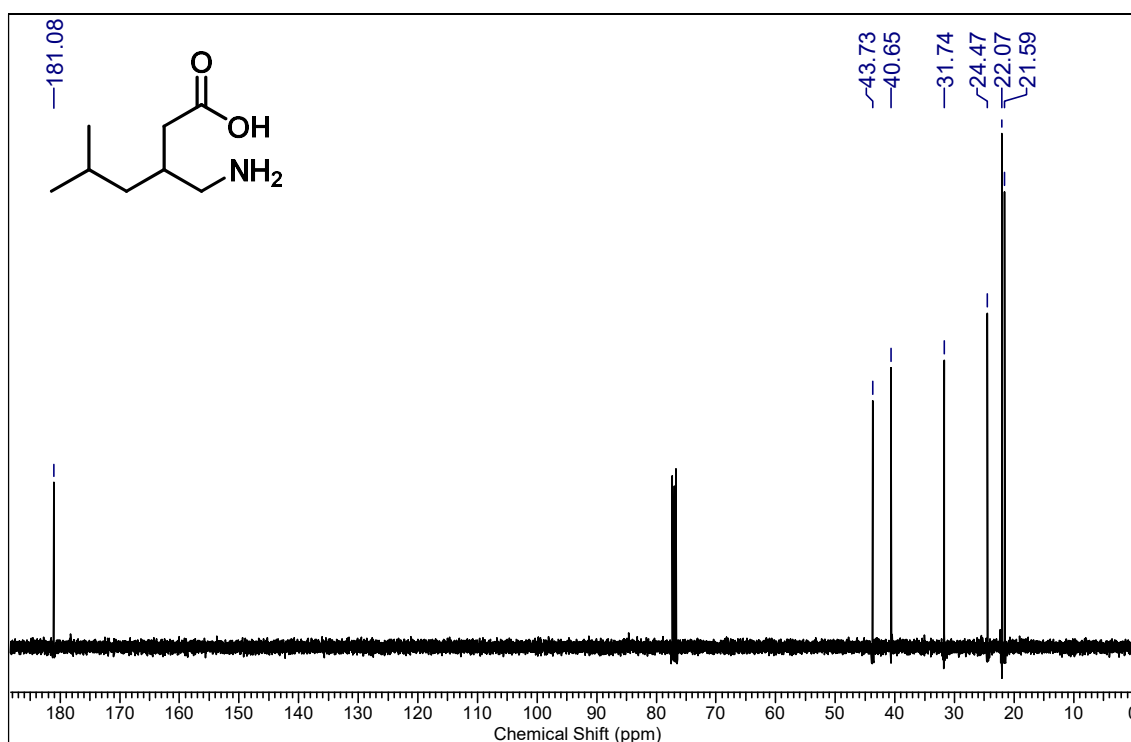


Figure S66. Spectrum of ¹³C NMR (75 MHz, D₂O, capillary CDCl₃) of Pregabalin 2a.

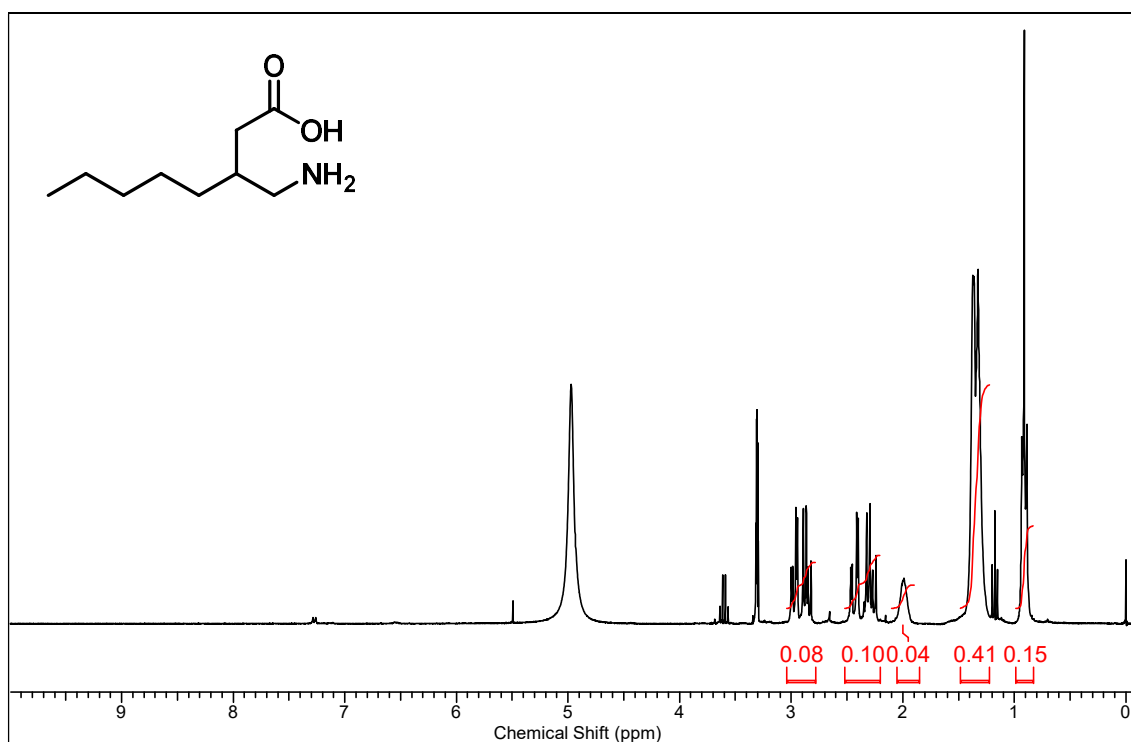


Figure S67. Spectrum of ^1H NMR (300 MHz, $\text{MeOH-}d_4$) of γ -amino acid **2b**.

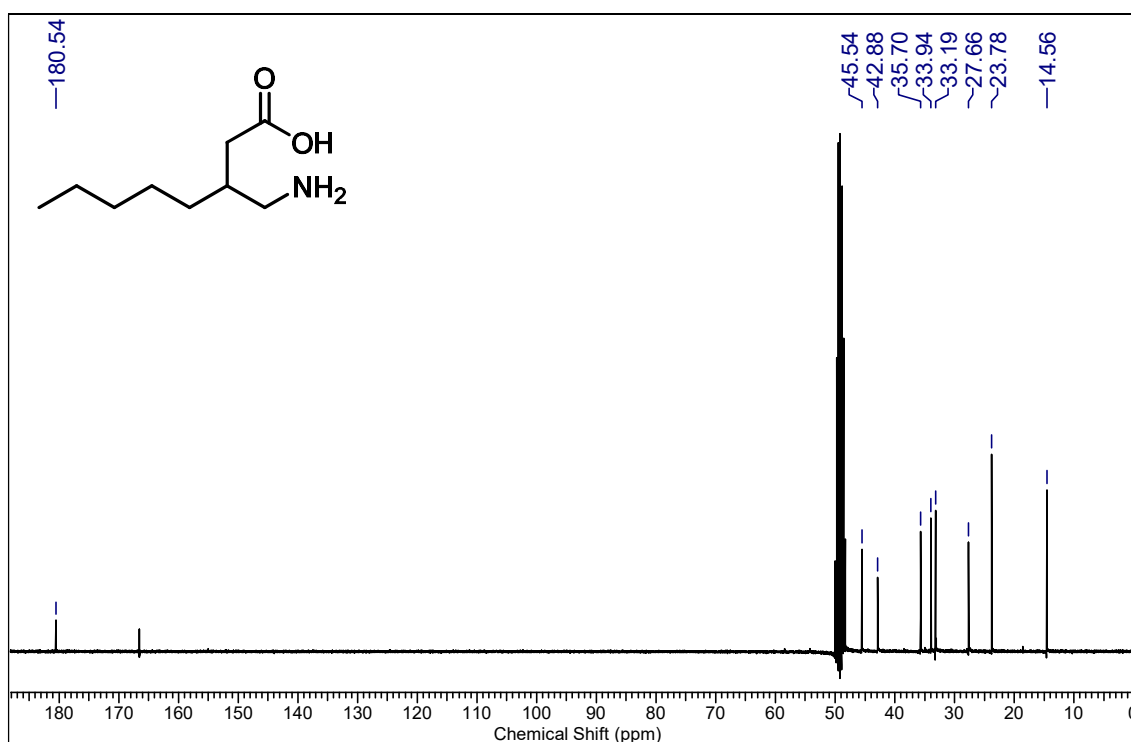


Figure S68. Spectrum of ^{13}C NMR (300 MHz, $\text{MeOH-}d_4$) of γ -amino acid **2b**.

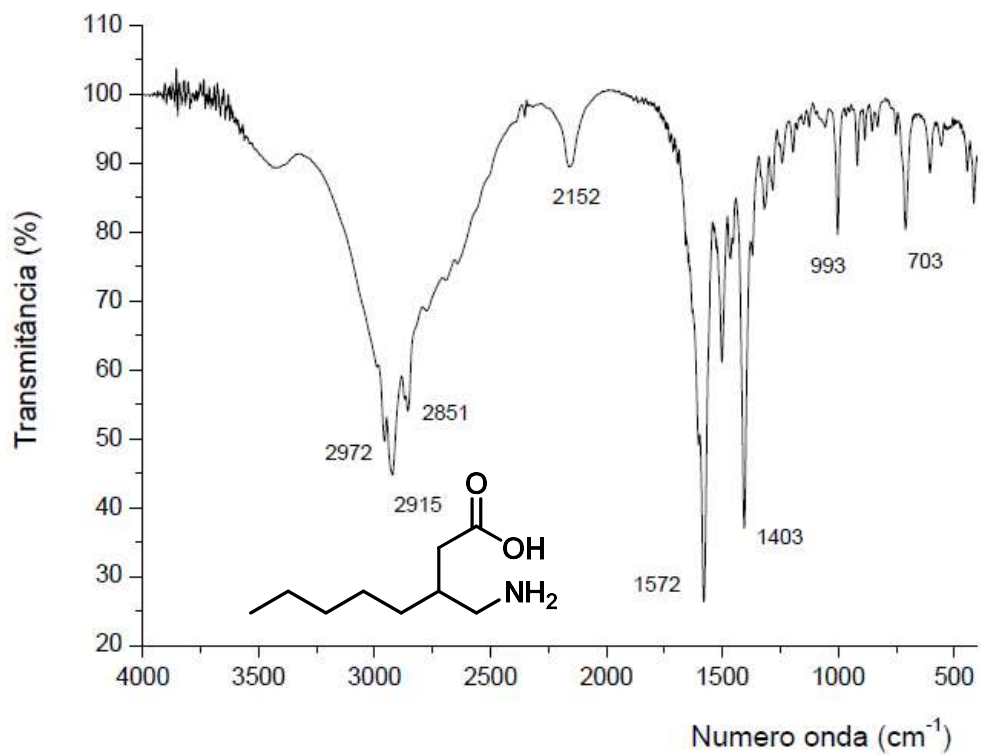


Figure S69. Spectrum of IR (KBr) of γ -nitro acid **2b**.

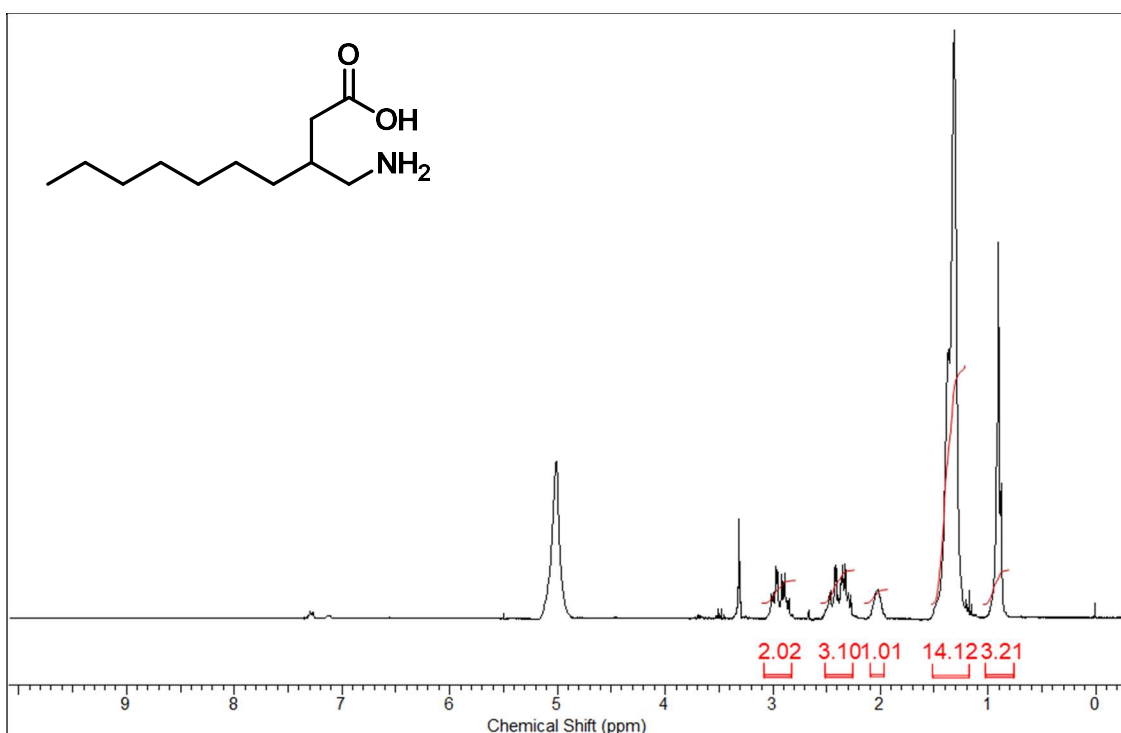


Figure S70. Spectrum of ^1H NMR (300 MHz, $\text{MeOH-}d_4$) of γ -amino acid **2c**.

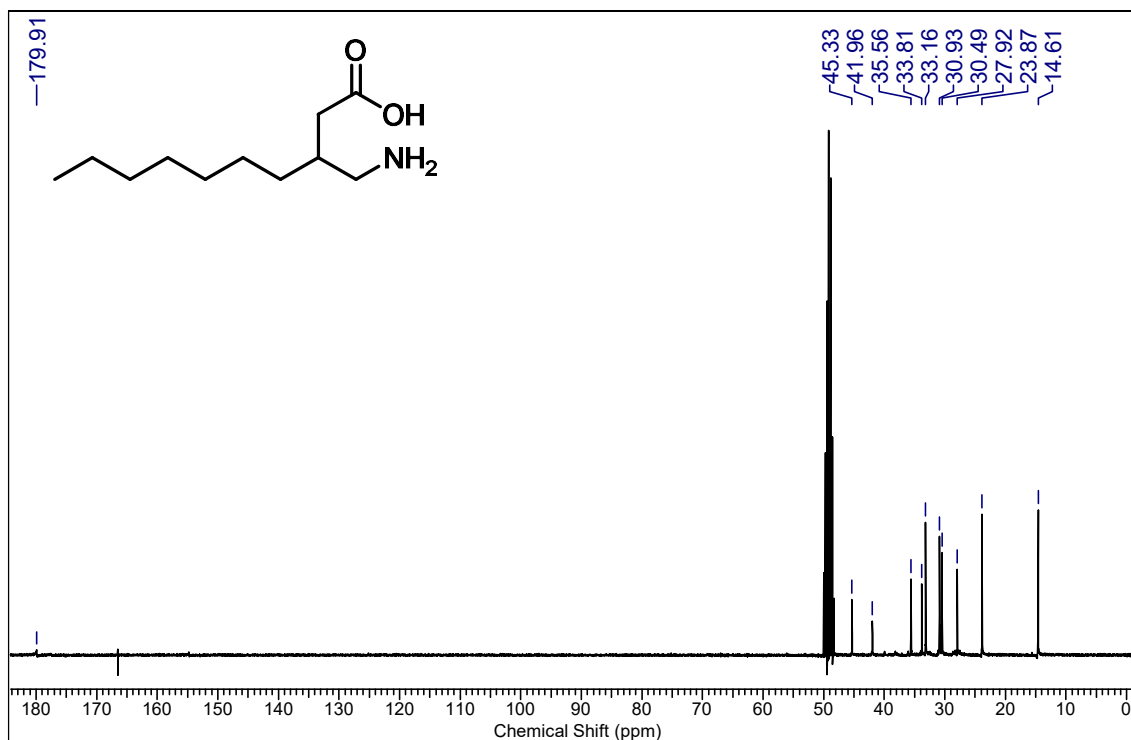


Figure S71. Spectrum of ^{13}C NMR (75 MHz, $\text{MeOH-}d_4$) of γ -amino acid **2c**.

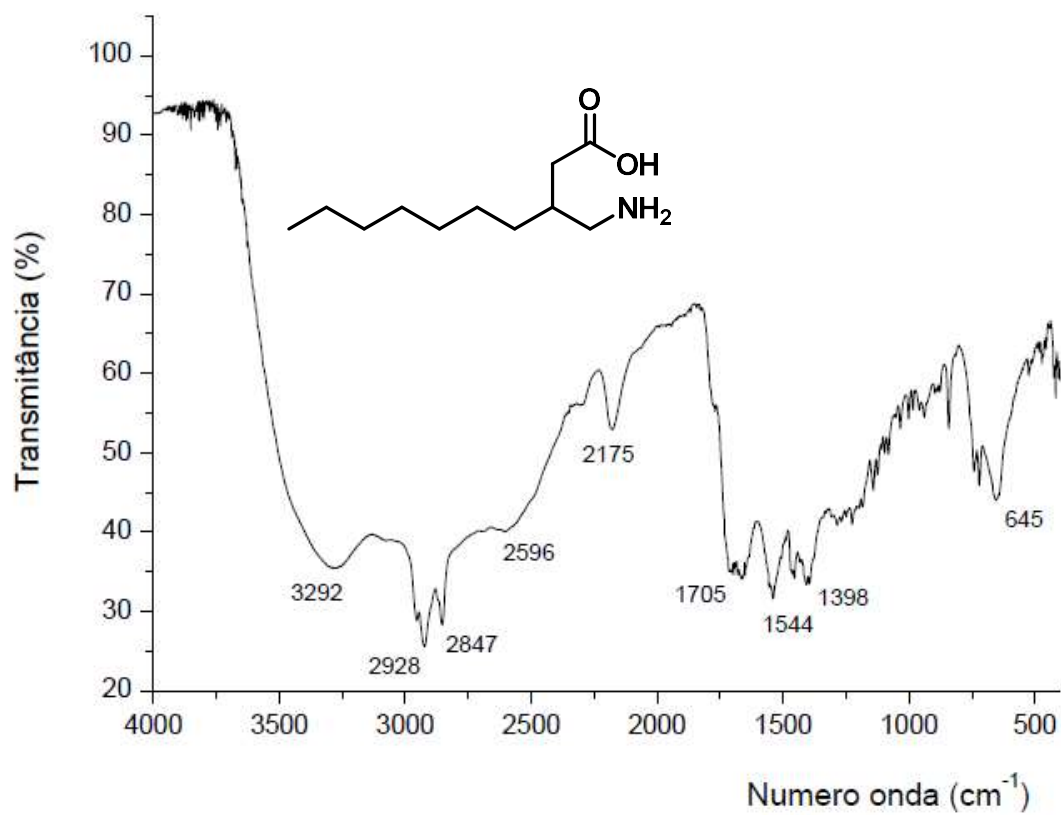


Figure S72. Spectrum of IR (KBr) of γ -nitro acid **2c**.

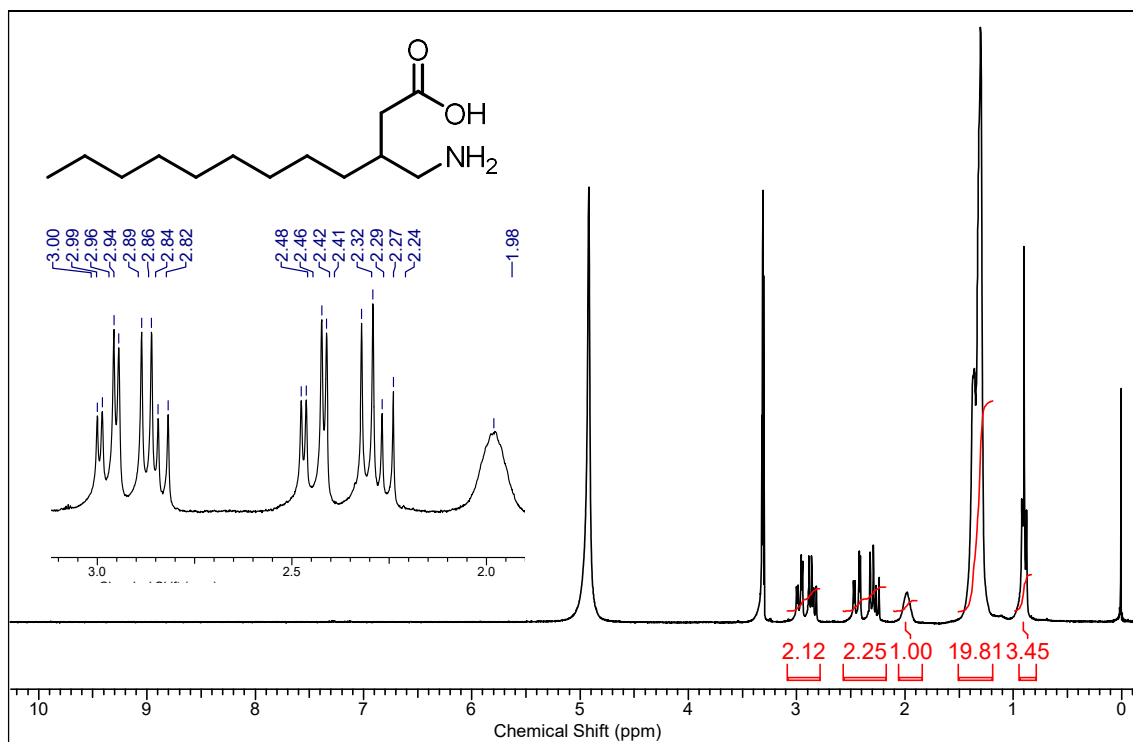


Figure S73. Spectrum of ^1H NMR (300 MHz, MeOH- d_4) of γ -amino acid **2d**.

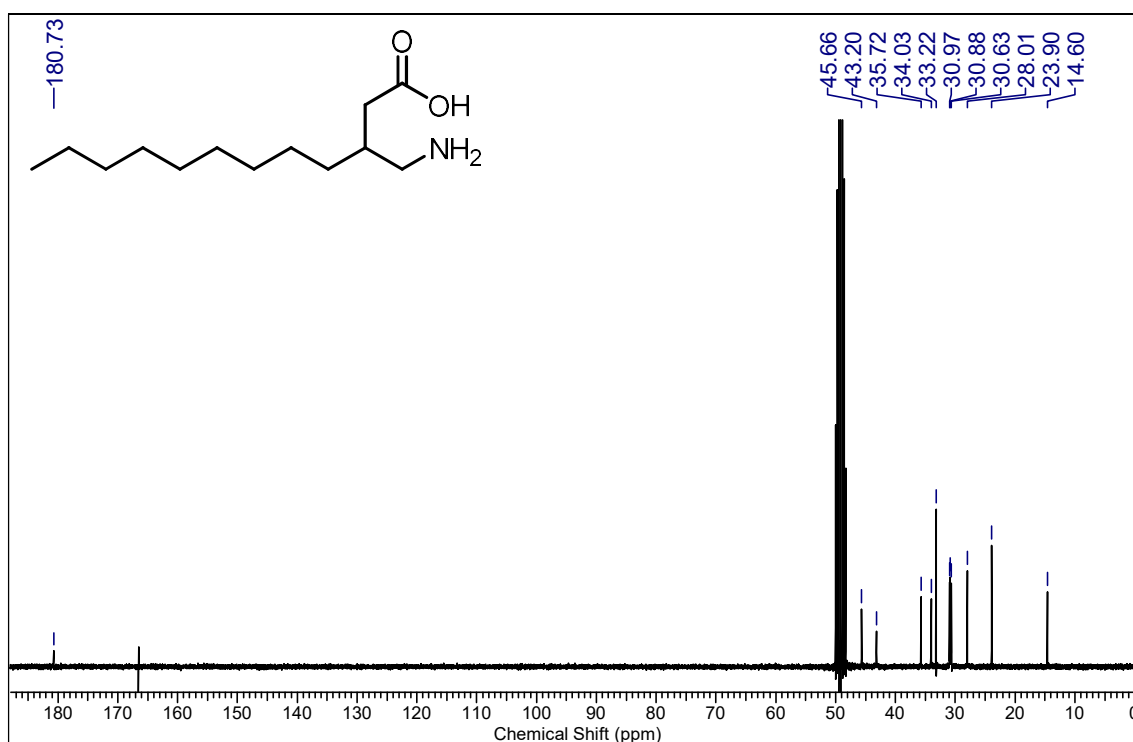


Figure S74. Spectrum of ^{13}C NMR (75 MHz, MeOH- d_4) of γ -amino acid **2d**.

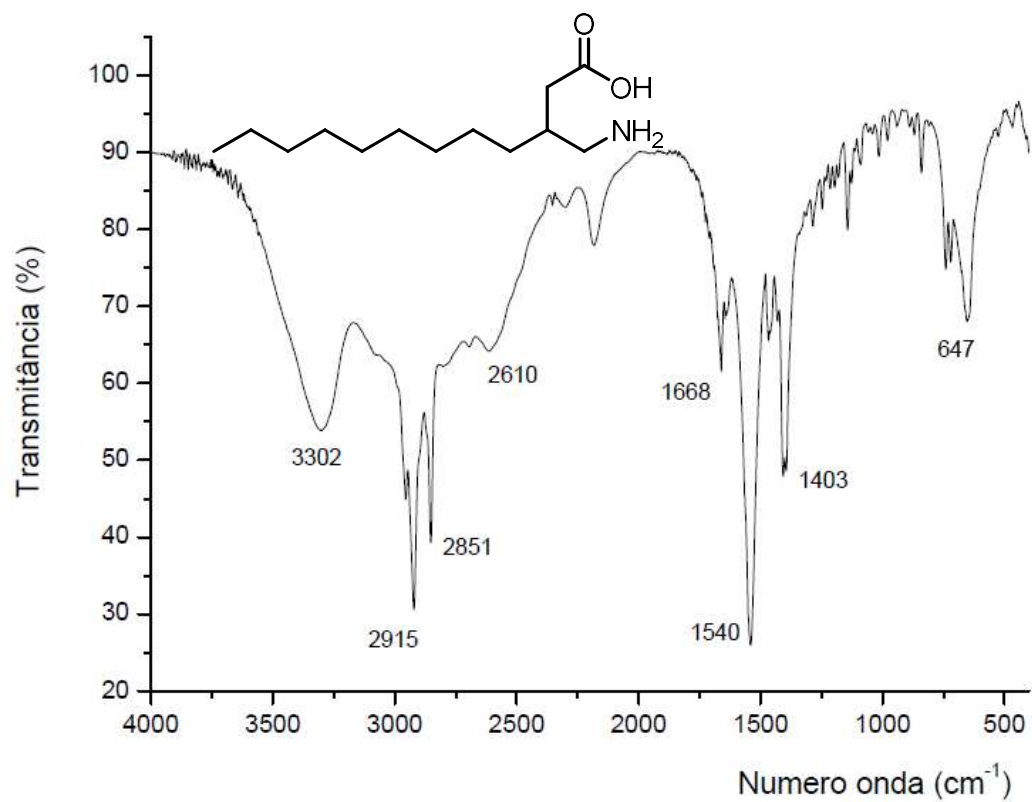


Figure S75. Spectrum of IR (KBr) of γ -nitro acid **2d**.

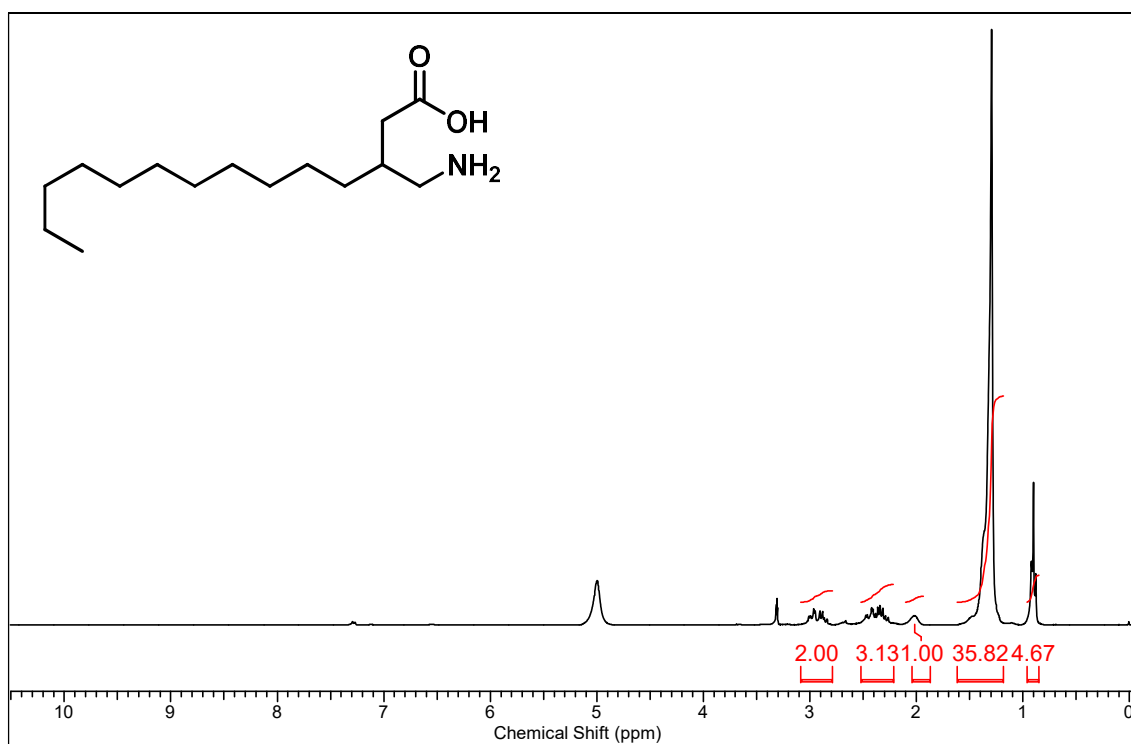


Figure S76. Spectrum of ^1H NMR (300 MHz, $\text{MeOH-}d_4$) of γ -amino acid **2e**.

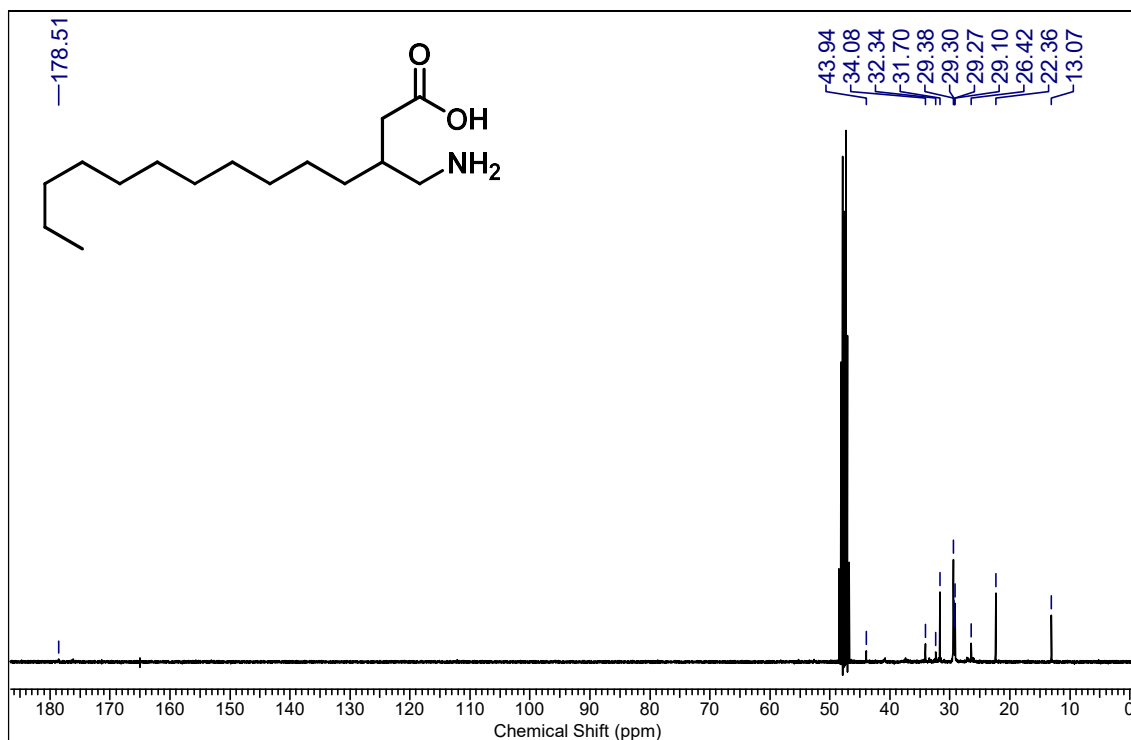


Figure S77. Spectrum of ^{13}C NMR (75 MHz, $\text{MeOH-}d_4$) of γ -amino acid **2e**.

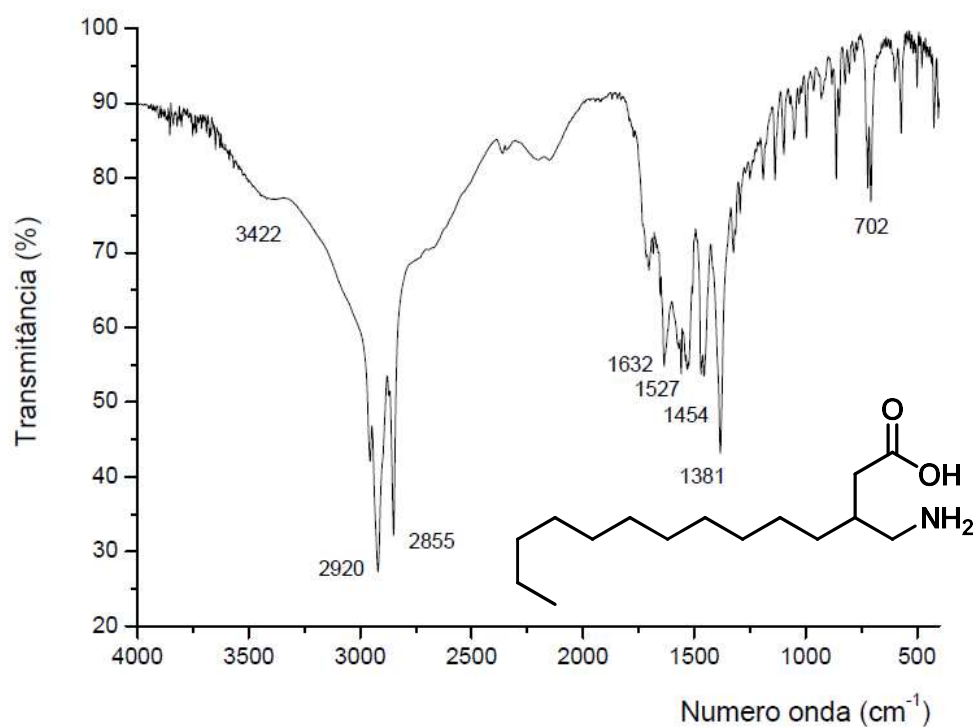


Figure S78. Spectrum of IR (KBr) of γ -nitro acid **2e**.

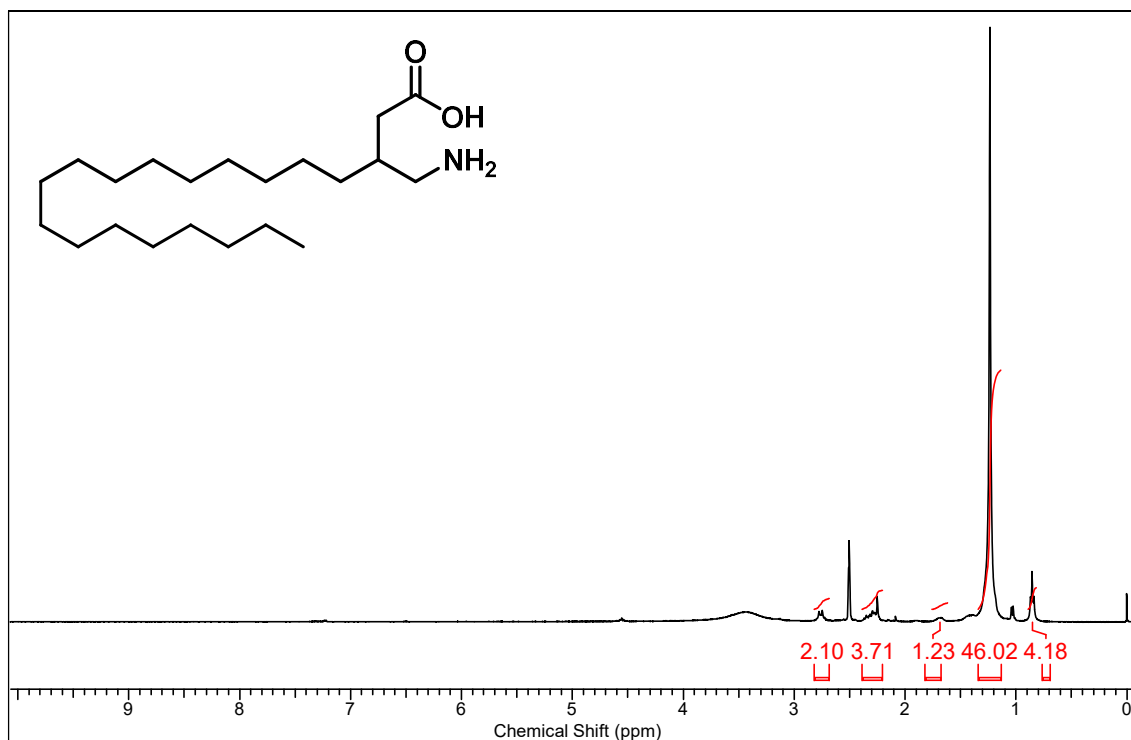


Figure S79. Spectrum of ^1H NMR (300 MHz, $\text{DMSO-}d_6$) of γ -amino acid **2g**.

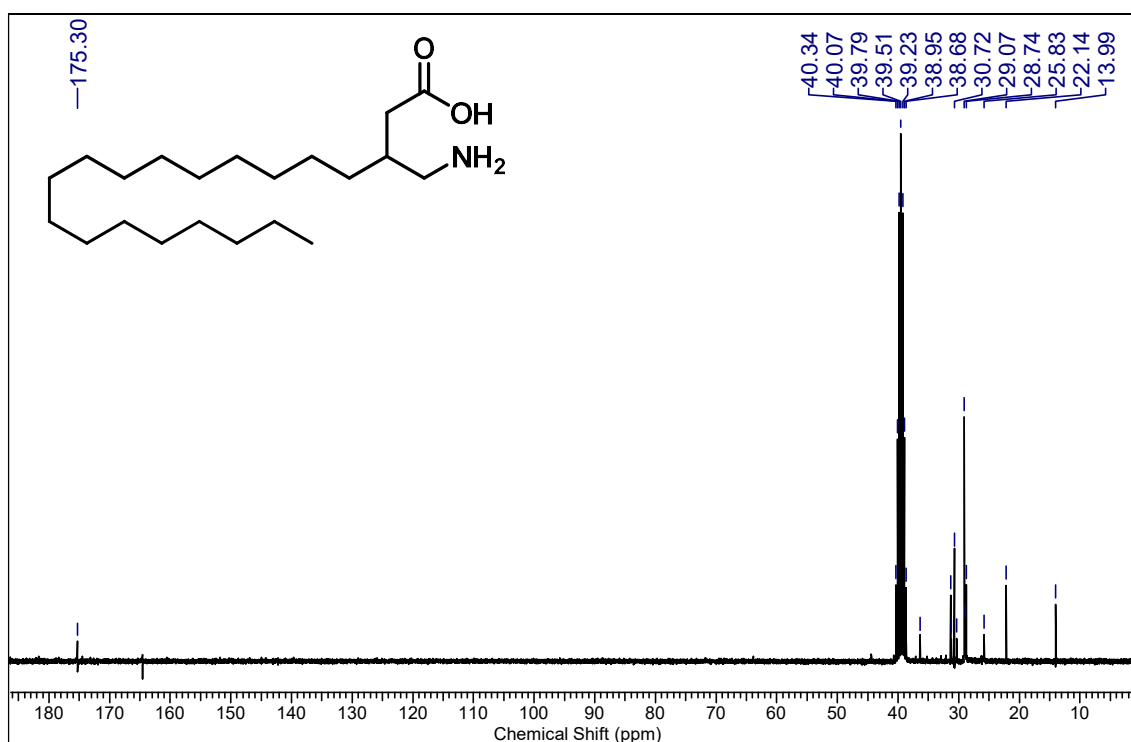


Figure S80. Spectrum of ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of γ -amino acid **2g**.