

**An efficient cyclization of Lapachol to new benzo[h]chromene hybrid
compounds: Stepwise vs one-pot esterification-click (CuAAC) study**

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Selected figures and spectra

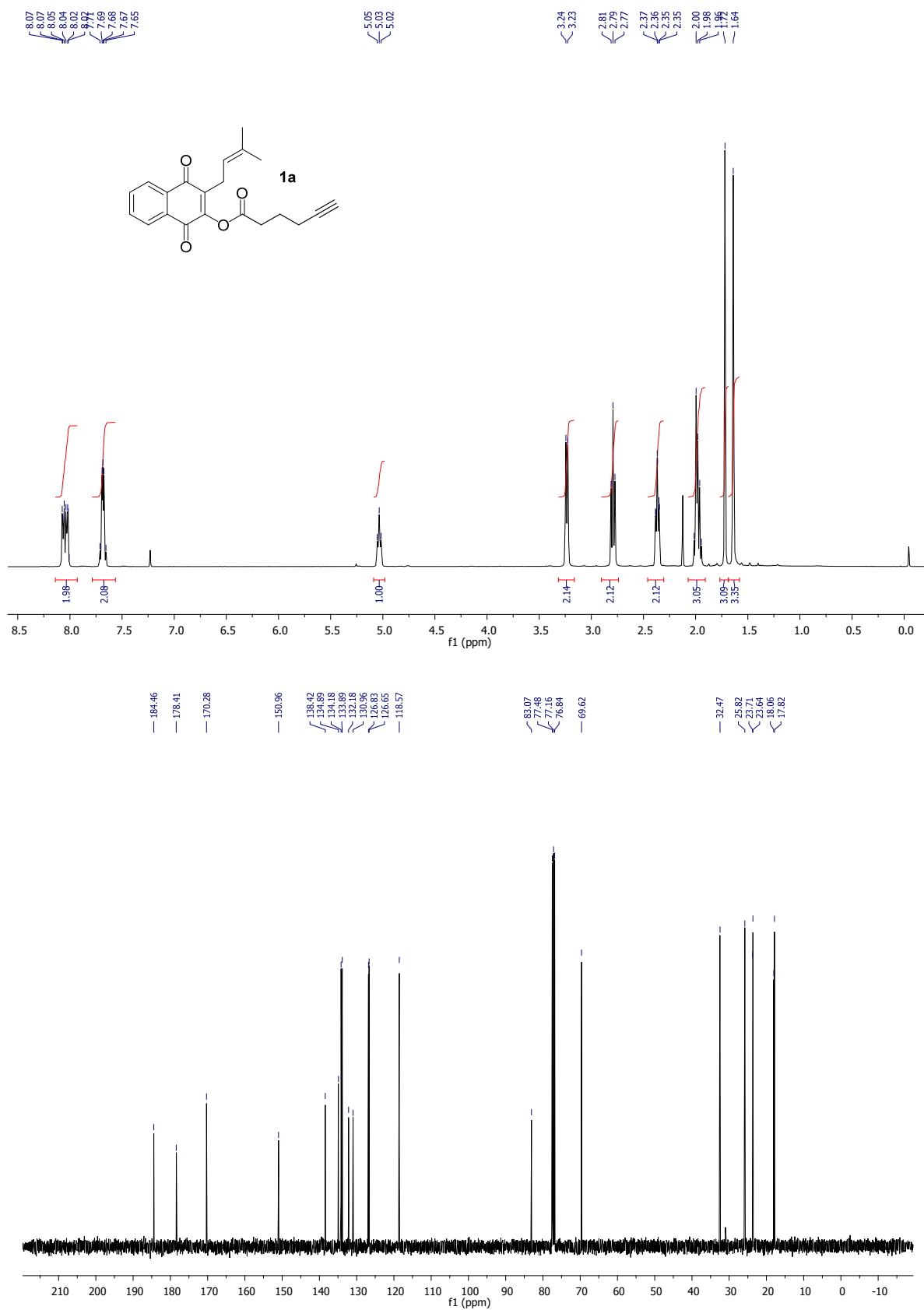


Figure 1. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **1a**.

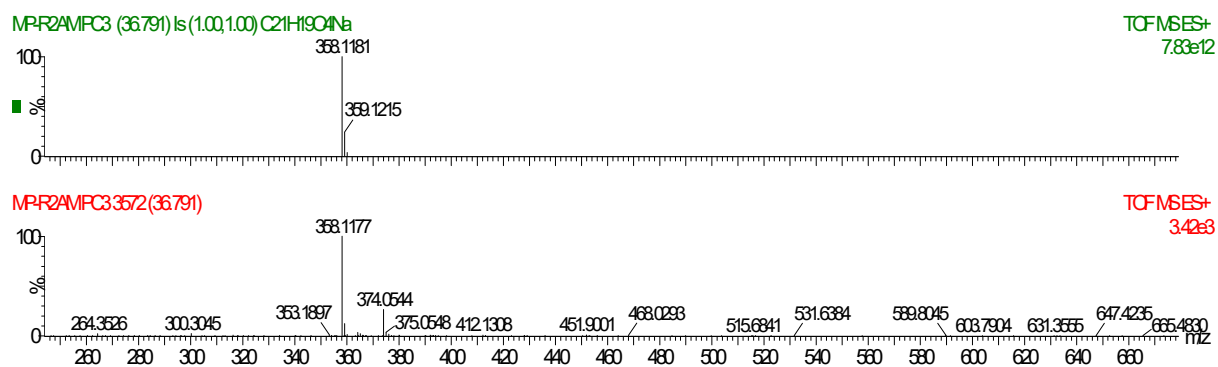


Figure 2. HREIMS spectrum of compound **1a**.

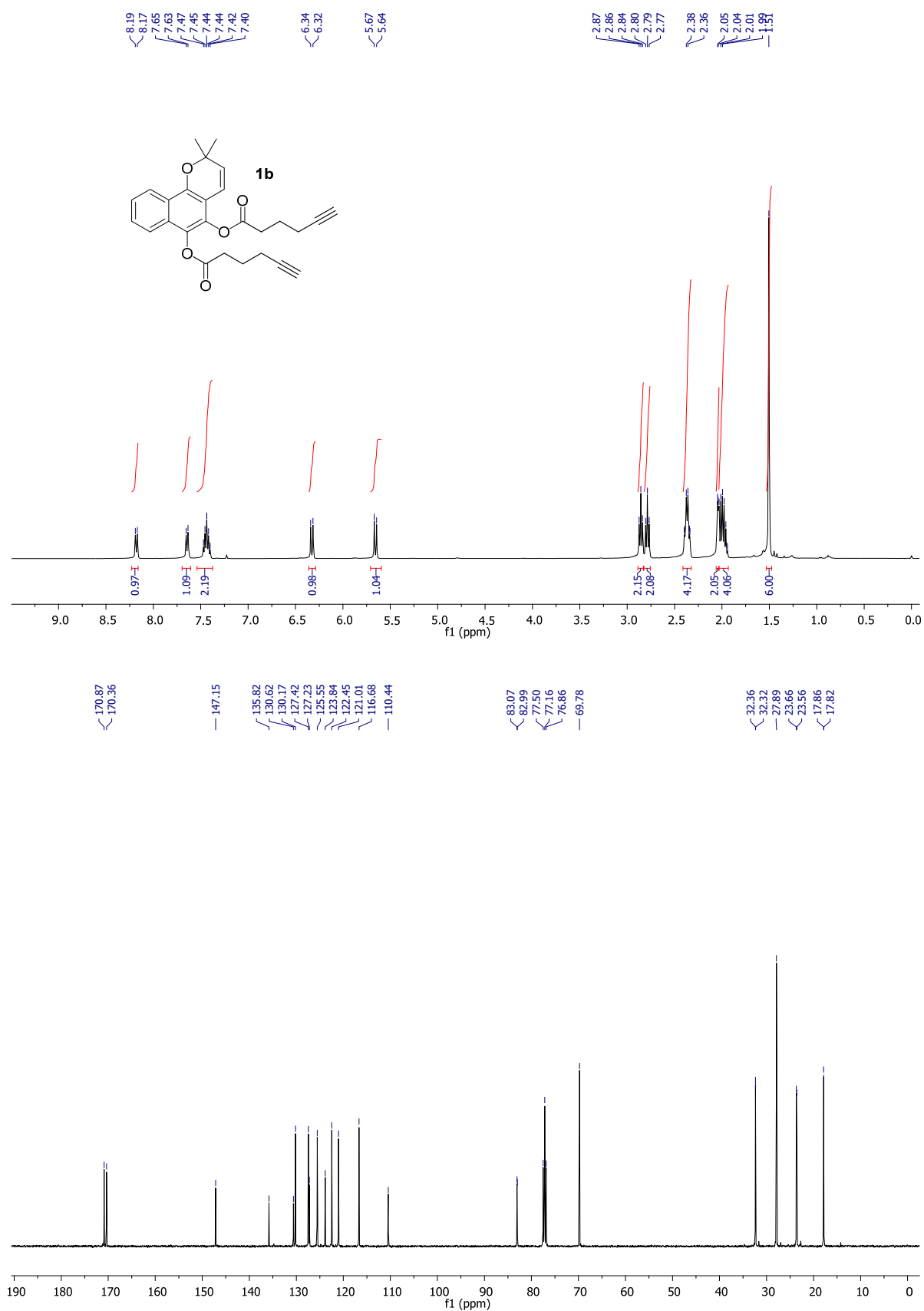


Figure 3. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **1b**.

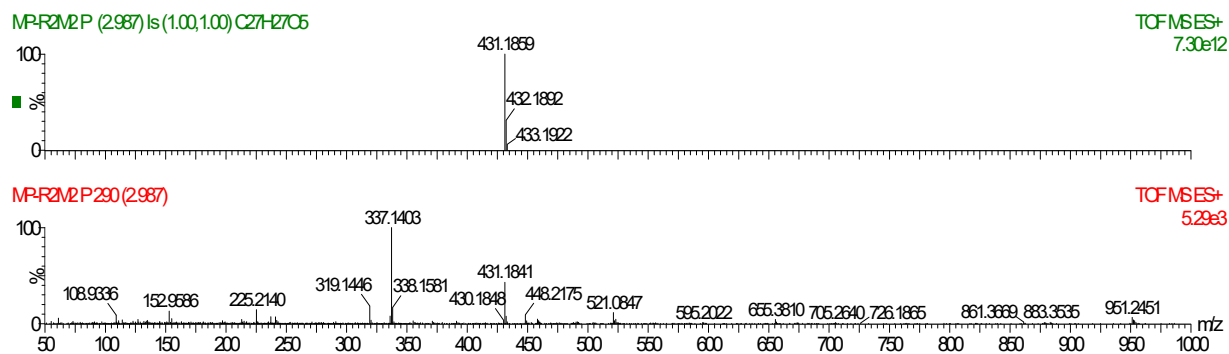


Figure 4. HREIMS spectrum of compound **1b**.

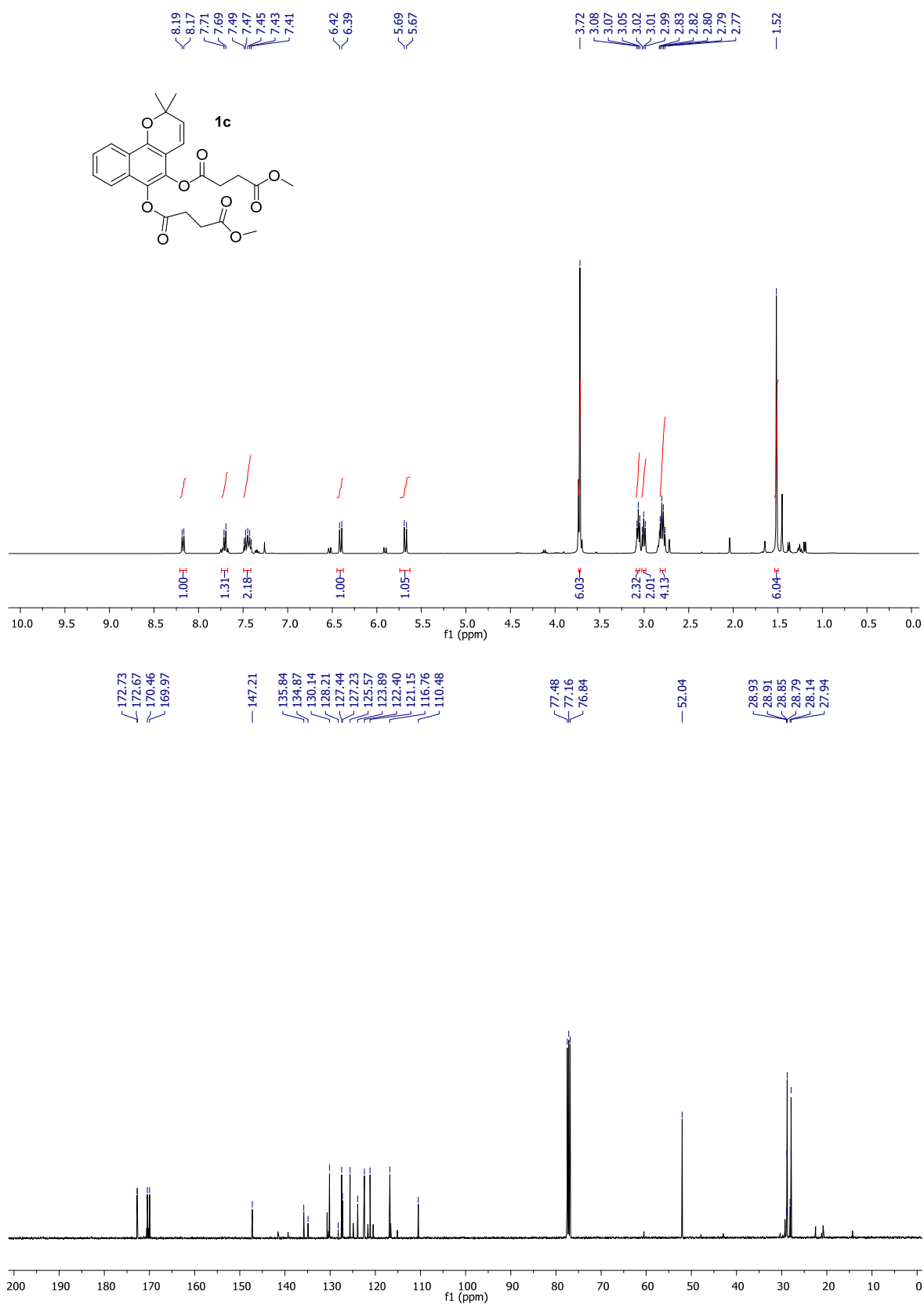


Figure 5. ^1H and ^{13}C NMR spectra in CDCl₃ of compound **1c**.

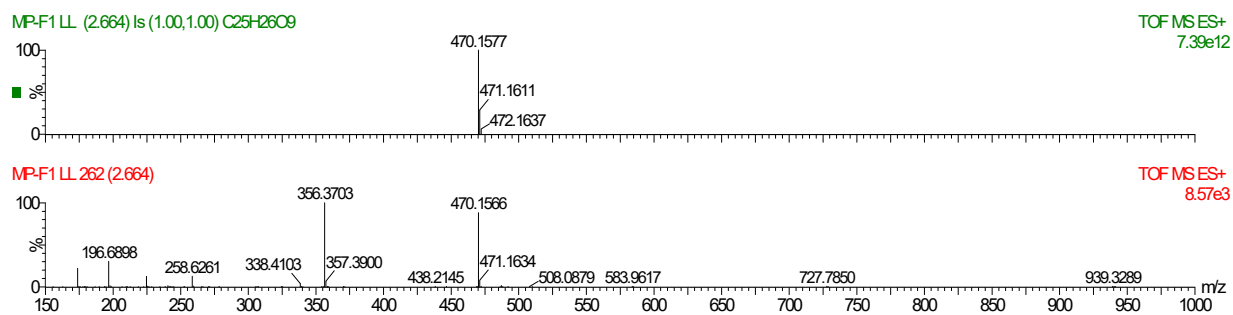


Figure 6. HREIMS spectrum of compound **1c**.

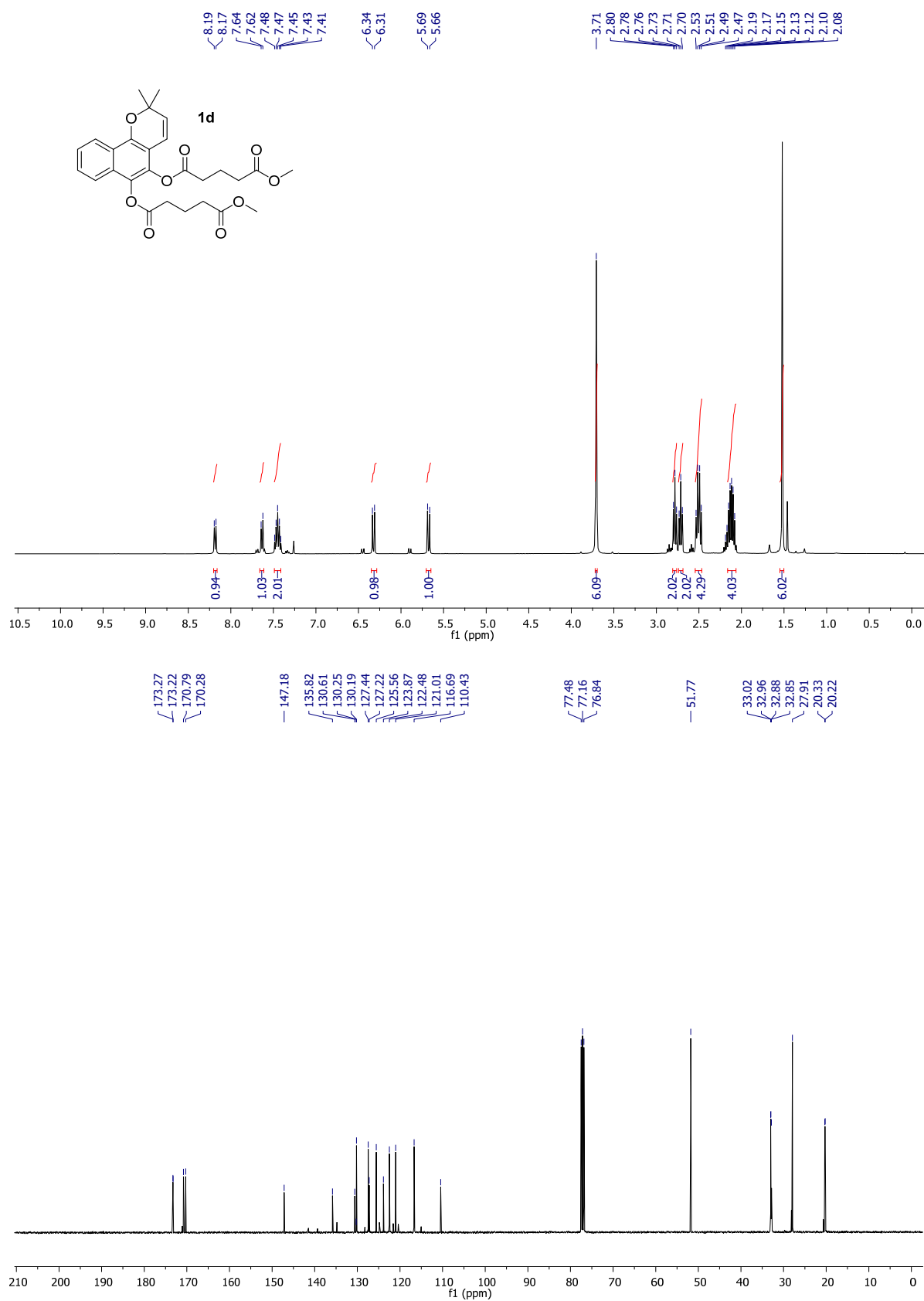


Figure 7. ¹H and ¹³C NMR spectra in CDCl₃ of compound **1d**.

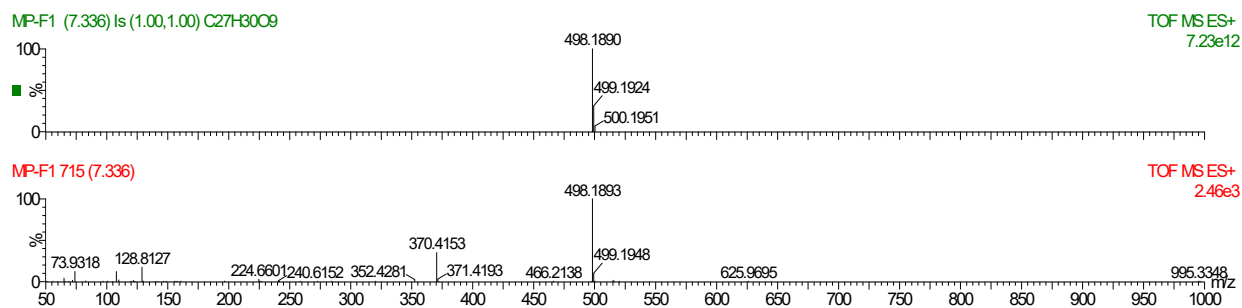


Figure 8. HREIMS spectrum of compound **1d**.

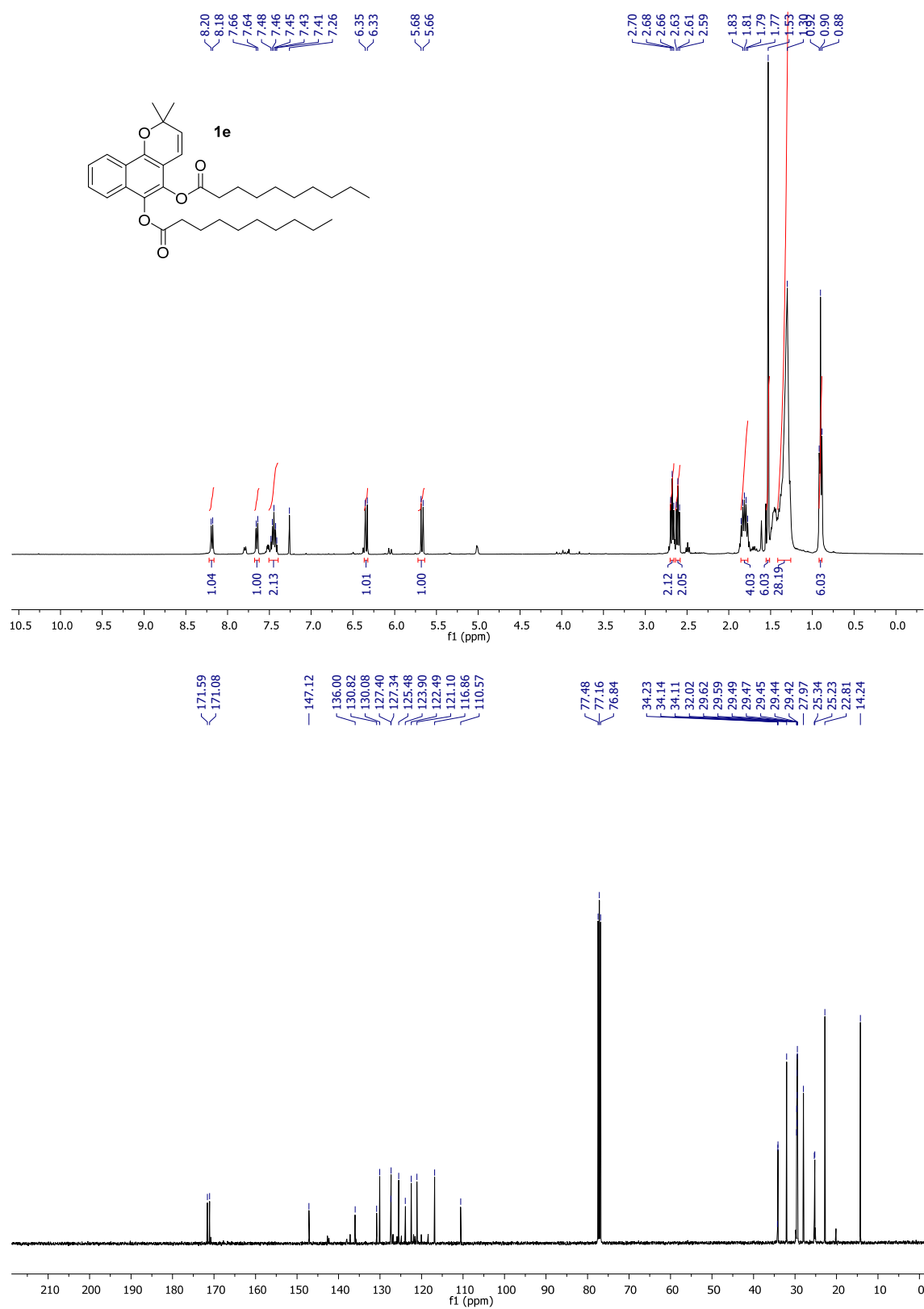


Figure 9. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **1e**.

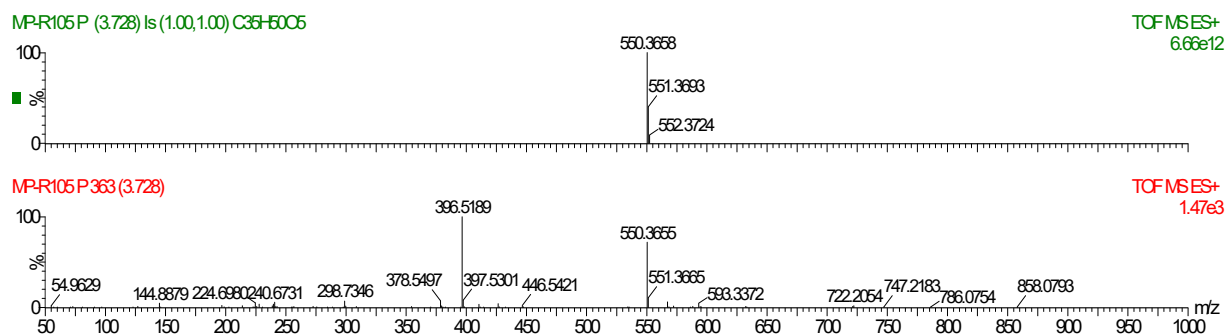


Figure 10. HREIMS spectrum of compound **1e**.

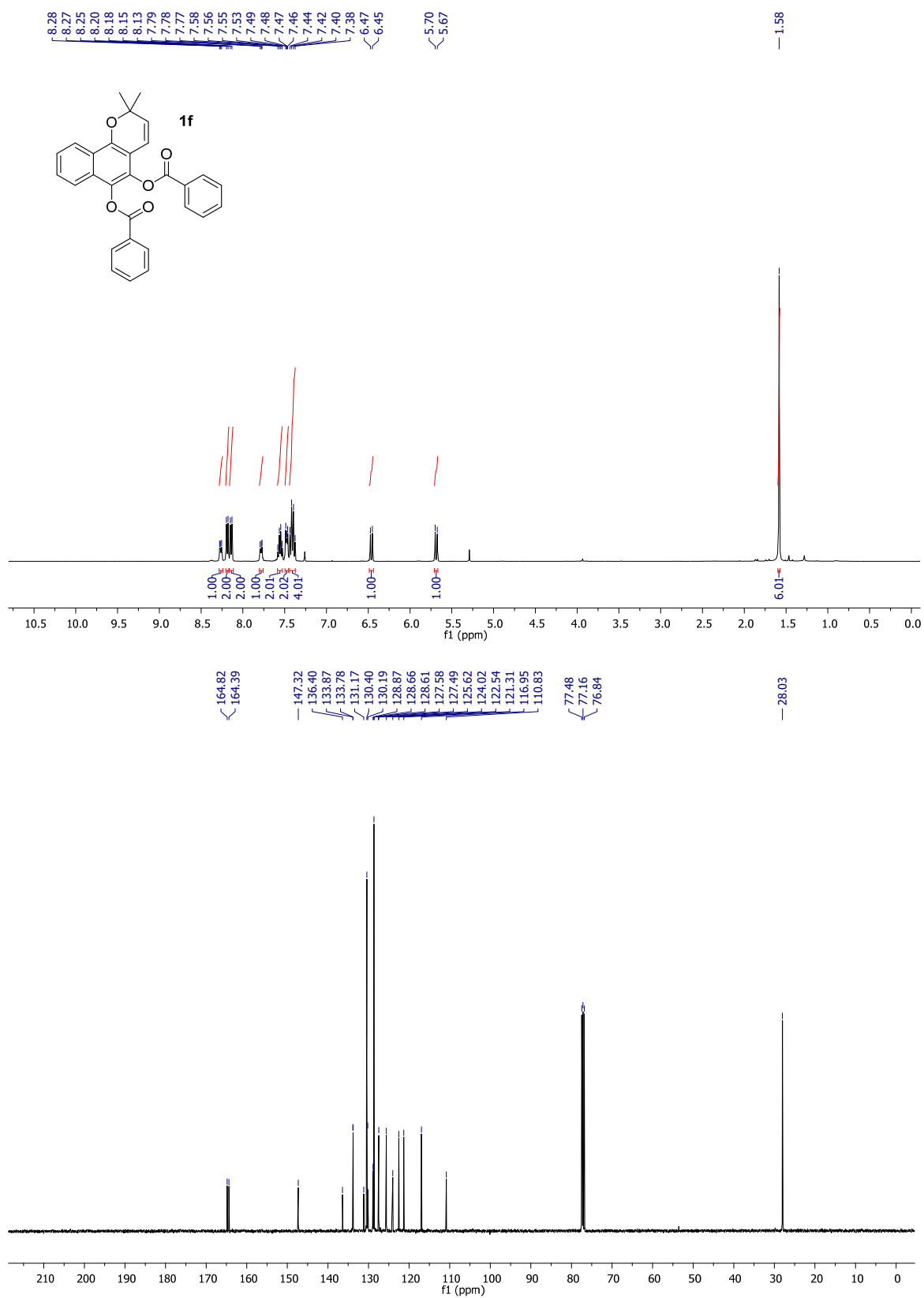


Figure 11. ^1H and ^{13}C NMR spectra in CDCl₃ of compound **1f**.

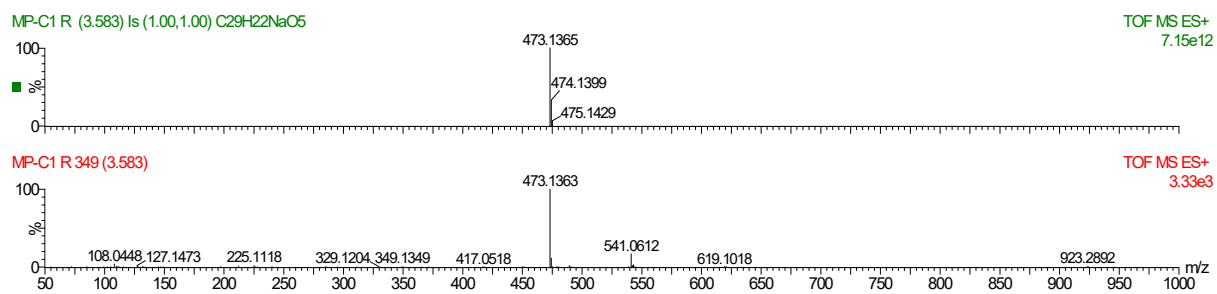


Figure 12. HREIMS spectrum of compound **1f**.

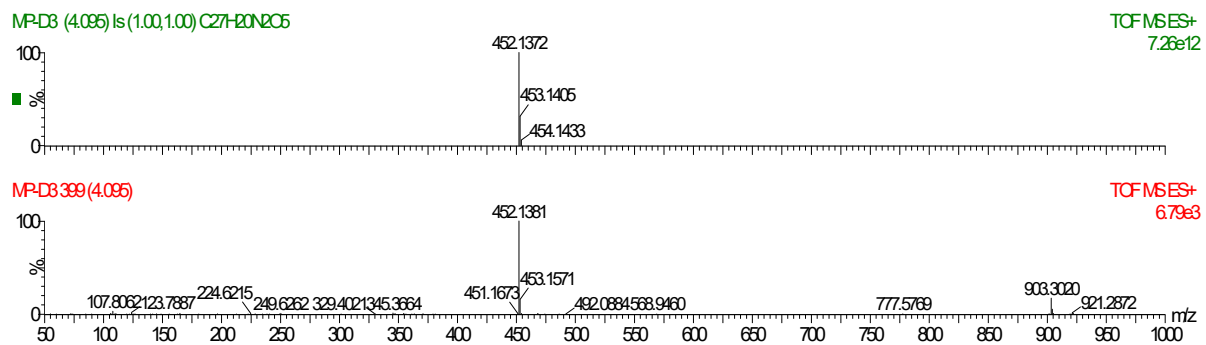


Figure 14. HREIMS spectrum of compound **1g**.

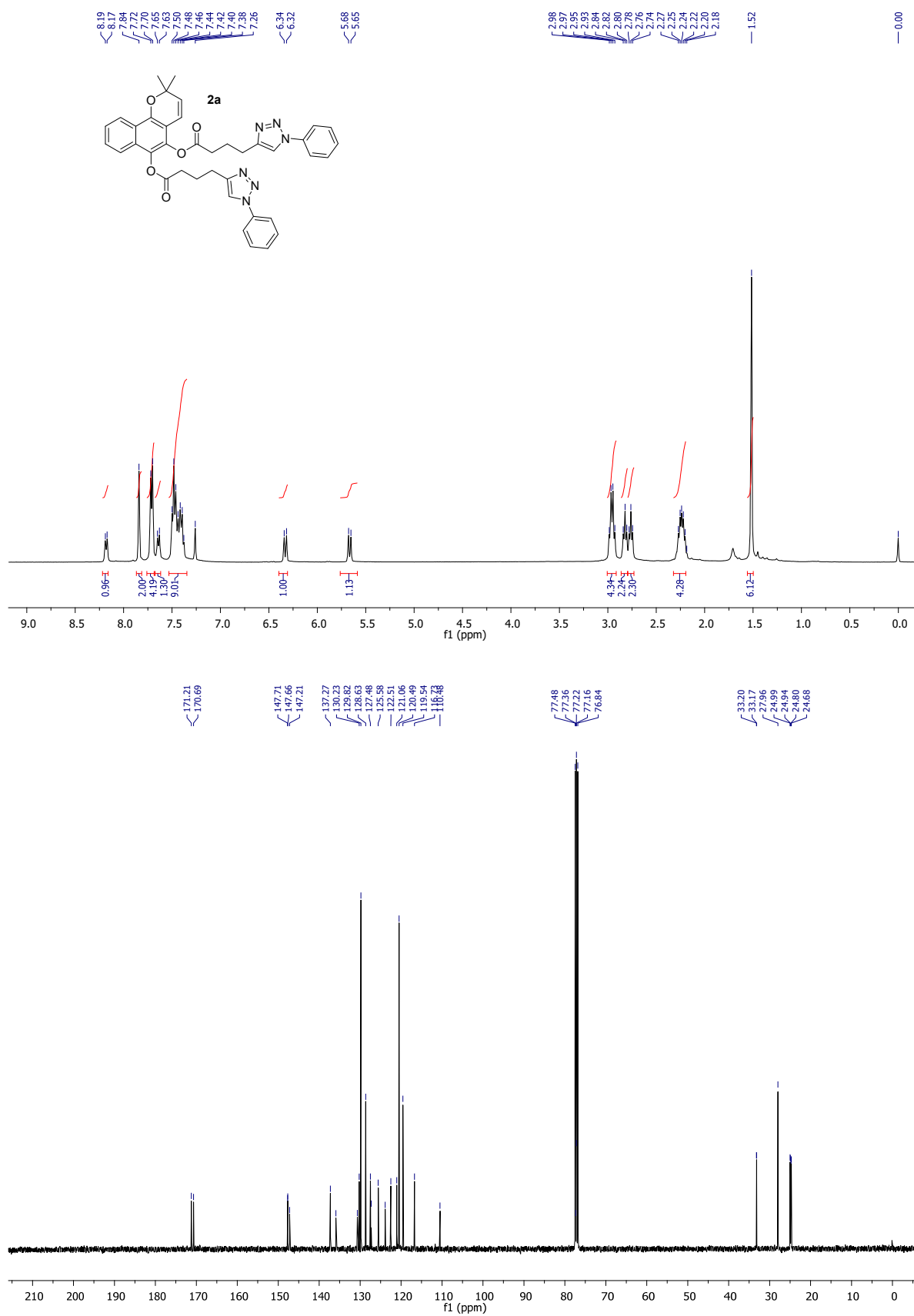


Figure 15. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **2a**.

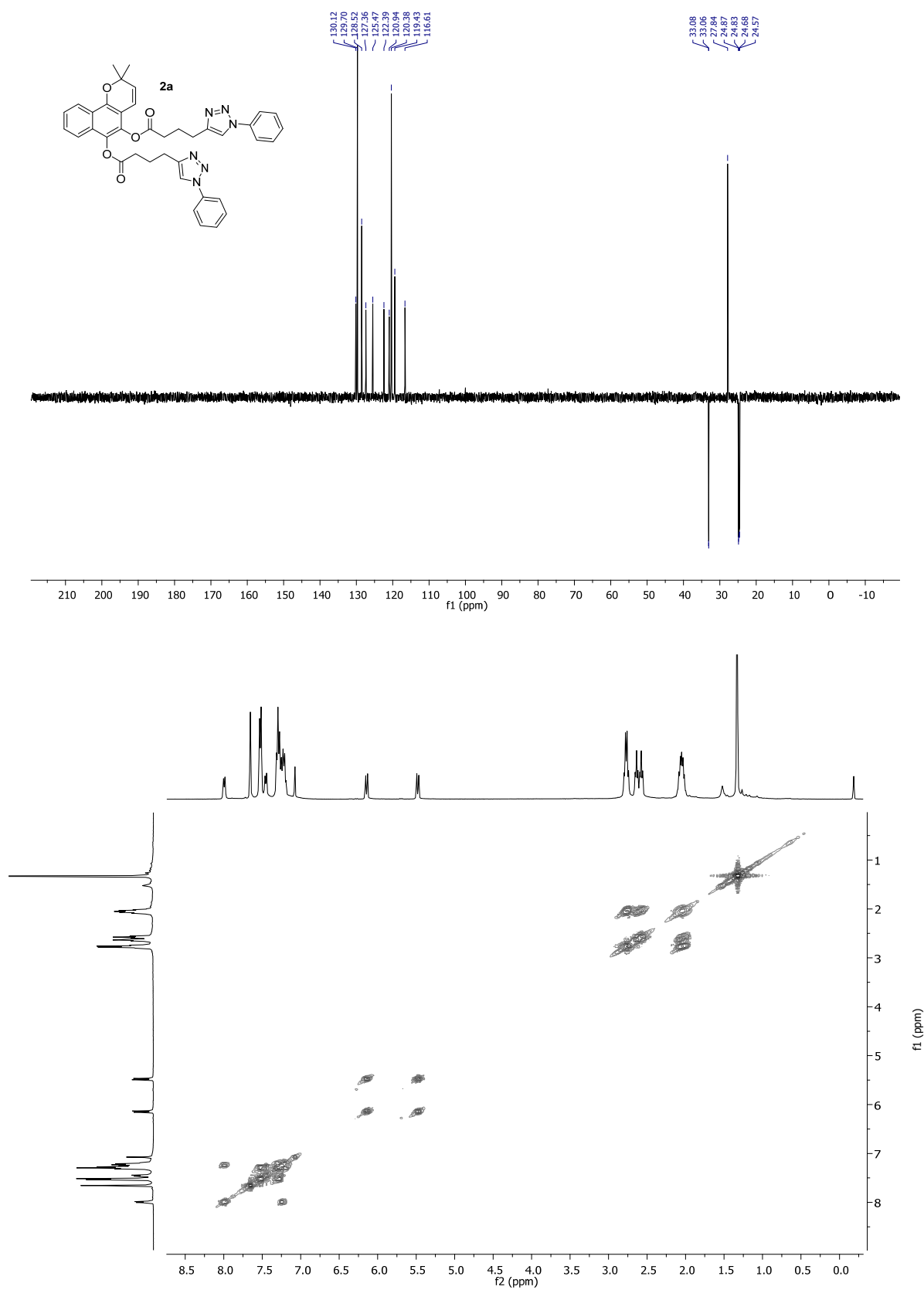


Figure 16. DEPT 135° and COSY spectra in CDCl₃ of compound **2a**.

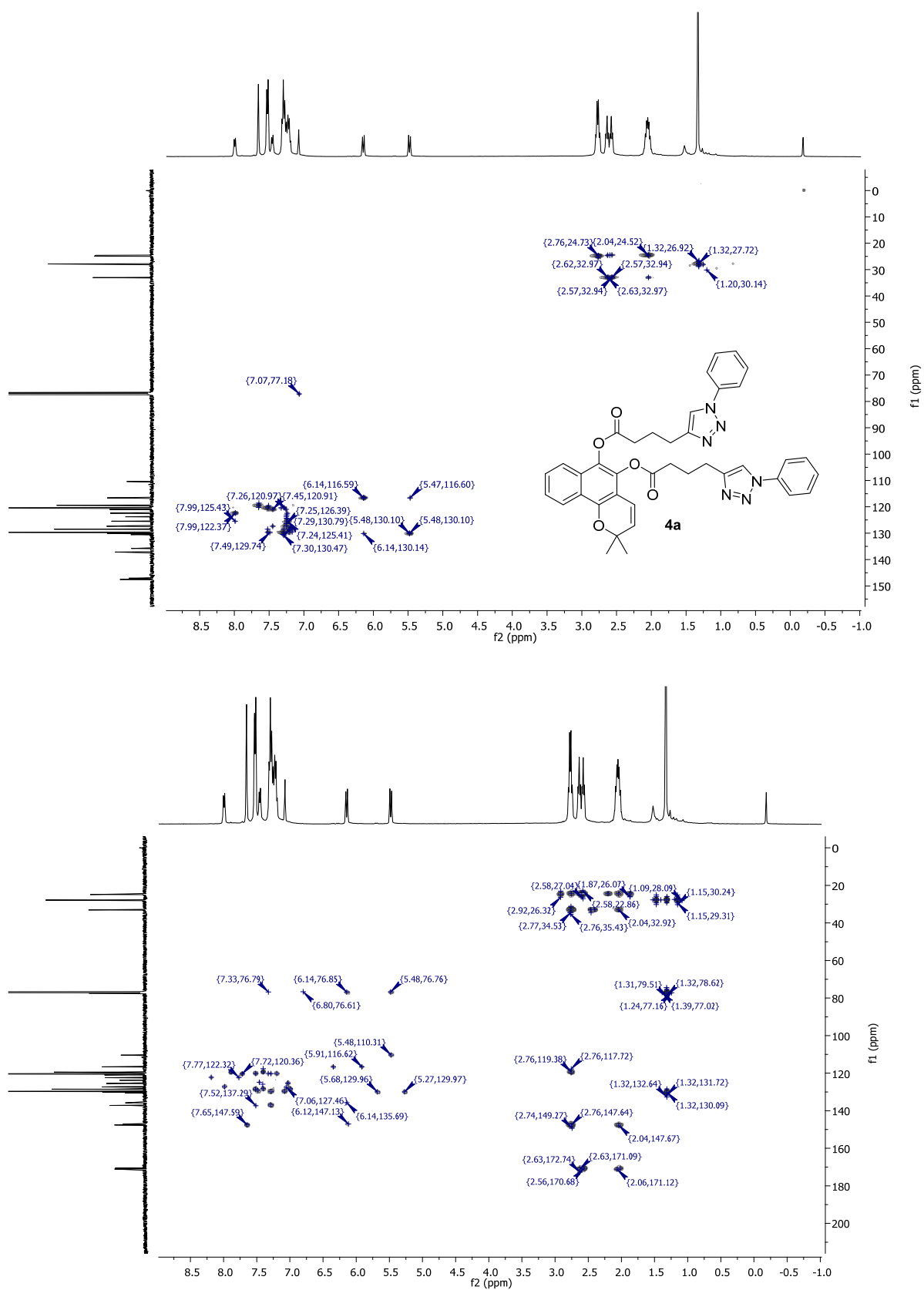


Figure 17. HSQC and HMBC spectra in CDCl_3 of compound **2a**.

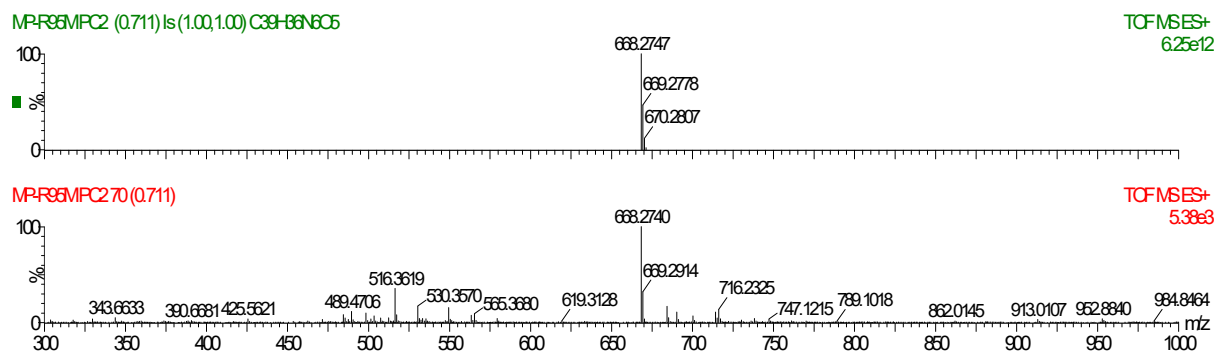


Figure 18. HREIMS spectrum of compound **2a**.

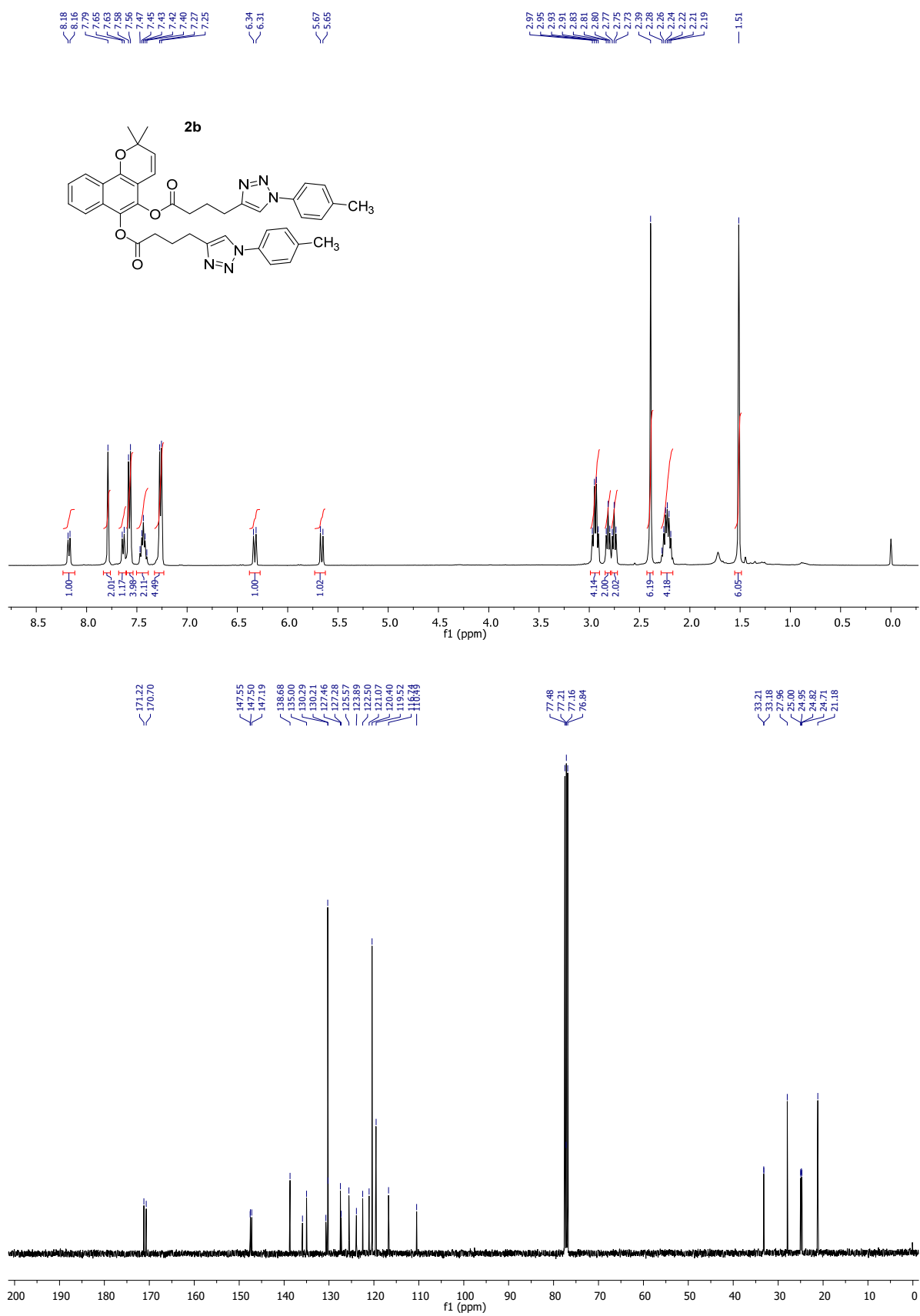


Figure 19. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **2b**.

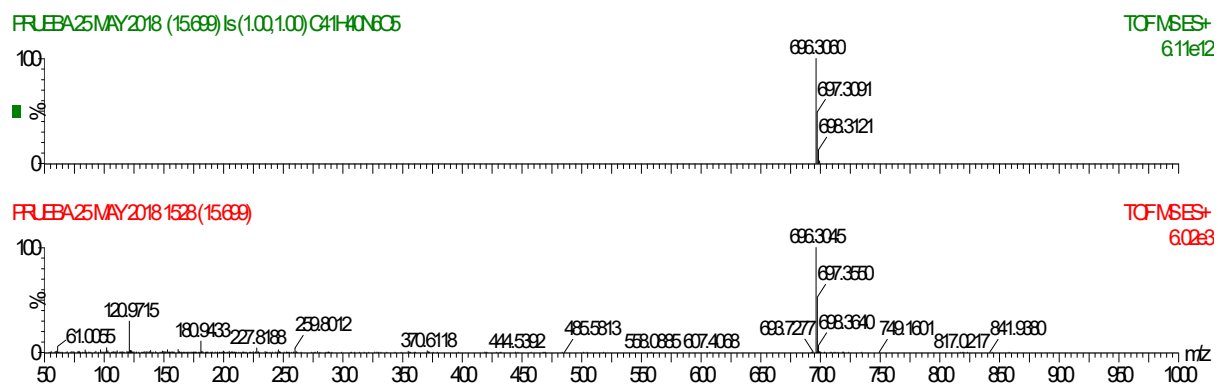


Figure 20. HREIMS spectrum of compound **2b**.

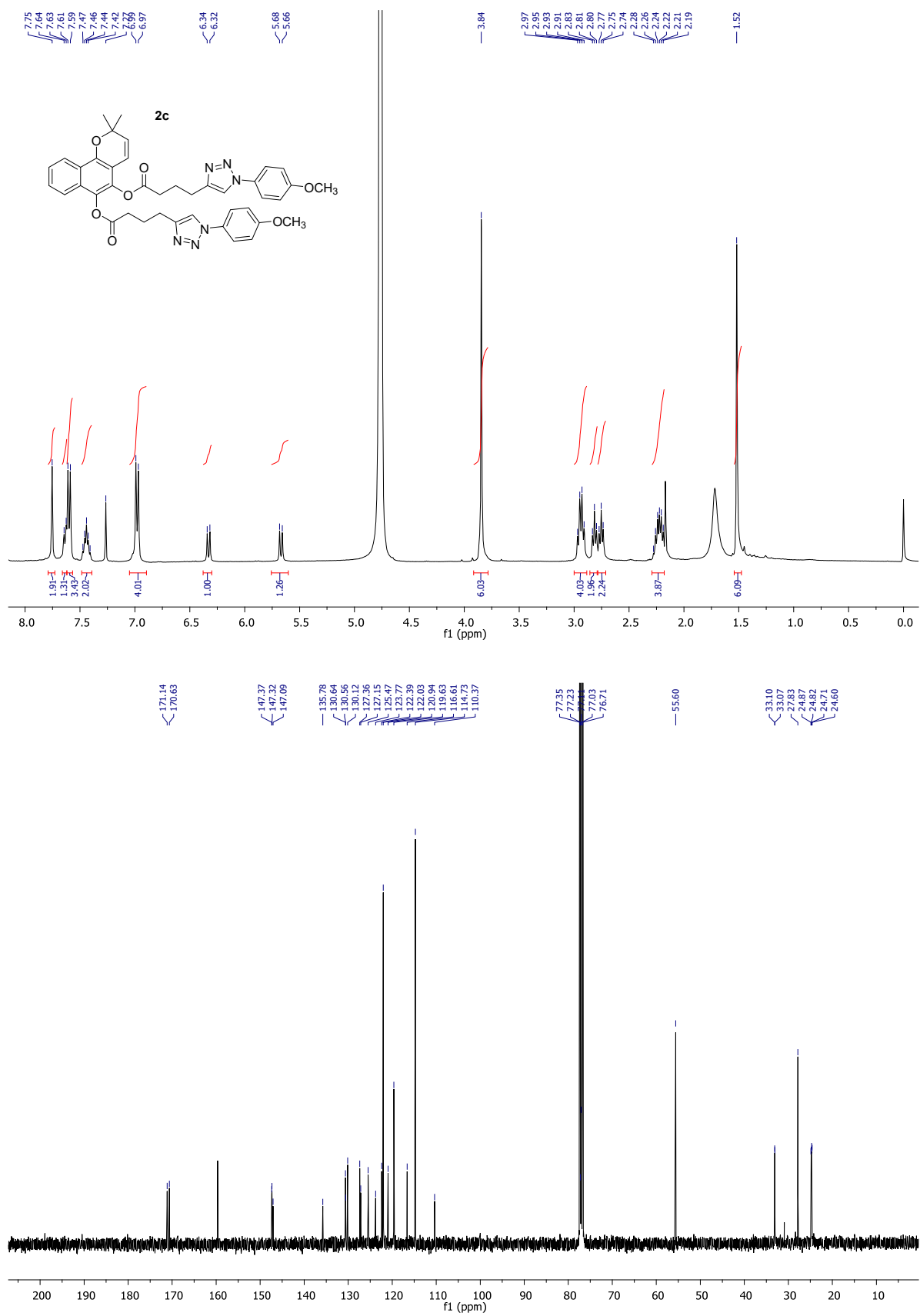
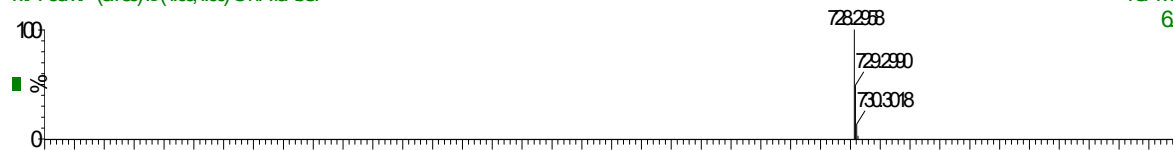


Figure 21. ¹H and ¹³C NMR spectra in CDCl₃ of compound **2c**.

MPRAMP (578) $\text{Is}(1.00,1.00) \text{C}_{41}\text{H}_{40}\text{N}_6\text{O}_7$

TOFMS ES+
6.08e12



MPRAMP 552 (5.78)

TOFMS ES+
6.19e12

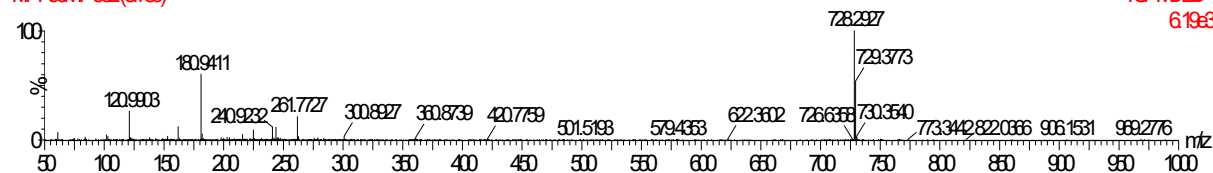


Figure 22. HREIMS spectrum of compound 2c.

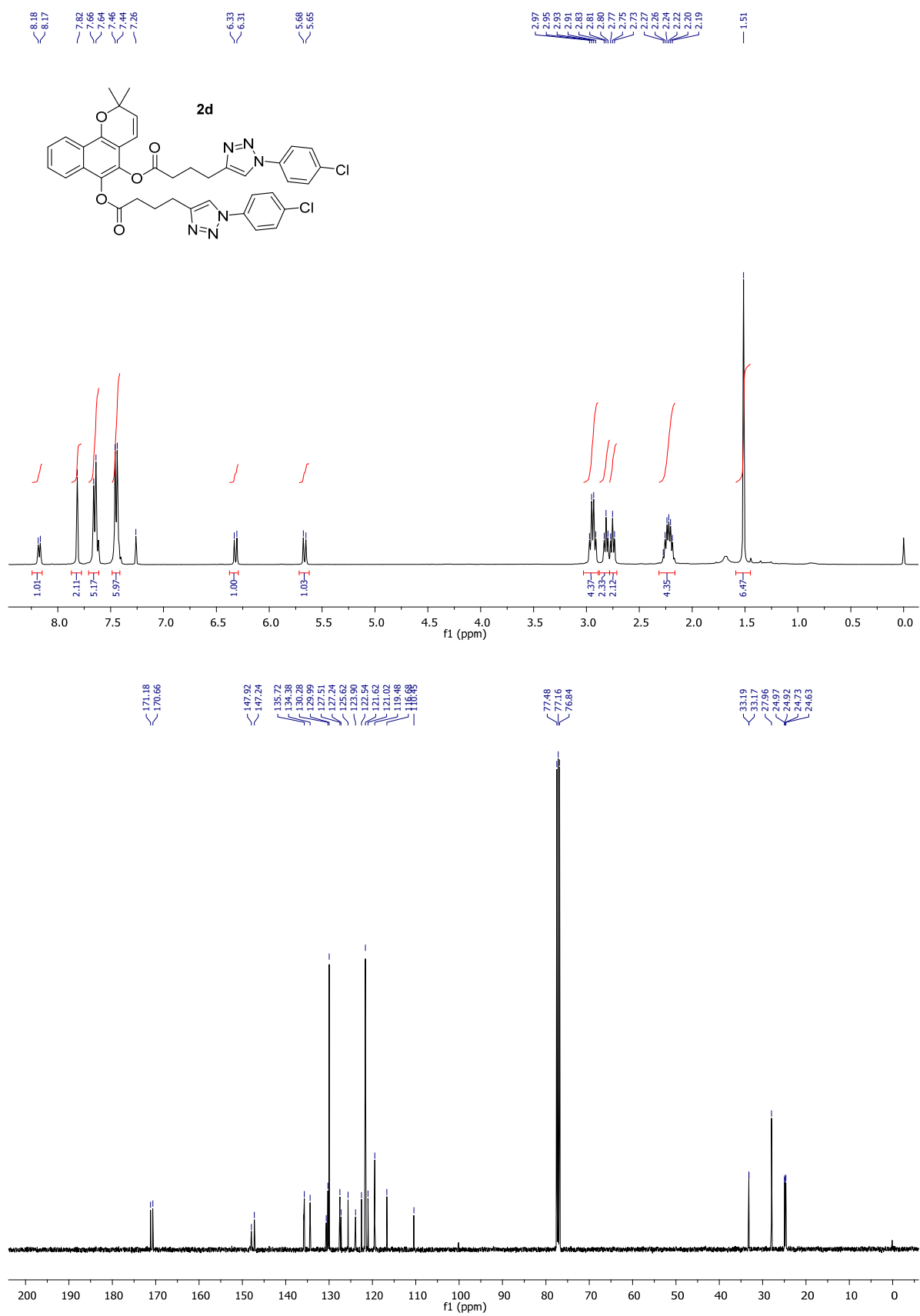


Figure 23. ¹H and ¹³C NMR spectra in CDCl₃ of compound **2d**.

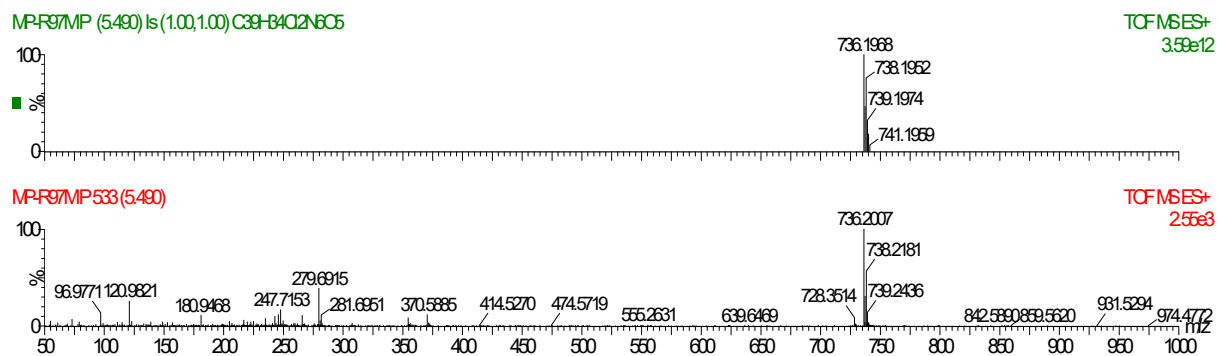


Figure 24. HREIMS spectrum of compound **2d**.

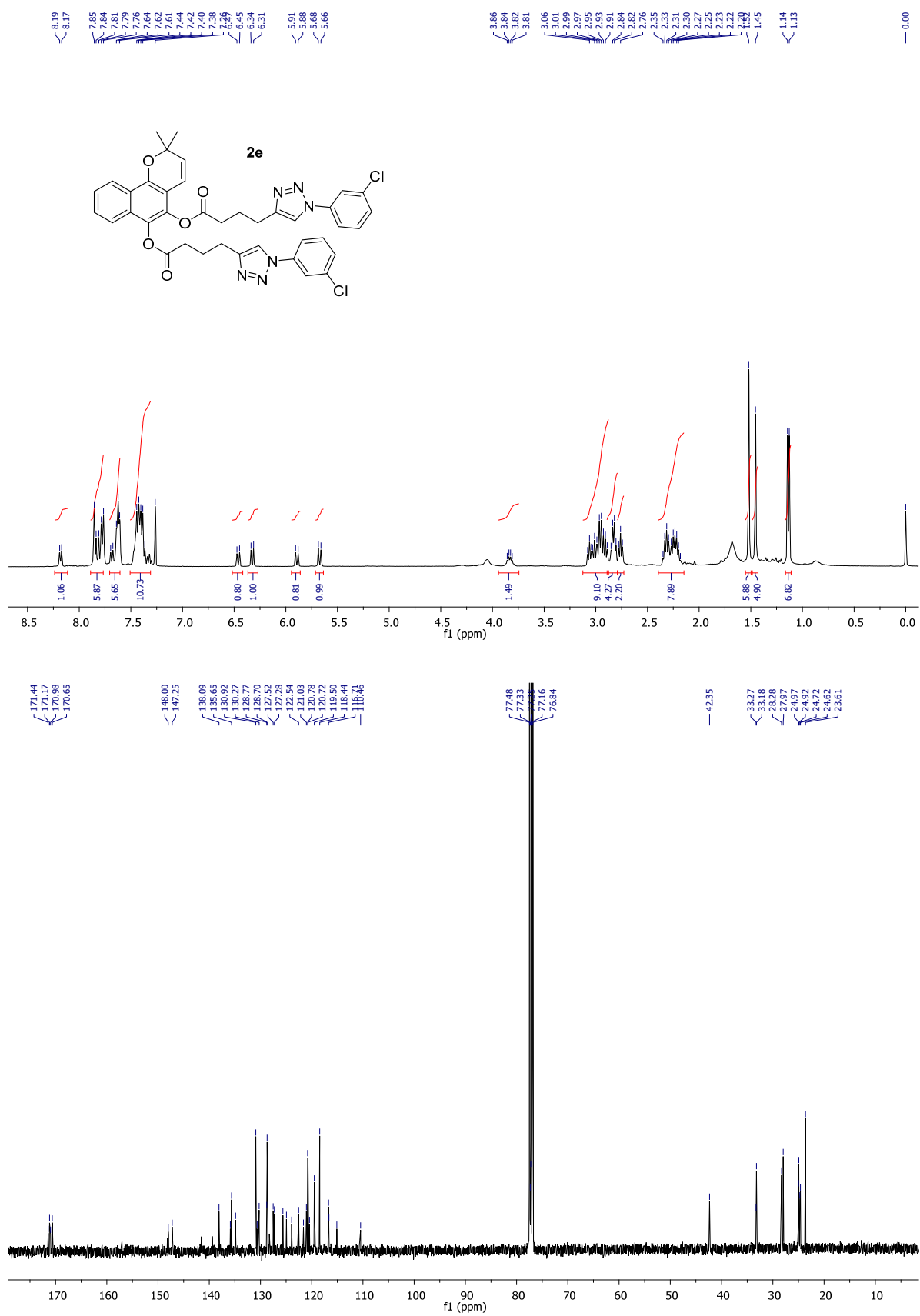


Figure 25. ¹H and ¹³C NMR spectra in CDCl₃ of compound **2e**.

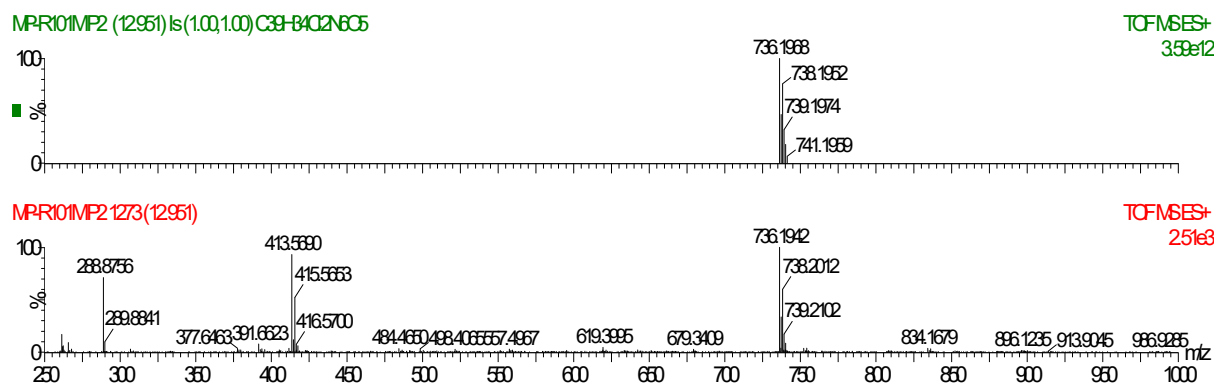


Figure 26. HREIMS spectrum of compound **2e**.

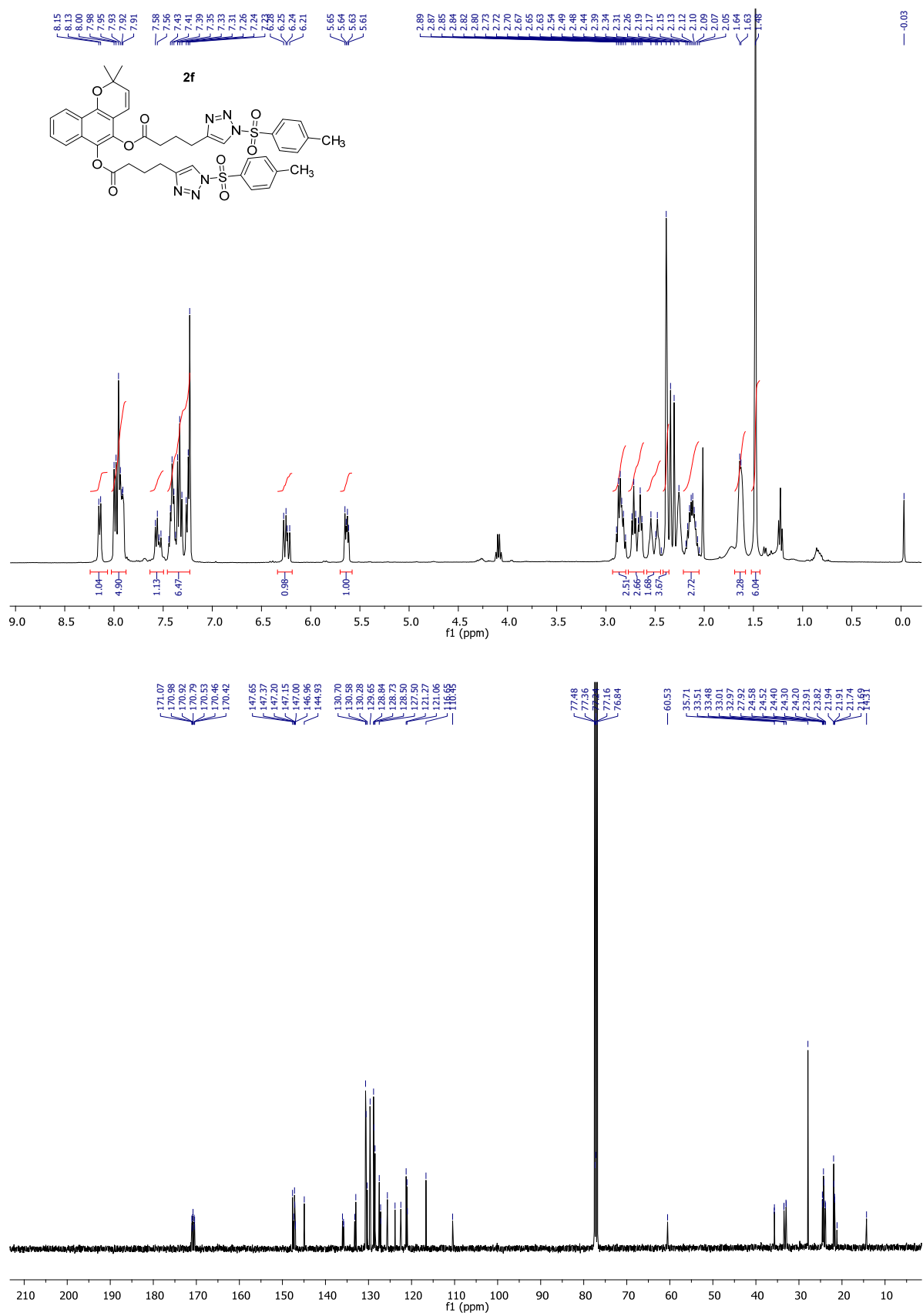


Figure 27. ¹H and ¹³C NMR spectra in CDCl₃ of compound 2f.

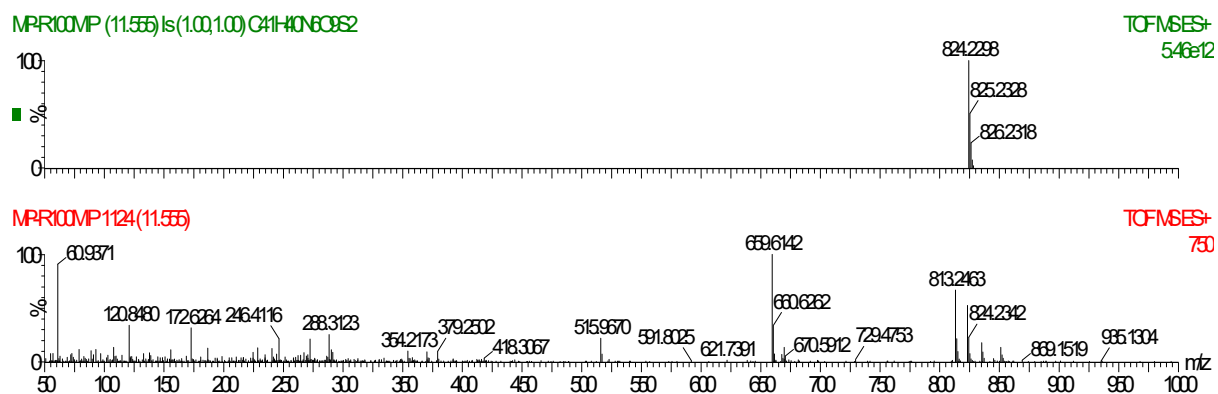


Figure 28. HREIMS spectrum of compound **2f**.

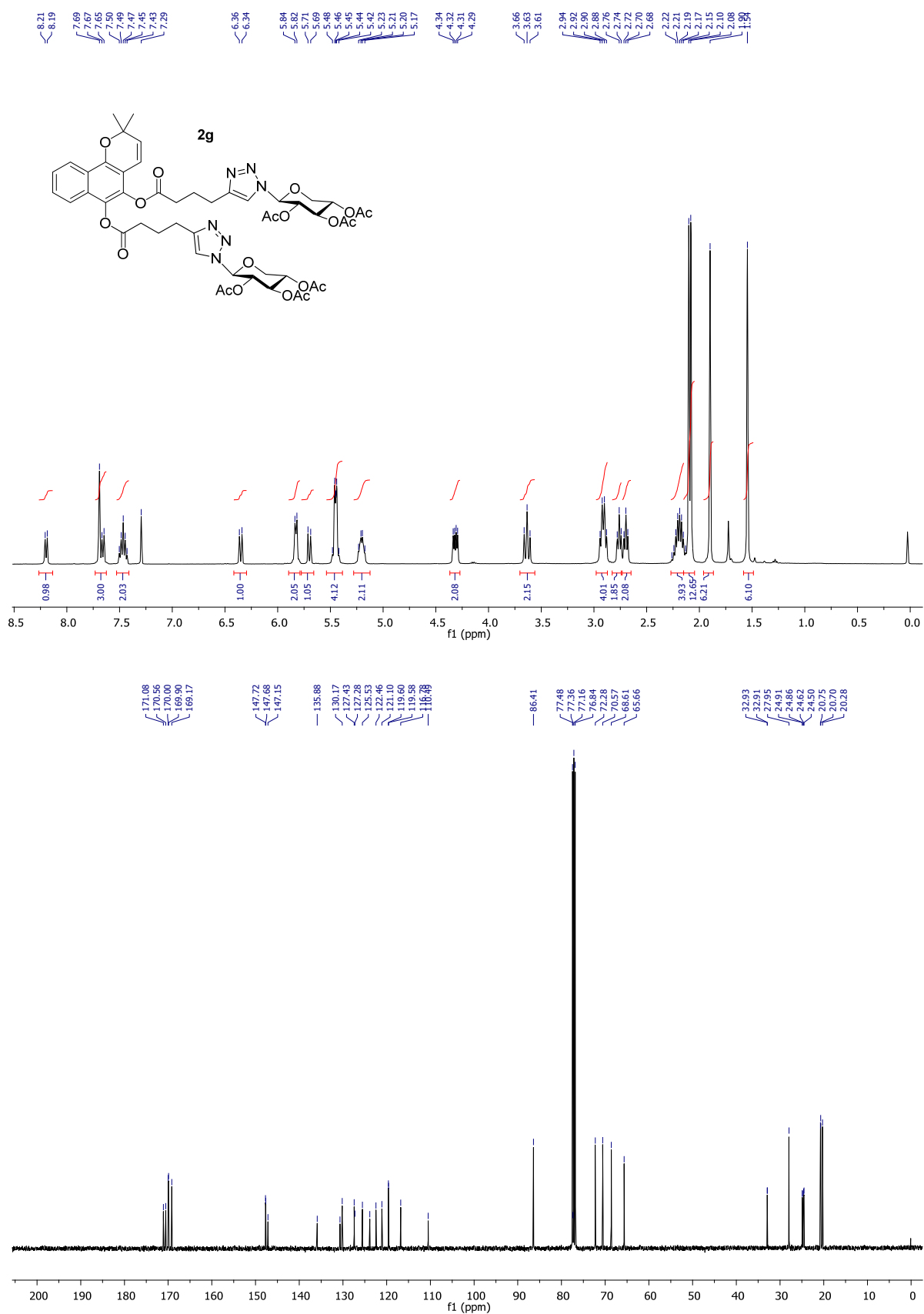


Figure 29. ¹H and ¹³C NMR spectra in CDCl₃ of compound **2g**.

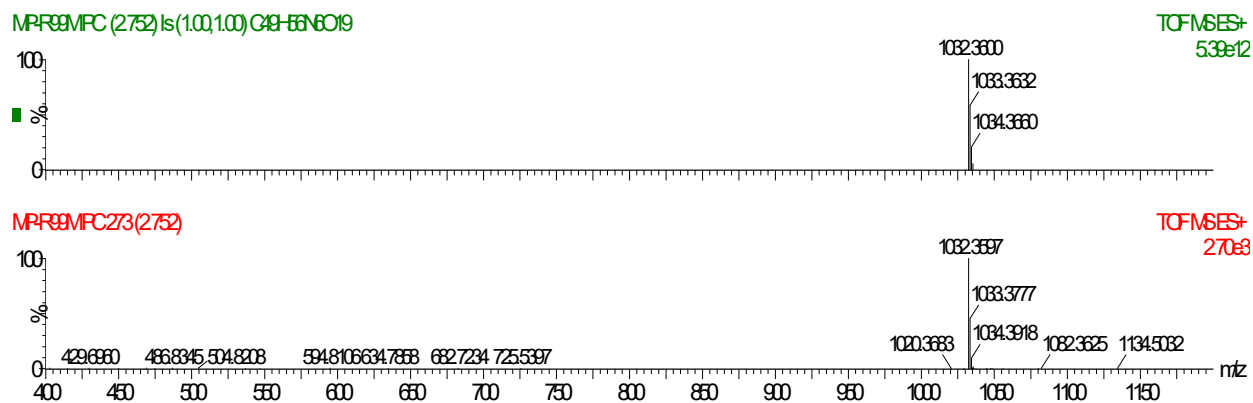


Figure 30. HREIMS spectrum of compound **2g**.

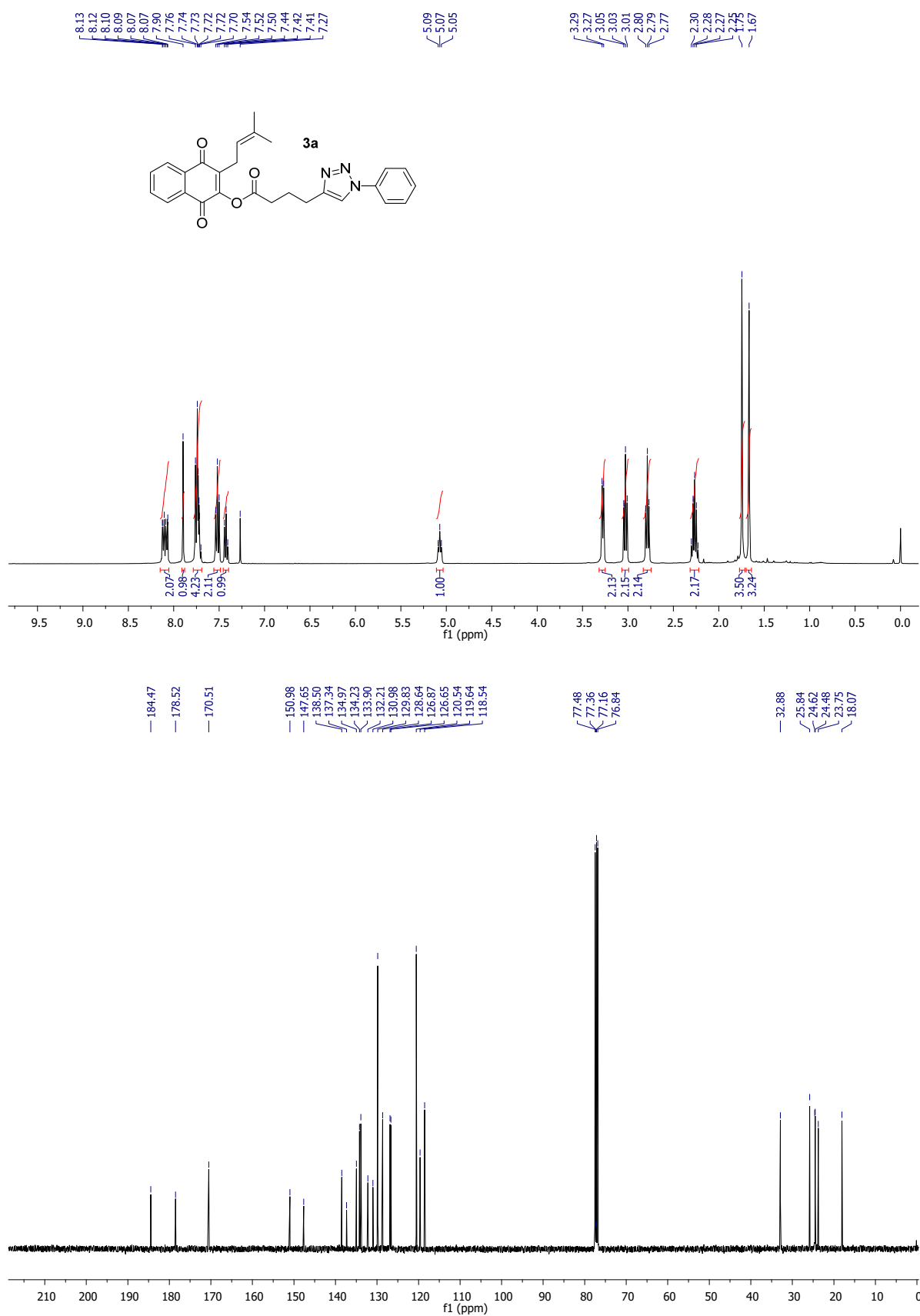


Figure 31. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **3a**.

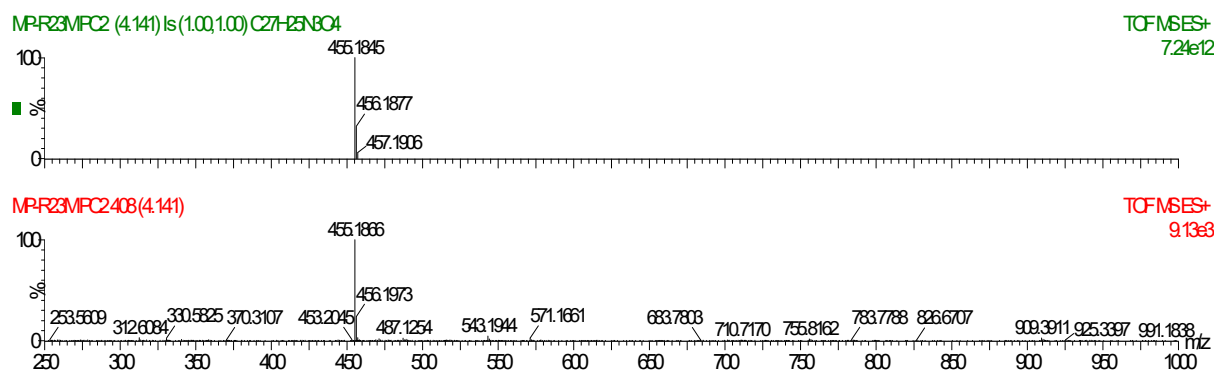


Figure 32. HREIMS spectrum of compound **3a**.

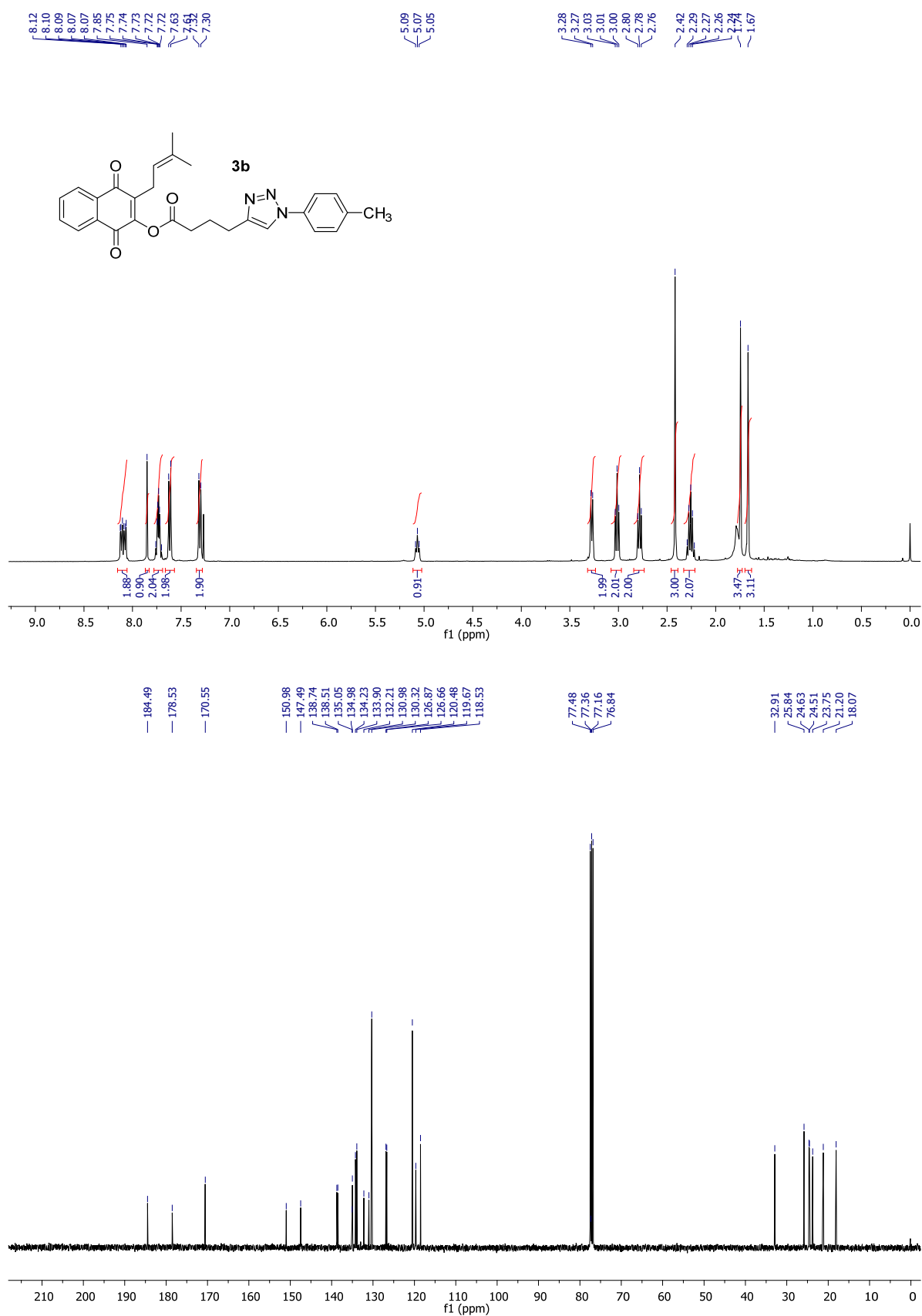


Figure 33. ¹H and ¹³C NMR spectra in CDCl₃ of compound **3b**.

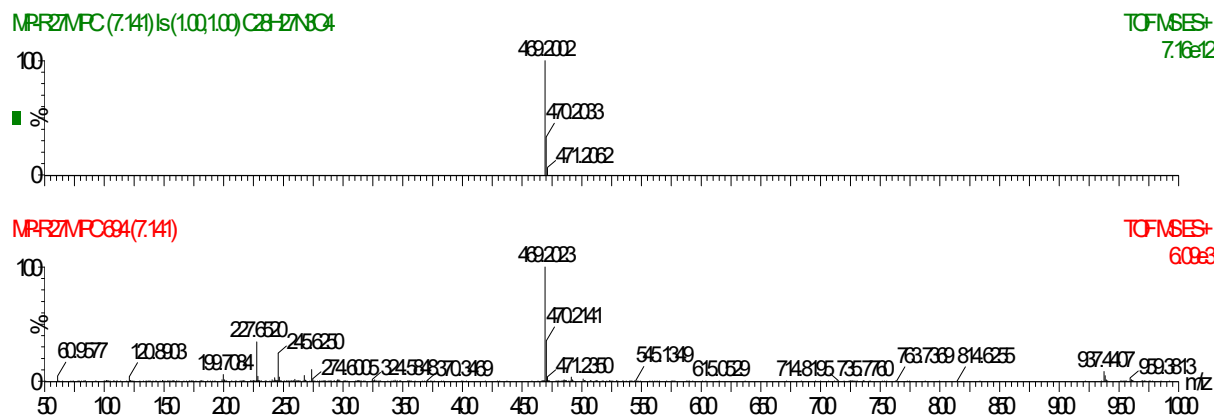


Figure 34. HREIMS spectrum of compound **3b**.

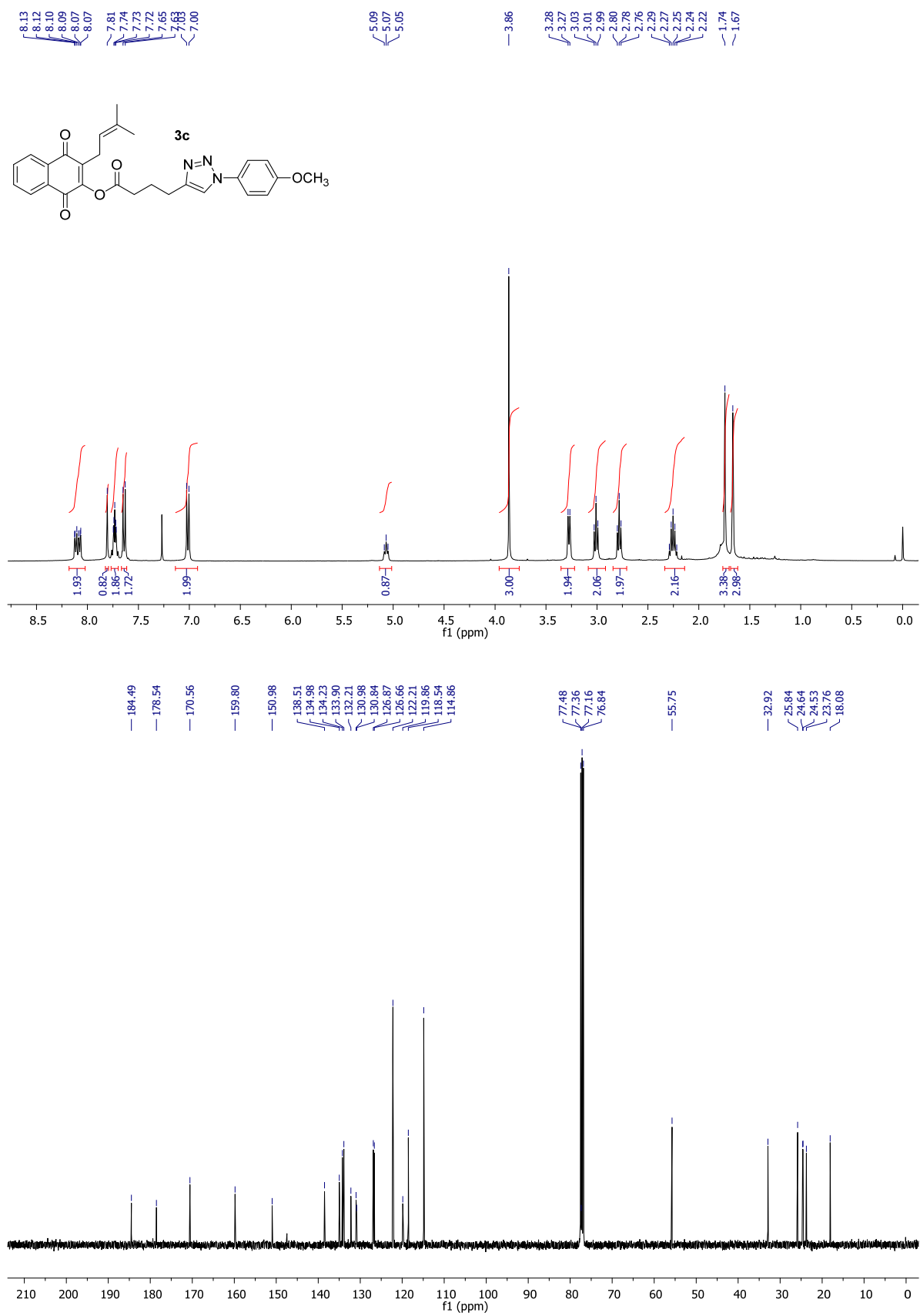
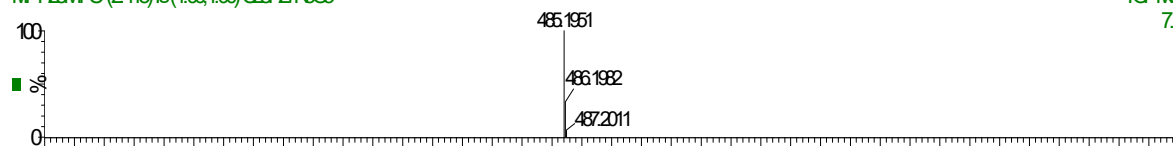


Figure 35. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **3c**.

MPR2MFC (2415) Is (1.00,1.00) C28H27NO5

TOFMS ES+
7.14e12



MPR2MFC 234 (2415)

TOFMS ES+
3.82e8

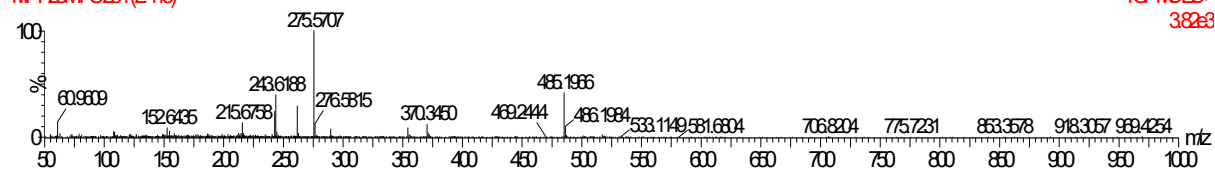


Figure 36. HREIMS spectrum of compound 3c.

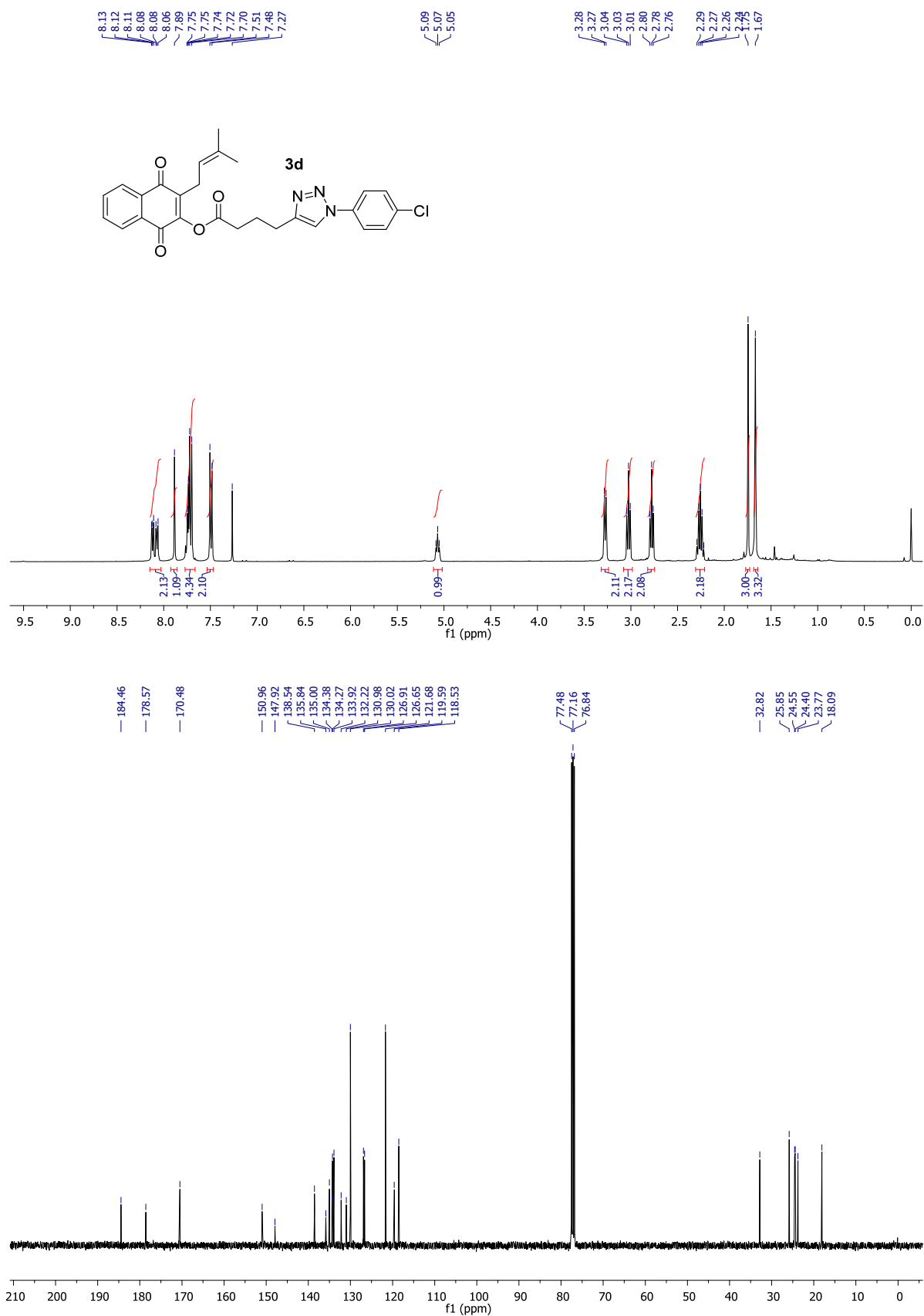


Figure 37. ¹H and ¹³C NMR spectra in CDCl₃ of compound **3d**.

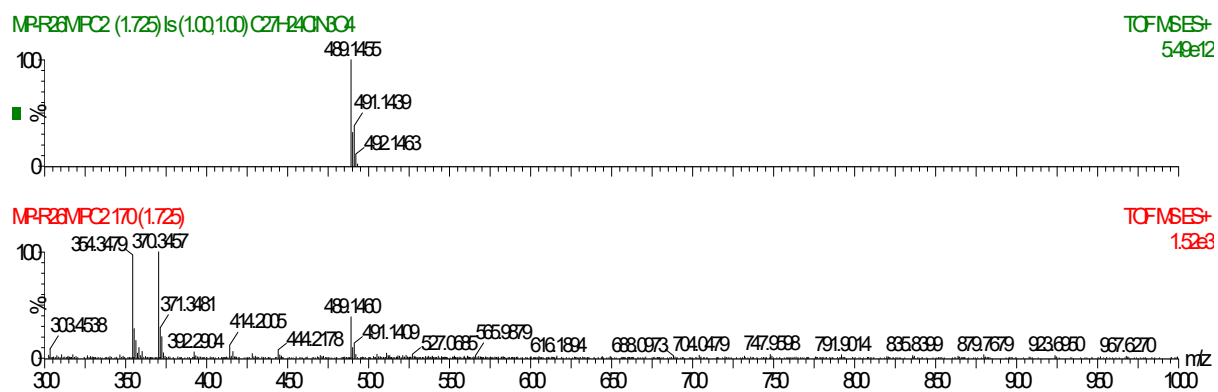


Figure 38. HREIMS spectrum of compound **3d**.

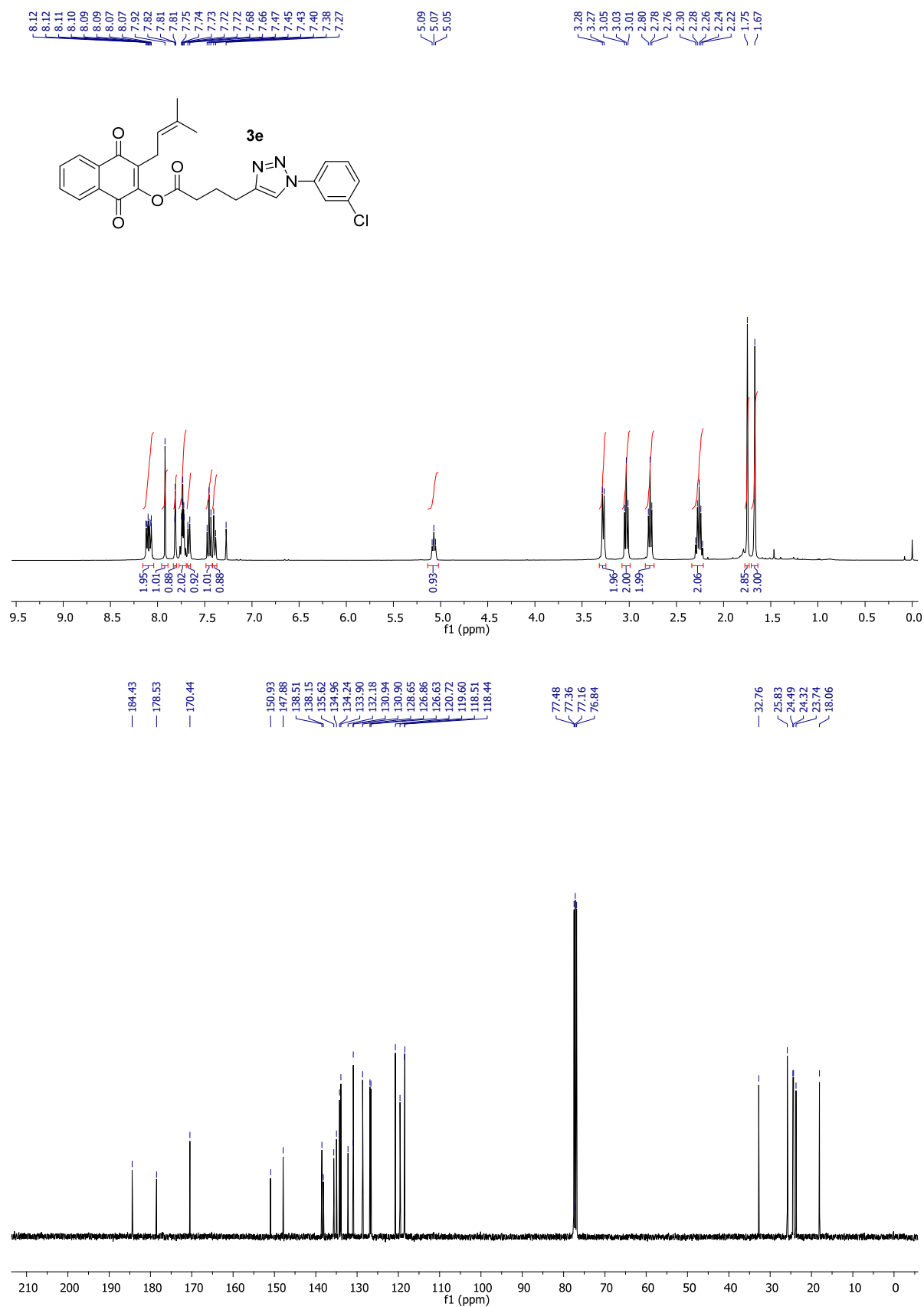


Figure 39. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **3e**.

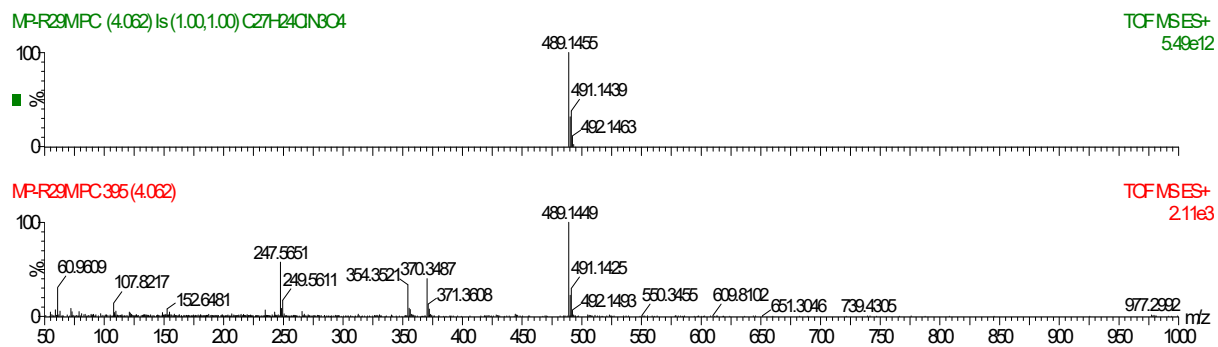


Figure 40. HREIMS spectrum of compound **3e**.

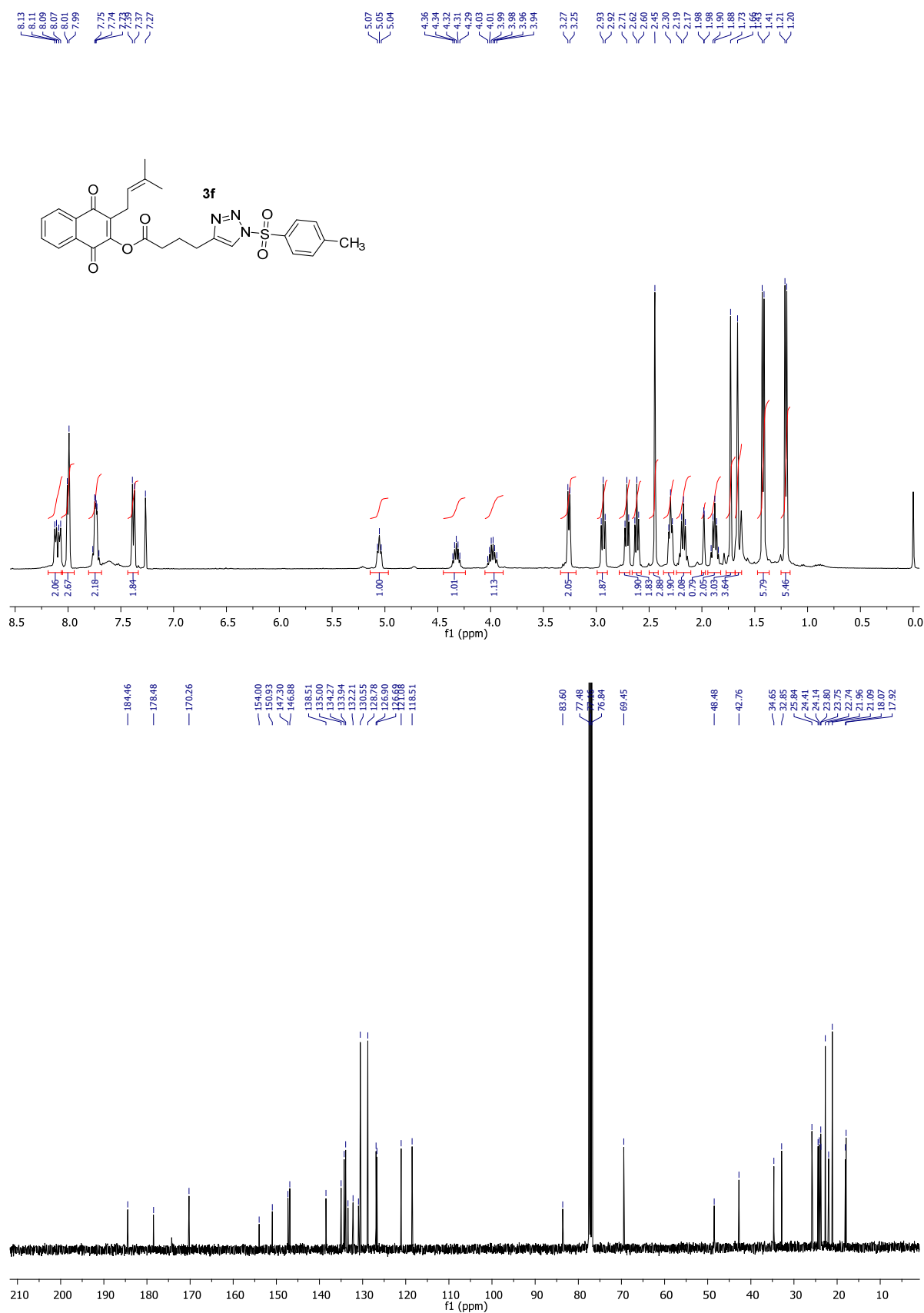


Figure 41. ^1H and ^{13}C NMR spectra in CDCl₃ of compound **3f**.

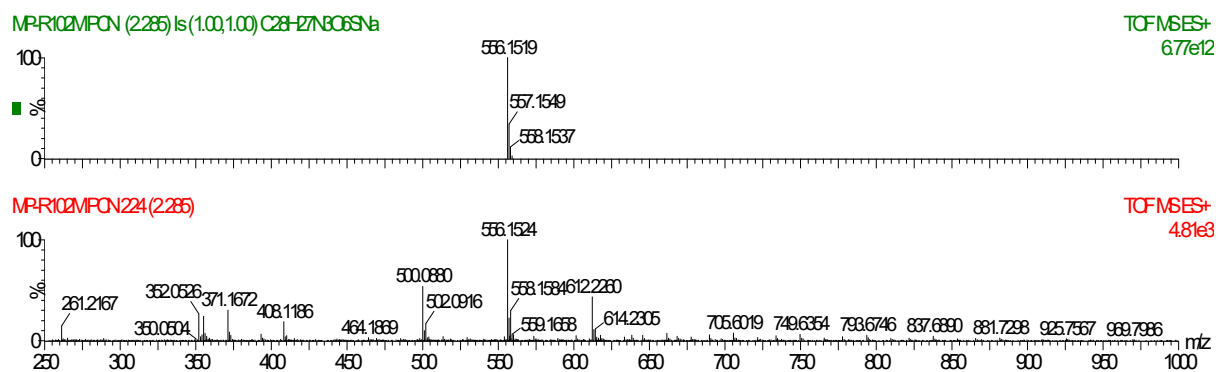


Figure 42. HREIMS spectrum of compound **3f**.

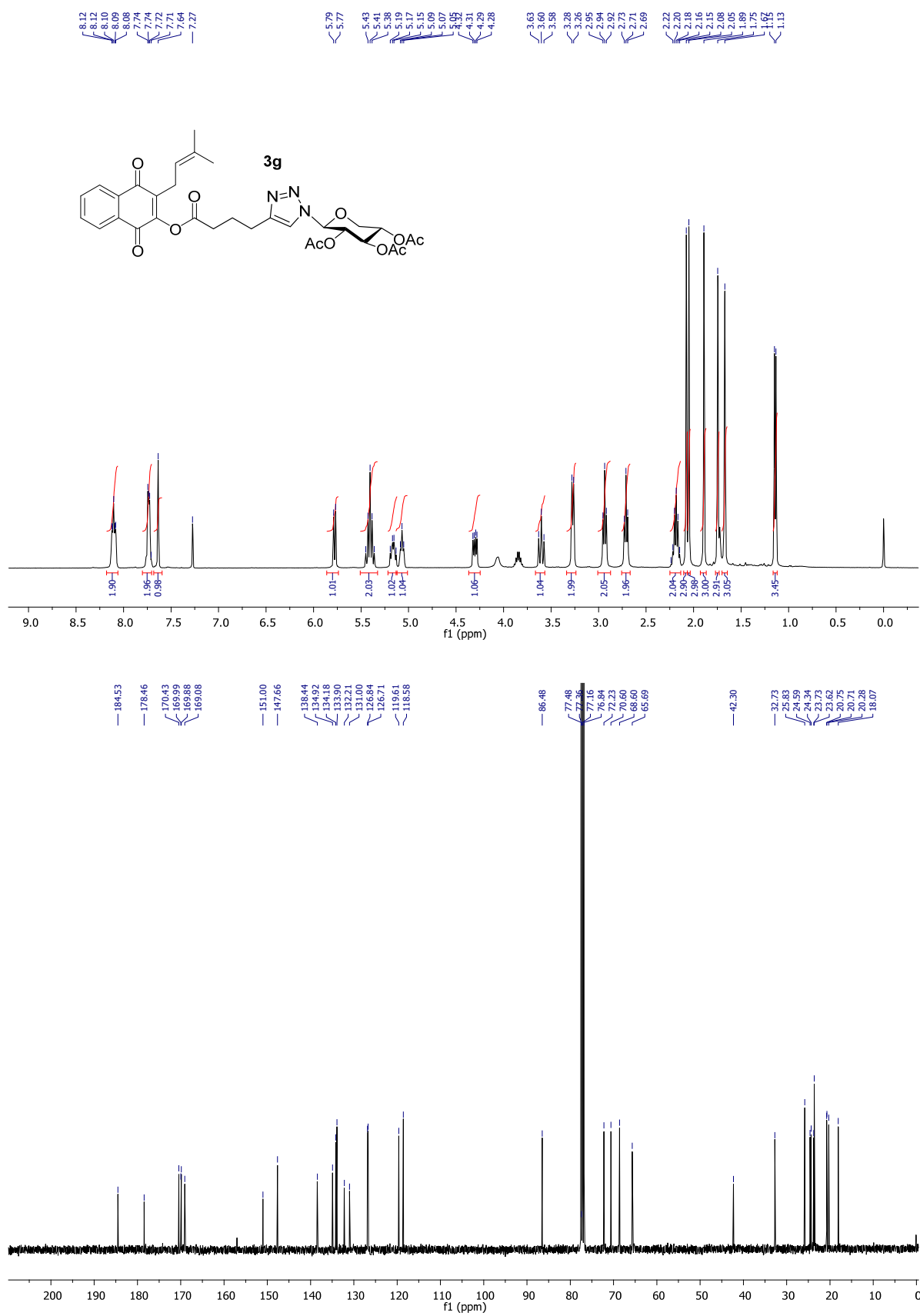


Figure 43. ^1H and ^{13}C NMR spectra in CDCl₃ of compound **3g**.

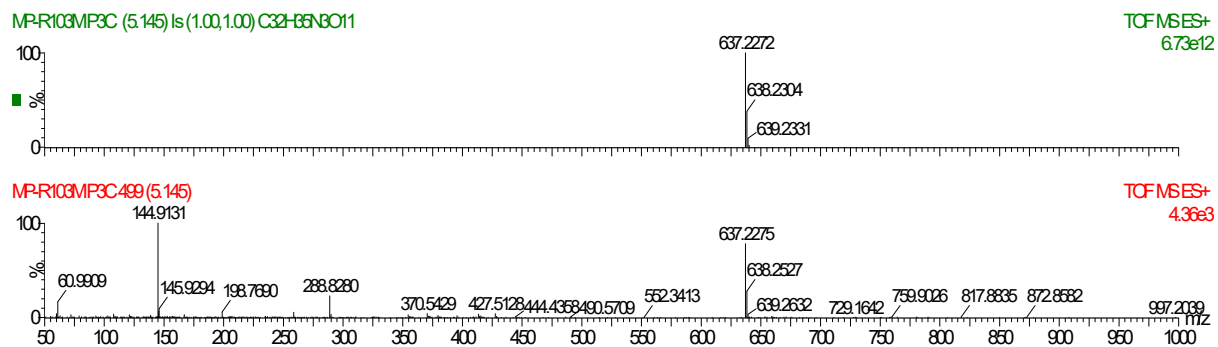


Figure 44. HREIMS spectrum of compound **3g**.

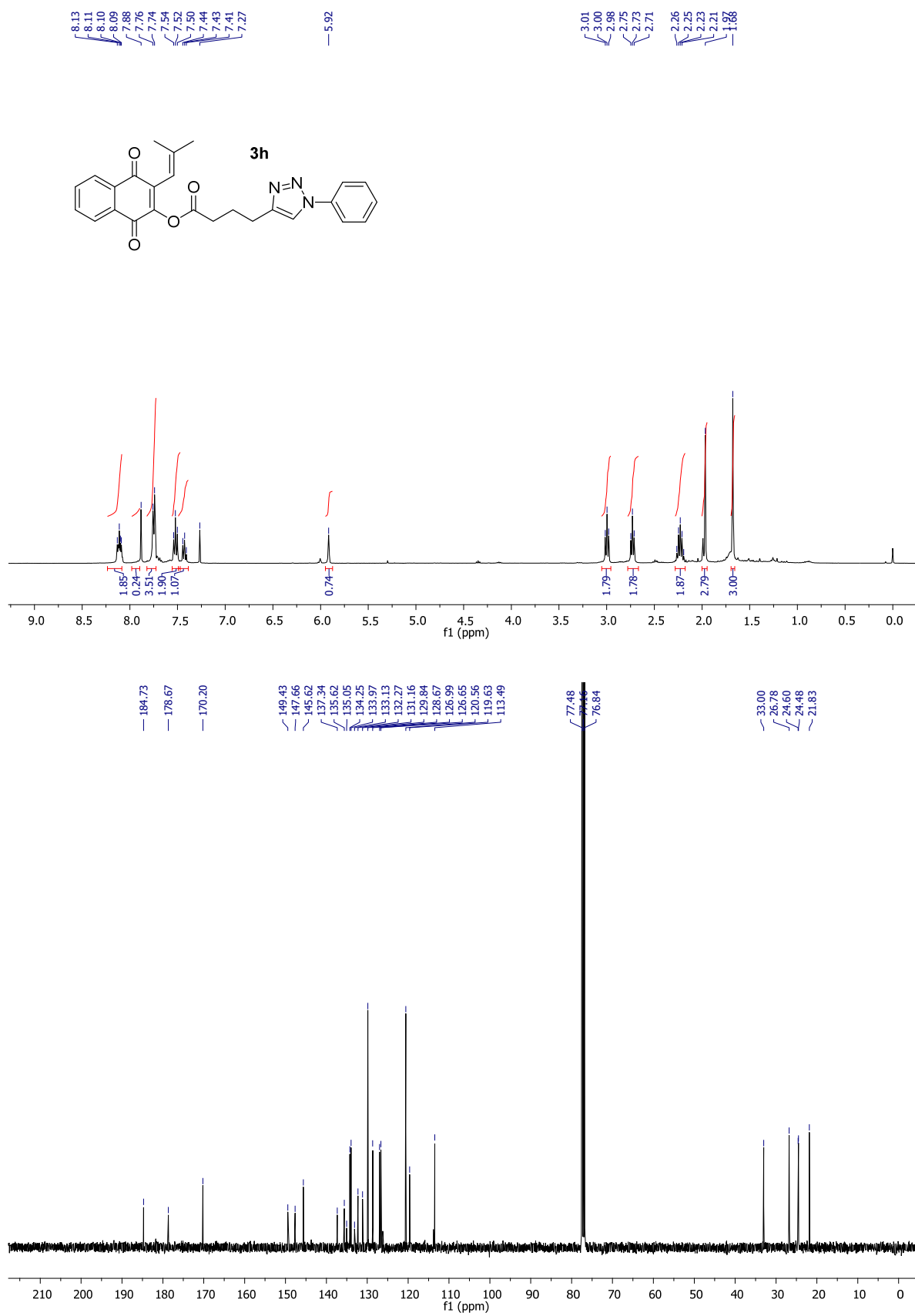


Figure 45. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **3h**.

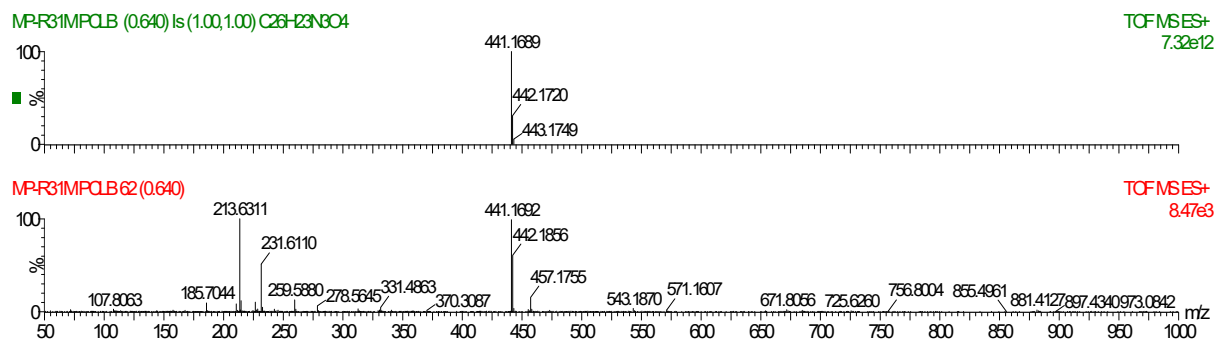


Figure 46. HREIMS spectrum of compound **3h**.

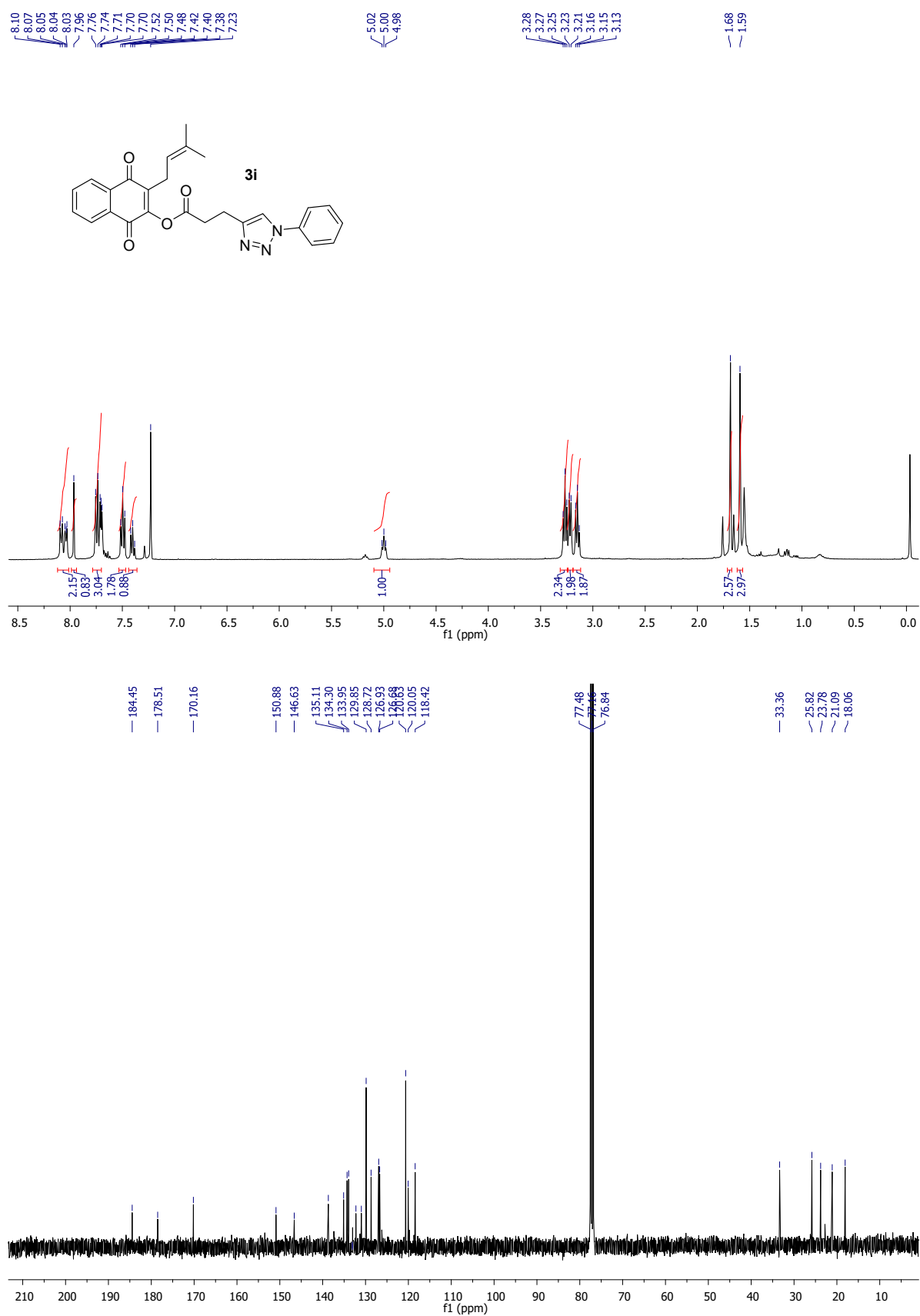


Figure 47. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **3i**.

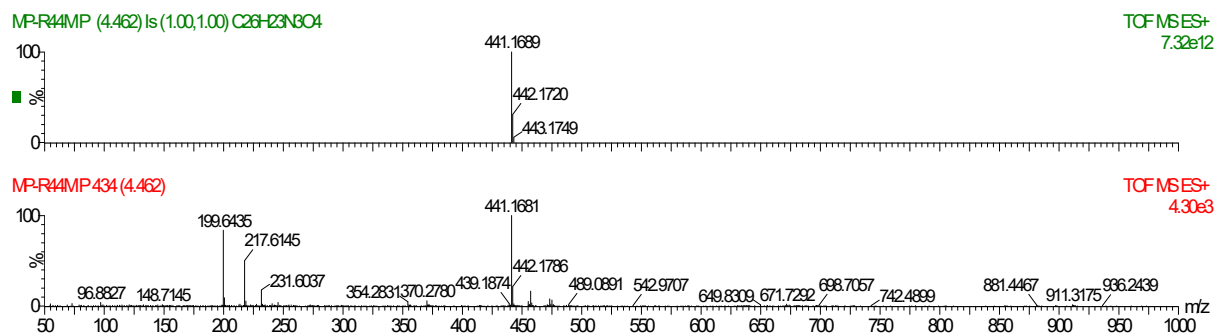


Figure 48. HREIMS spectrum of compound **3i**.

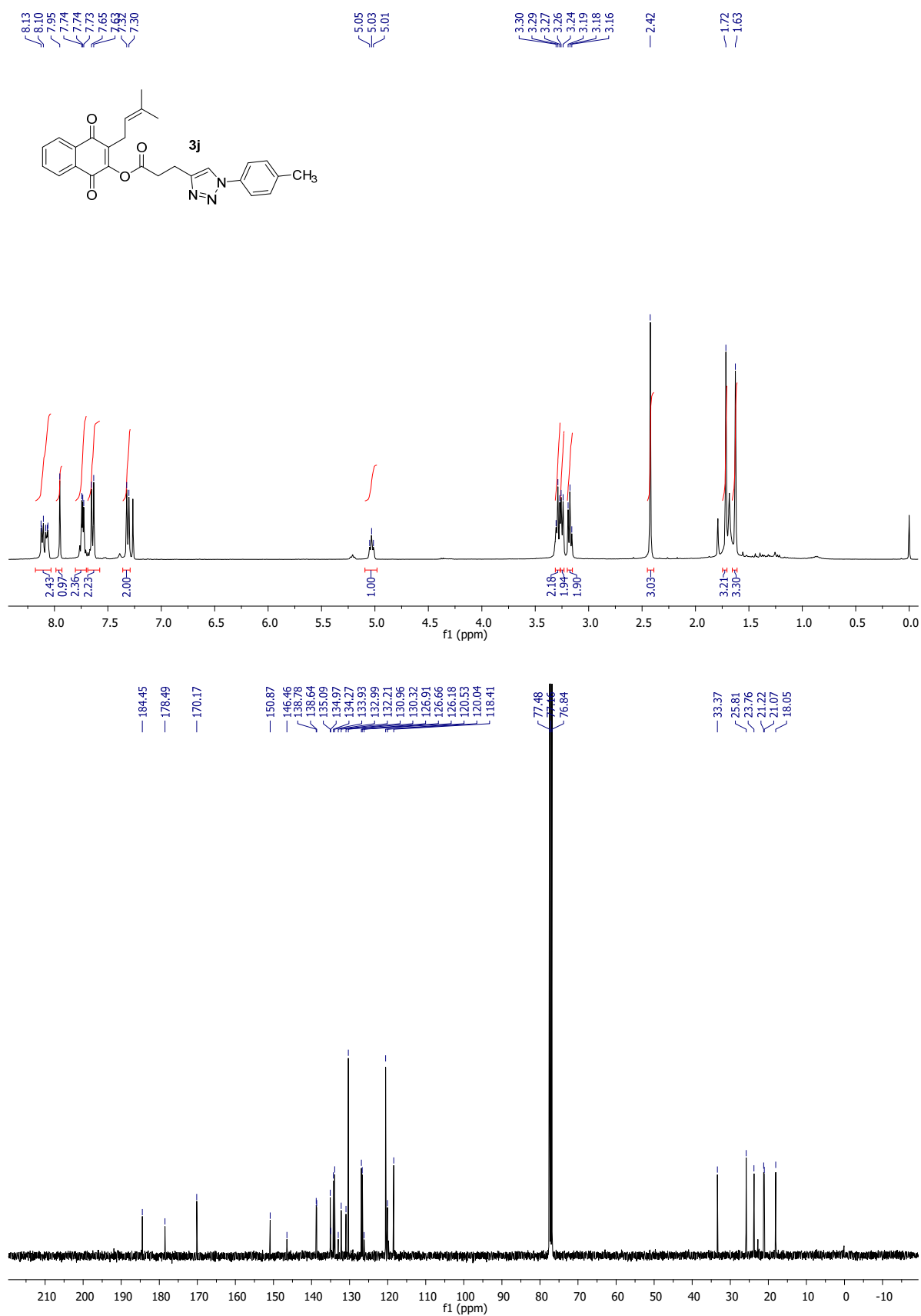


Figure 49. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **3j**.

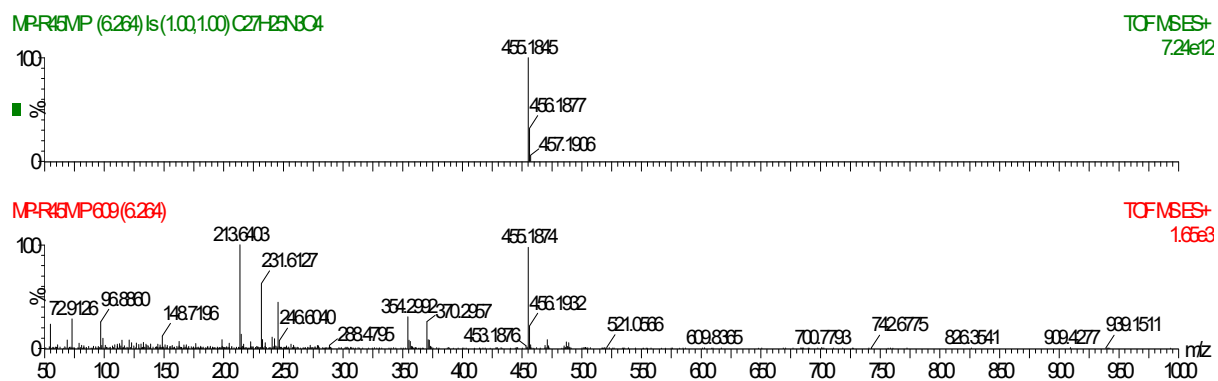


Figure 50. HREIMS spectrum of compound **3j**.

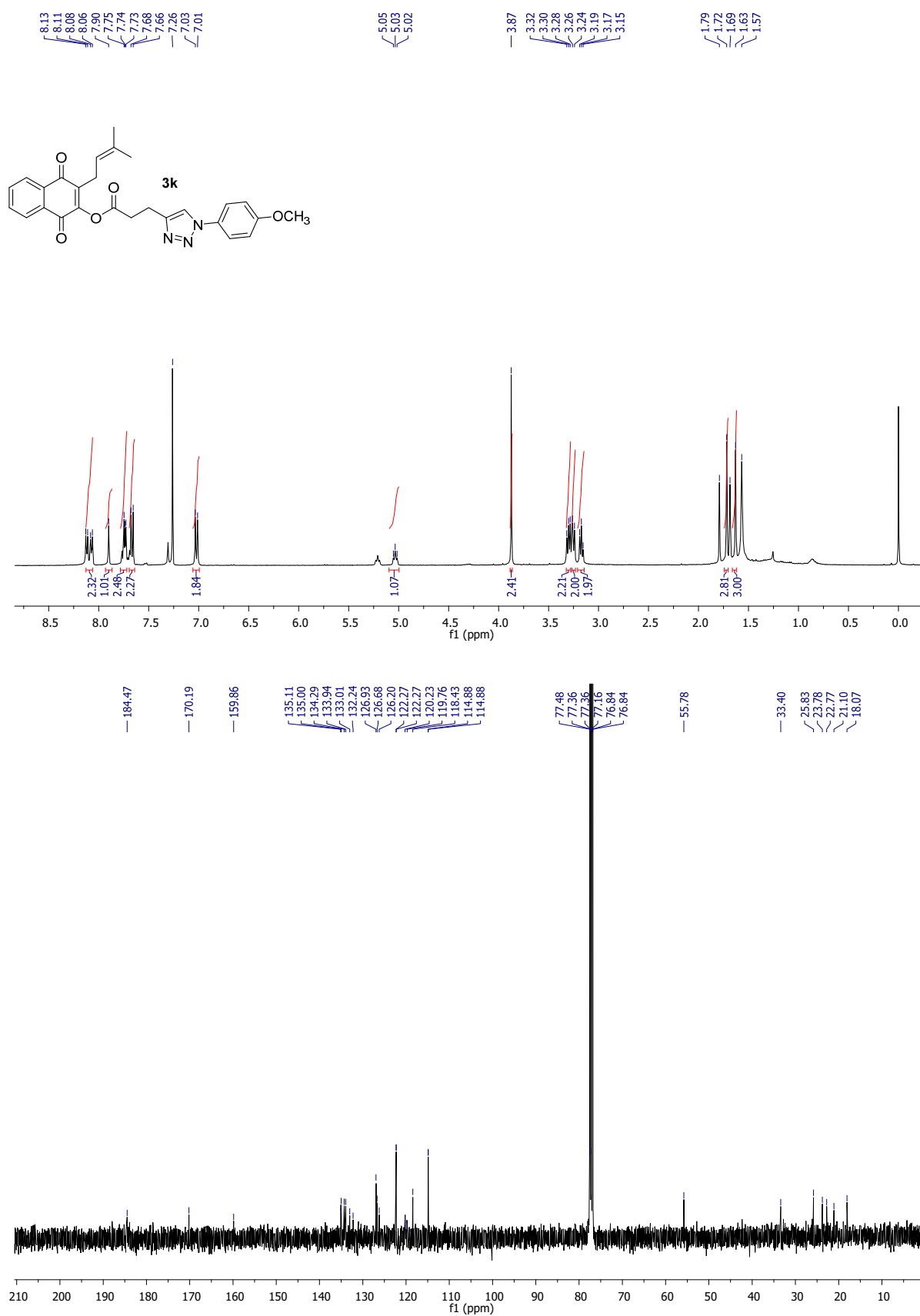


Figure 51. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **3k**.

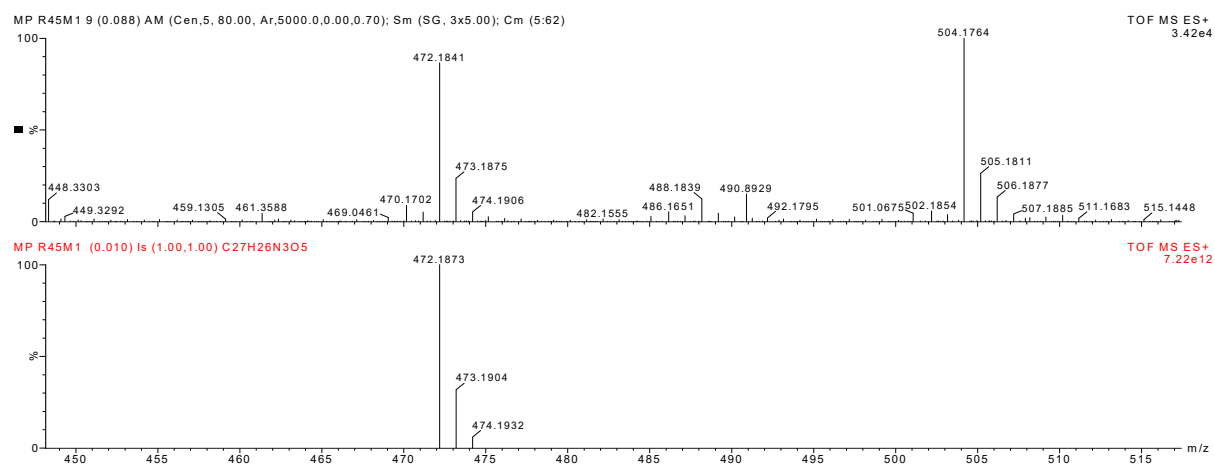


Figure 52. HREIMS spectrum of compound **3k**.

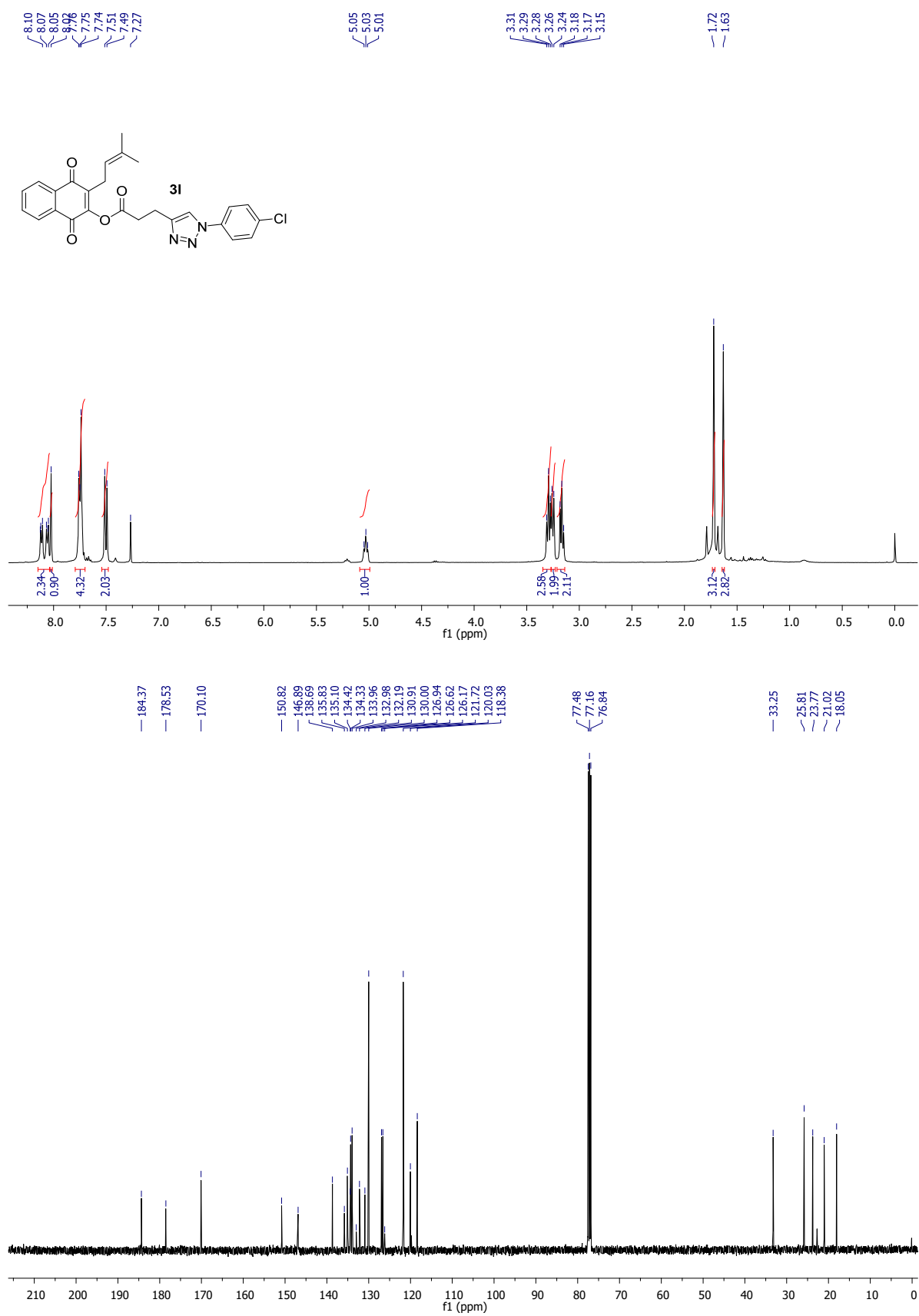


Figure 53. ^1H and ^{13}C NMR spectra in CDCl_3 of compound **31**.

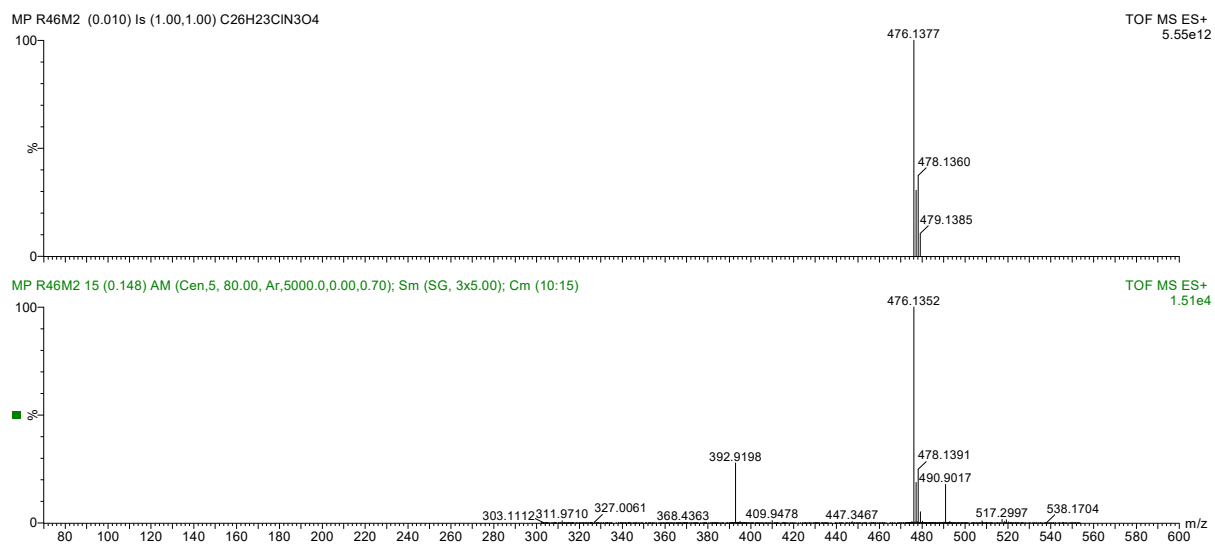


Figure 54. HREIMS spectrum of compound **31**.

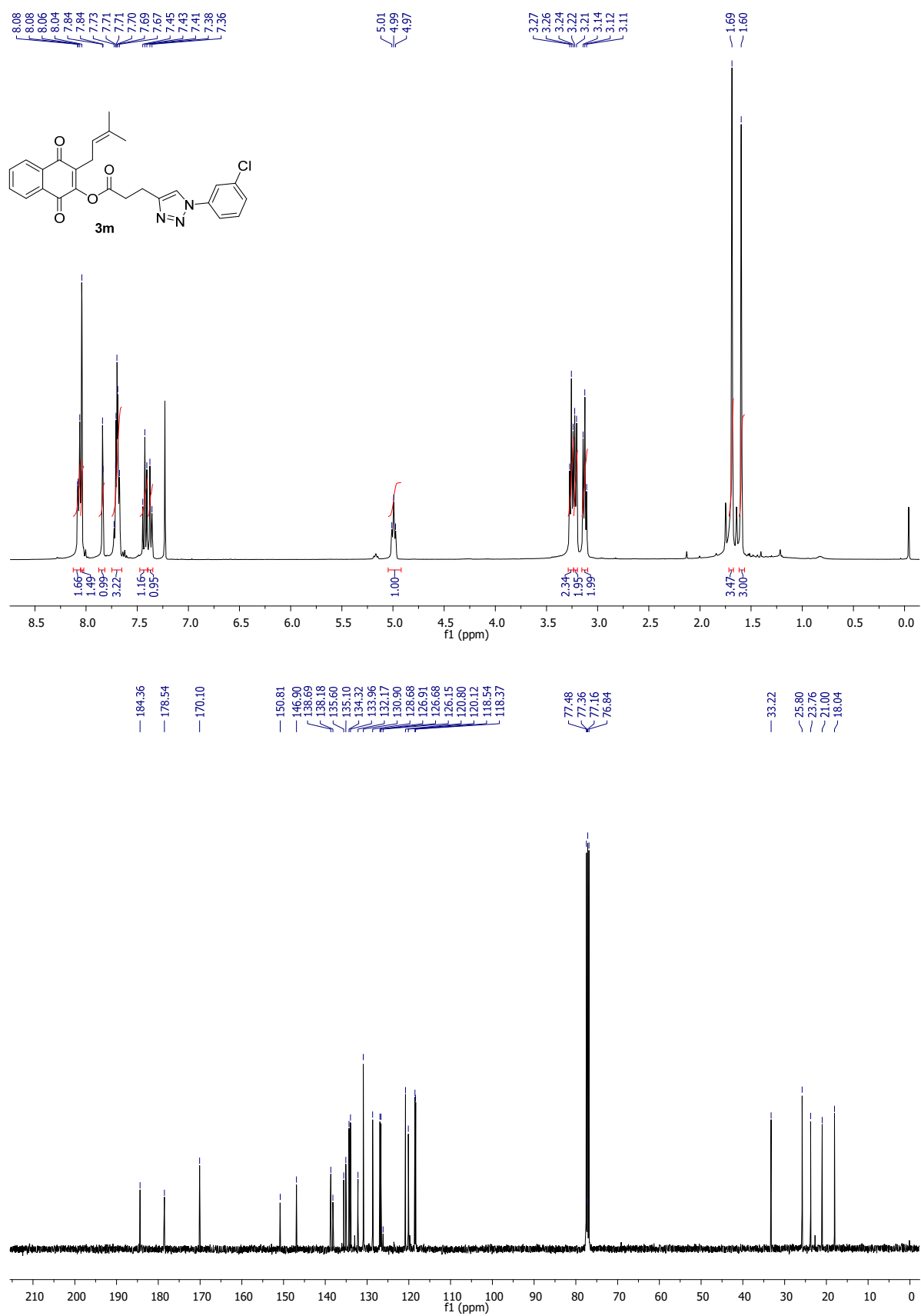


Figure 55. ^1H and ^{13}C NMR spectra in CDCl₃ of compound **3m**.

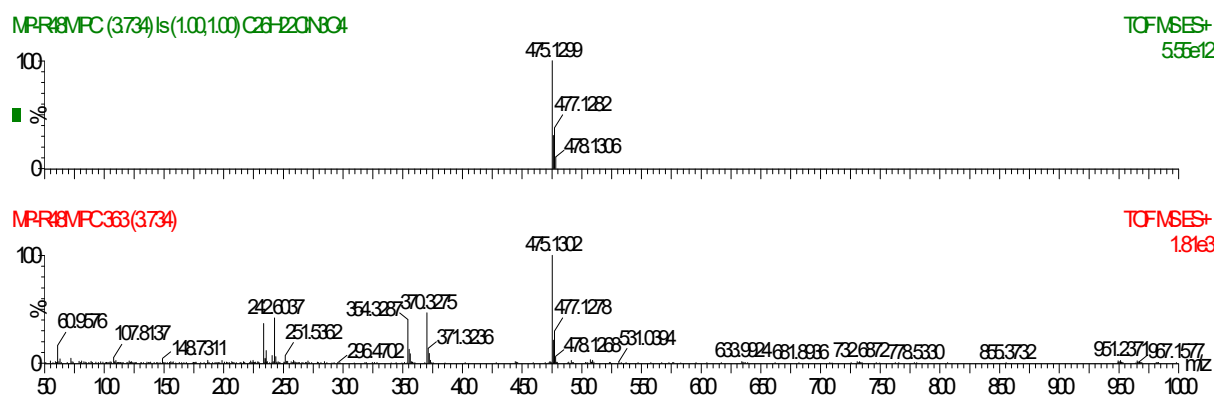


Figure 56. HREIMS spectrum of compound **3m**.