

Supplementary Information

Synthesis, *in vitro* Antifungal Activity and Molecular Modeling Studies of New Mannich Bases Derived from Lawsone

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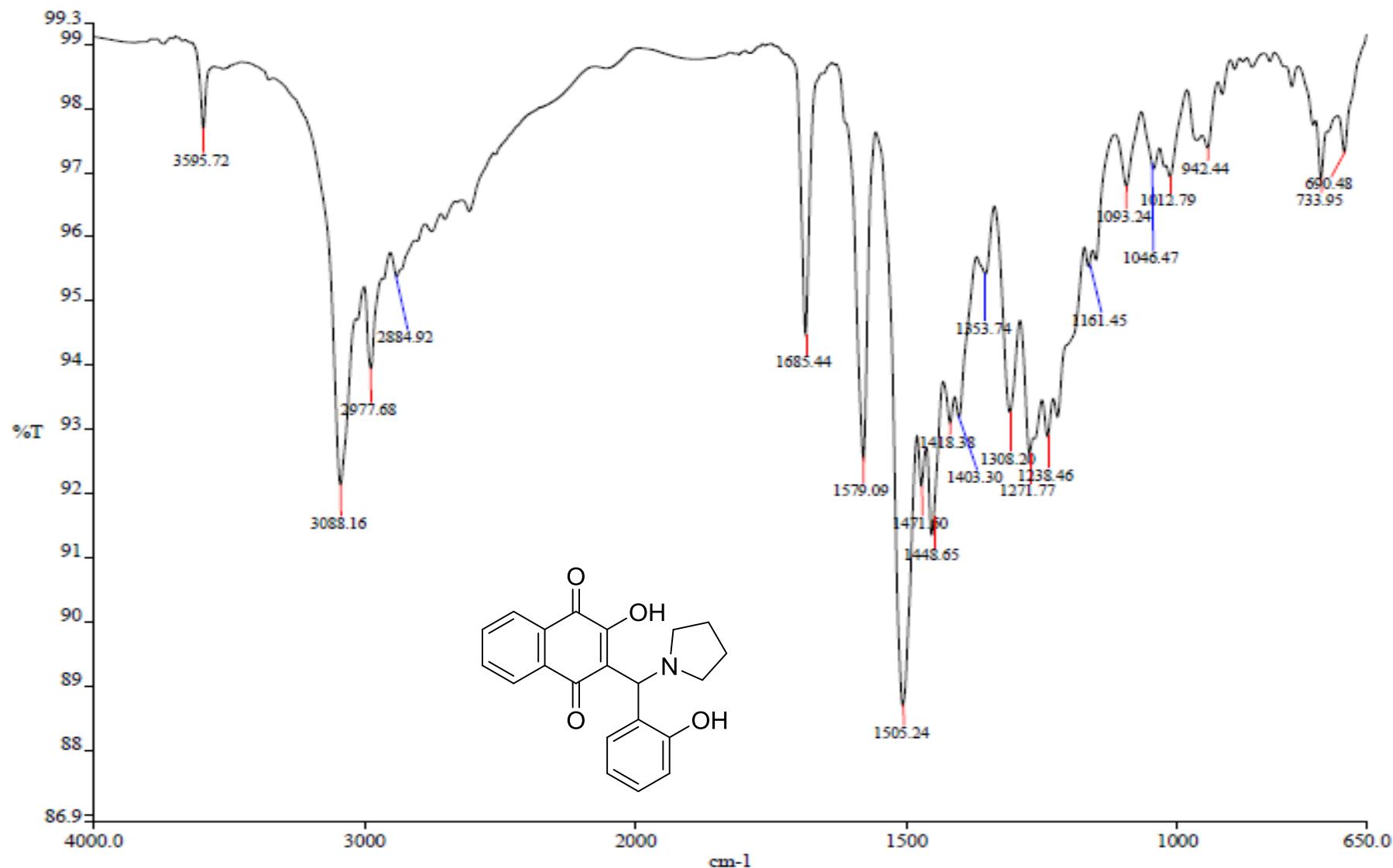


Figure S1. Infrared spectrum (ATR) of compound 4.

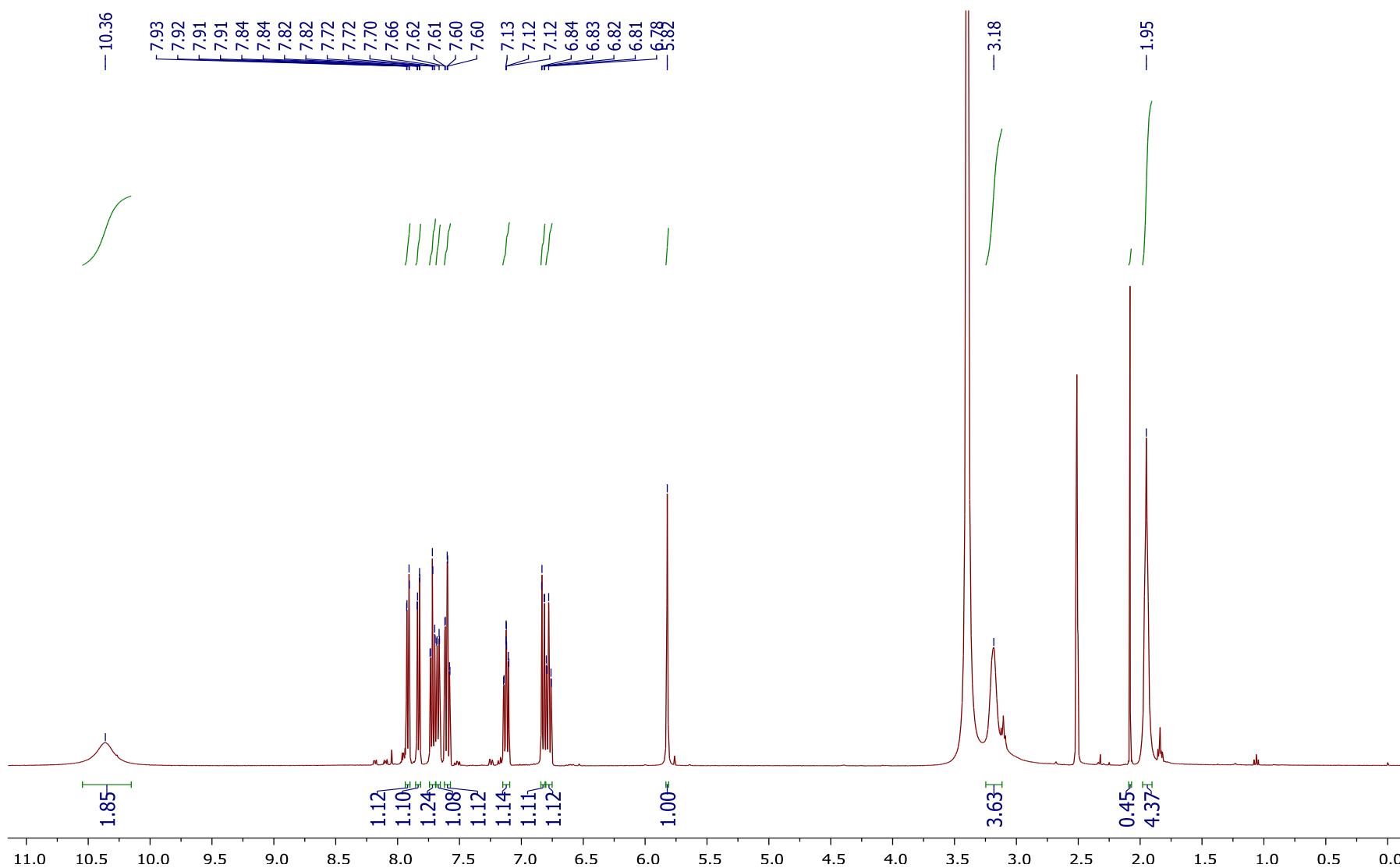


Figure S2. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 4.

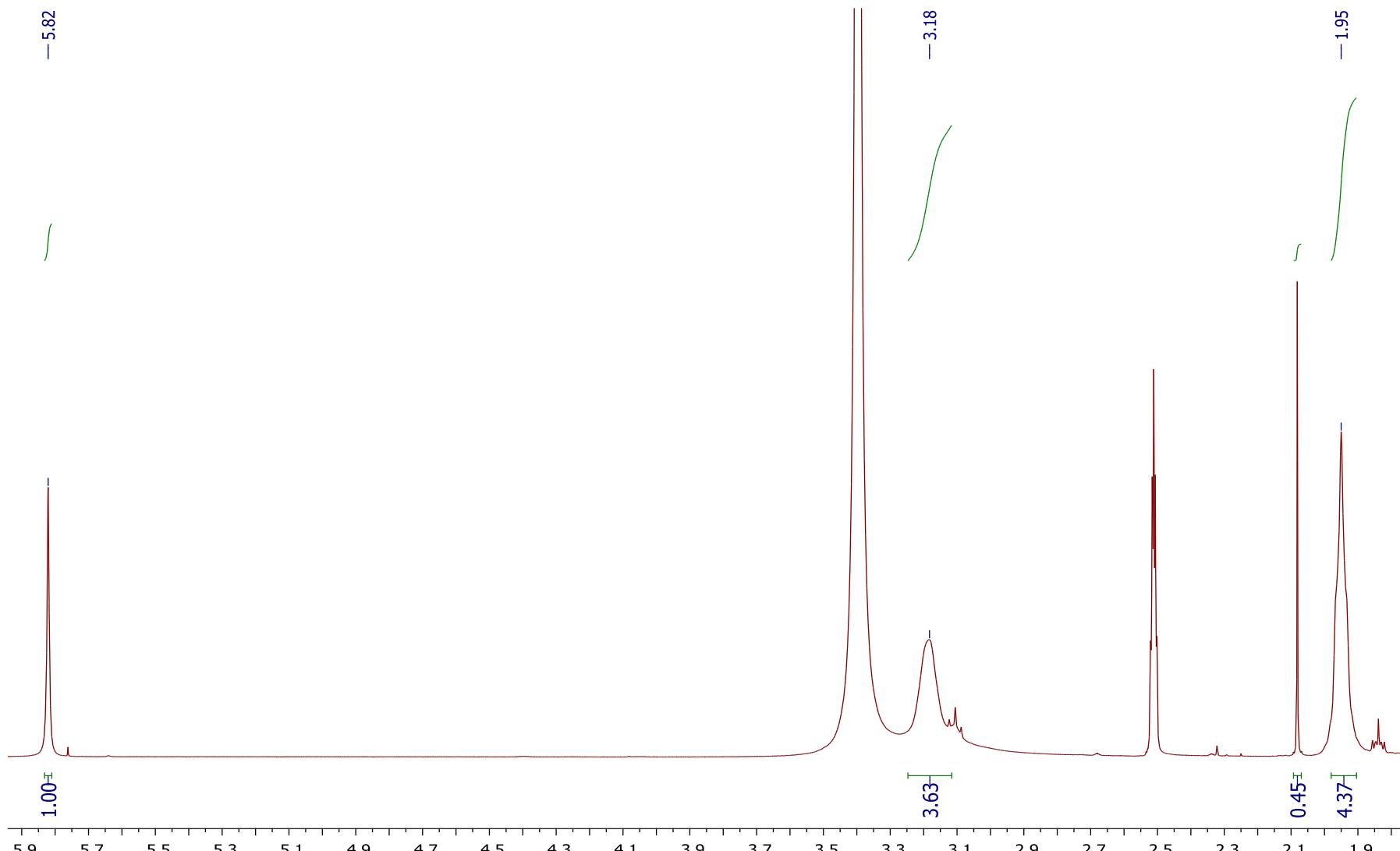


Figure S3. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aliphatic region of compound 4.

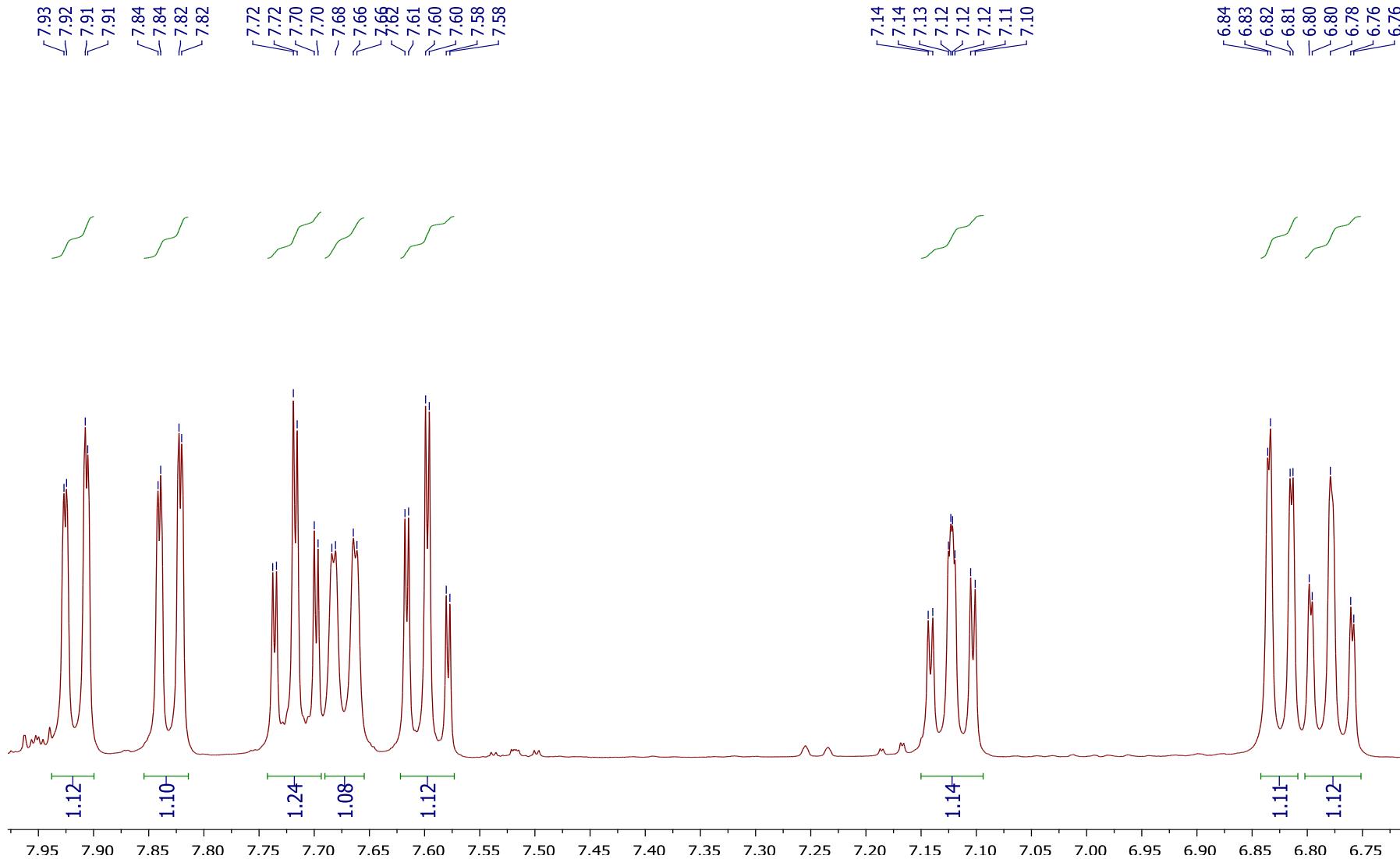


Figure S4. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aromatic region of compound 4.

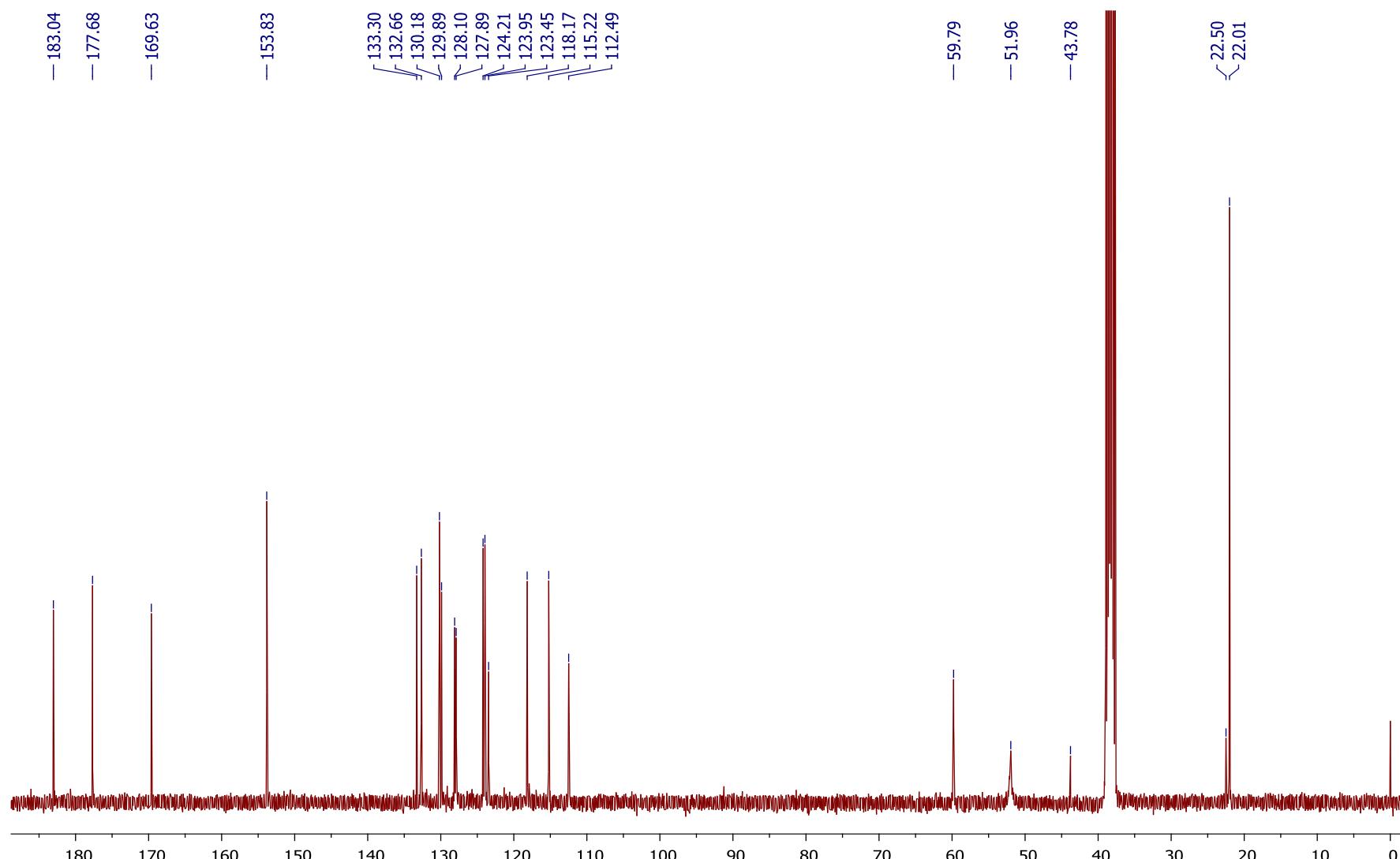


Figure S5. ^{13}C NMR spectrum (101 MHz, $\text{DMSO}-d_6$) of compound 4.

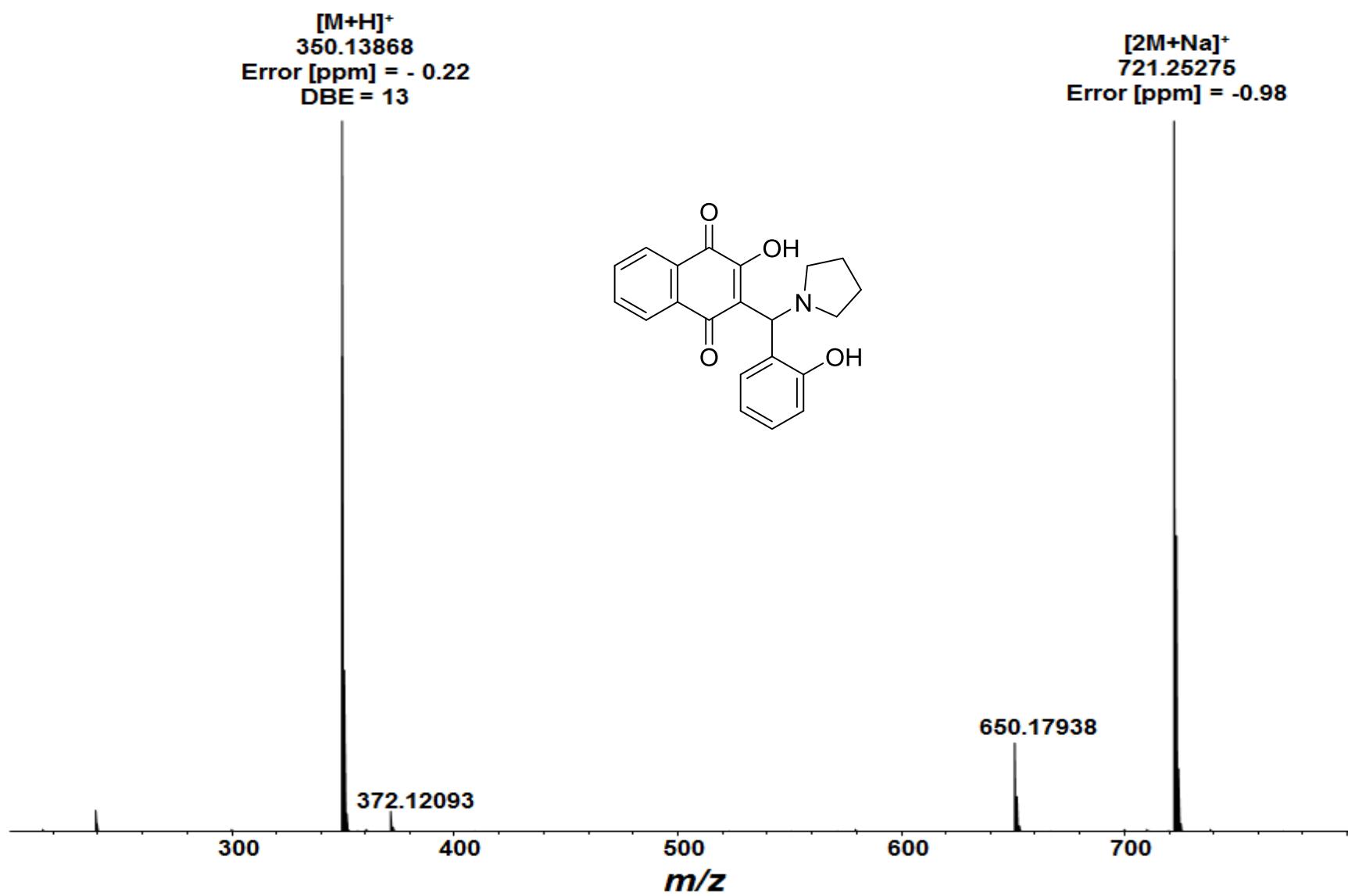


Figure S6. ESI(+)-FT-ICR mass spectrum of compound 4.

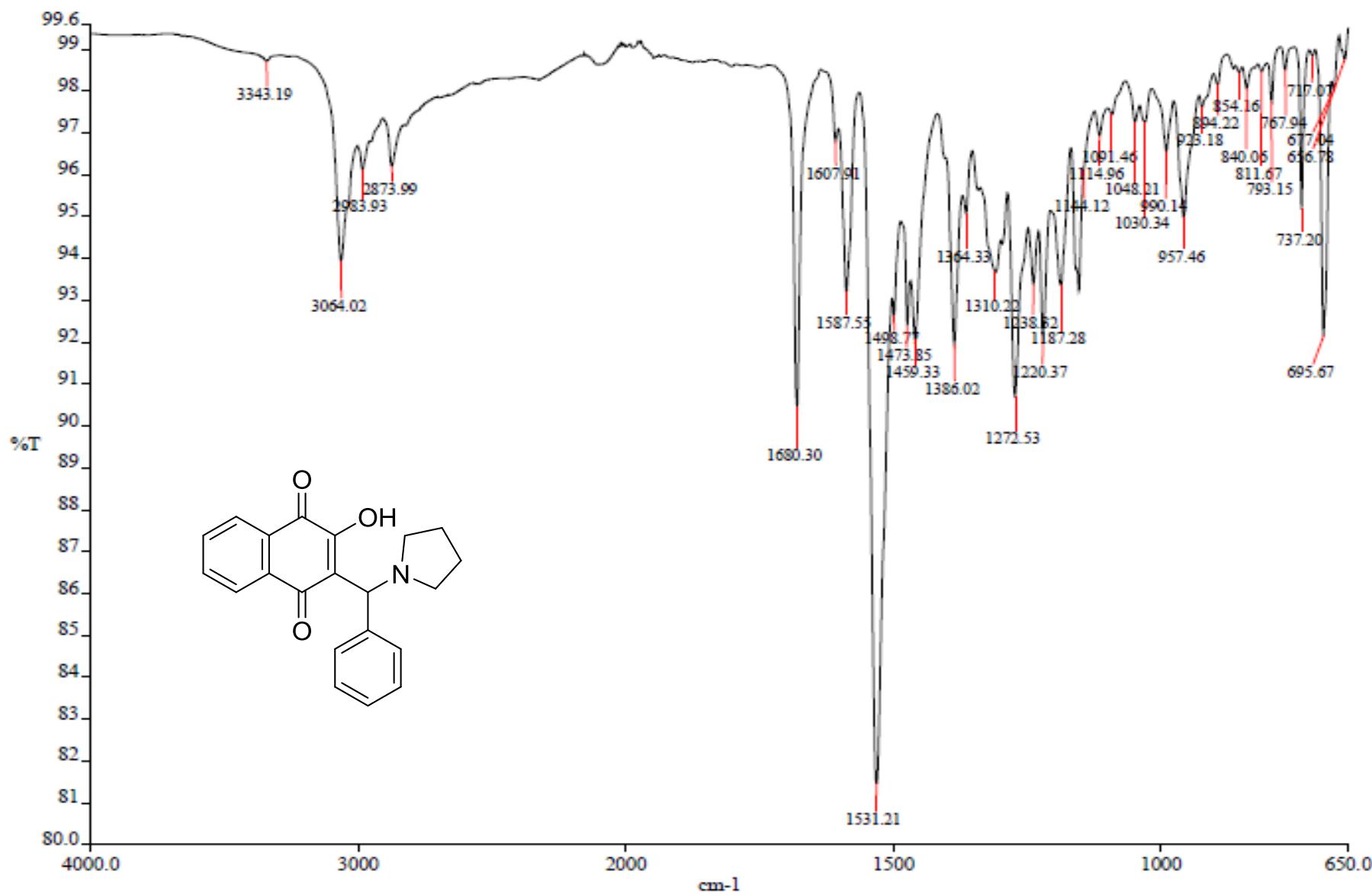


Figure S7. Infrared spectrum (ATR) of compound 5.

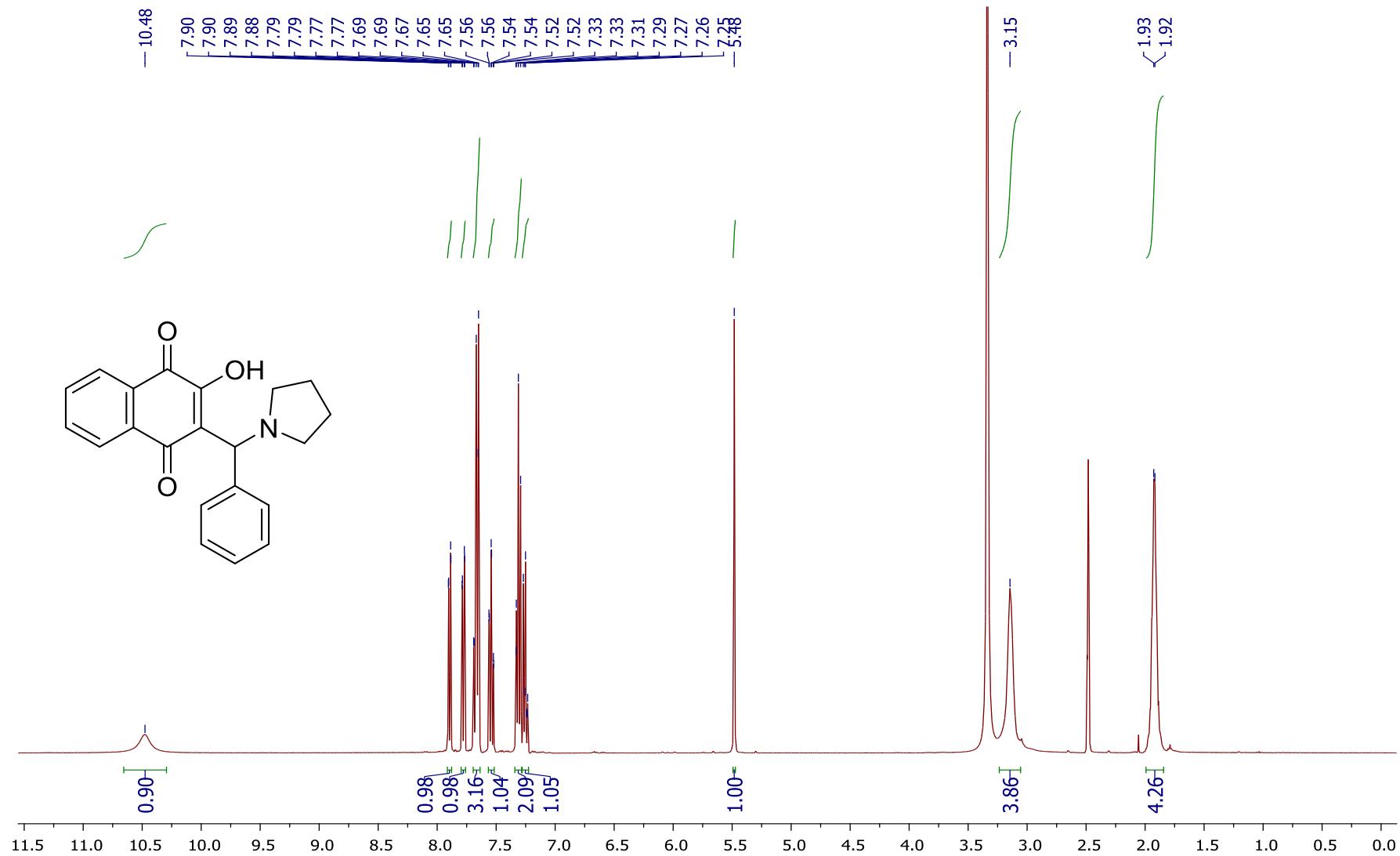


Figure S8. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **5**.

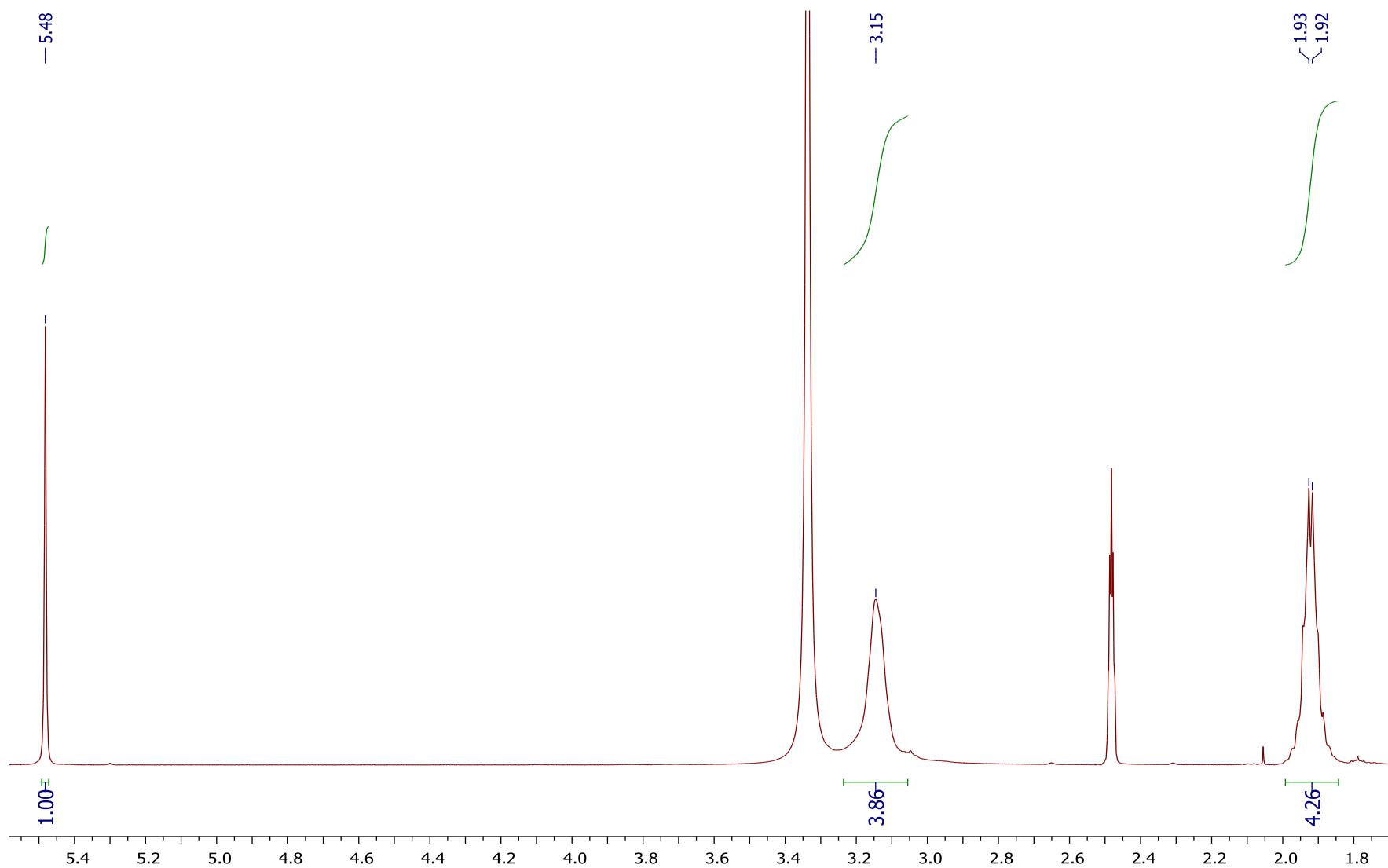


Figure S9. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aliphatic region of compound 5.

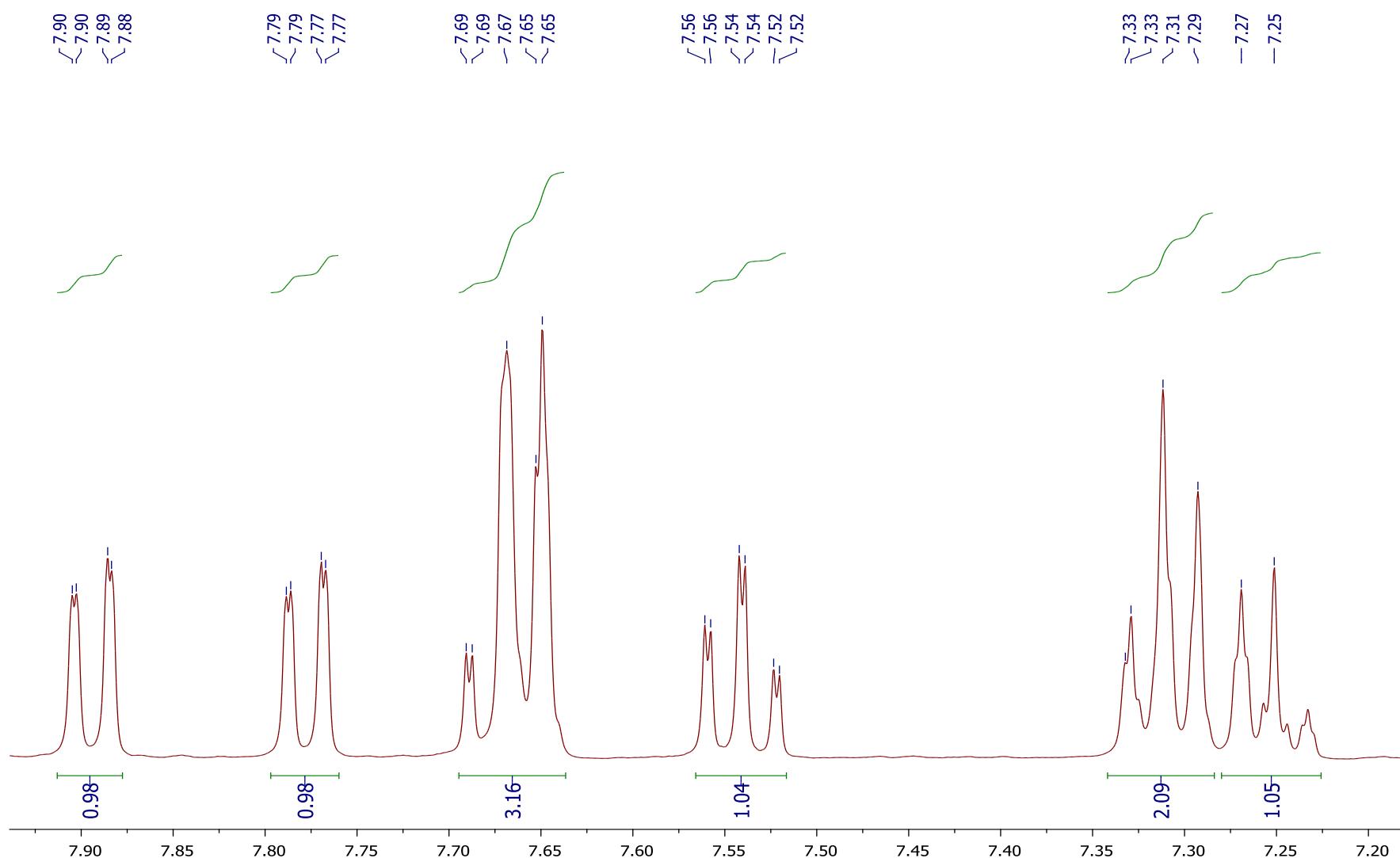


Figure S10. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aromatic region of compound 5.

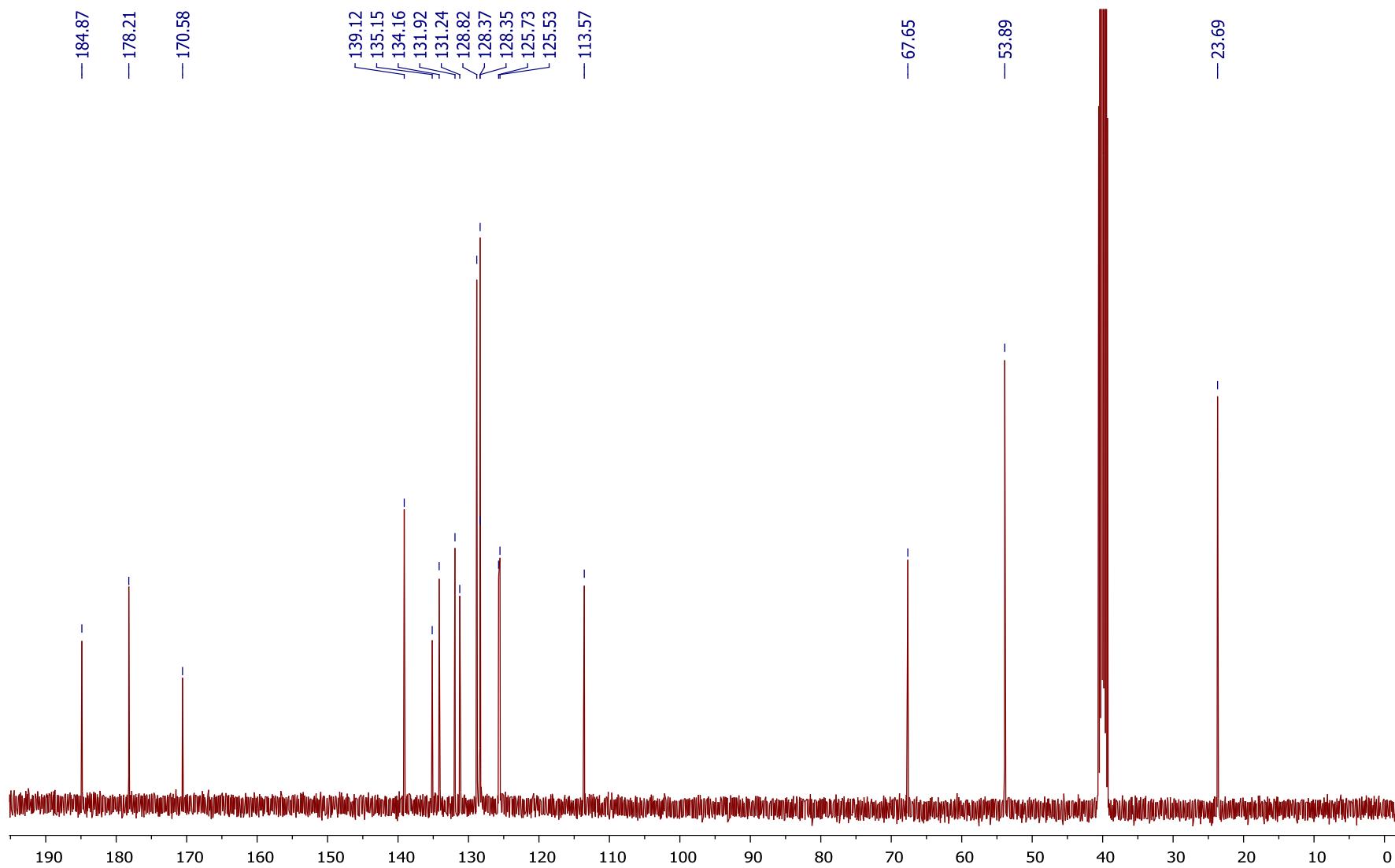


Figure S11. ^{13}C NMR spectrum (101 MHz, $\text{DMSO}-d_6$) of compound 5.

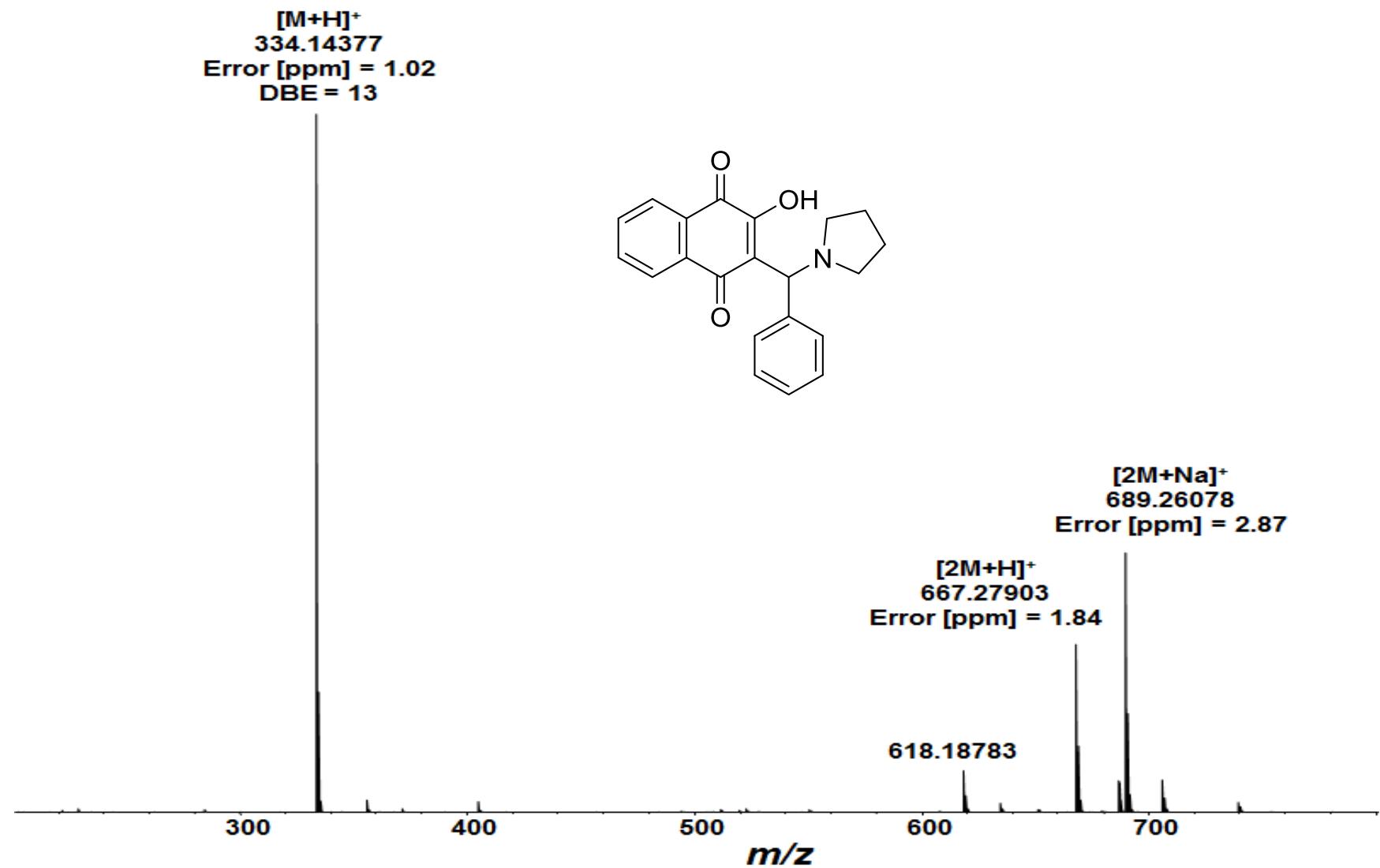


Figure S12. ESI(+) -FT-ICR mass spectrum of compound 5.

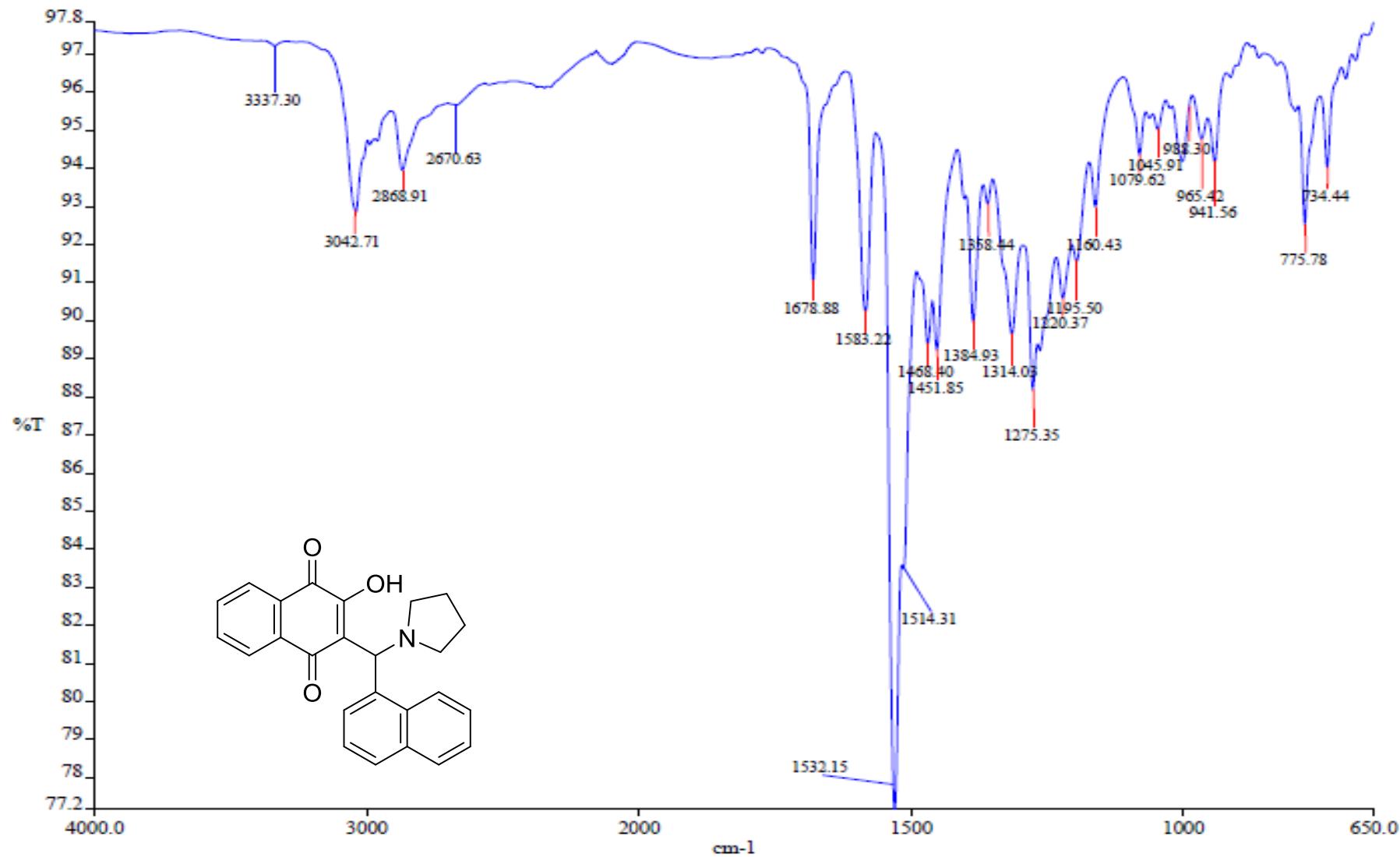


Figure S13. Infrared spectrum (ATR) of compound 6.

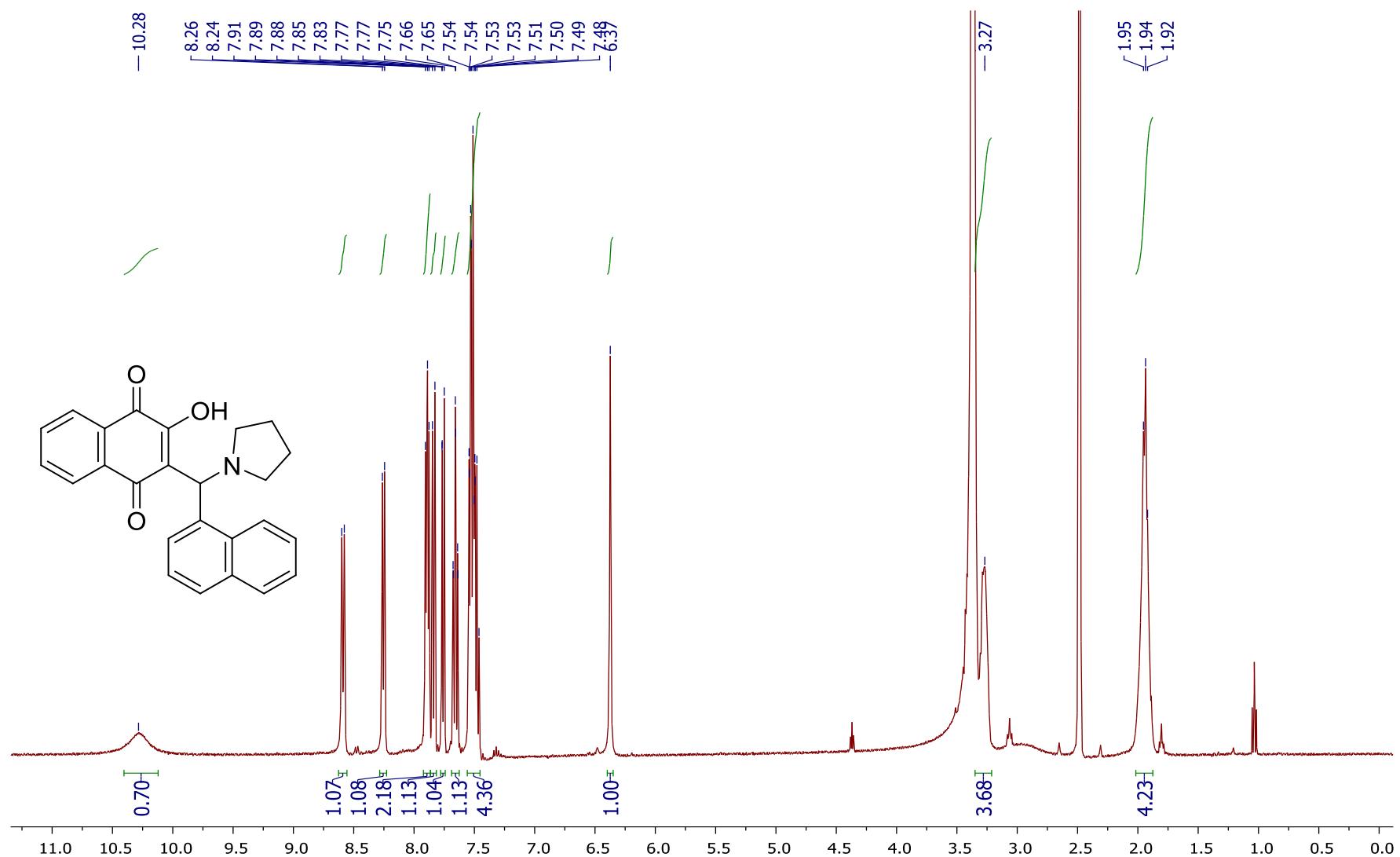


Figure S14. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 6.

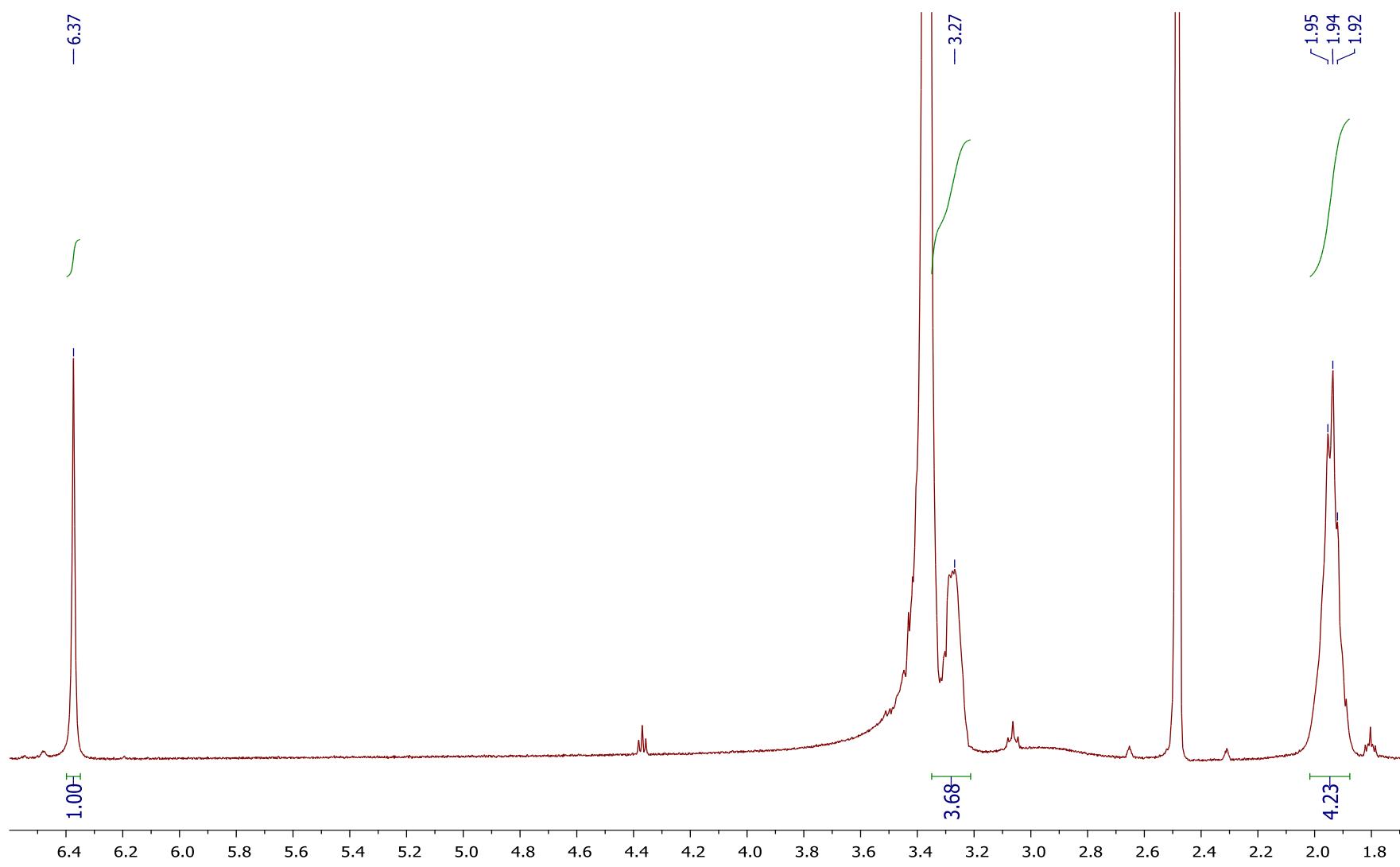


Figure S15. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aliphatic region of compound **6**.

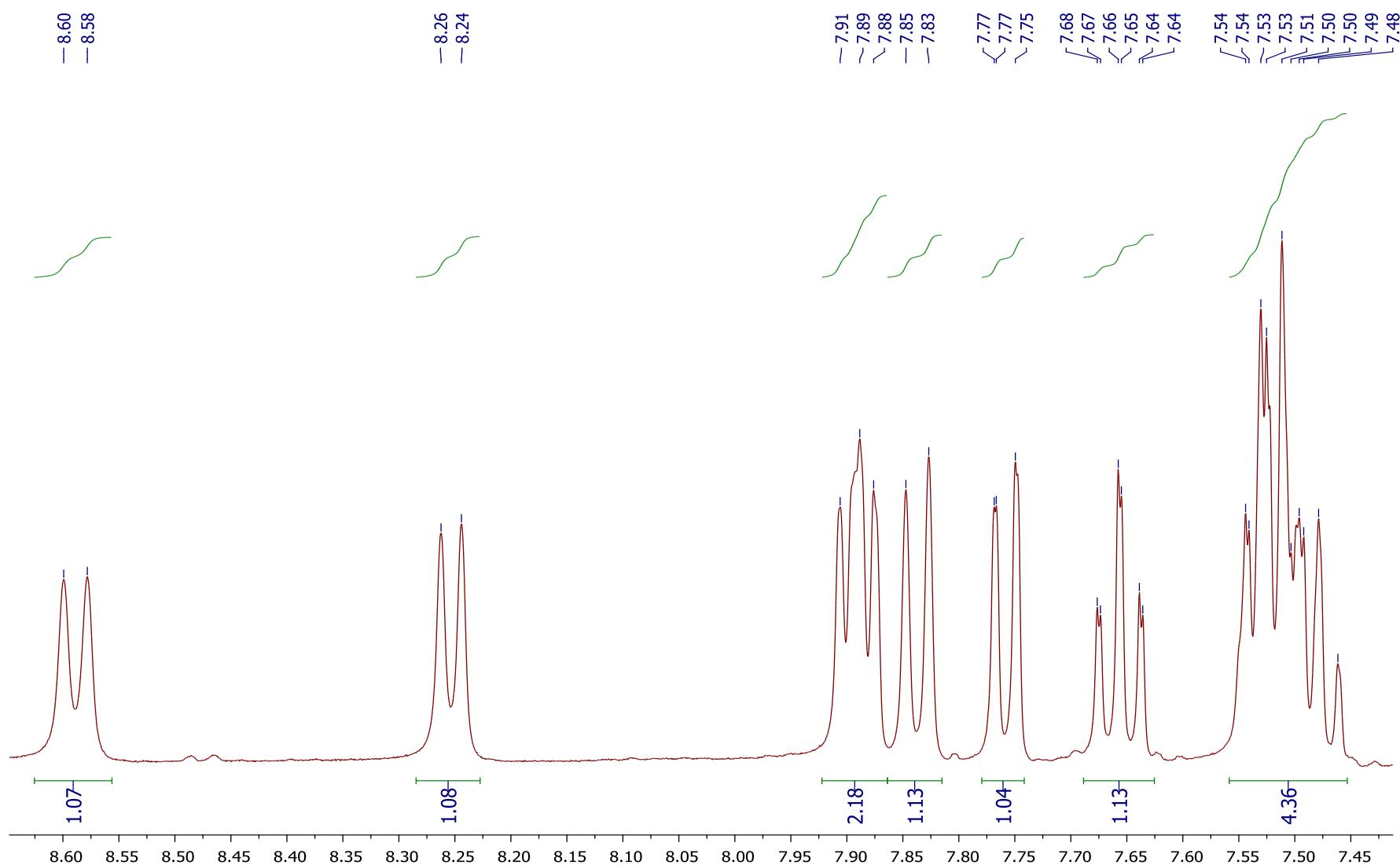


Figure S16. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aromatic region of compound 6.

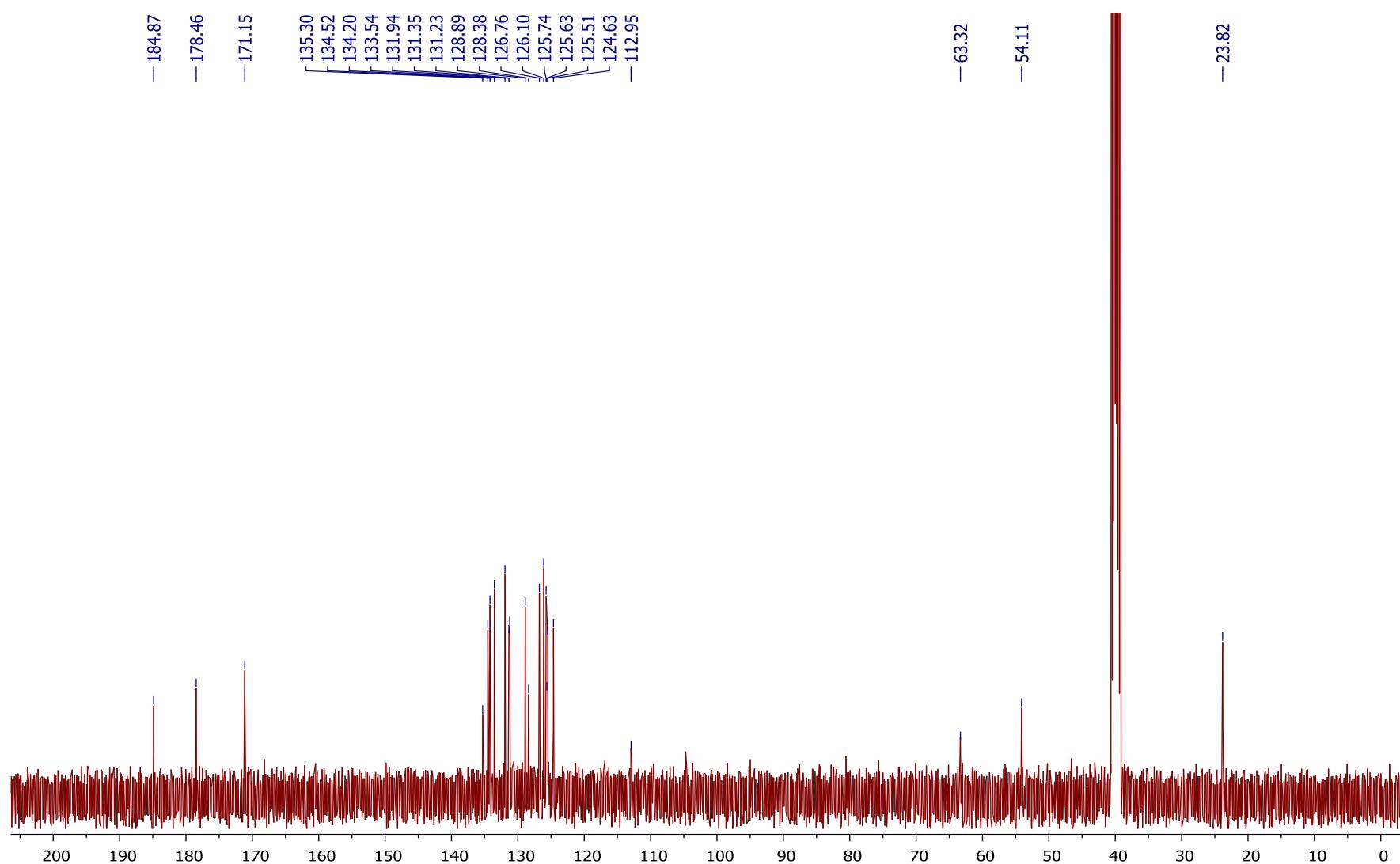


Figure S17. ^{13}C NMR spectrum (101 MHz, DMSO- d_6) of compound 6.

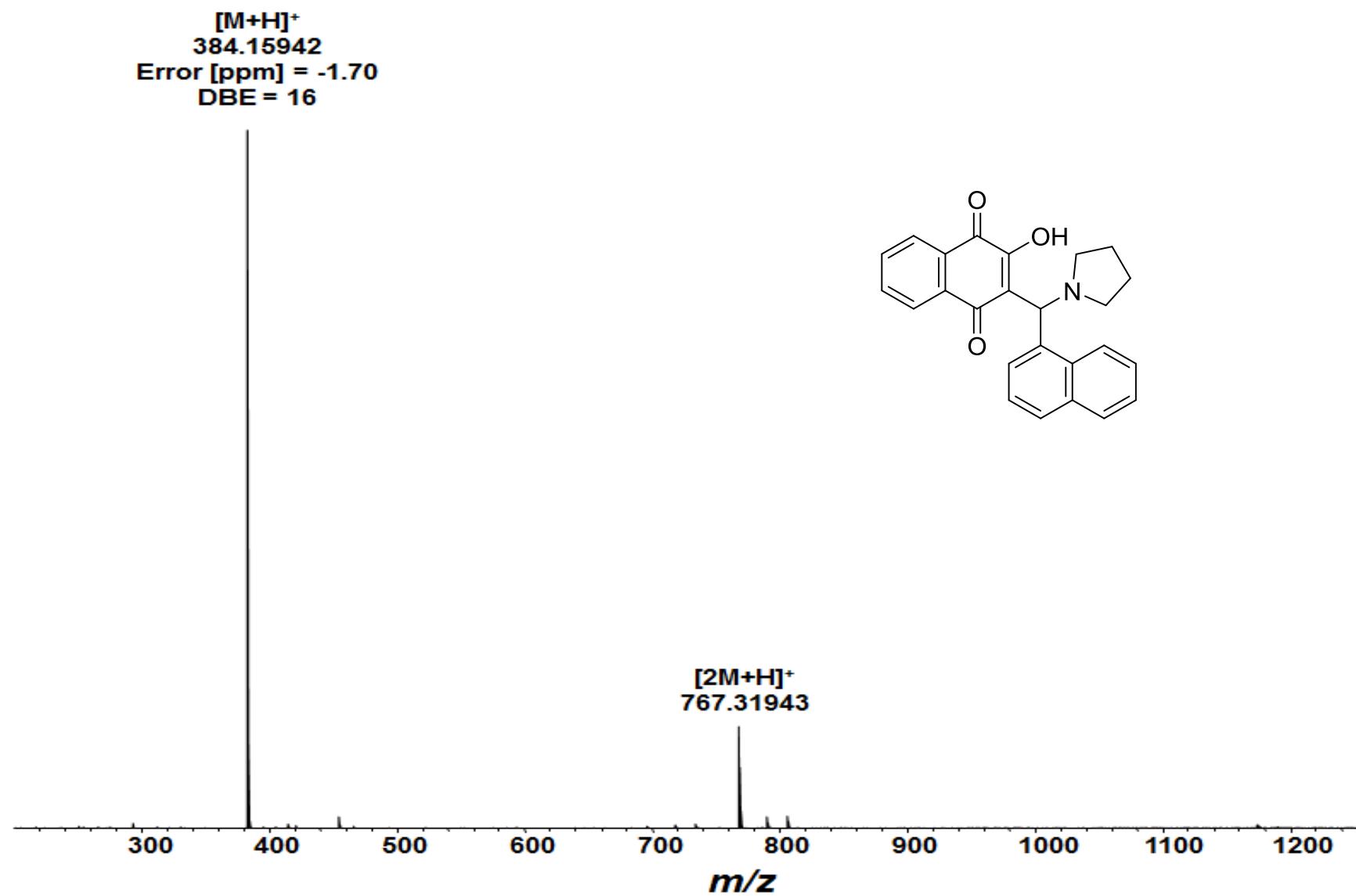


Figure S18. ESI(+) -FT-ICR mass spectrum of compound 6.

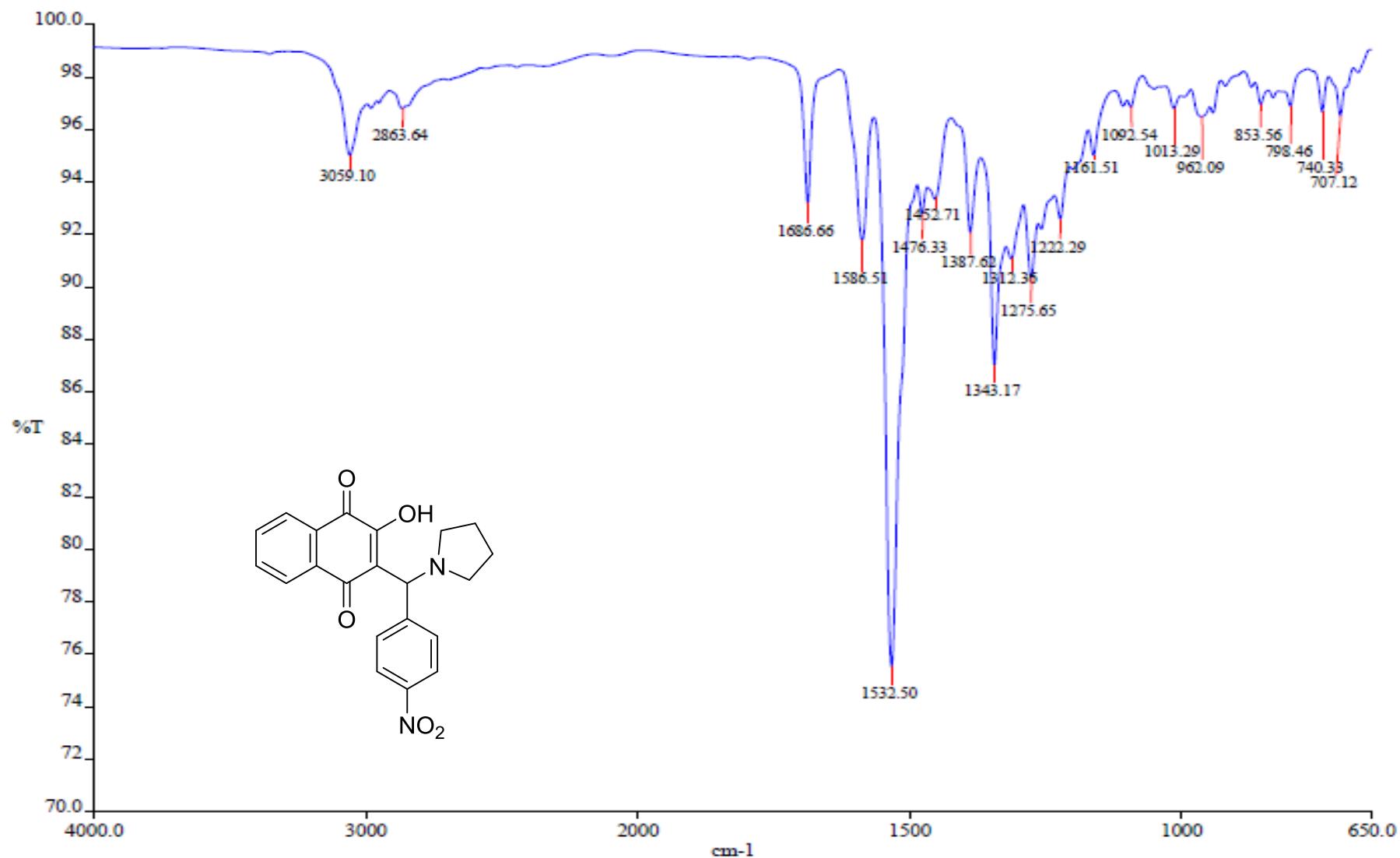


Figure S19. Infrared spectrum (ATR) of compound 7.

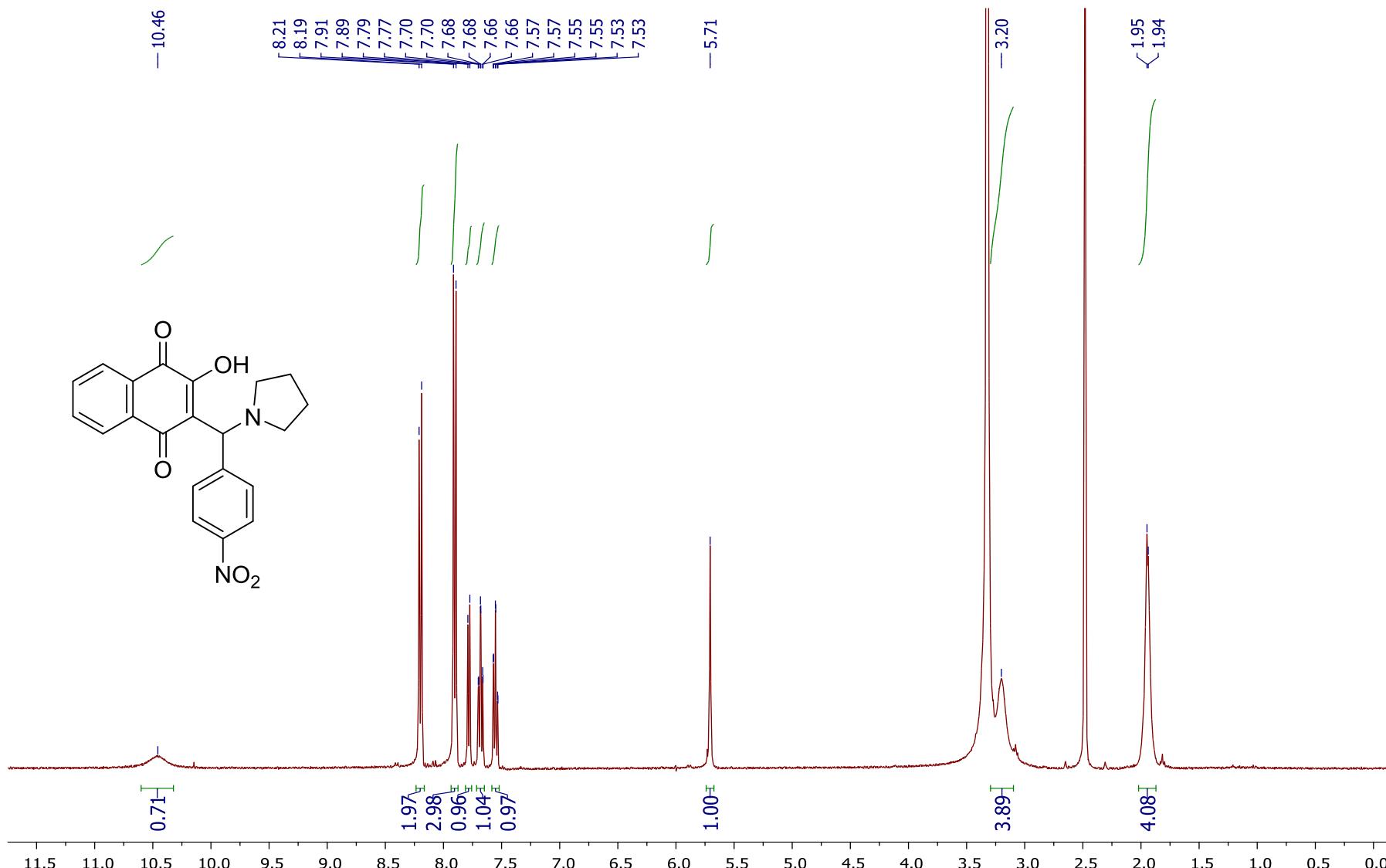


Figure S20. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 7.

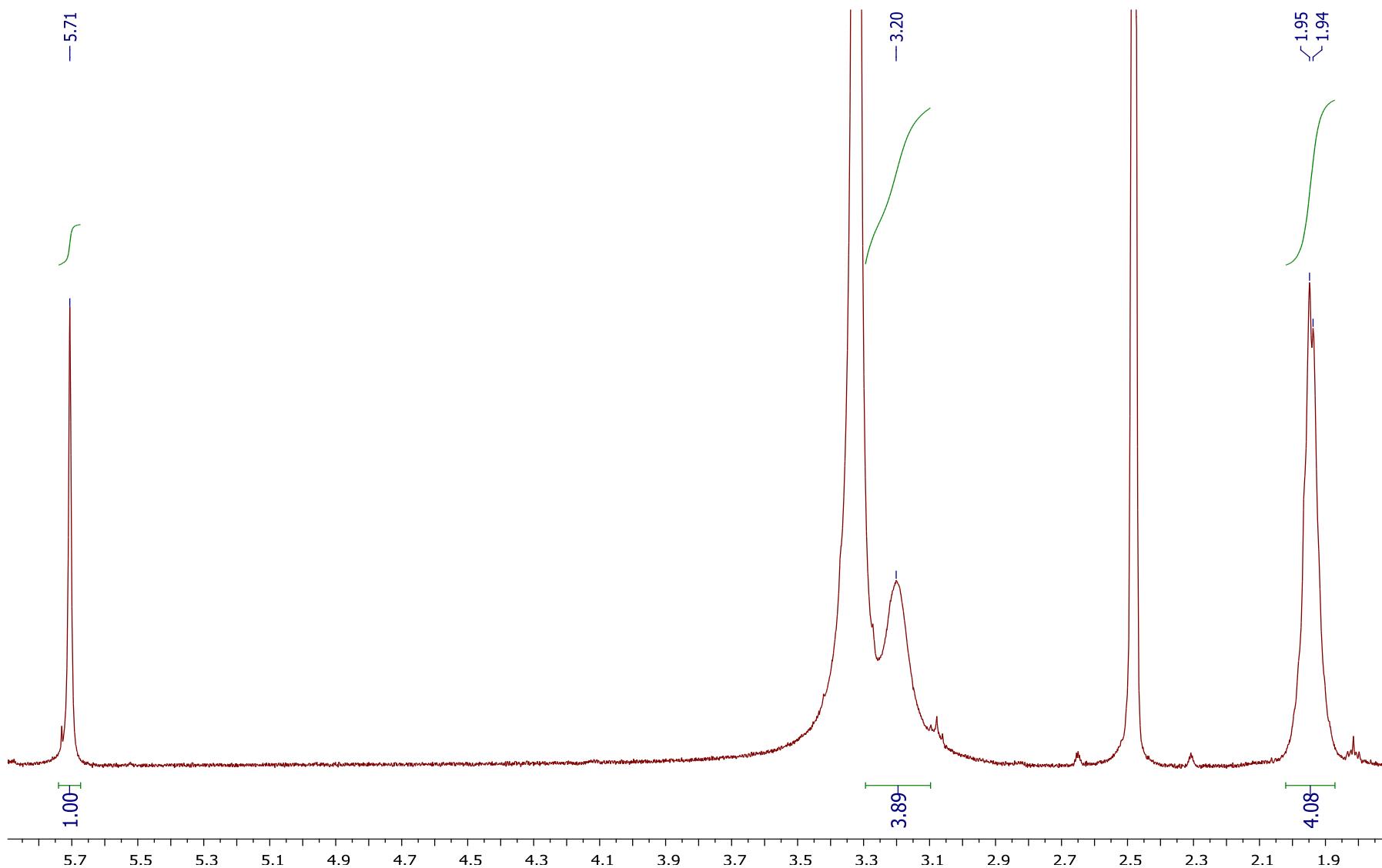


Figure S21. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aliphatic region of compound 7.

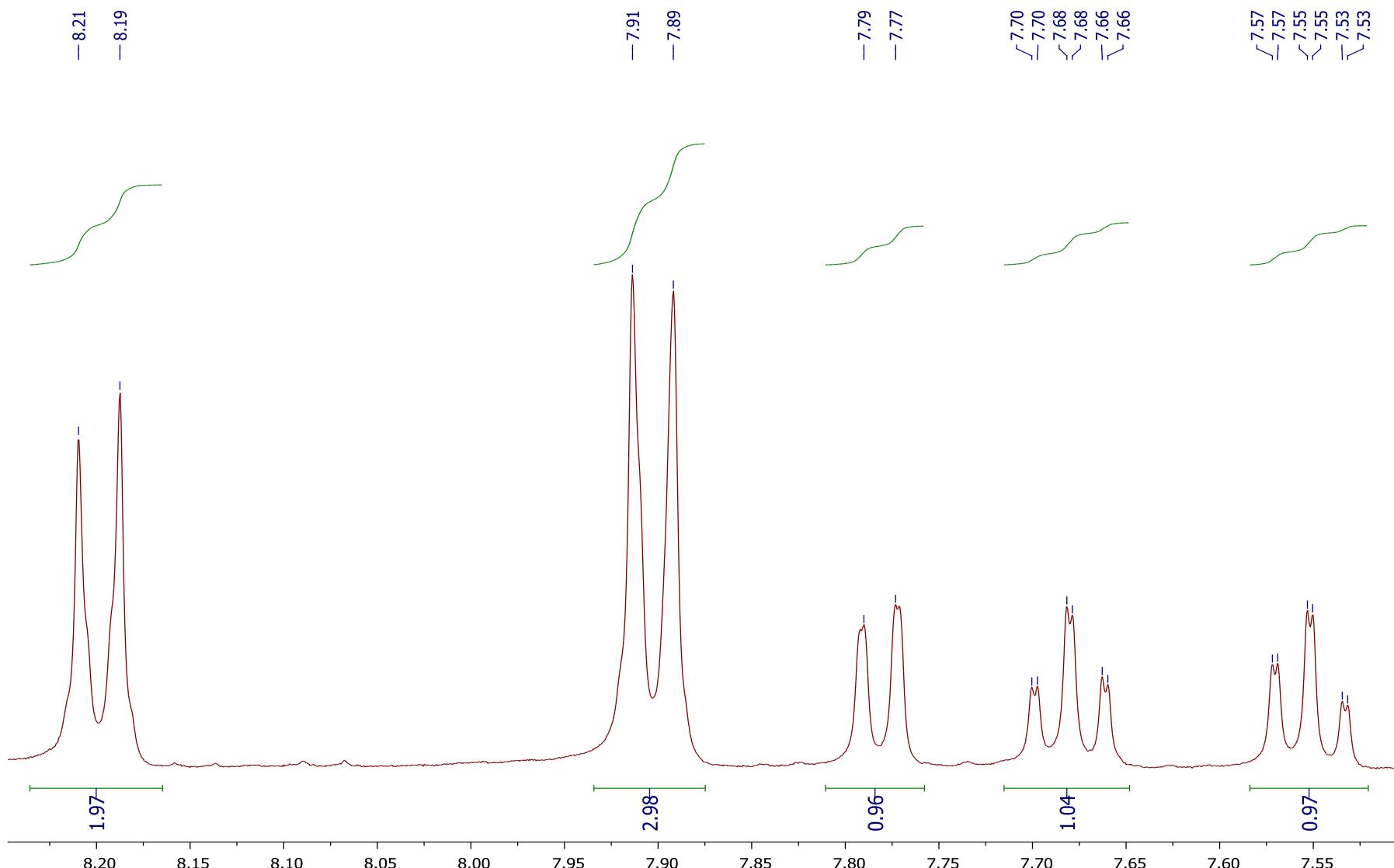


Figure S22. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aromatic region of compound 7.

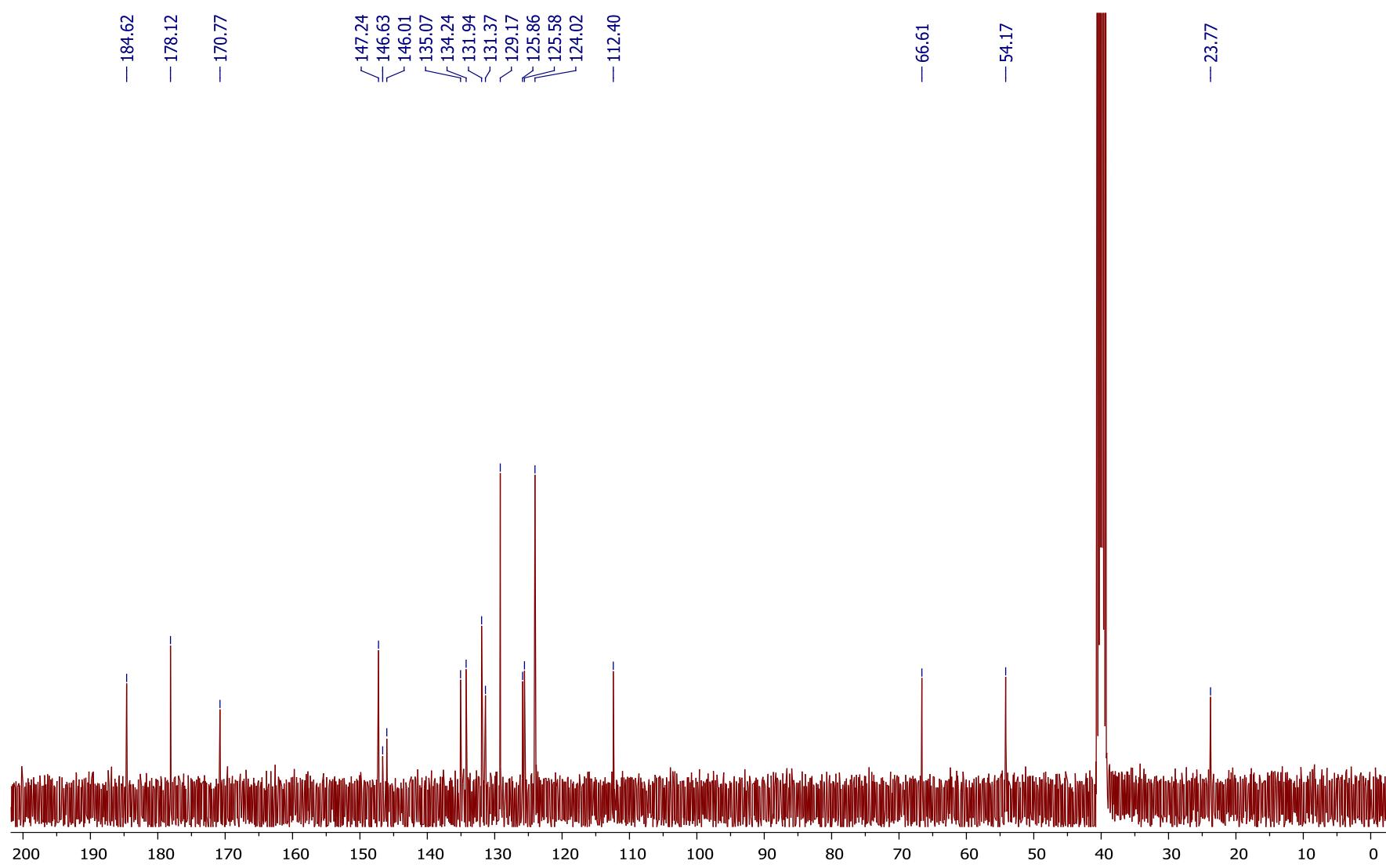


Figure S23. ^{13}C NMR spectrum (101 MHz, $\text{DMSO}-d_6$) of compound 7.

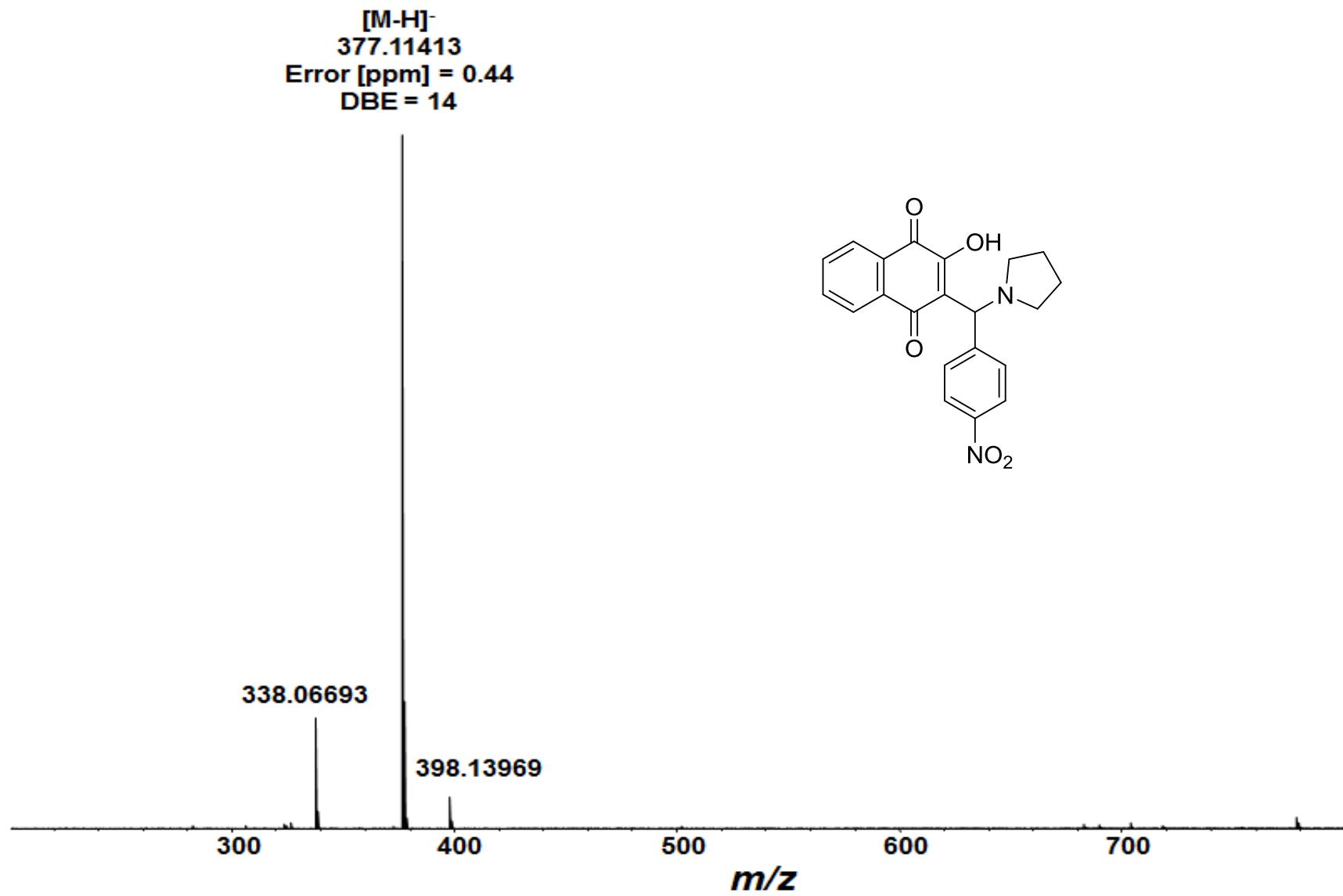


Figure S24. ESI(-)-FT-ICR mass spectrum of compound 7.

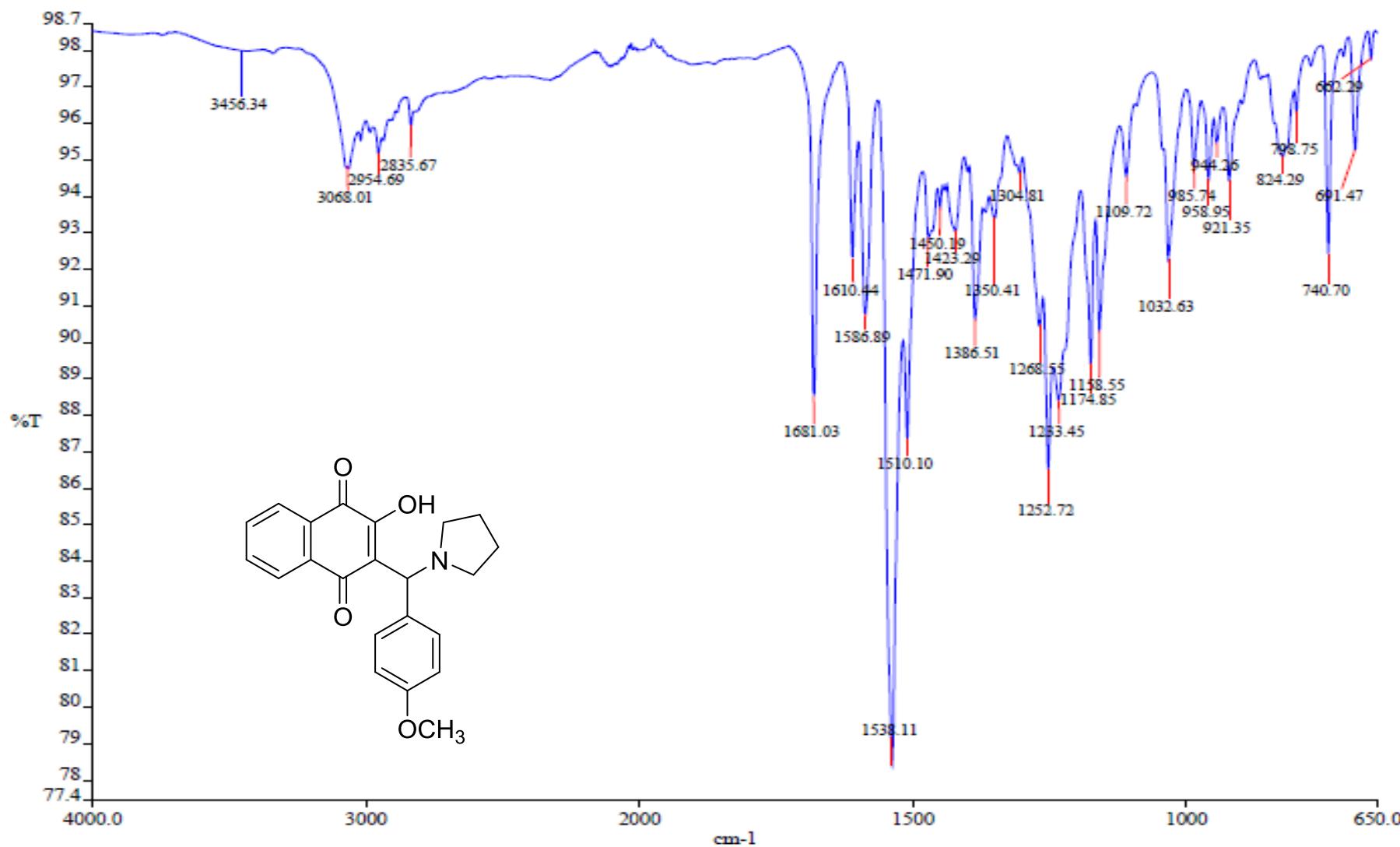


Figure S25. Infrared spectrum (ATR) of compound 8.

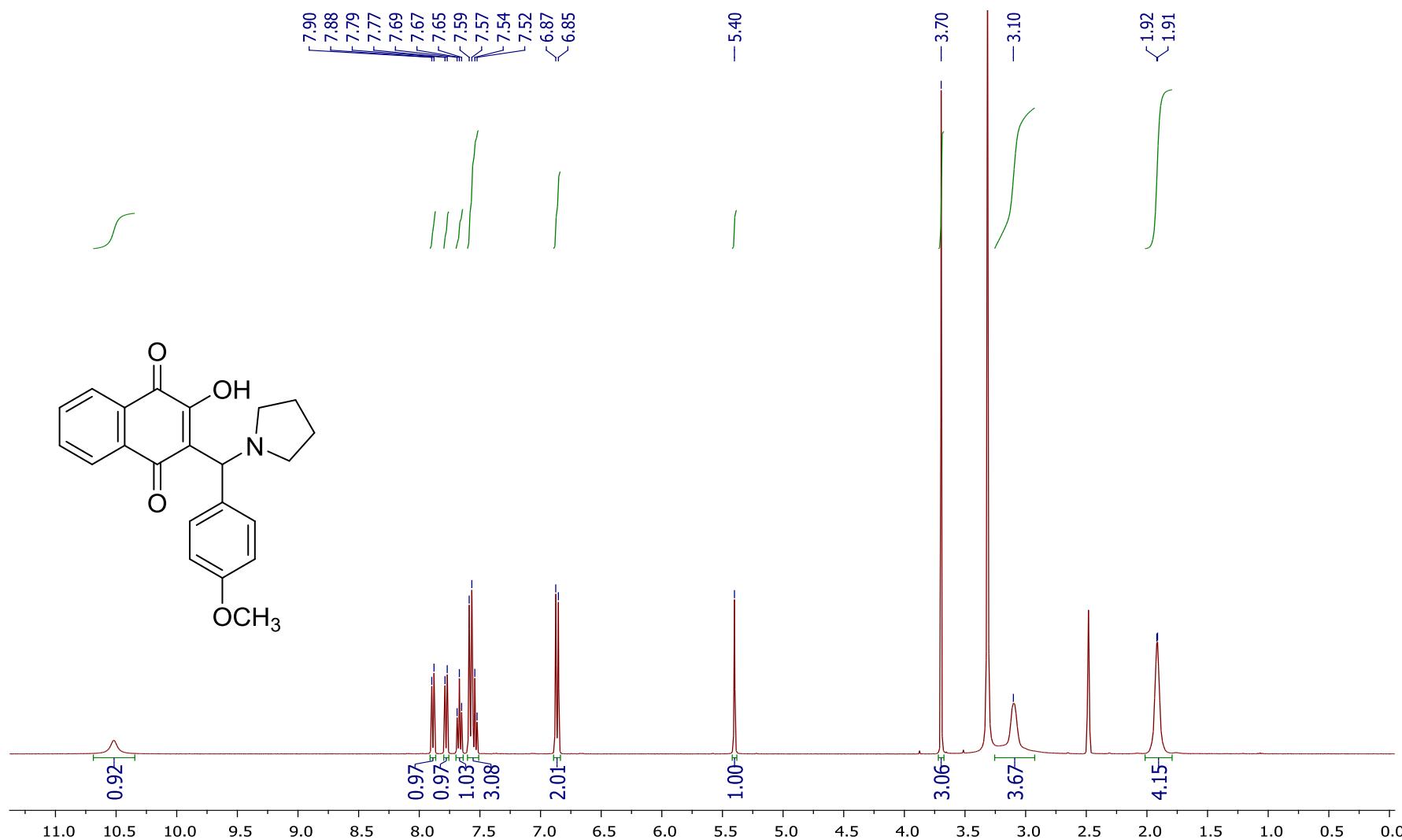


Figure S26. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 8.

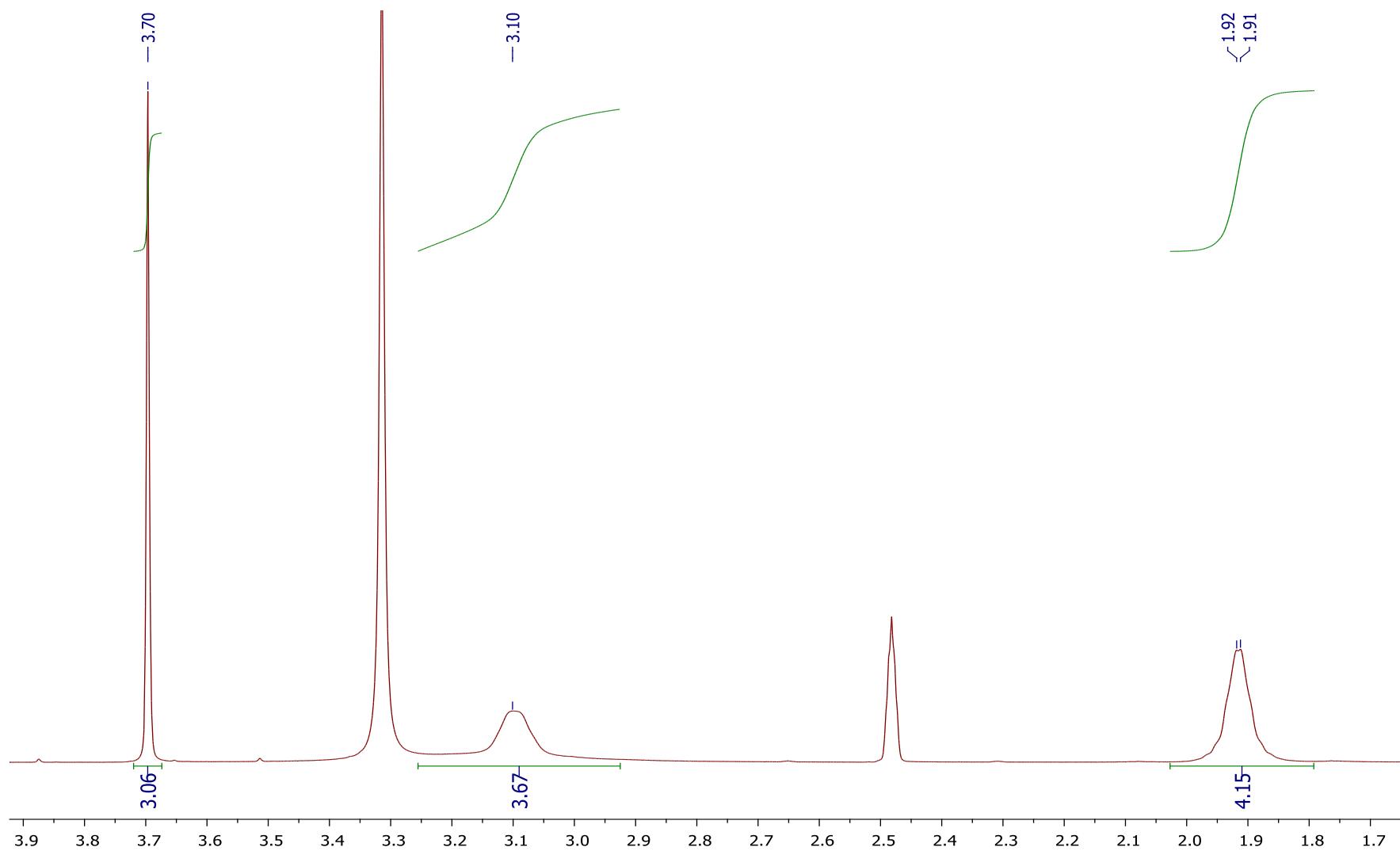


Figure S27. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aliphatic region of compound 8.

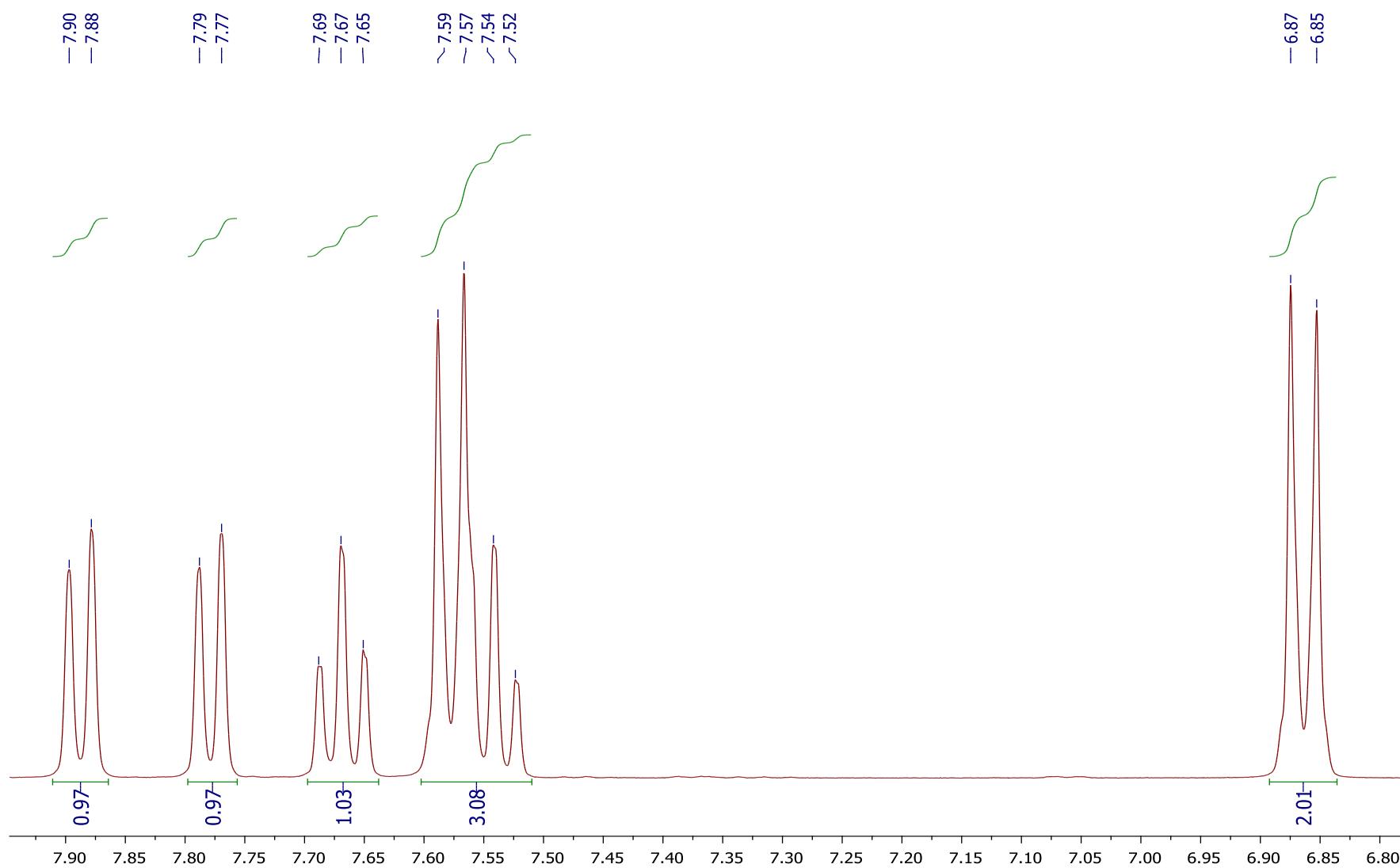


Figure S28. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aromatic region of compound 8.

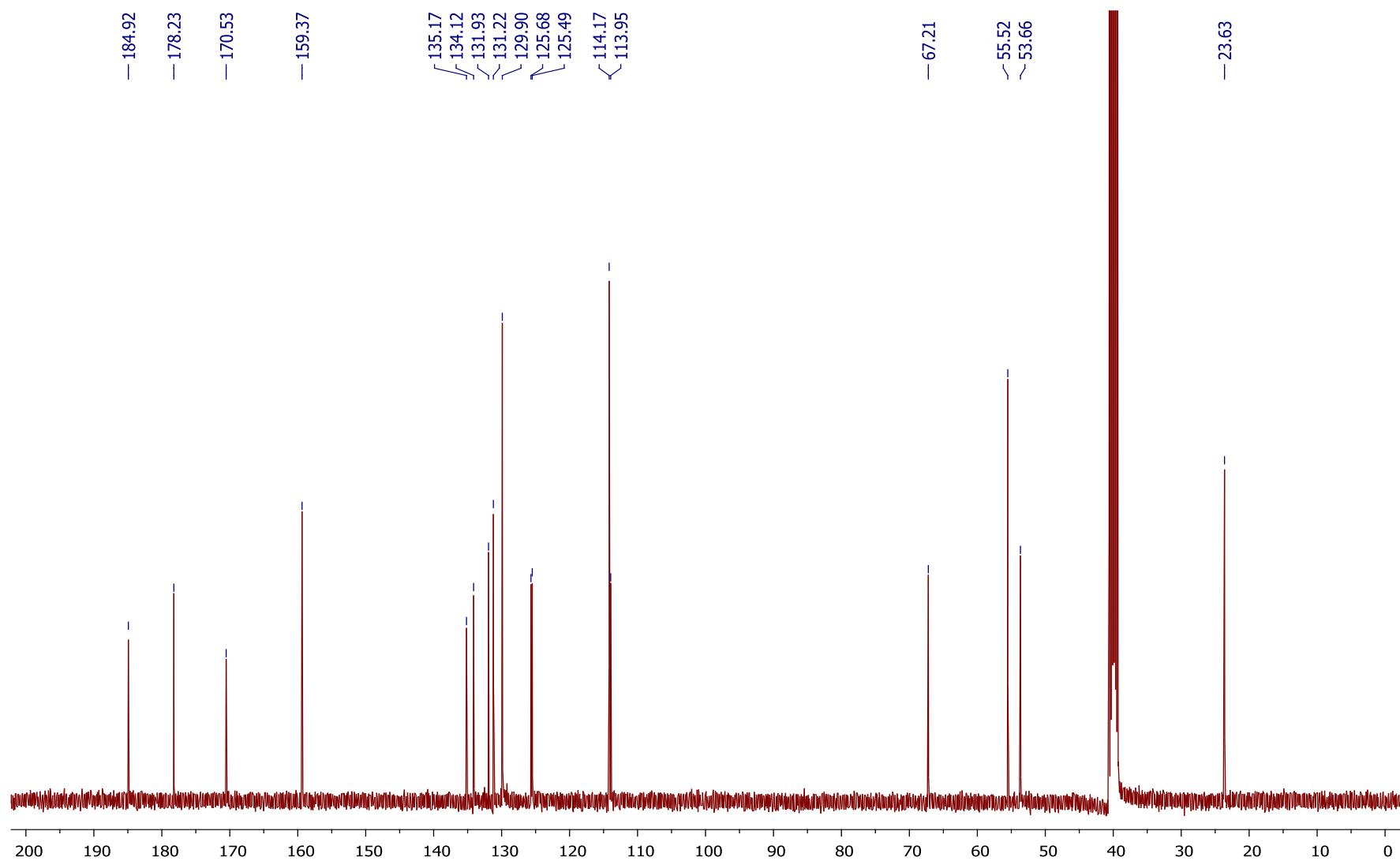


Figure S29. ^{13}C NMR spectrum (101 MHz, DMSO- d_6) of compound 8.

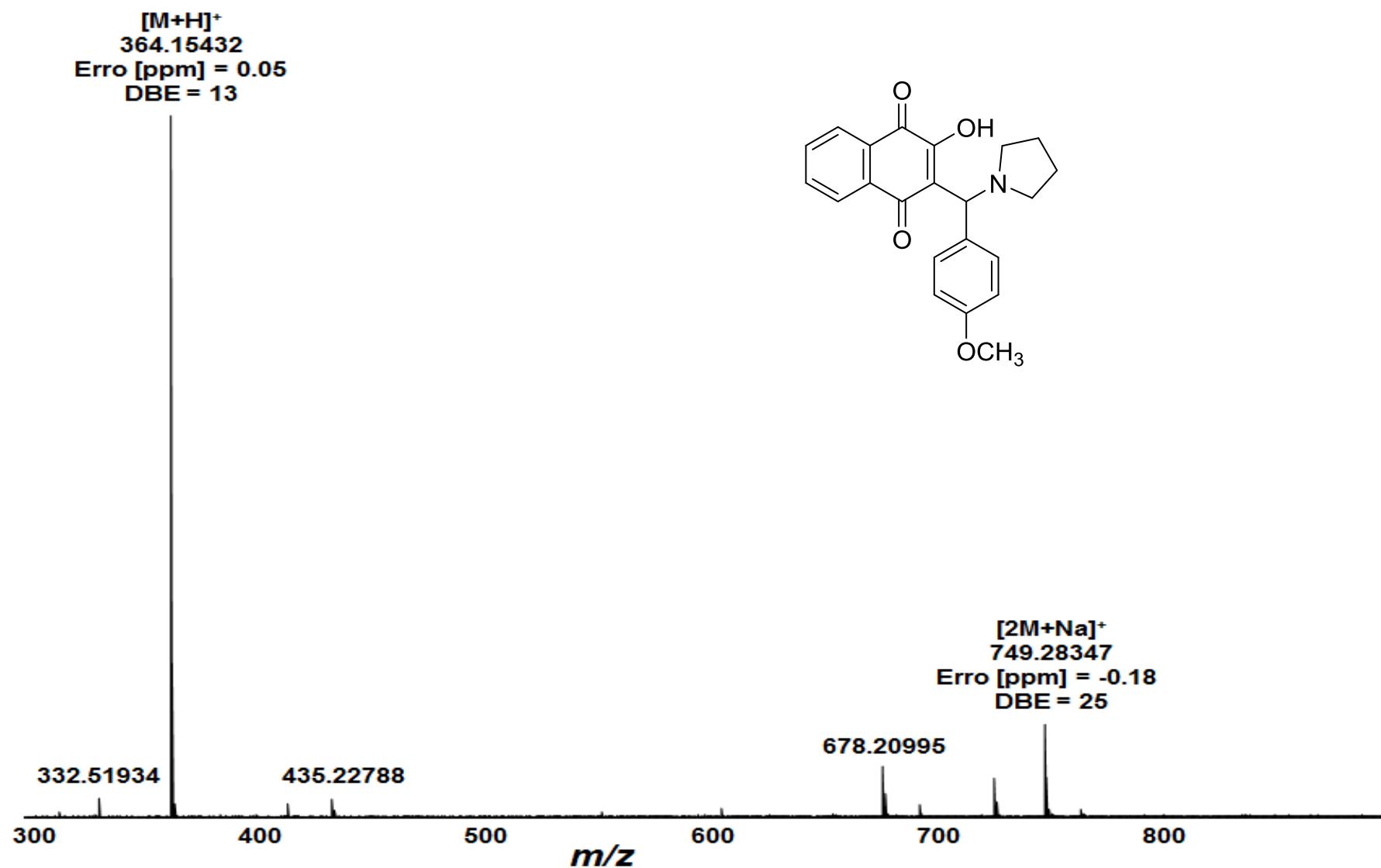


Figure S30. ESI(+) -FT-ICR mass spectrum of compound 8.

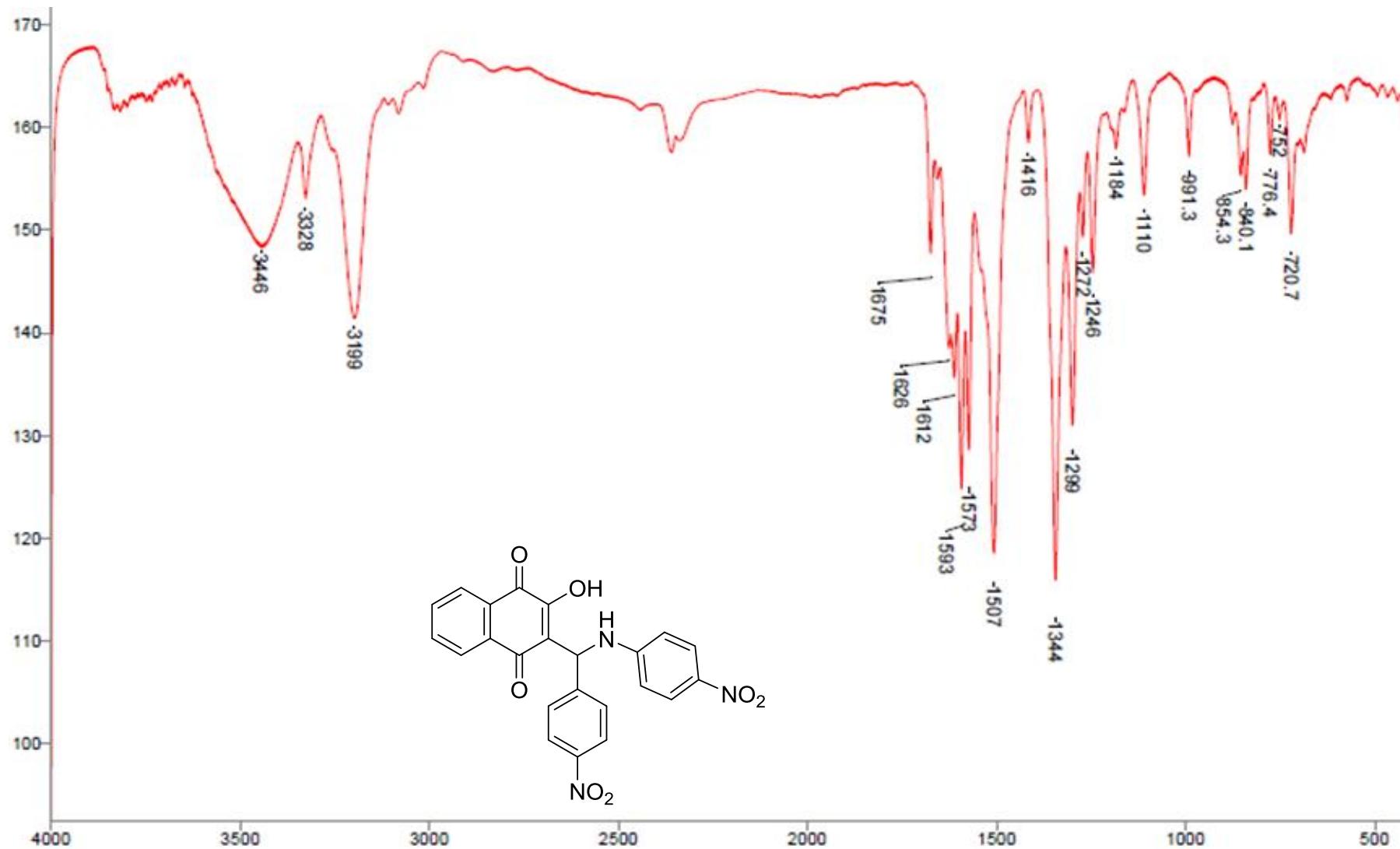


Figure S31. Infrared spectrum (KBr) of compound 10.

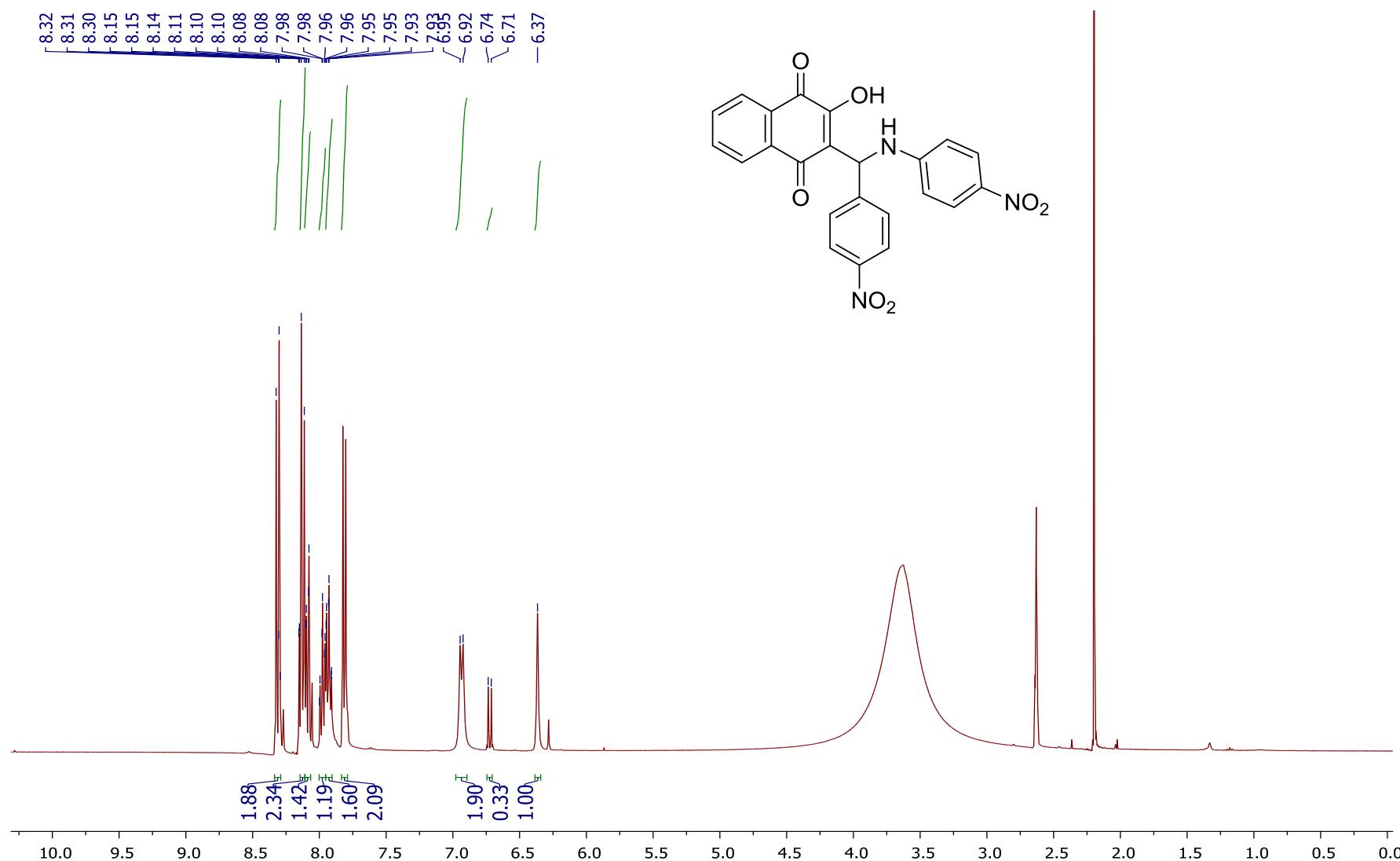


Figure S32. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **10**.

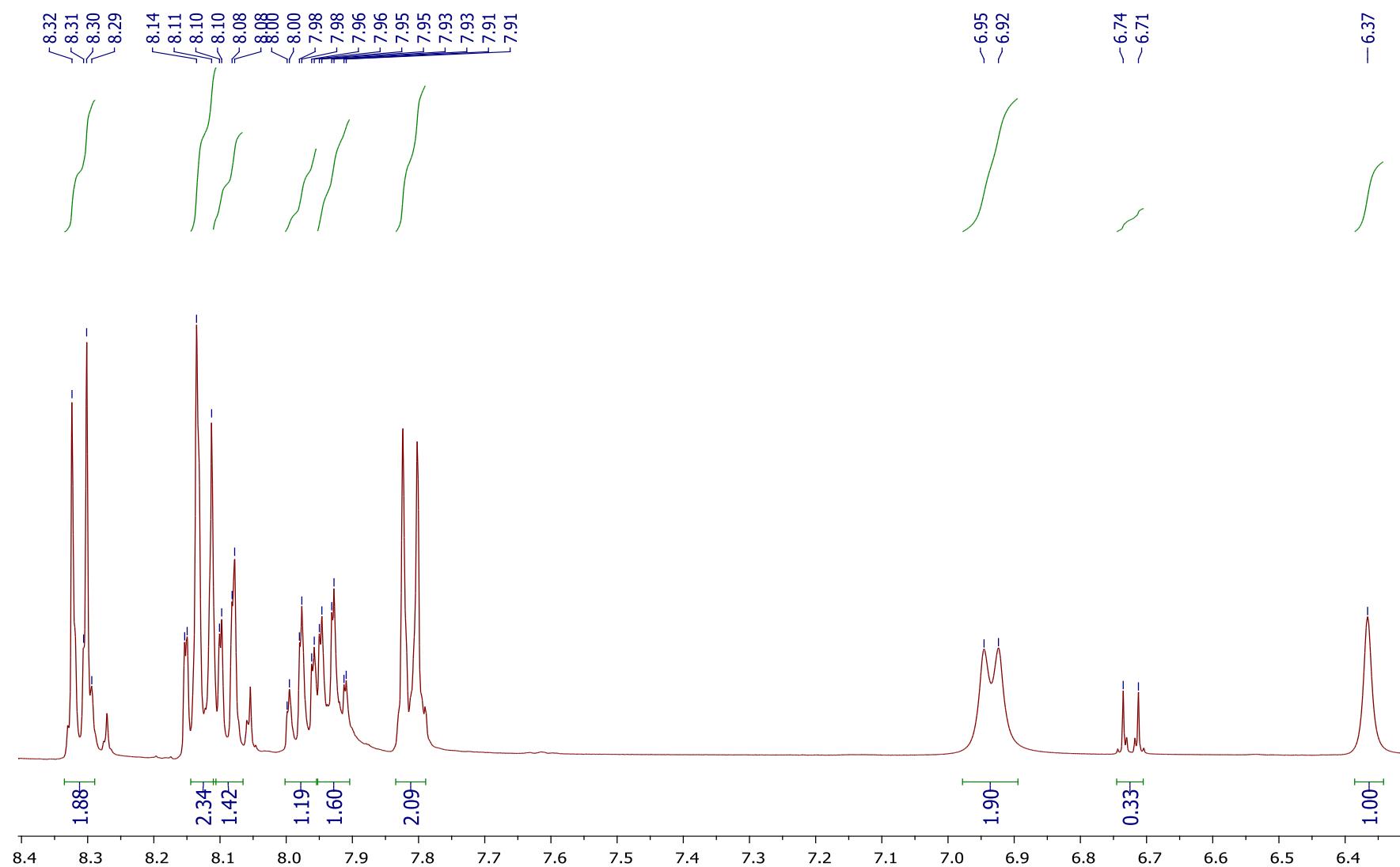


Figure S33. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aromatic region of compound 10.

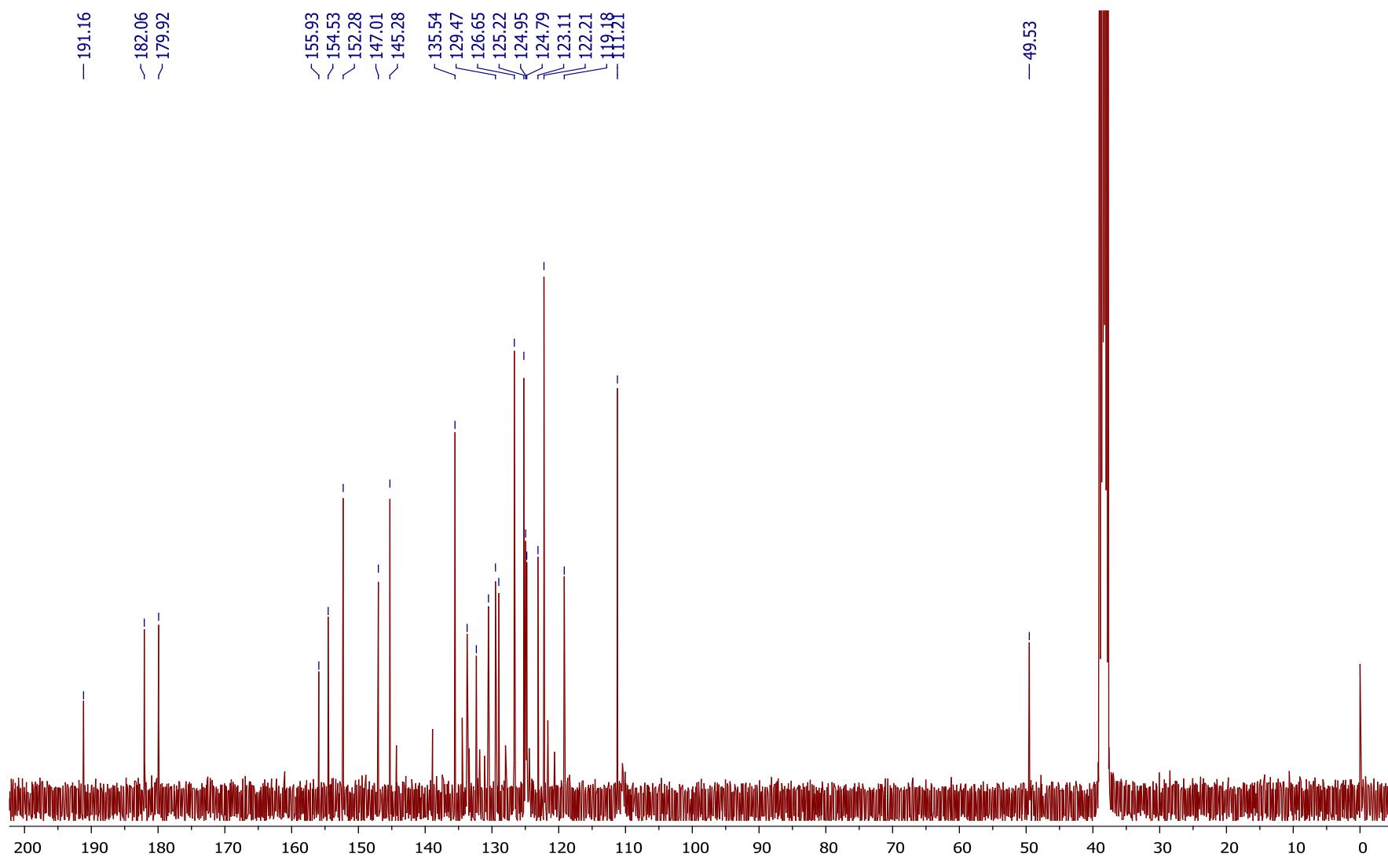


Figure S34. ^{13}C NMR spectrum (101 MHz, $\text{DMSO}-d_6$) of compound **10**.

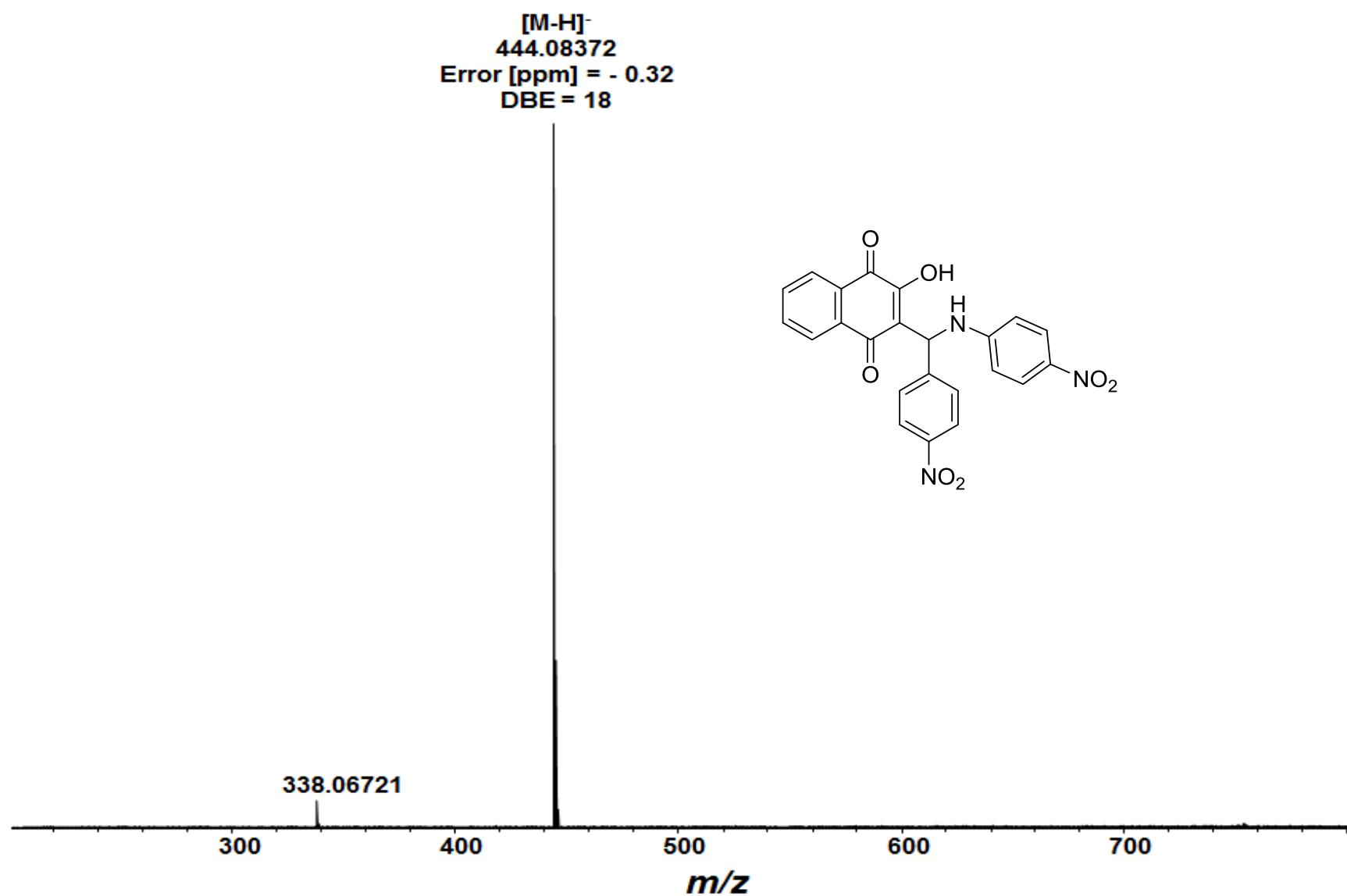


Figure S35. ESI(-)-FT-ICR mass spectrum of compound 10.

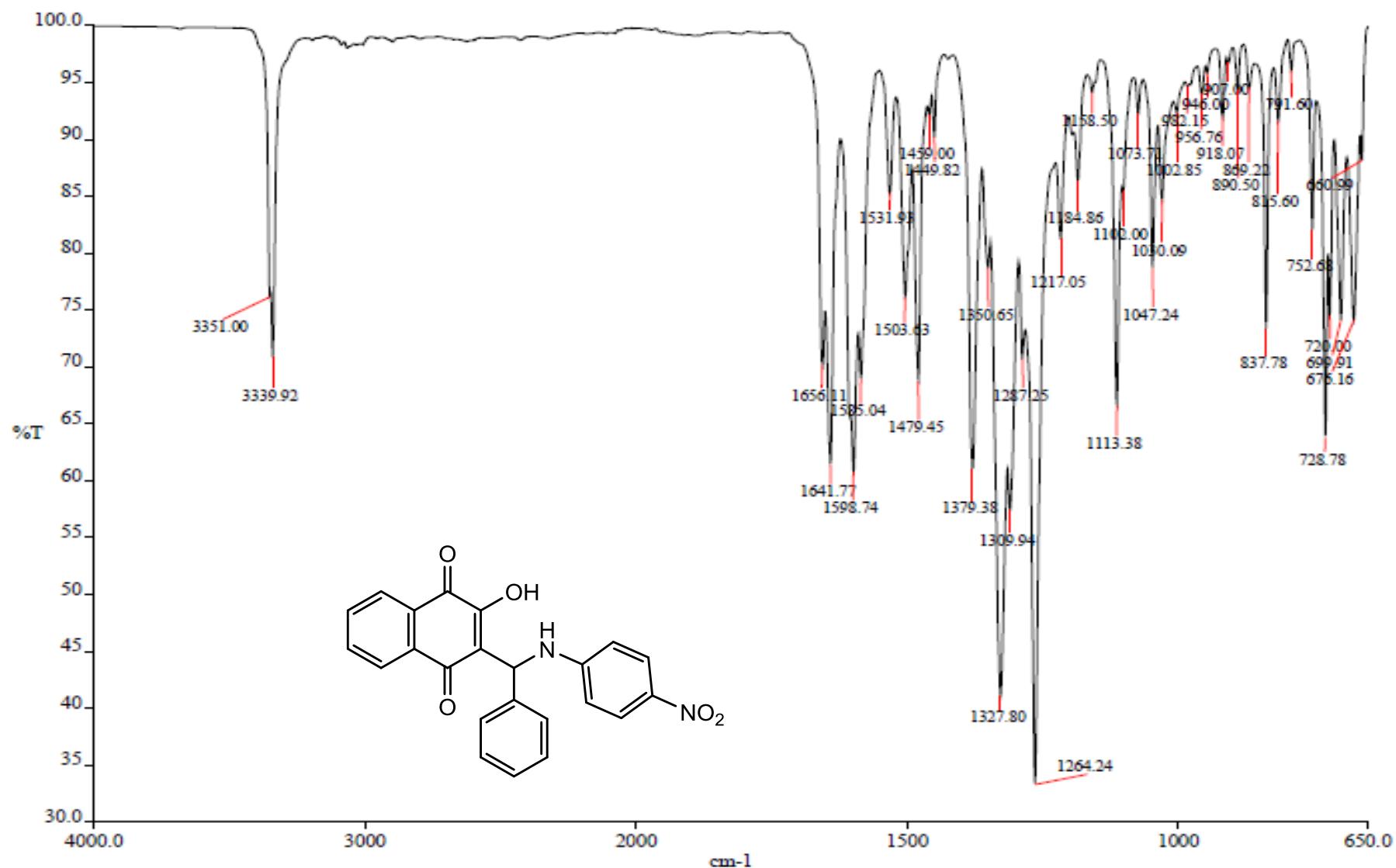


Figure S36. Infrared spectrum (ATR) of compound 11.

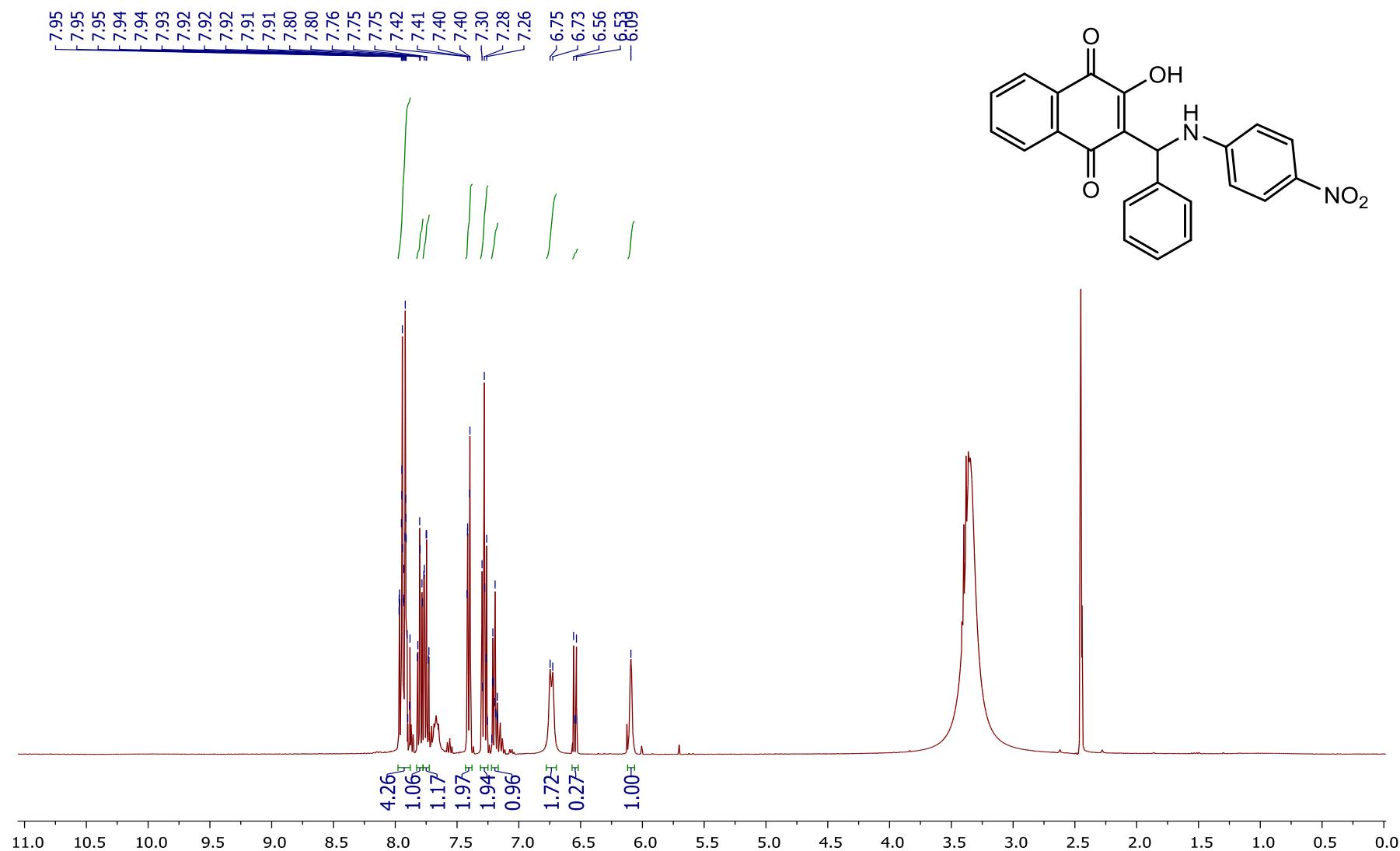


Figure S37. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound 11.

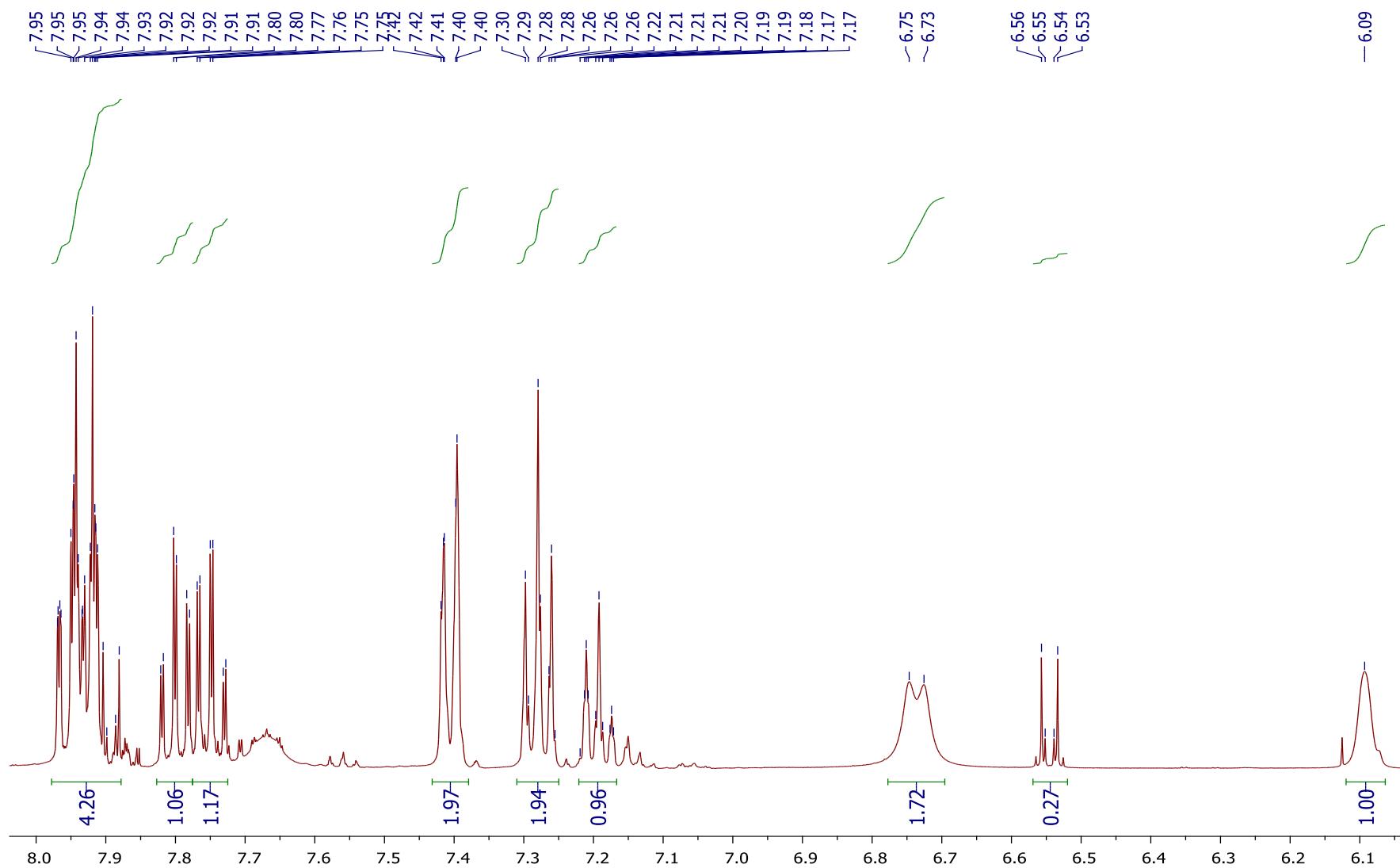


Figure S38. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aromatic region of compound 11.

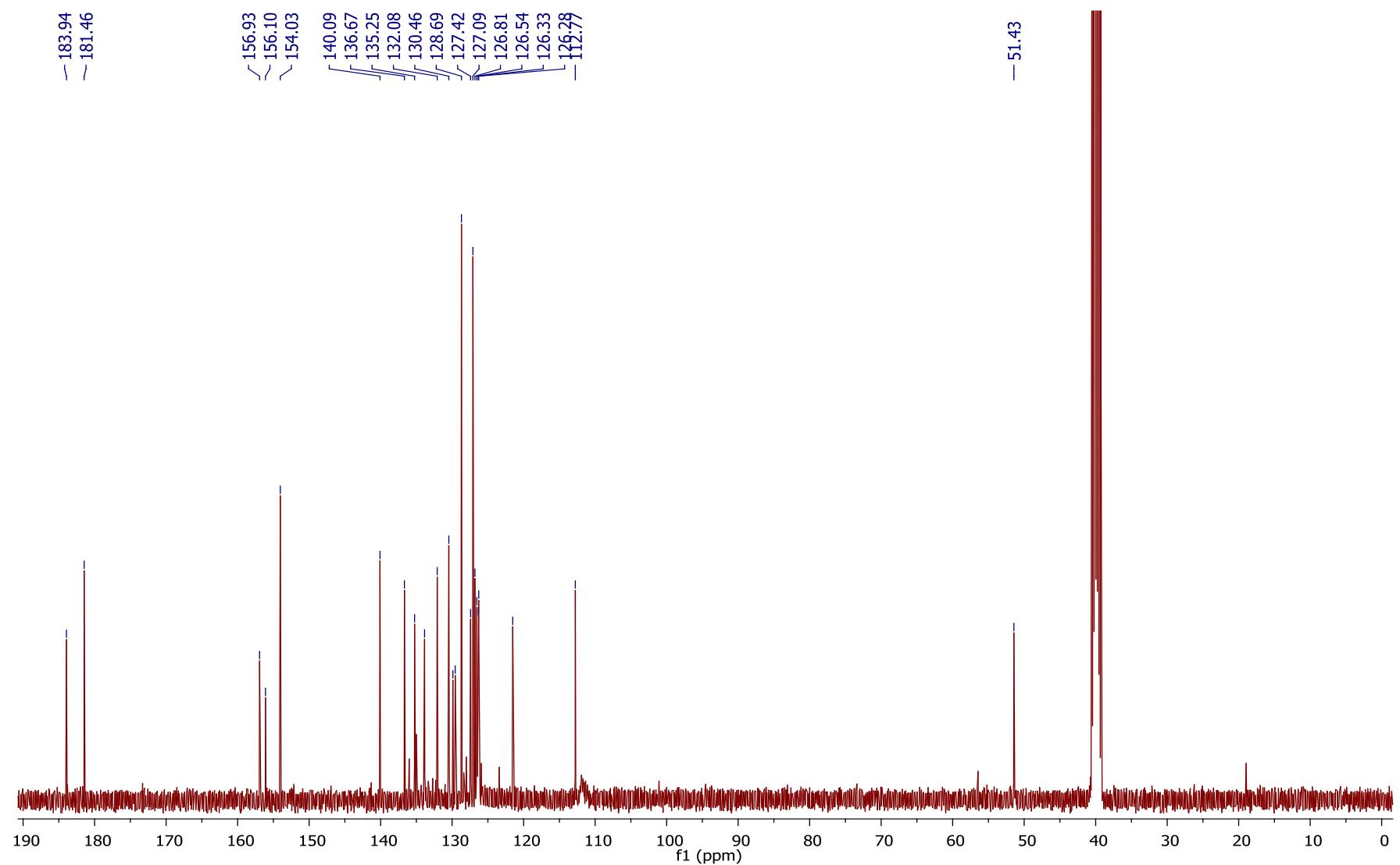


Figure S39. ^{13}C NMR spectrum (101 MHz, $\text{DMSO}-d_6$) of compound **11**.

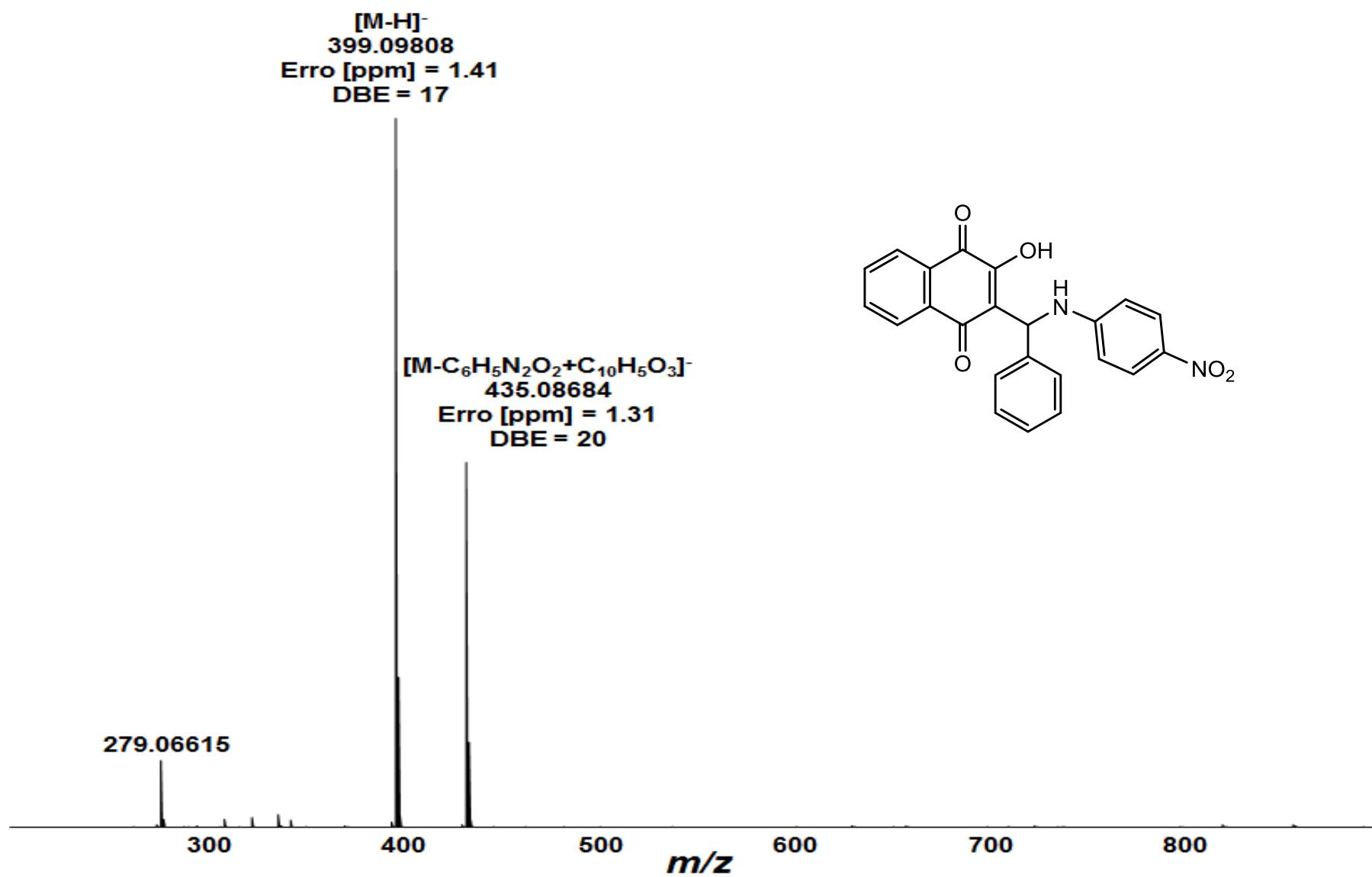


Figure S40. ESI(-)-FT-ICR mass spectrum of compound 11.

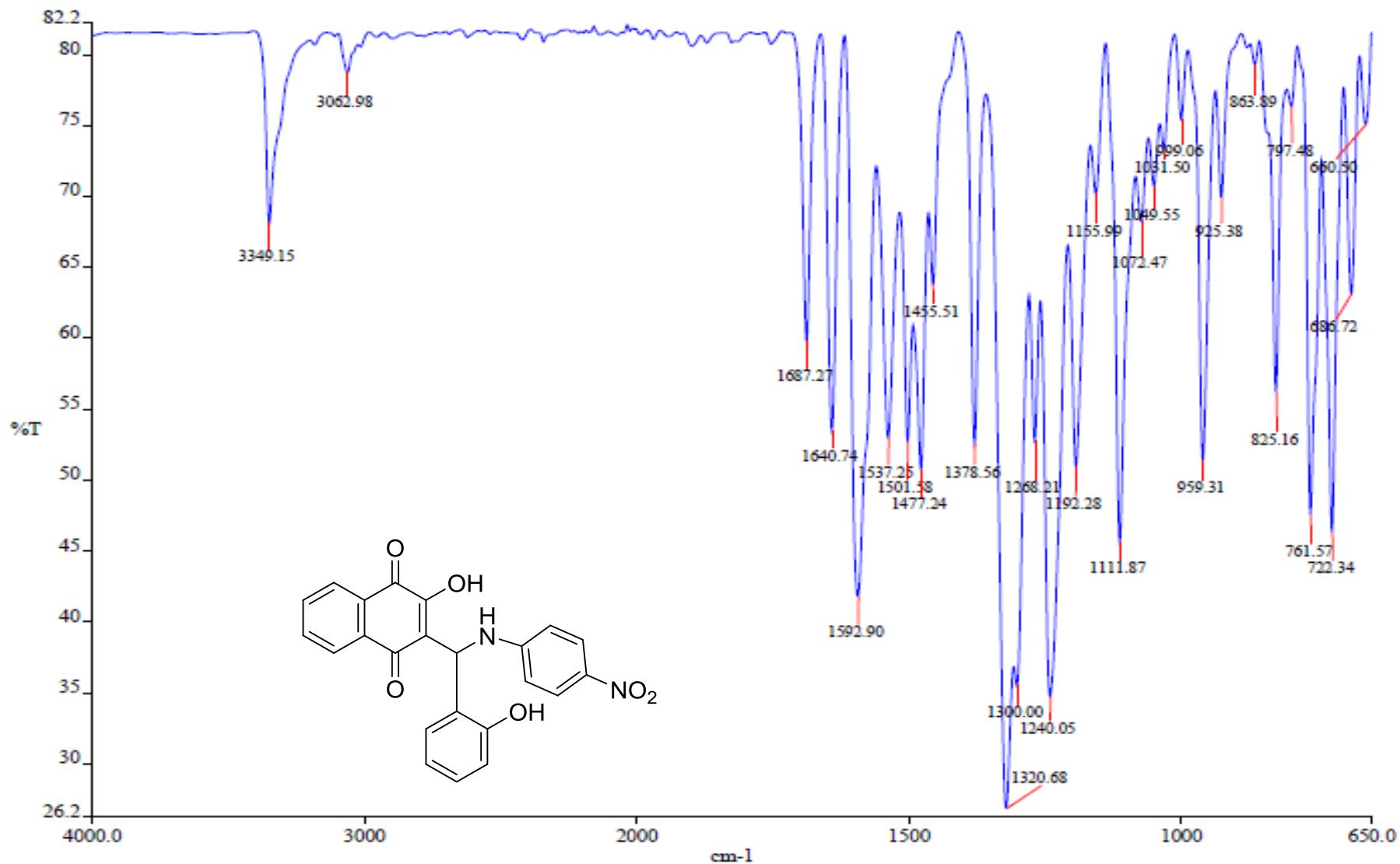


Figure S41. Infrared spectrum (ATR) of compound 12.

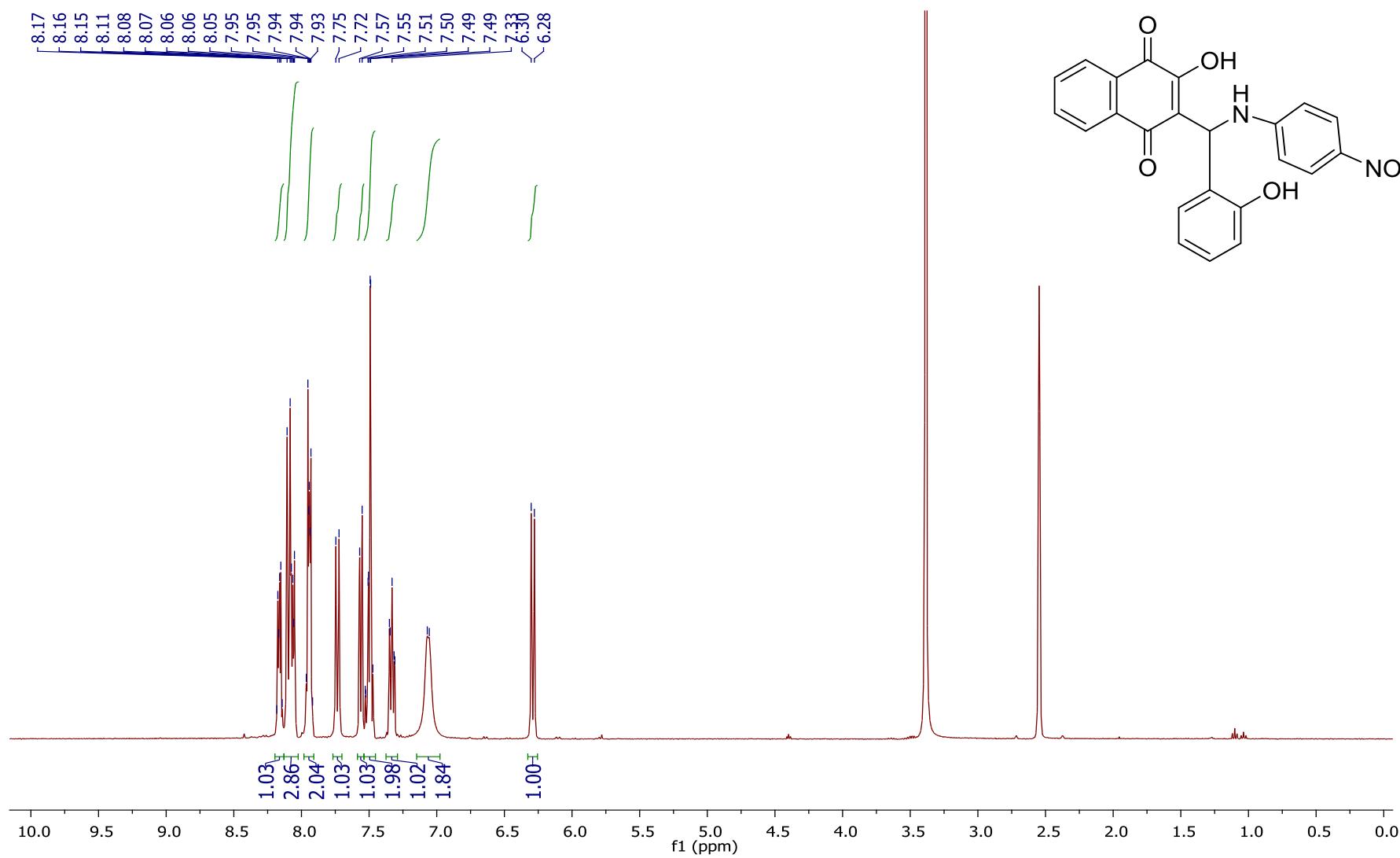


Figure S42. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 12.

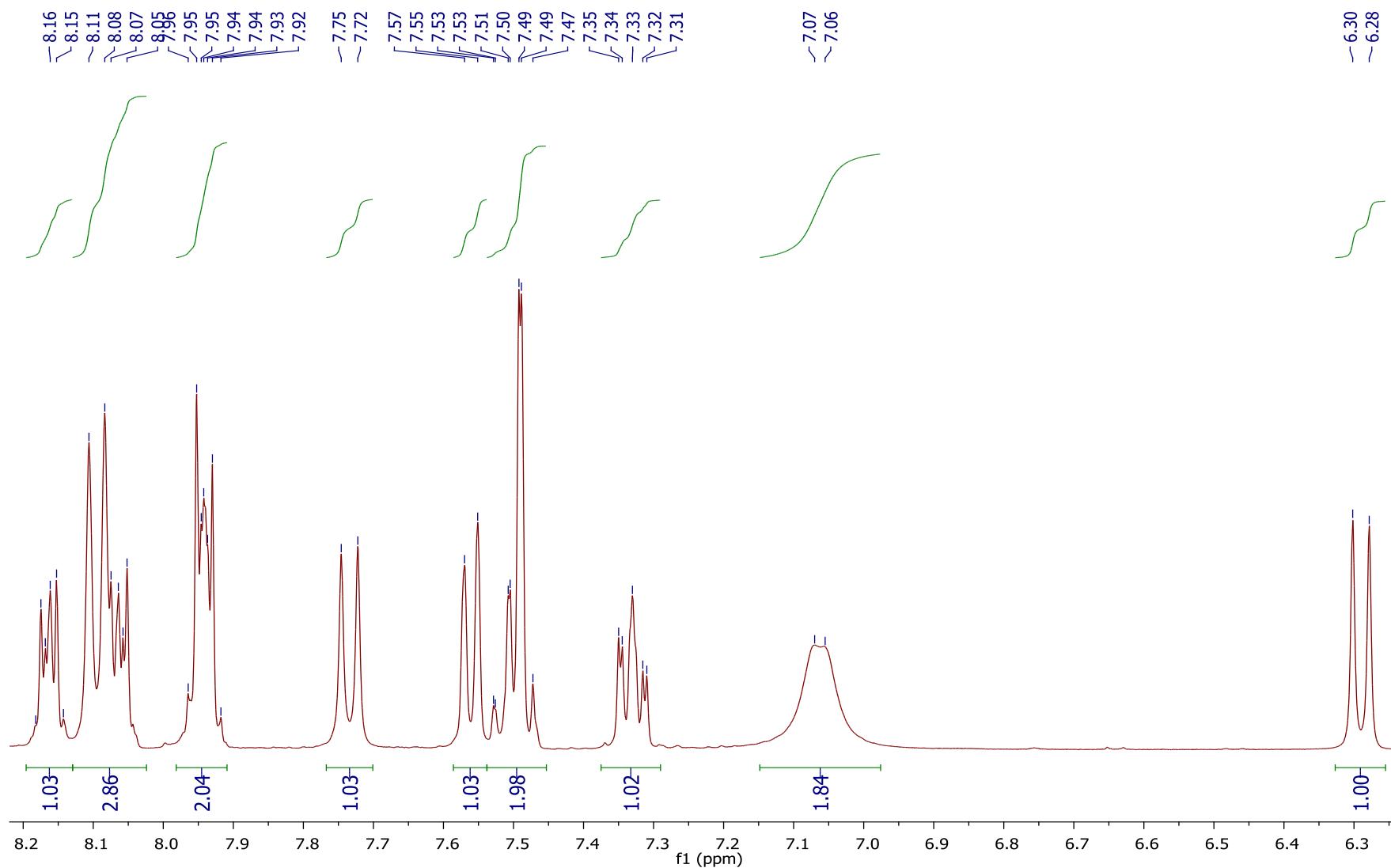


Figure S43. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aromatic region of compound **12**.

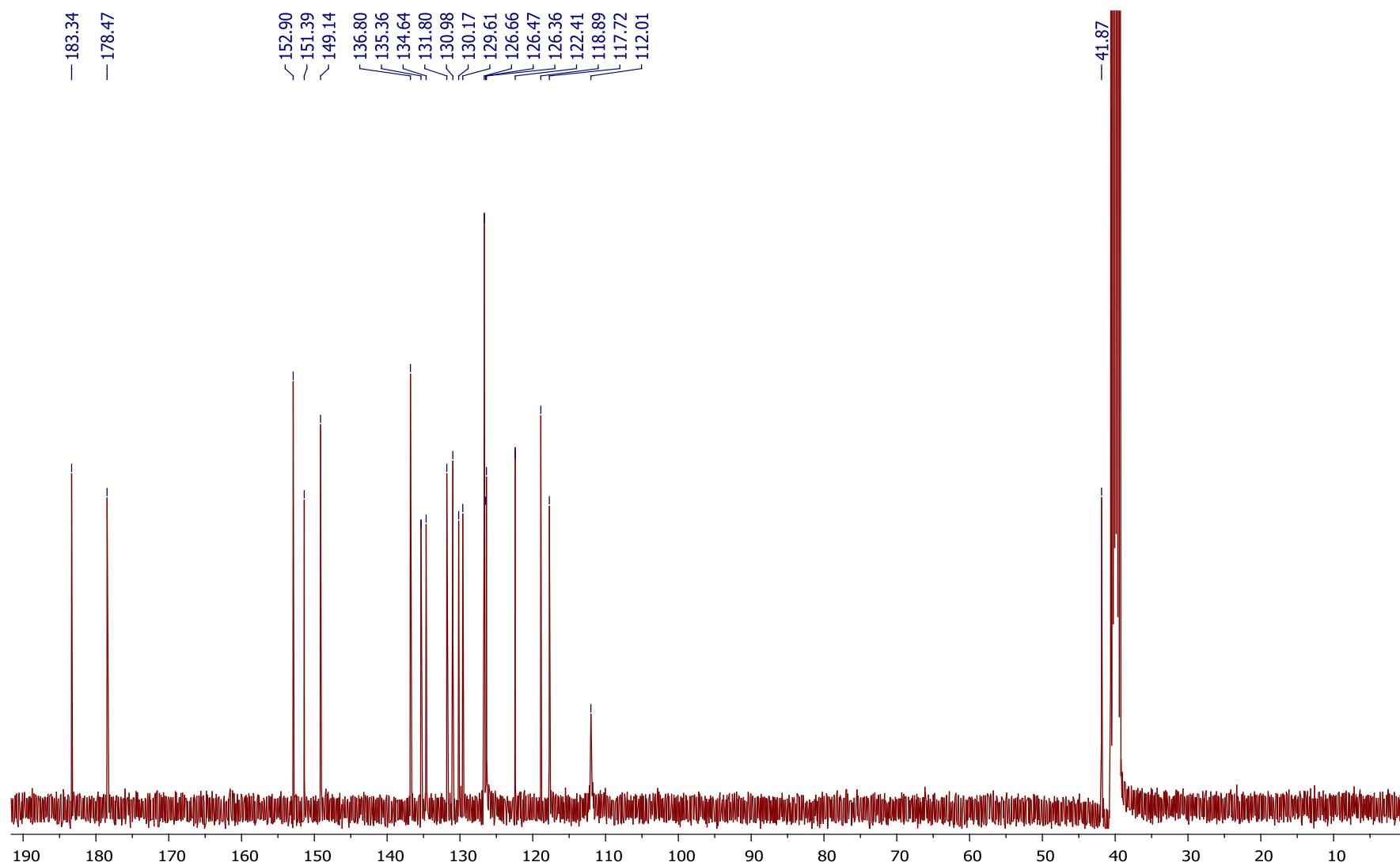


Figure S44. ^{13}C NMR spectrum (101 MHz, $\text{DMSO}-d_6$) of compound **12**.

[M-2H-OH]
397.08265
Err = 0.88
DBE = 17

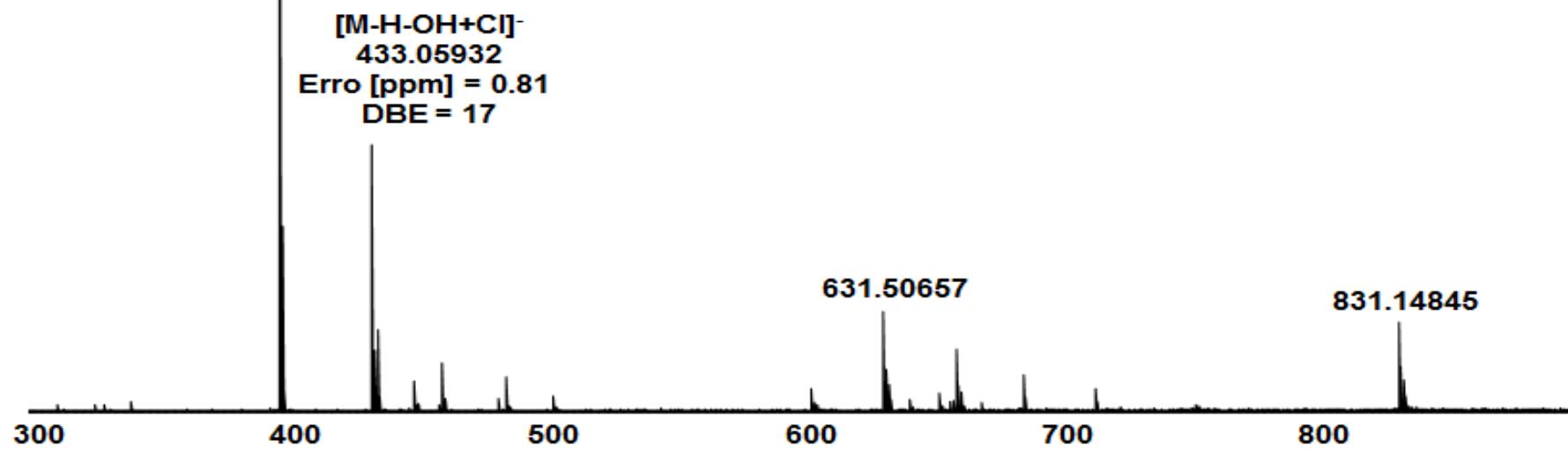
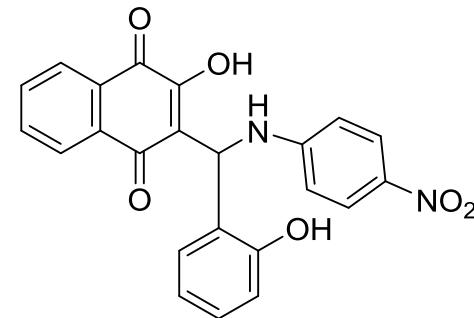


Figure S45. ESI(-)-FT-ICR mass spectrum of compound 12.

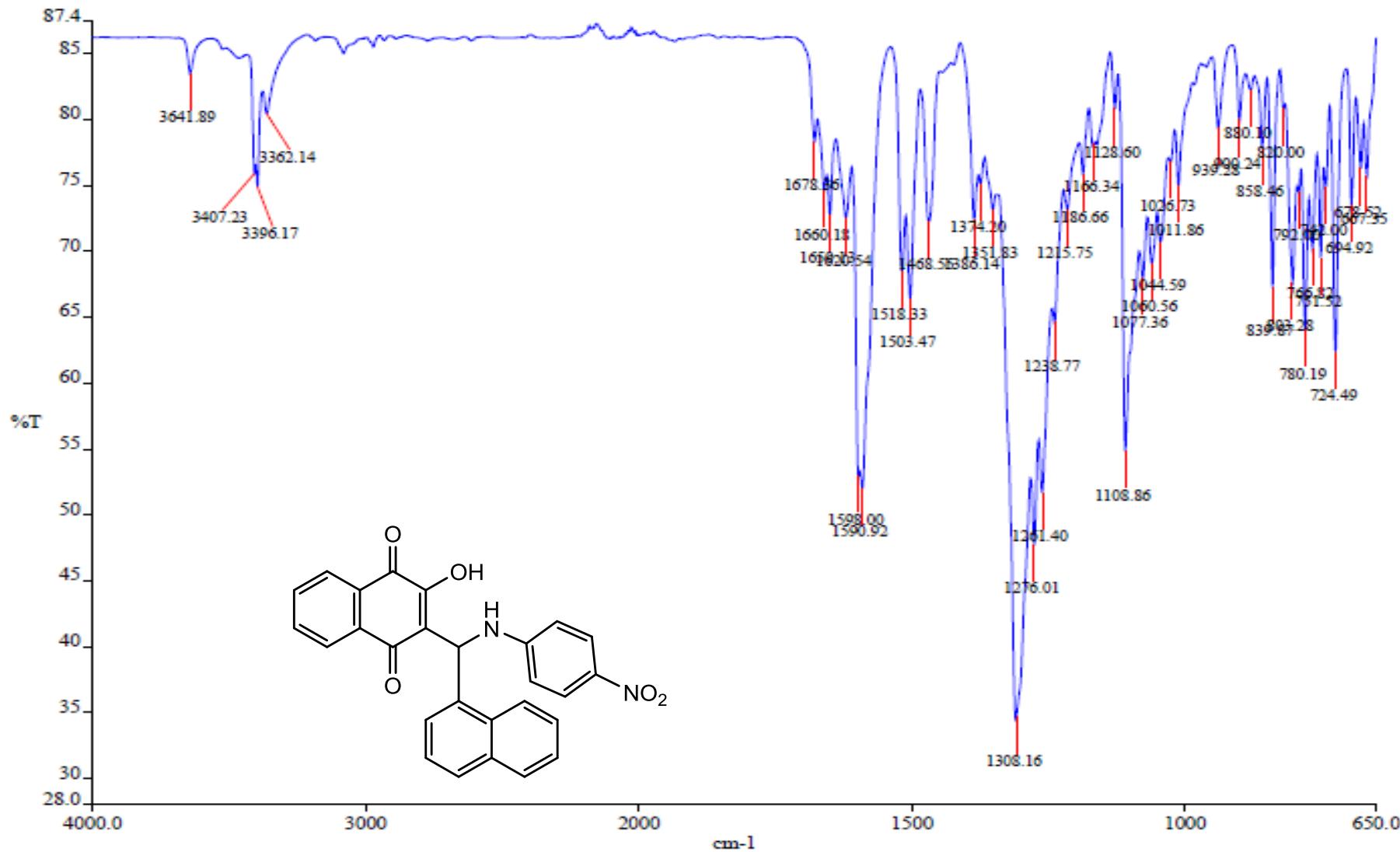


Figure S46. Infrared spectrum (ATR) of compound 13.

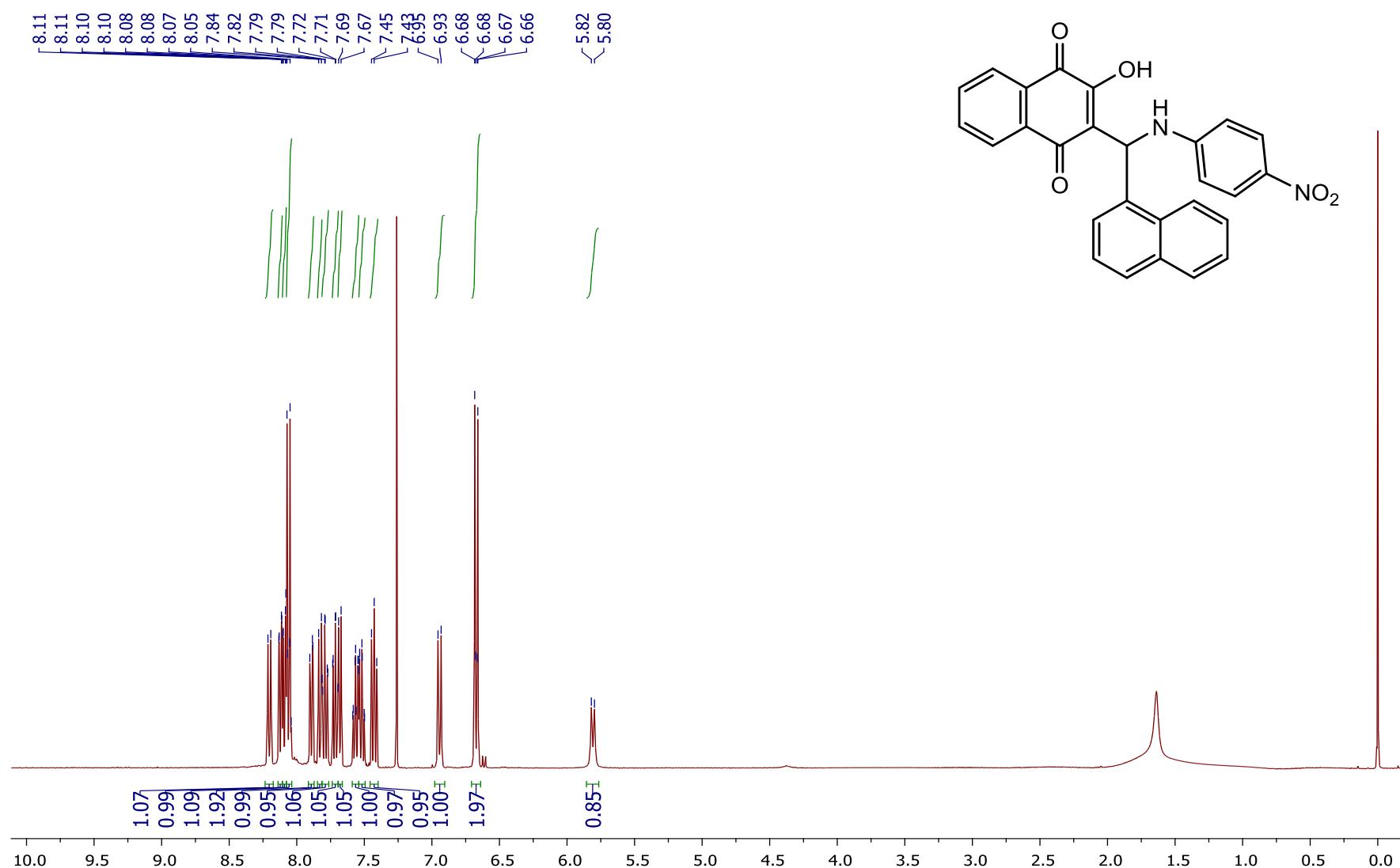


Figure S47. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 13.

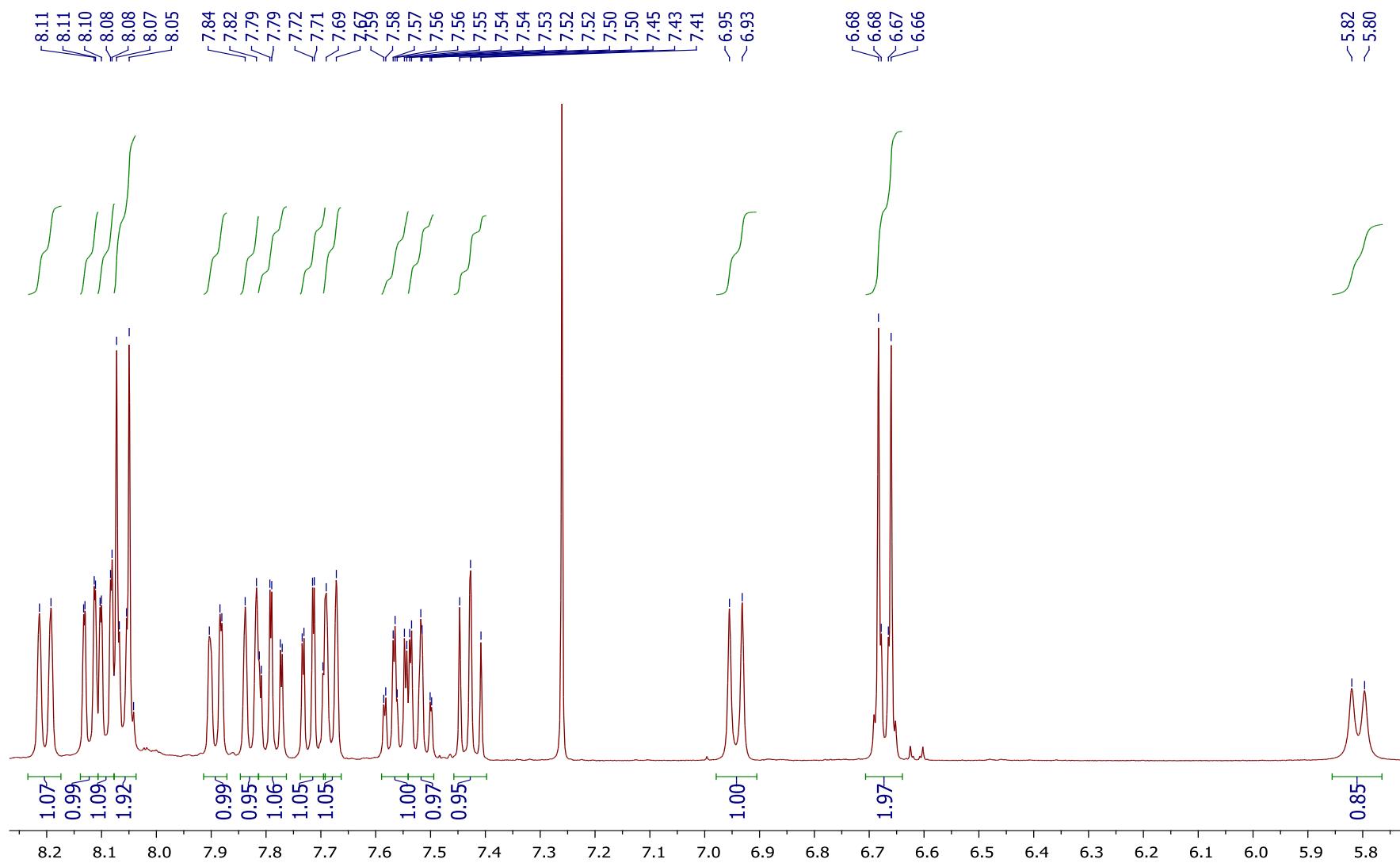


Figure S48. ^1H NMR spectrum (400 MHz, CDCl_3) of aromatic region of compound 13.

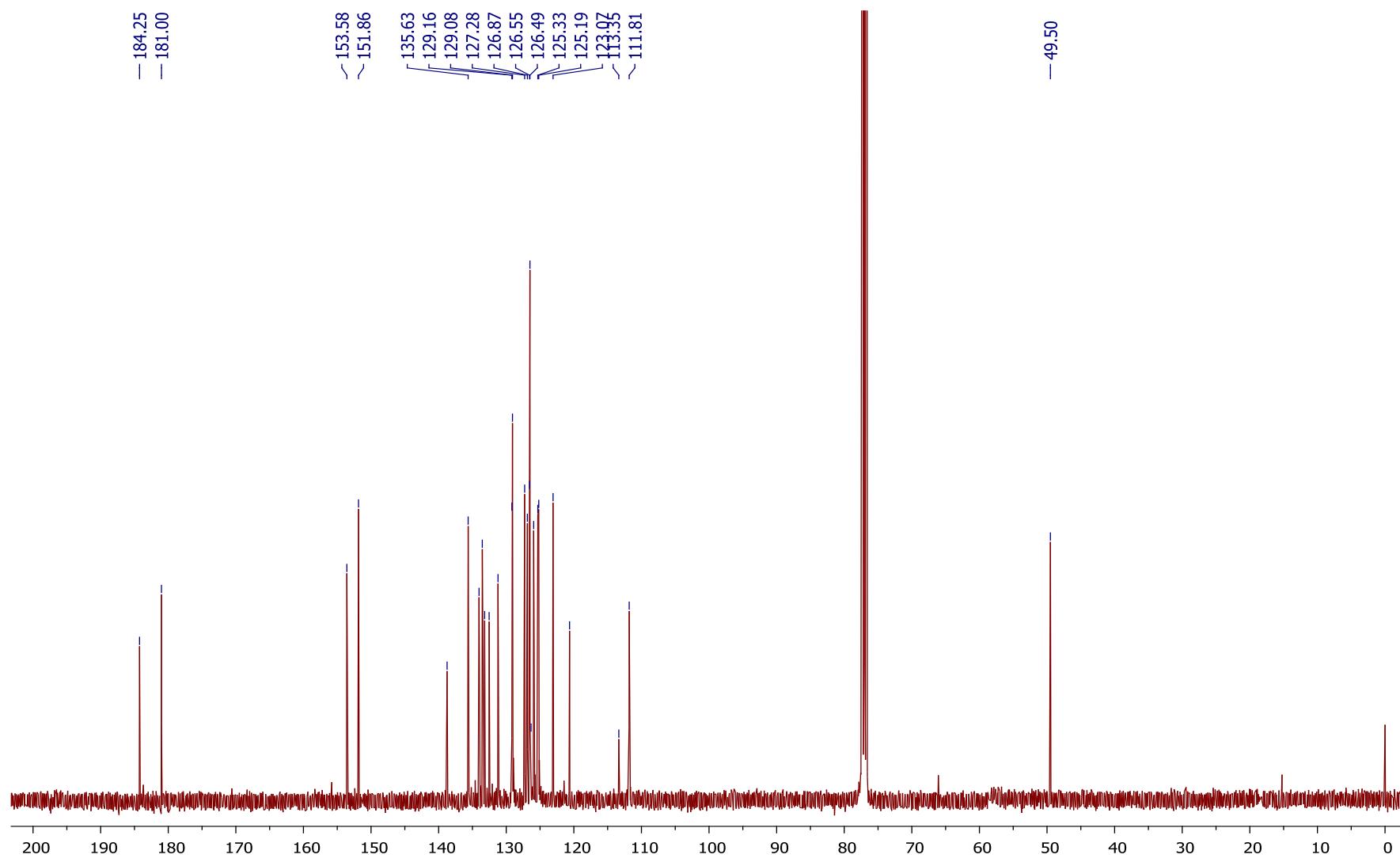


Figure S49. ^{13}C NMR spectrum (101 MHz, CDCl_3) of compound **13**.

$[M-C_6H_5N_2O_2+OH]^-$

329.08162

Erro [ppm] = 0.94

DBE = 18

$[M-H]^-$

449.11367

Erro [ppm] = 1.39

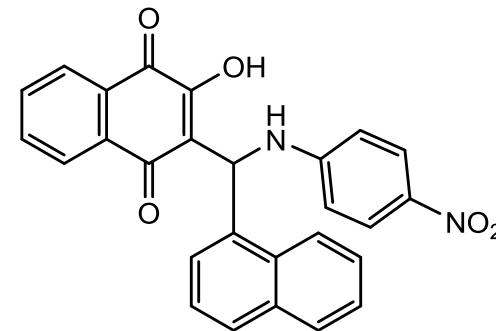
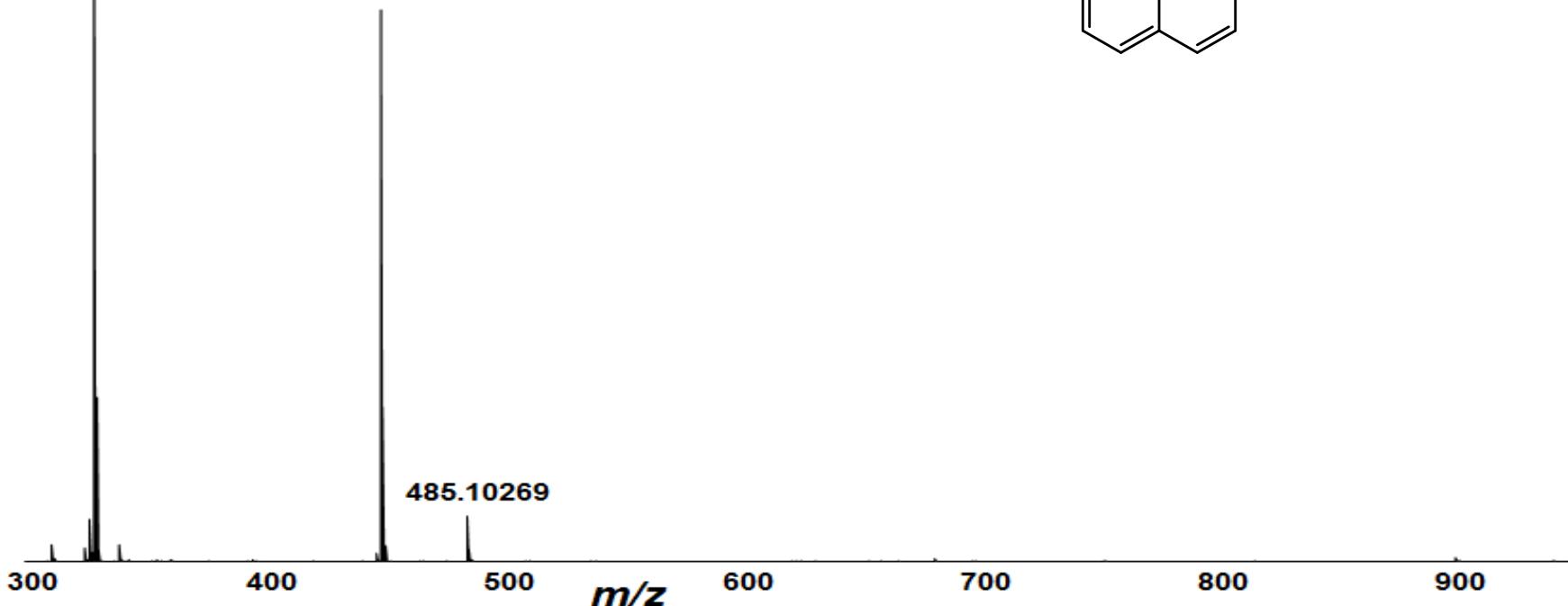


Figure S50. ESI(-)-FT-ICR mass spectrum of compound 13.

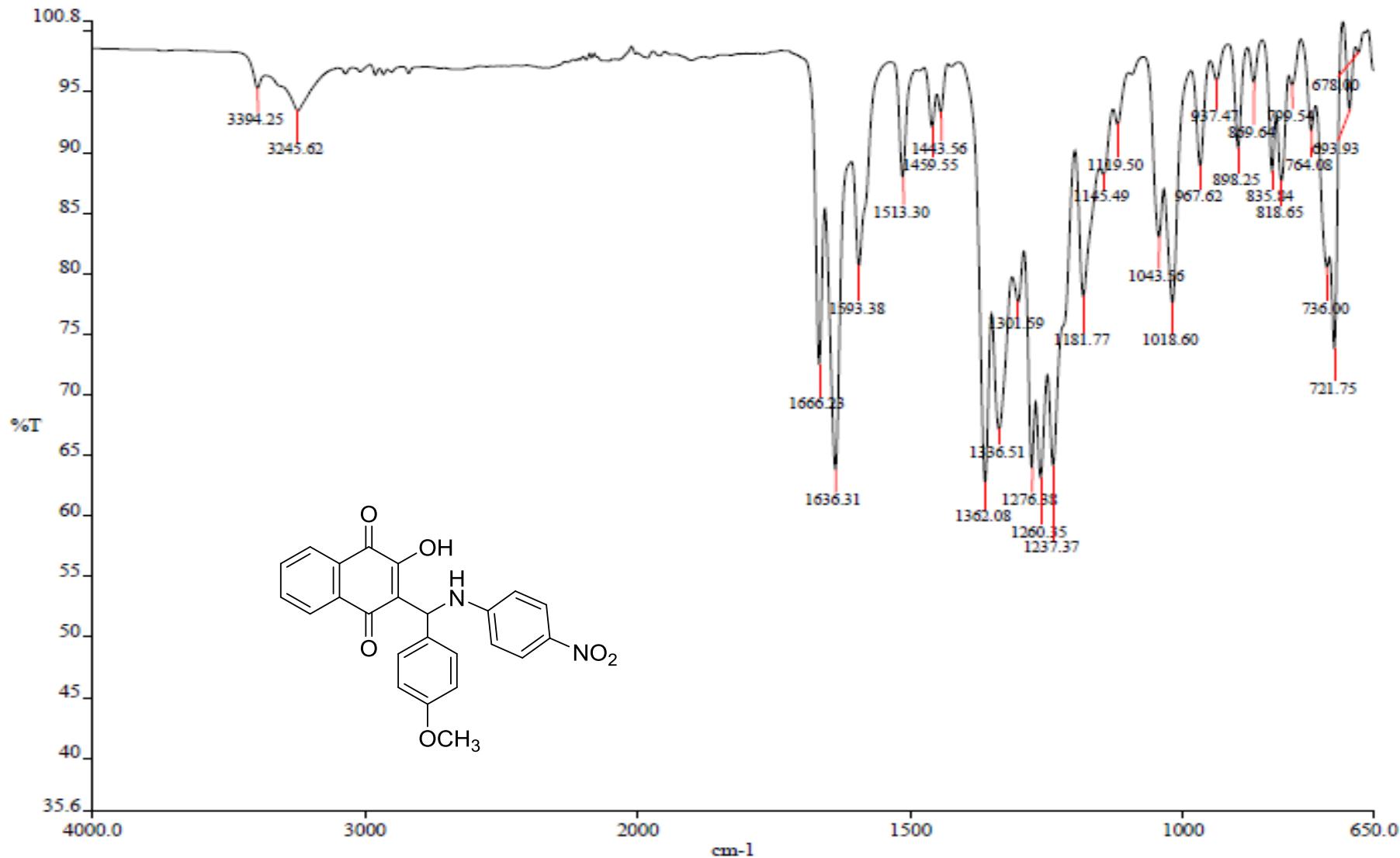


Figure S51. Infrared spectrum (ATR) of compound 14.

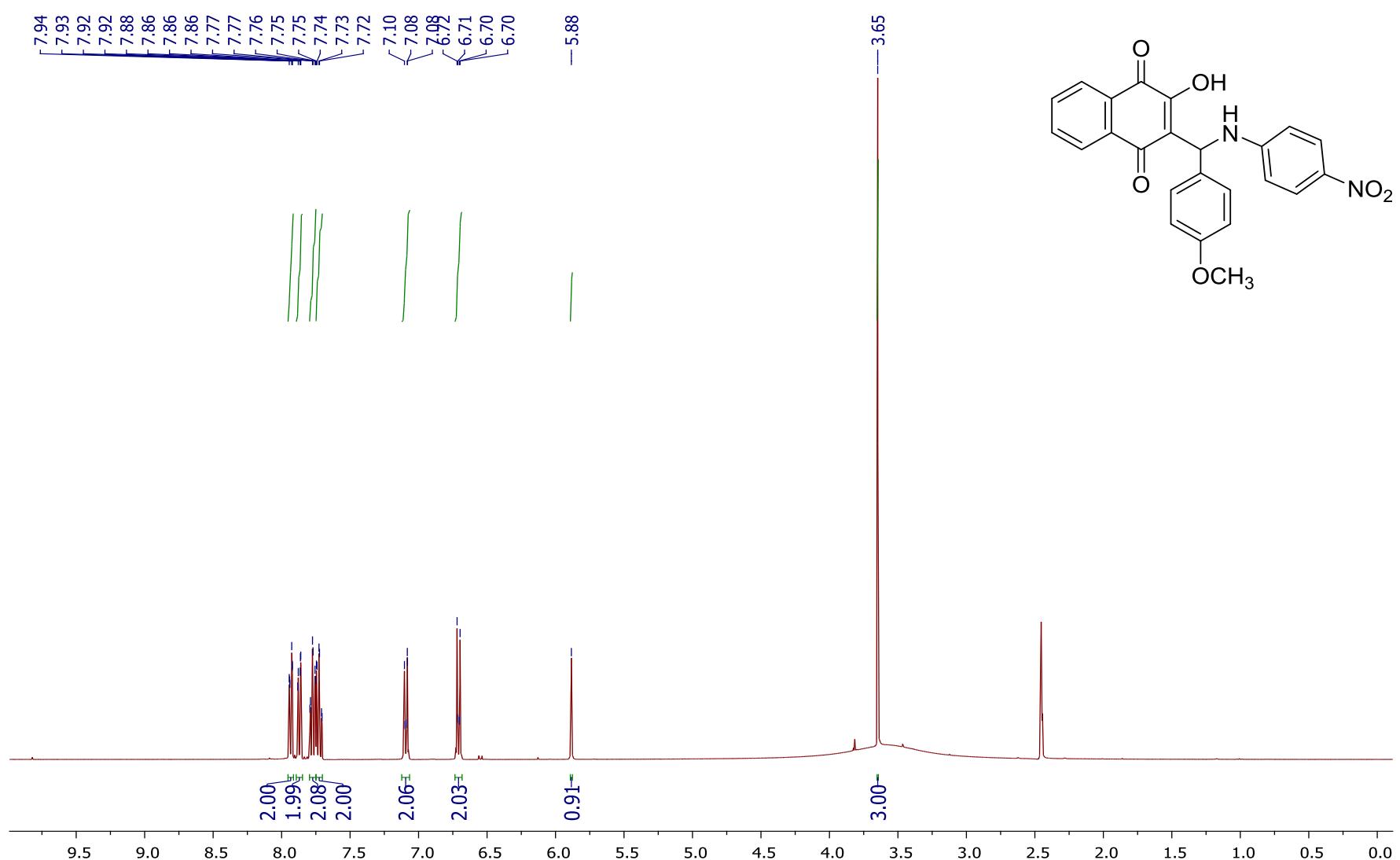


Figure S52. ¹H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 14.

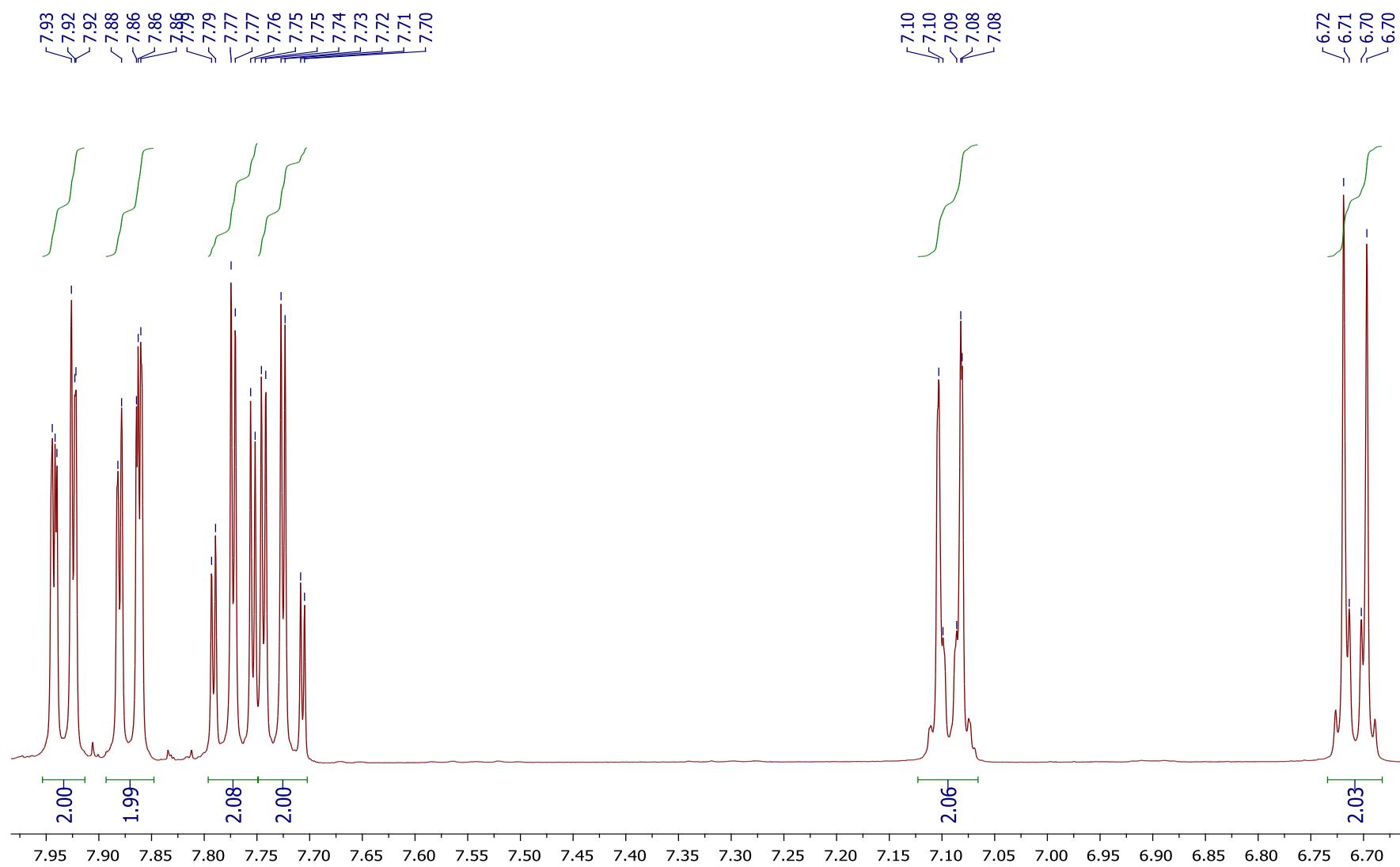


Figure S53. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aromatic region of compound 14.

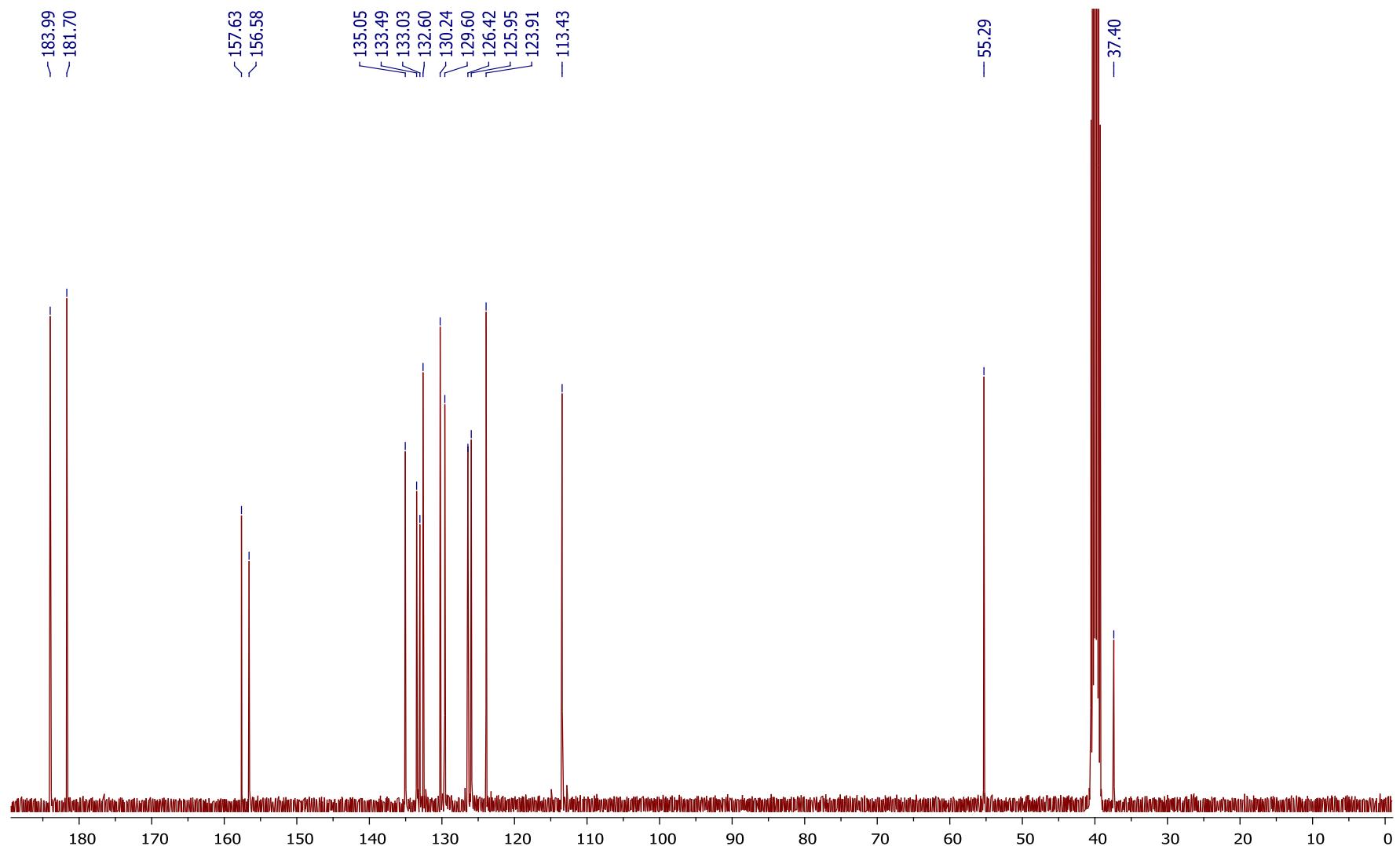


Figure S54. ^{13}C NMR spectrum (101 MHz, $\text{DMSO}-d_6$) of compound 14.

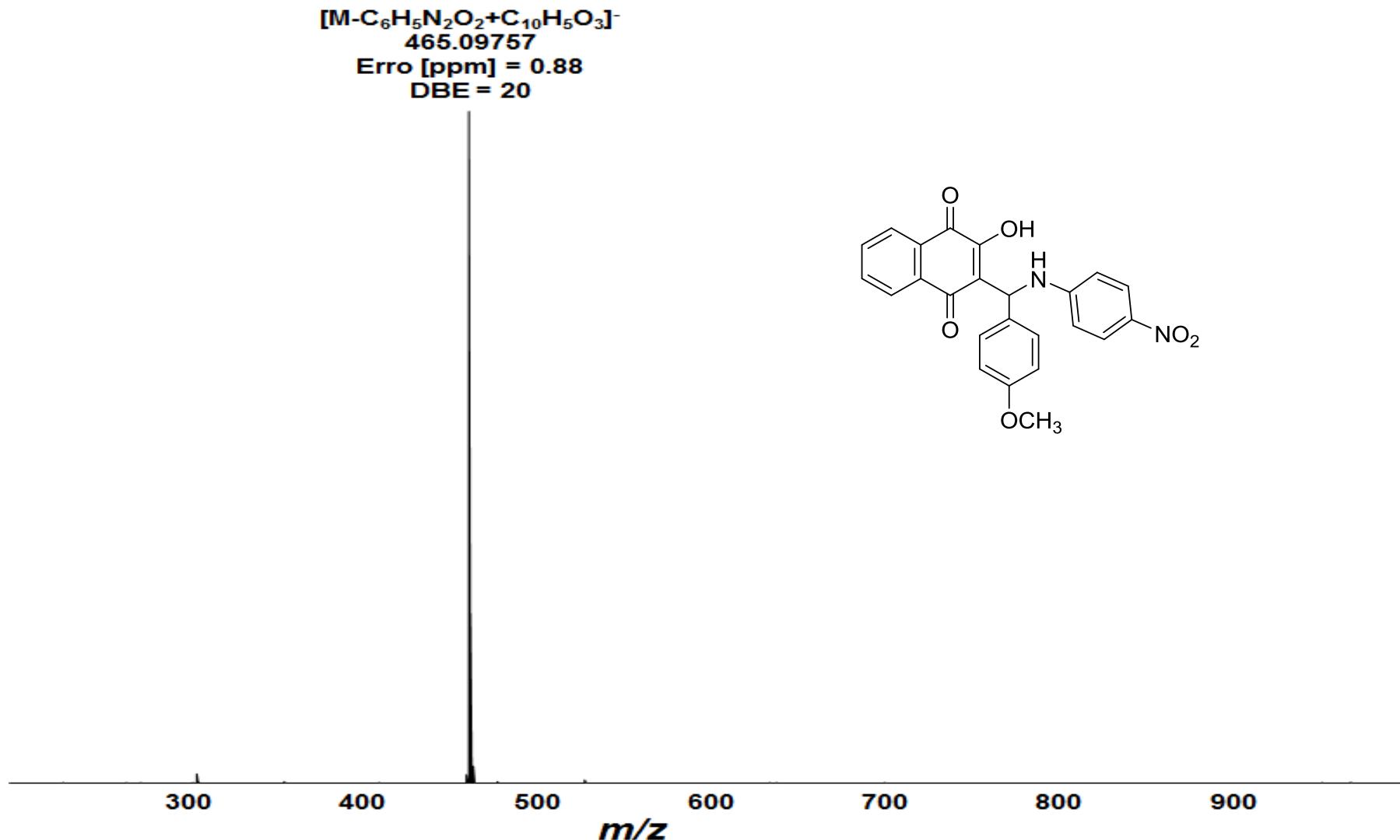


Figure S55. ESI(-)-FT-ICR mass spectrum of compound 14.

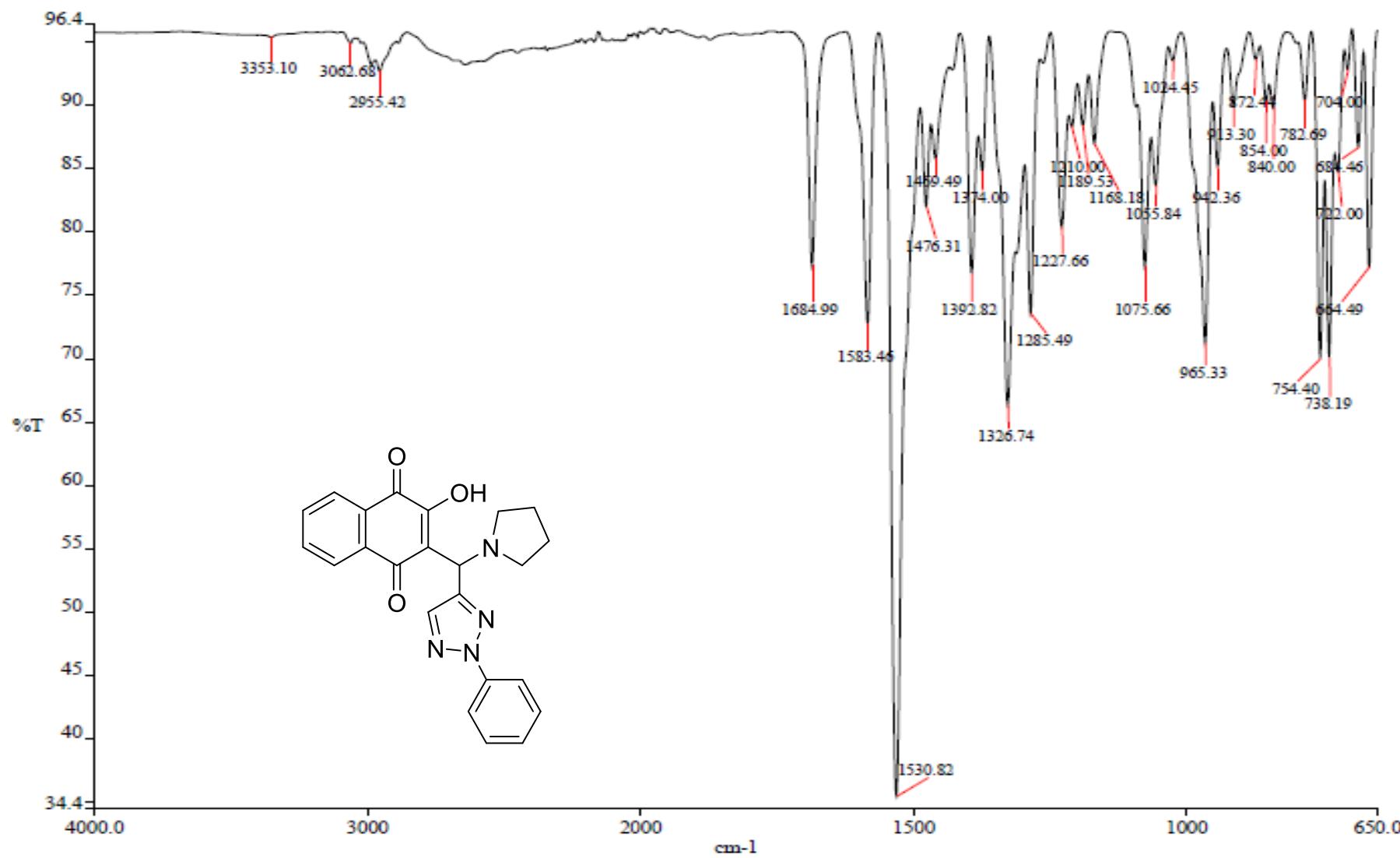


Figure S56. Infrared spectrum (ATR) of compound 16.

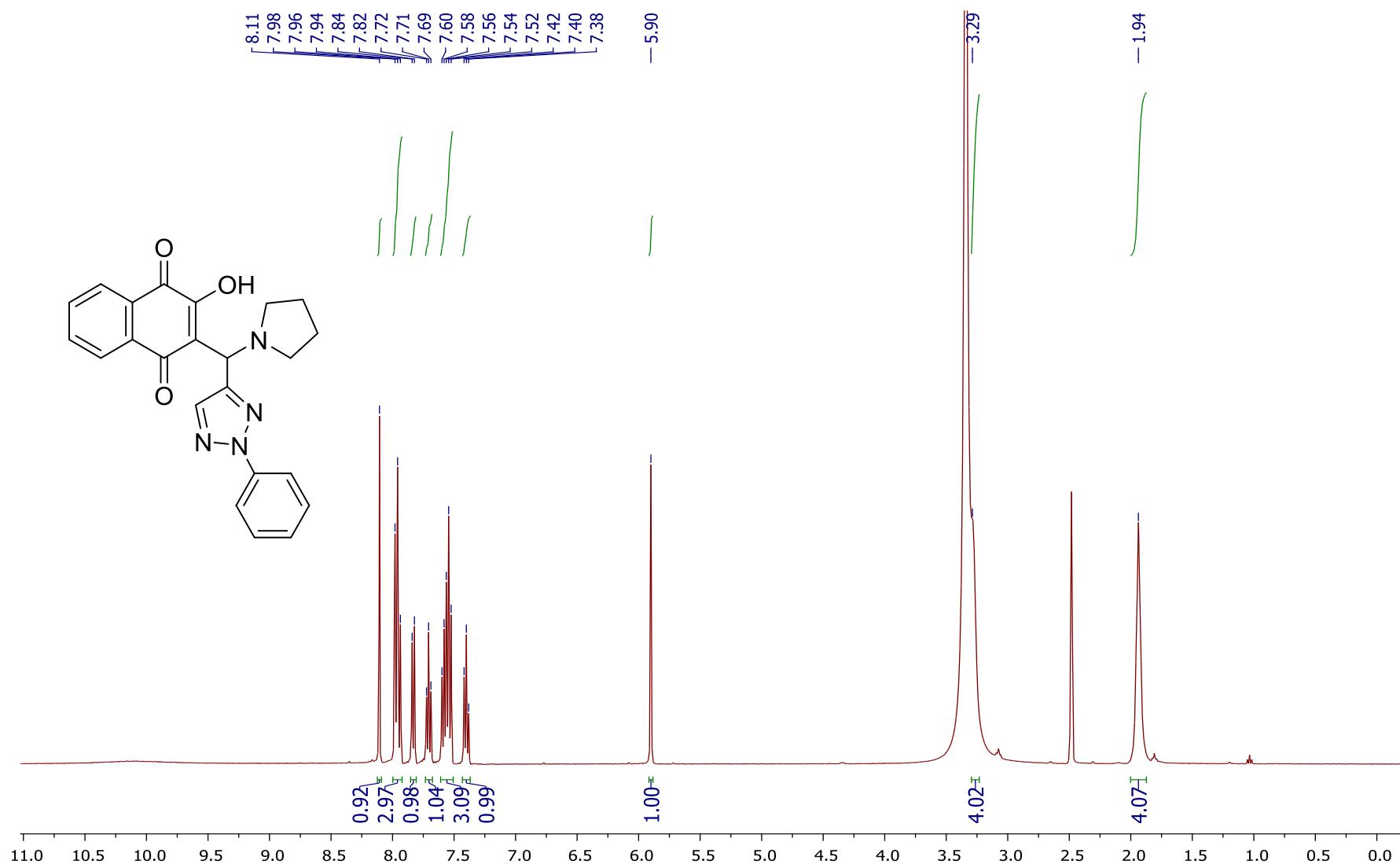


Figure S57. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 16.

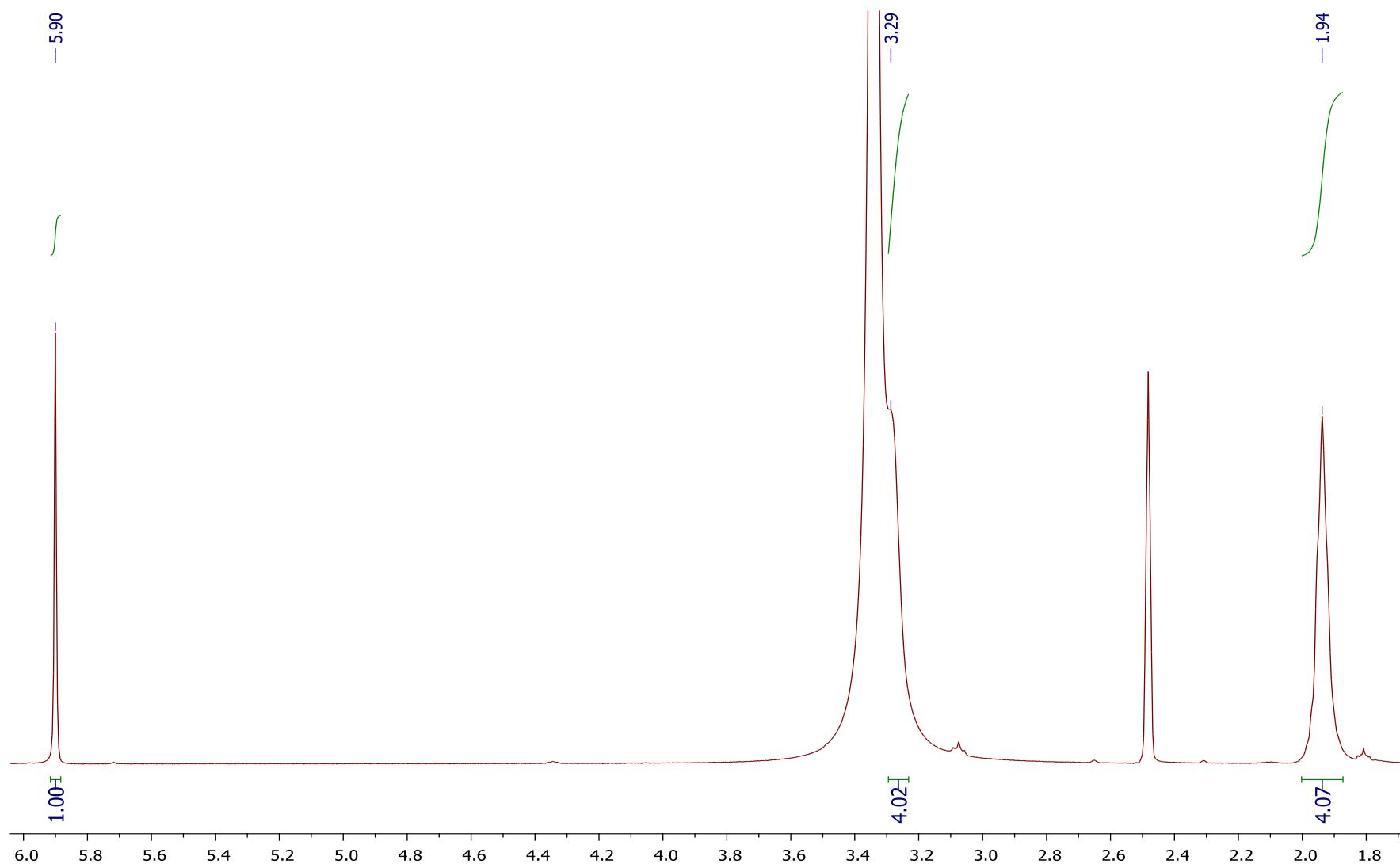


Figure S58. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aliphatic region of compound **16**.

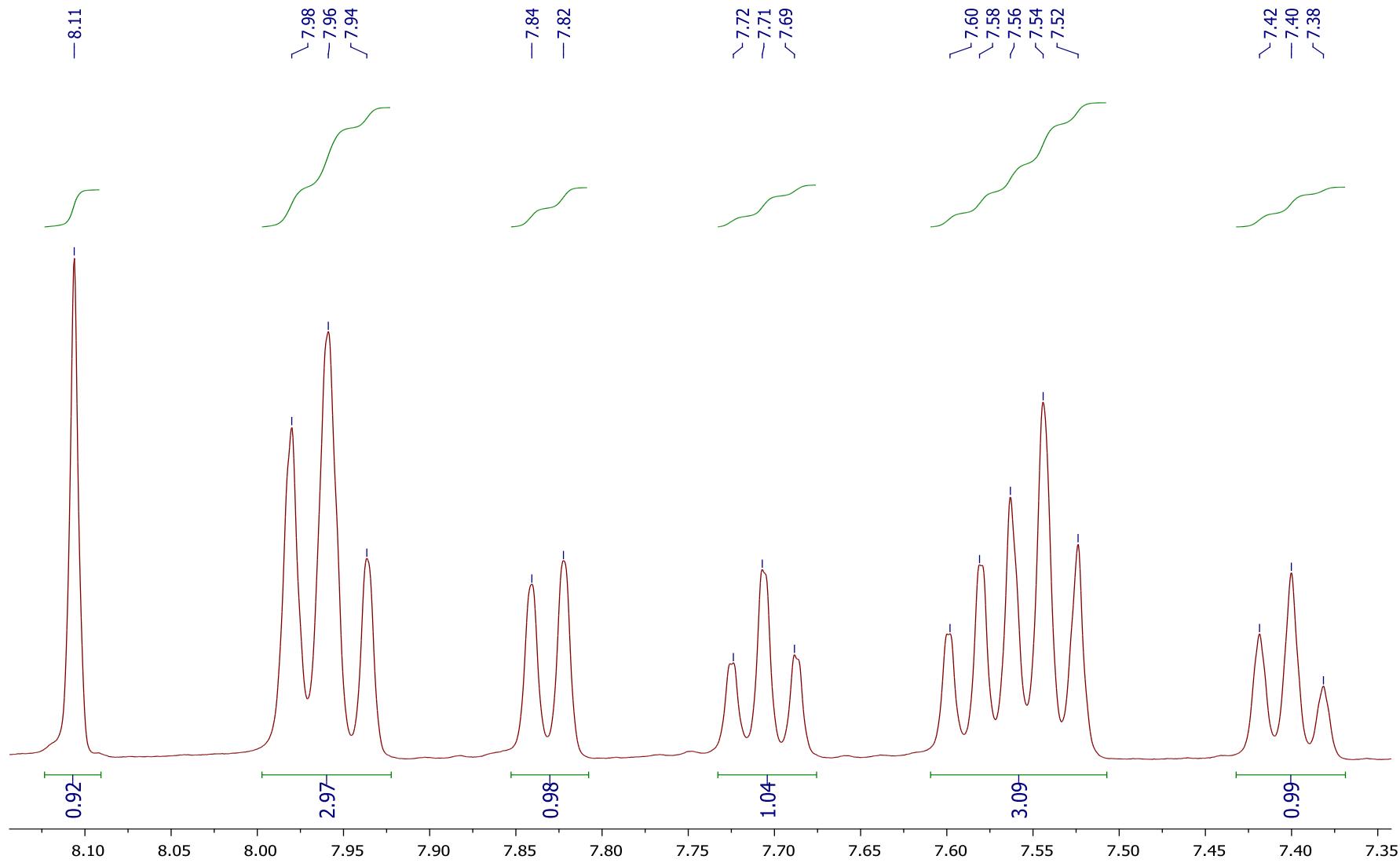


Figure S59. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of aromatic region of compound 16.

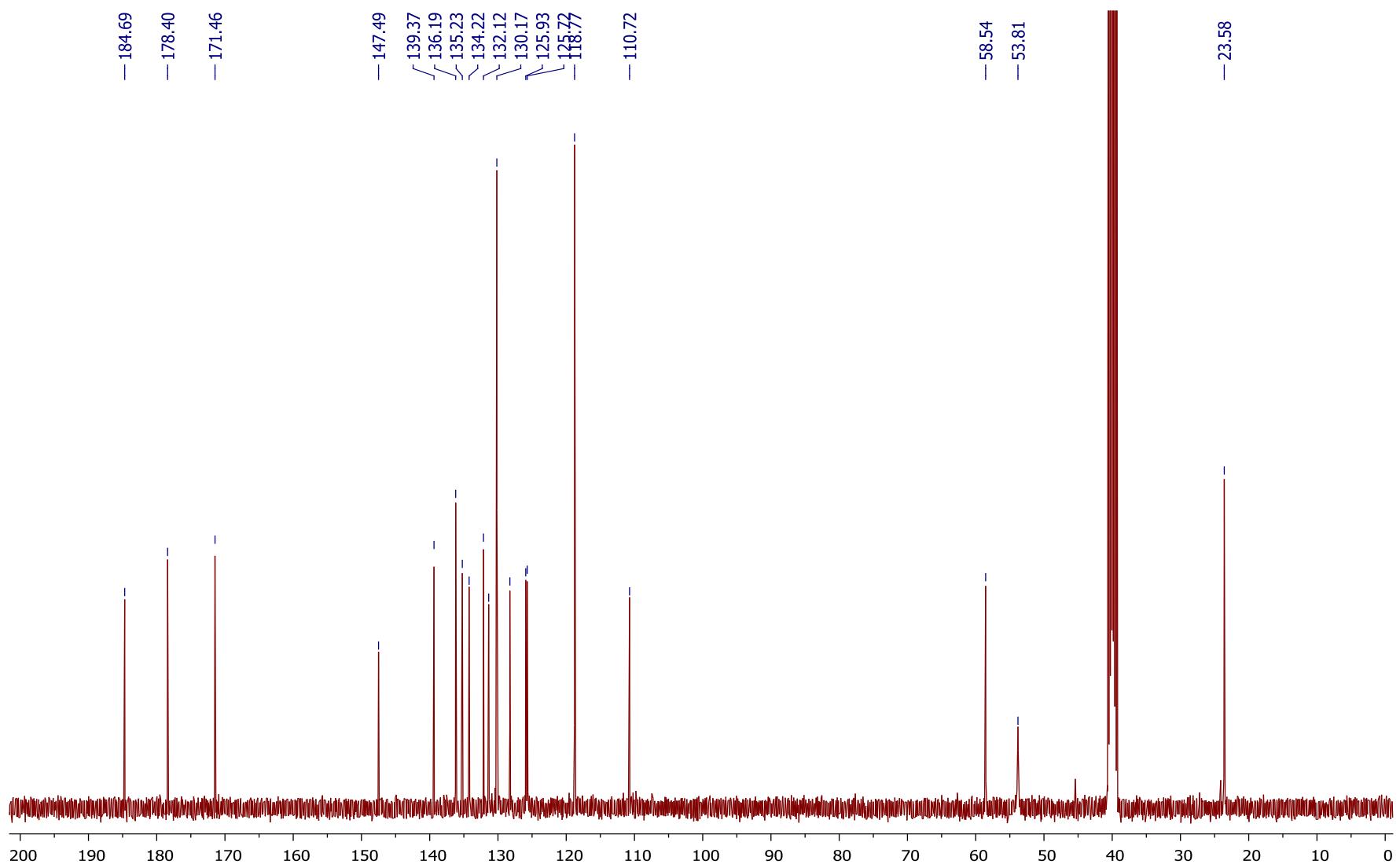


Figure S60. ^{13}C NMR spectrum (101 MHz, $\text{DMSO}-d_6$) of compound **16**.

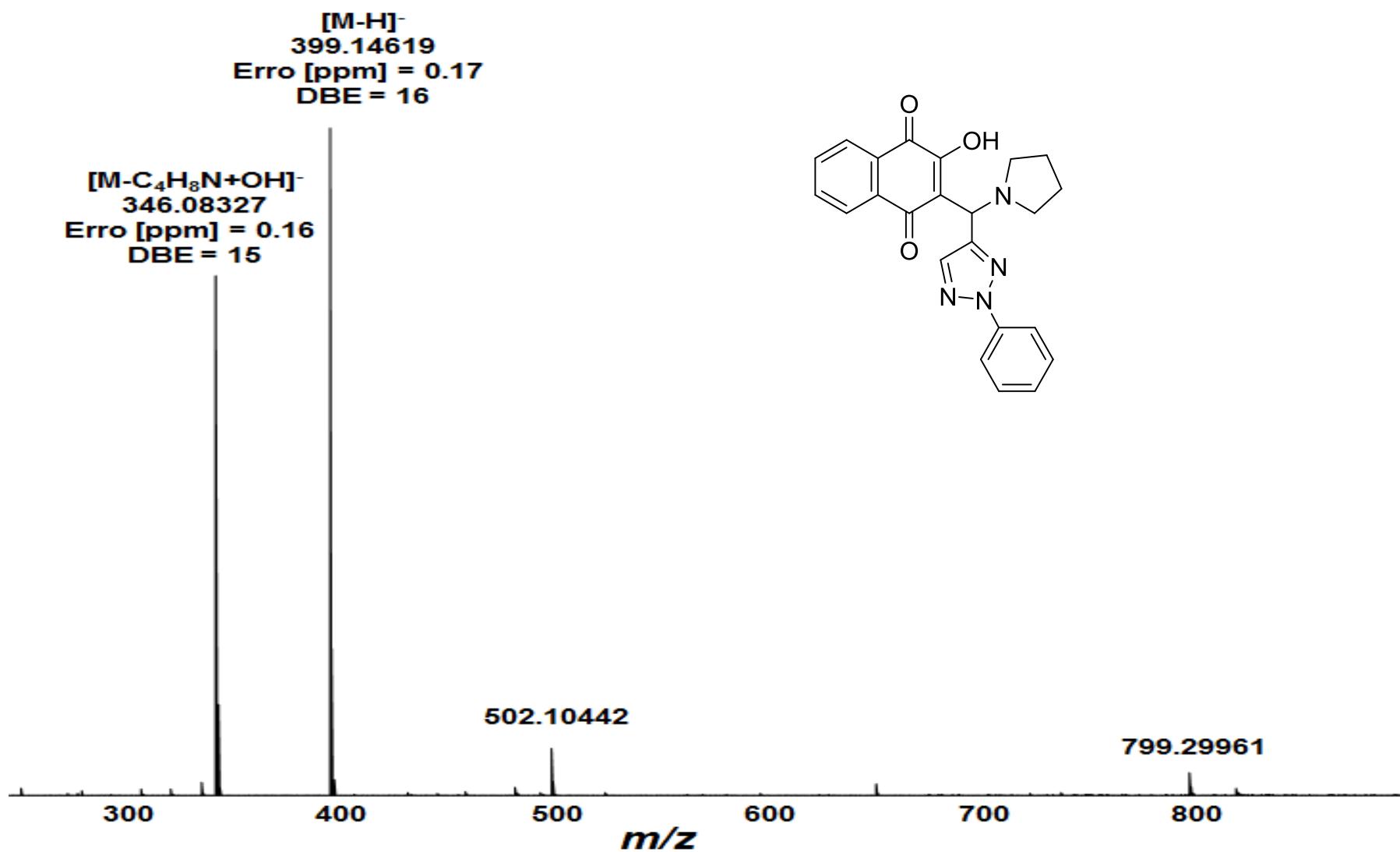


Figure S61. ESI(-)-FT-ICR mass spectrum of compound 16.

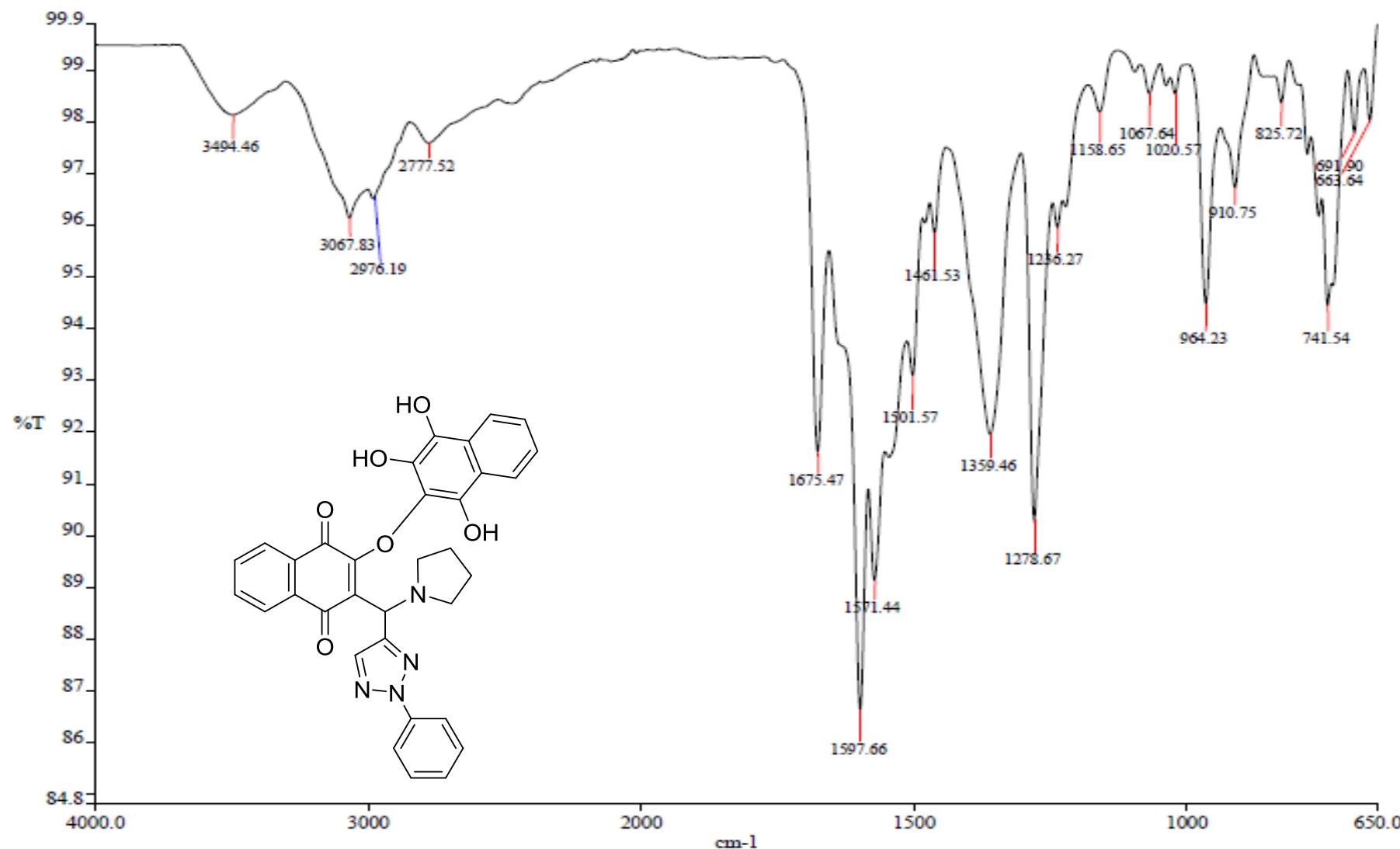


Figure S62. Infrared spectrum (KBr) of compound 17.

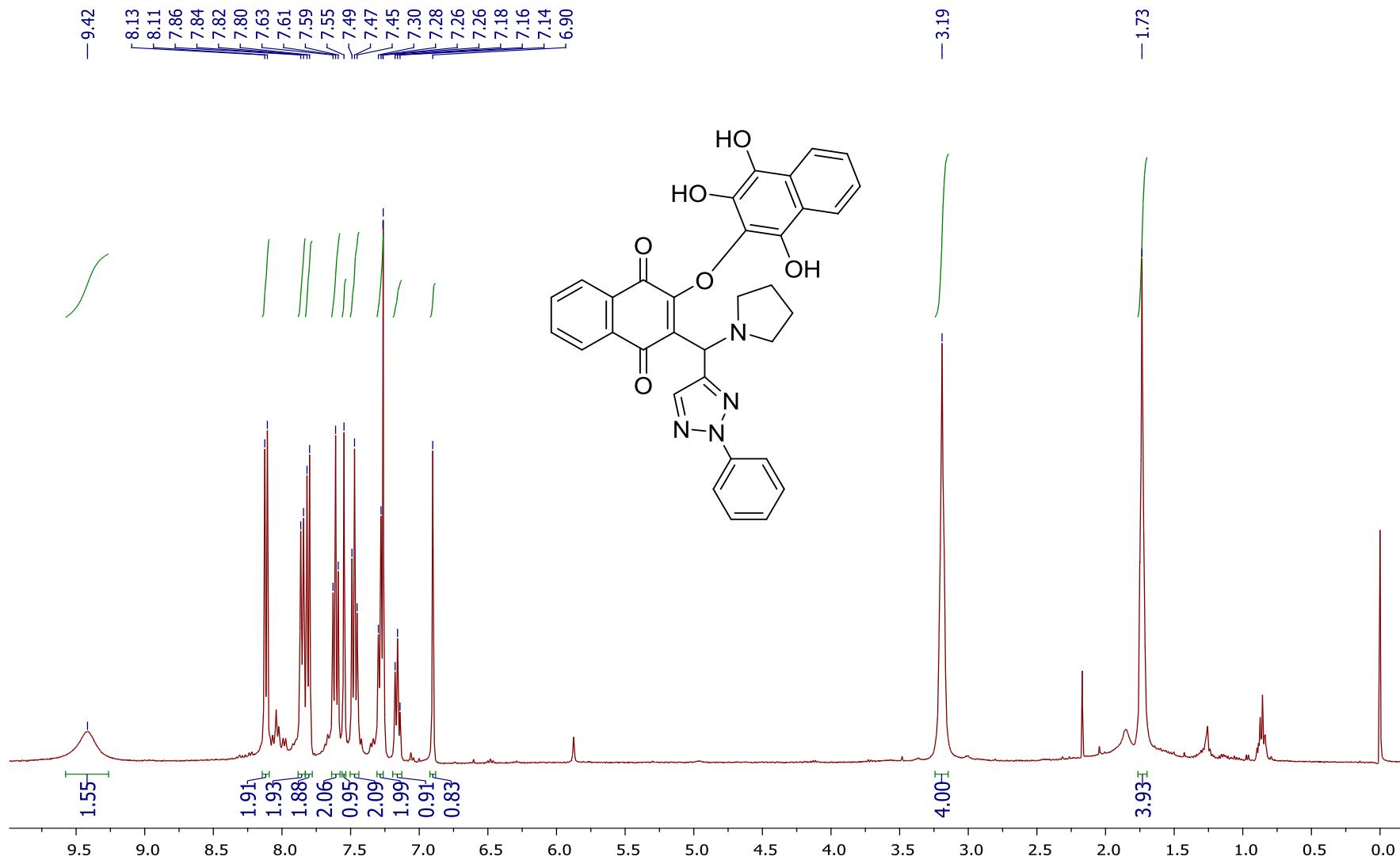


Figure S63. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 17.

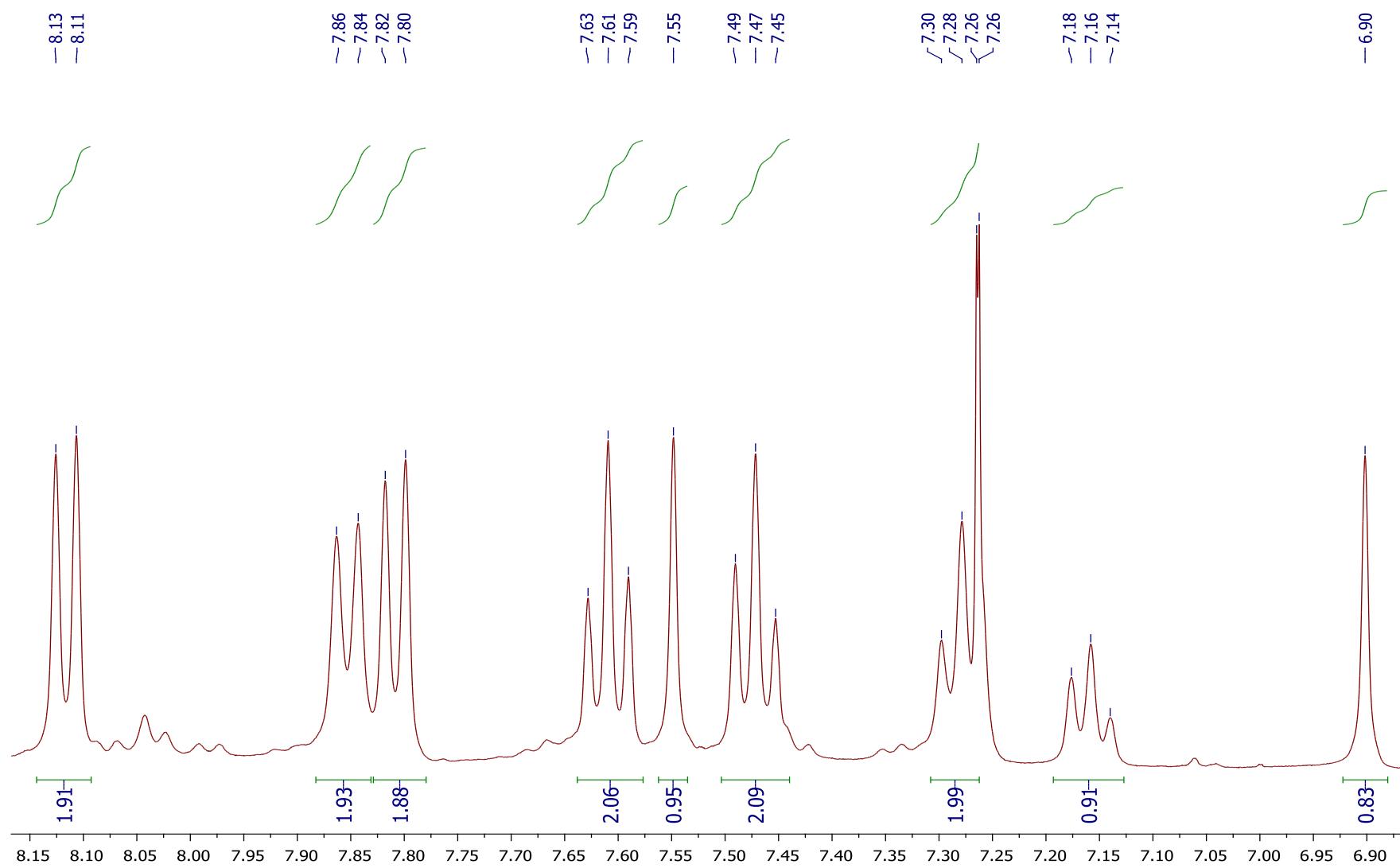


Figure S64. ^1H NMR spectrum (400 MHz, CDCl_3) of aromatic region of compound 17.

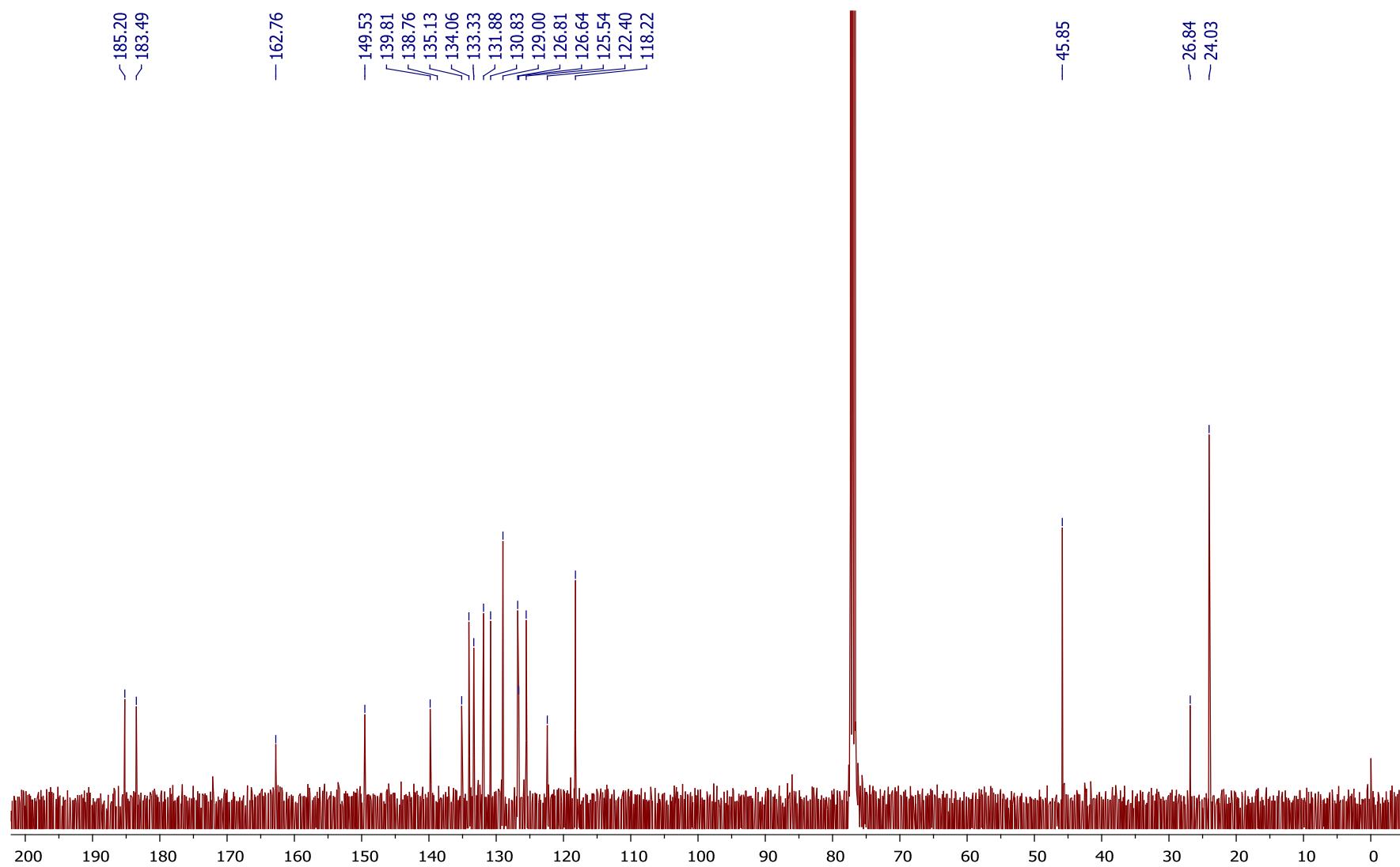


Figure S65. ^{13}C NMR spectrum (101 MHz, CDCl_3) of compound 17.

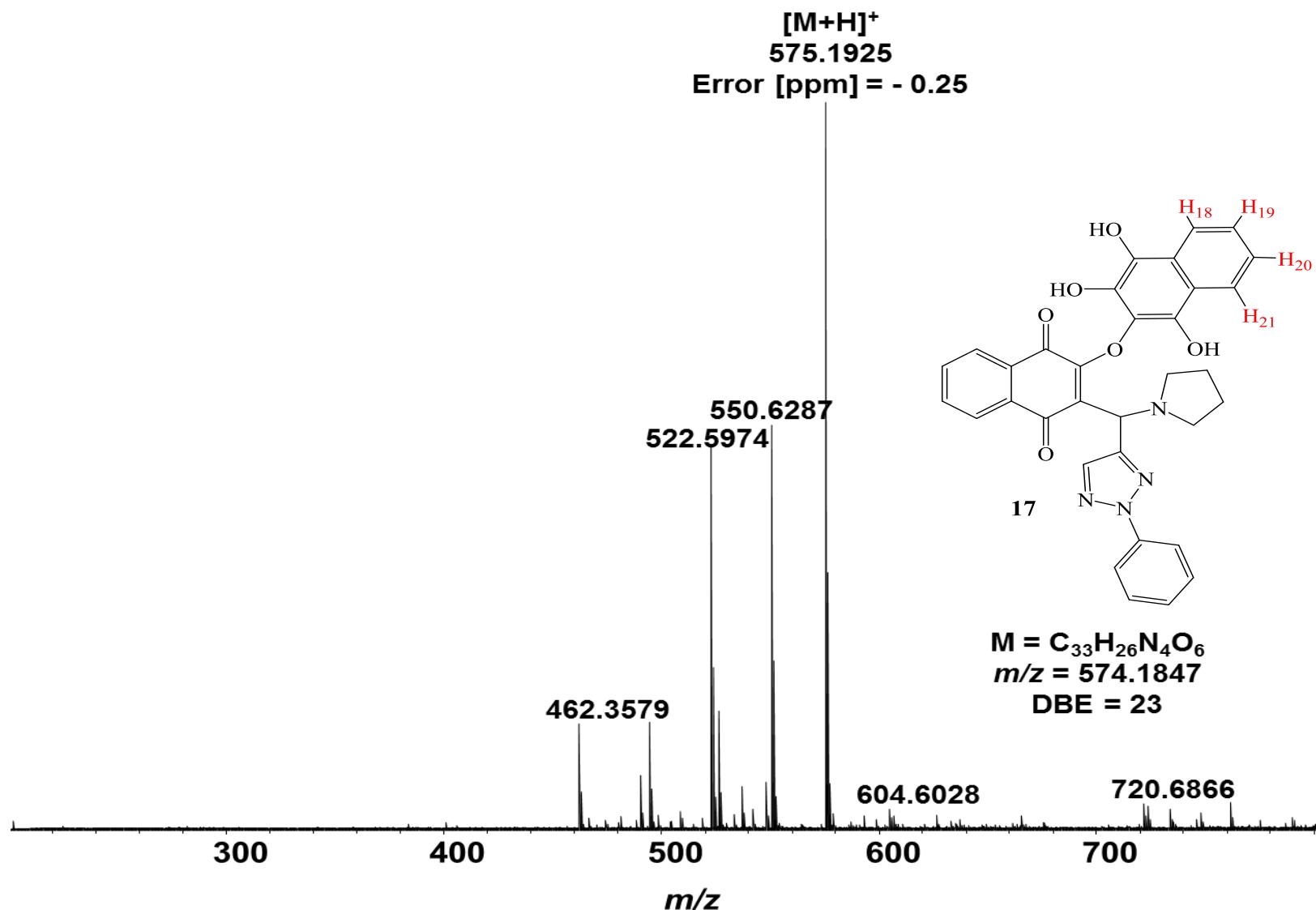


Figure S66. ESI(+) -FT-ICR mass spectrum of compound 17.

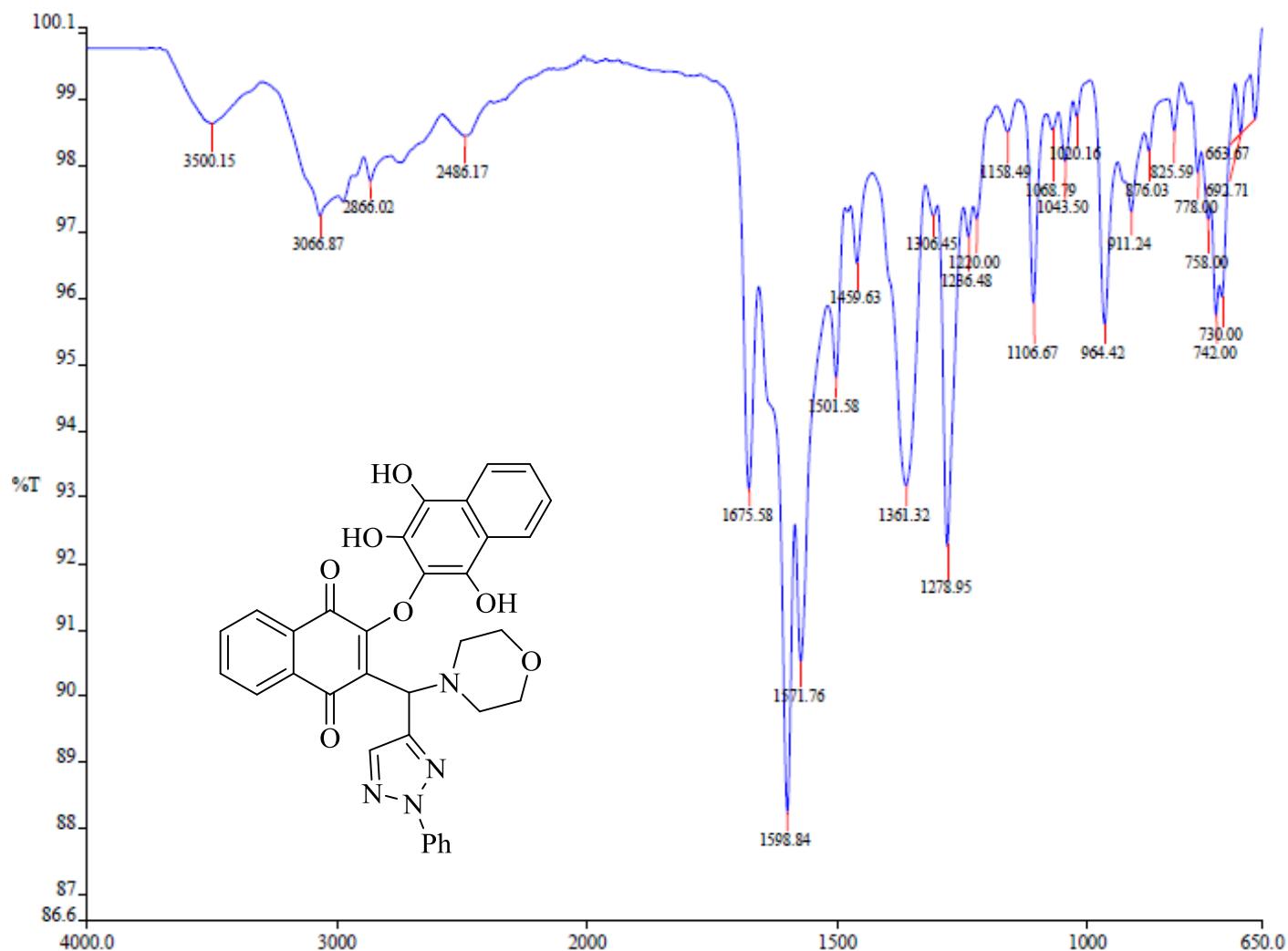


Figure S67. Infrared spectrum (ATR) of compound 23.

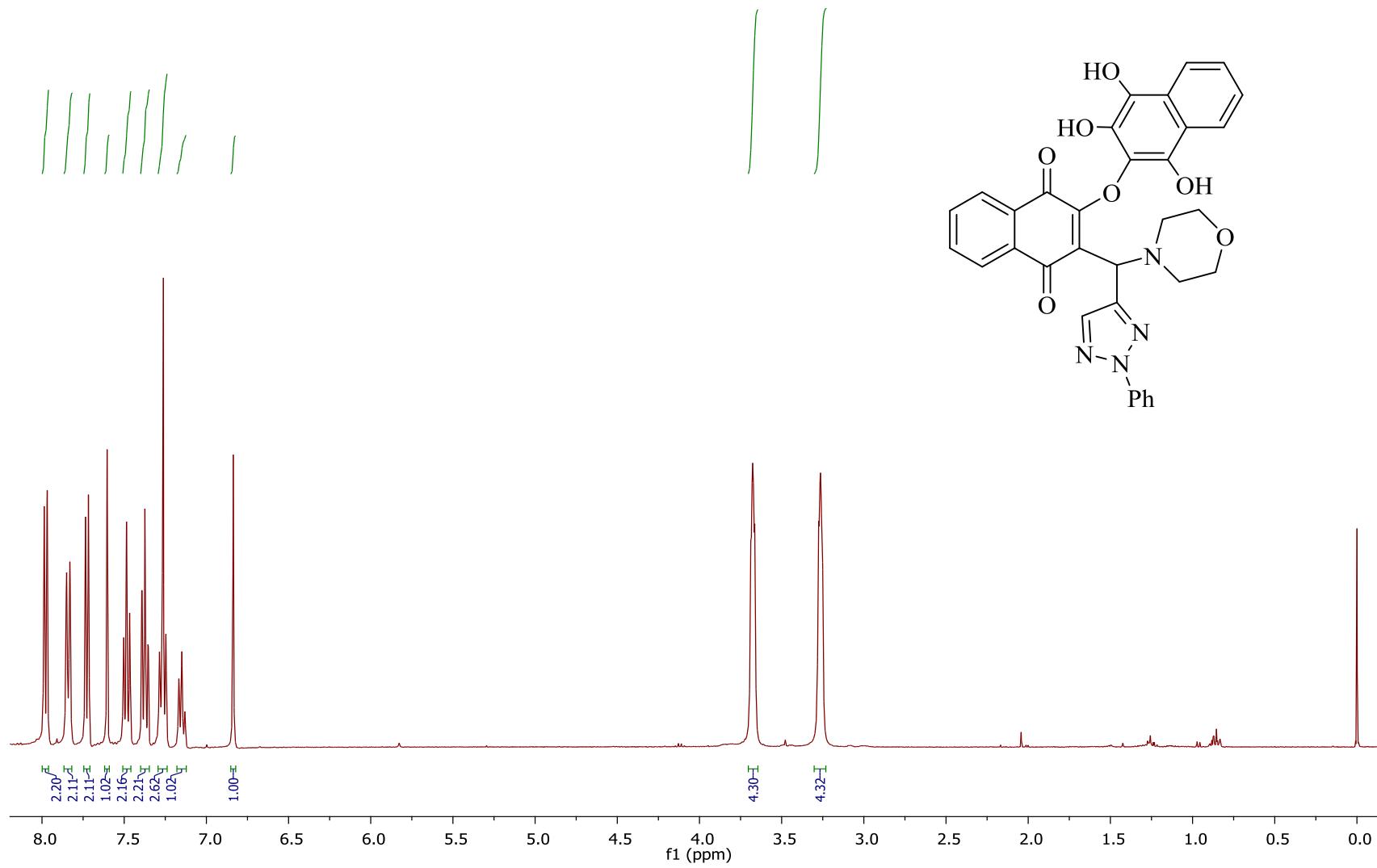


Figure S68. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 23.

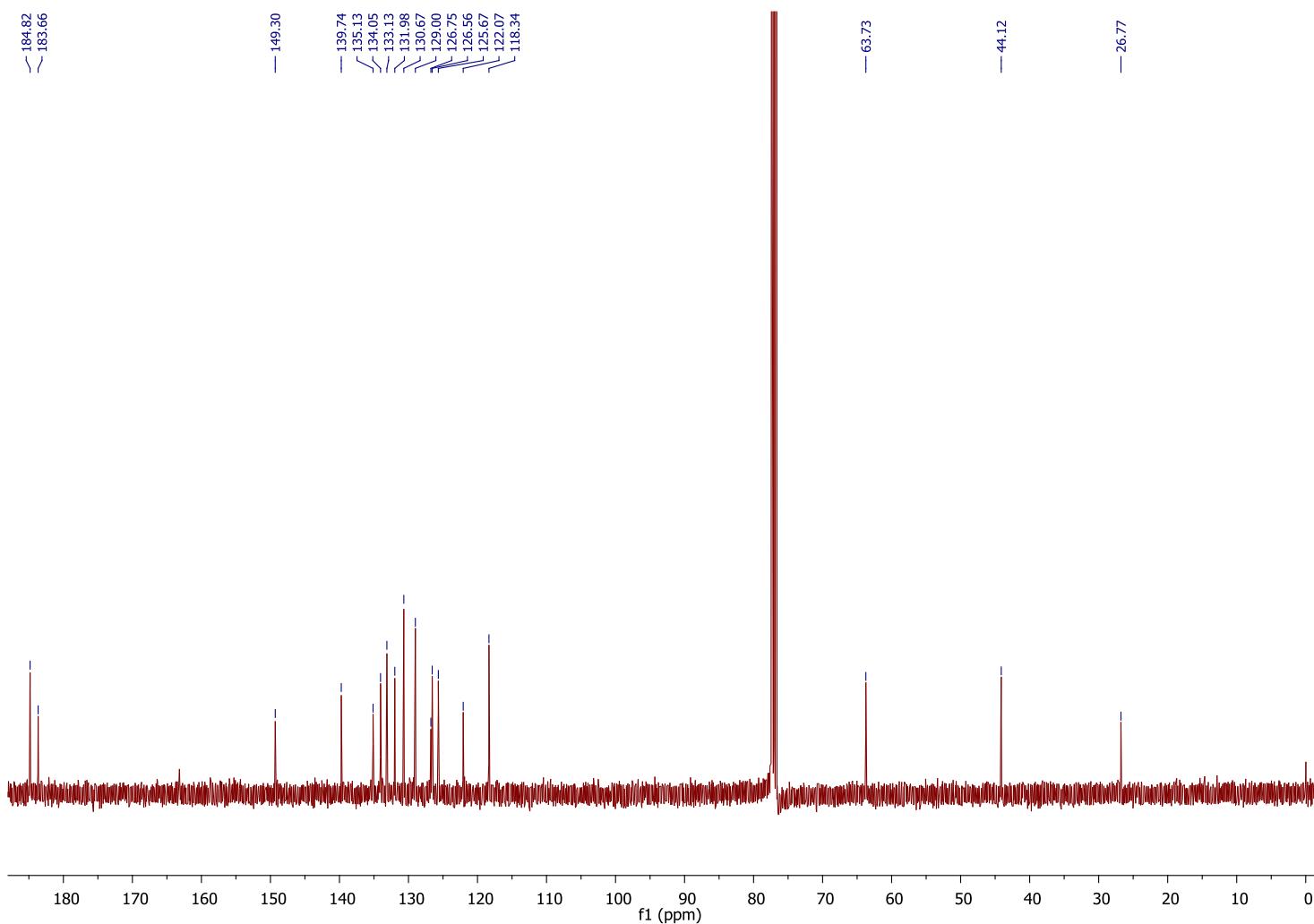


Figure S69. ^{13}C NMR spectrum (101 MHz, CDCl_3) of compound **23**.

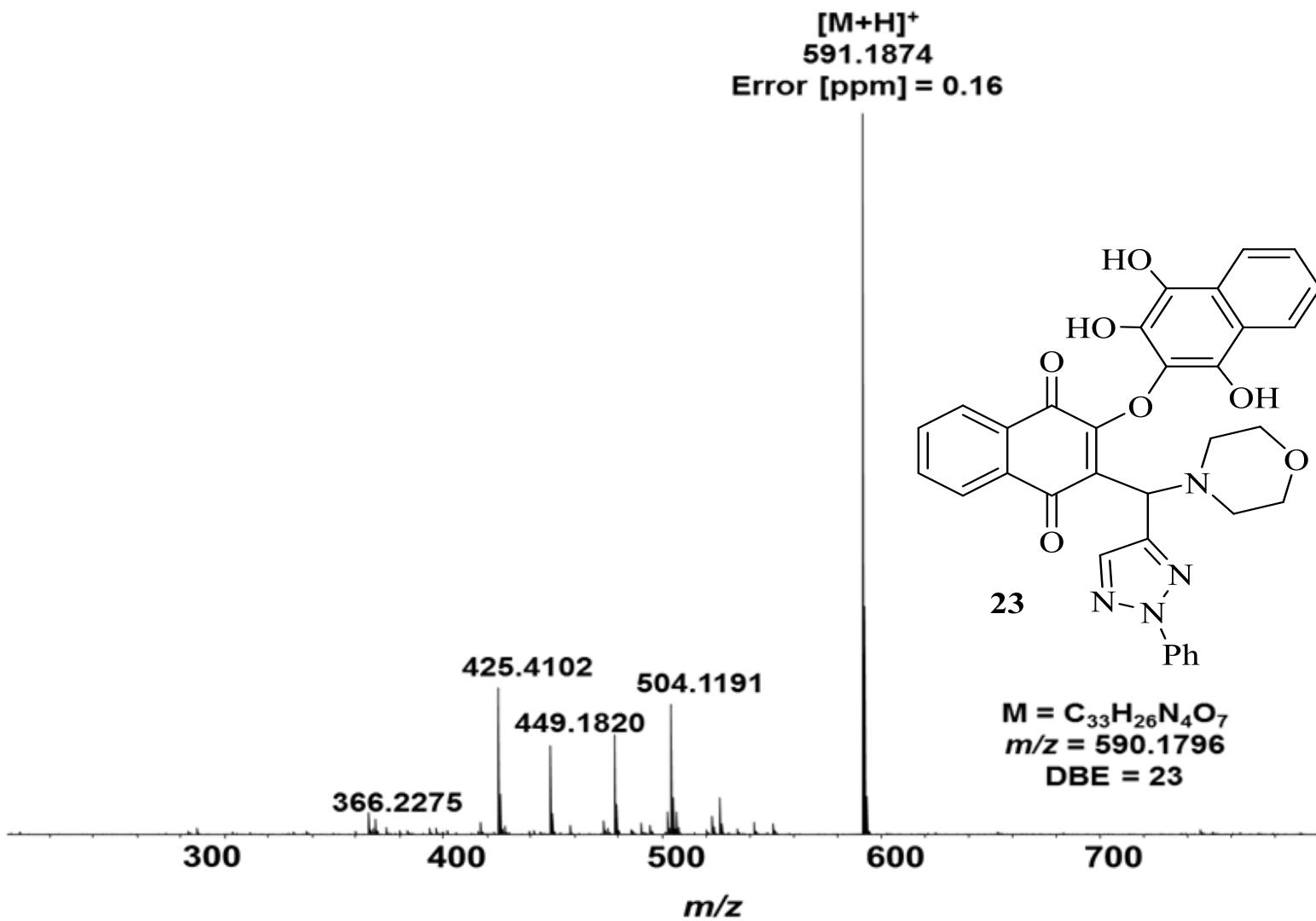


Figure S70. ESI(+)-FT-ICR mass spectrum of compound **23**.