

# Synthesis of New 2-*N,N'*-dialkylamino-1,4-naphthoquinone Derivatives: Concerning the Reactivity of Lapachol with Secondary Amines

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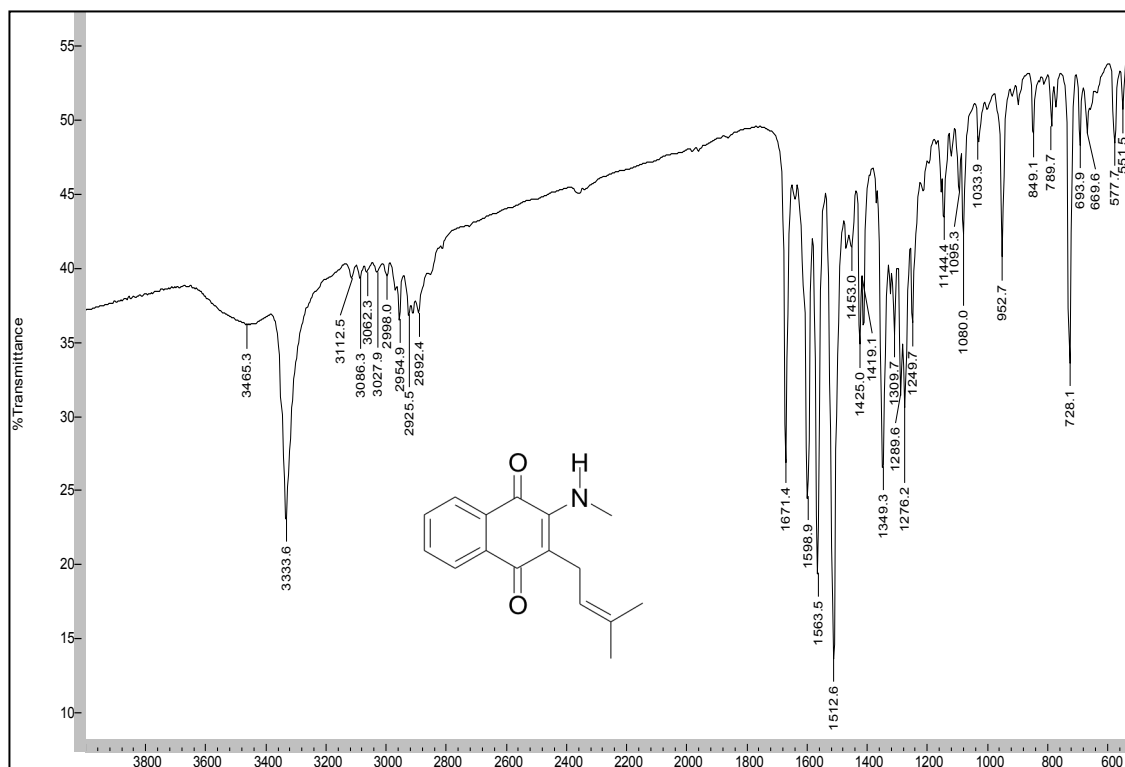


Figure S1. Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of compound 1i

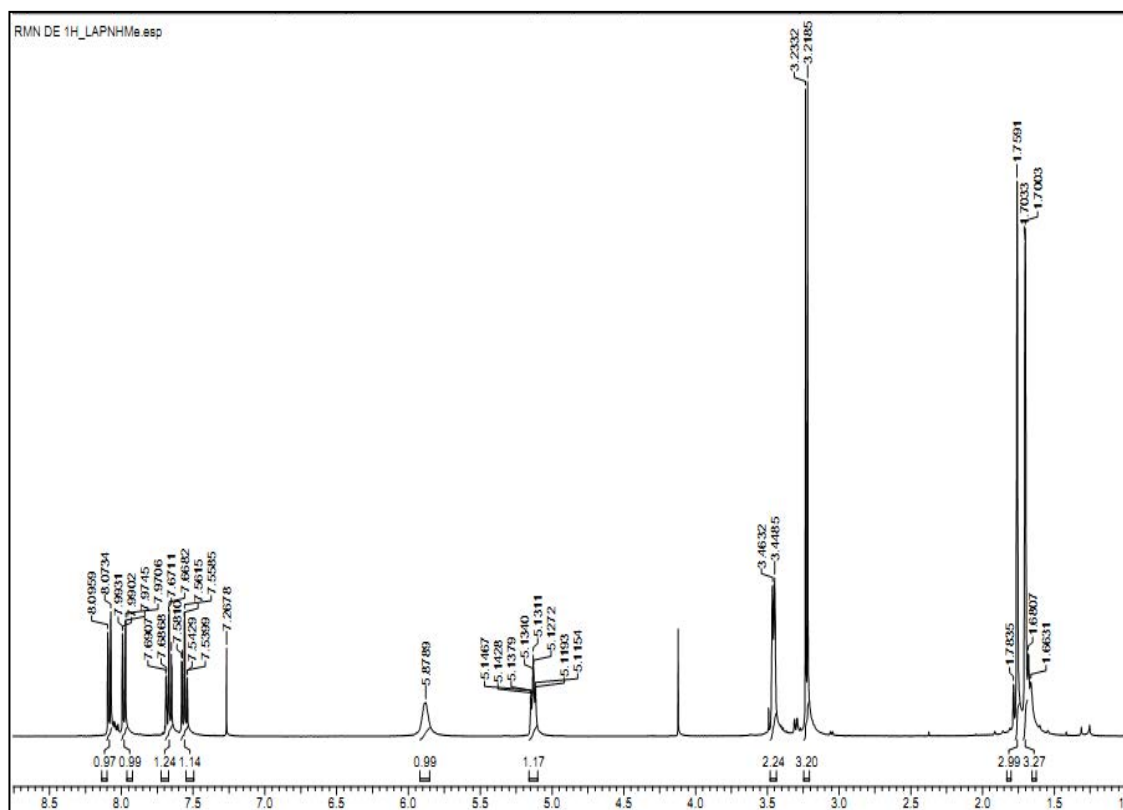


Figure S2.  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 400 MHz) of compound **1i**

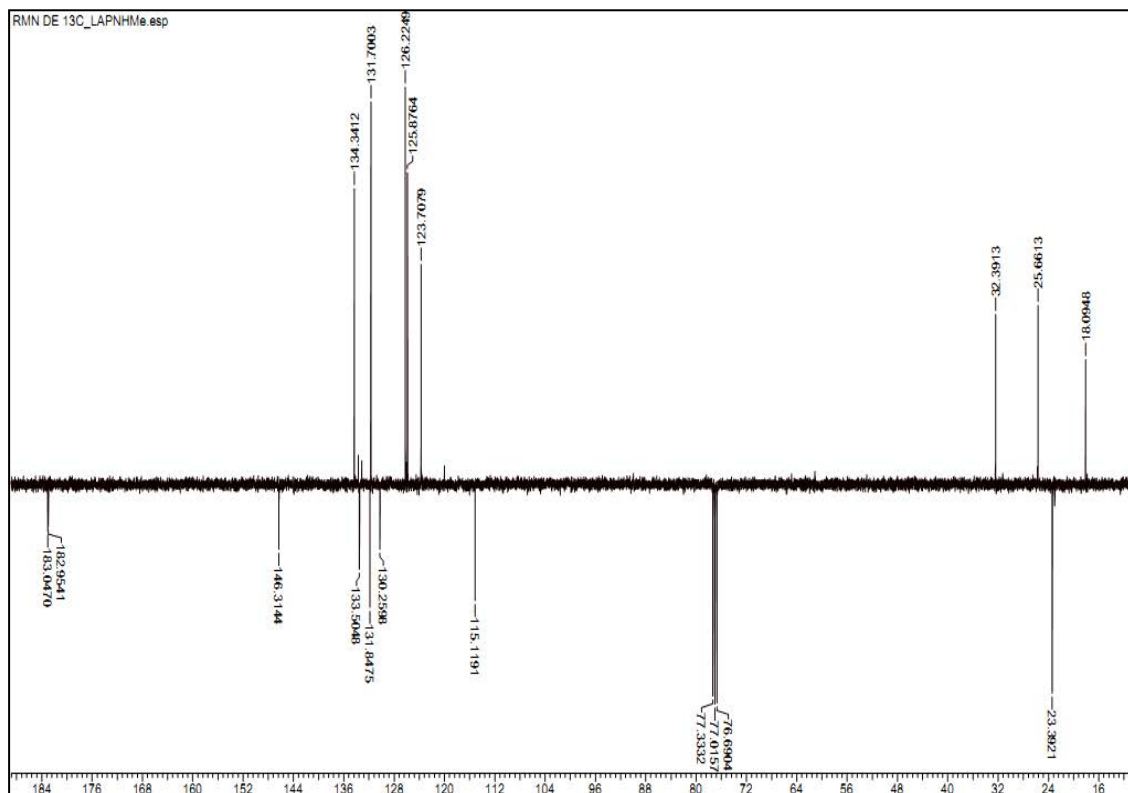


Figure S3.  $^{13}\text{C}$  NMR (APT) spectrum ( $\text{CDCl}_3$ , 100 MHz) of compound **1i**

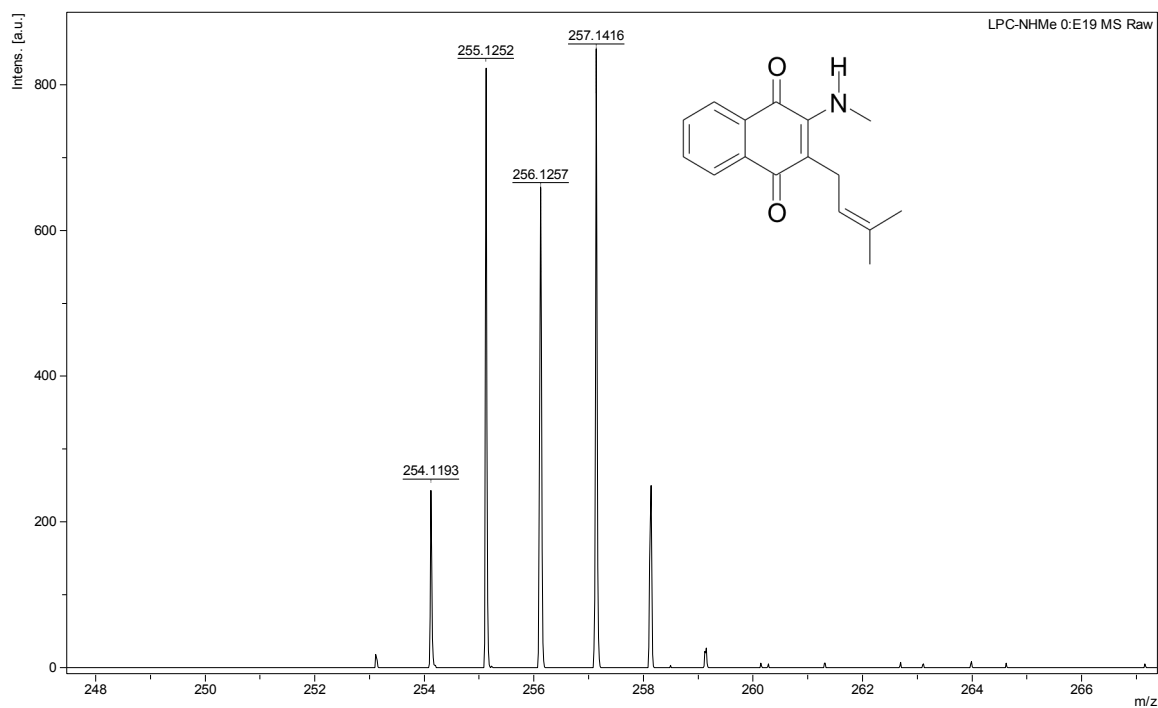


Figure S4. High resolution mass spectra of compound **1i**

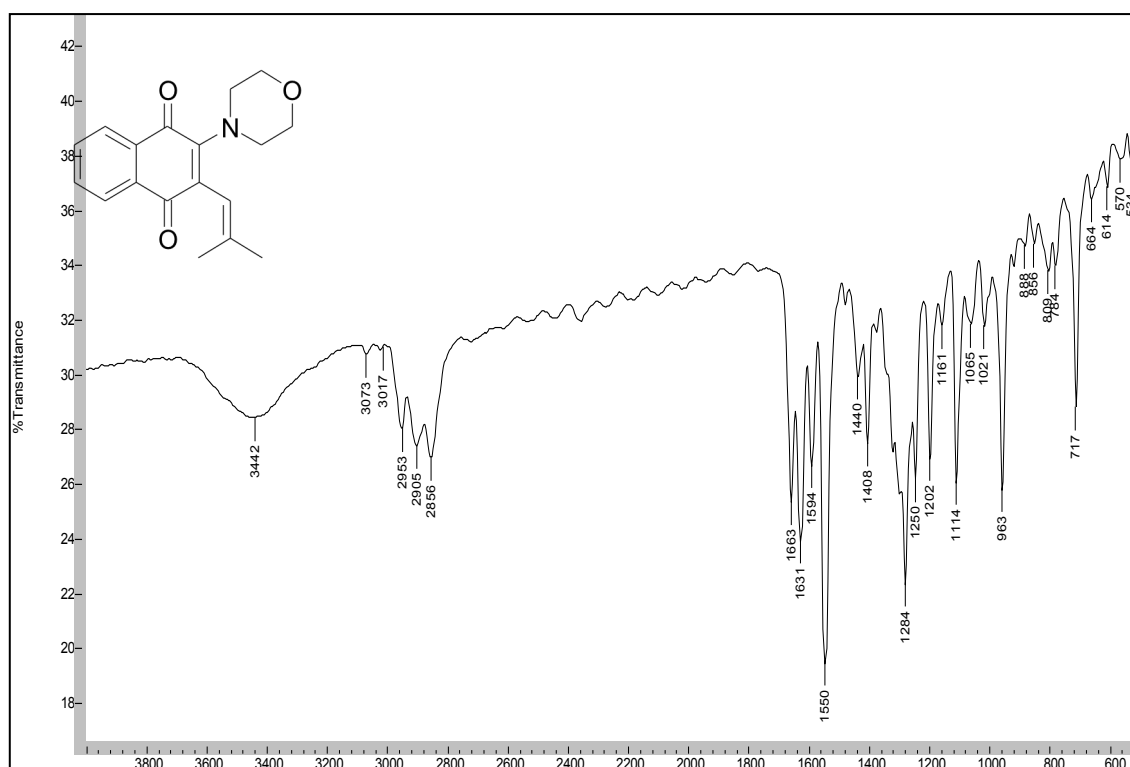


Figure S5. Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of compound **5b**

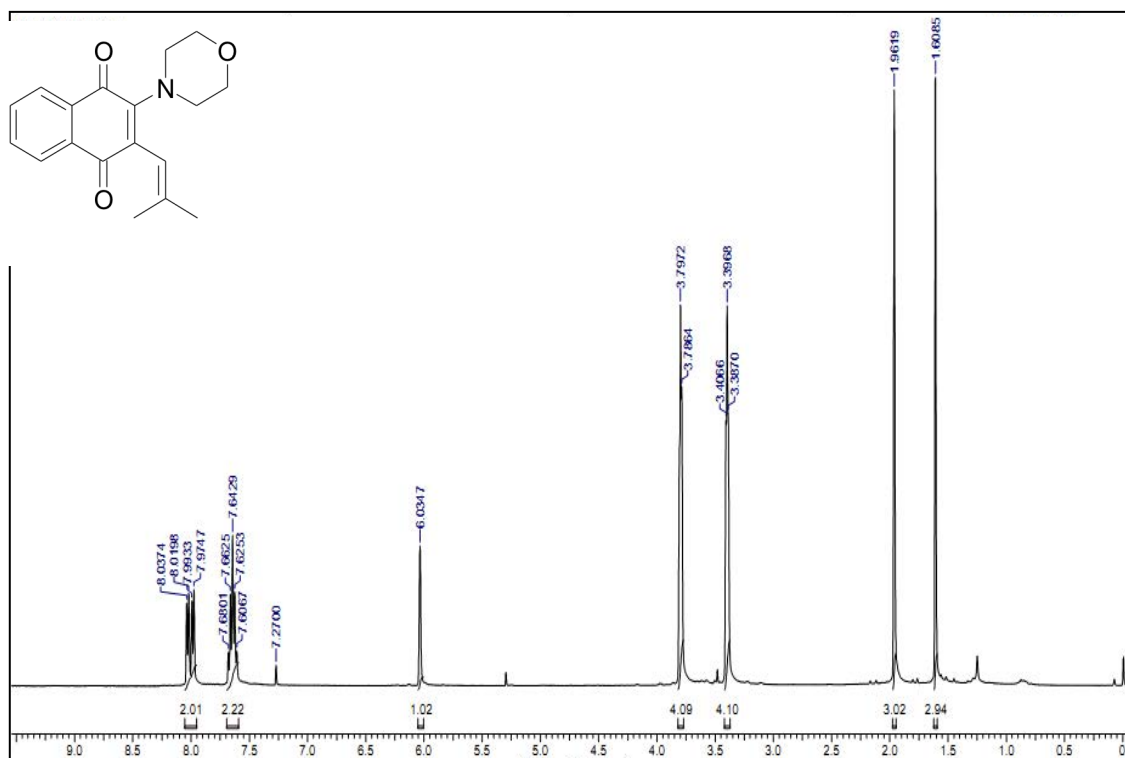


Figure S6. <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 400 MHz) of compound 5b

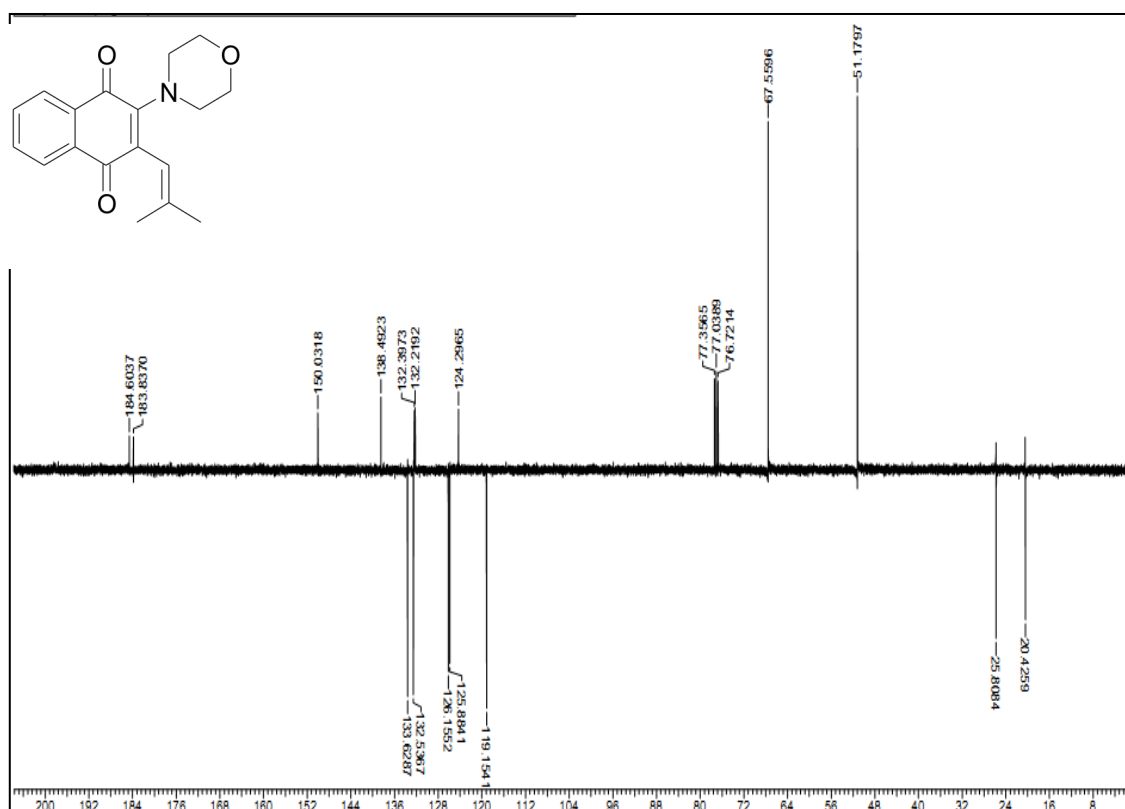


Figure S7. <sup>13</sup>C NMR (APT) spectrum (CDCl<sub>3</sub>, 100 MHz) of compound 5b

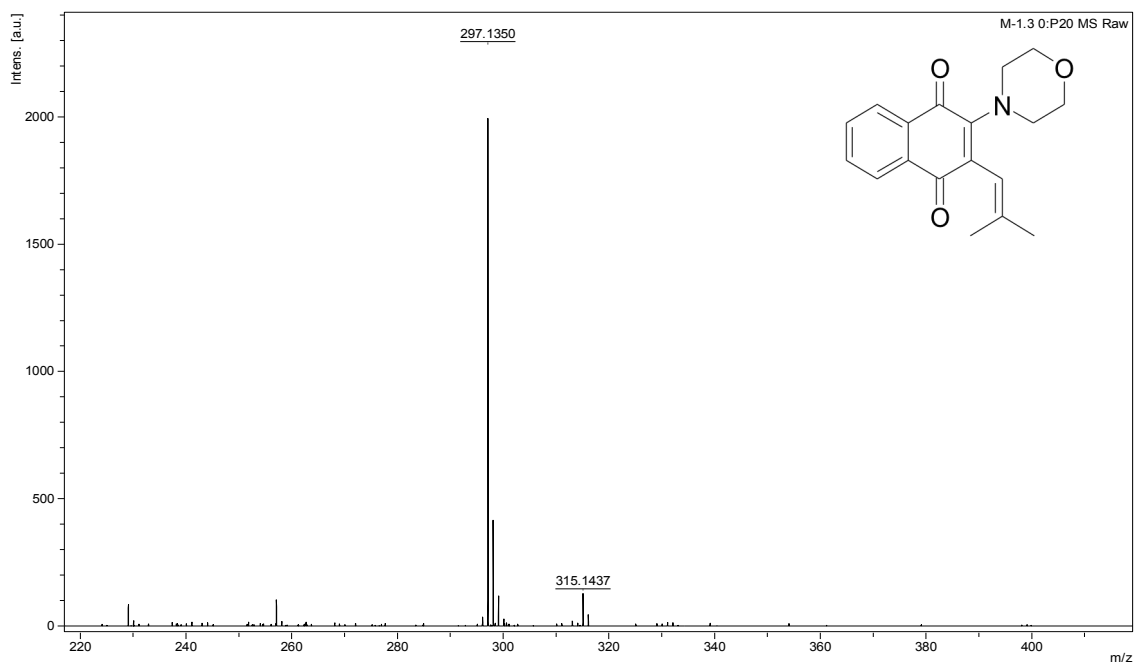


Figure S8. High resolution mass spectra of compound 5b

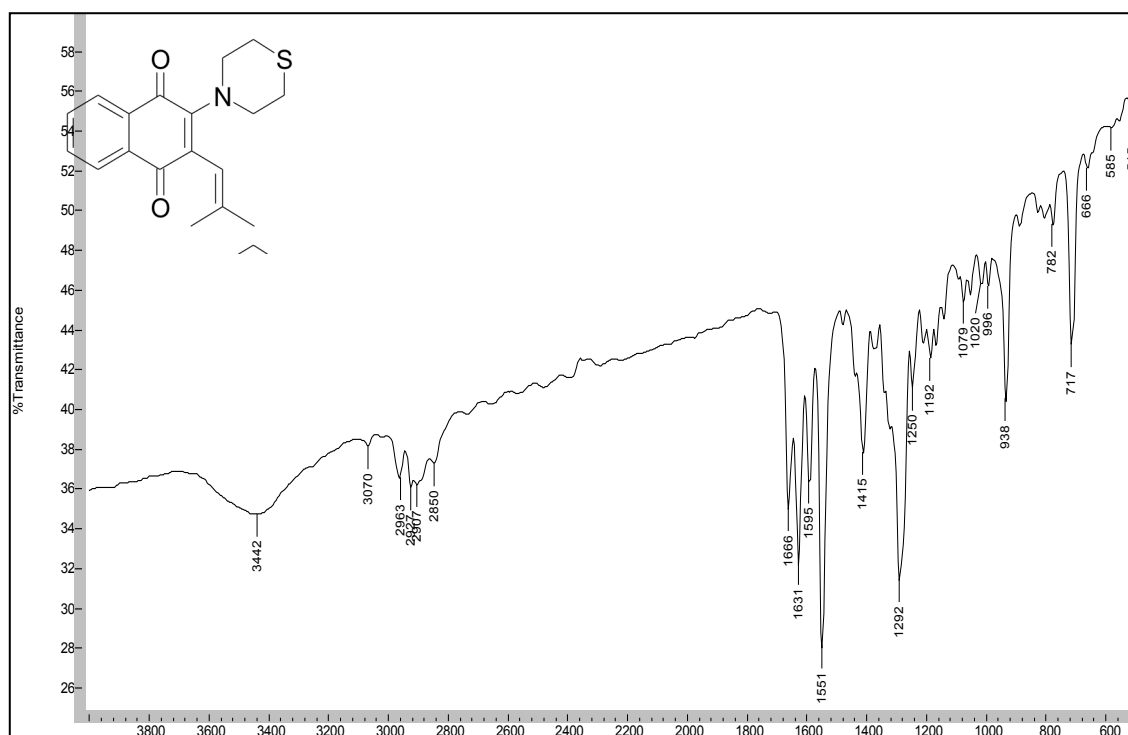


Figure S9. Infrared spectrum (KBr, cm<sup>-1</sup>) of compound 5c

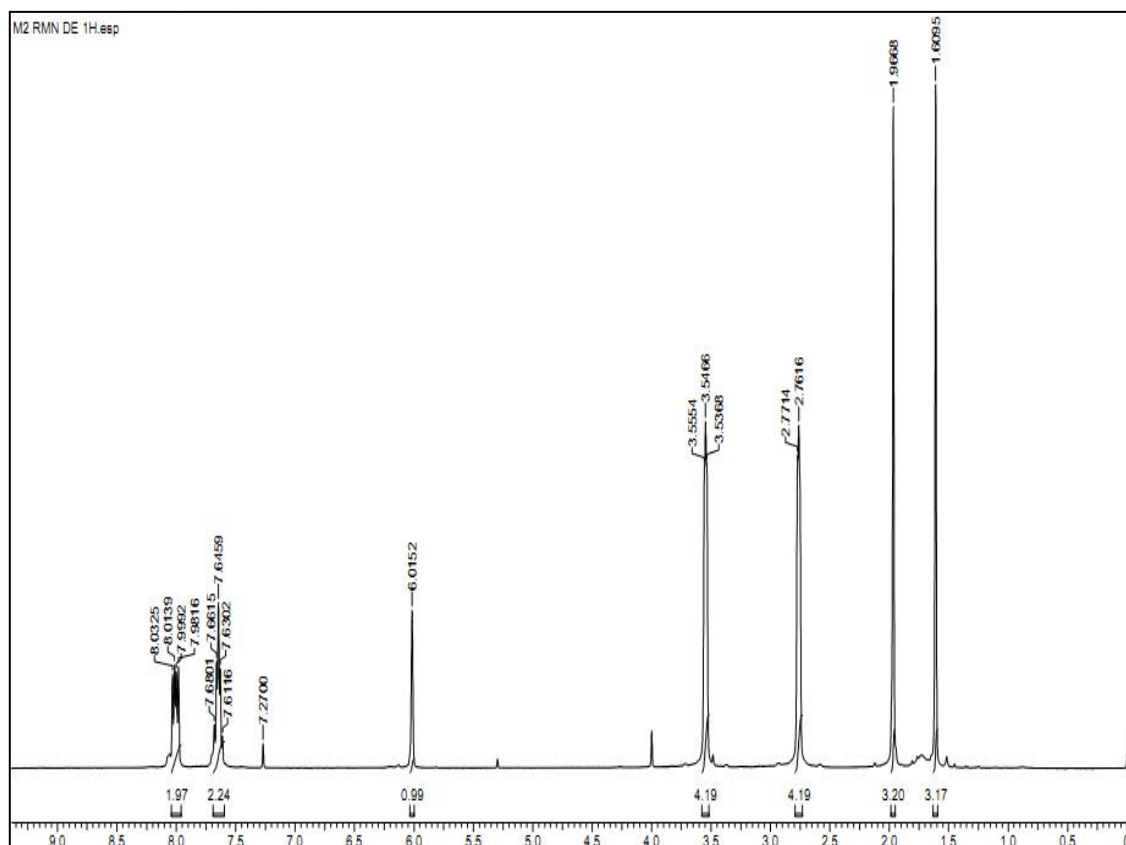


Figure S10.  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 400 MHz) of compound **5c**

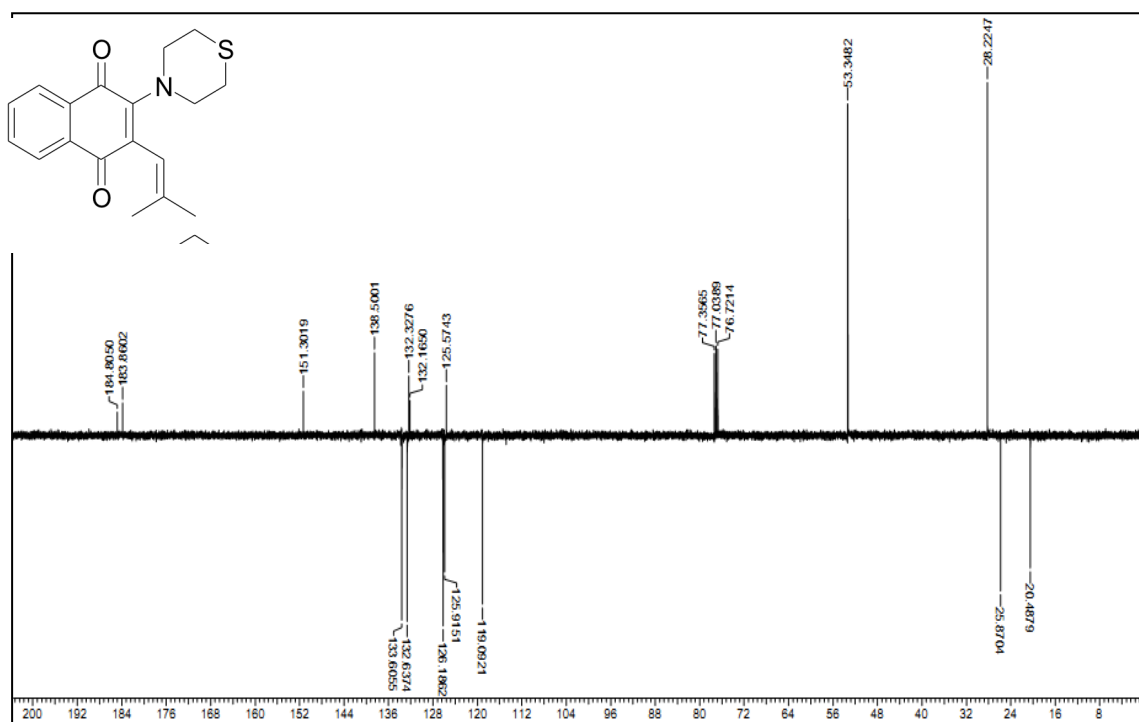


Figure S11.  $^{13}\text{C}$  NMR (APT) spectrum ( $\text{CDCl}_3$ , 100 MHz) of compound **5c**

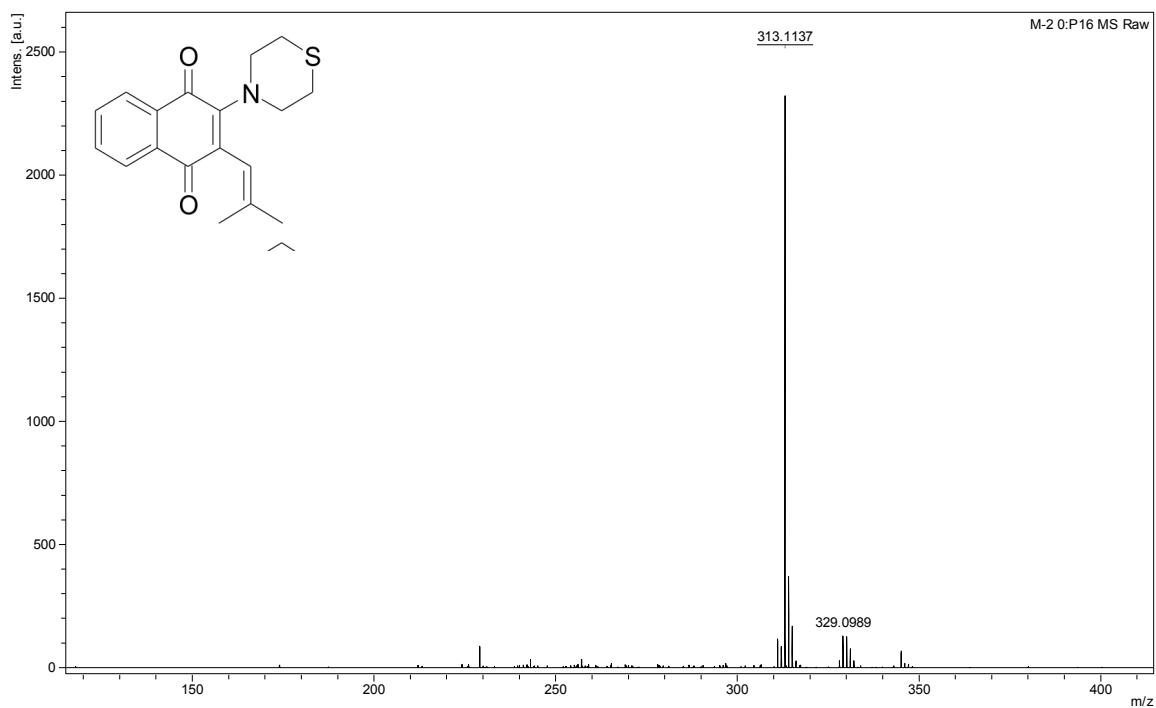


Figure S12. High resolution mass spectra of compound 5c

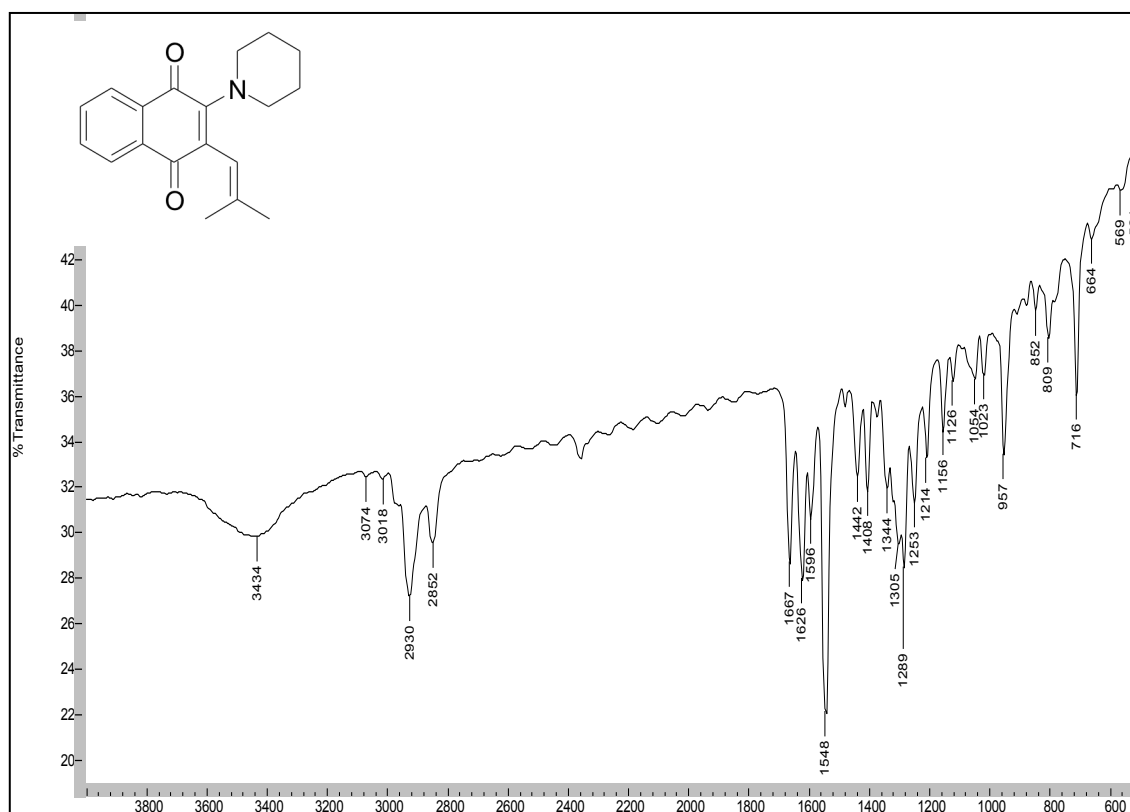


Figure S13. Infrared spectrum (KBr, cm<sup>-1</sup>) of compound 5d

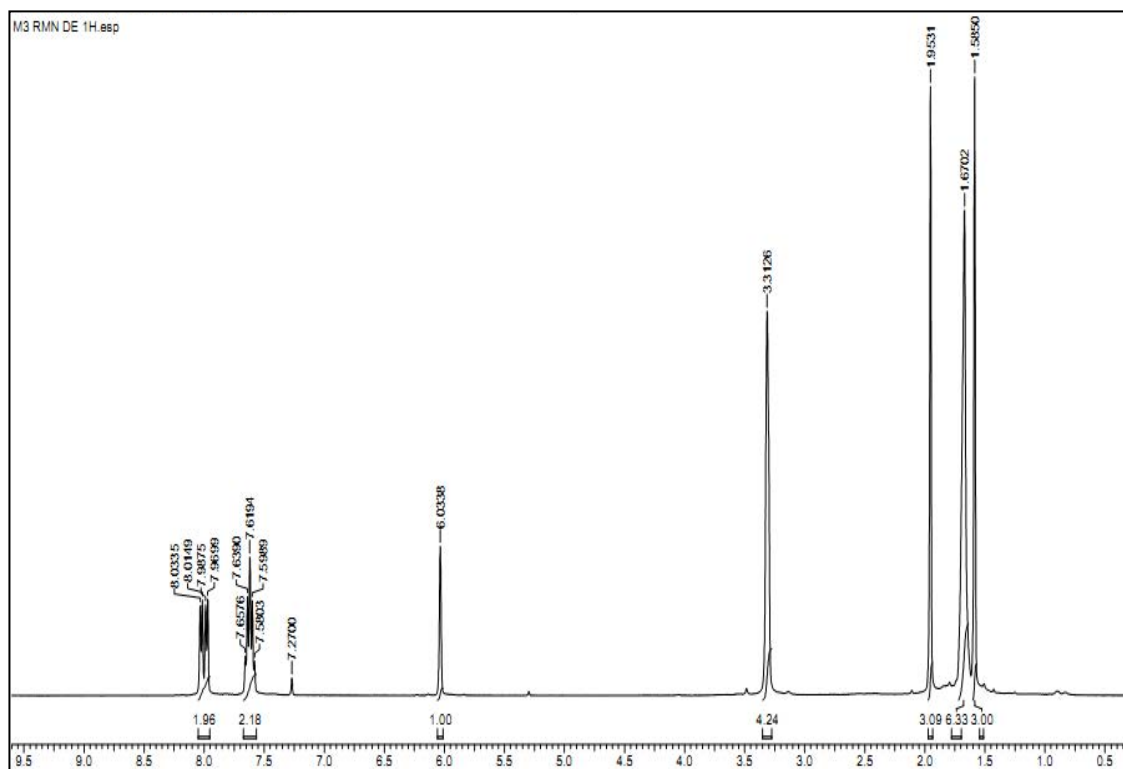


Figure S14.  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 400 MHz) of compound **5d**

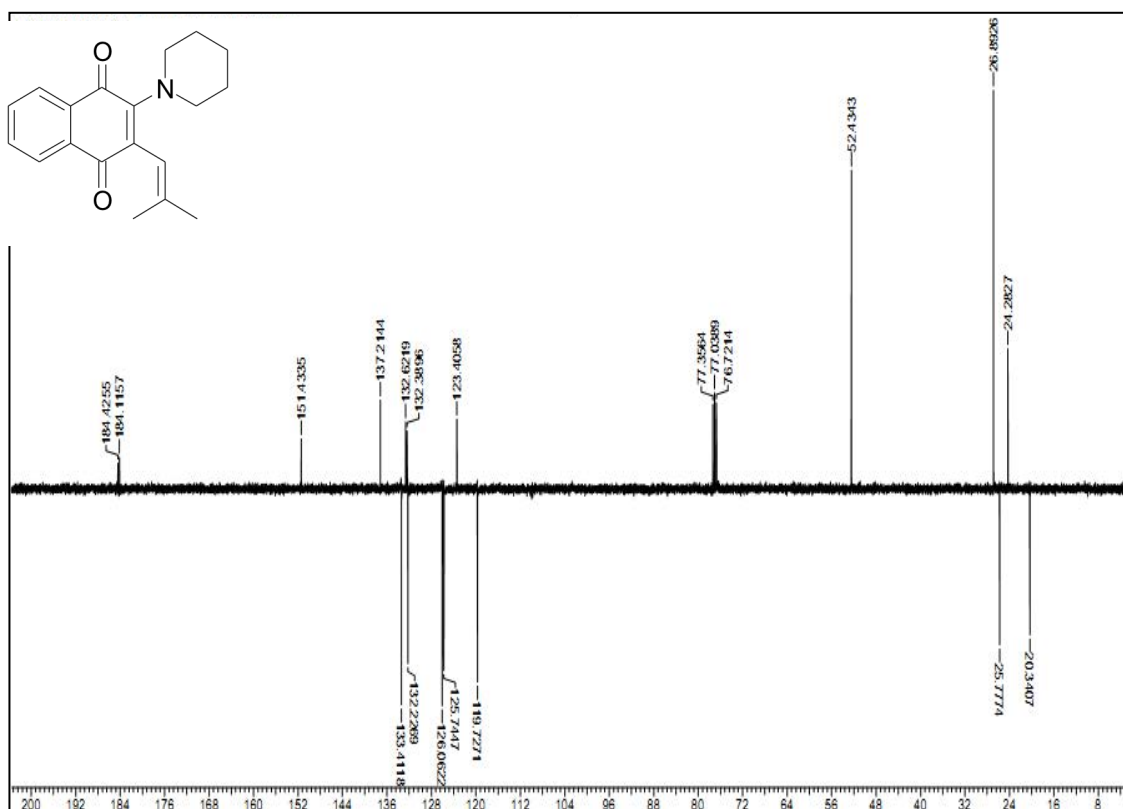


Figure S15.  $^{13}\text{C}$  NMR (APT) spectrum ( $\text{CDCl}_3$ , 100 MHz) of compound **5d**



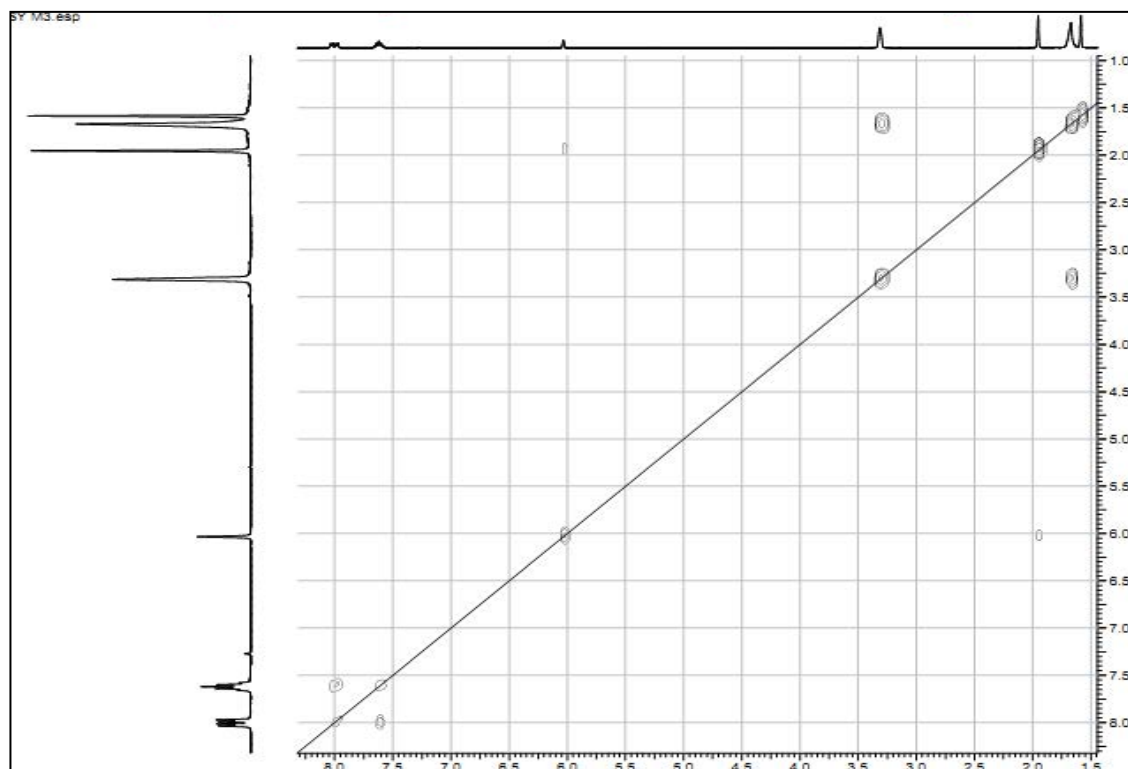


Figure S16. COSY spectrum of compound **5d**

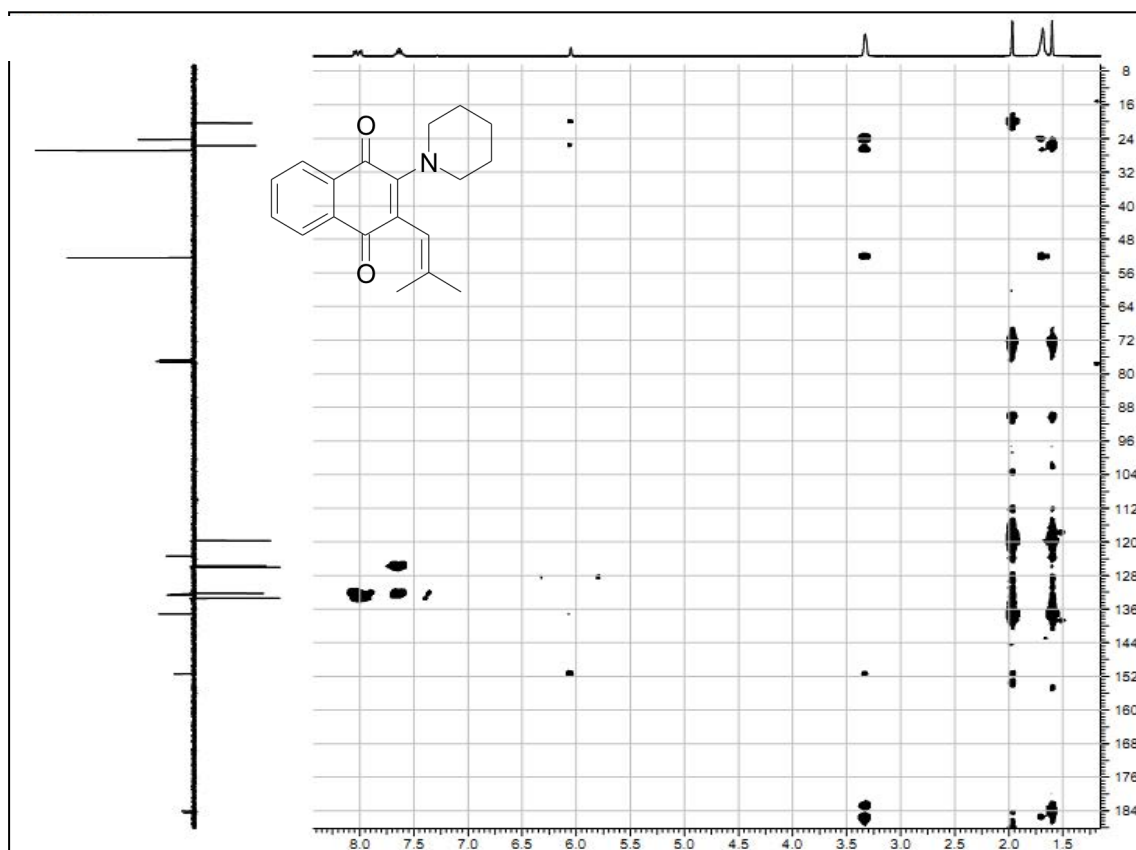


Figure S17. HMBC spectrum of compound **5d**

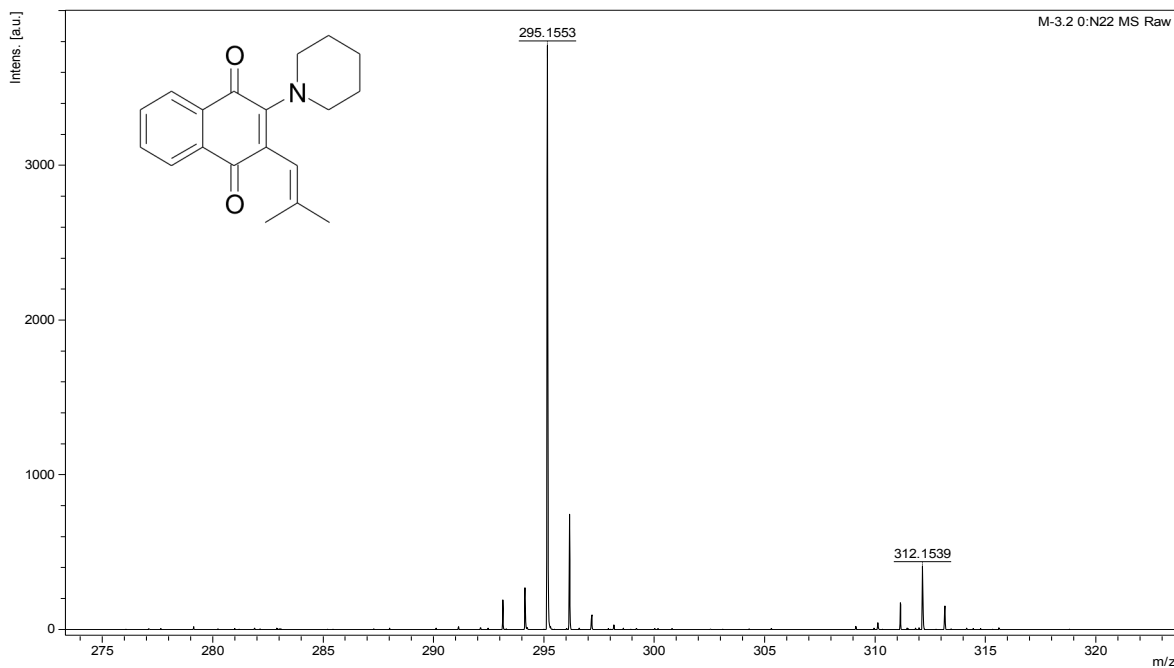
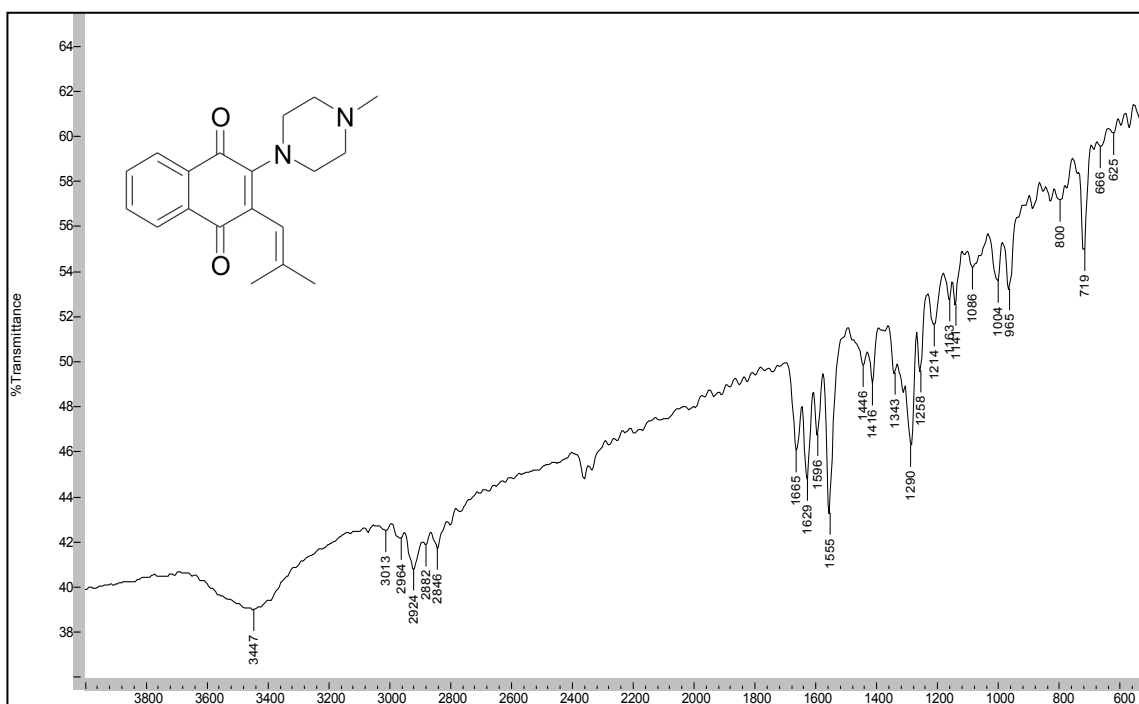


Figure S18. High resolution mass spectra of compound 5d

Figure S19. Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of compound 5e

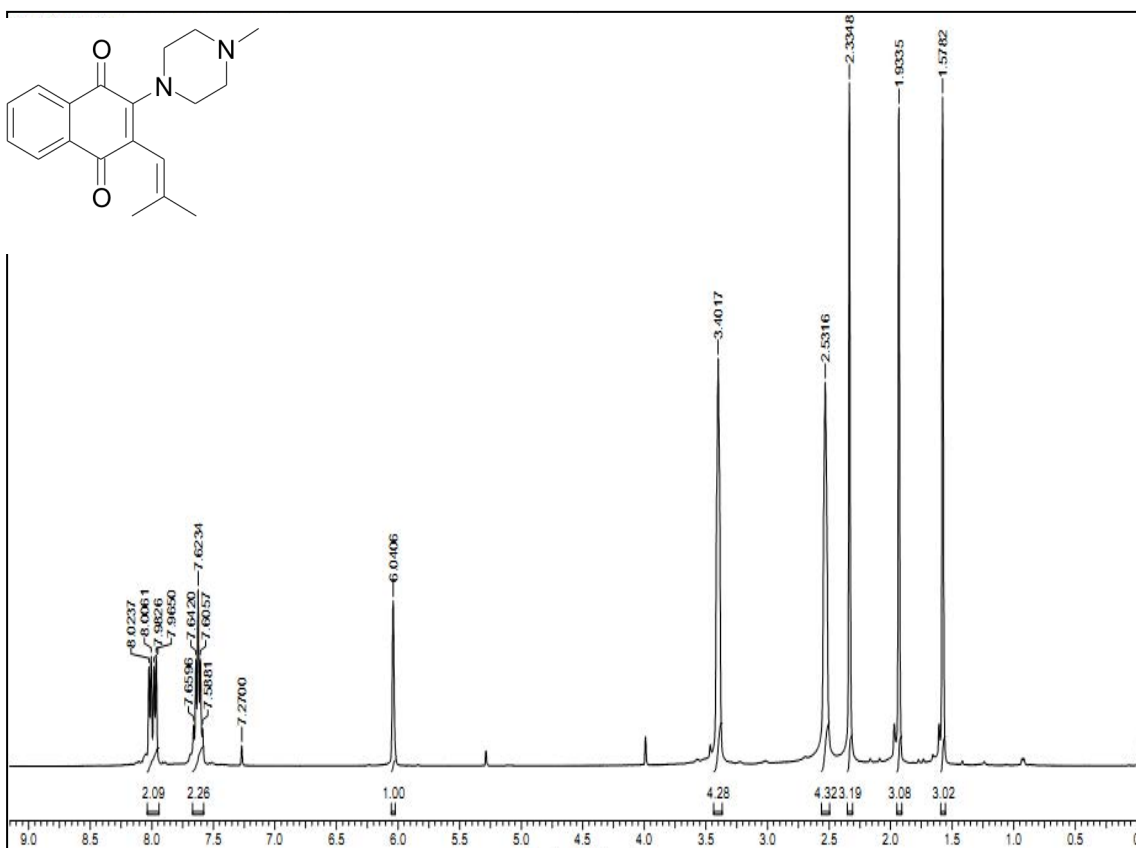


Figure S20.  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 400 MHz) of compound 5e

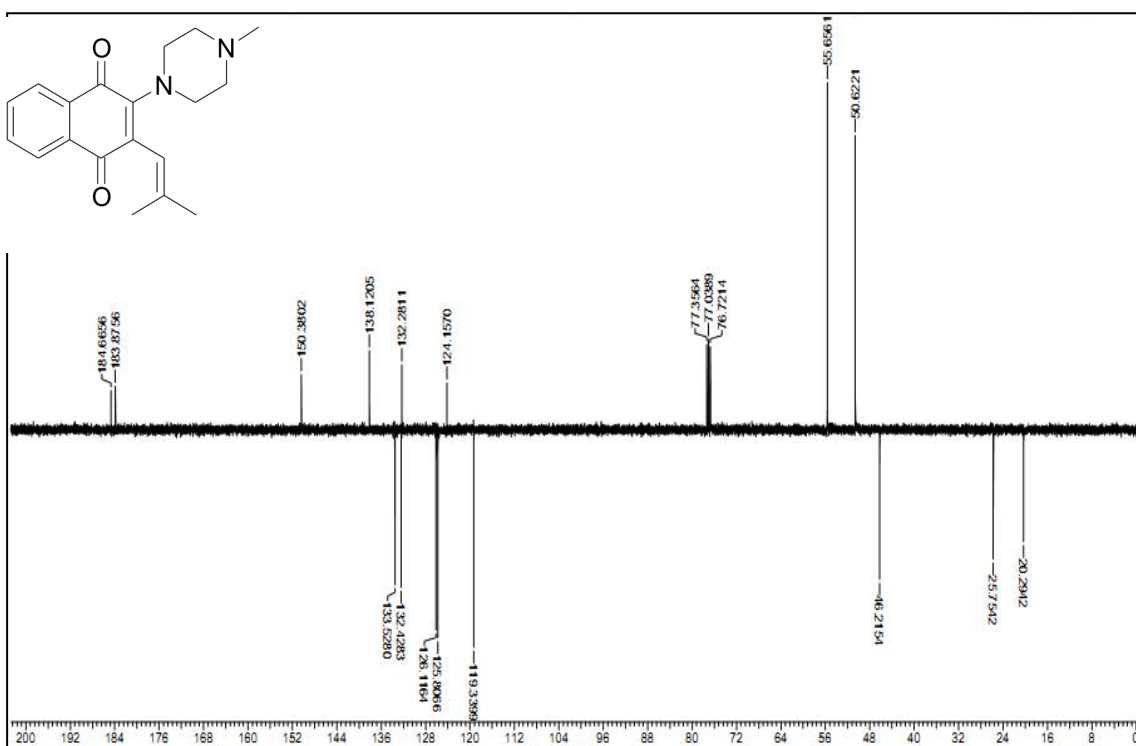


Figure S21.  $^{13}\text{C}$  NMR (APT) spectrum ( $\text{CDCl}_3$ , 100 MHz) of compound 5e

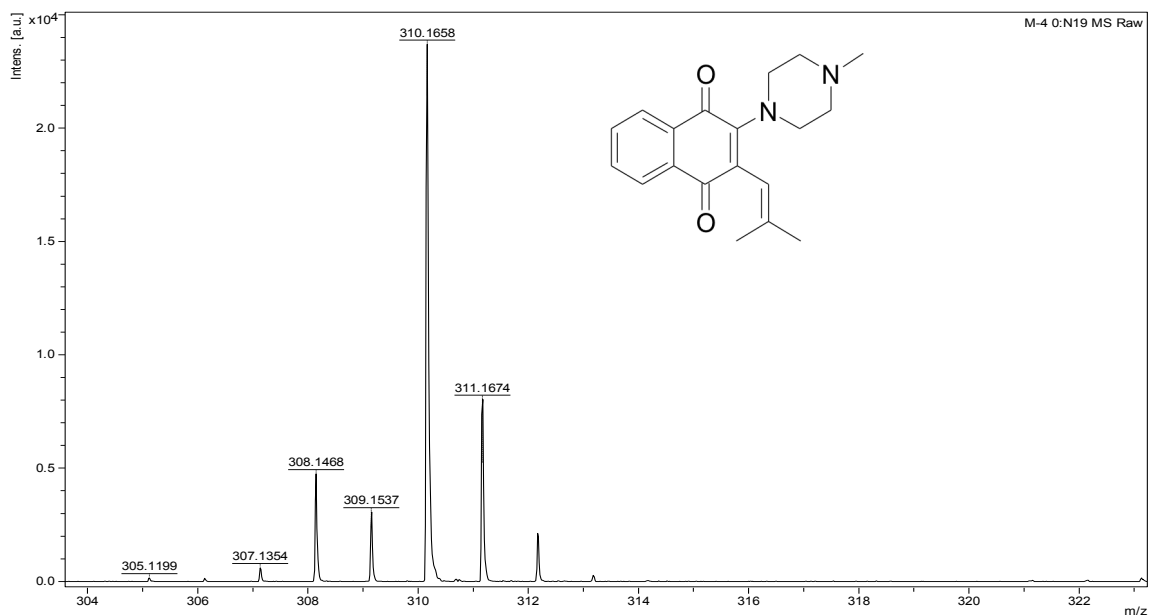


Figure S22. High resolution mass spectra of compound 5e

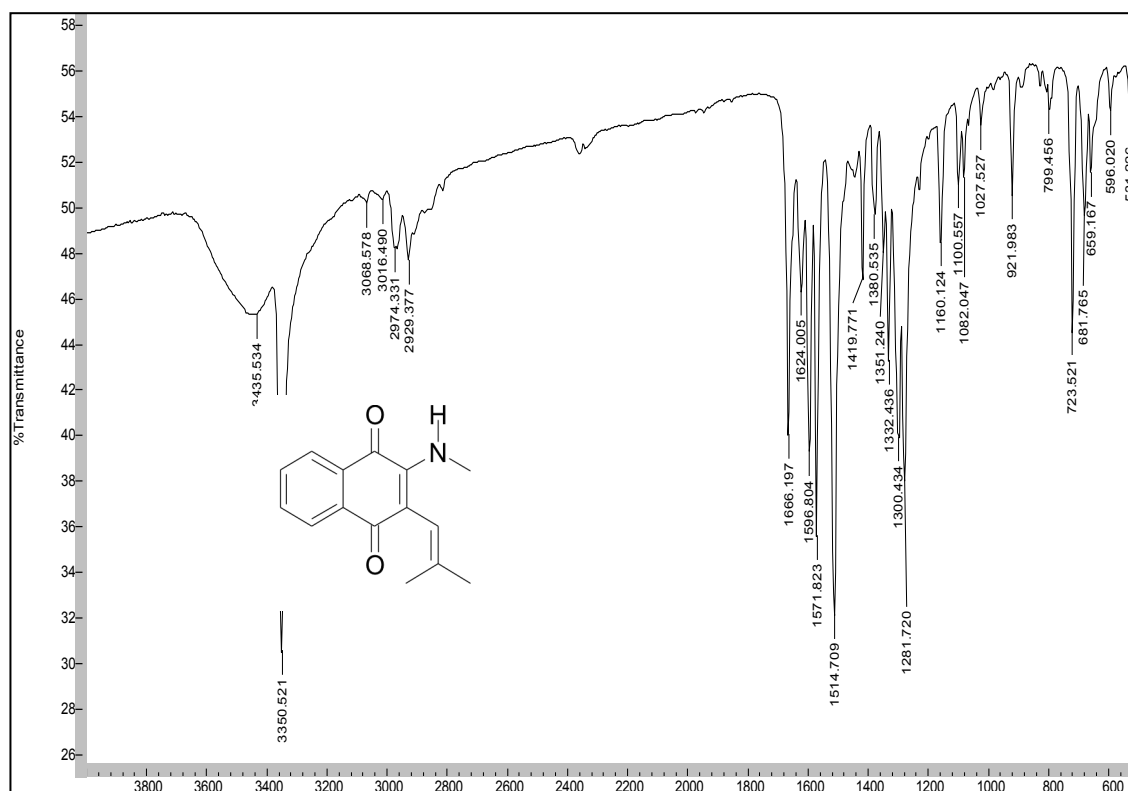


Figure S23. Infrared spectrum (KBr, cm<sup>-1</sup>) of compound 5i

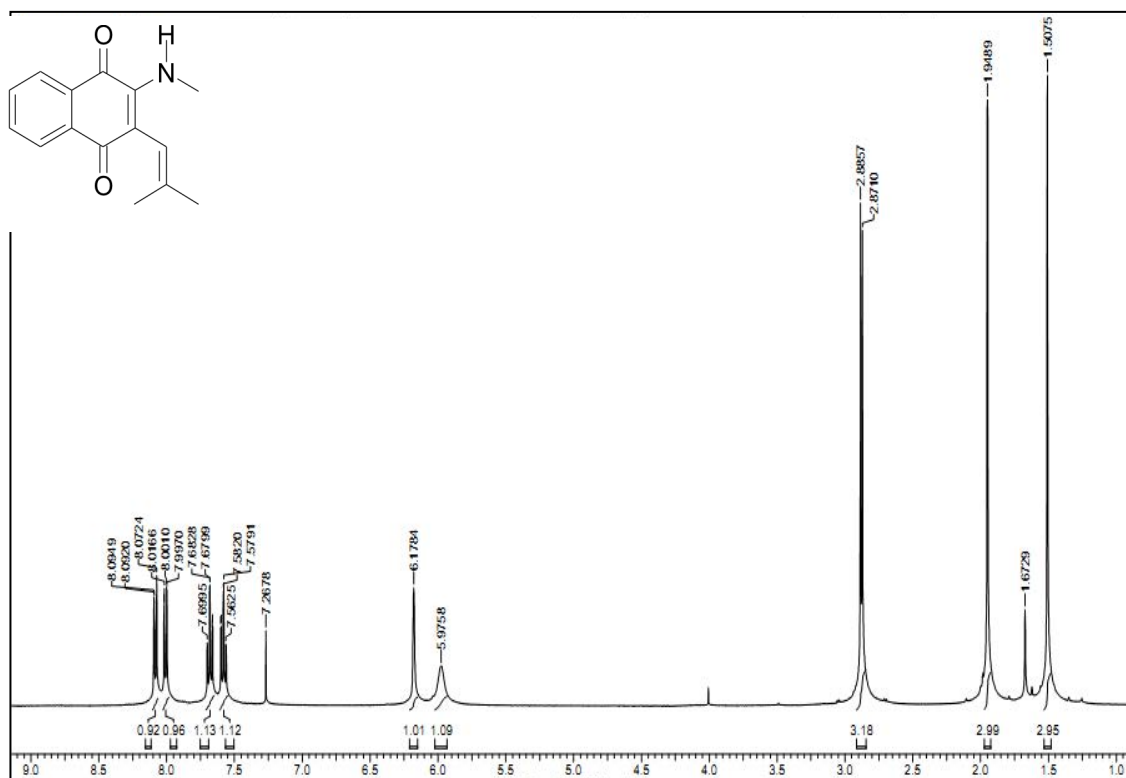


Figure S24.  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 400 MHz) of compound 5i

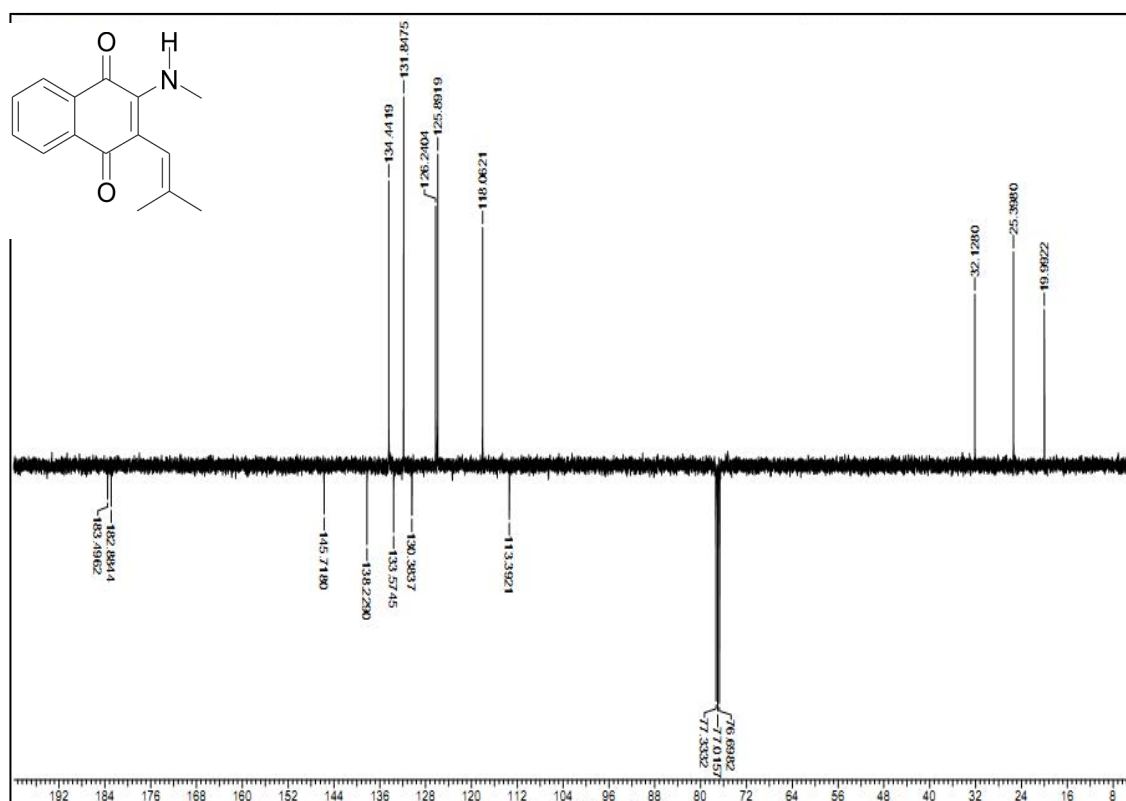


Figure S25.  $^{13}\text{C}$  NMR (APT) spectrum ( $\text{CDCl}_3$ , 100 MHz) of compound 5i

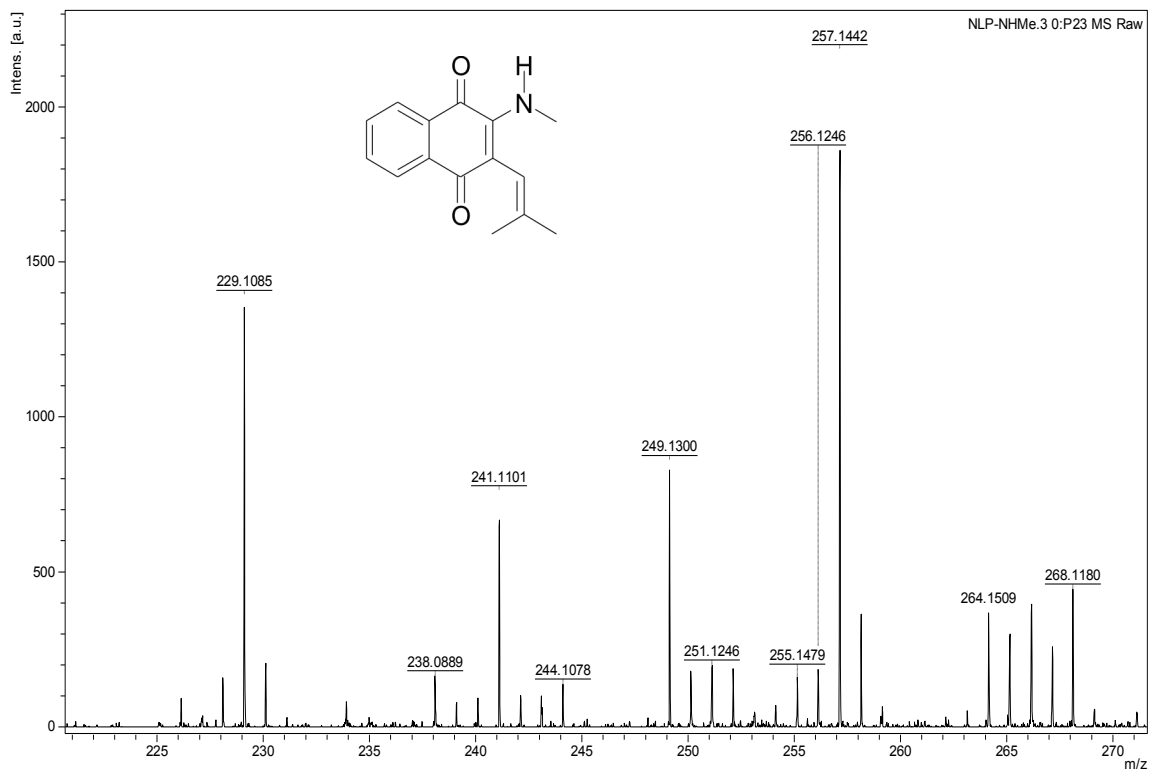


Figure 26. High resolution mass spectra of compound 5i

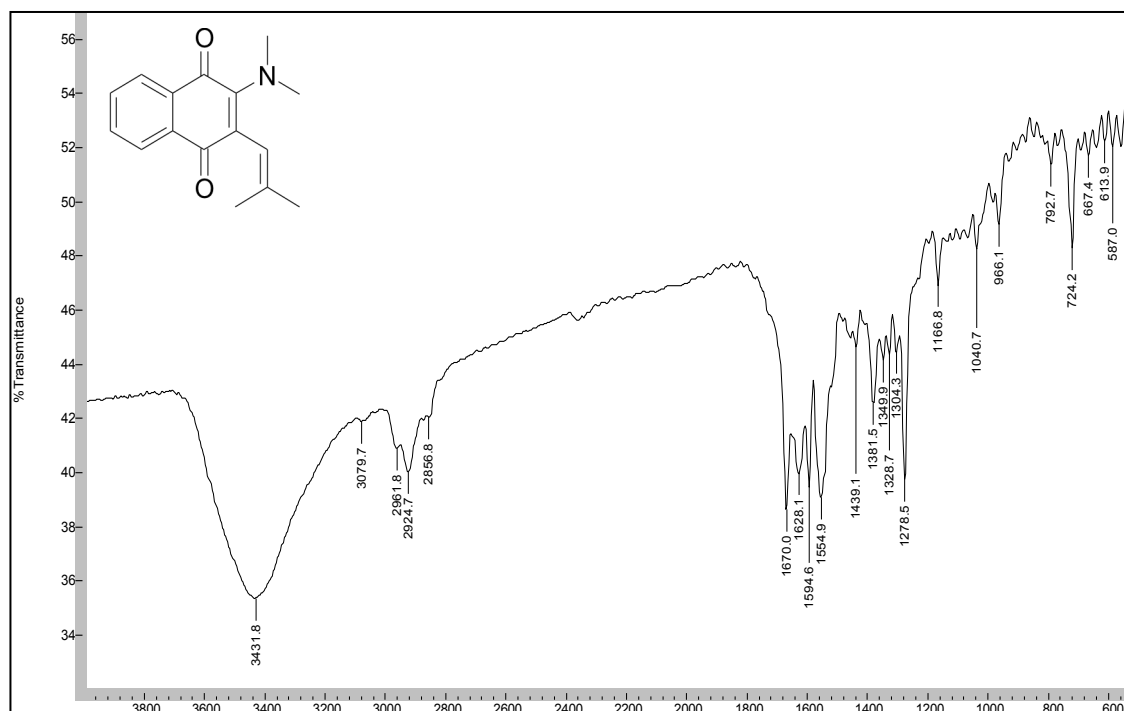


Figure S27. Infrared spectrum (KBr, cm<sup>-1</sup>) of compound 5j

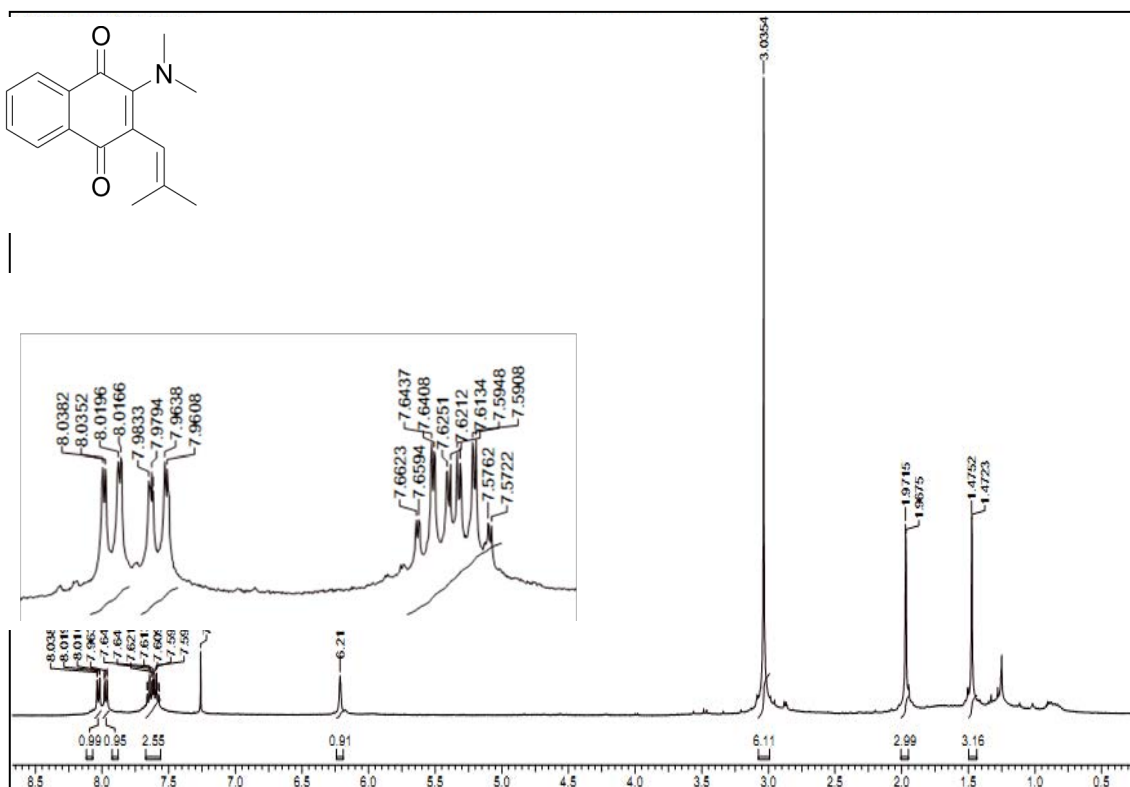


Figure S28.  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 400 MHz) of compound 5j

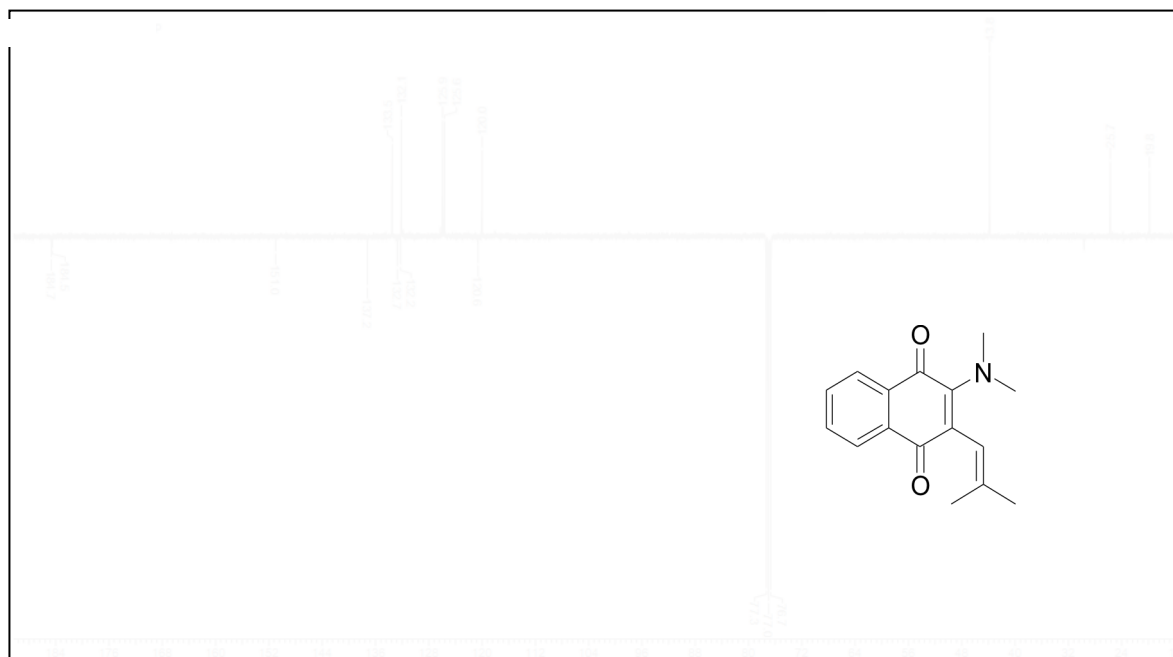


Figure S29.  $^{13}\text{C}$  NMR (APT) spectrum ( $\text{CDCl}_3$ , 100 MHz) of compound 5j

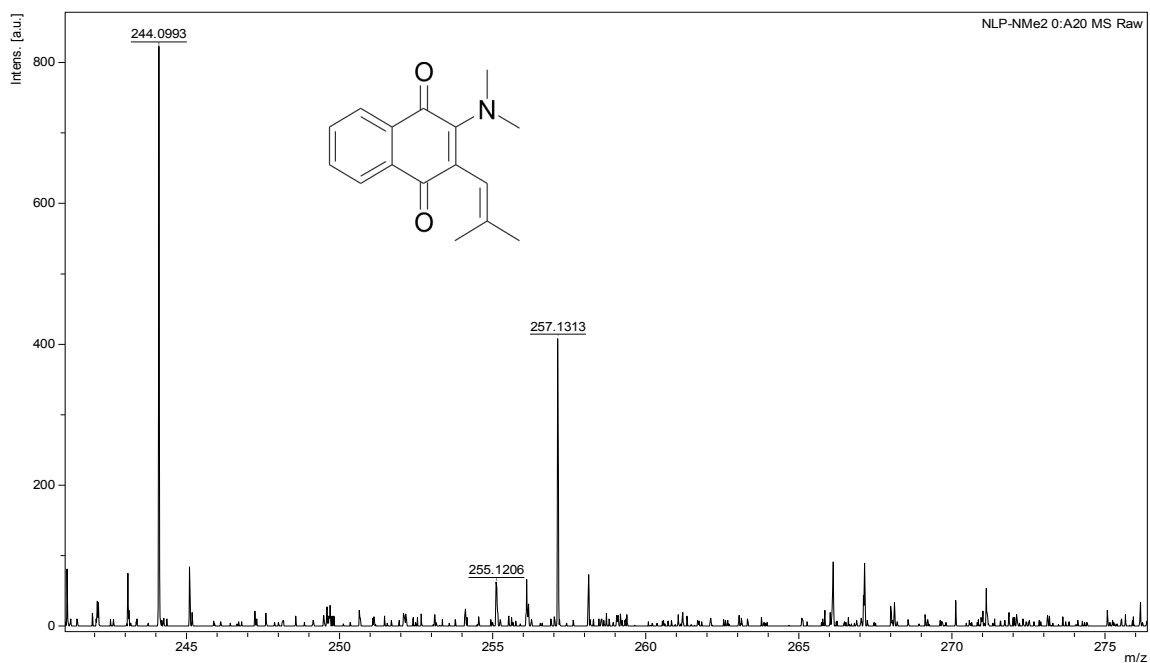


Figure 30. High resolution mass spectra of compound **5j**

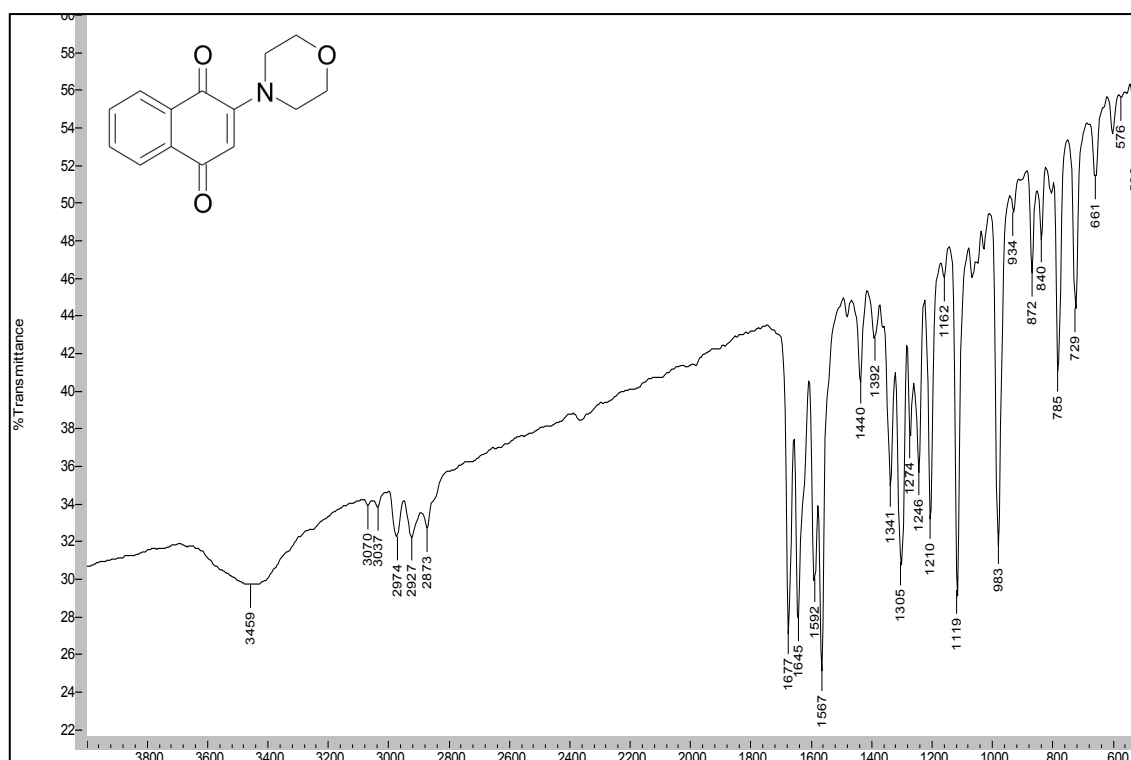


Figure S31. Infrared spectrum ( $\text{KBr}$ ,  $\text{cm}^{-1}$ ) of compound **6b**



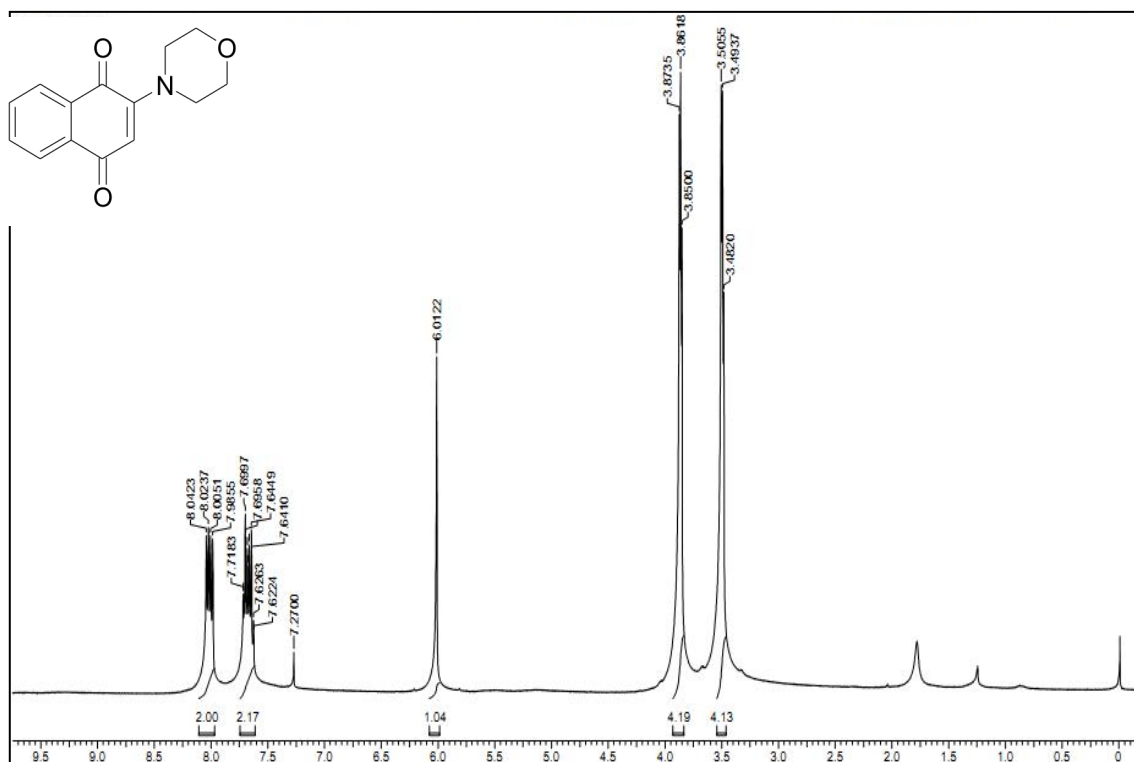


Figure S32. <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 400 MHz) of compound 6b

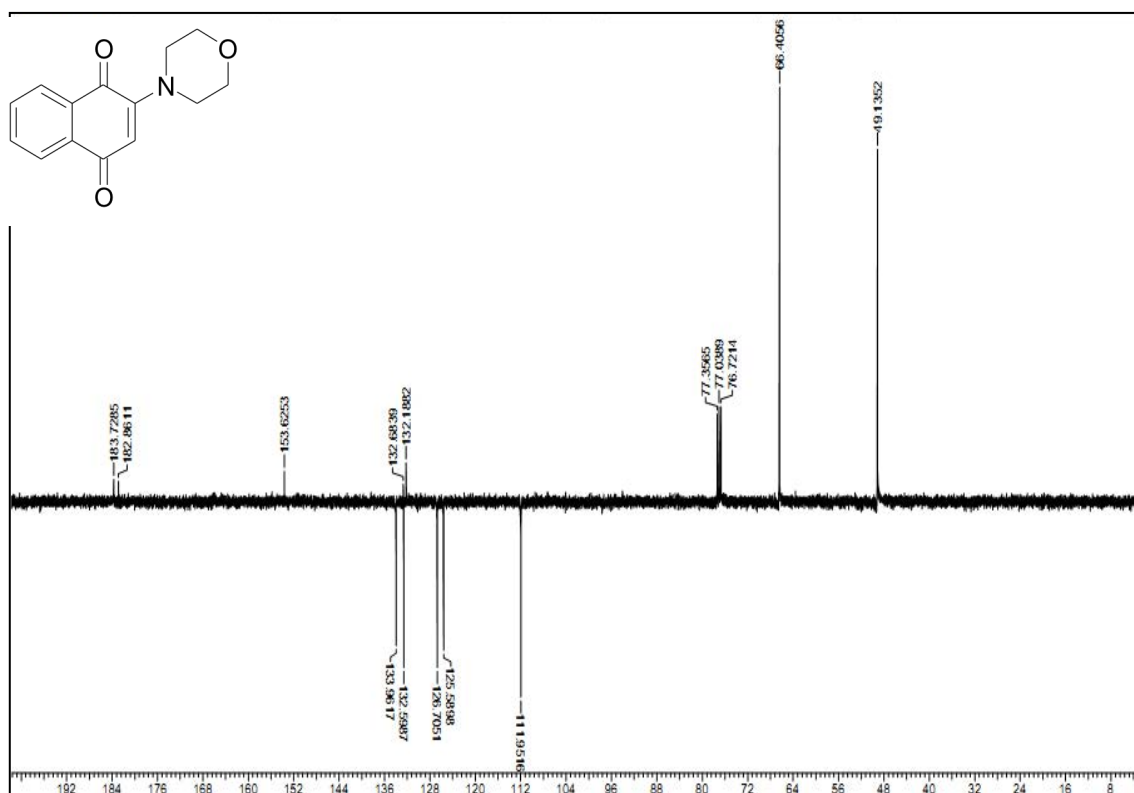


Figure S33. <sup>13</sup>C NMR (APT) spectrum (CDCl<sub>3</sub>, 100 MHz) of compound 6b

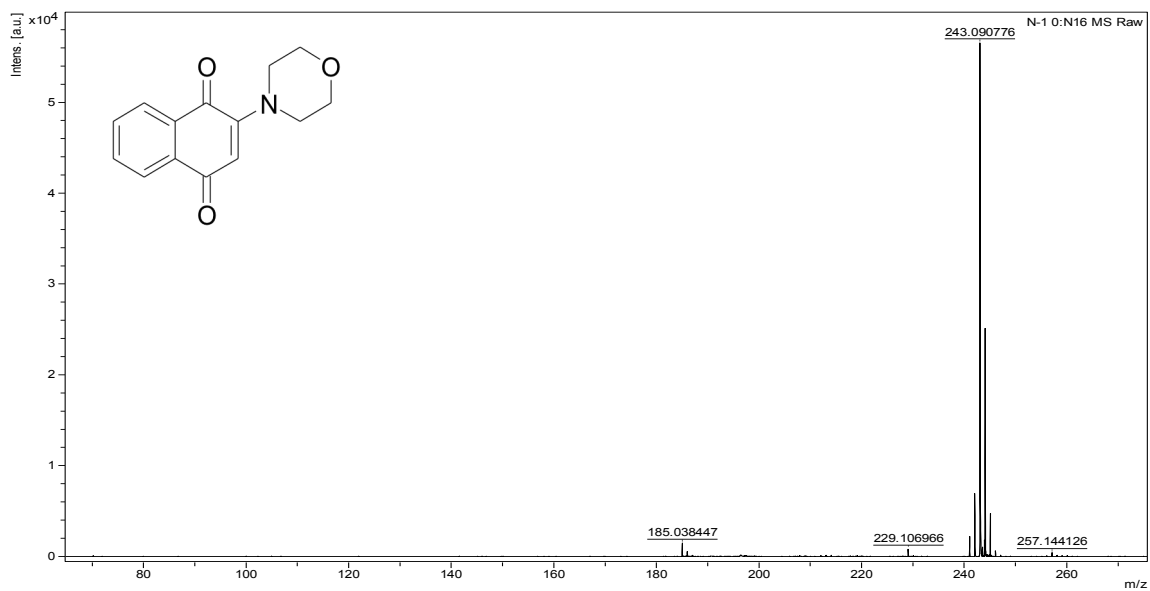


Figure S34. High resolution mass spectra of compound **6b**

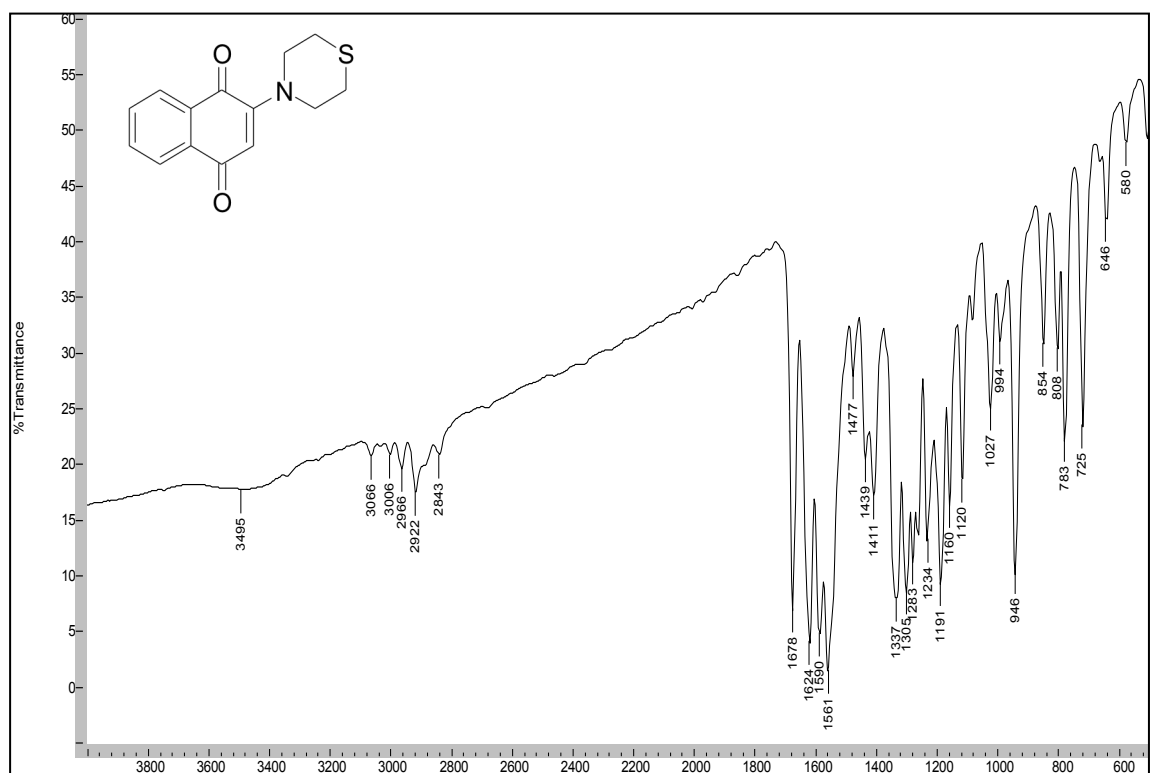


Figure S35. Infrared spectrum ( $\text{KBr}$ ,  $\text{cm}^{-1}$ ) of compound **6c**



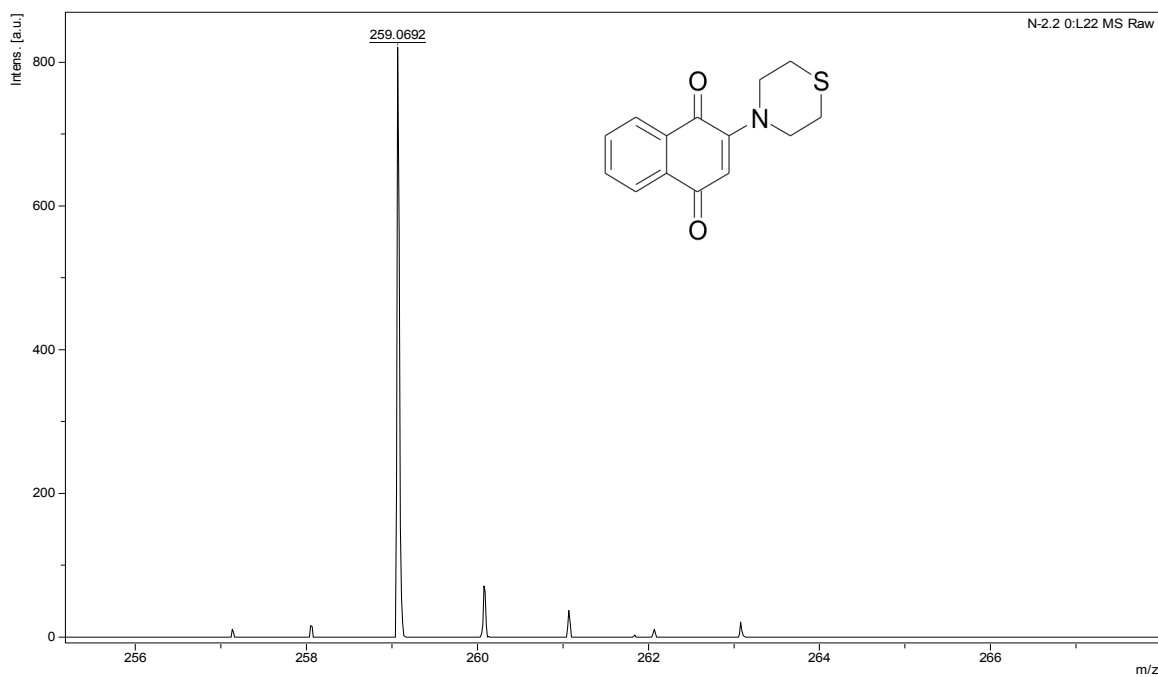


Figure S38. High resolution mass spectra of compound **6c**

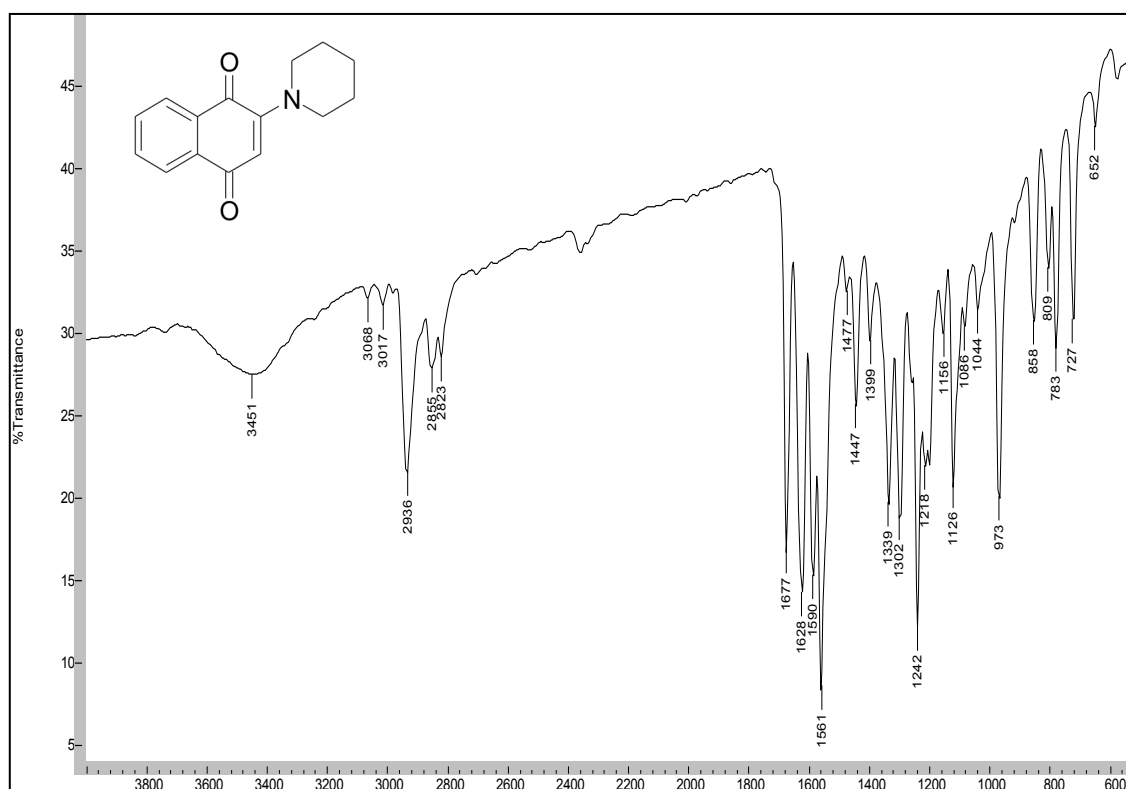


Figure S39. Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of compound **6d**

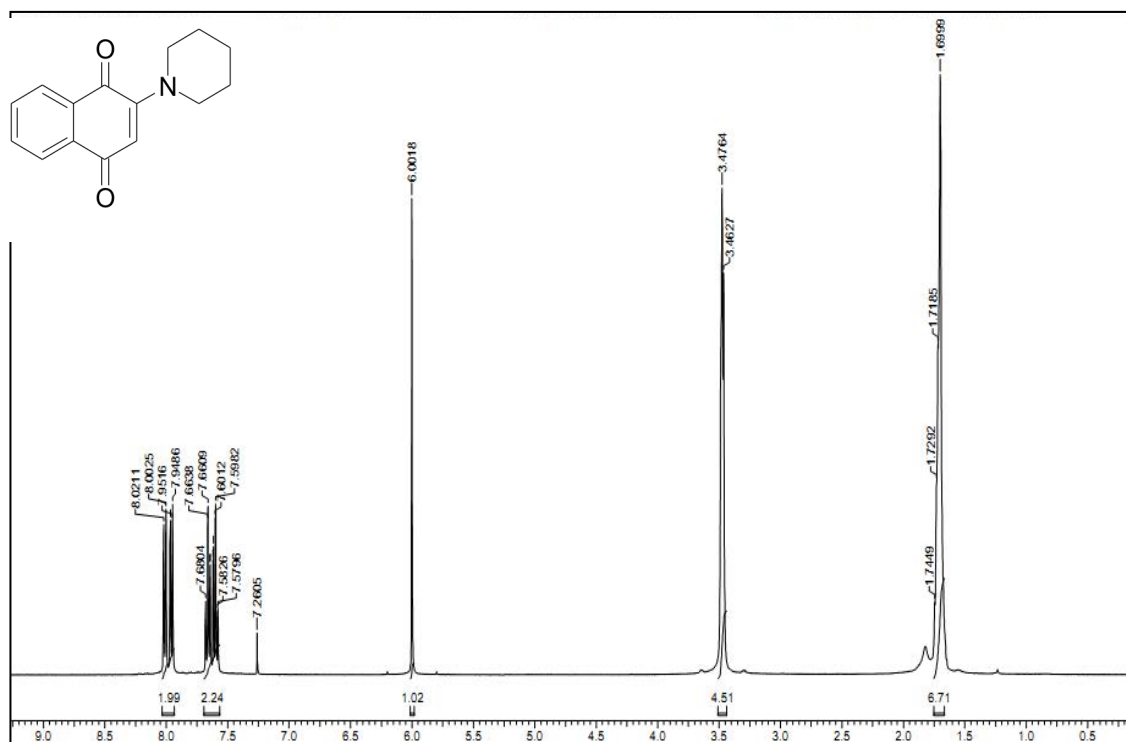


Figure S40. <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 400 MHz) of compound 6d

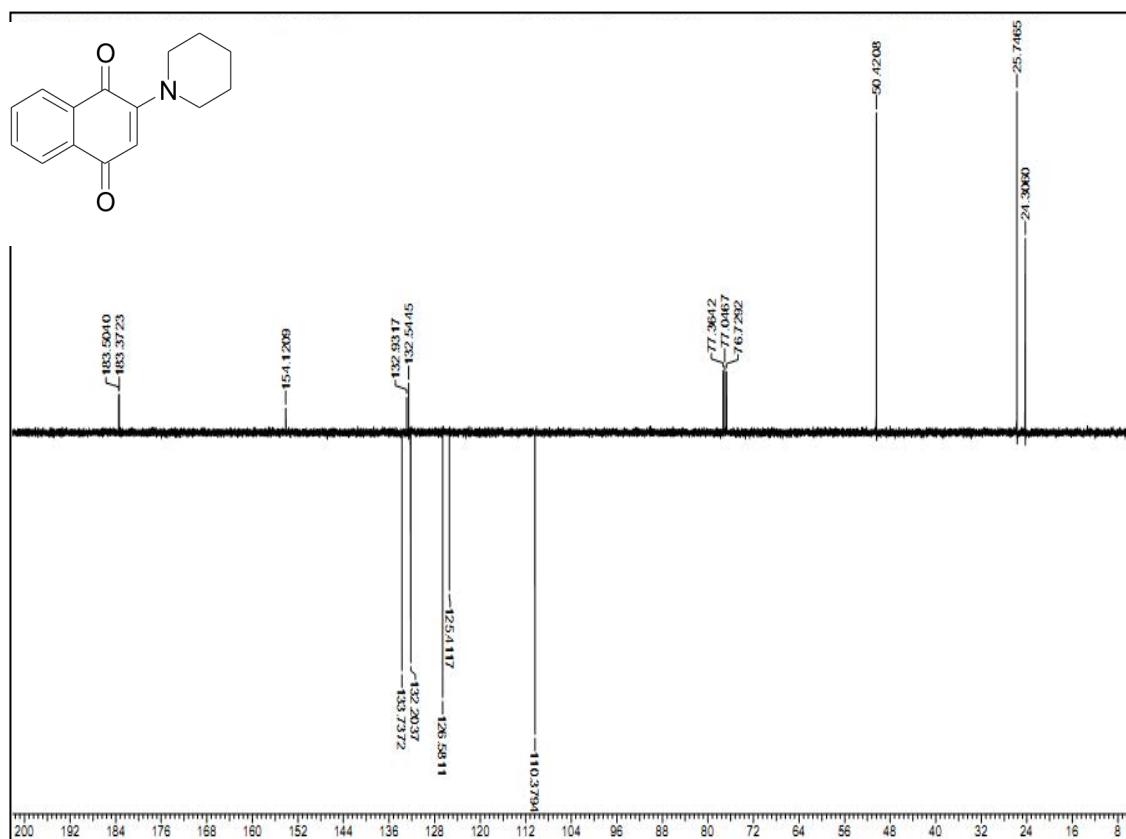
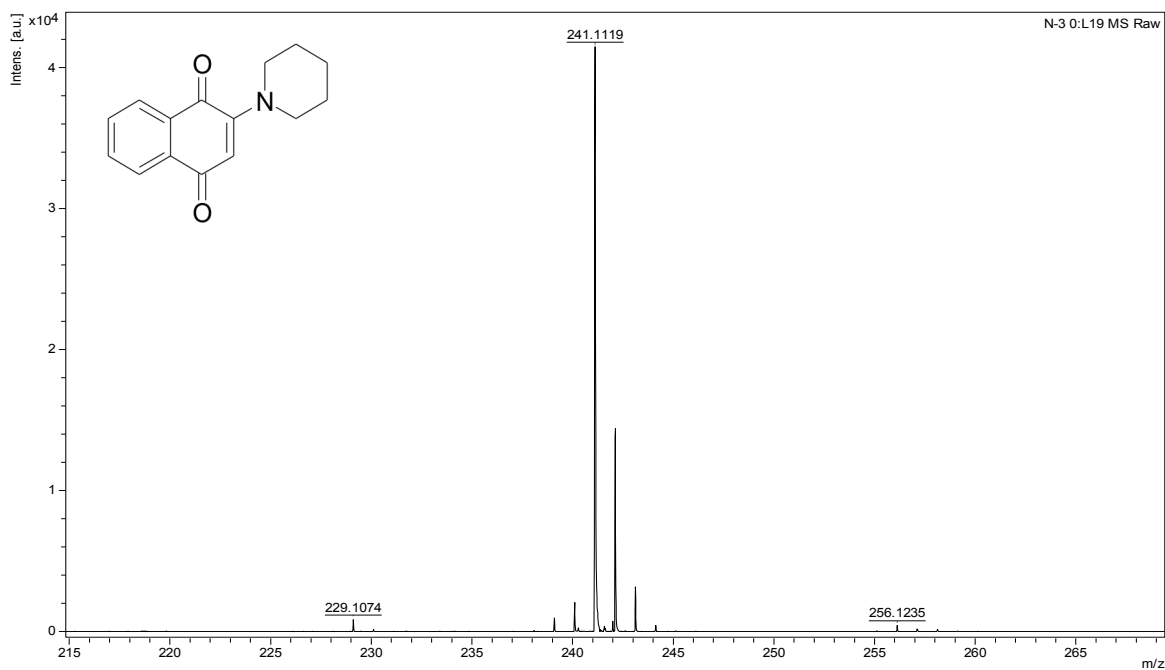
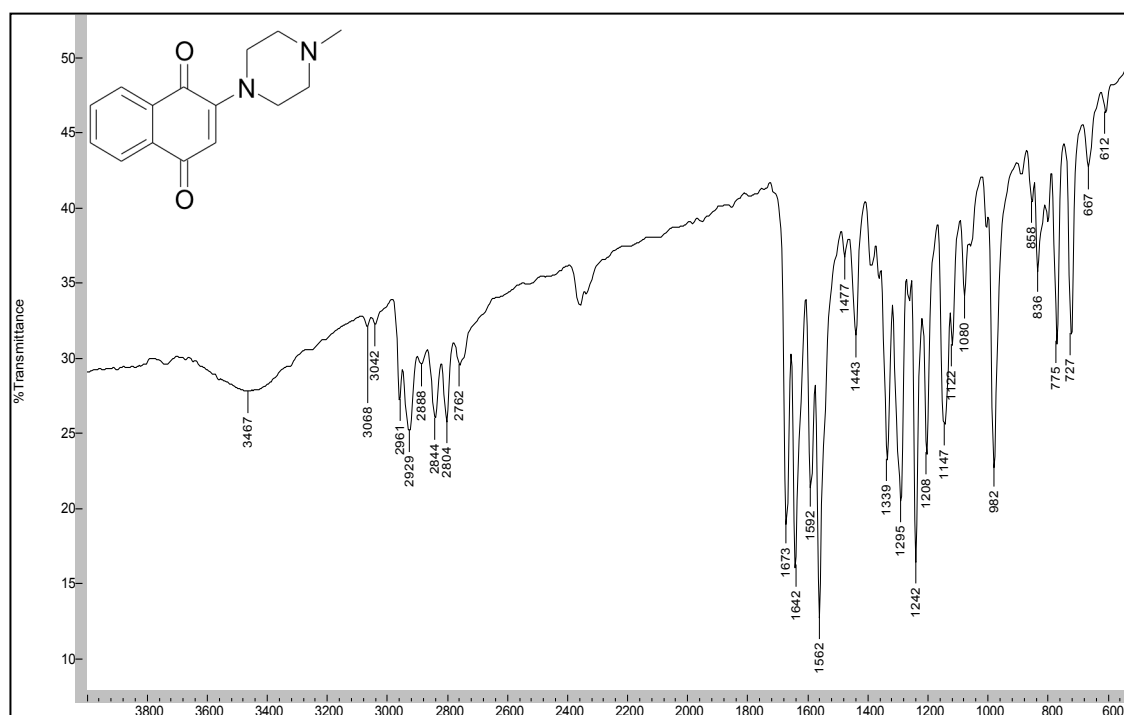


Figure S41. <sup>13</sup>C NMR (APT) spectrum (CDCl<sub>3</sub>, 100 MHz) of compound 6d

Figure S42. High resolution mass spectra of compound **6d**Figure S43. Infrared spectrum ( $\text{KBr}$ ,  $\text{cm}^{-1}$ ) of compound **6e**

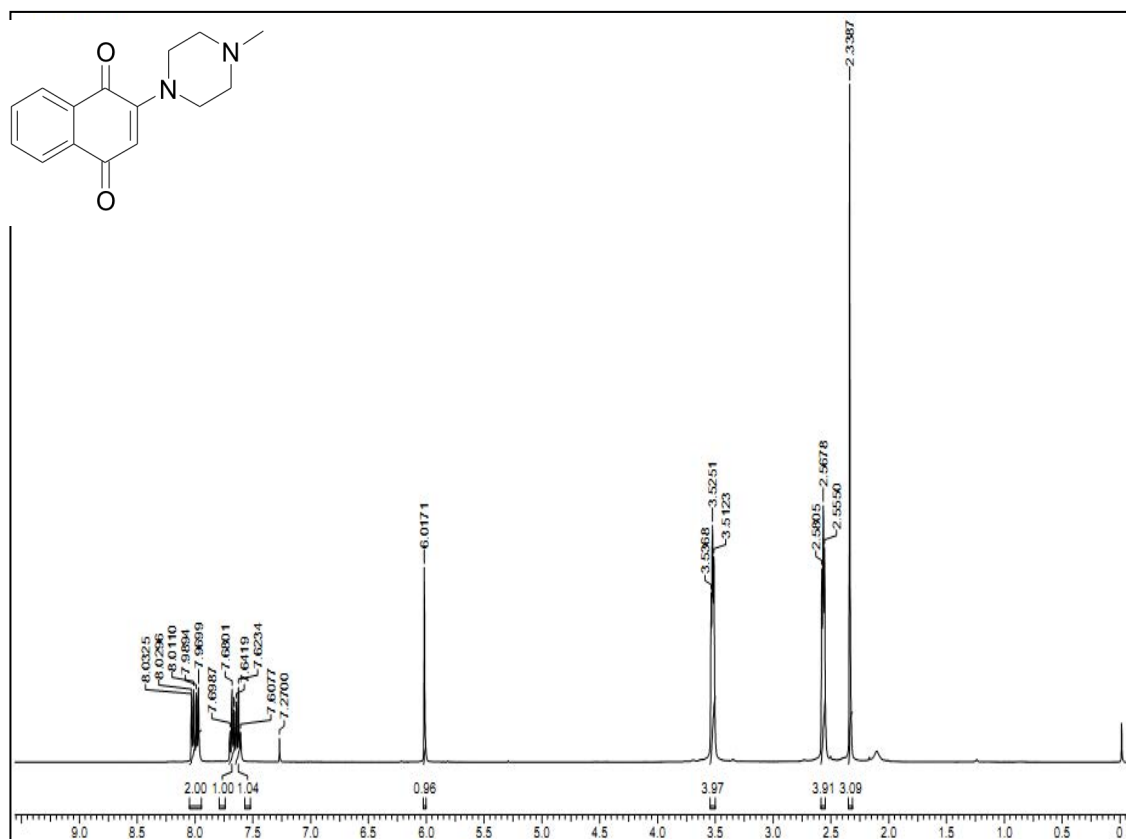


Figure S44.  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 400 MHz) of compound 6e

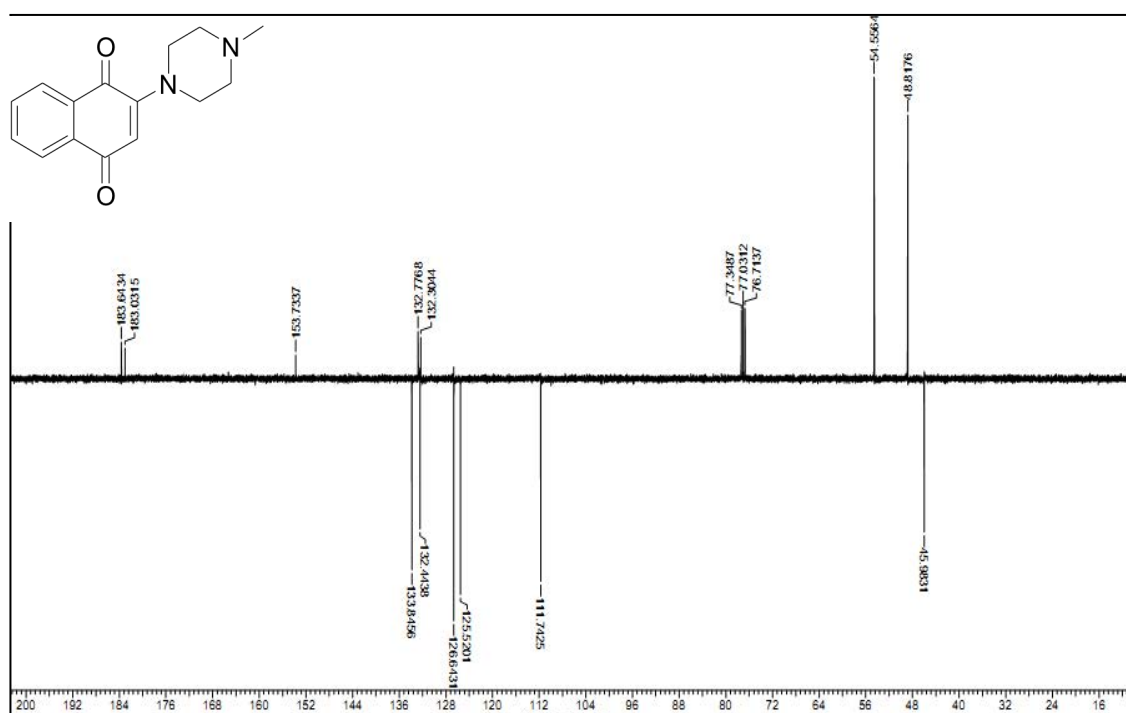


Figure S45.  $^{13}\text{C}$  NMR (APT) spectrum ( $\text{CDCl}_3$ , 100 MHz) of compound 6e

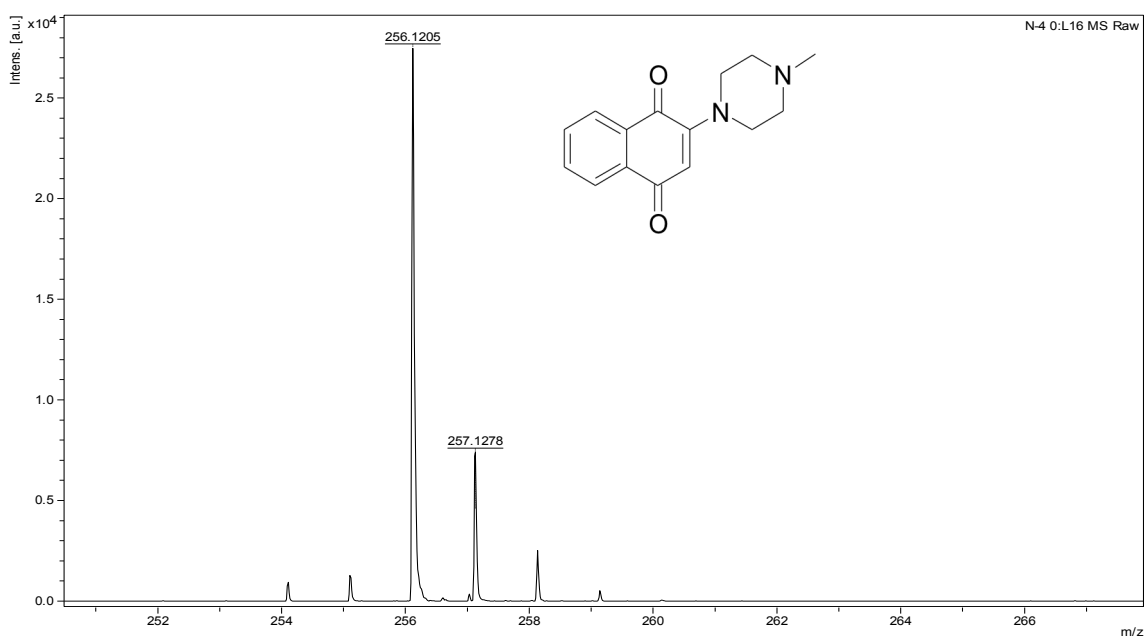


Figure S46. High resolution mass spectra of compound 6e

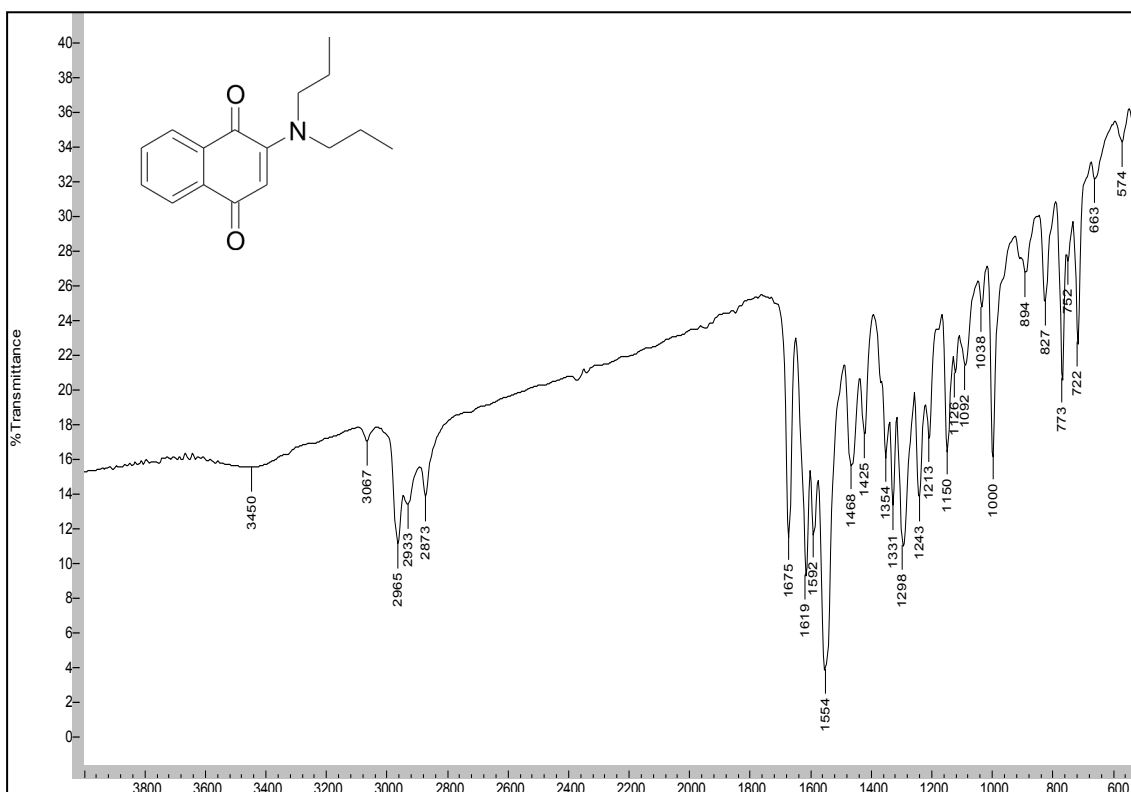


Figure S47. Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of compound 6f



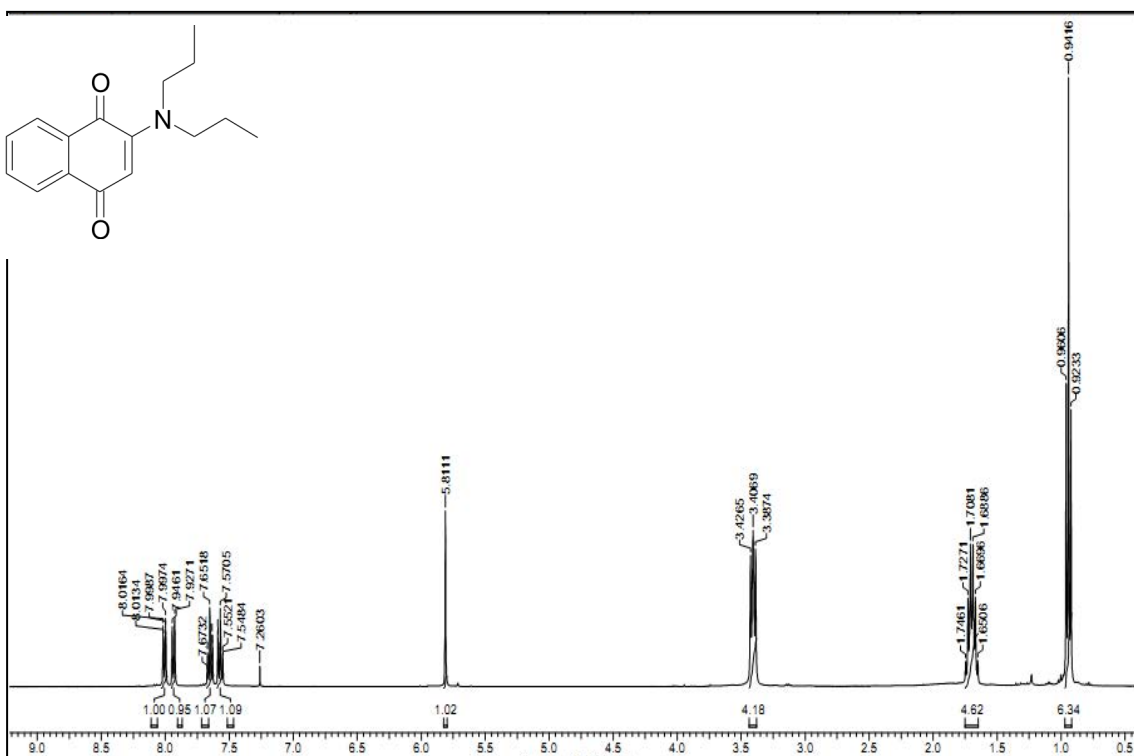


Figure S48. <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 400 MHz) of compound 6f

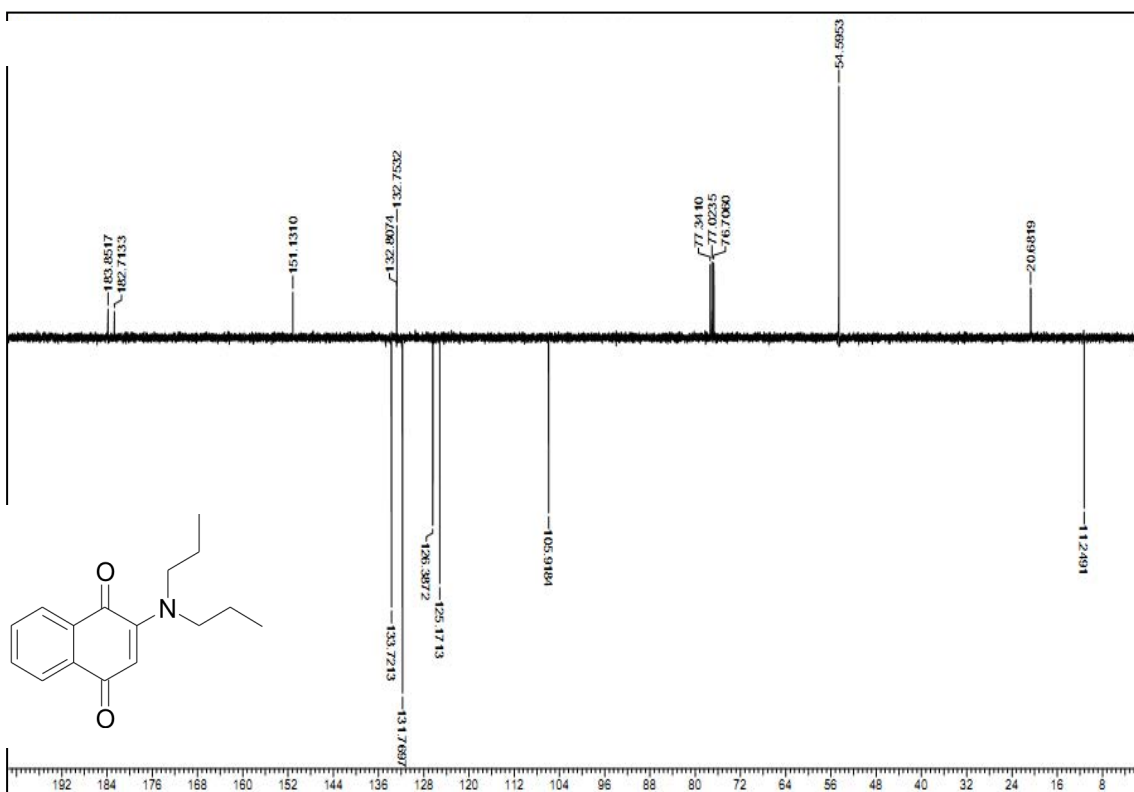


Figure S49. <sup>13</sup>C NMR (APT) spectrum (CDCl<sub>3</sub>, 100 MHz) of compound 6f

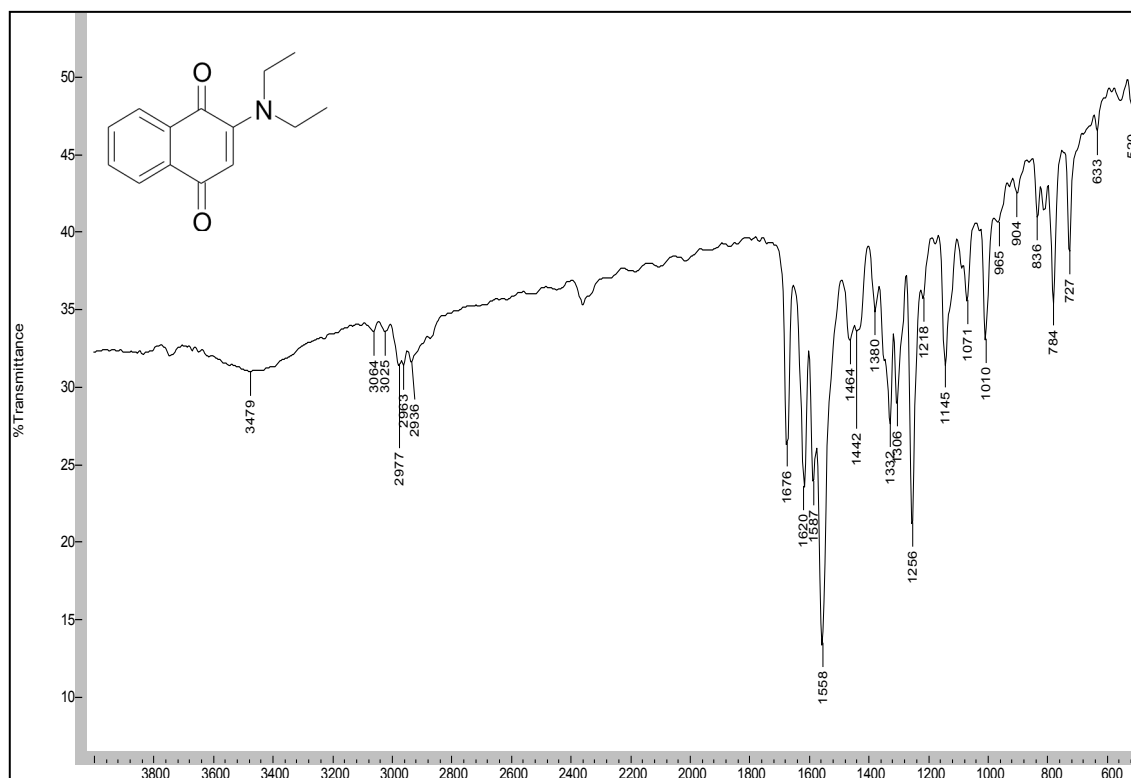


Figure S50. Infrared spectrum (KBr, cm<sup>-1</sup>) of compound **6g**

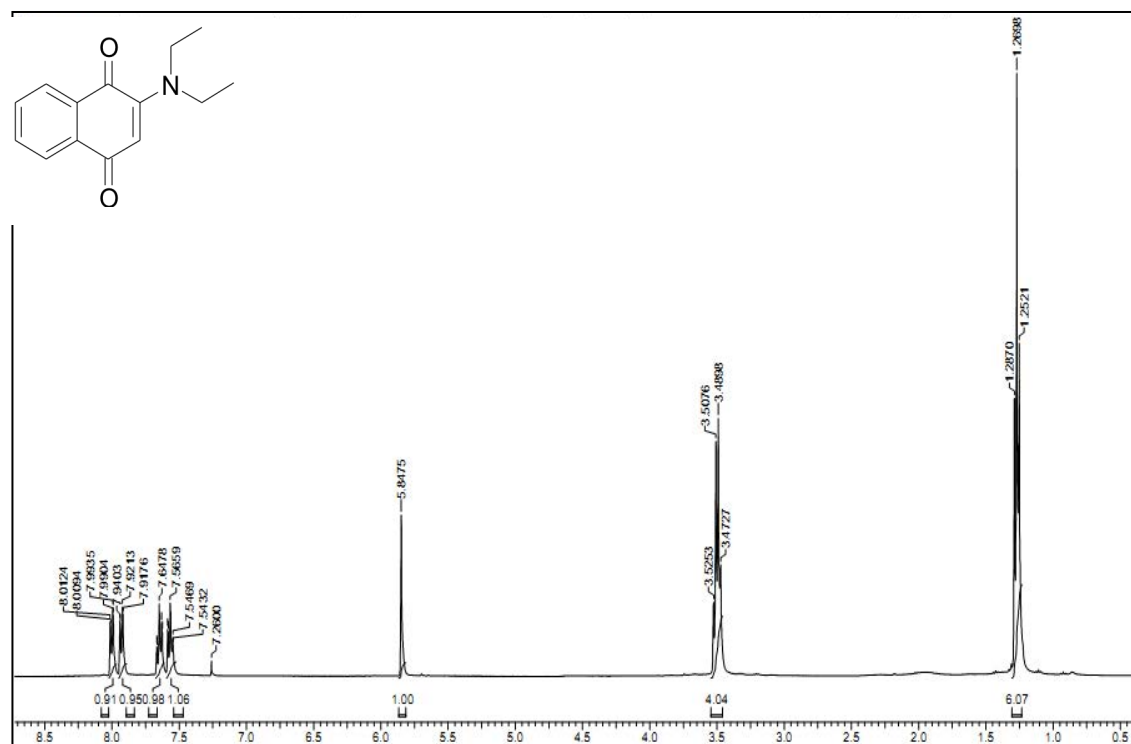


Figure S51. <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 400 MHz) of compound **6g**

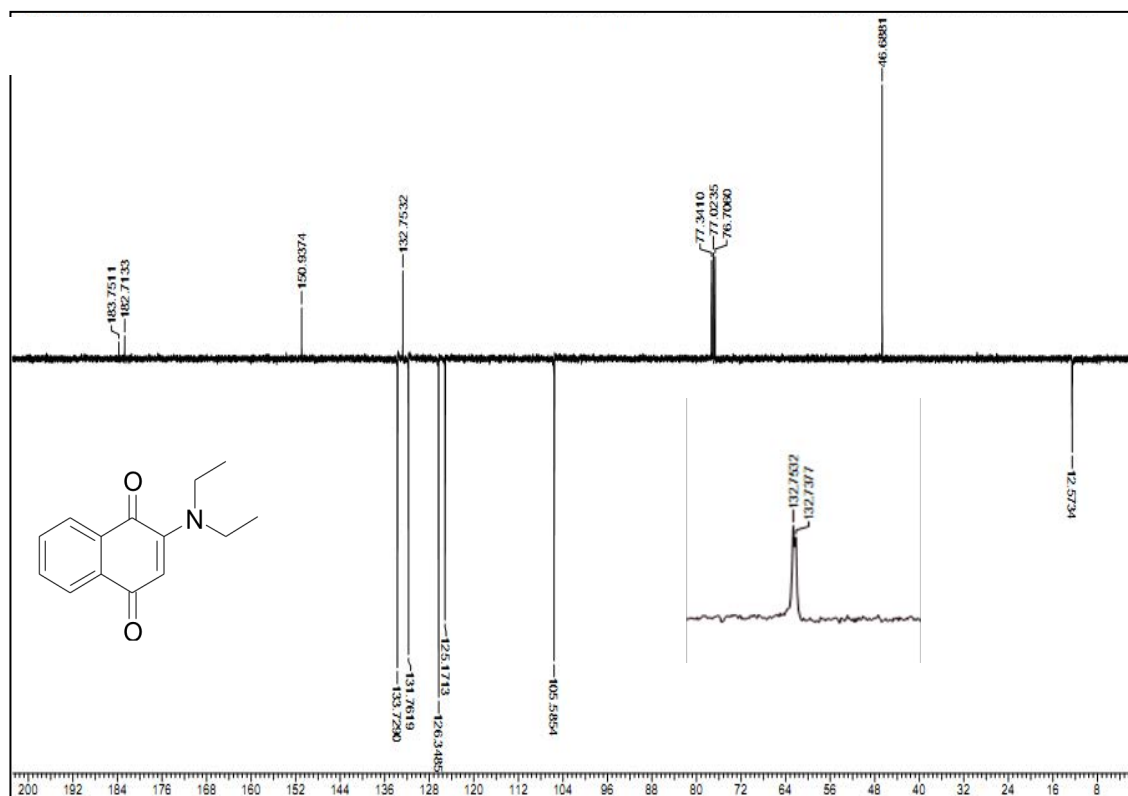


Figure S52.  $^{13}\text{C}$  NMR (APT) spectrum ( $\text{CDCl}_3$ , 100 MHz) of compound **6g**

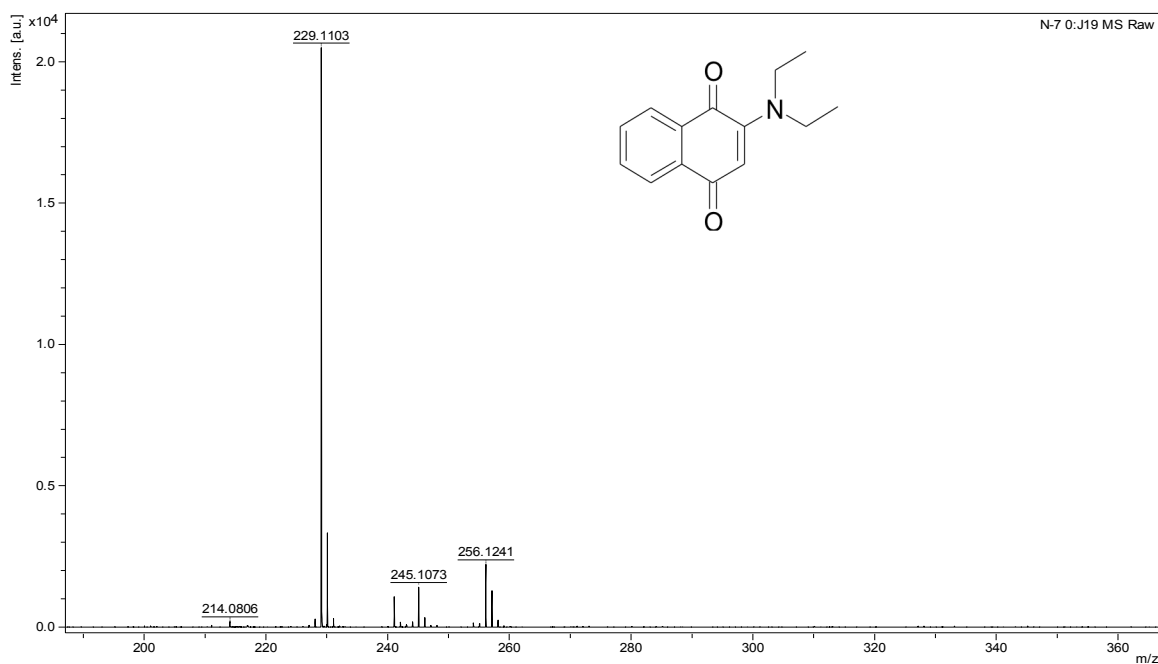


Figure S53. High resolution mass spectra of compound **6g**

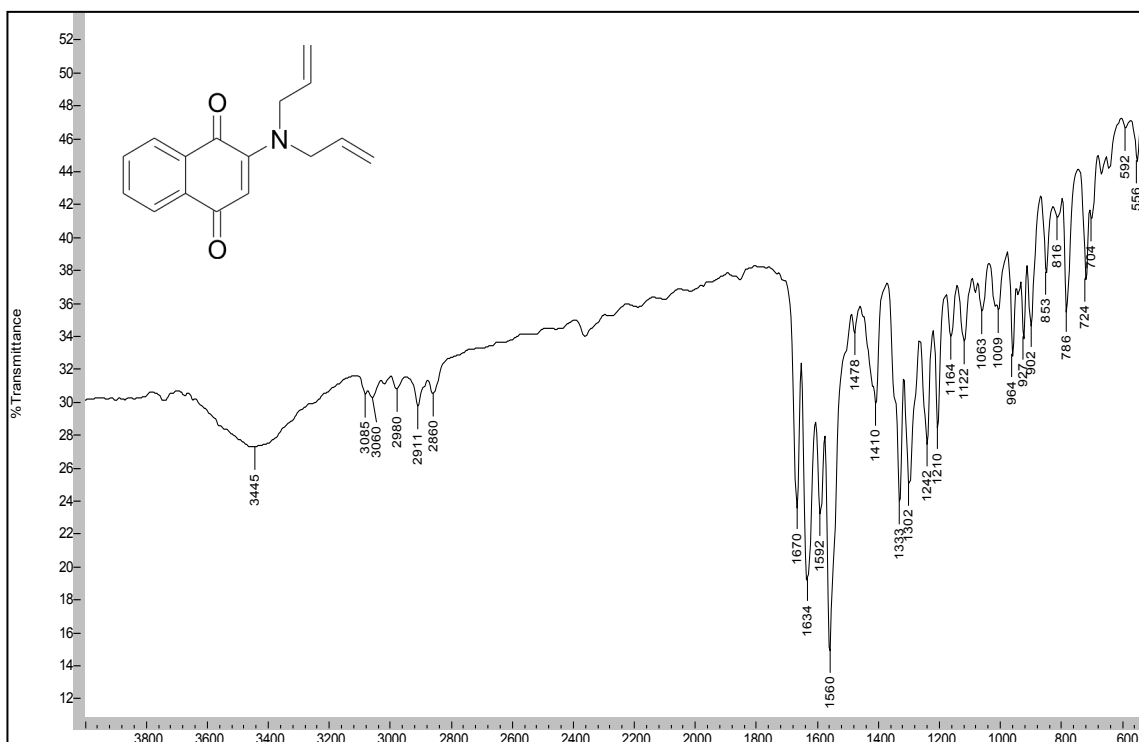


Figure S54. Infrared spectrum (KBr, cm<sup>-1</sup>) of compound 6h

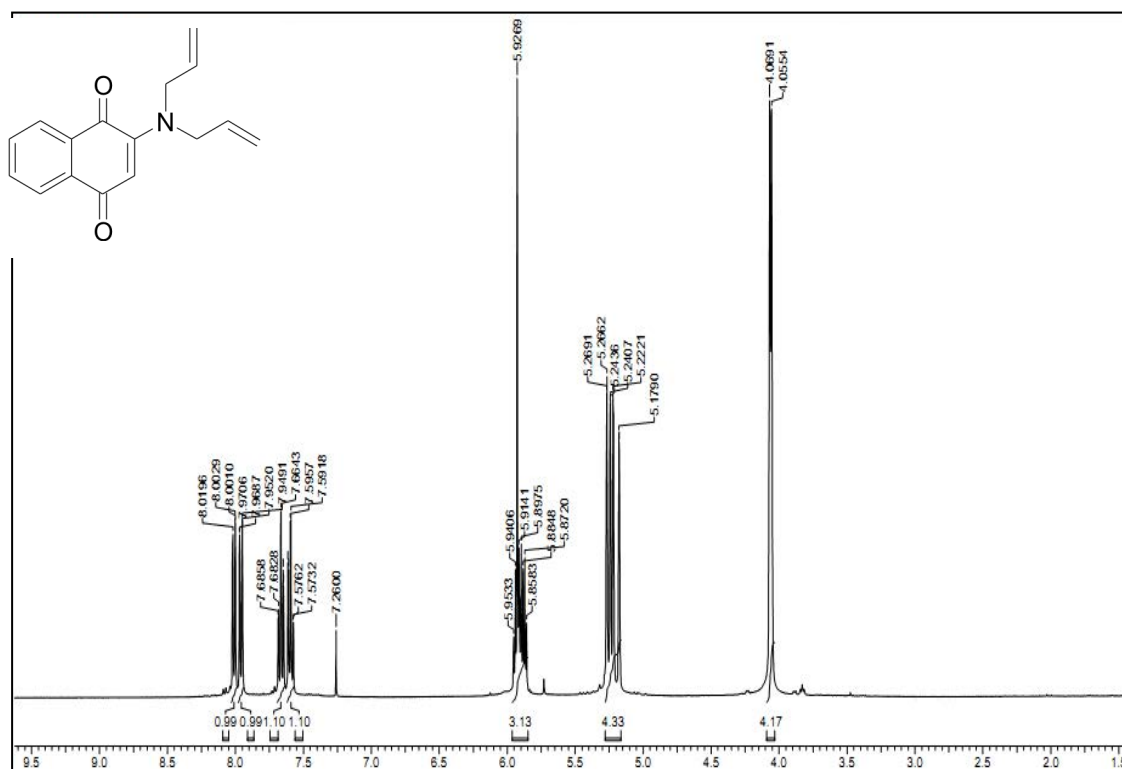


Figure S55. <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 400 MHz) of compound 6h.

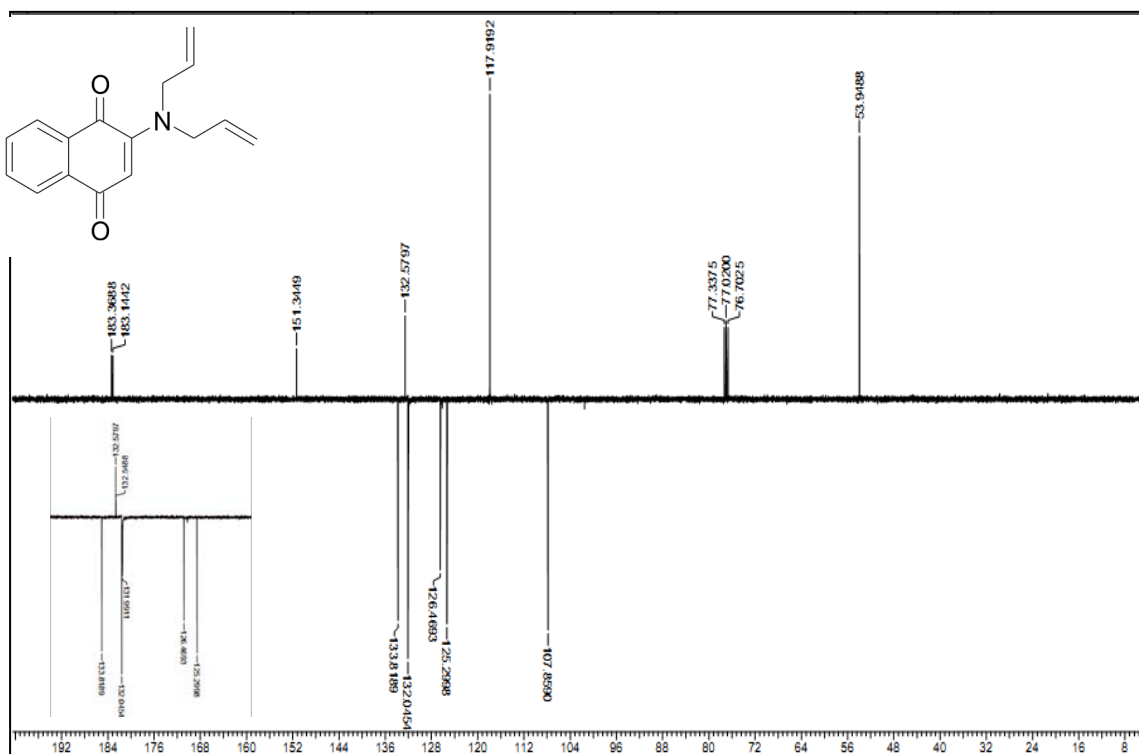


Figure S56.  $^{13}\text{C}$  NMR (APT) spectrum ( $\text{CDCl}_3$ , 100 MHz) of compound 6h

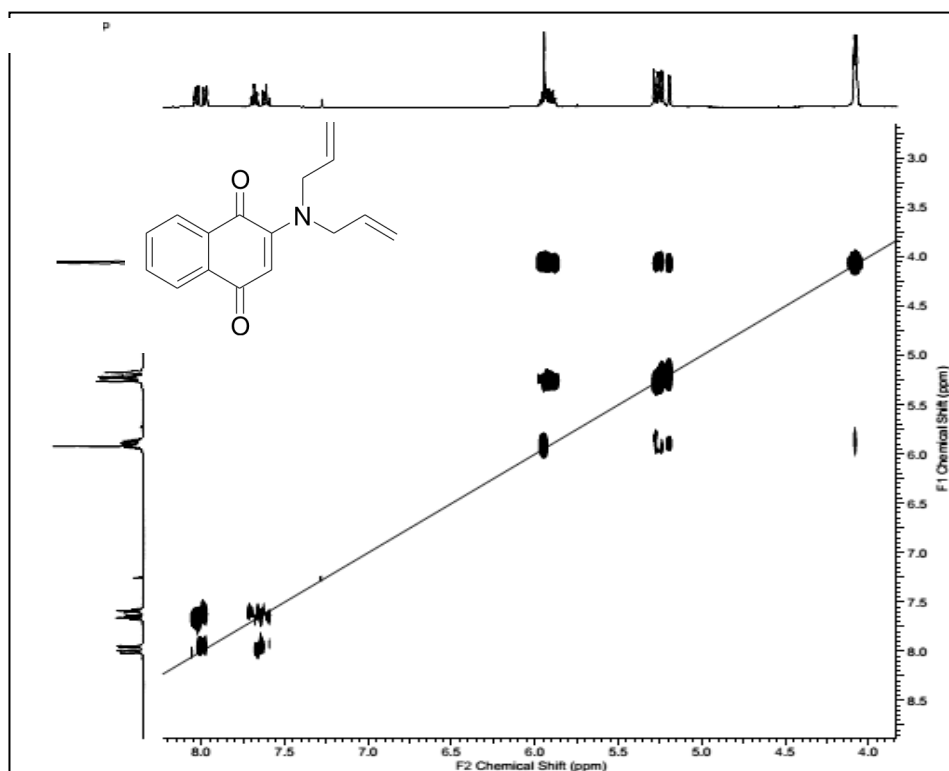


Figure S57. COSY spectrum of compound 6h.

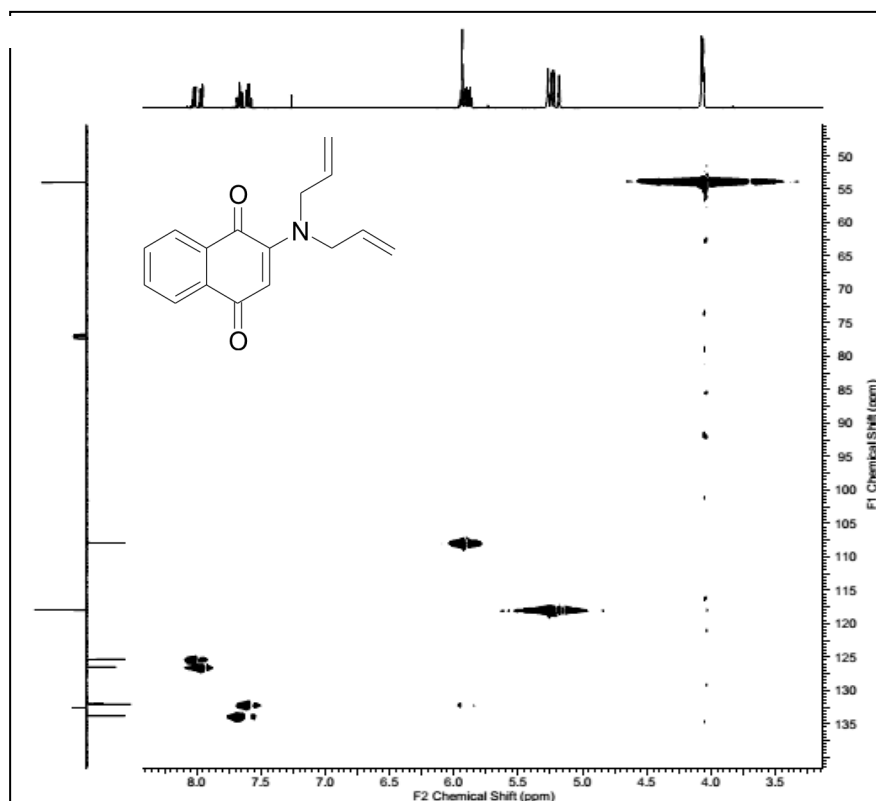


Figure S58. HMQC spectrum of compound 6h

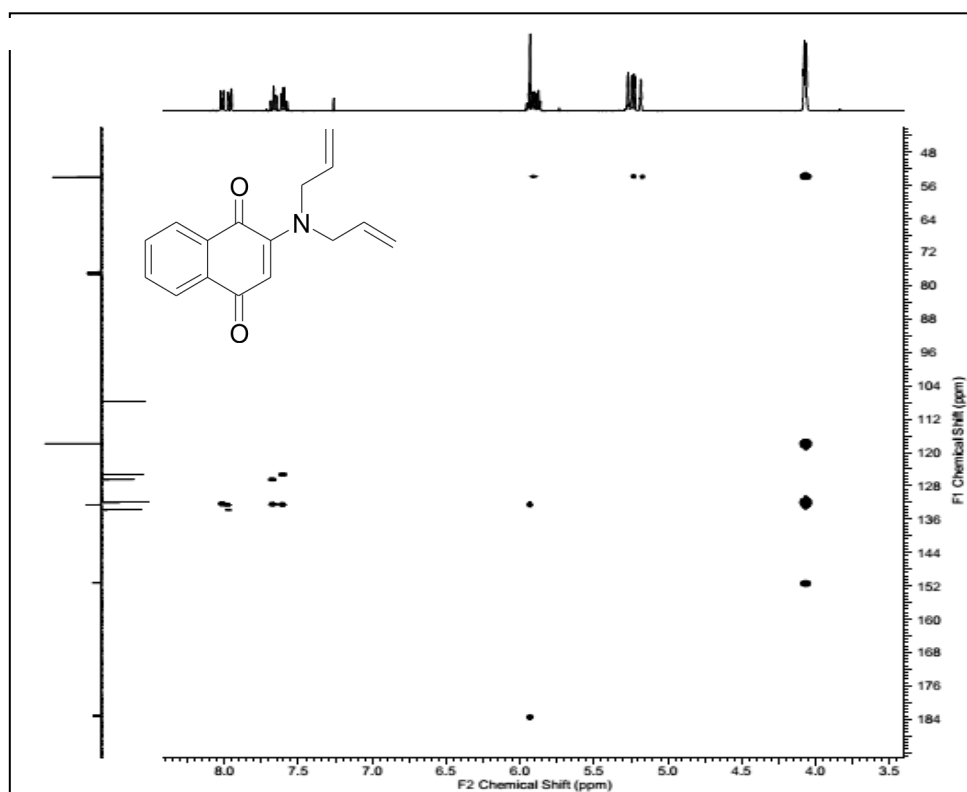


Figure S59. HMBC spectrum of compound 6h.

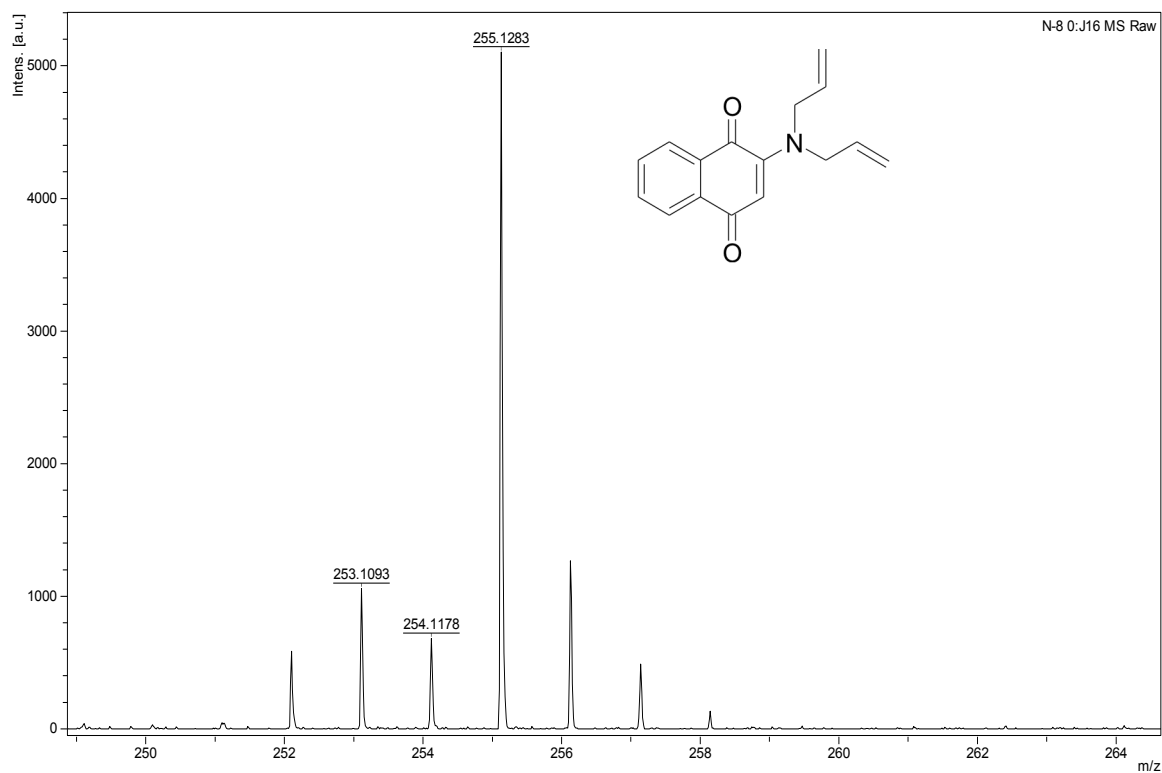


Figure 60. High resolution mass spectra of compound 6h

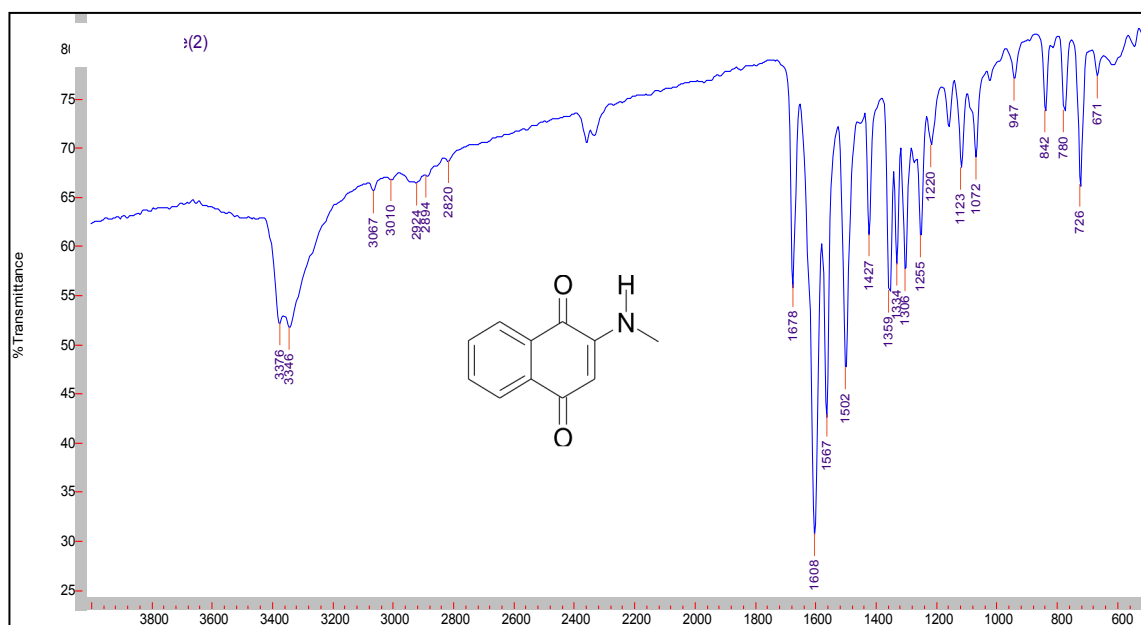


Figure S61. Infrared spectrum (KBr,  $\text{cm}^{-1}$ ) of compound 6i.

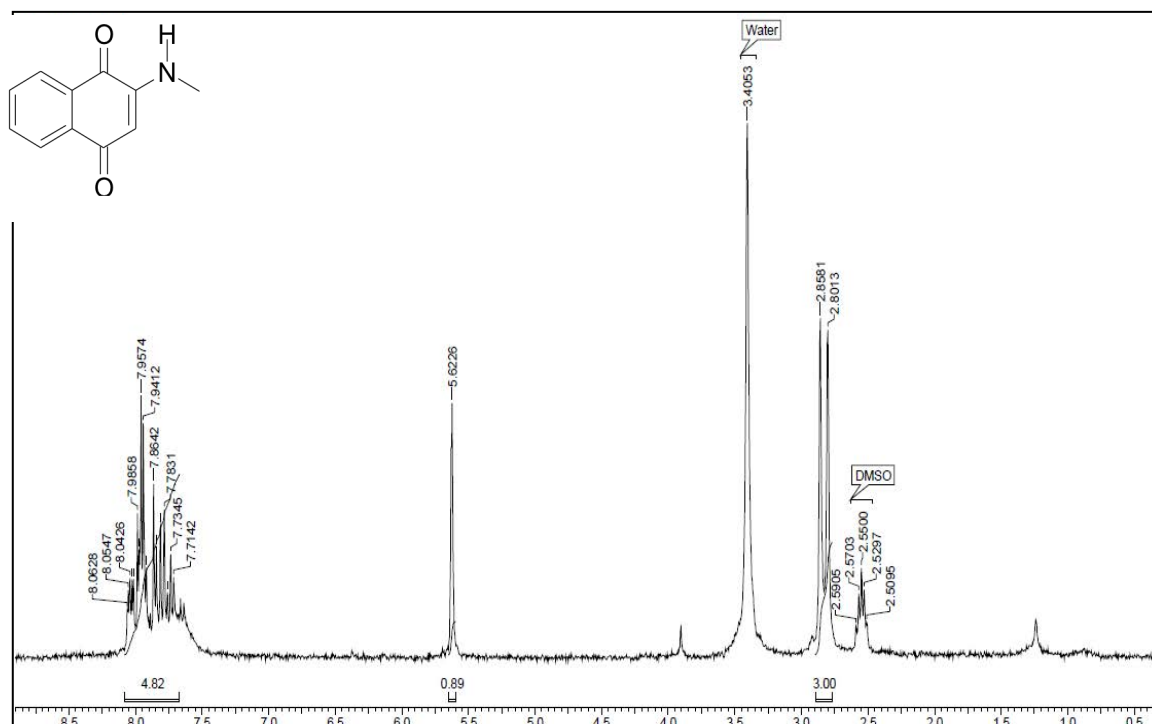


Figure 62. <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>, 90 MHz) of compound 6i

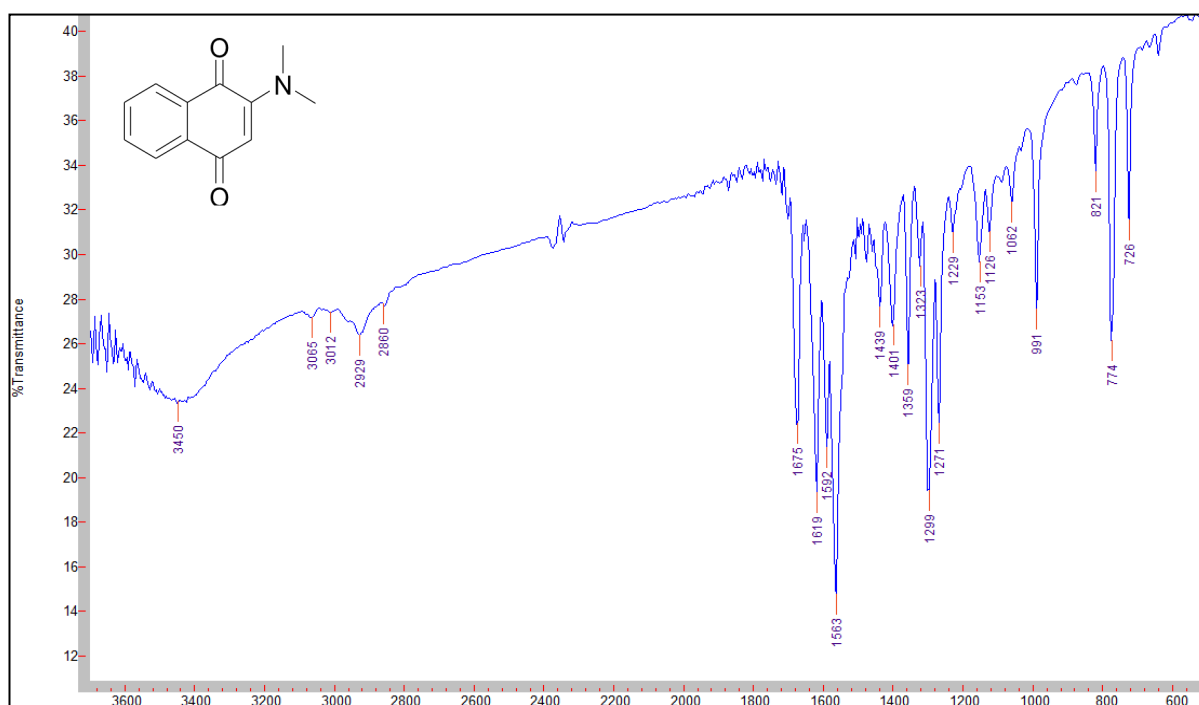


Figure 63. IR (KBr, cm<sup>-1</sup>) of compound 6j.



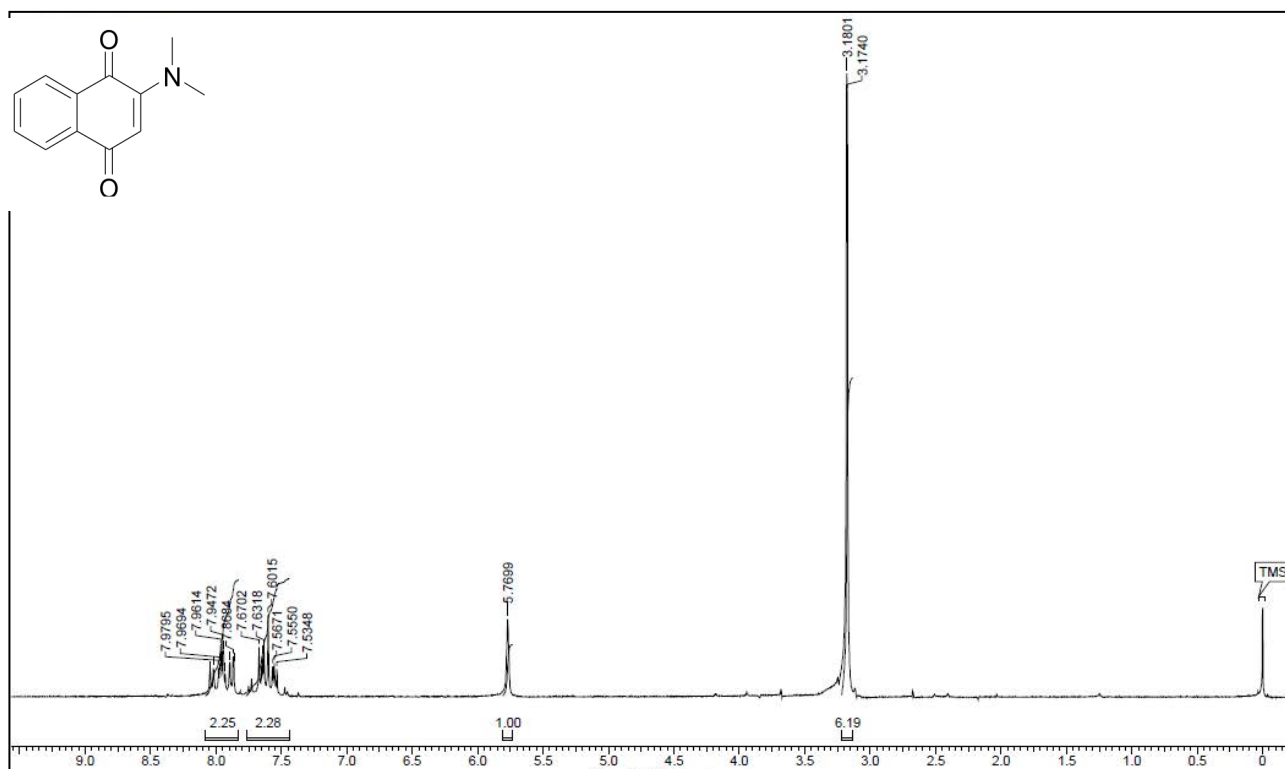


Figure 64.  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 90 MHz) of compound 6j

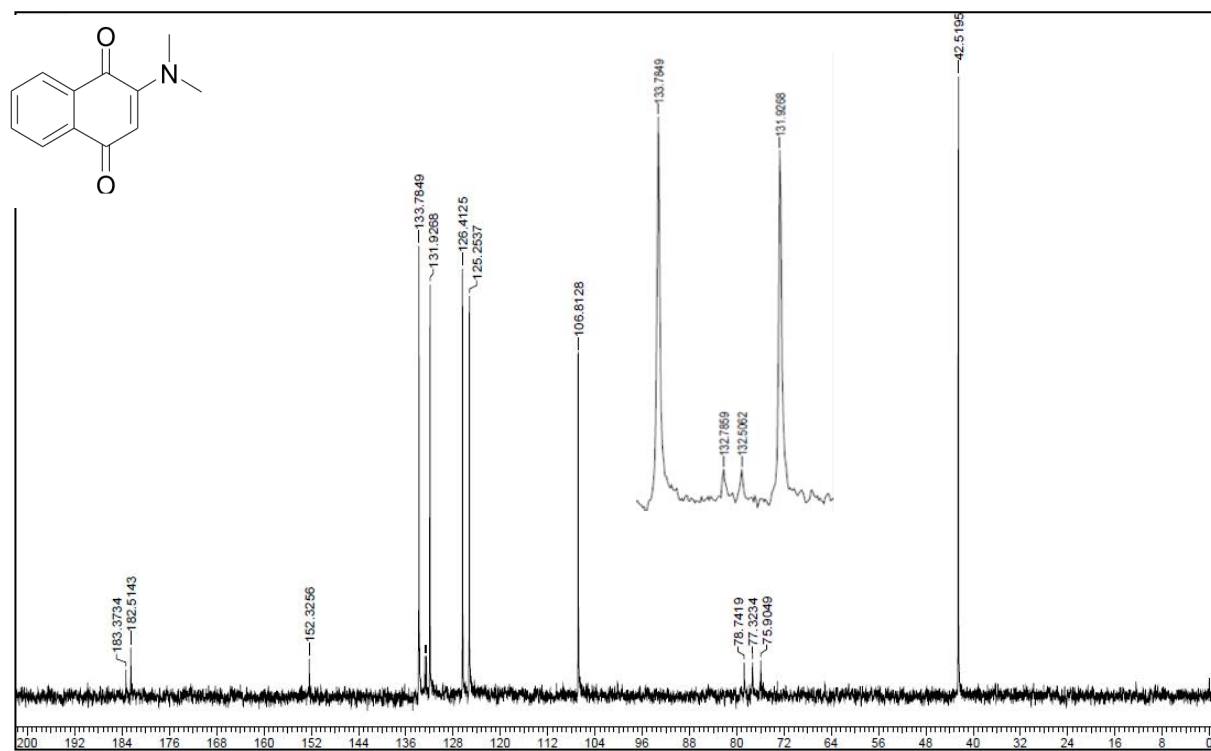


Figure S65.  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 22.73 MHz) of compound 6j