

Supplementary Information

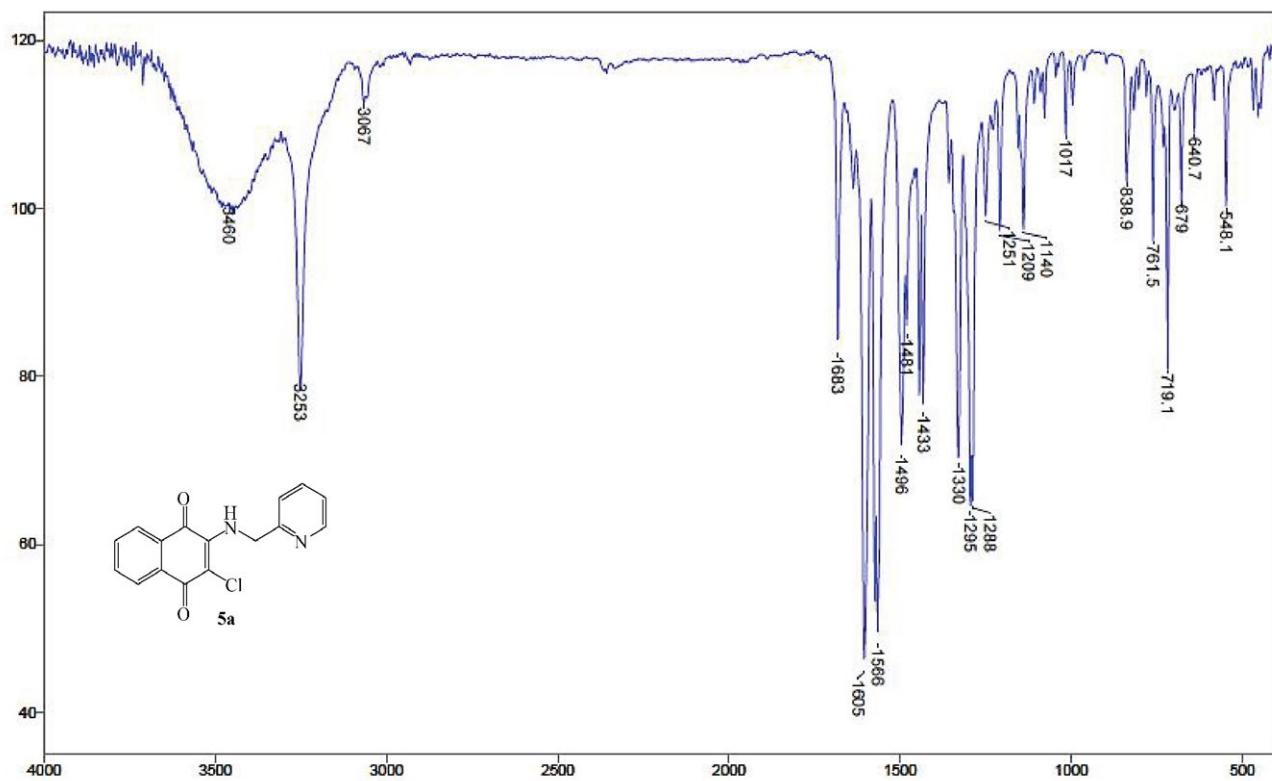
Synthesis, Antitumor Activity and Docking of 2,3-(Substituted)-1,4-Naphthoquinone Derivatives Containing Nitrogen, Oxygen and Sulfur

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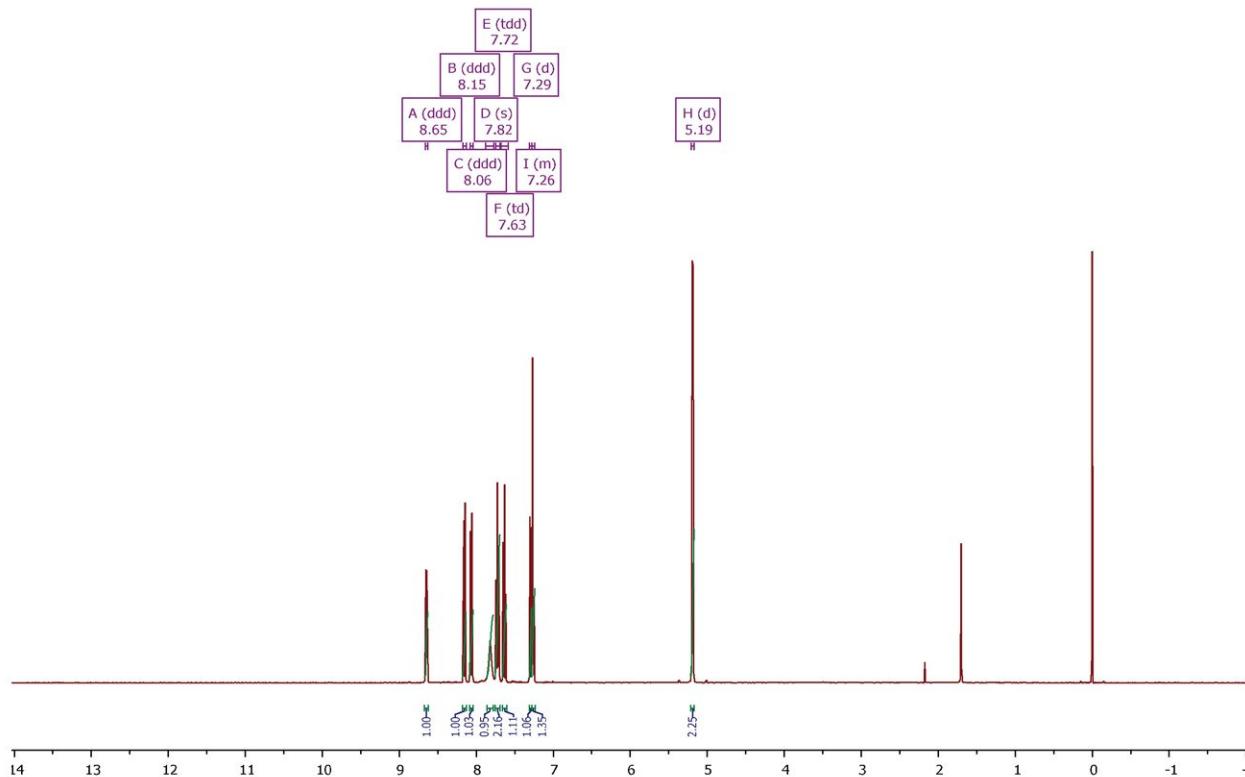


Figure S2. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **5a**.

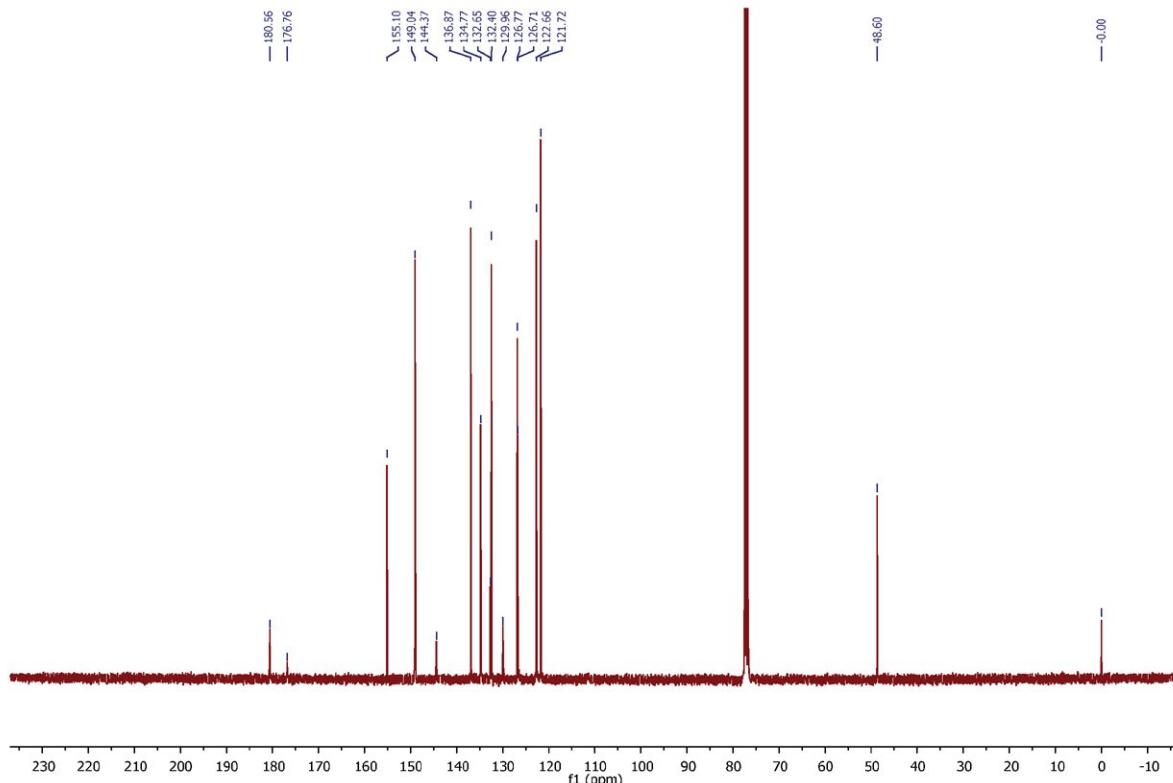
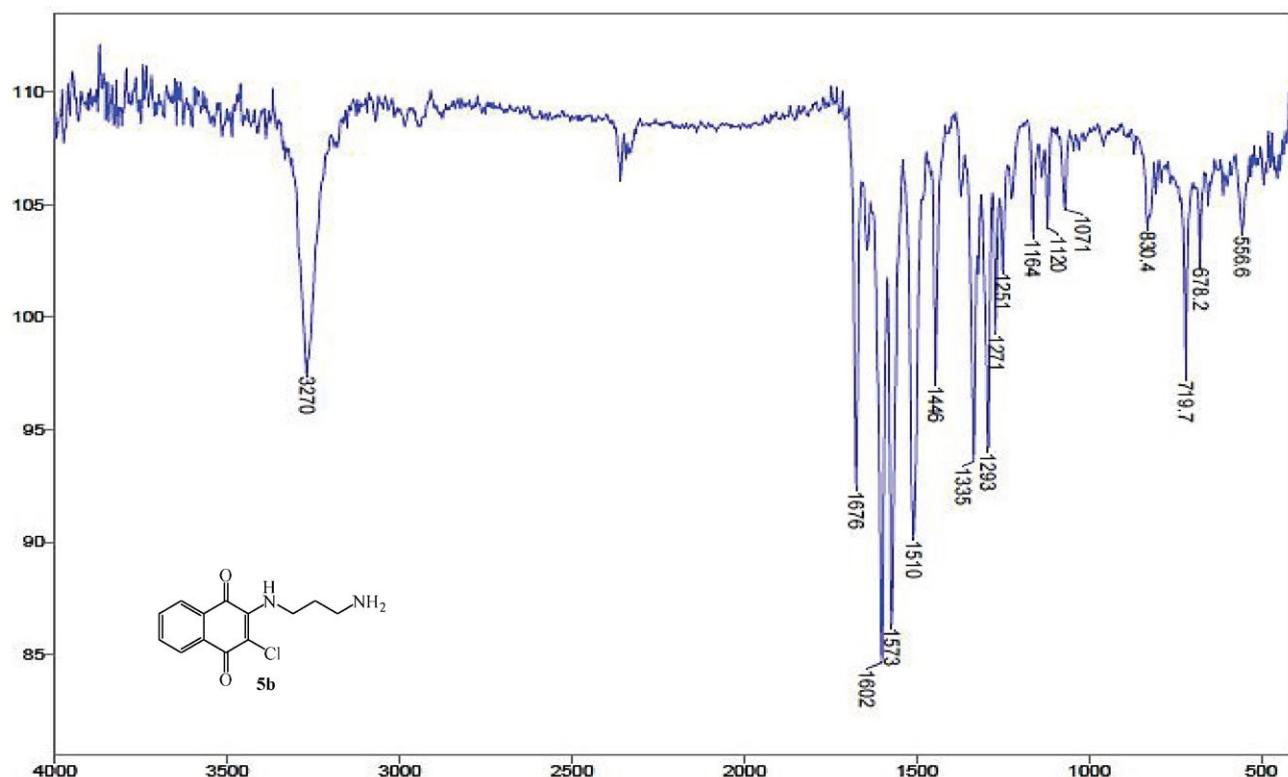
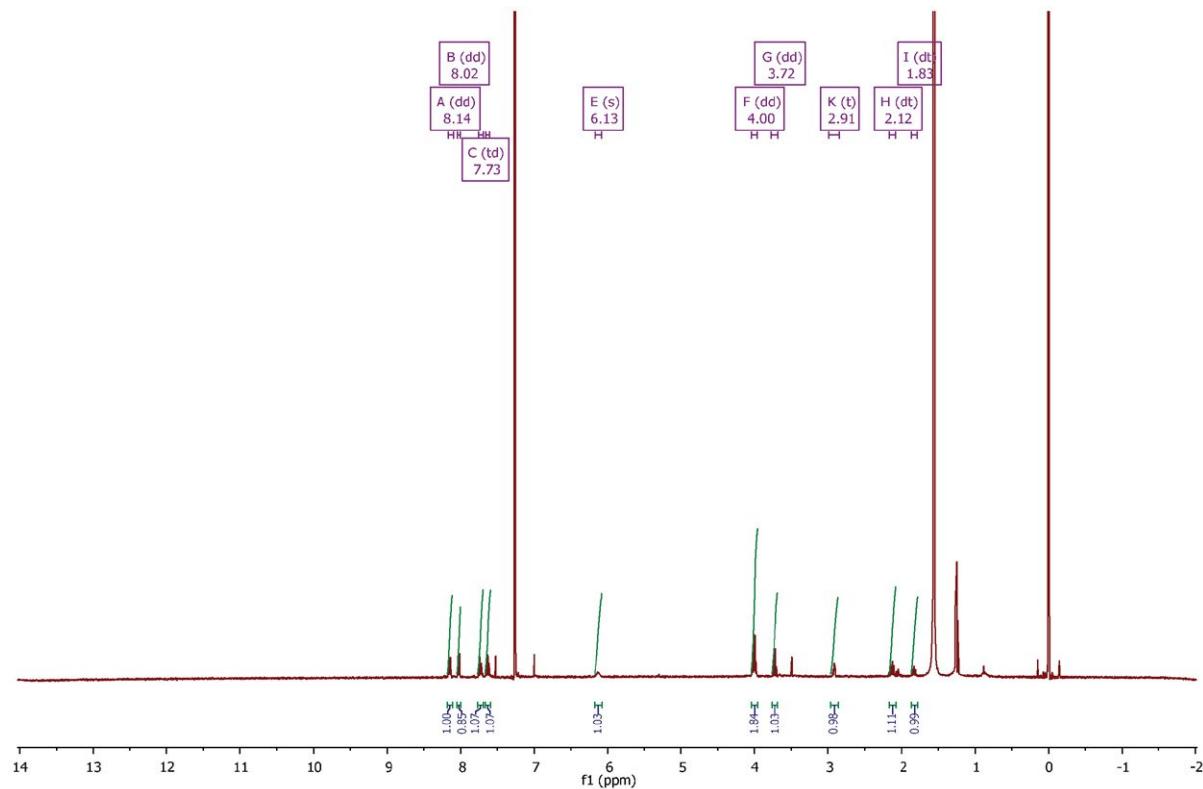


Figure S3. ^{13}C NMR spectrum (101 MHz, CDCl_3) of Compound **5a**.

**Figure S4.** Infrared spectrum (KBr) of compound **5b**.**Figure S5.** ¹H NMR spectrum (400 MHz, CDCl₃) of compound **5b**.

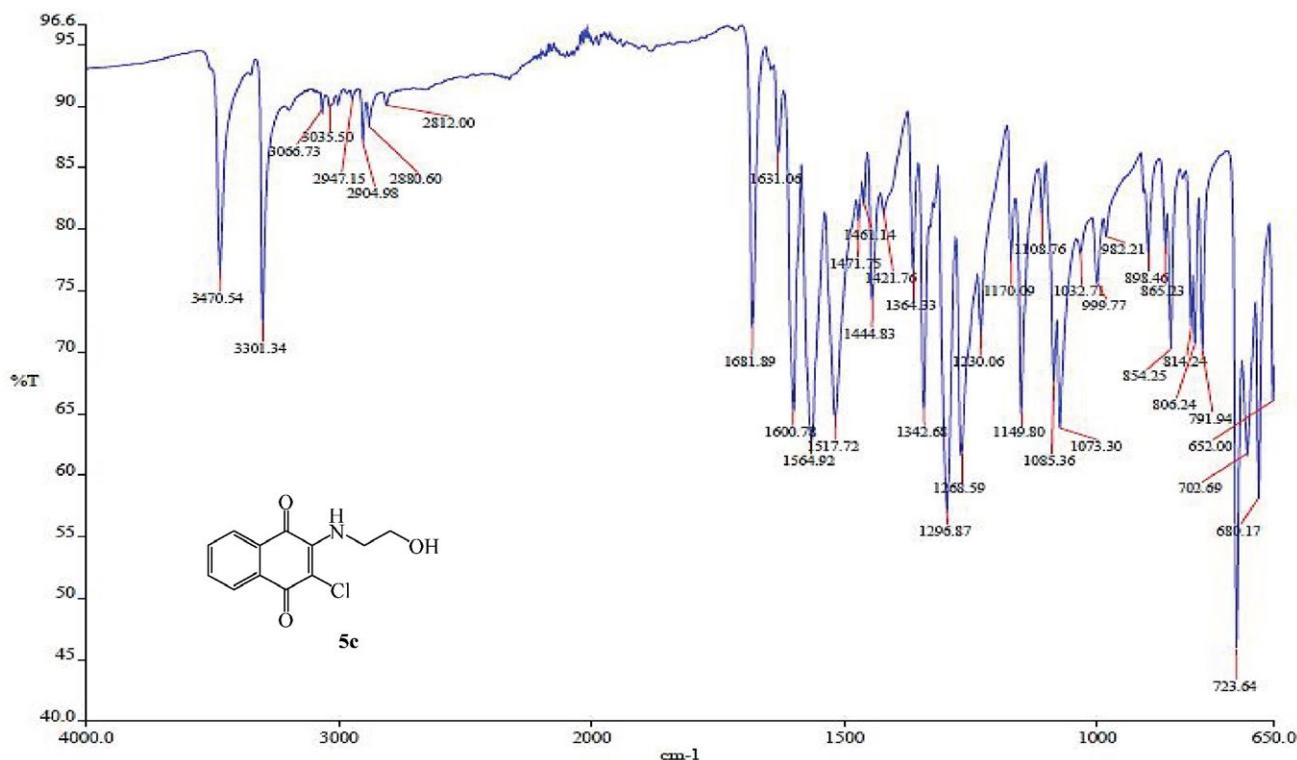


Figure S6. Infrared spectrum (KBr) of compound **5c**.

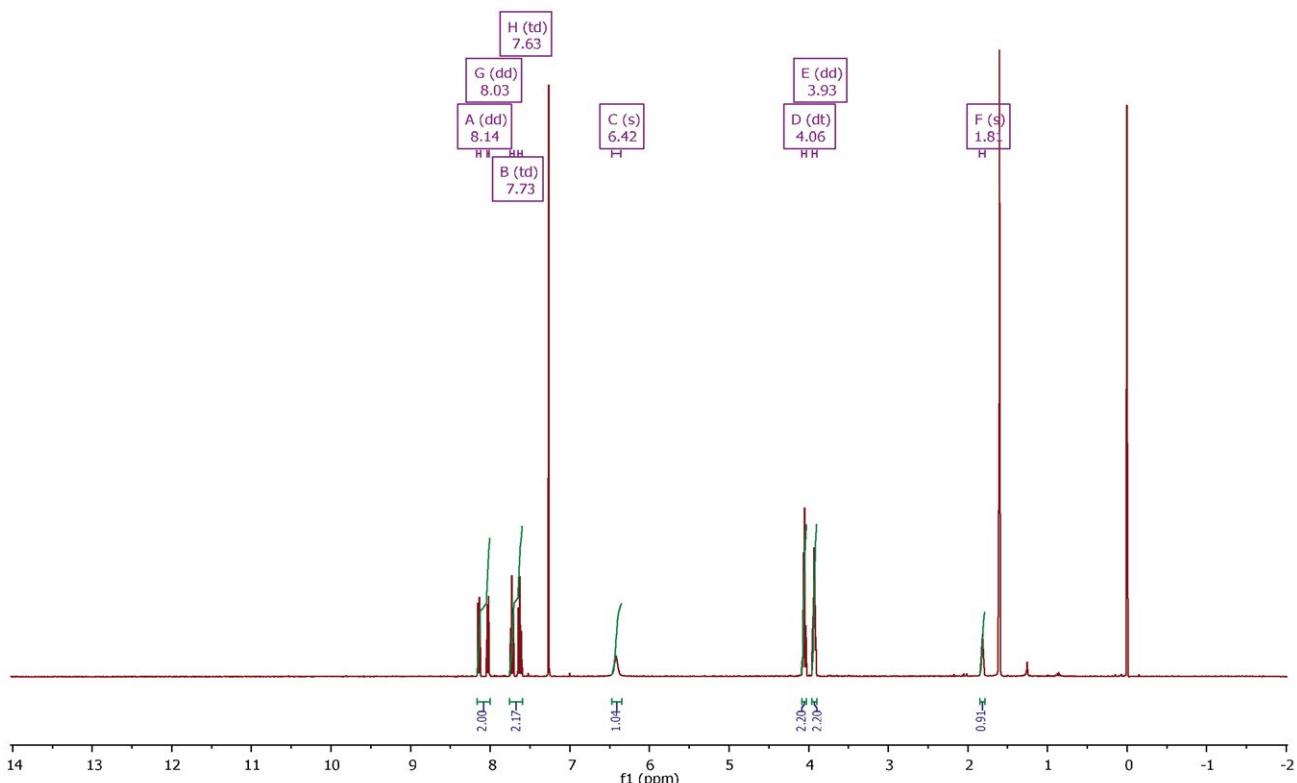


Figure S7. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **5c**.

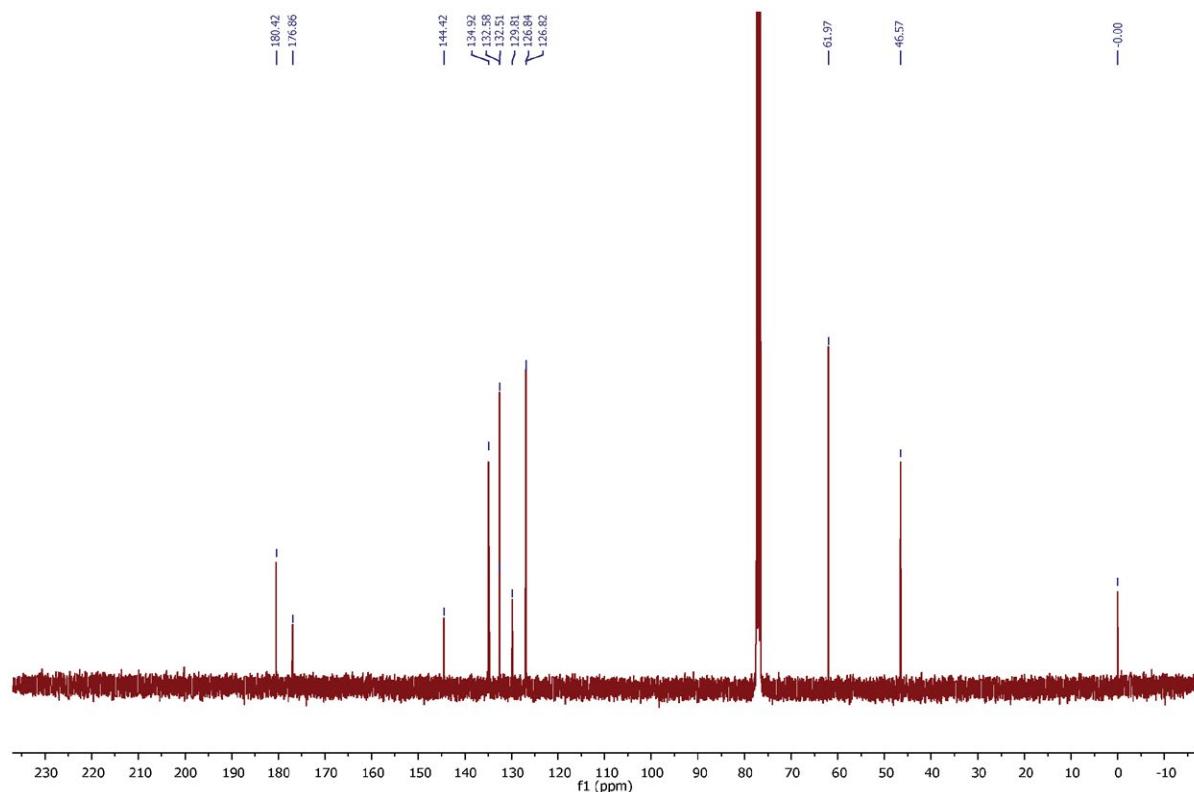


Figure S8. ¹³C NMR spectrum (101 MHz, CDCl₃) of compound 5c.

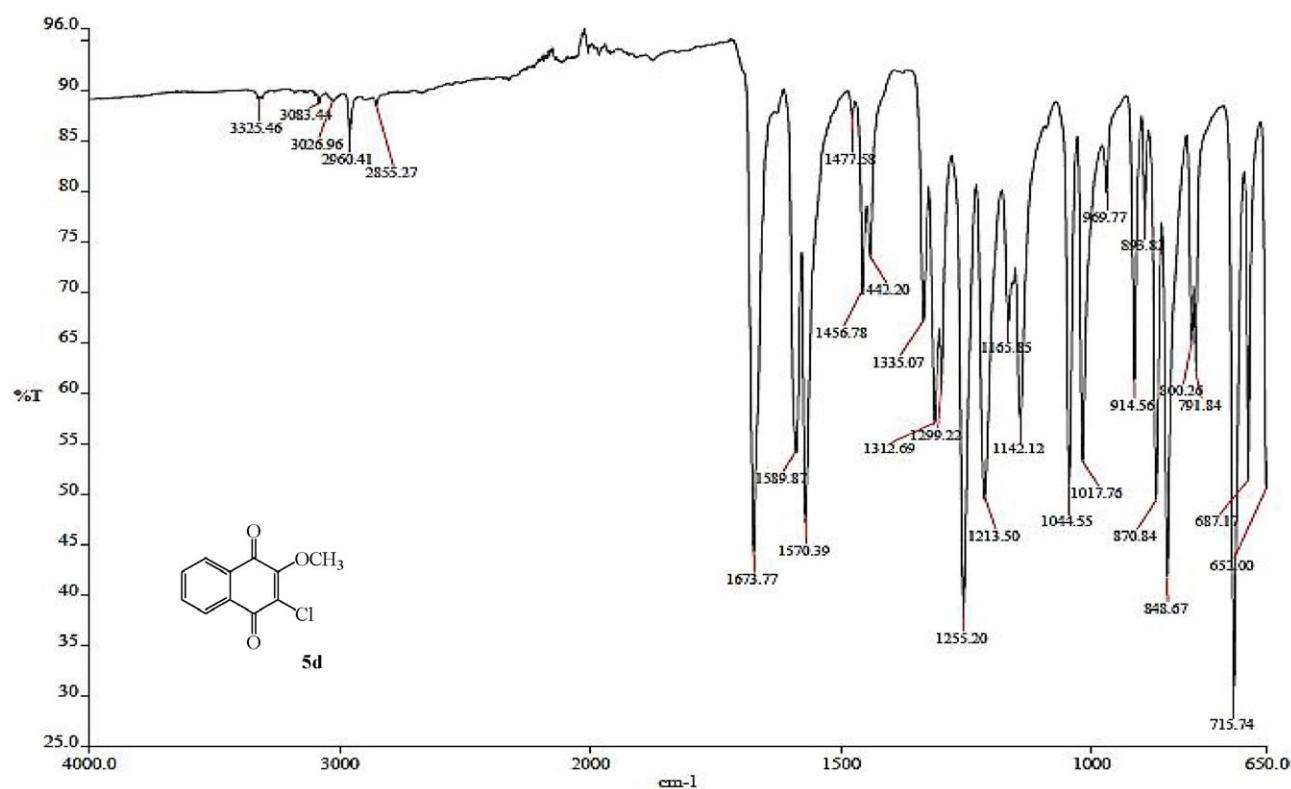


Figure S9. Infrared spectrum (KBr) of compound 5d.

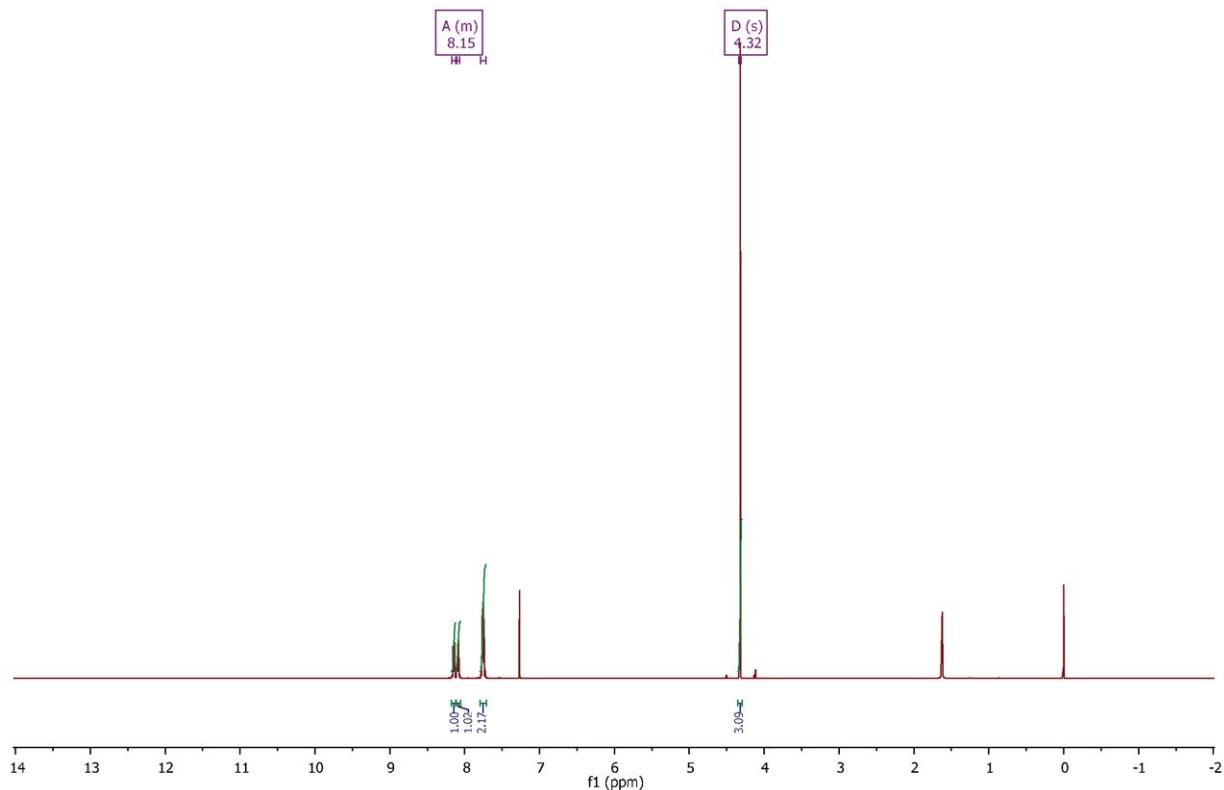


Figure S10. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **5d**.

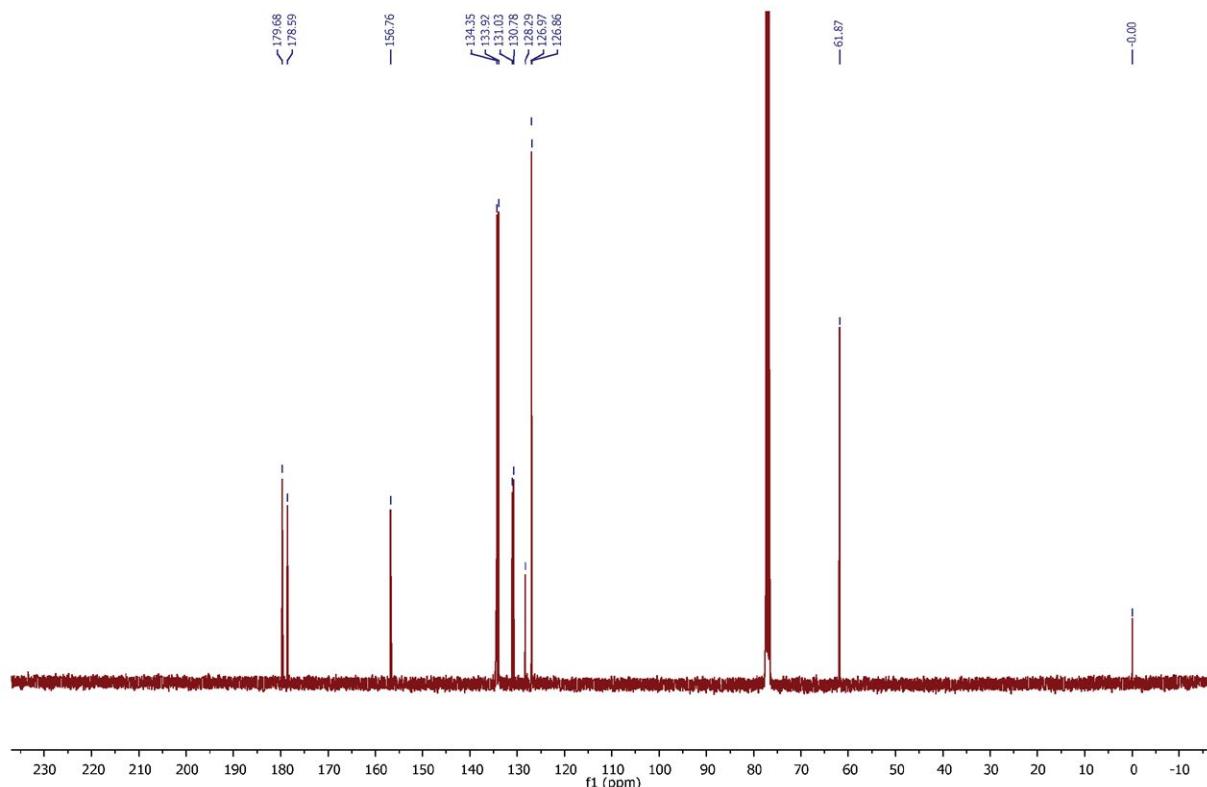
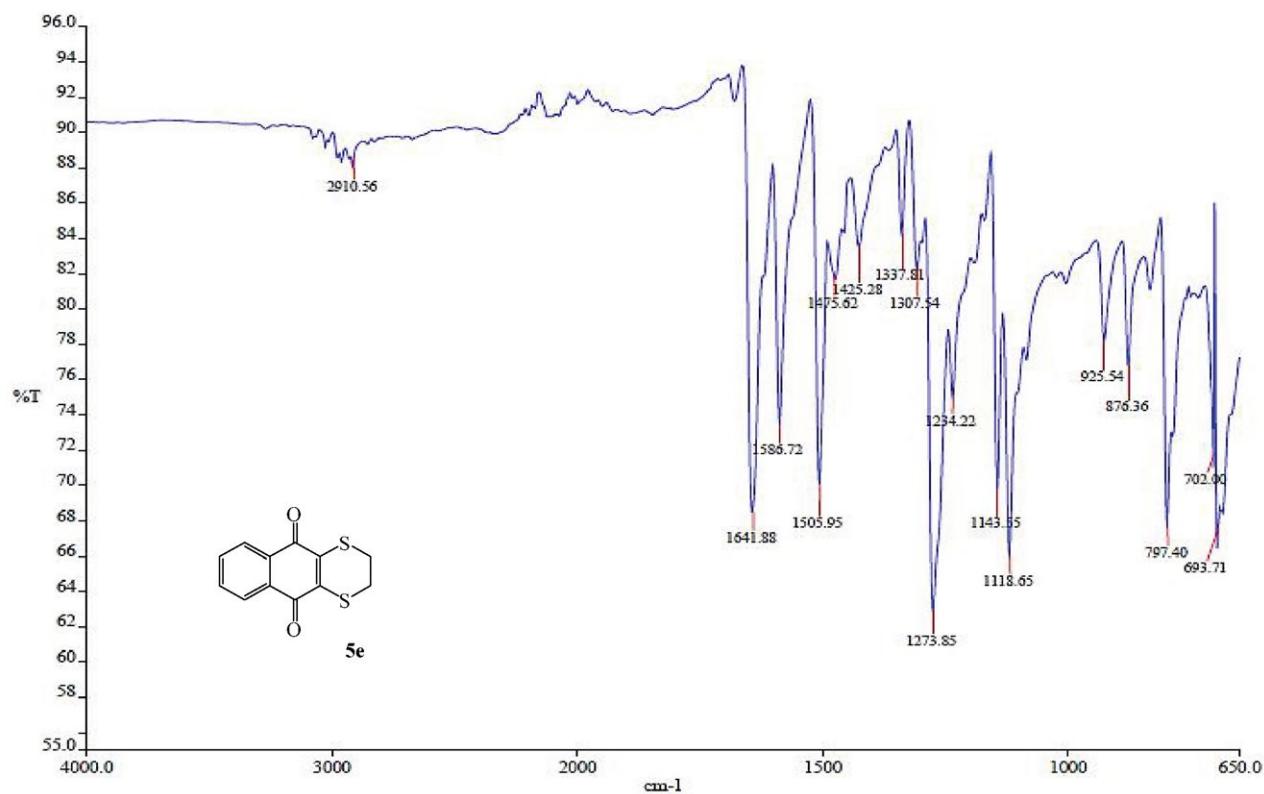
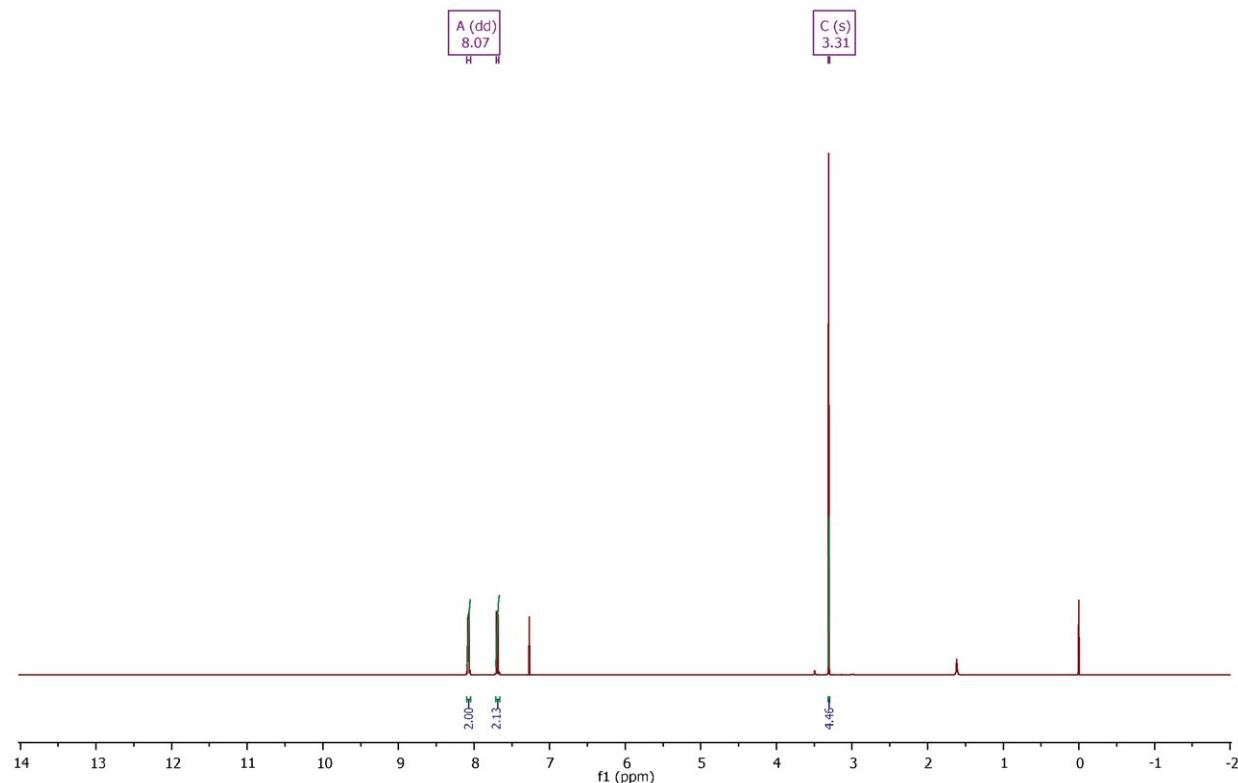


Figure S11. ^{13}C NMR spectrum (101 MHz, CDCl_3) of compound **5d**.

**Figure S12.** Infrared spectrum (KBr) of compound **5e**.**Figure S13.** ¹H NMR spectrum (400 MHz, CDCl₃) of compound **5e**.

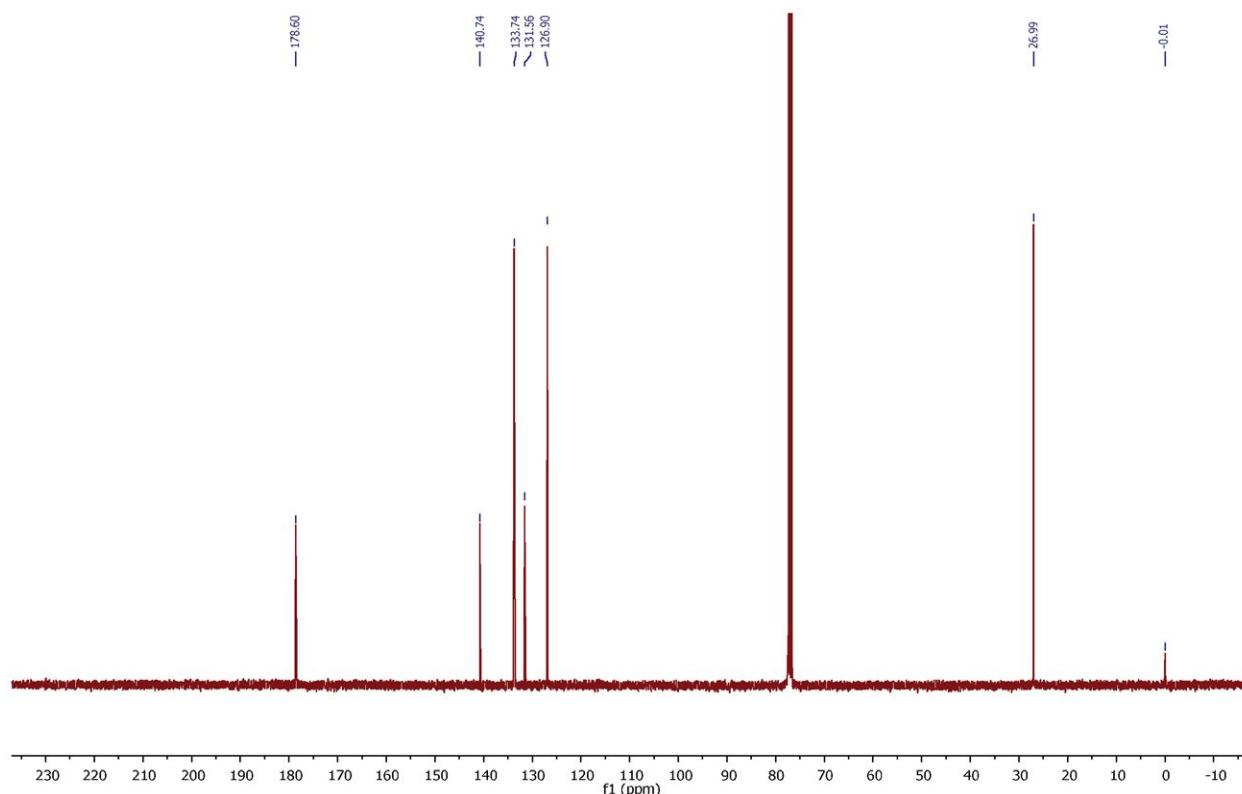


Figure S14. ¹³C NMR spectrum (101 MHz, CDCl₃) of Compound 5e.

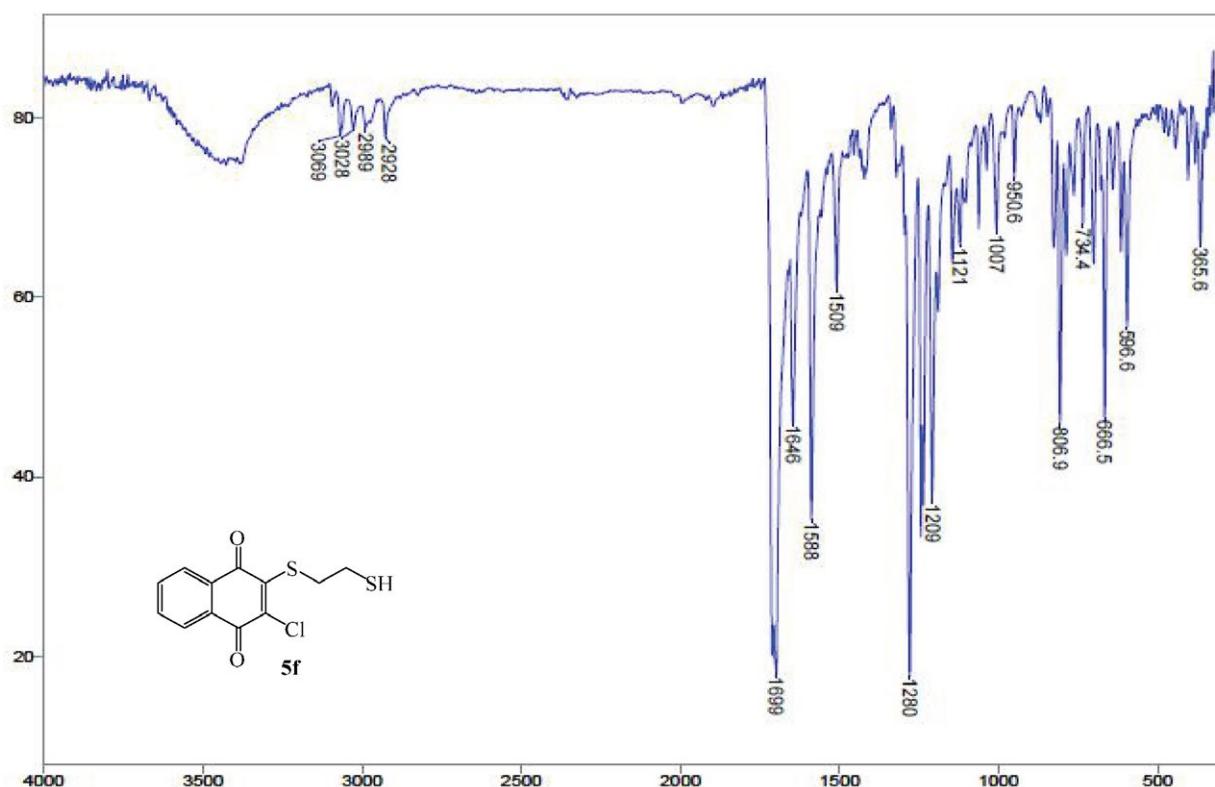


Figure S15. Infrared spectrum (KBr) of compound 5f.

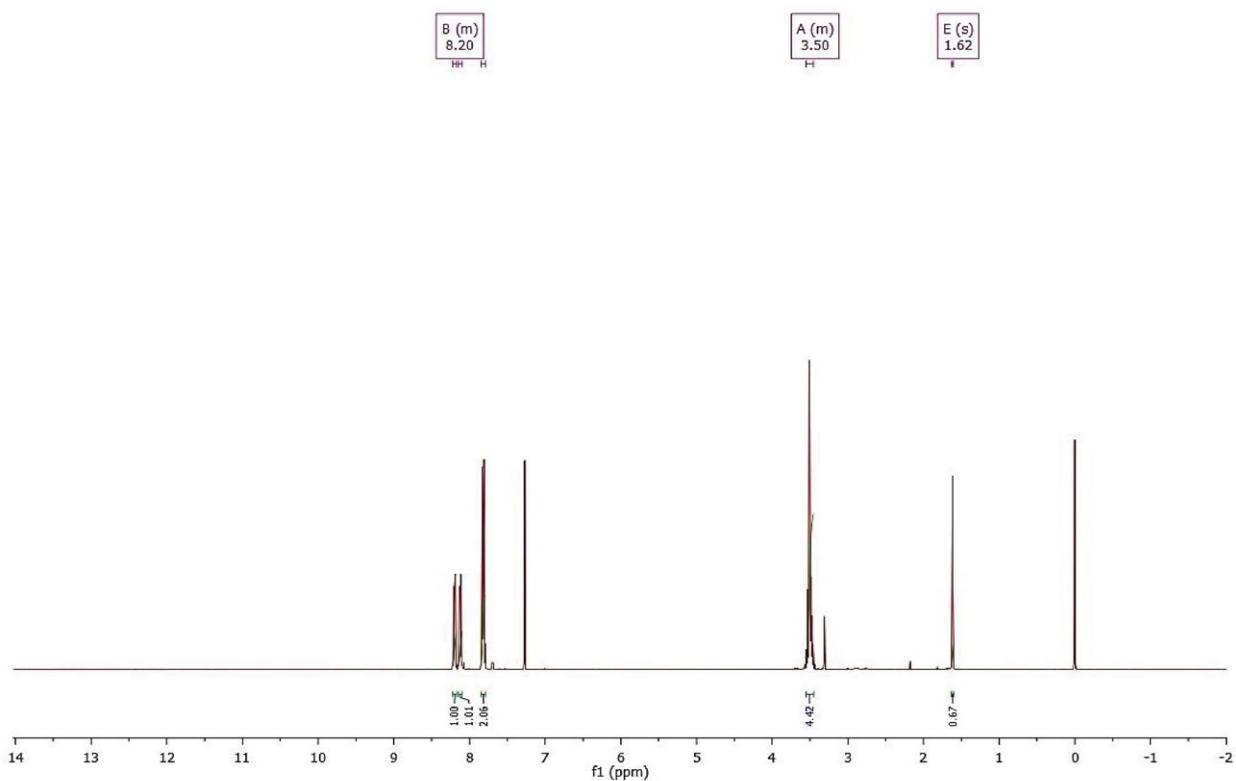


Figure S16. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **5f**.

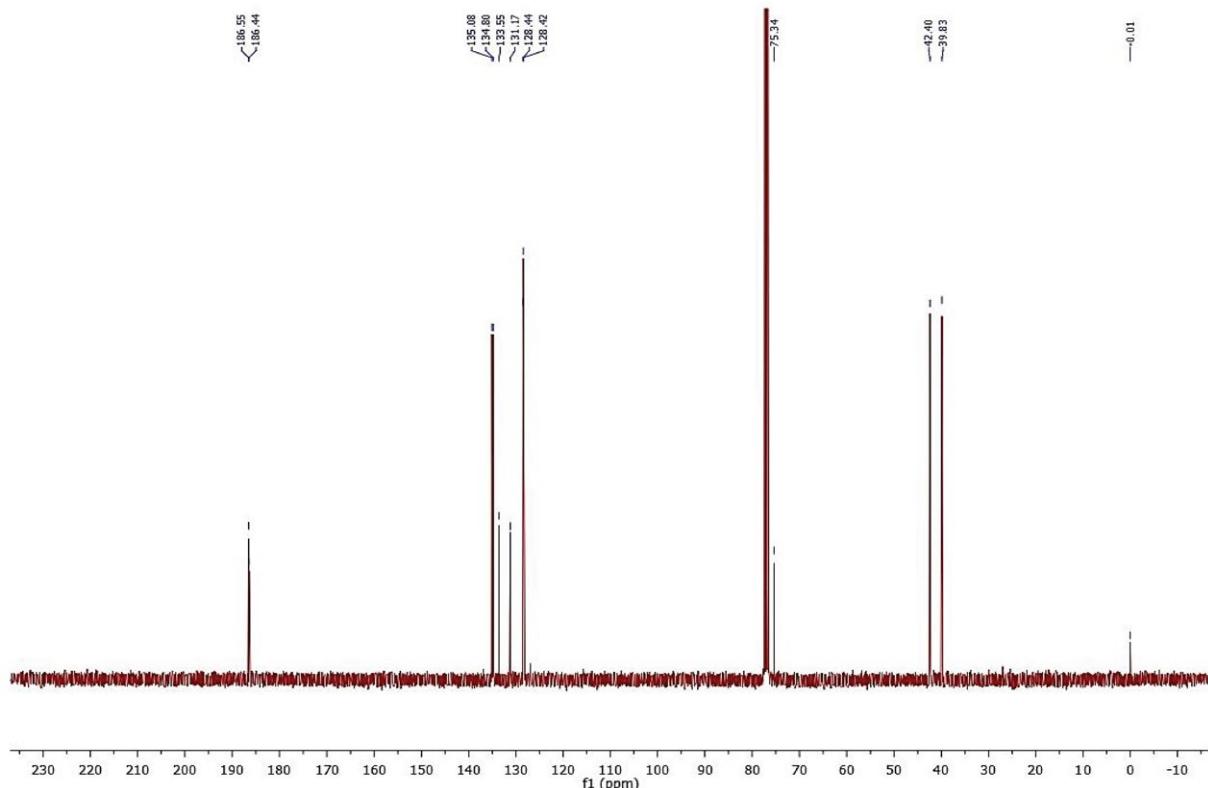


Figure S17. ^{13}C NMR spectrum (101 MHz, CDCl_3) of compound **5f**.

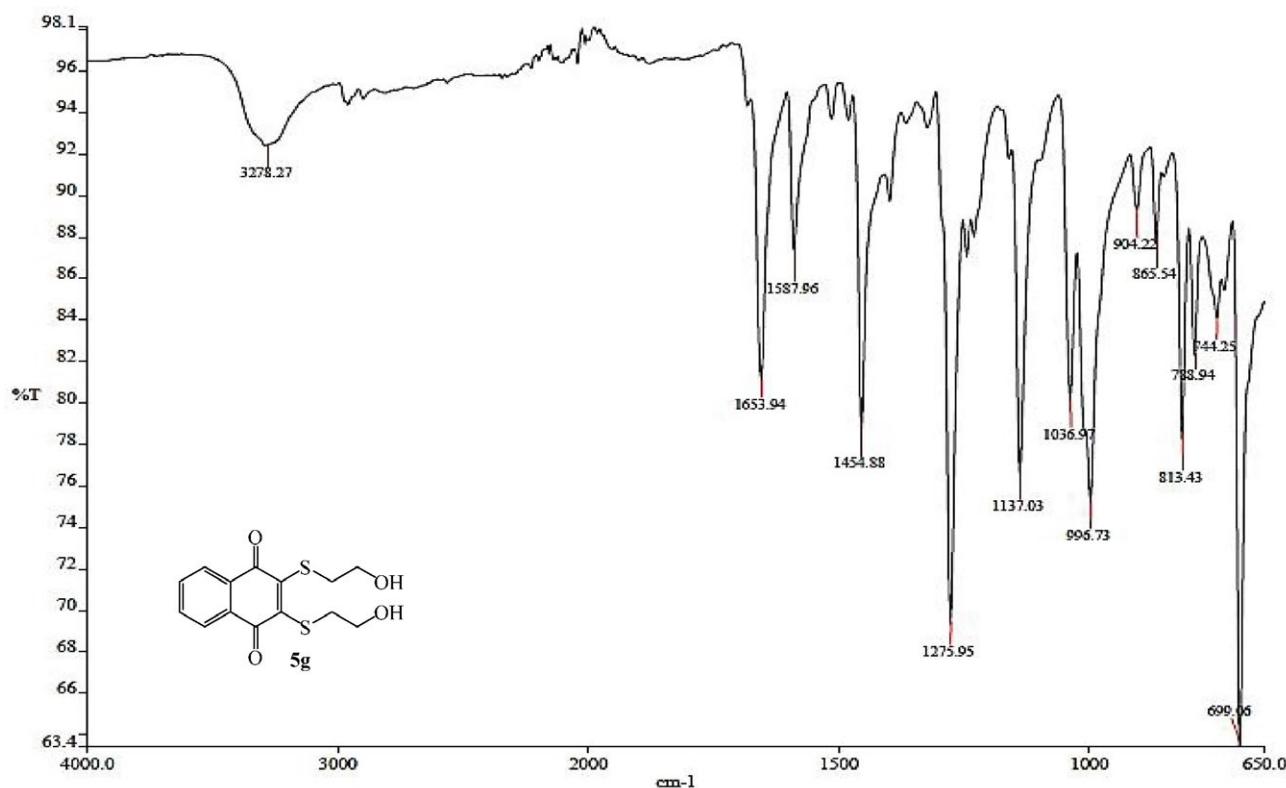


Figure S18. Infrared spectrum (KBr) of compound **5g**.

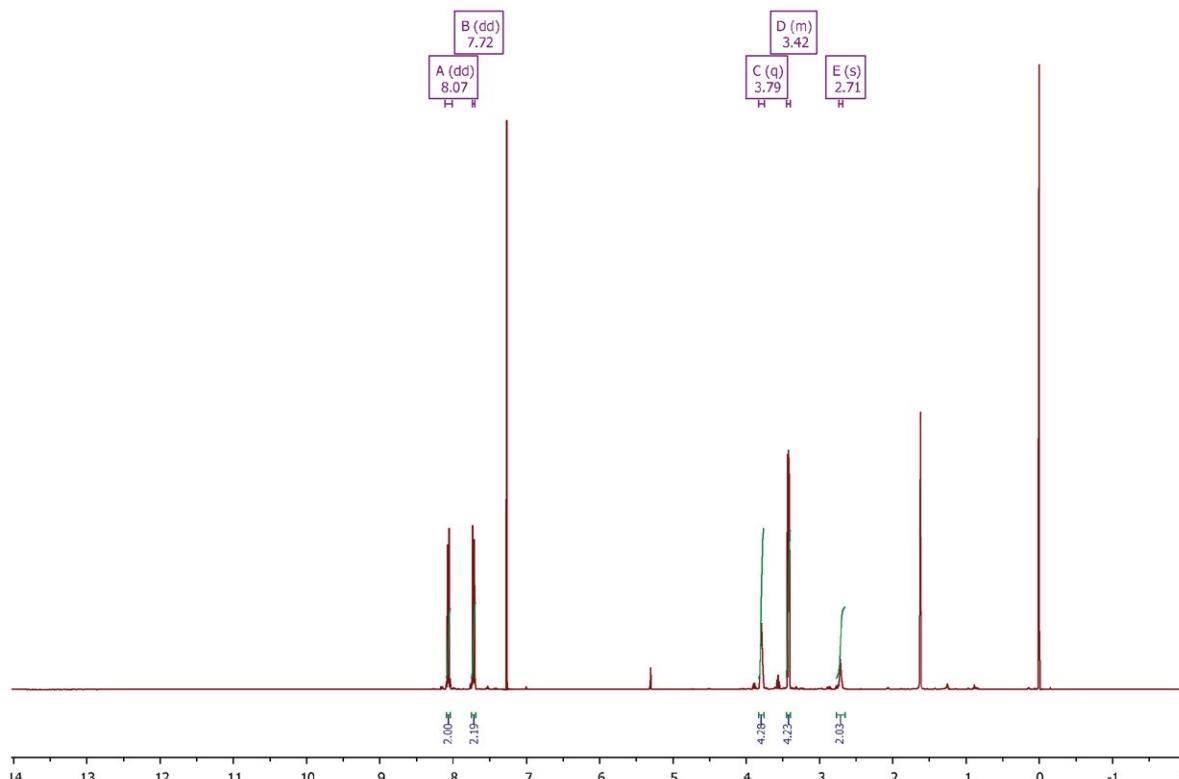


Figure S19. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **5g**.

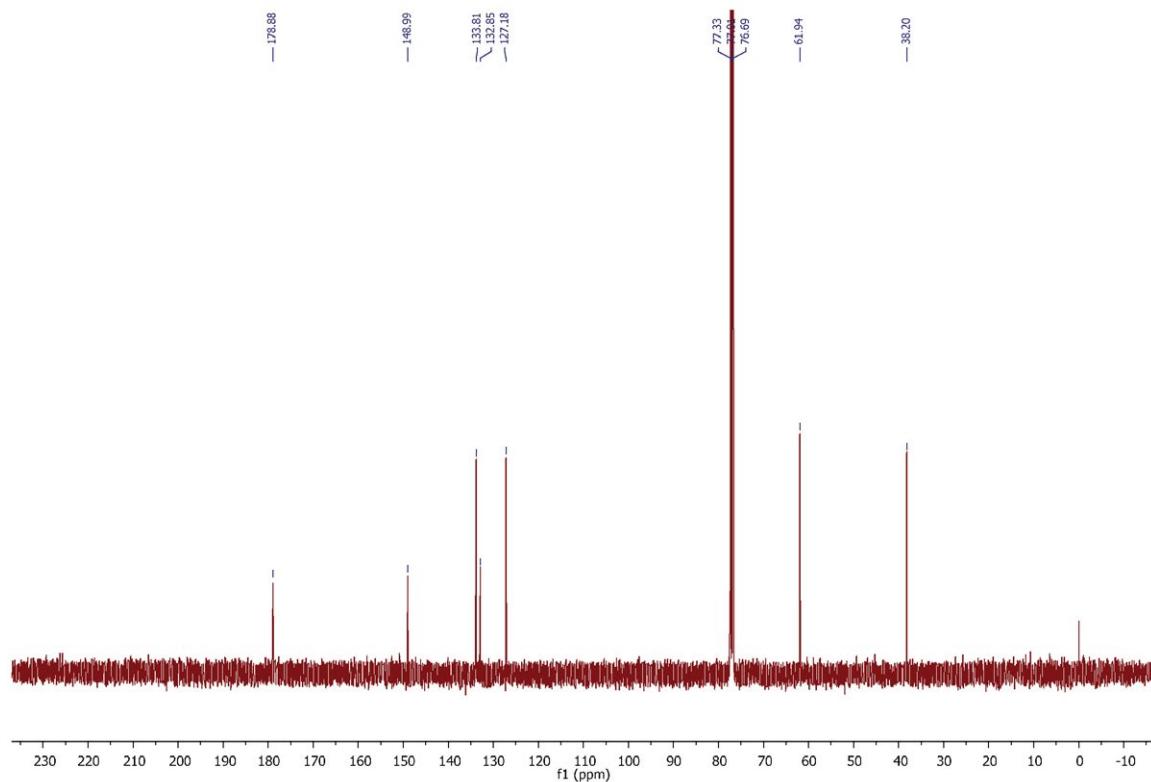


Figure S20. ^{13}C NMR spectrum (101 MHz, CDCl_3) of compound **5g**.

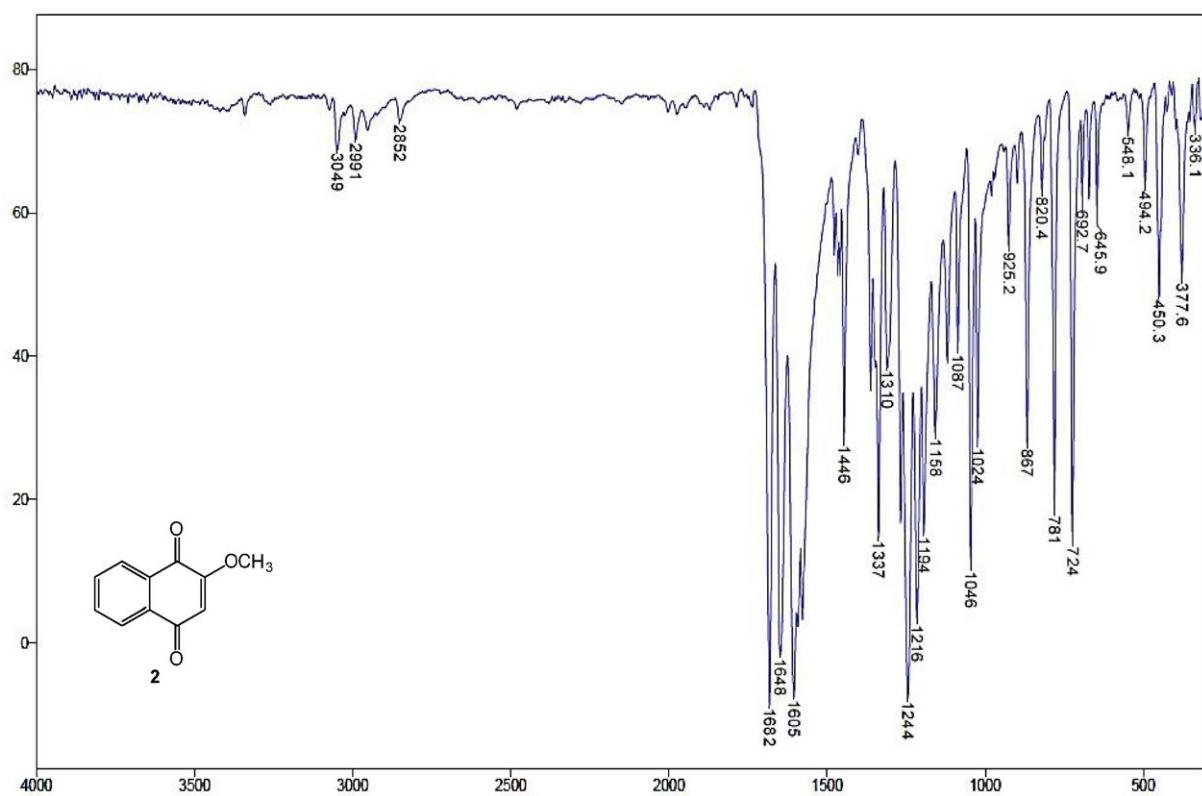


Figure S21. Infrared spectrum (KBr) of compound 2.

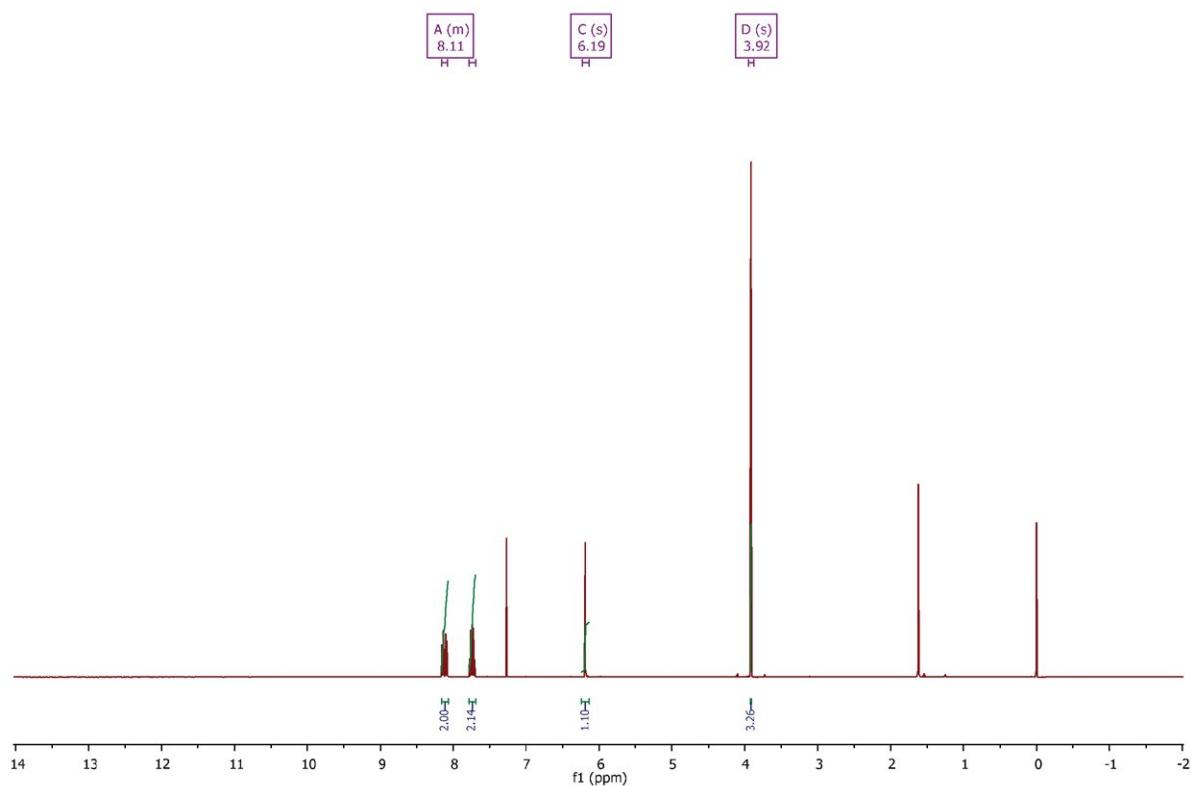


Figure S22. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 2.

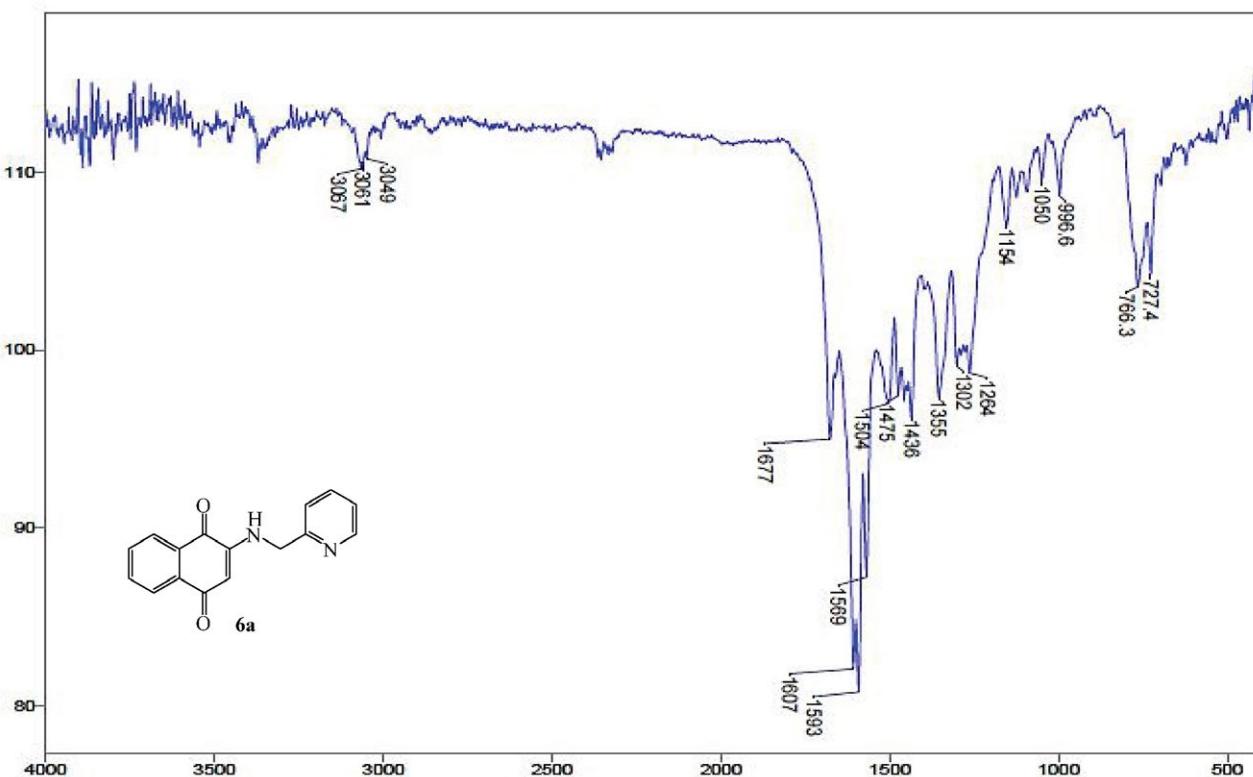
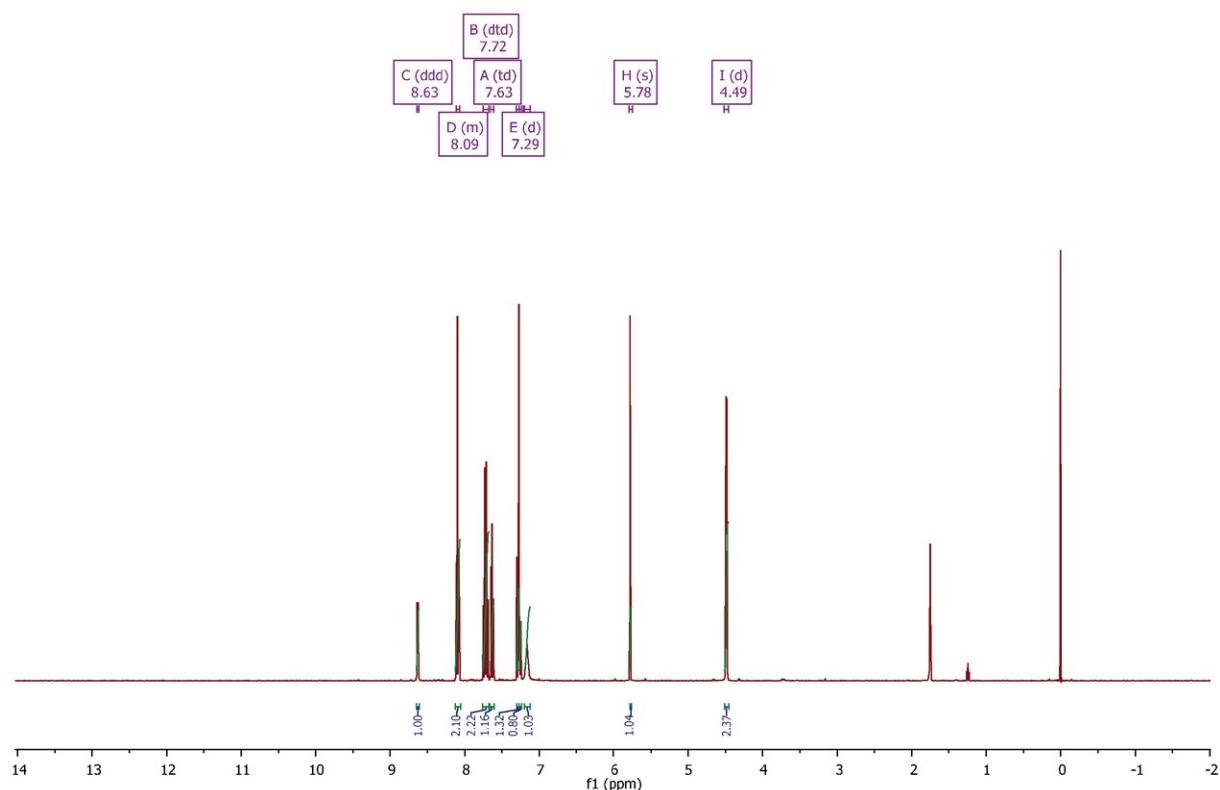
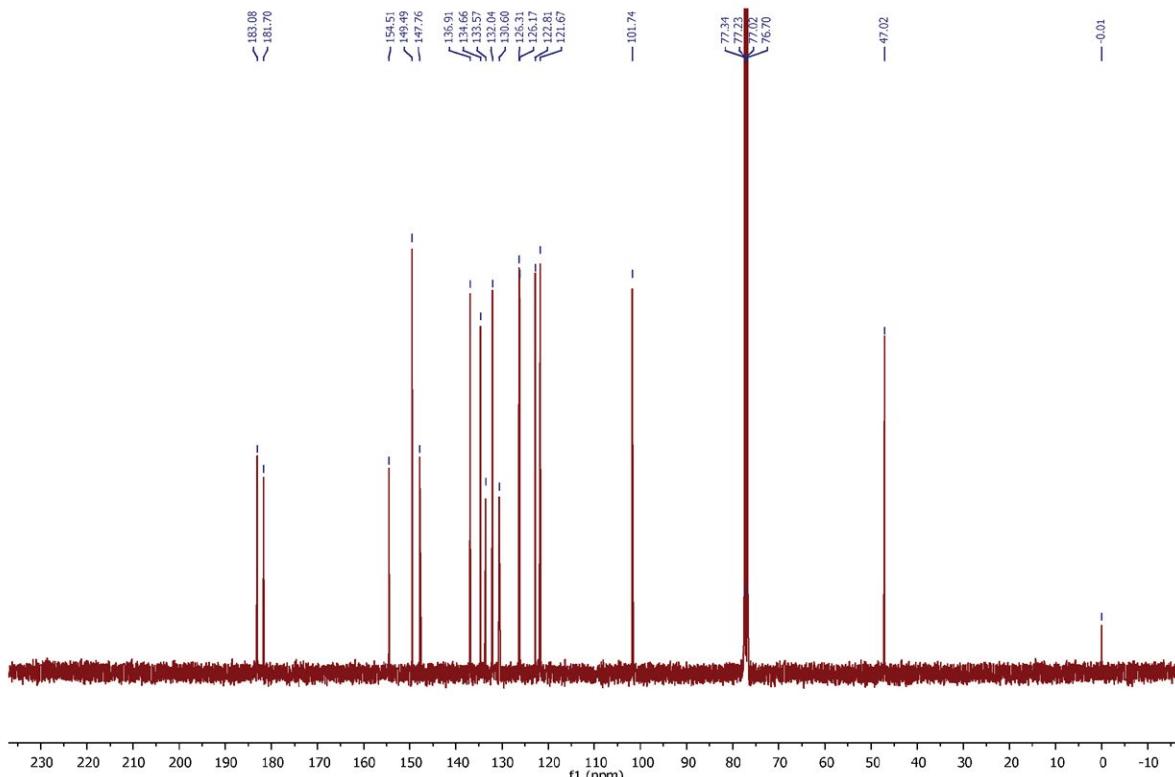


Figure S23. Infrared spectrum (KBr) of compound 6a.

**Figure S24.** ^1H NMR spectrum (400 MHz, CDCl_3) of compound **6a**.**Figure S25.** ^{13}C NMR spectrum (101 MHz, CDCl_3) of compound **6a**.

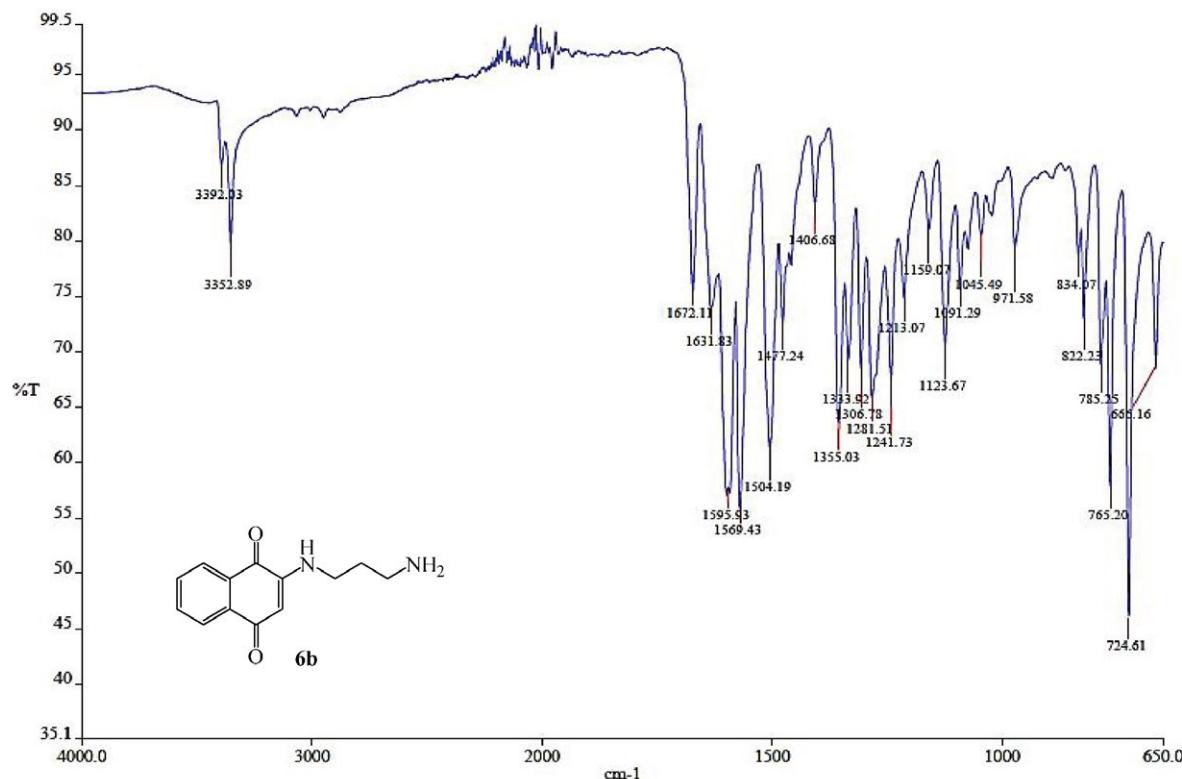


Figure S26. Infrared spectrum (KBr) of compound **6b**.

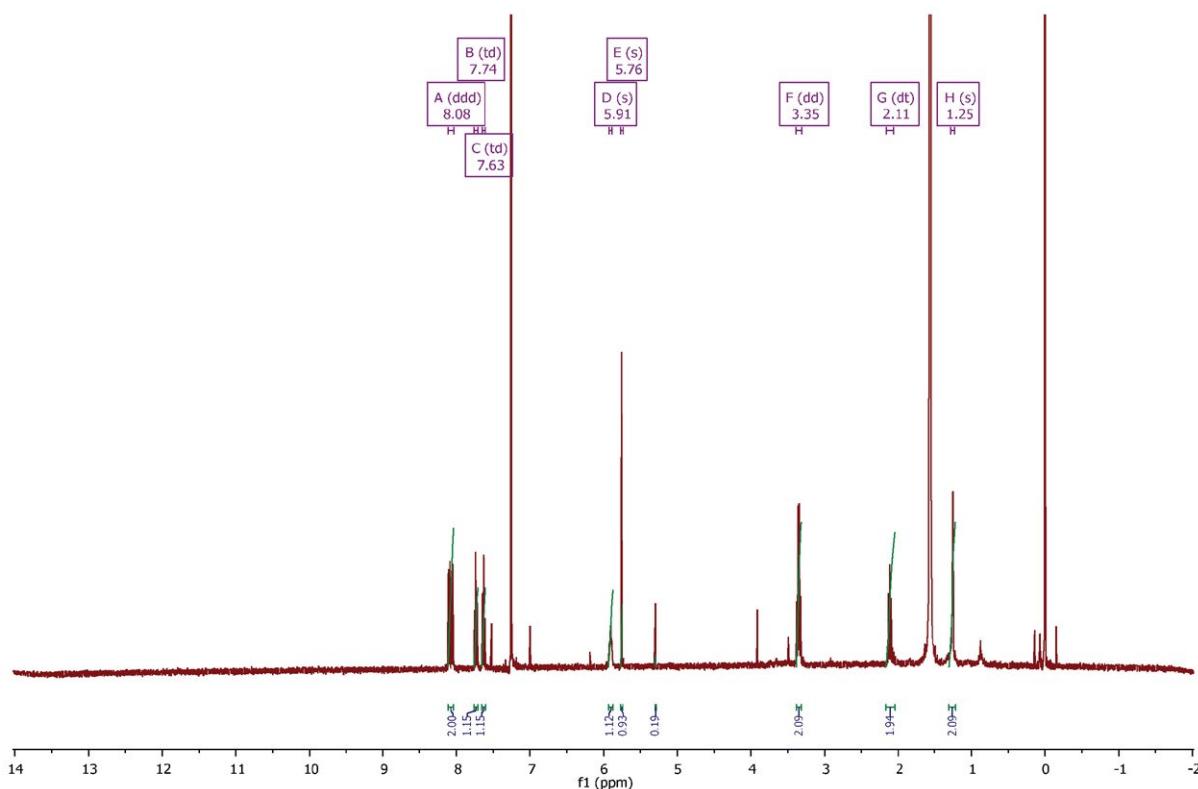
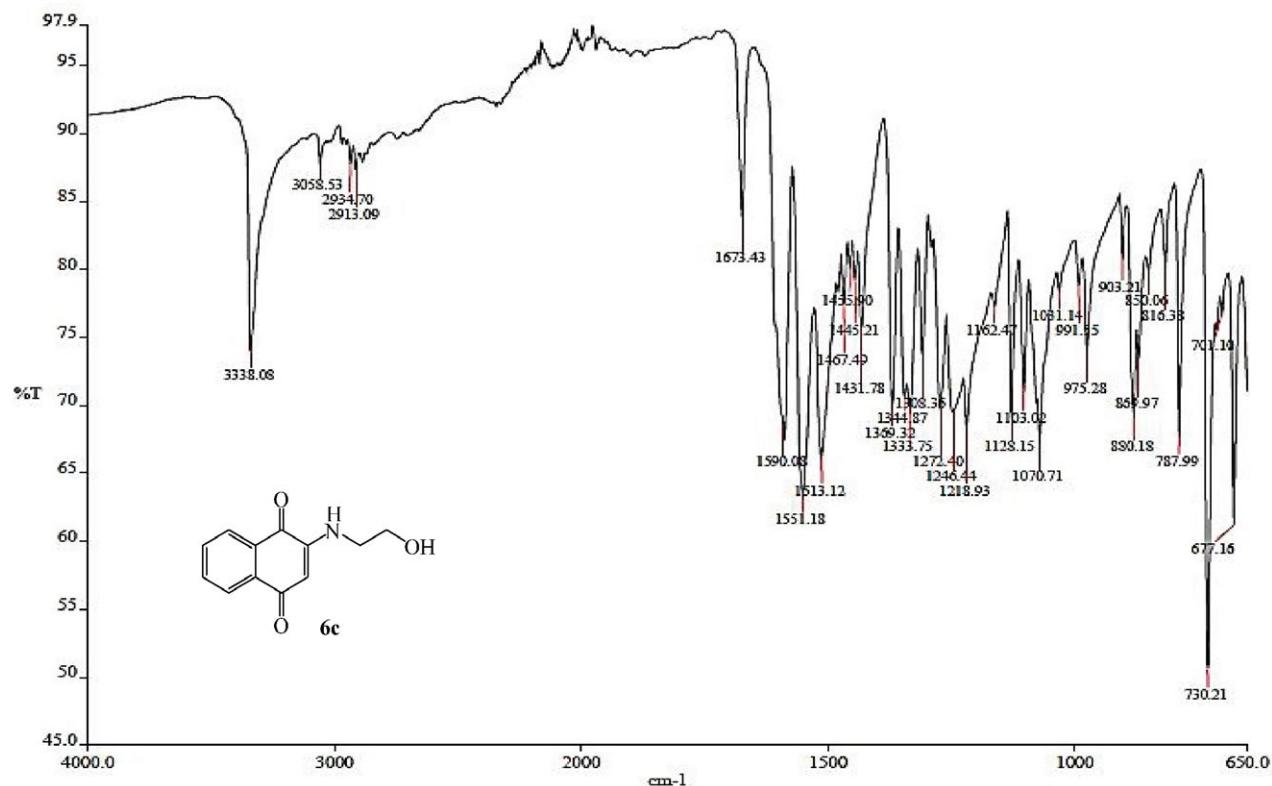
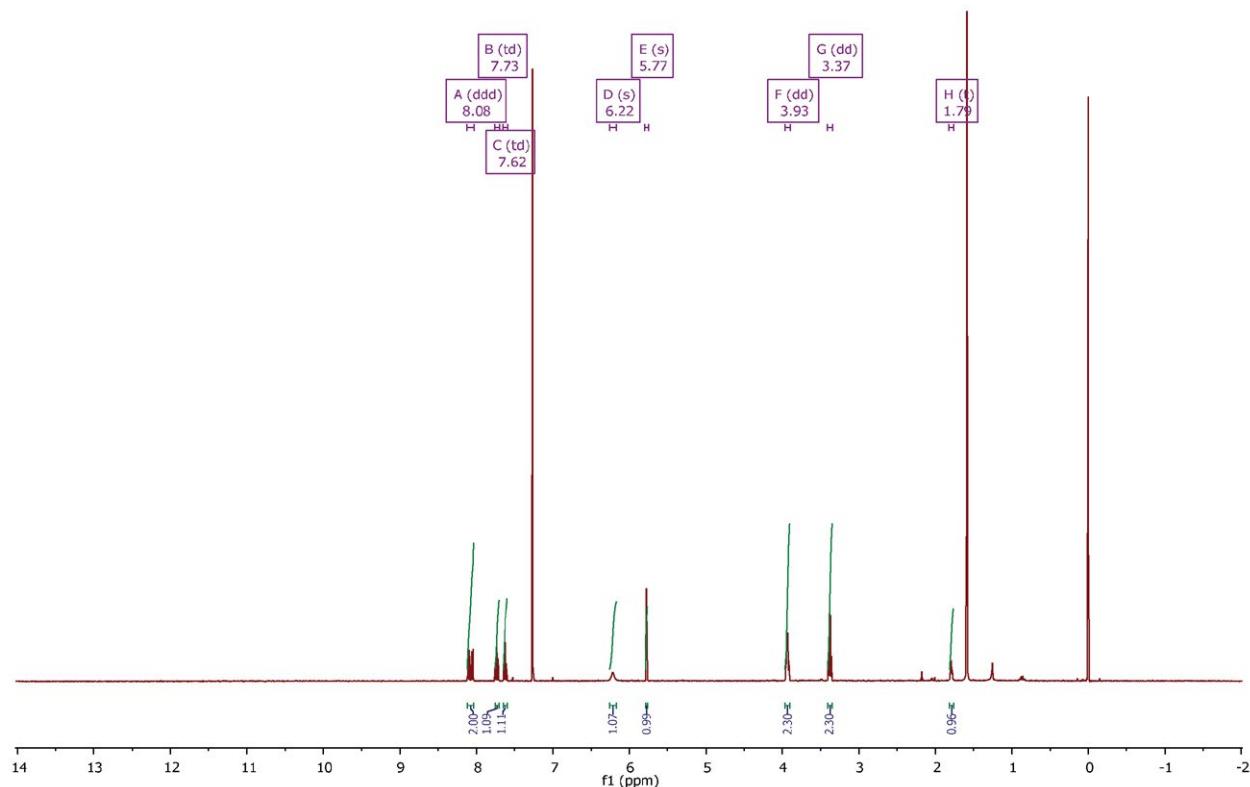


Figure S27. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **6b**.

**Figure S28.** Infrared spectrum (KBr) of compound **6c**.**Figure S29.** ¹H NMR spectrum (400 MHz, CDCl₃) of compound **6c**.

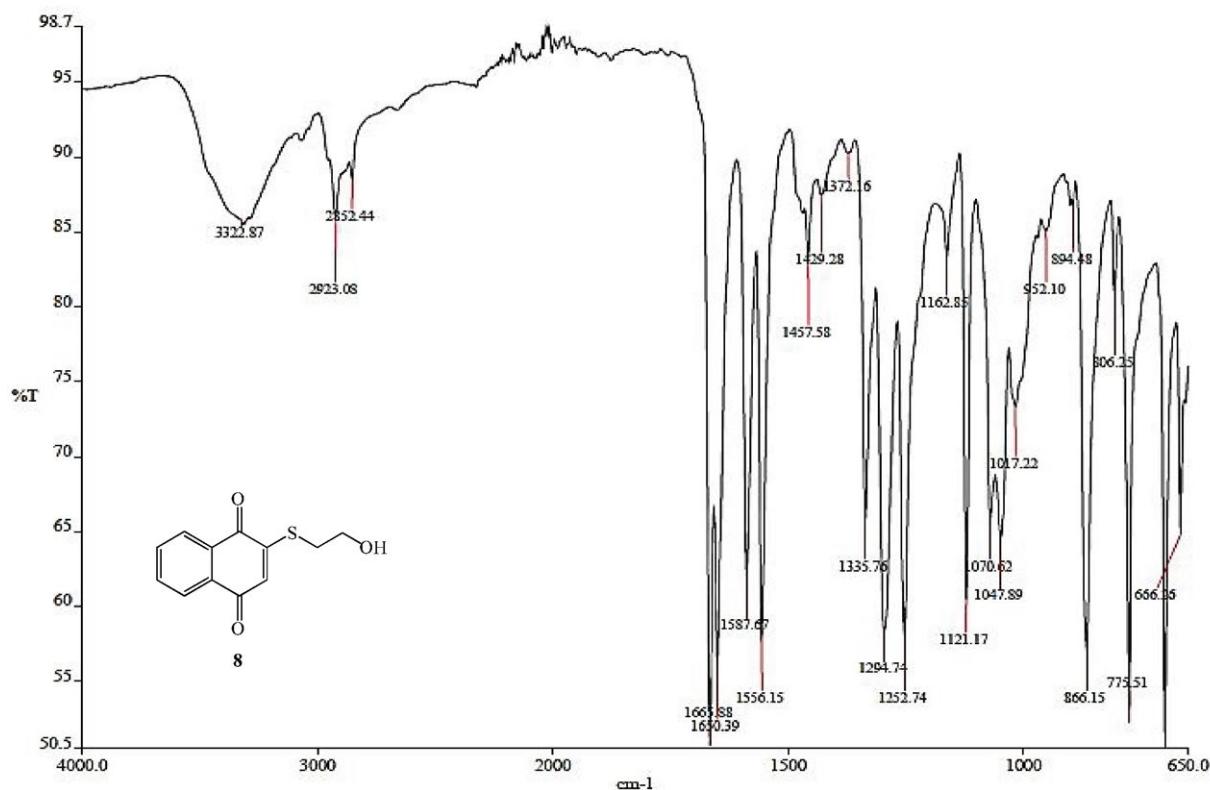


Figure S30. Infrared spectrum (KBr) of compound **8**.

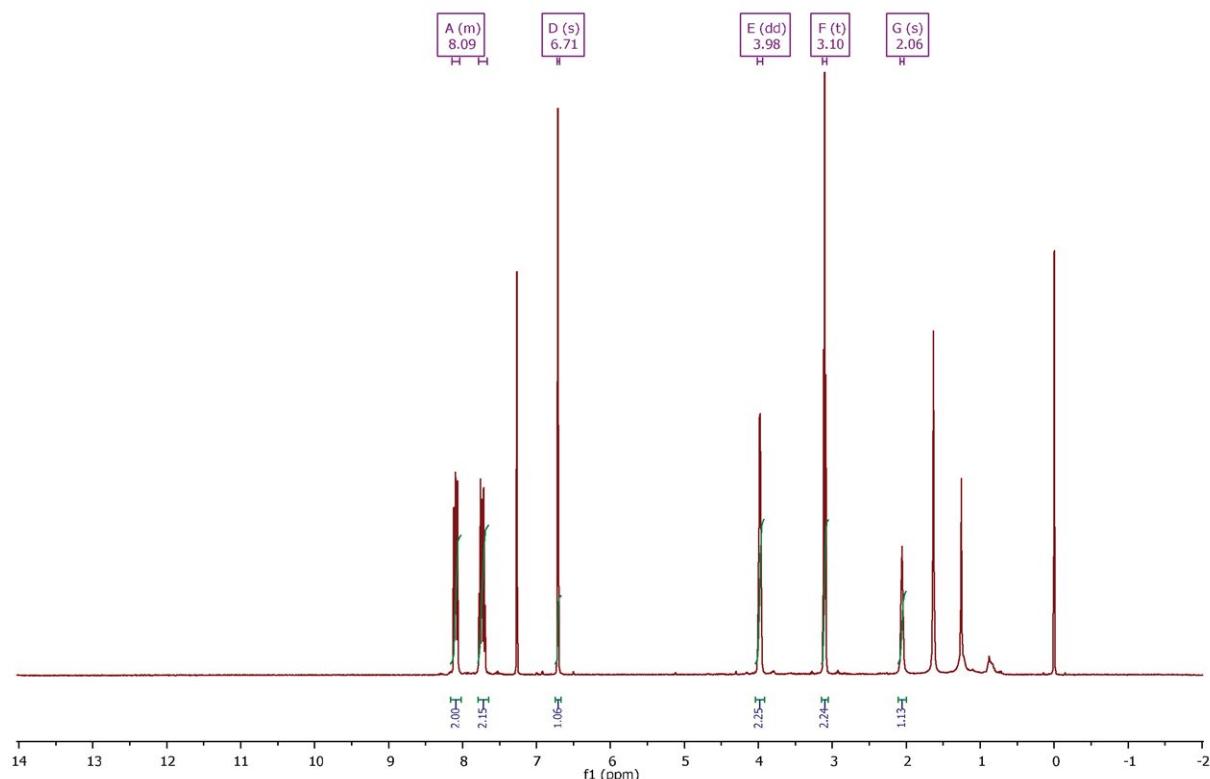


Figure S31. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **8**.

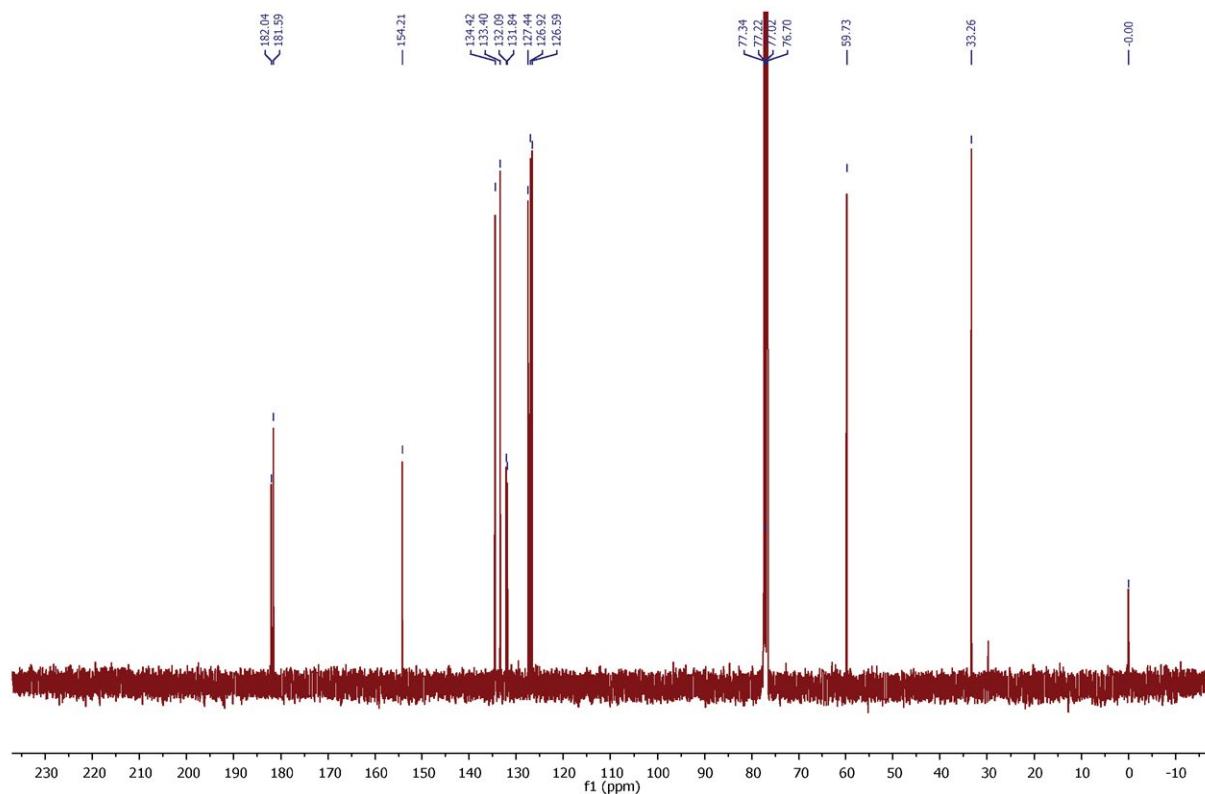


Figure S32. ¹³C NMR spectrum (101 MHz, CDCl₃) of compound 8.

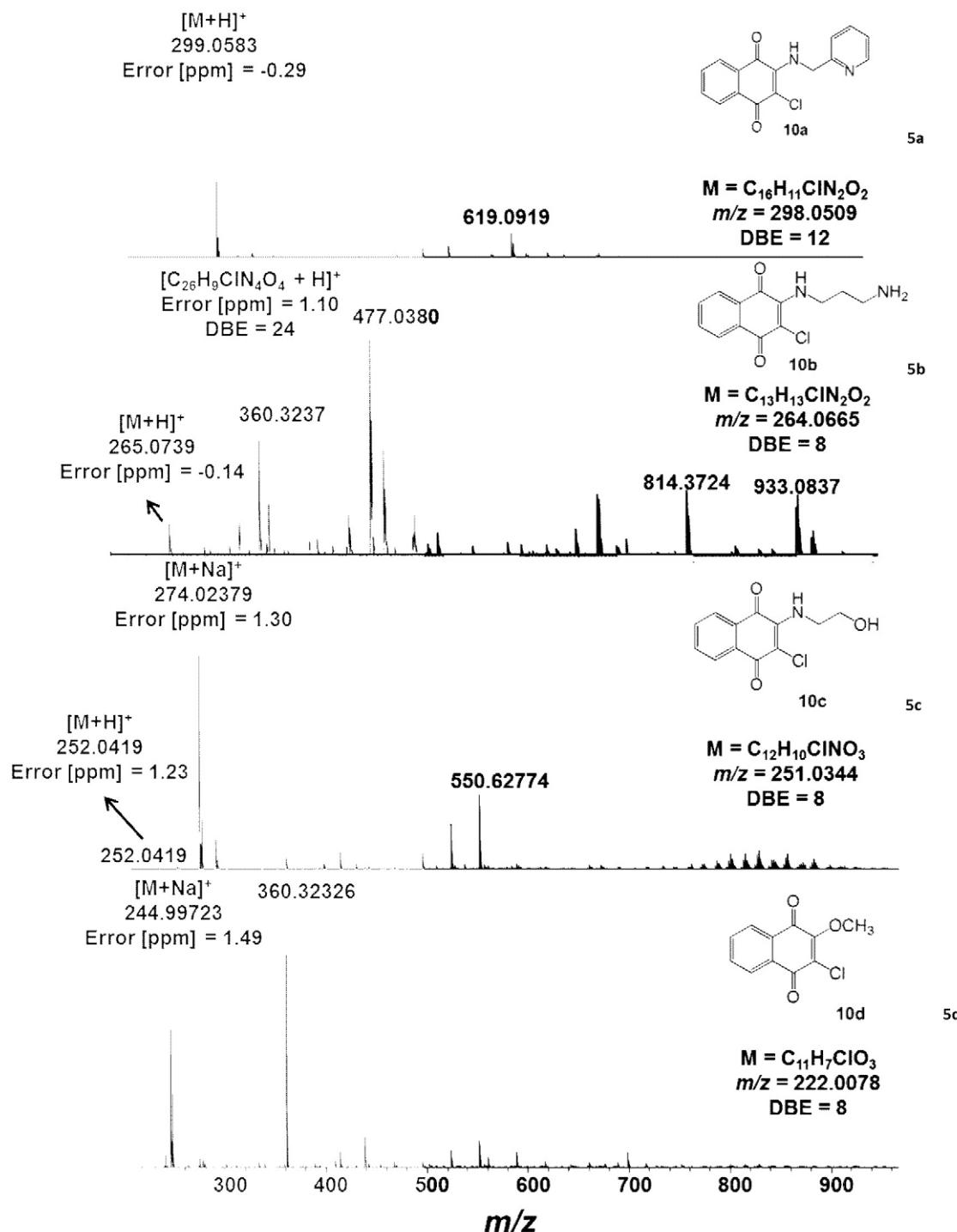


Figure S33. ESI(+)-FT-ICR MS spectra for compounds 5a-d.

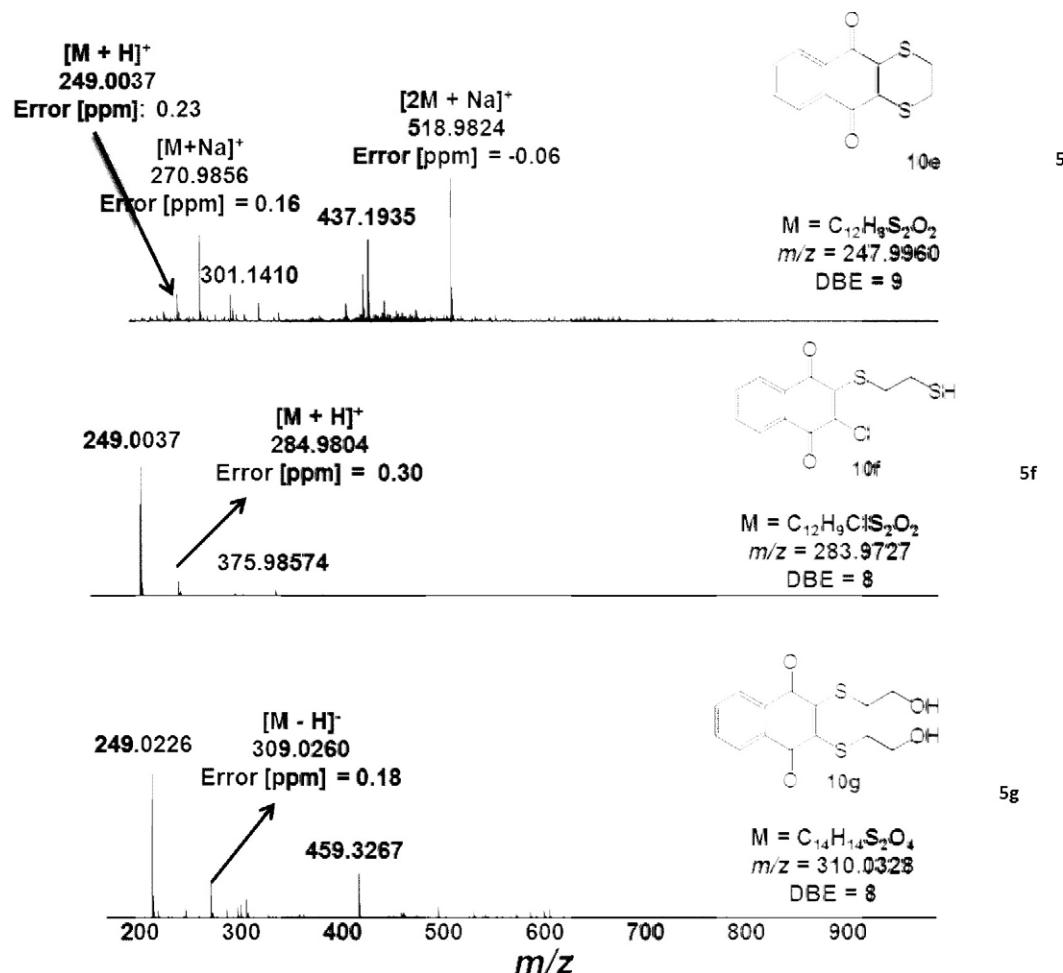


Figure S34. ESI(\pm)-FT-ICR MS spectra for compounds 5e-g.

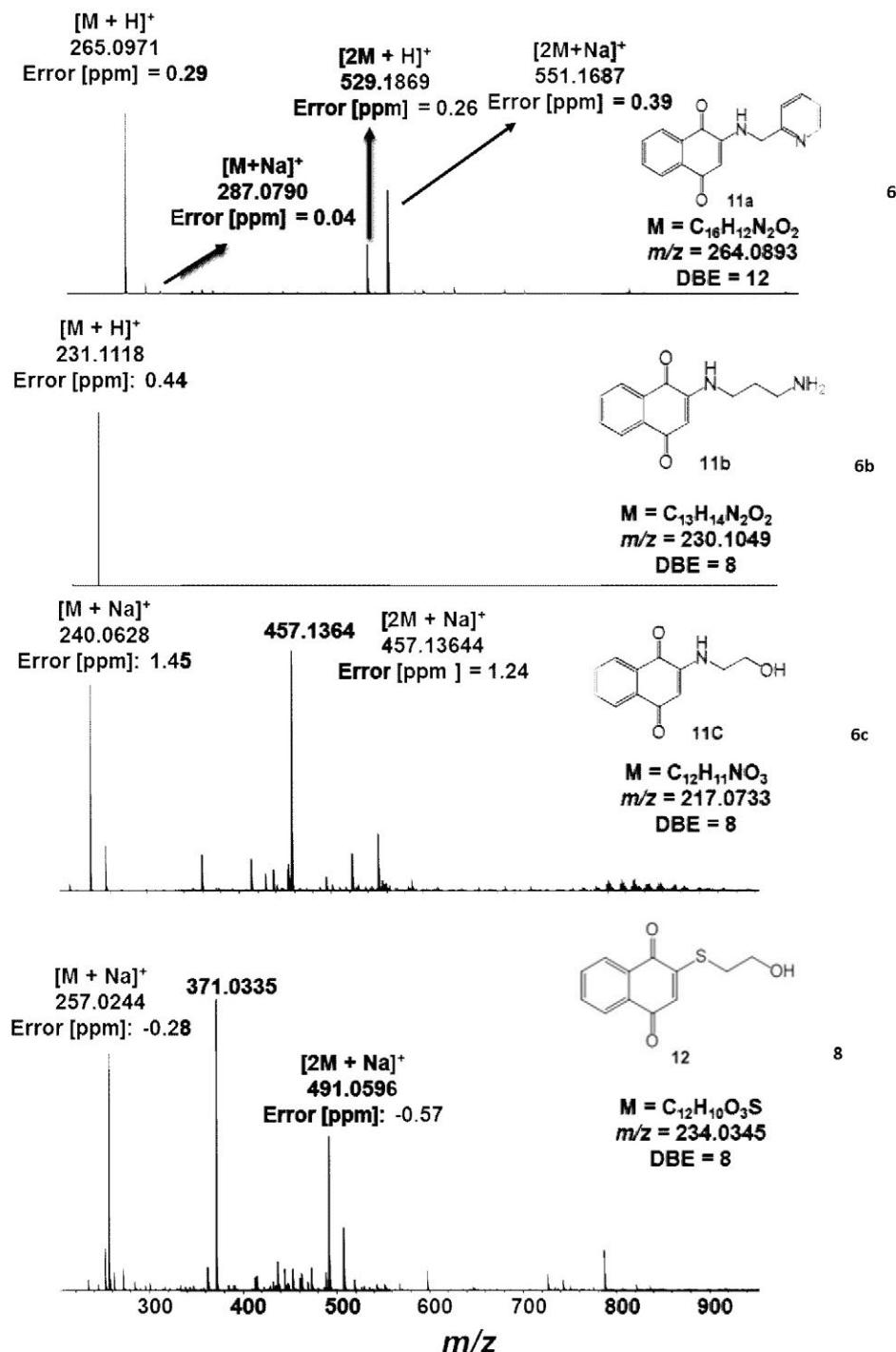


Figure S35. ESI(+) FT-ICR MS spectra for compounds 6a-c and 8.