

Figure S1. The <sup>1</sup>H NMR spectrum of compound 3 (400 MHz, solvent DMSO-*d*<sub>6</sub>)

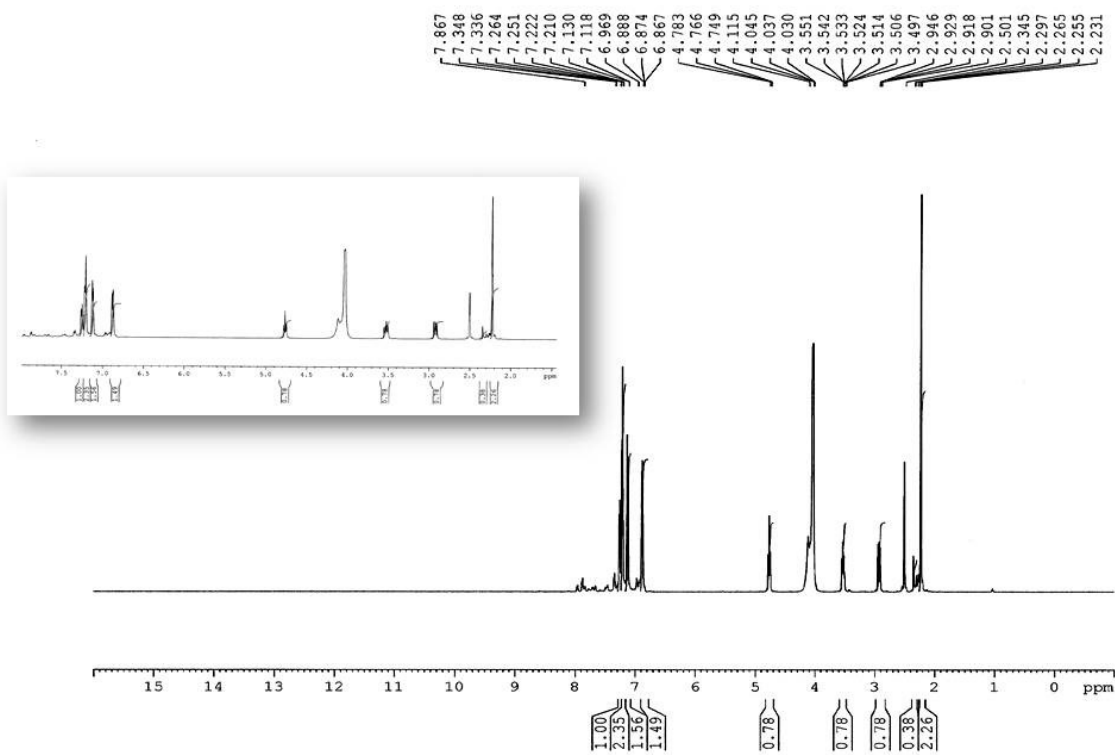
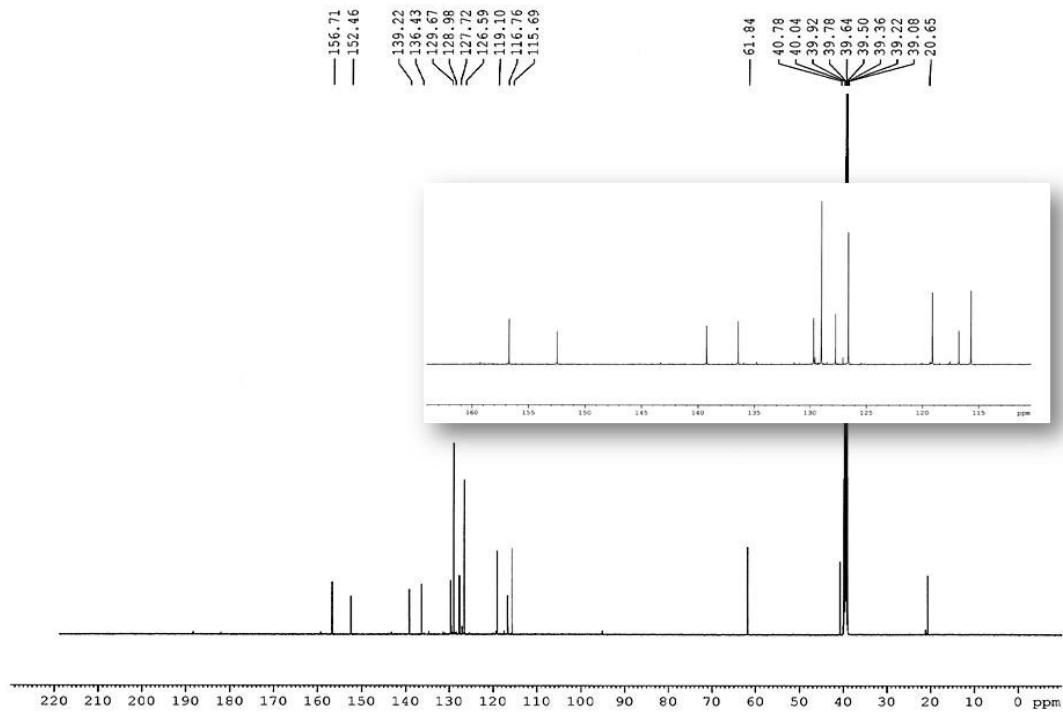
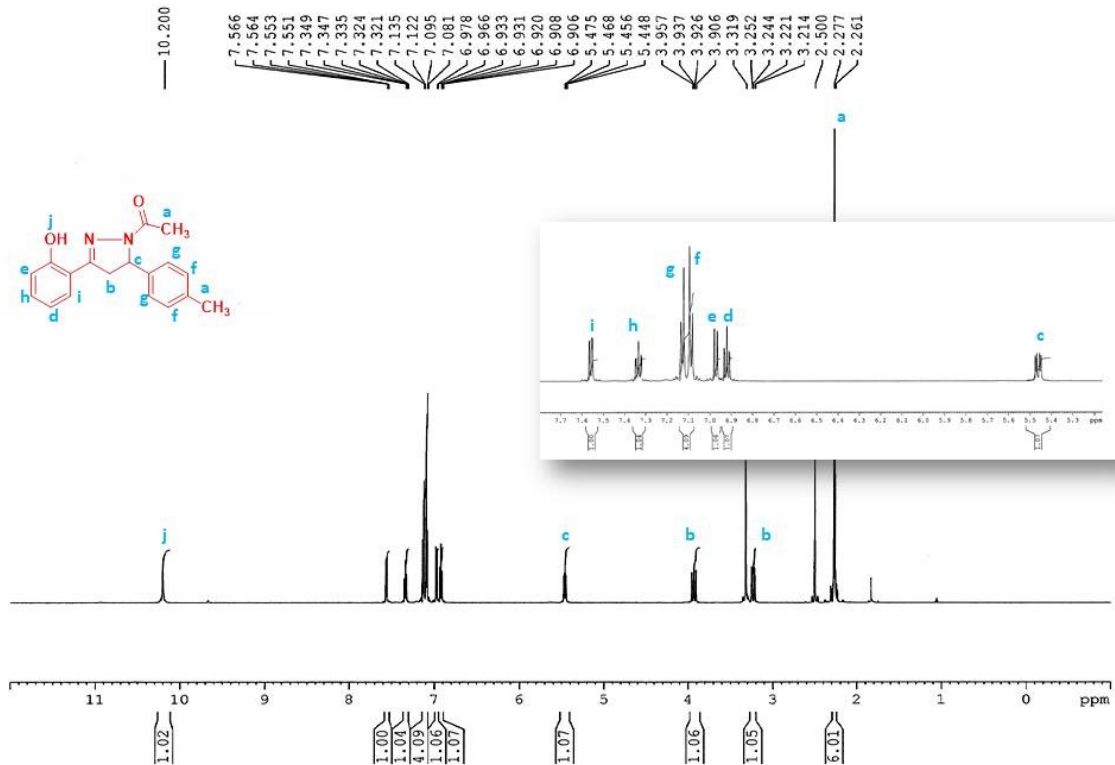


Figure S2. The D<sub>2</sub>O <sup>1</sup>H NMR spectrum of compound 3 (400 MHz, solvent DMSO-*d*<sub>6</sub>)



**Figure S3.** The  $^{13}\text{C}$  NMR spectrum of compound **3** (100 MHz, solvent  $\text{DMSO-}d_6$ )



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

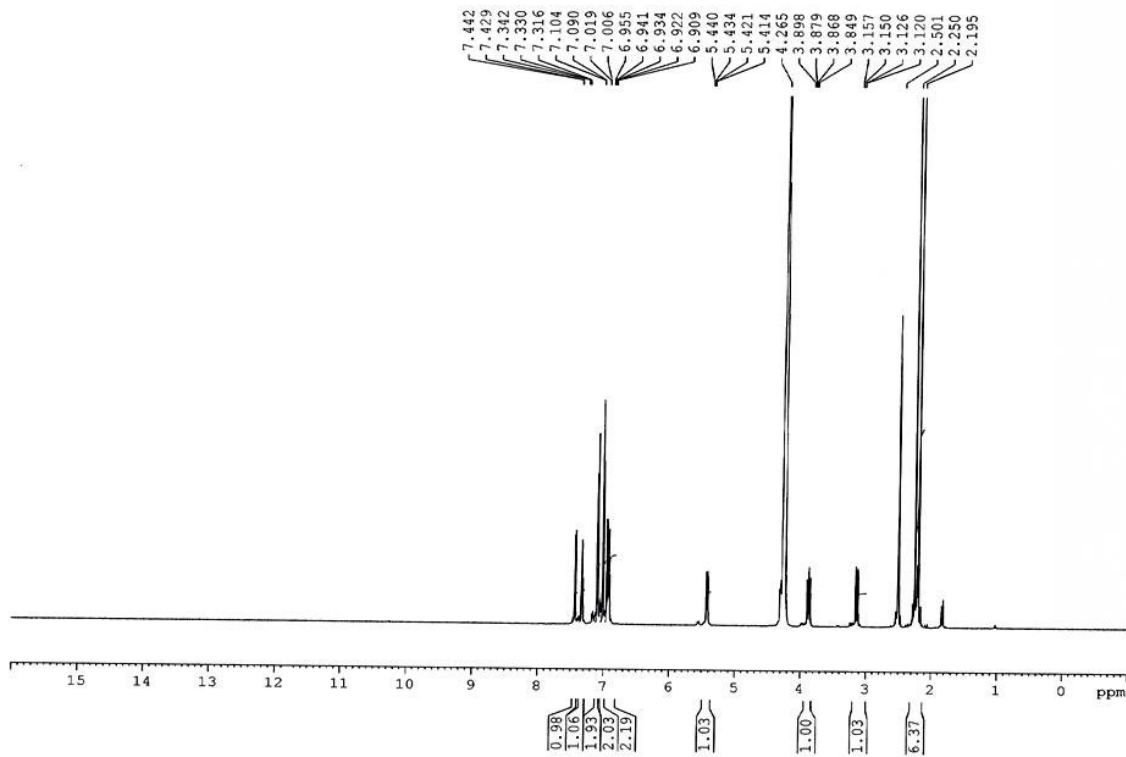


Figure S5. The  $D_2O$   $^1H$  NMR spectrum of compound **4** (400 MHz, solvent  $DMSO-d_6$ )

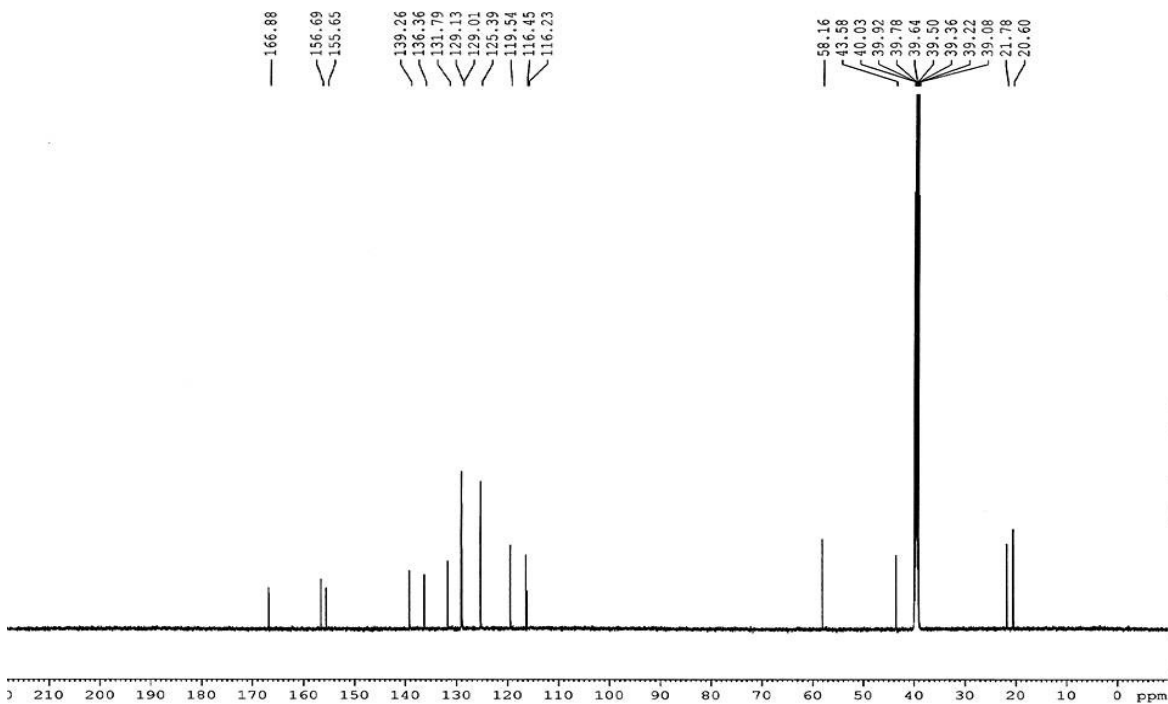
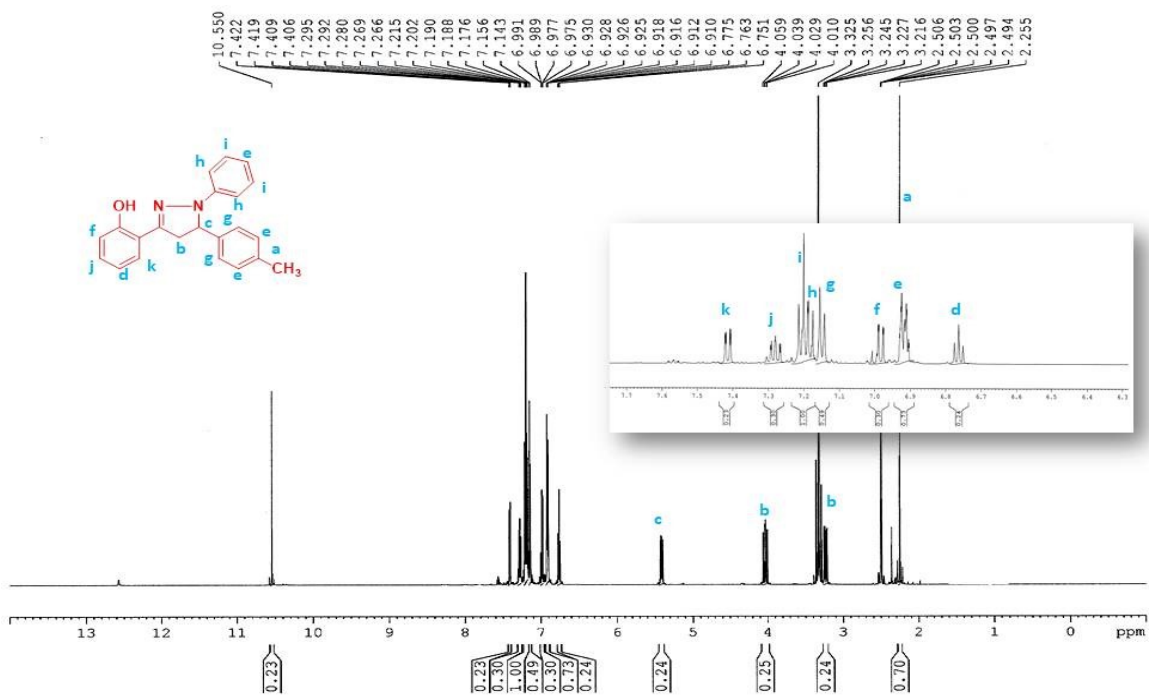
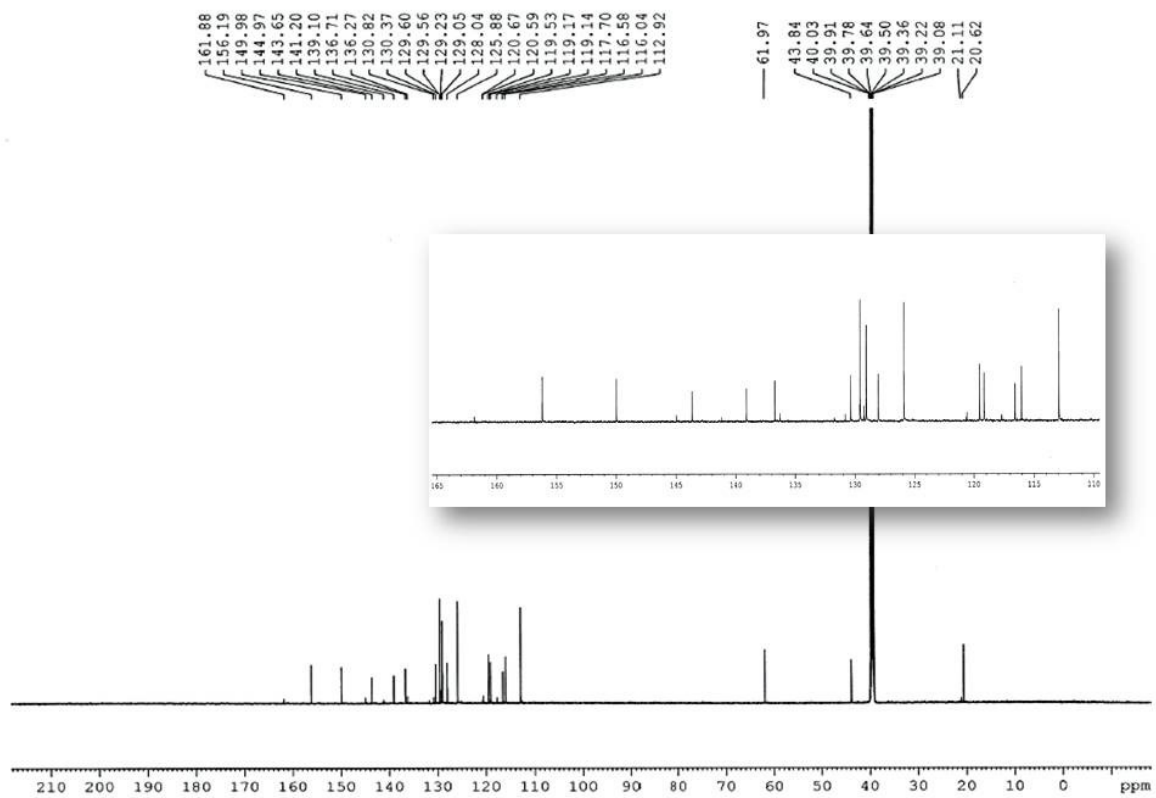


Figure S6. The  $^{13}C$  NMR spectrum of compound **4** (100 MHz, solvent  $DMSO-d_6$ )



**Figure S7.** The <sup>1</sup>H NMR spectrum of compound **6a** (400 MHz, solvent DMSO-*d*<sub>6</sub>)



**Figure S8.** The <sup>13</sup>C NMR spectrum of compound **6a** (100 MHz, solvent DMSO-*d*<sub>6</sub>)

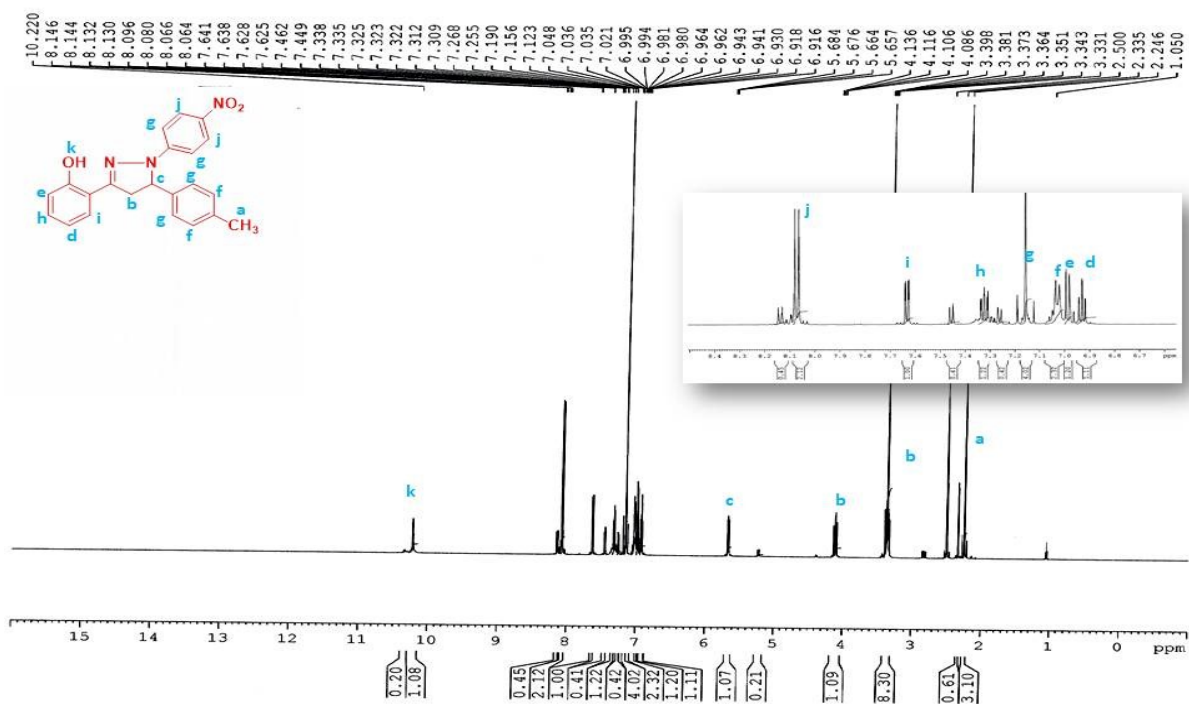


Figure S9. The  $^1\text{H}$  NMR spectrum of compound **6b** (400 MHz, solvent  $\text{DMSO}-d_6$ )

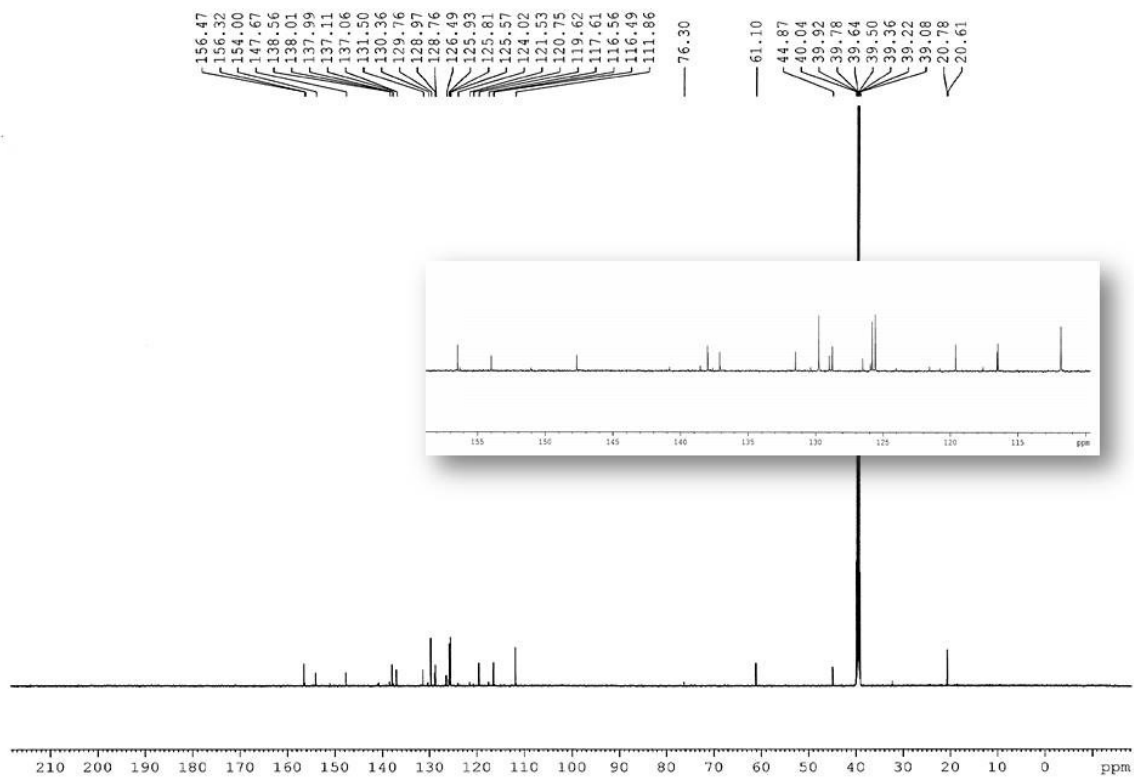


Figure S10. The  $^{13}\text{C}$  NMR spectrum of compound **6b** (100 MHz, solvent  $\text{DMSO}-d_6$ )

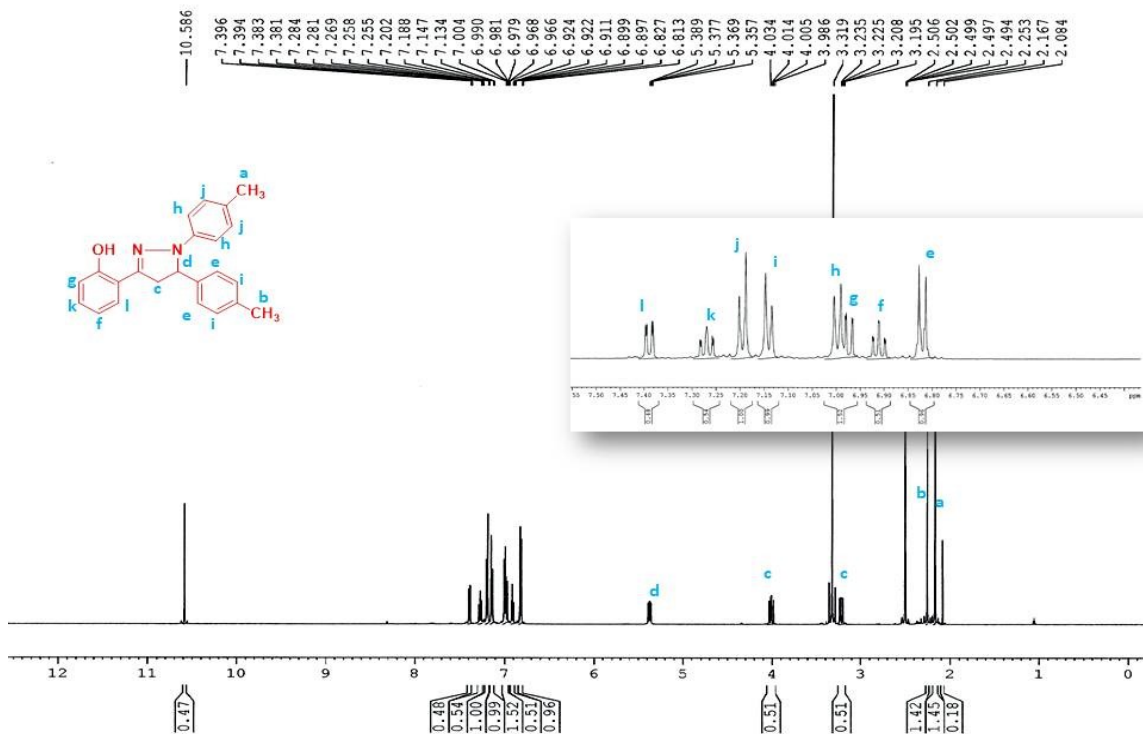


Figure S11. The <sup>1</sup>H NMR spectrum of compound **6c** (400 MHz, solvent DMSO-*d*<sub>6</sub>)

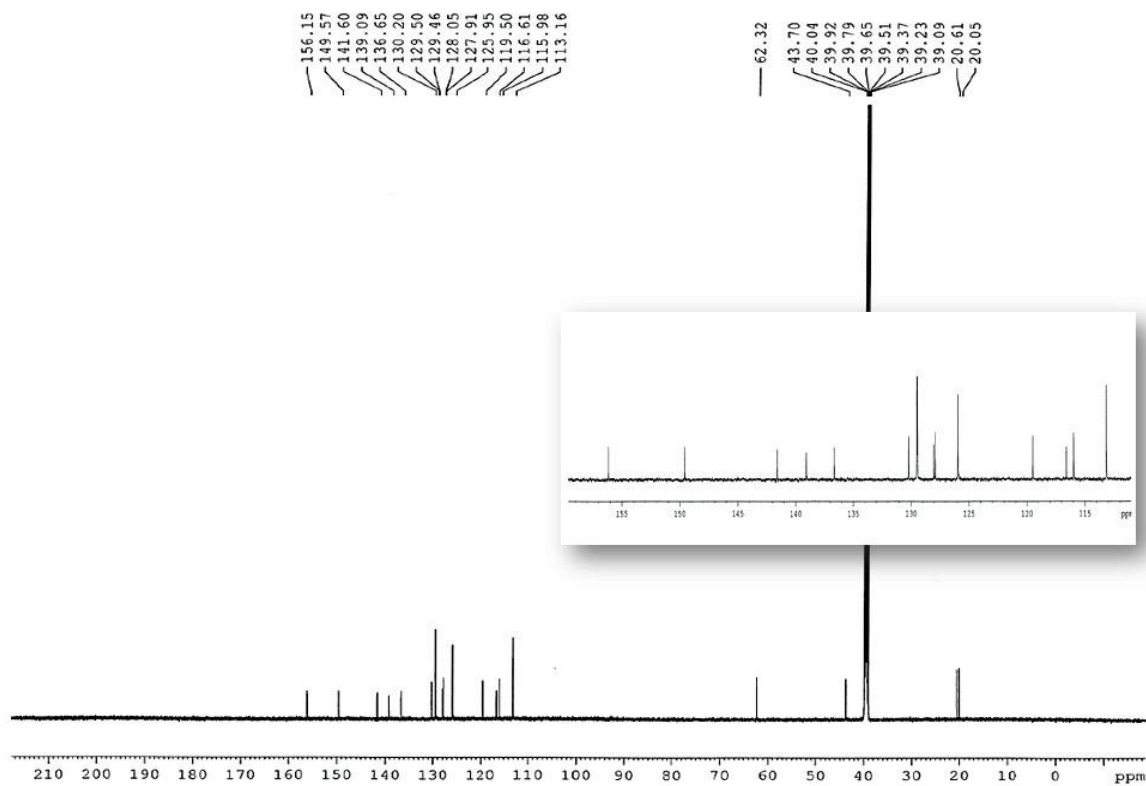


Figure S12. The <sup>13</sup>C NMR spectrum of compound **6c** (100 MHz, solvent DMSO-*d*<sub>6</sub>)

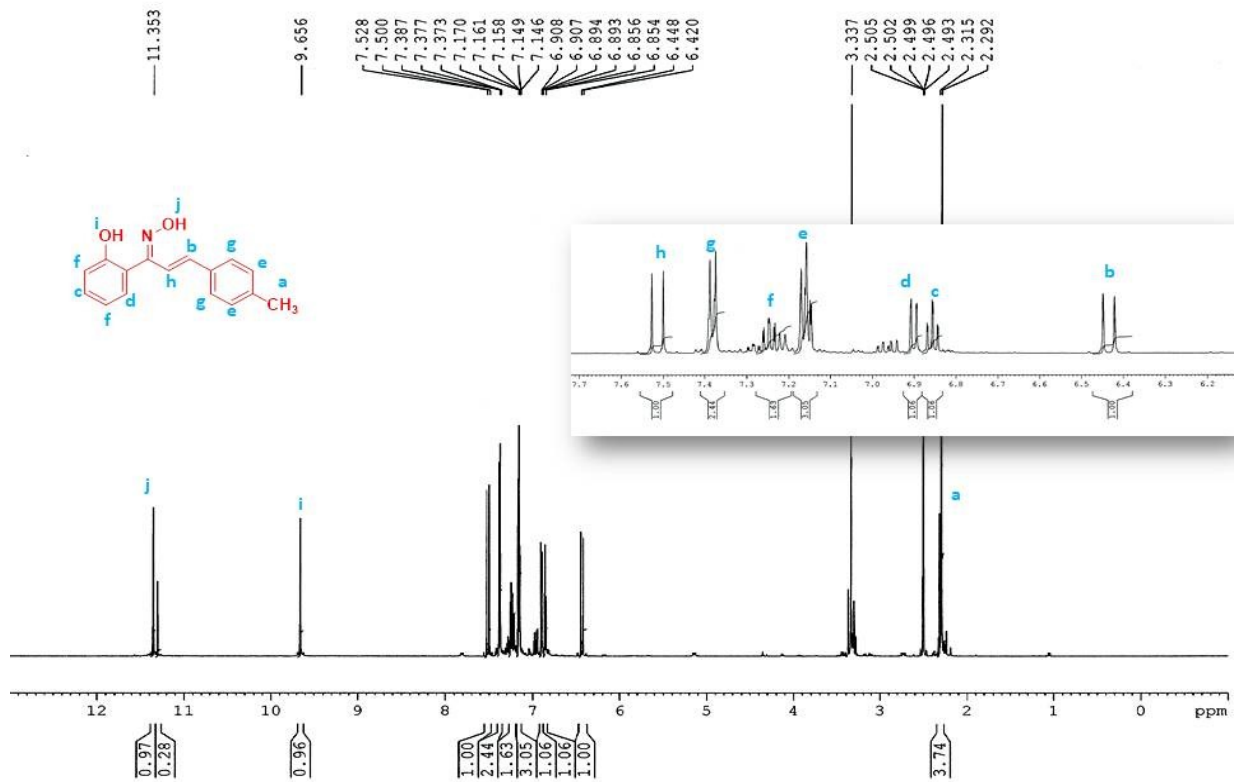


Figure S13. The <sup>1</sup>H NMR spectrum of compound 8 (400 MHz, solvent DMSO-*d*<sub>6</sub>)

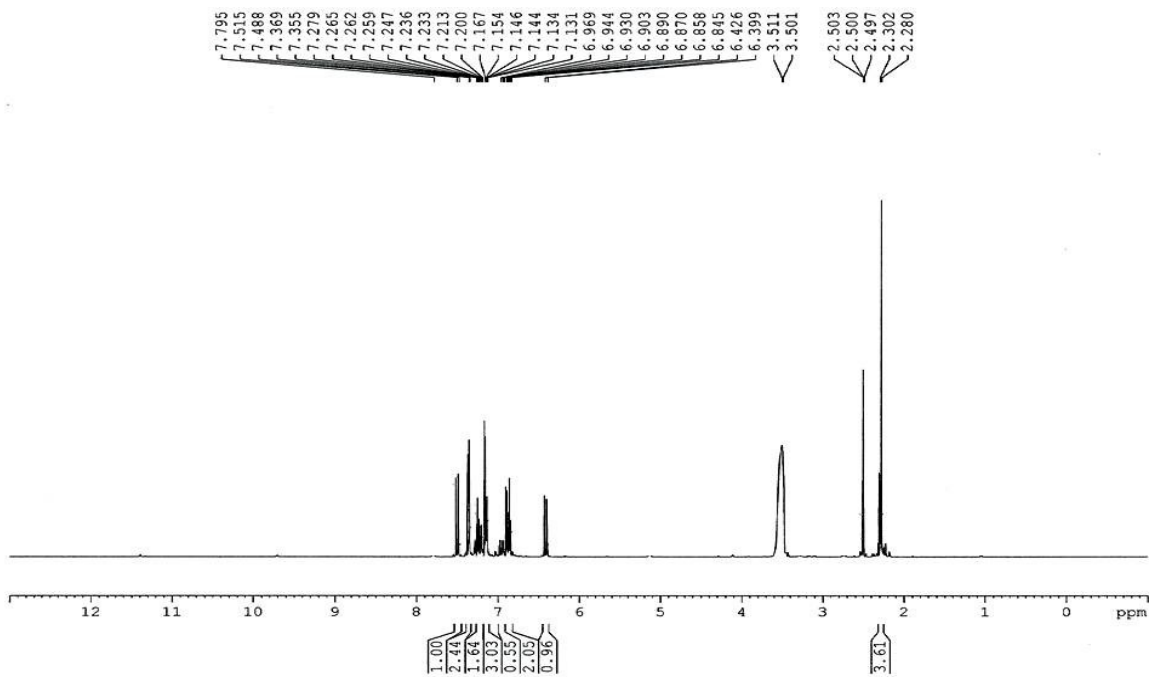


Figure S14. The D<sub>2</sub>O <sup>1</sup>H NMR spectrum of compound 8 (400 MHz, solvent DMSO-*d*<sub>6</sub>)



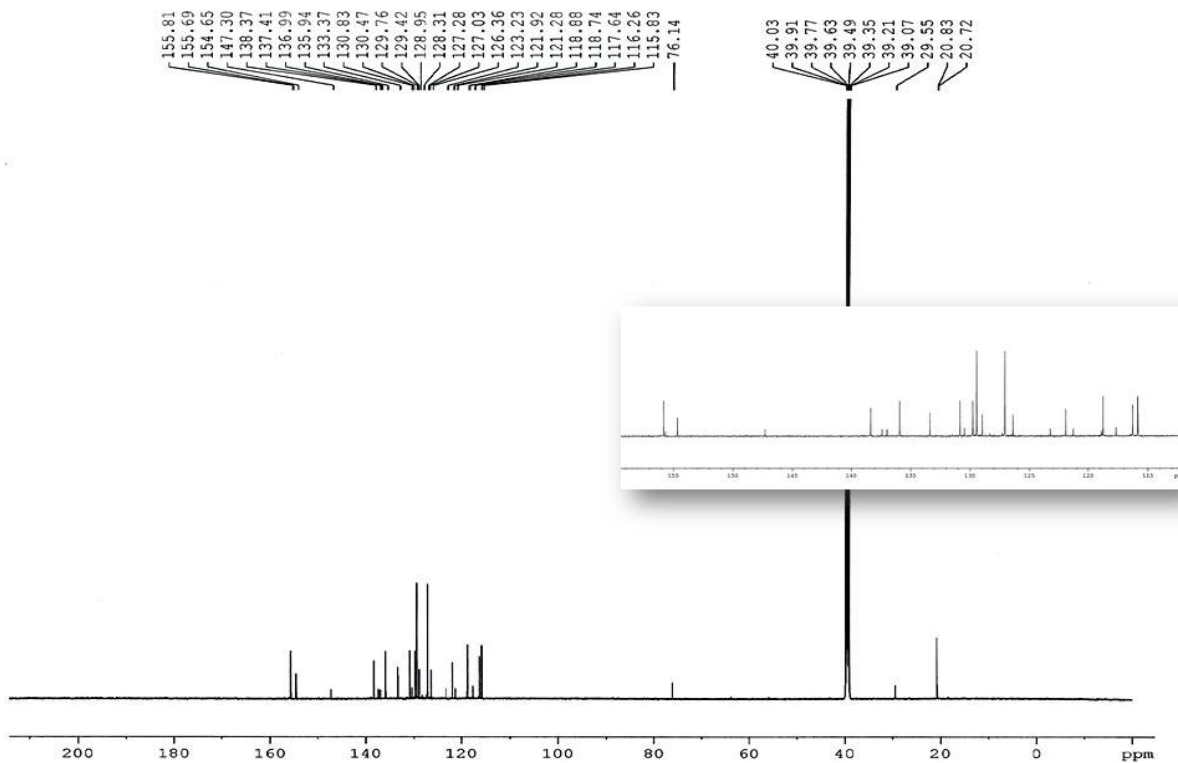


Figure S15. The  $^{13}\text{C}$  NMR spectrum of compound **8** (100 MHz, solvent  $\text{DMSO}-d_6$ )

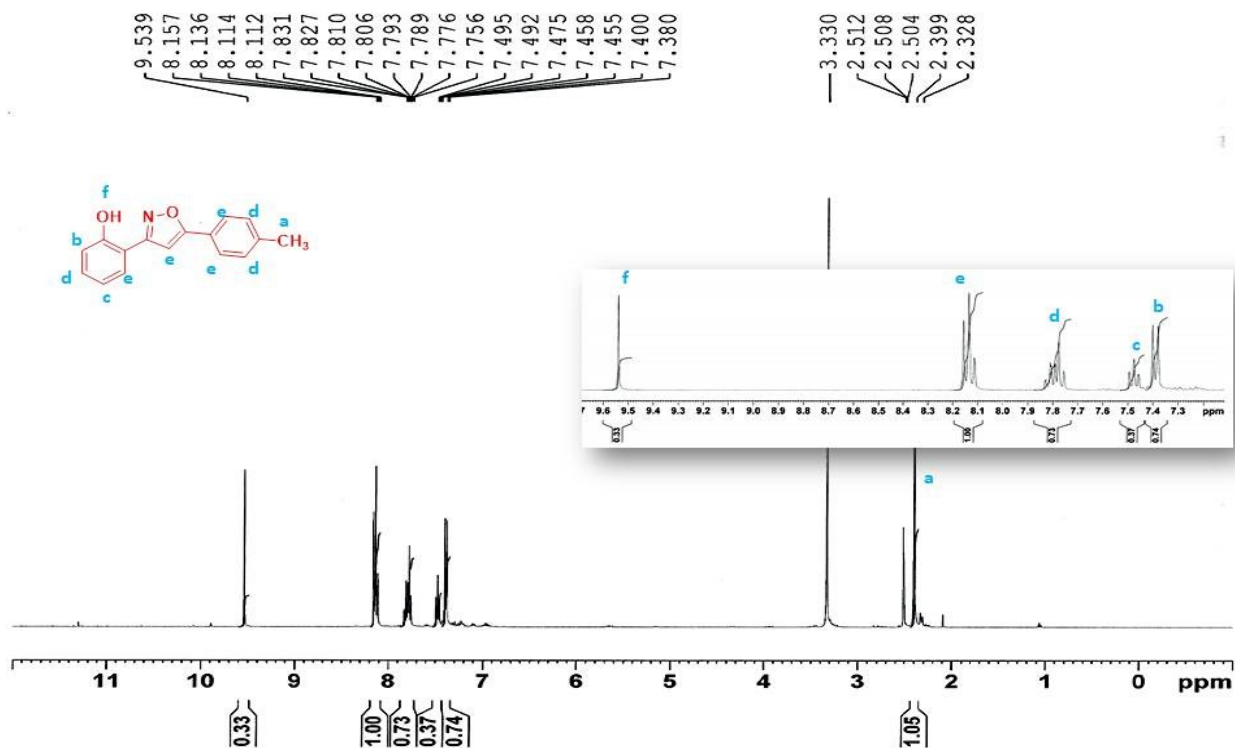
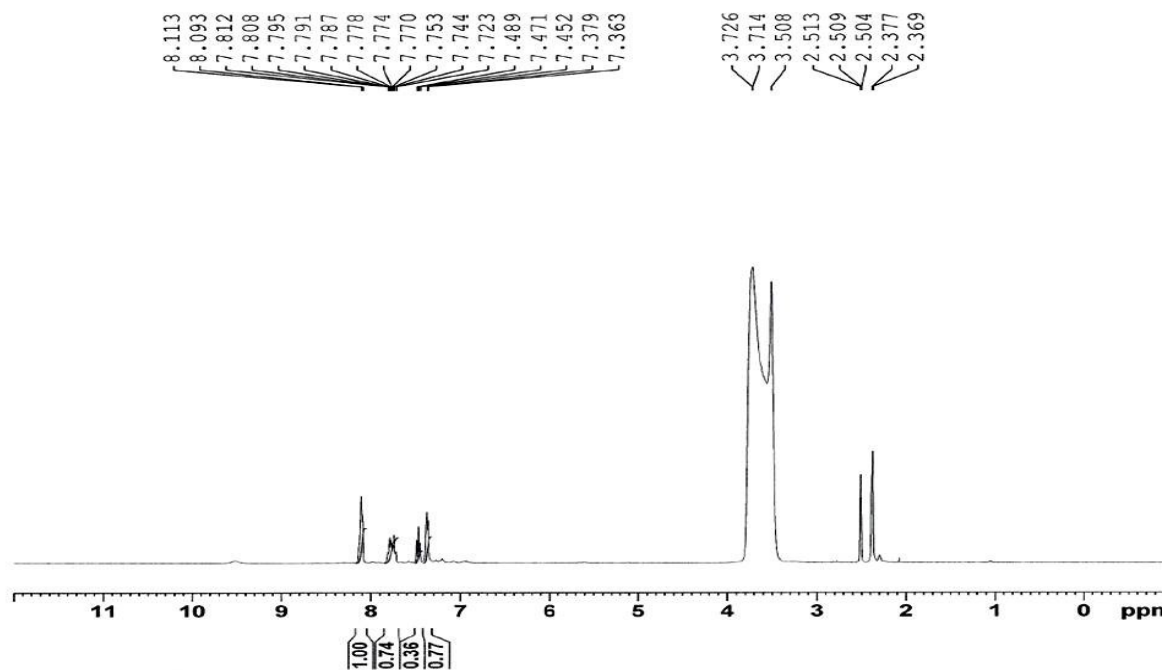
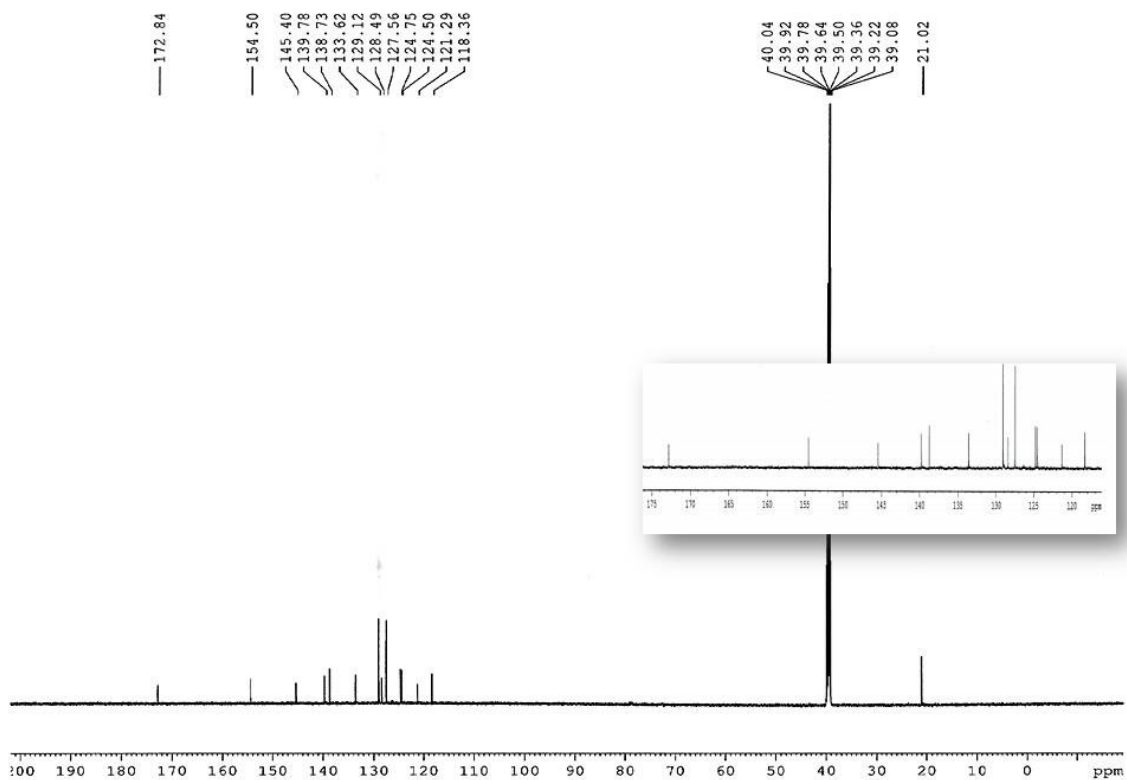


Figure S16. The  $^1\text{H}$  NMR spectrum of compound **9** (400 MHz, solvent  $\text{DMSO}-d_6$ )





**Figure S17.** The  $D_2O$   $^1H$  NMR spectrum of compound **9** (400 MHz, solvent  $DMSO-d_6$ )



**Figure S18.** The  $^{13}C$  NMR spectrum of compound **9** (100 MHz, solvent  $DMSO-d_6$ )

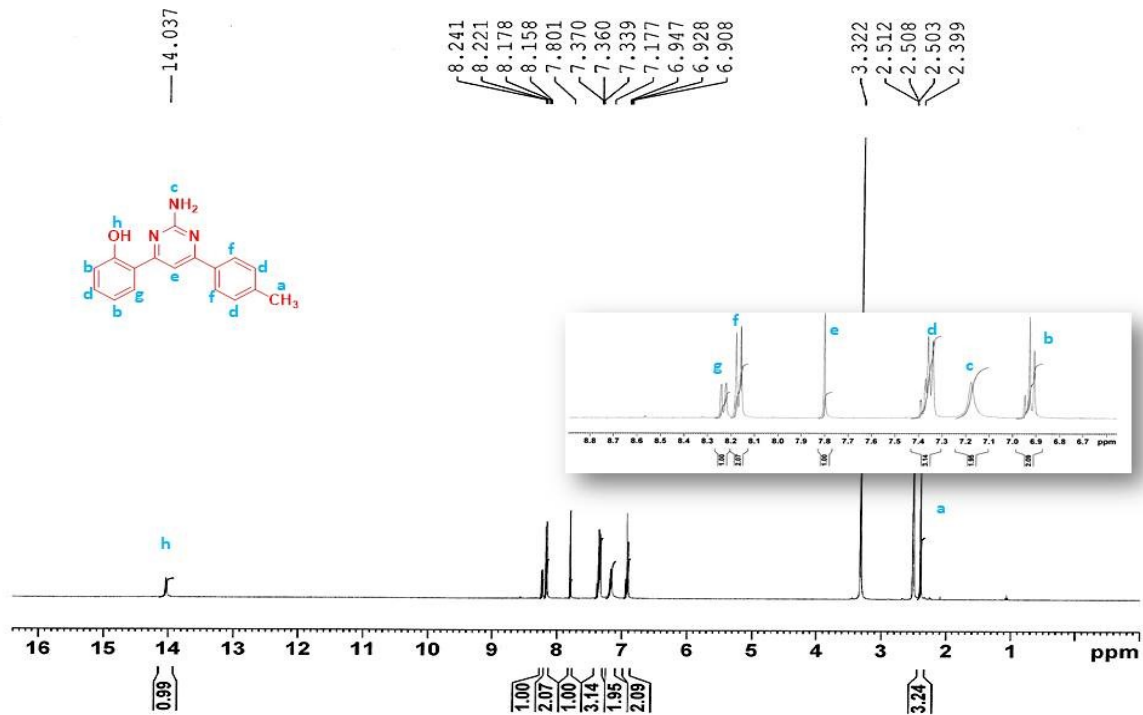


Figure S19. The <sup>1</sup>H NMR spectrum of compound 11 (400 MHz, solvent DMSO-*d*<sub>6</sub>)

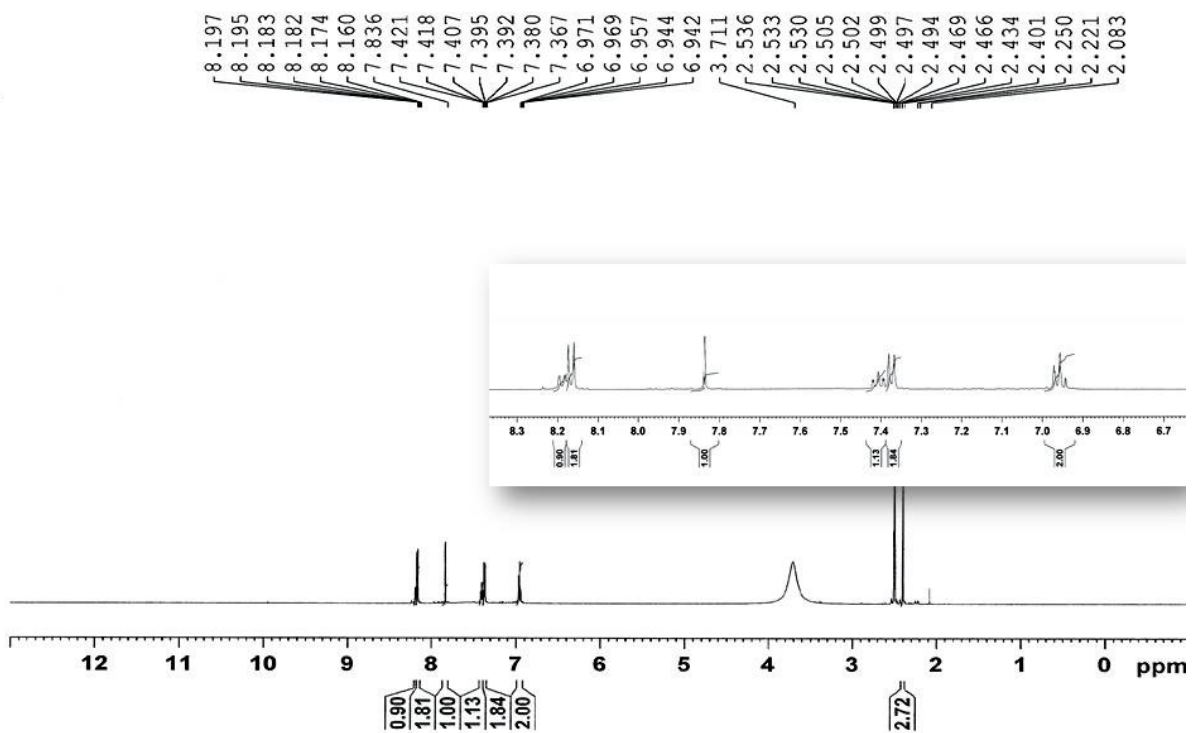


Figure S20. The D<sub>2</sub>O <sup>1</sup>H NMR spectrum of compound 11 (400 MHz, solvent DMSO-*d*<sub>6</sub>)

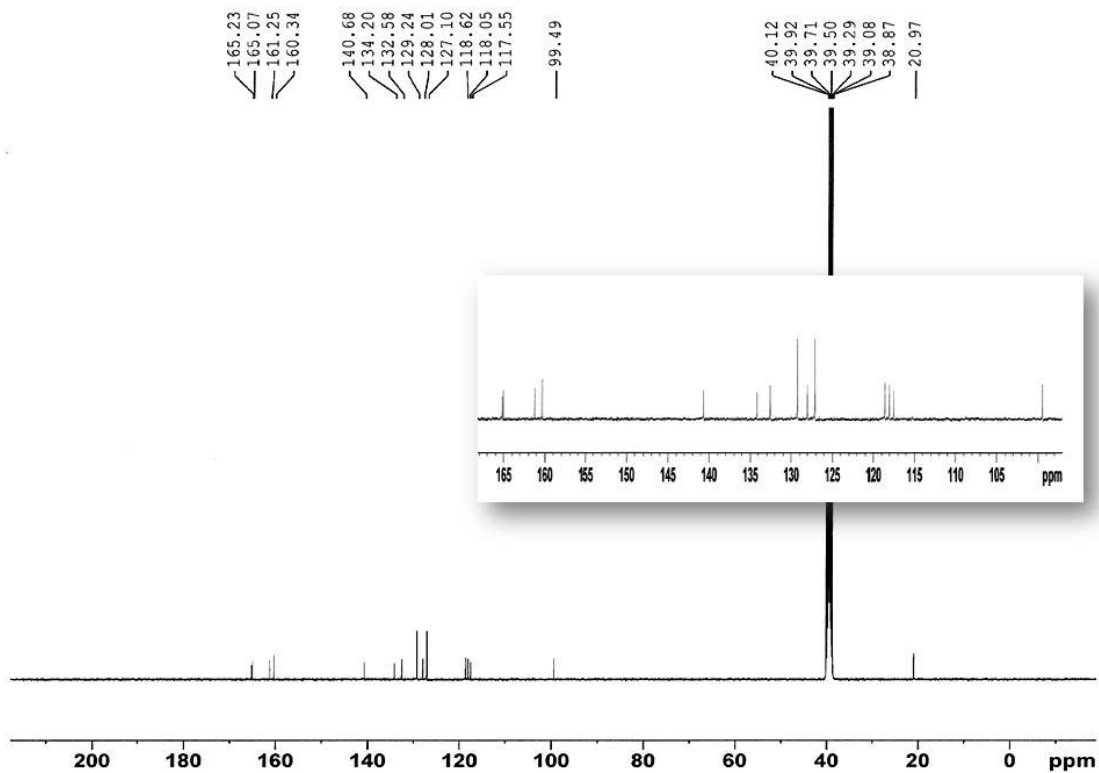


Figure S21. The  $^{13}\text{C}$  NMR spectrum of compound **11** (100 MHz, solvent  $\text{DMSO}-d_6$ )

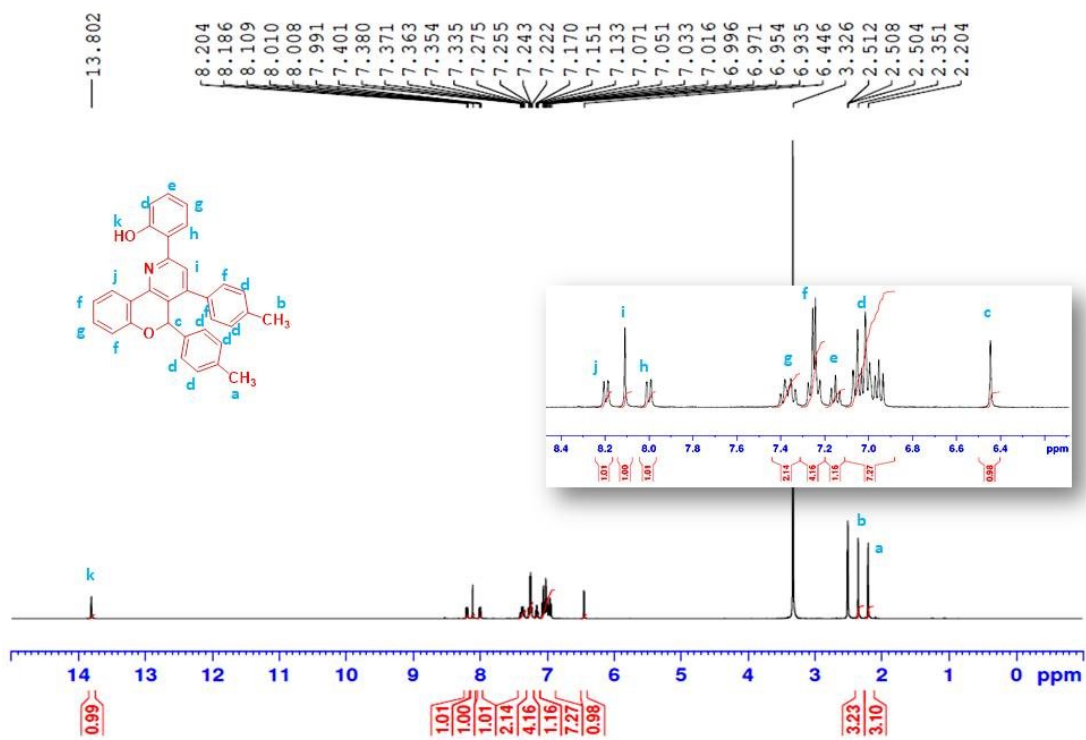


Figure S22. The  $^1\text{H}$  NMR spectrum of compound **13** (400 MHz, solvent  $\text{DMSO}-d_6$ )

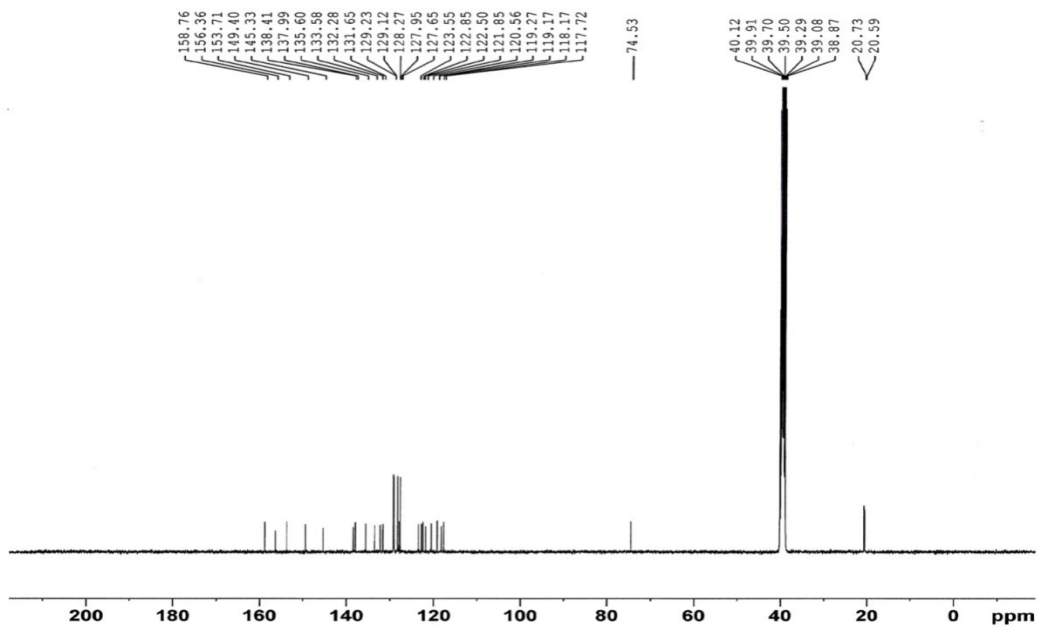


Figure S23. The  $^{13}\text{C}$  NMR spectrum of compound **13** (100 MHz, solvent  $\text{DMSO-}d_6$ )

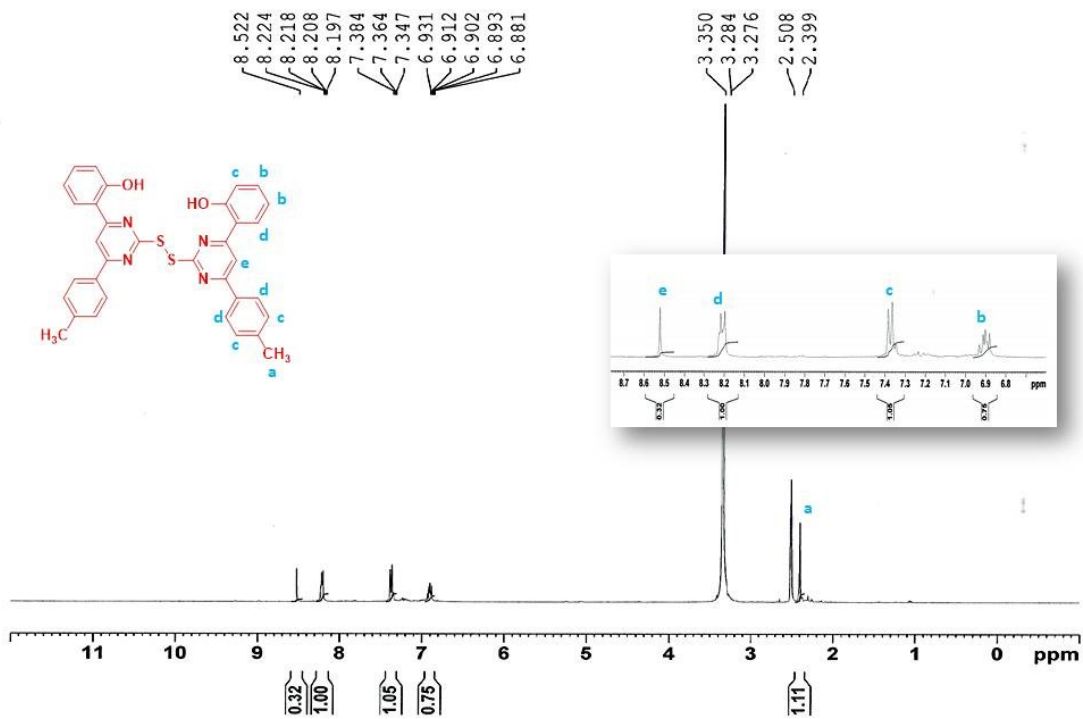


Figure S24. The  $^1\text{H}$  NMR spectrum of compound **15** (400 MHz, solvent  $\text{DMSO-}d_6$ )

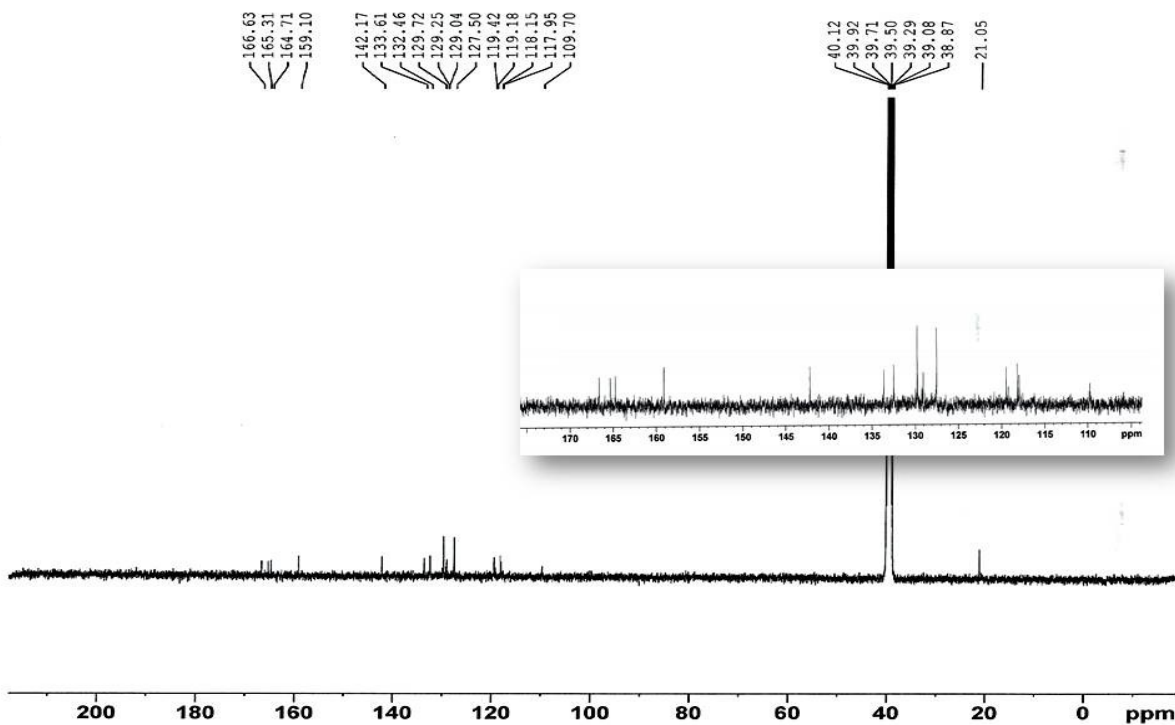


Figure S25. The  $^{13}\text{C}$  NMR spectrum of compound **15** (100 MHz, solvent  $\text{DMSO-}d_6$ )

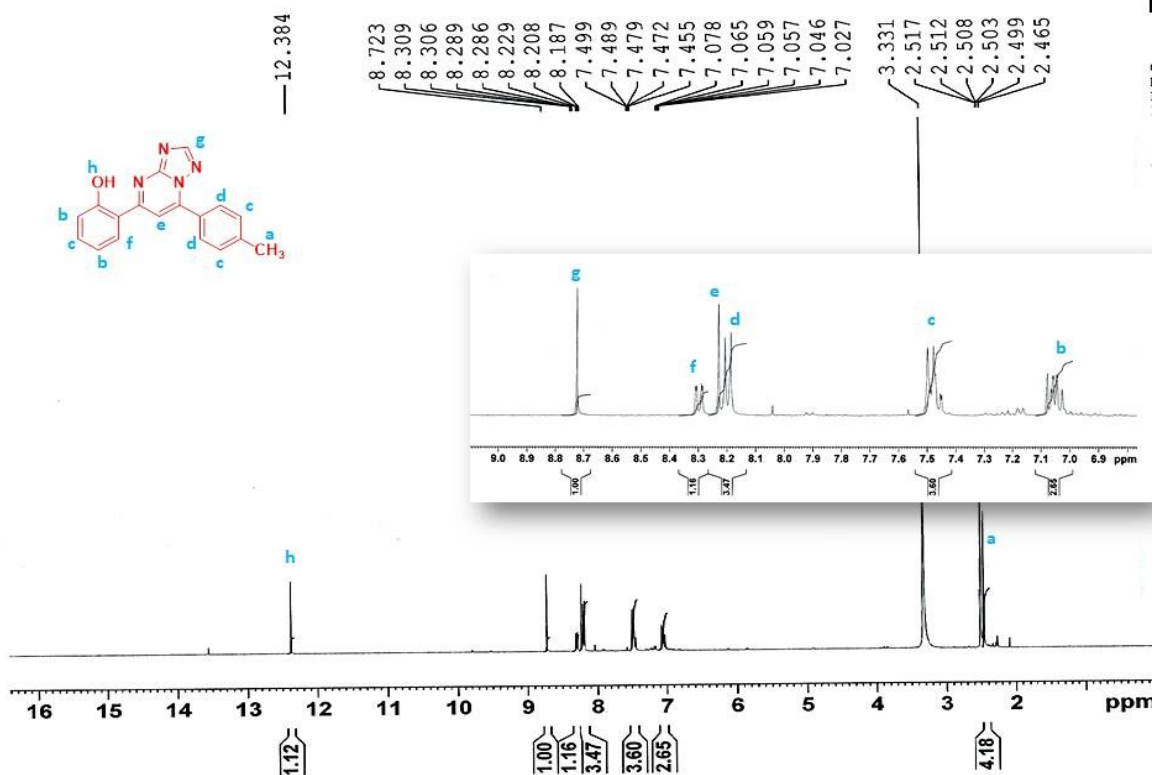


Figure S26. The  $^1\text{H}$  NMR spectrum of compound **17** (400 MHz, solvent  $\text{DMSO-}d_6$ )

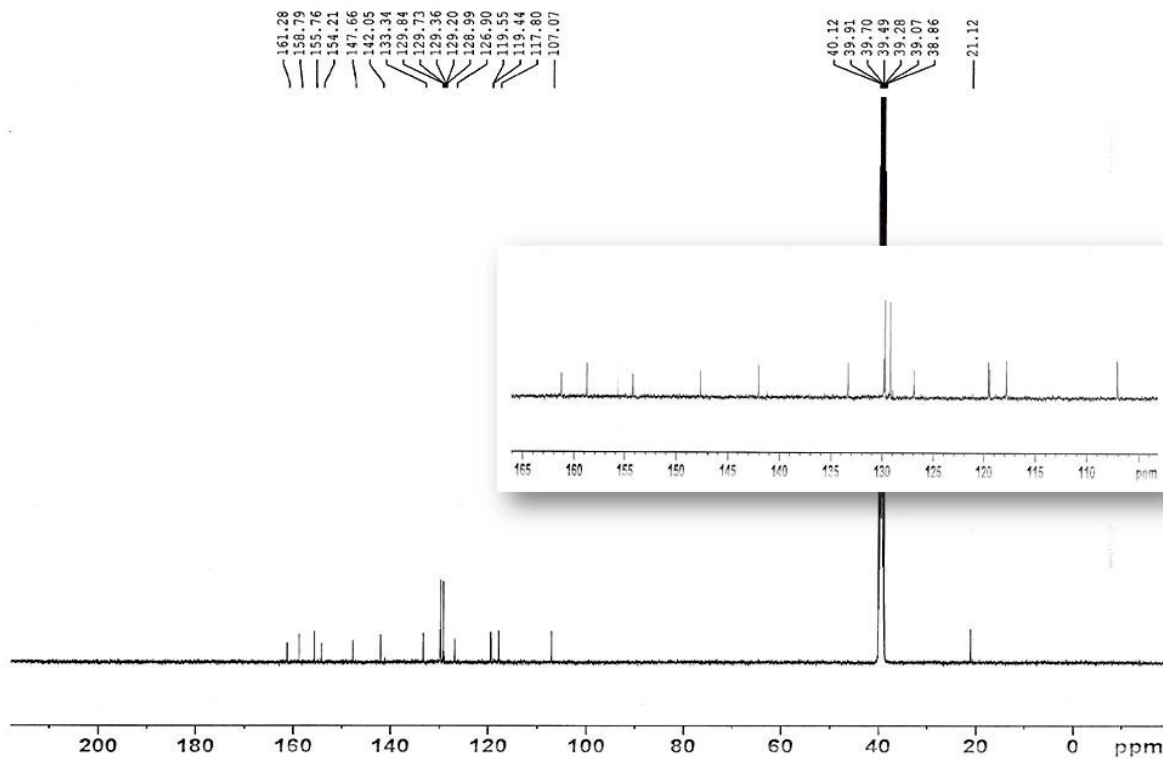


Figure S27. The  $^{13}\text{C}$  NMR spectrum of compound **17** (100 MHz, solvent  $\text{DMSO-}d_6$ )

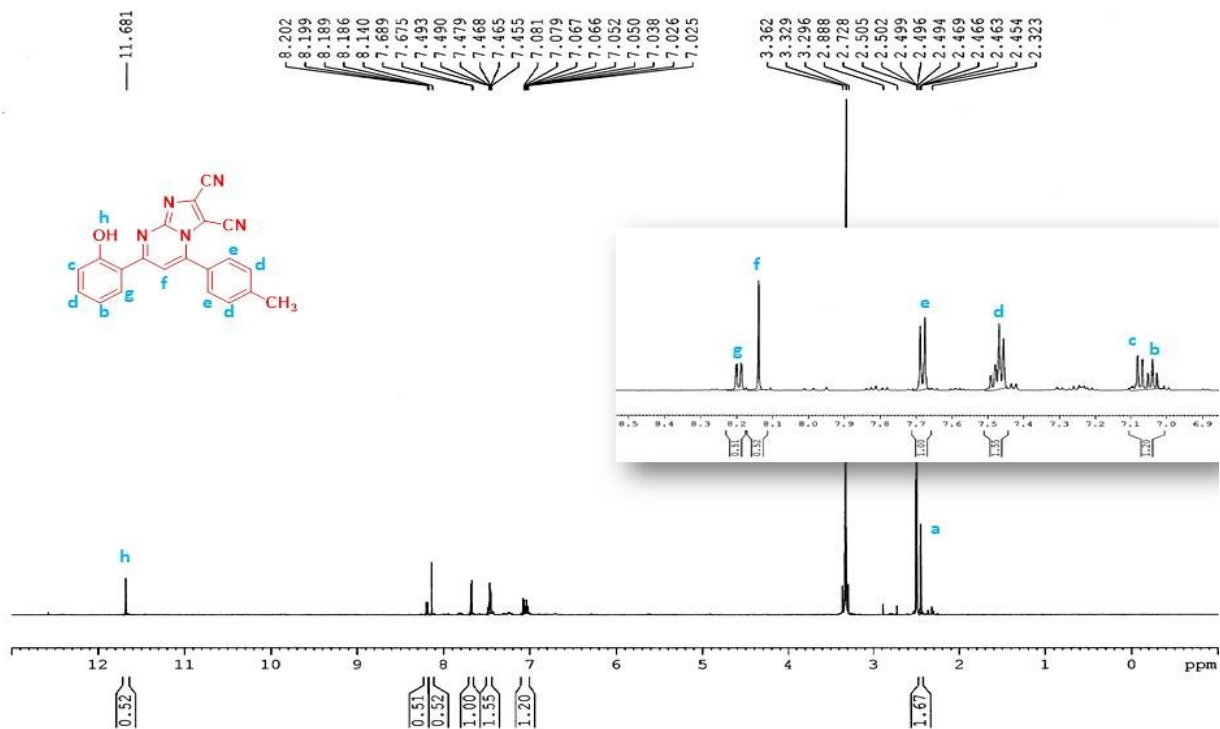


Figure S28. The  $^1\text{H}$  NMR spectrum of compound **19** (400 MHz, solvent  $\text{DMSO-}d_6$ )

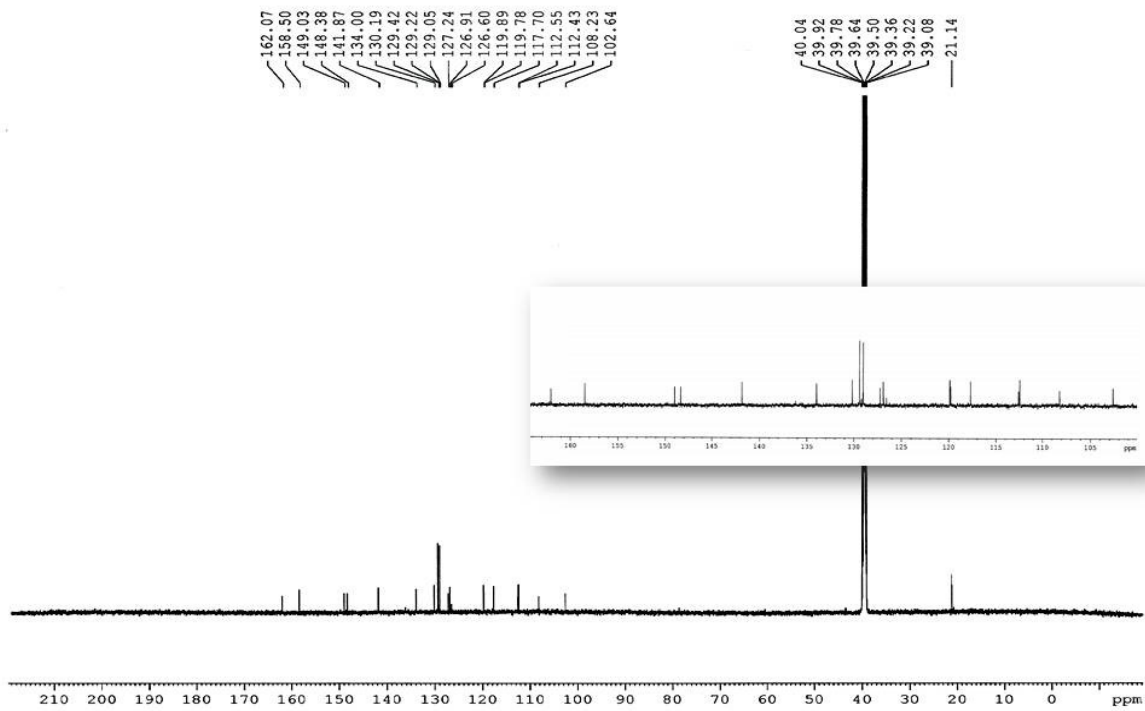


Figure S29. The  $^{13}\text{C}$  NMR spectrum of compound **19** (100 MHz, solvent  $\text{DMSO}-d_6$ )

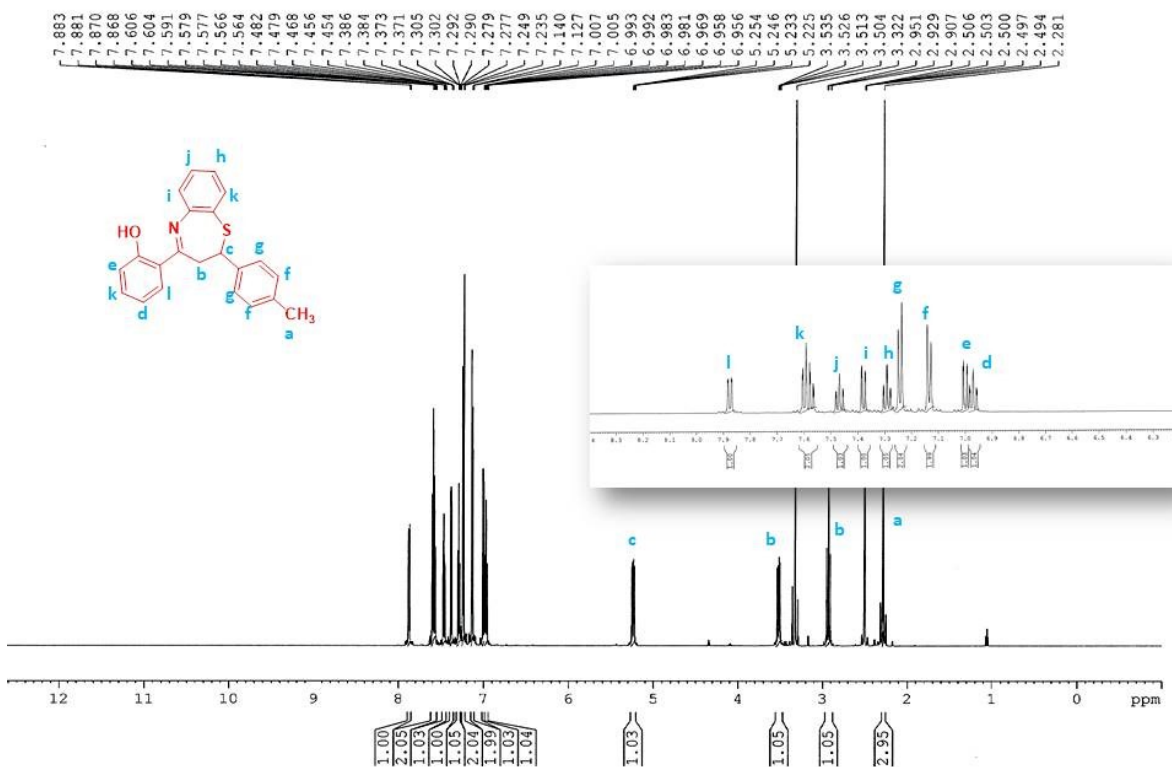
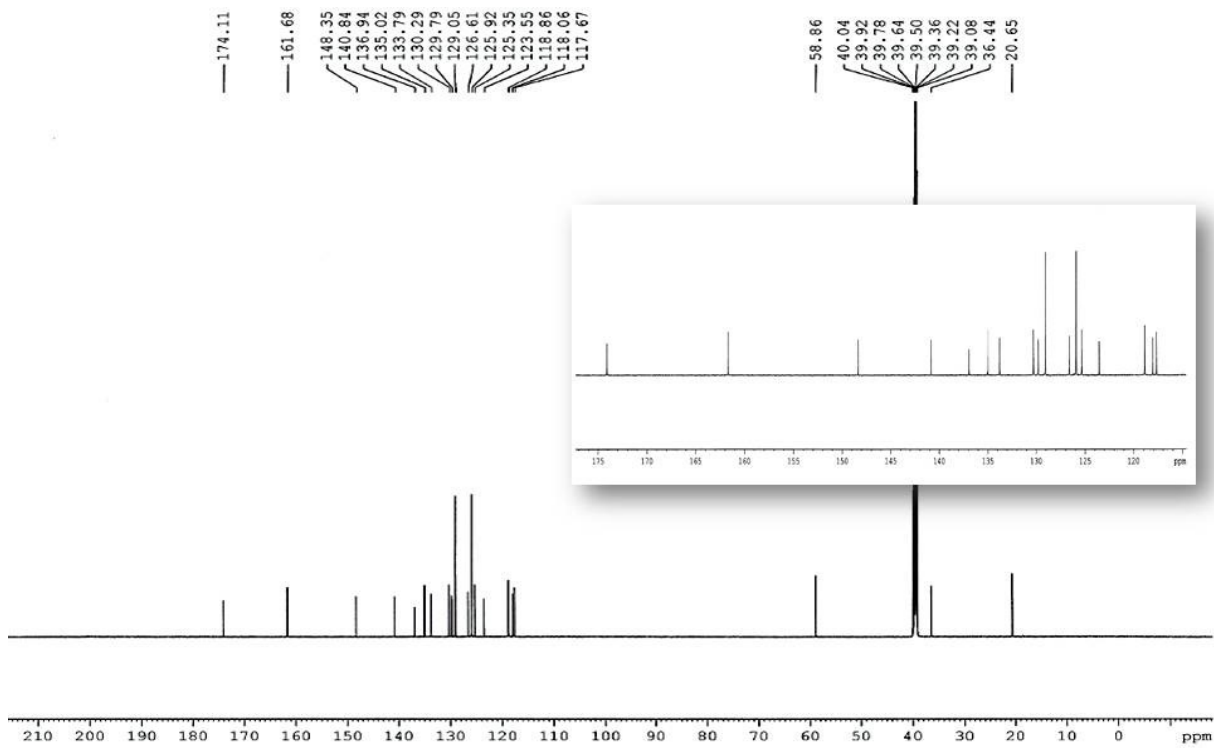
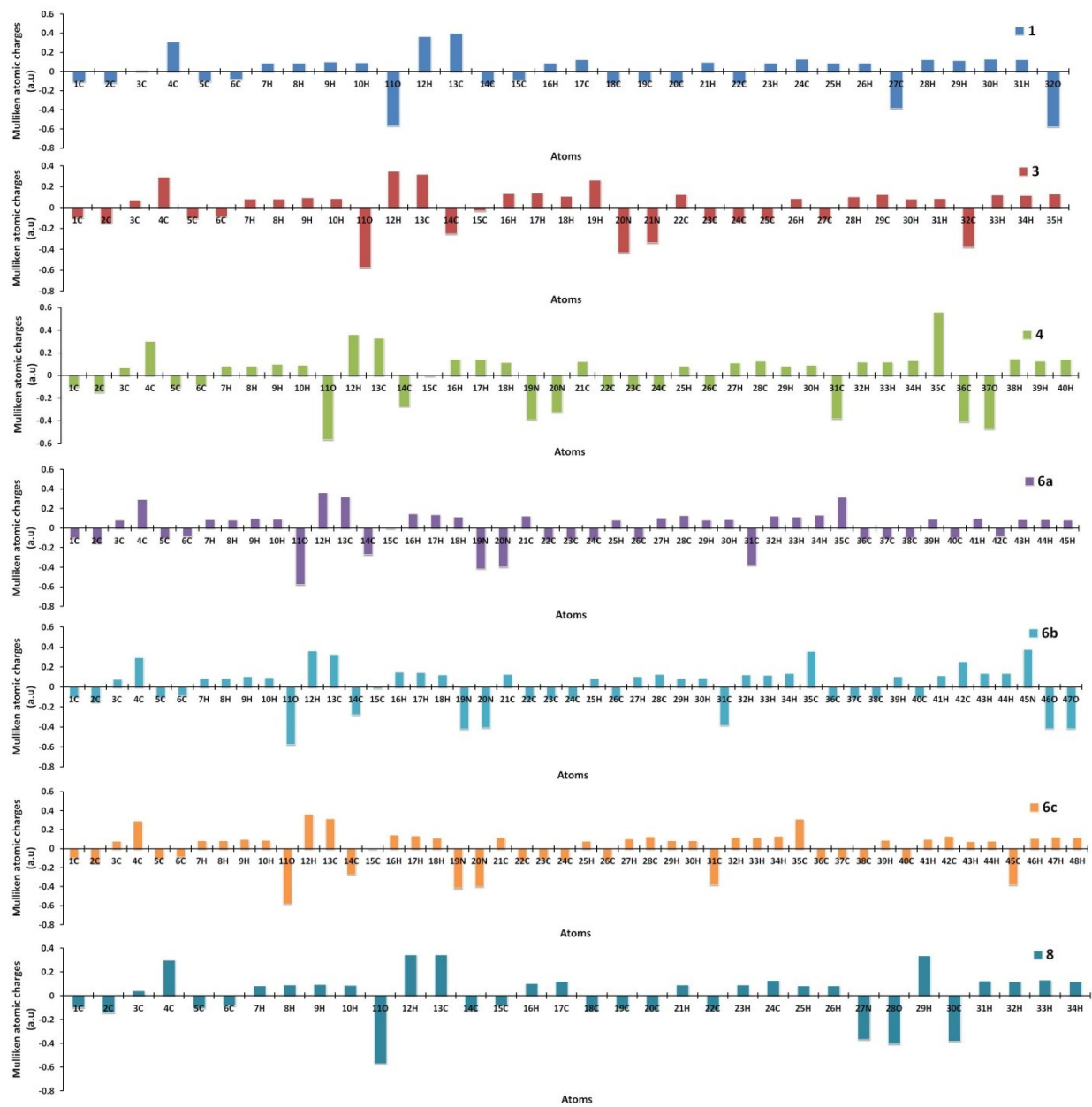


Figure S30. The  $^1\text{H}$  NMR spectrum of compound **21** (400 MHz, solvent  $\text{DMSO}-d_6$ )

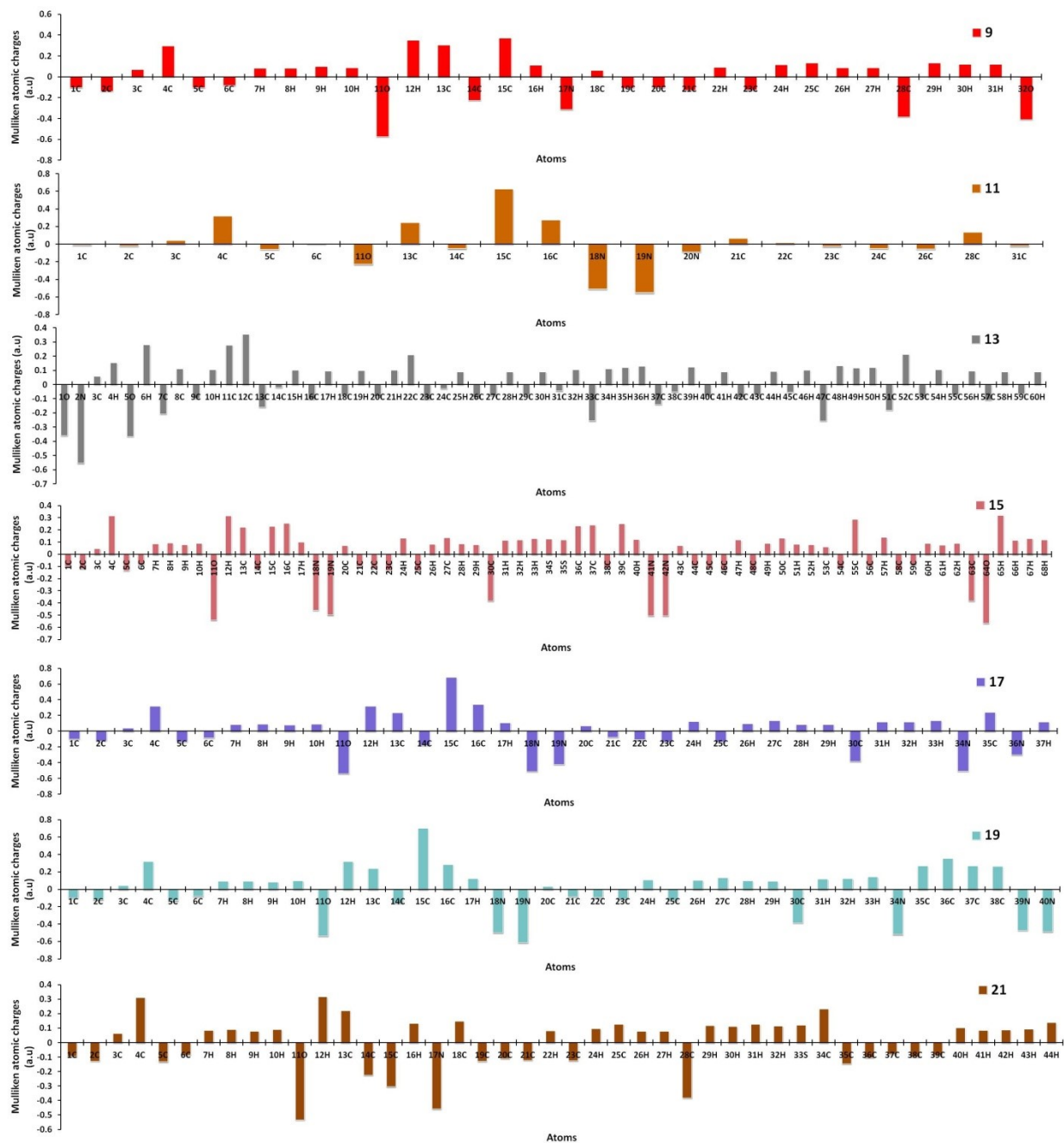




**Figure S31.** The  $^{13}\text{C}$  NMR spectrum of compound **21** (100 MHz, solvent  $\text{DMSO-}d_6$ )



**Figure S32.** Distribution of calculated Mulliken charges for compounds **1**, **3**, **4**, **6a**, **6b**, **6c** and **8**.



**Figure S33.** Distribution of calculated Mulliken charges for compounds 9, 11, 13, 15, 17, 19 and 21.