

Supplementary information

Structure, tautomerism, and radical scavenging activity of Schiff bases and hydrazones of gossypol

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NMR spectra

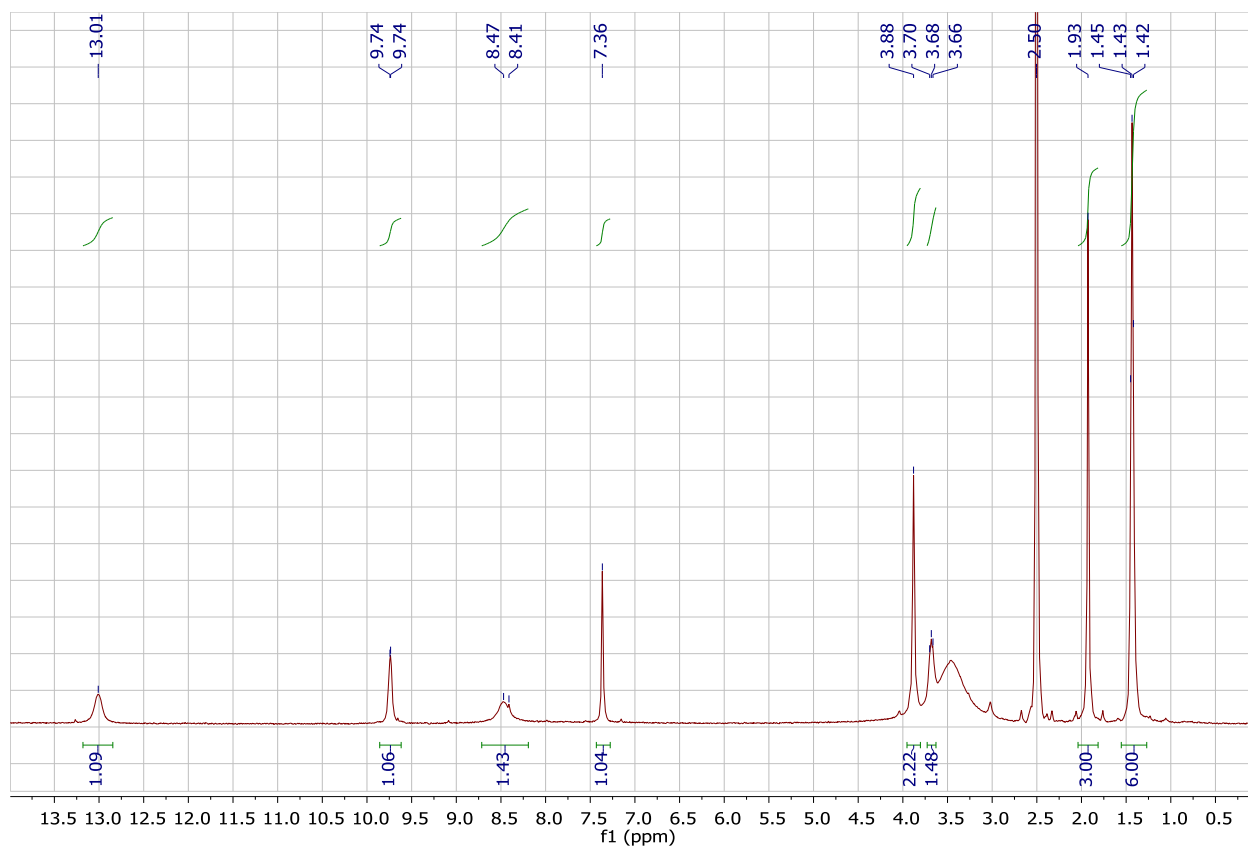


Fig. S1. ¹H NMR spectrum of compound **1** in DMSO-d₆.

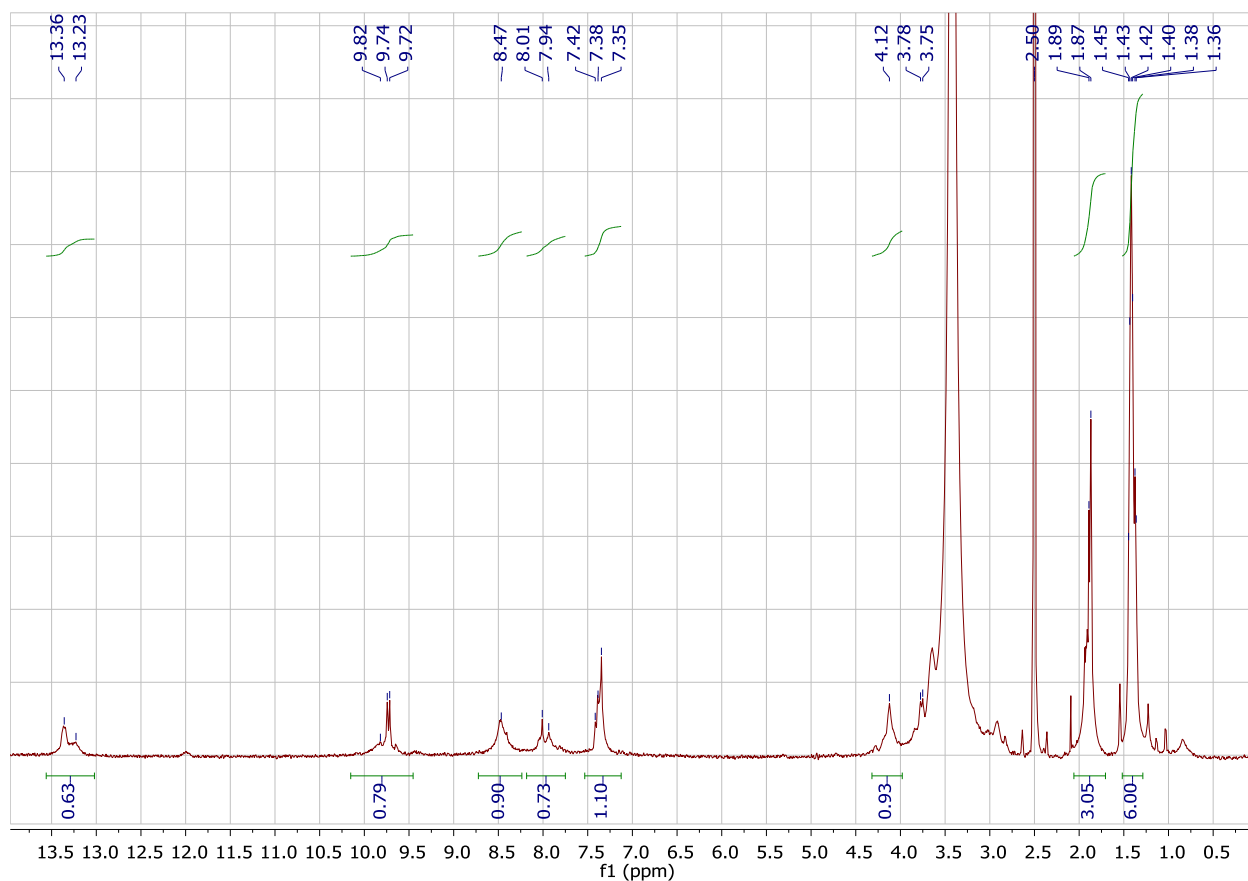
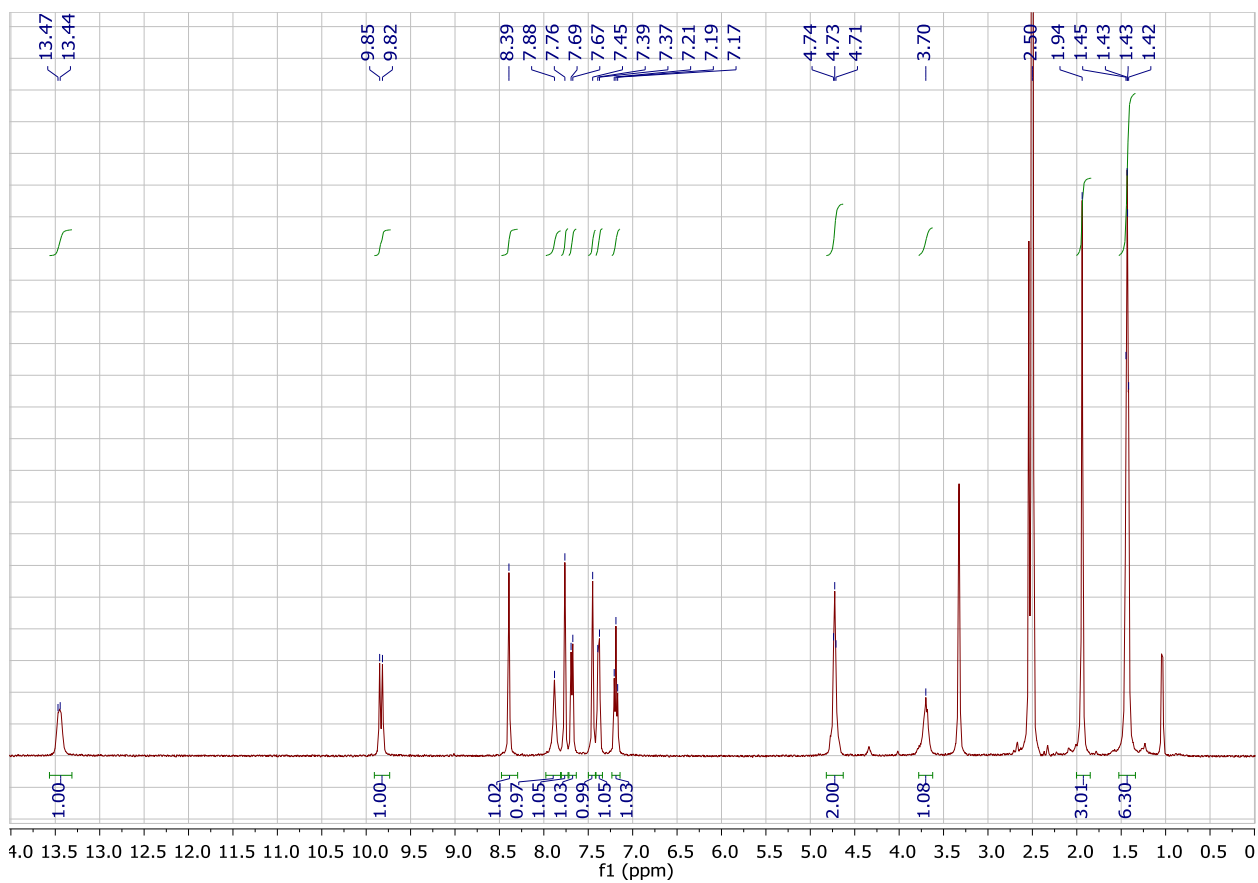
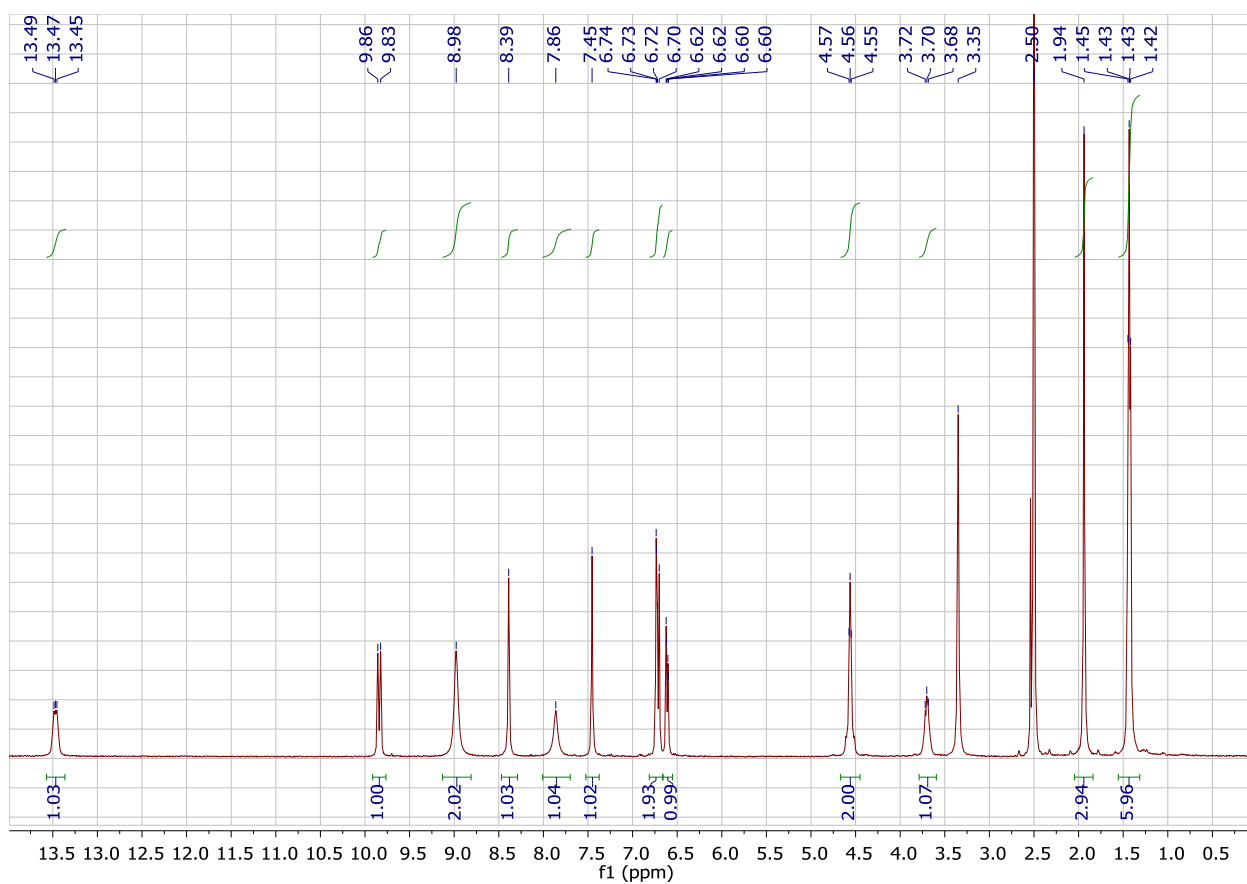


Fig. S2. ¹H NMR spectrum of compound **2** in DMSO-d₆.



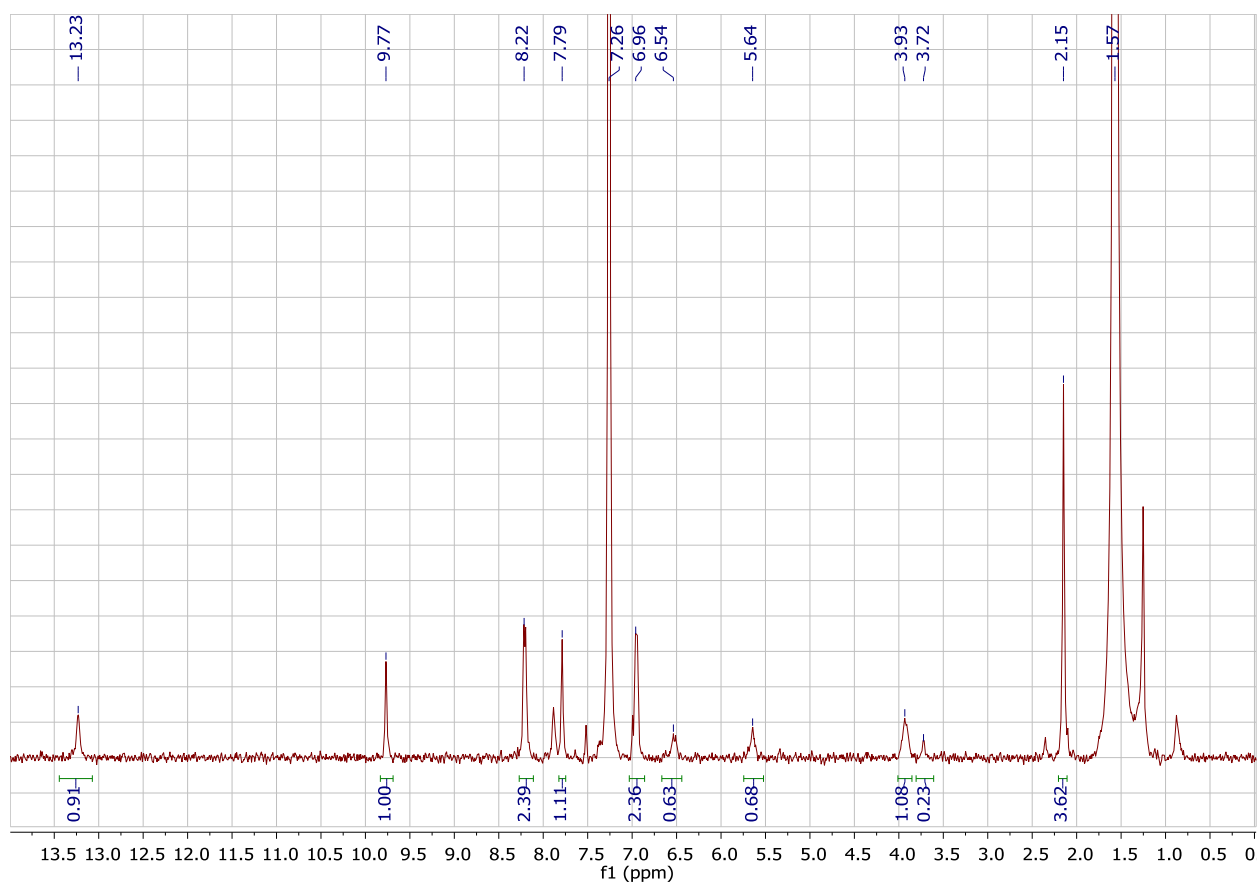


Fig. S5. ¹H NMR spectrum of compound **5** in CDCl₃.

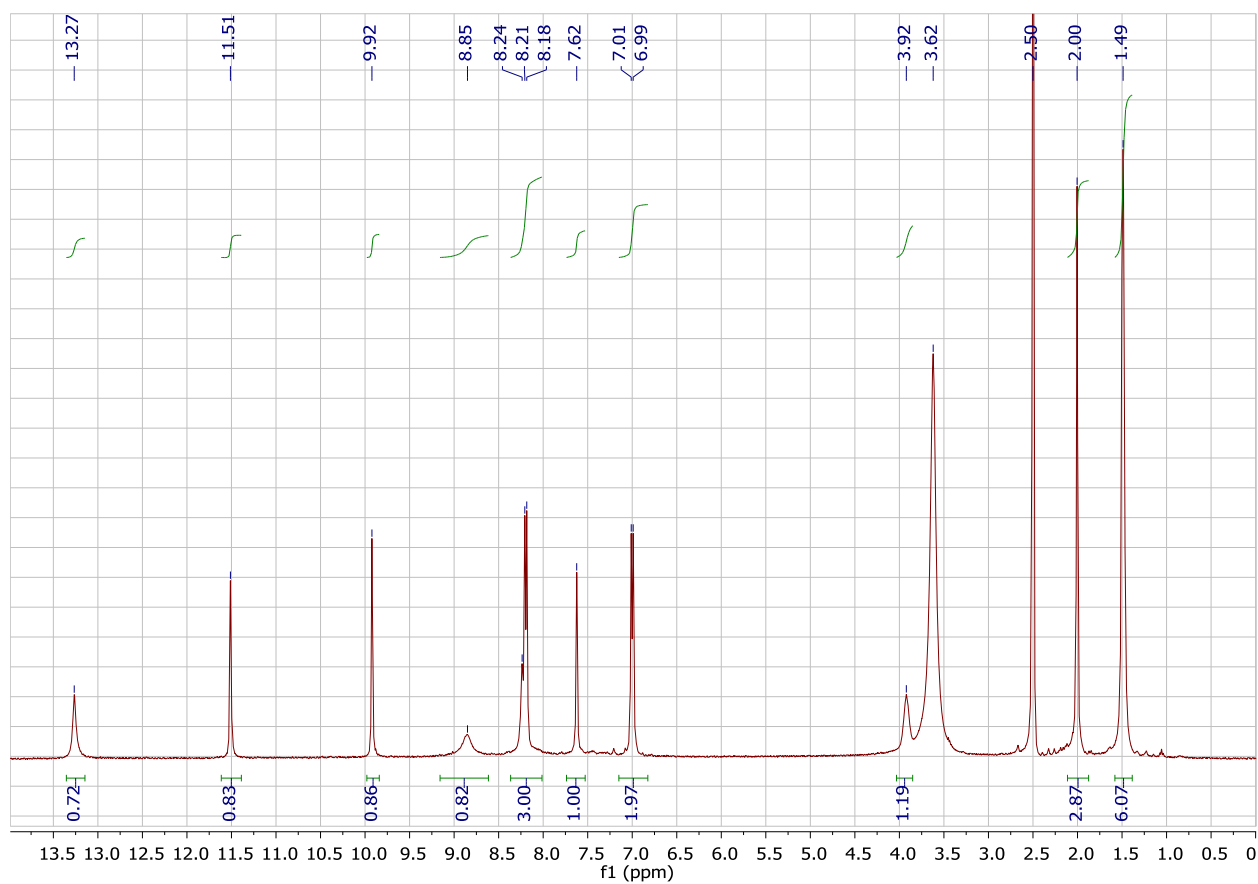


Fig. S6. ¹H NMR spectrum of compound **5** in DMSO-d₆.

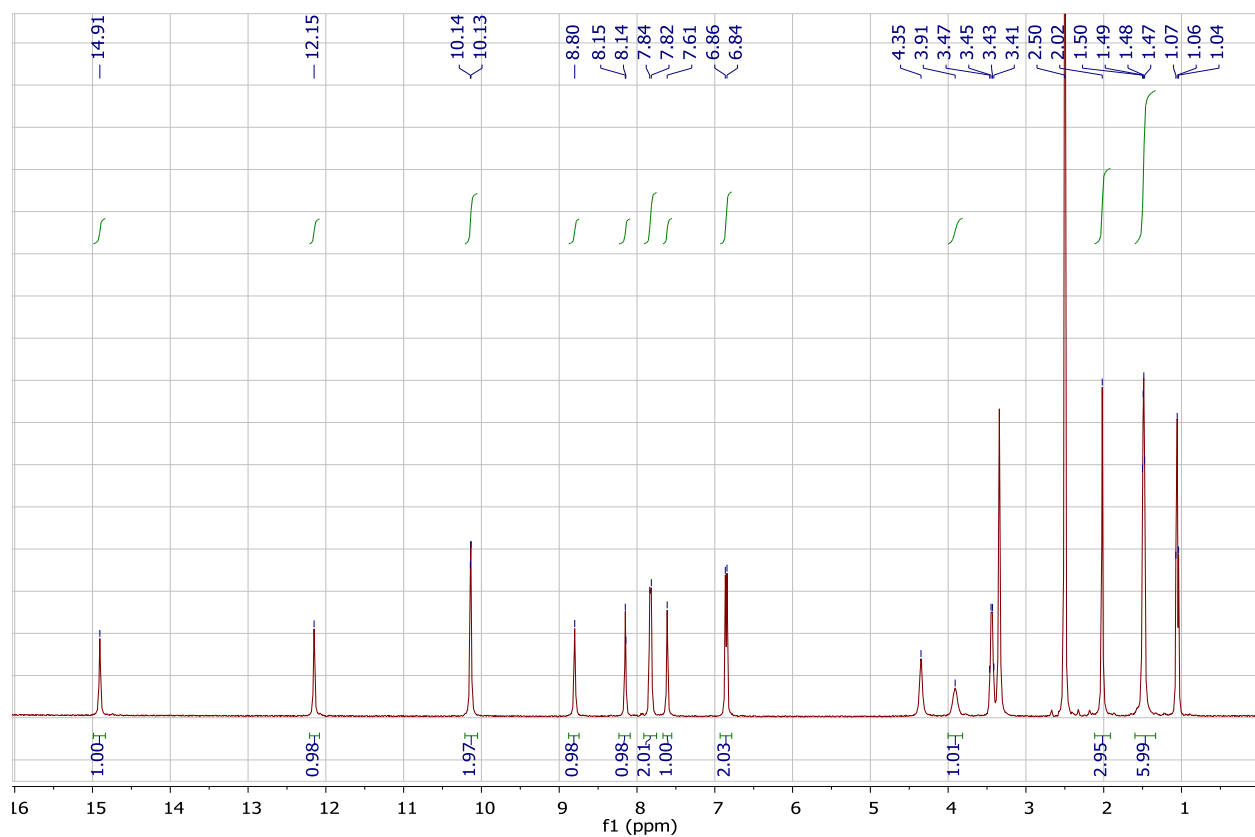


Fig. S7. ^1H NMR spectrum of compound **6** in DMSO- d_6 . (The chemical shifts at $\delta=1.06$ ppm, $\delta=3.45$ ppm, and $\delta=4.35$ ppm are assigned to residual signals of ethanol. The compound was subjected to additional drying before further studies).

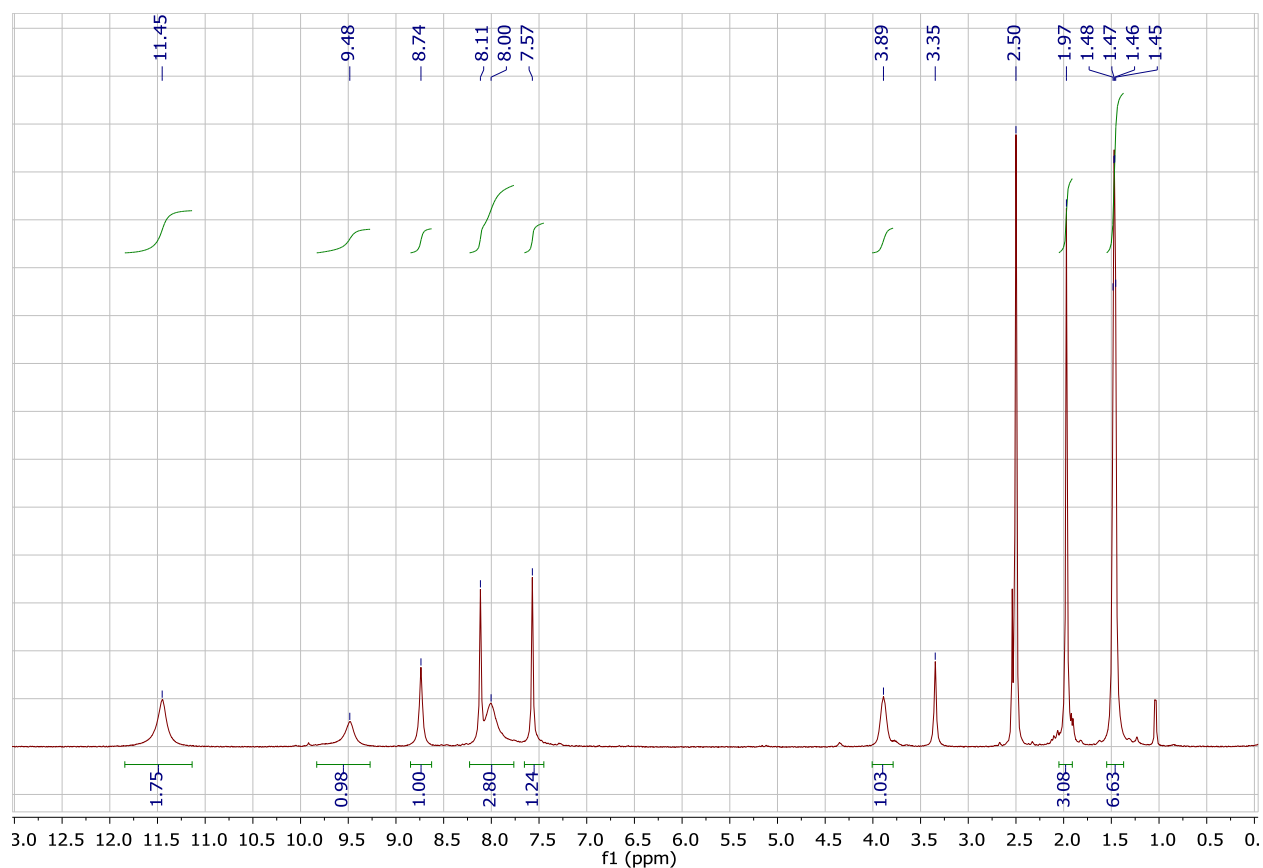


Fig. S8. ^1H NMR spectrum of compound **7** in DMSO- d_6 .

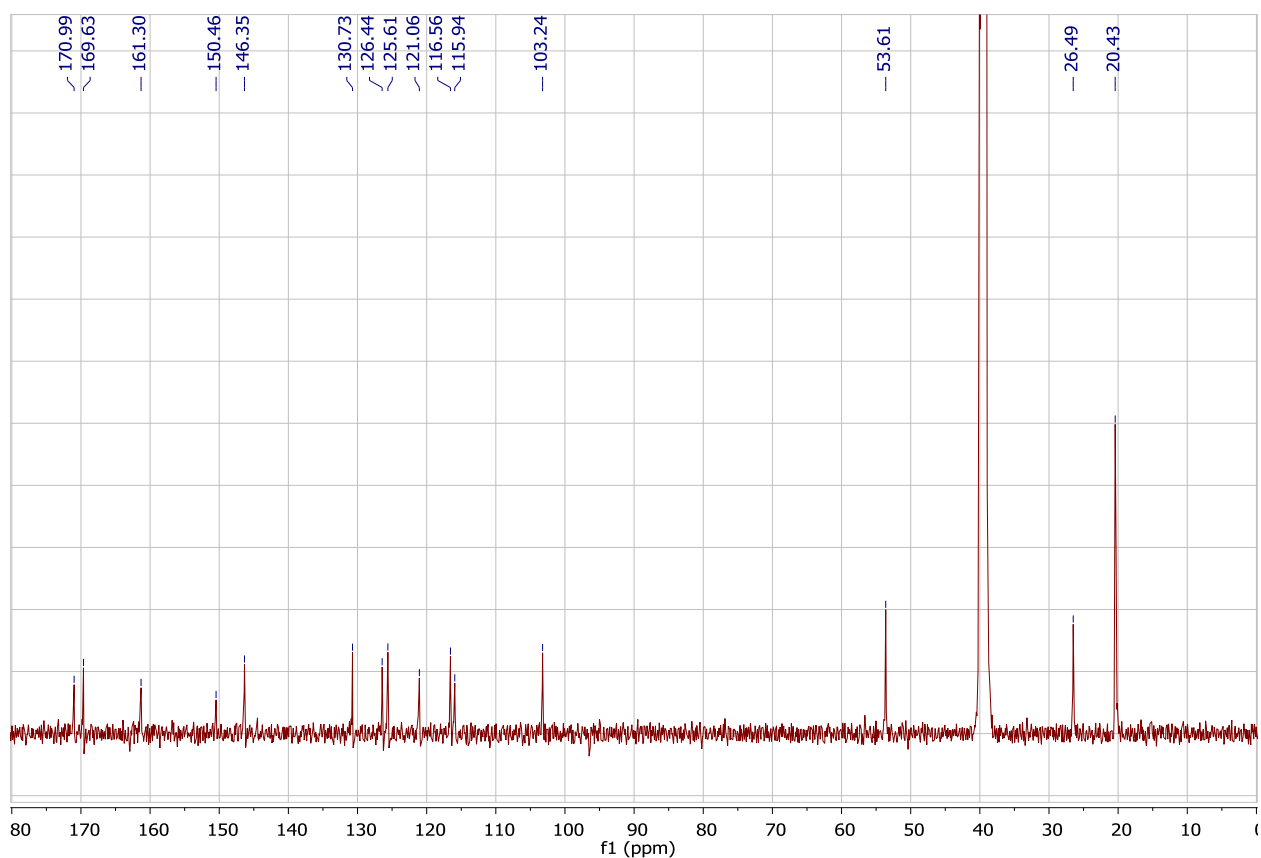


Fig. S9. ¹³C NMR spectrum of compound **1** in DMSO-d₆.

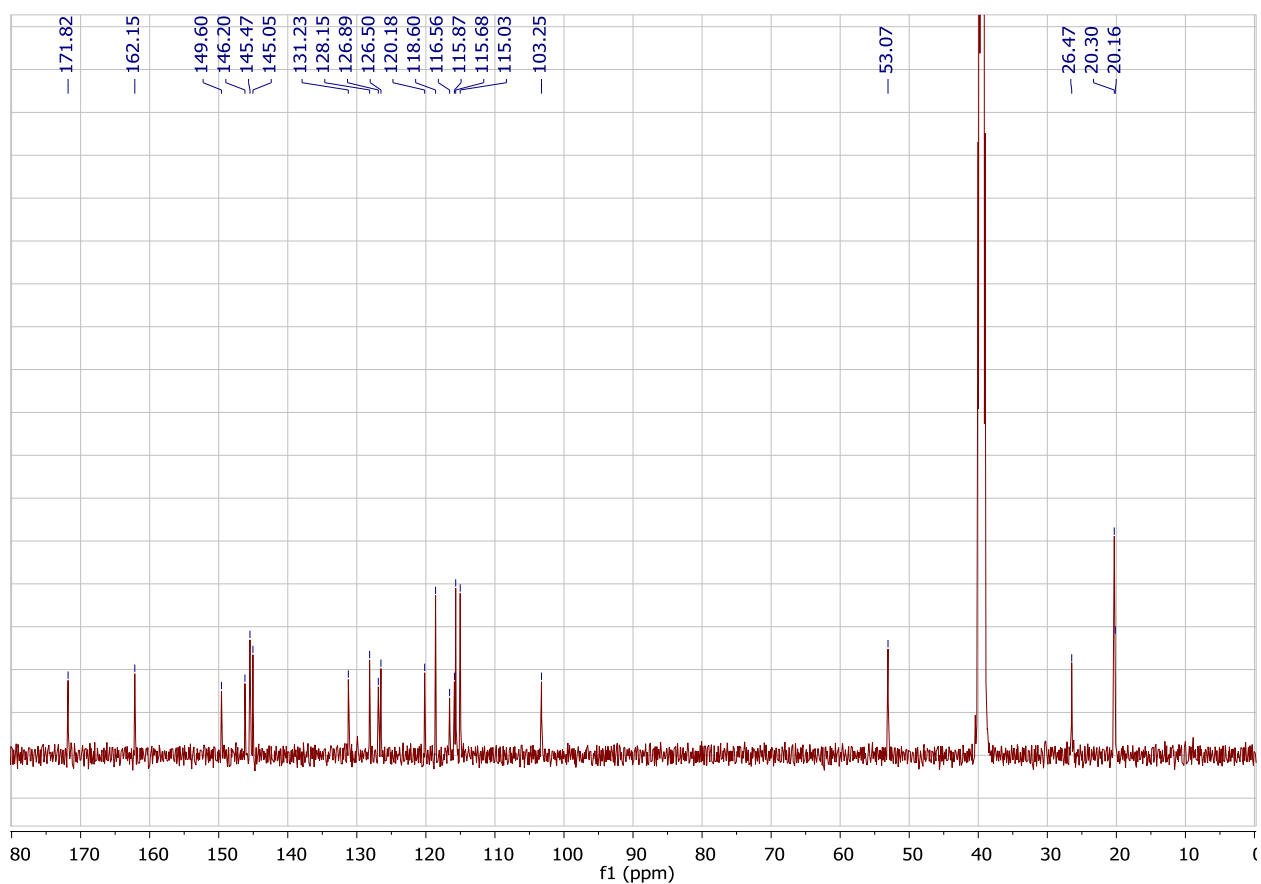


Fig. S10. ¹³C NMR spectrum of compound **3** in DMSO-d₆.

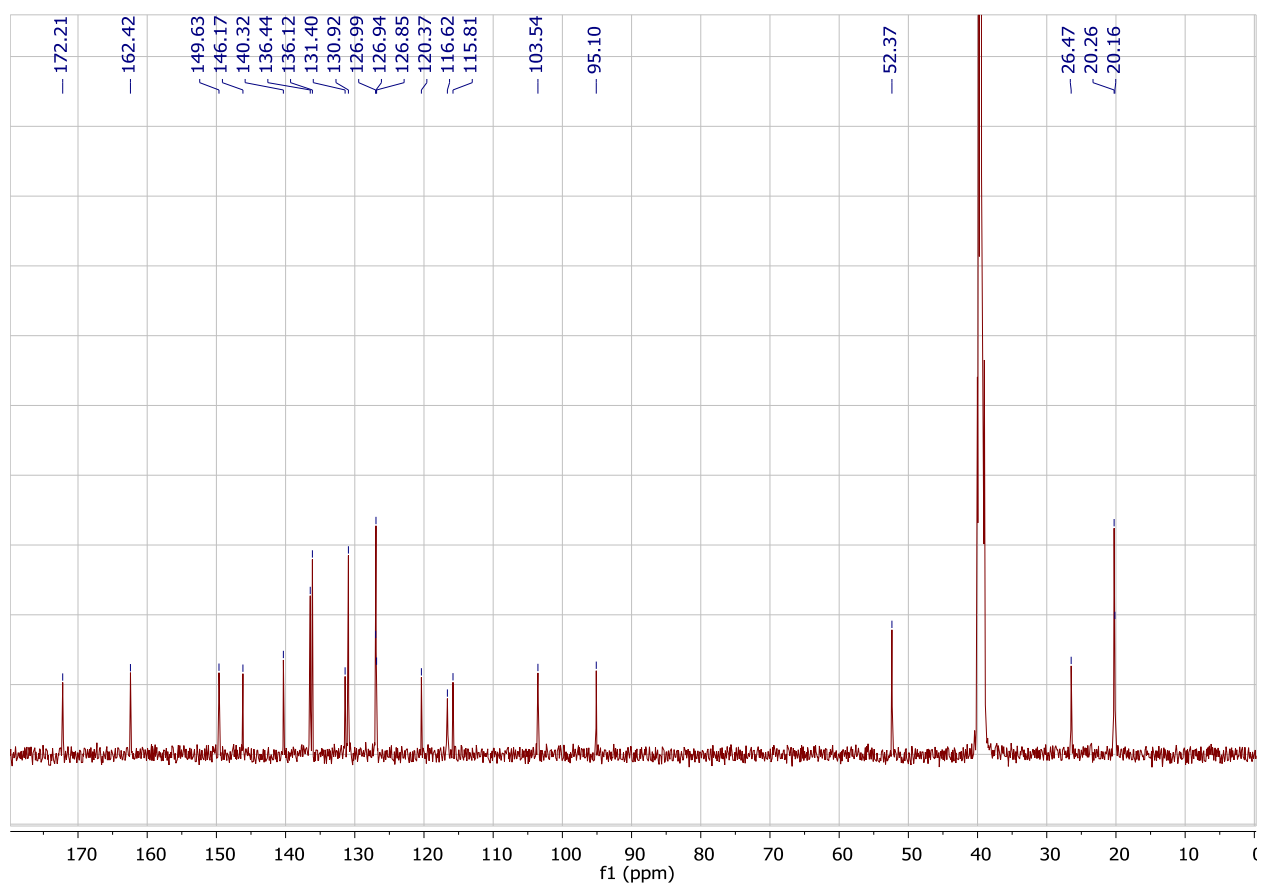


Fig. S11. ¹³C NMR spectrum of compound **4** in DMSO-d₆.

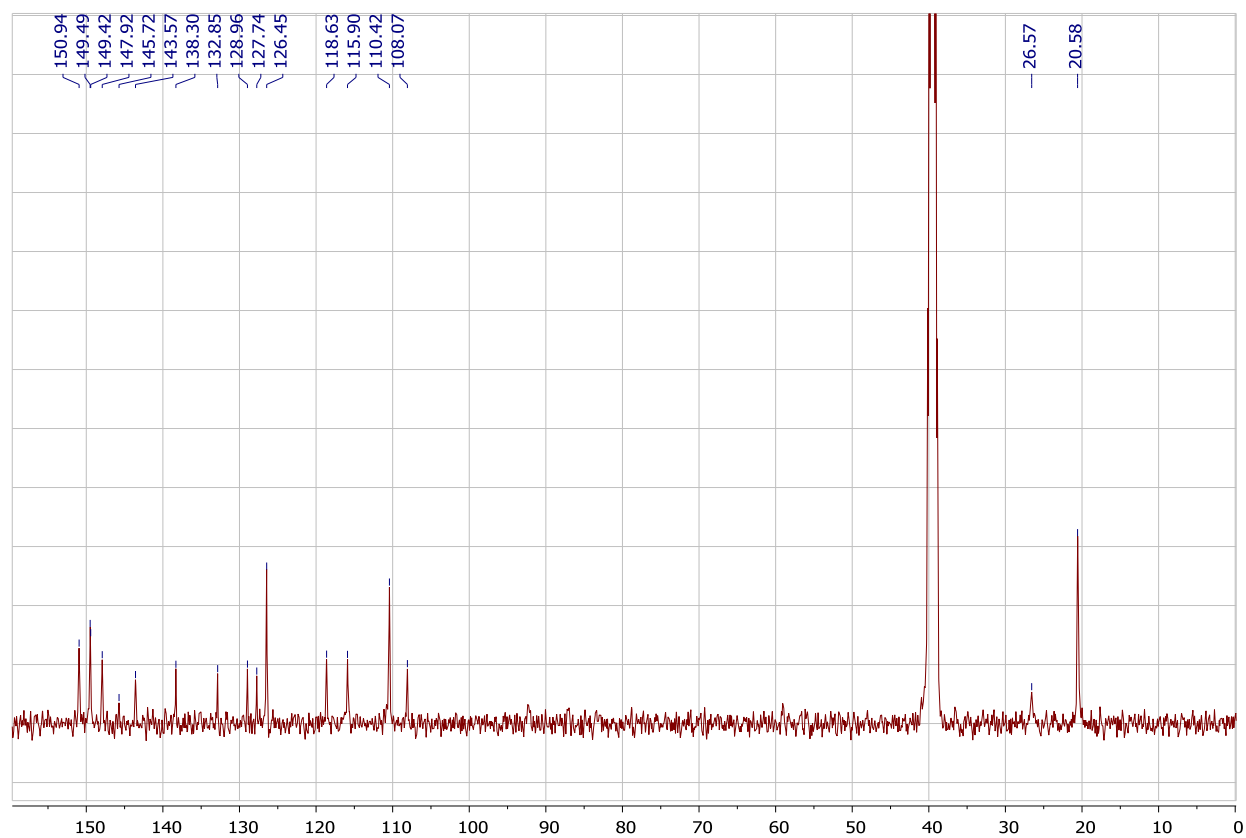


Fig. S12. ¹³C NMR spectrum of compound **5** in DMSO-d₆.

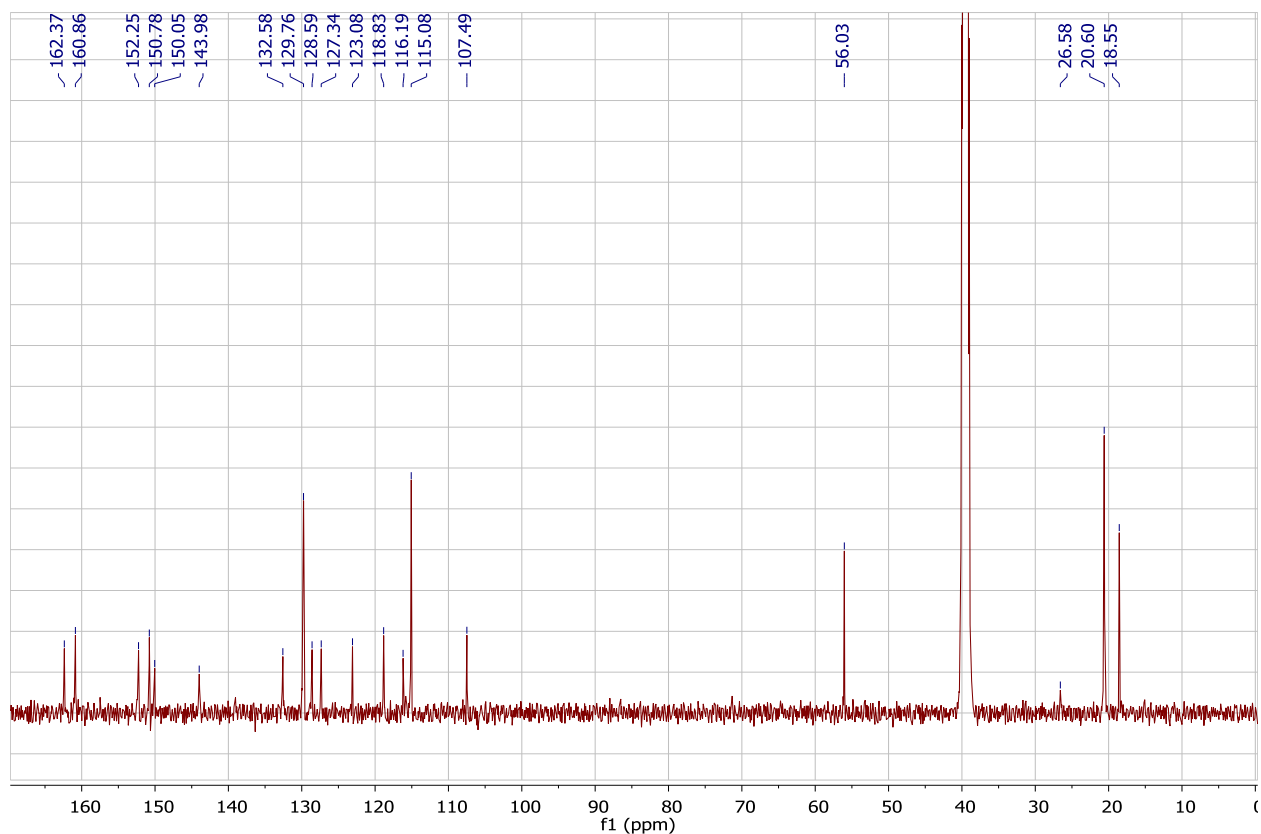


Fig. S13. ^{13}C NMR spectrum of compound **6** in DMSO- d_6 . (The chemical shifts at $\delta=18.55$ ppm and $\delta=56.03$ ppm are assigned to residual signals of ethanol. The compound was subjected to additional drying before further studies).

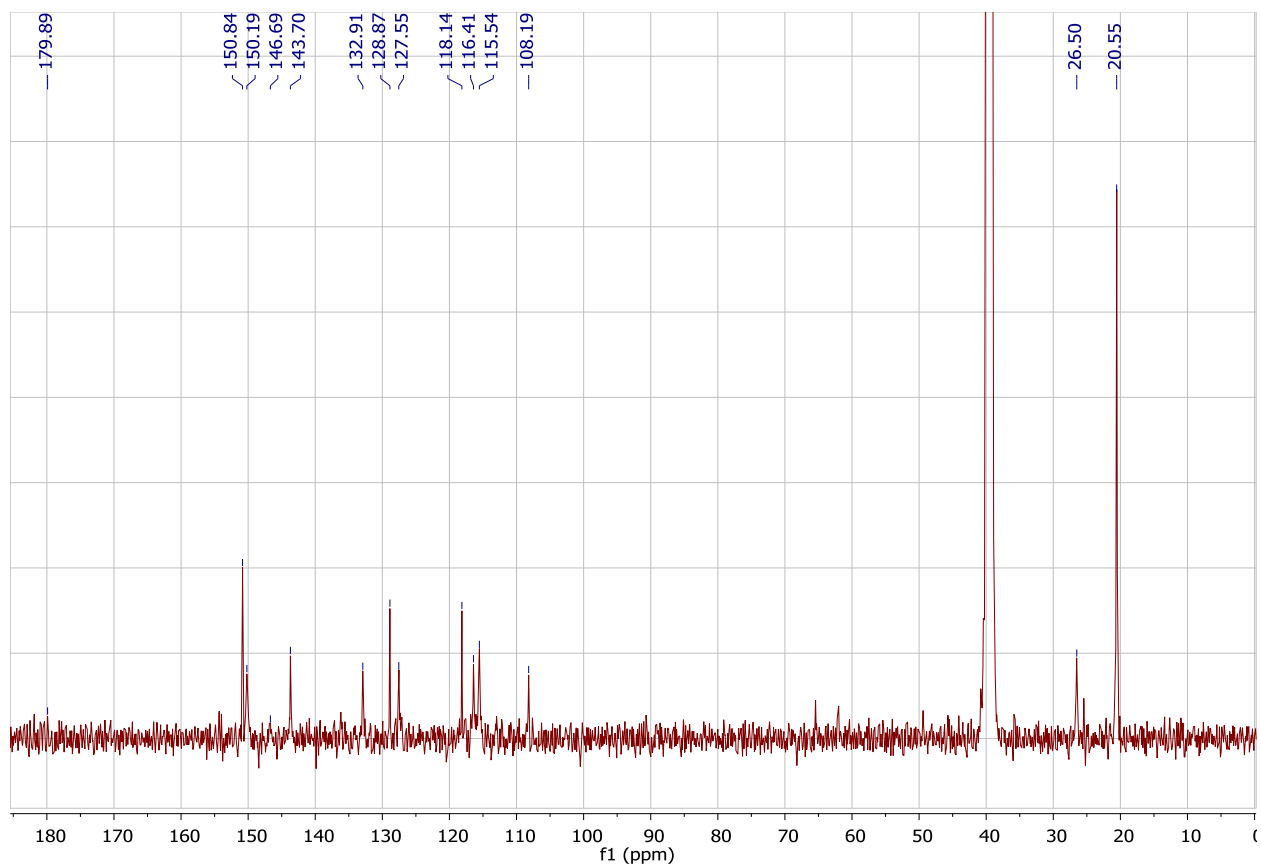


Fig. S14. ^{13}C NMR spectrum of compound **7** in DMSO- d_6 .

FT-IR spectra

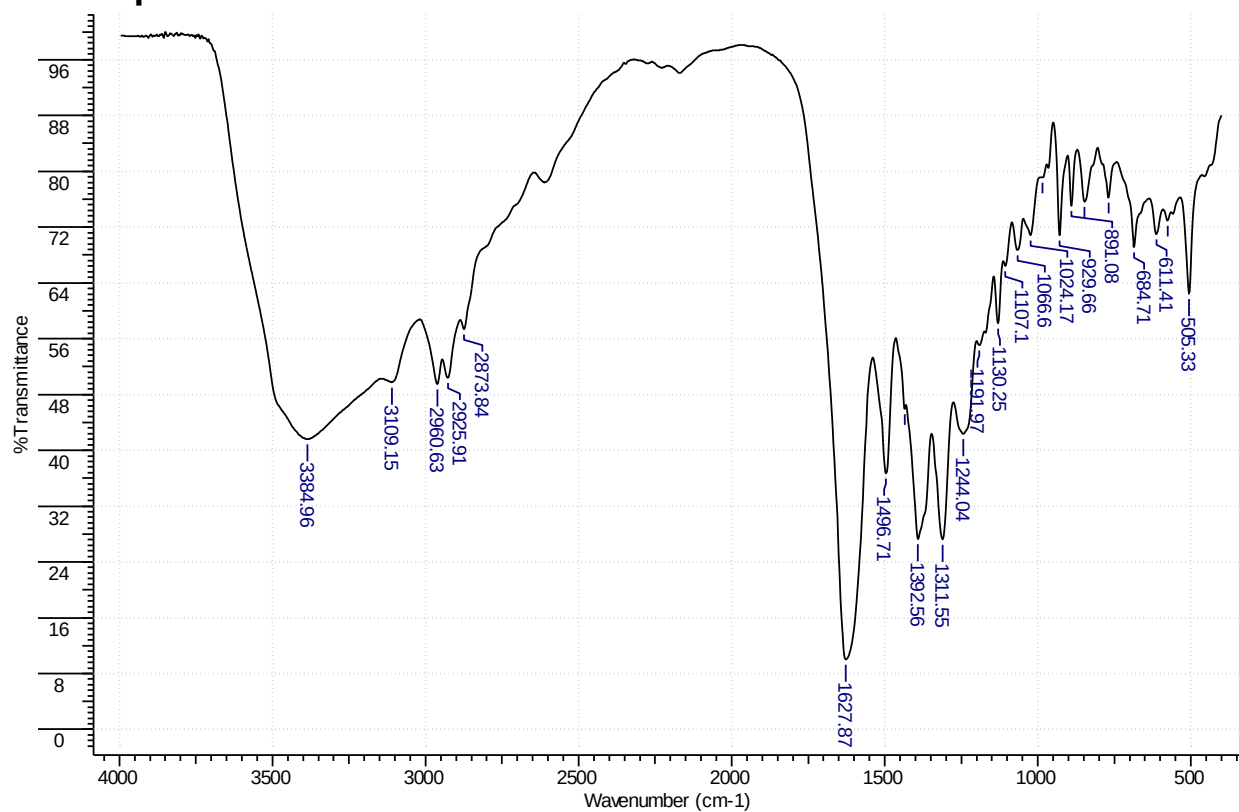


Fig. S15. FT-IR spectrum of compound **1** in KBr.

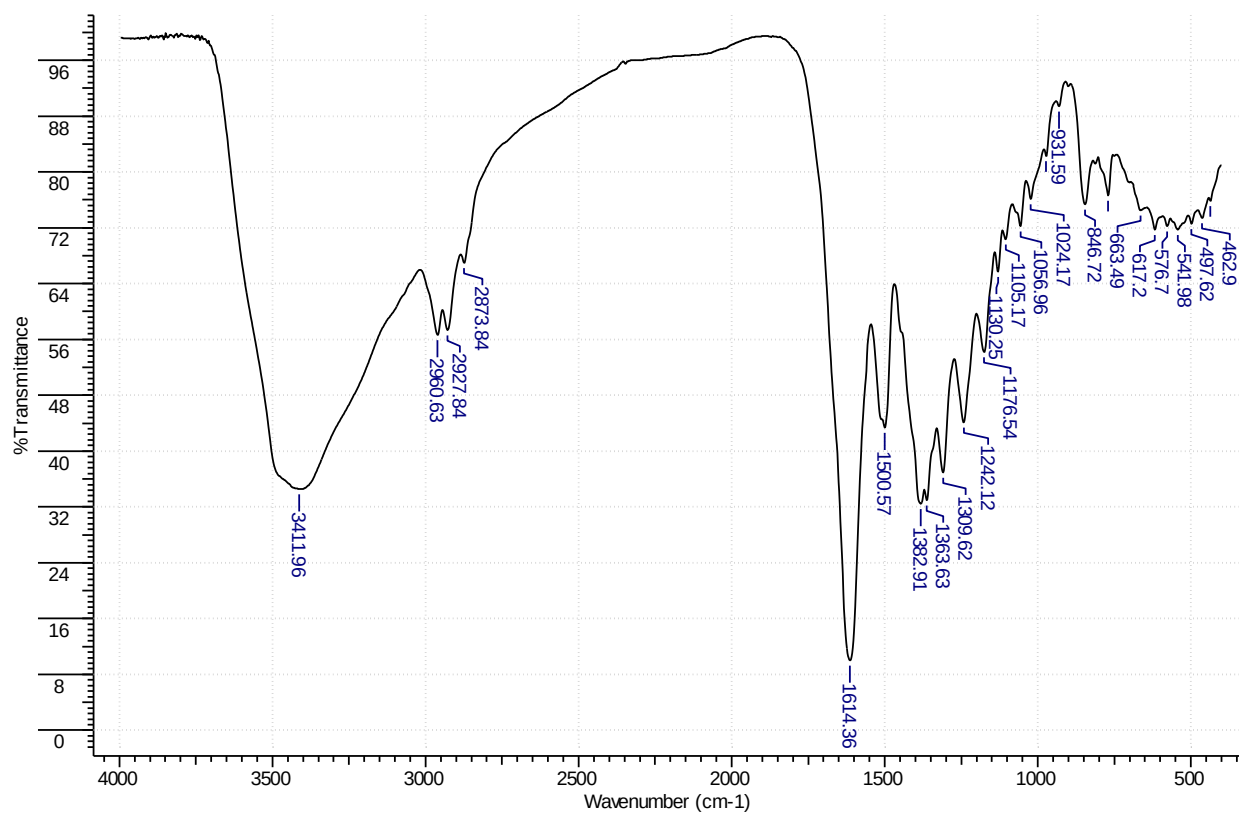


Fig. S16. FT-IR spectrum of compound **2** in KBr.

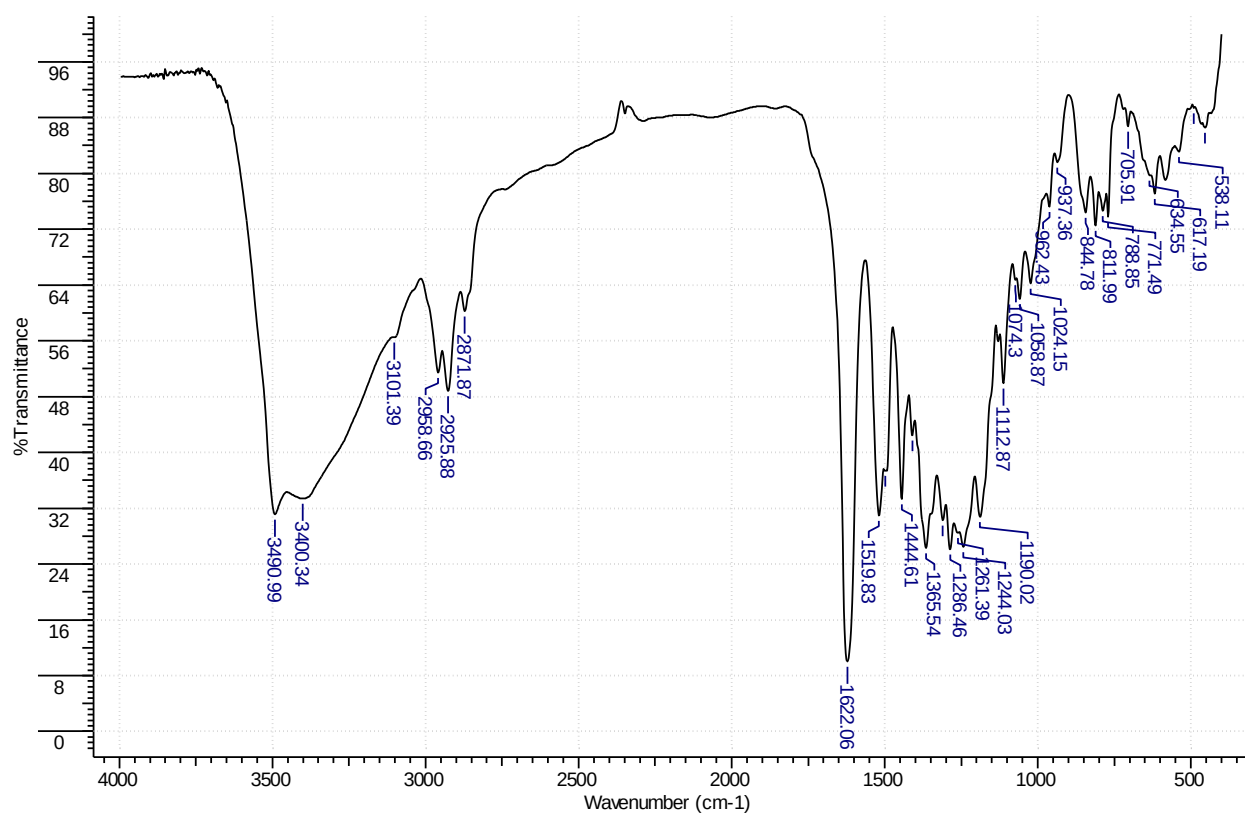


Fig. S17. FT-IR spectrum of compound **3** in KBr.

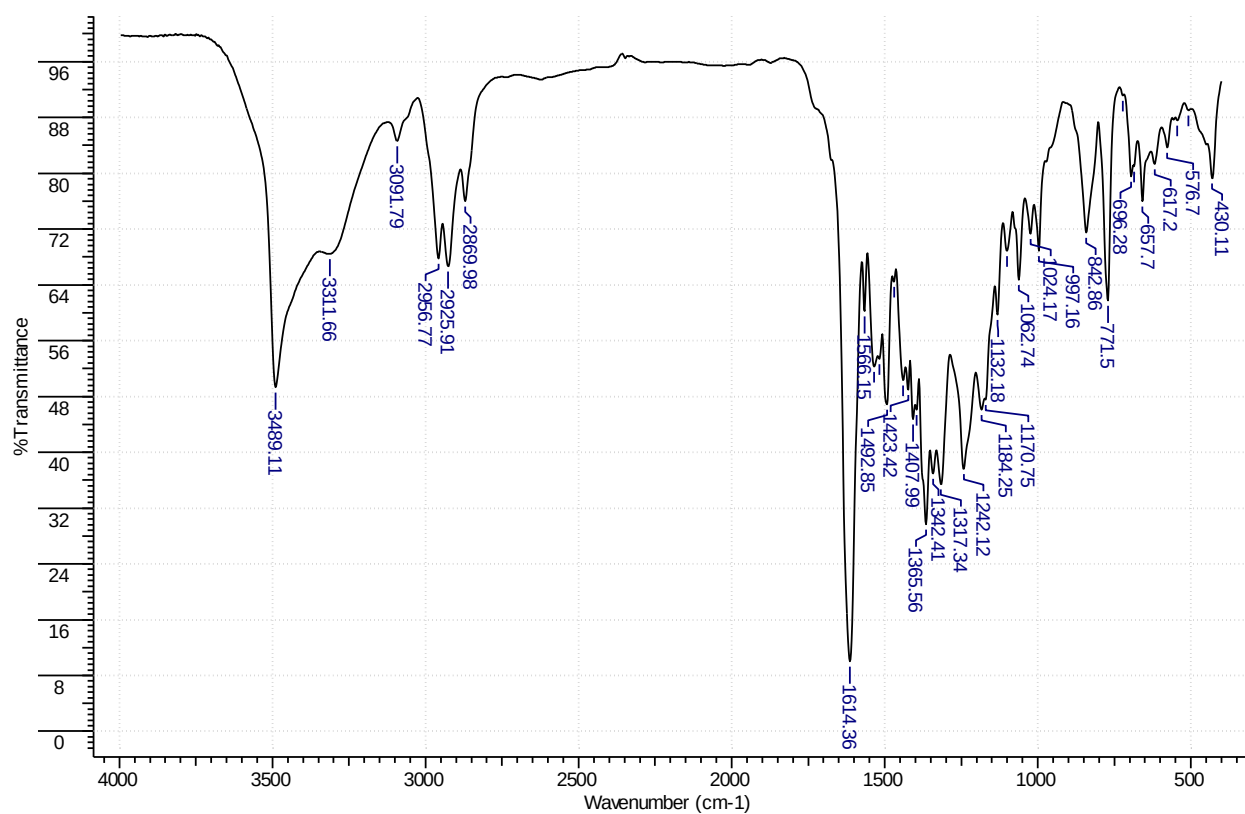


Fig. S18. FT-IR spectrum of compound **4** in KBr.

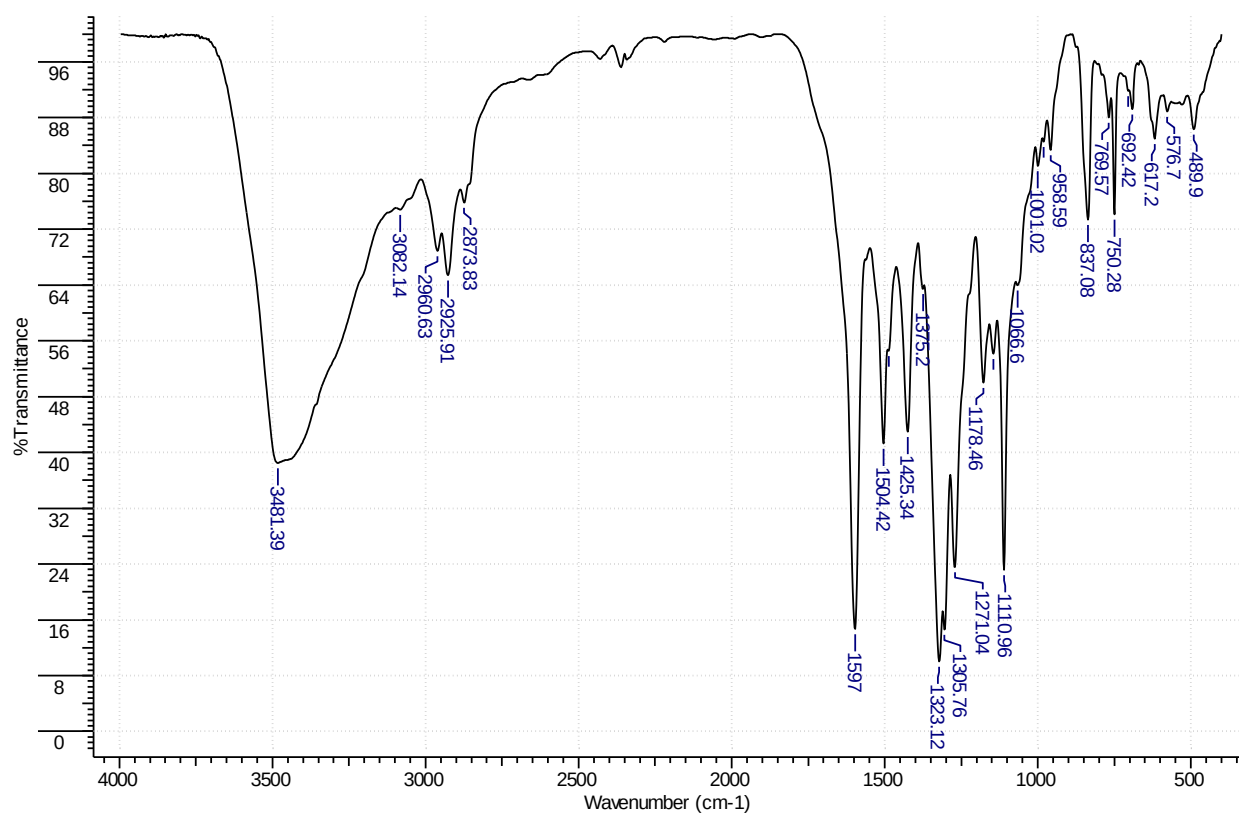


Fig. S19. FT-IR spectrum of compound **5** in KBr.

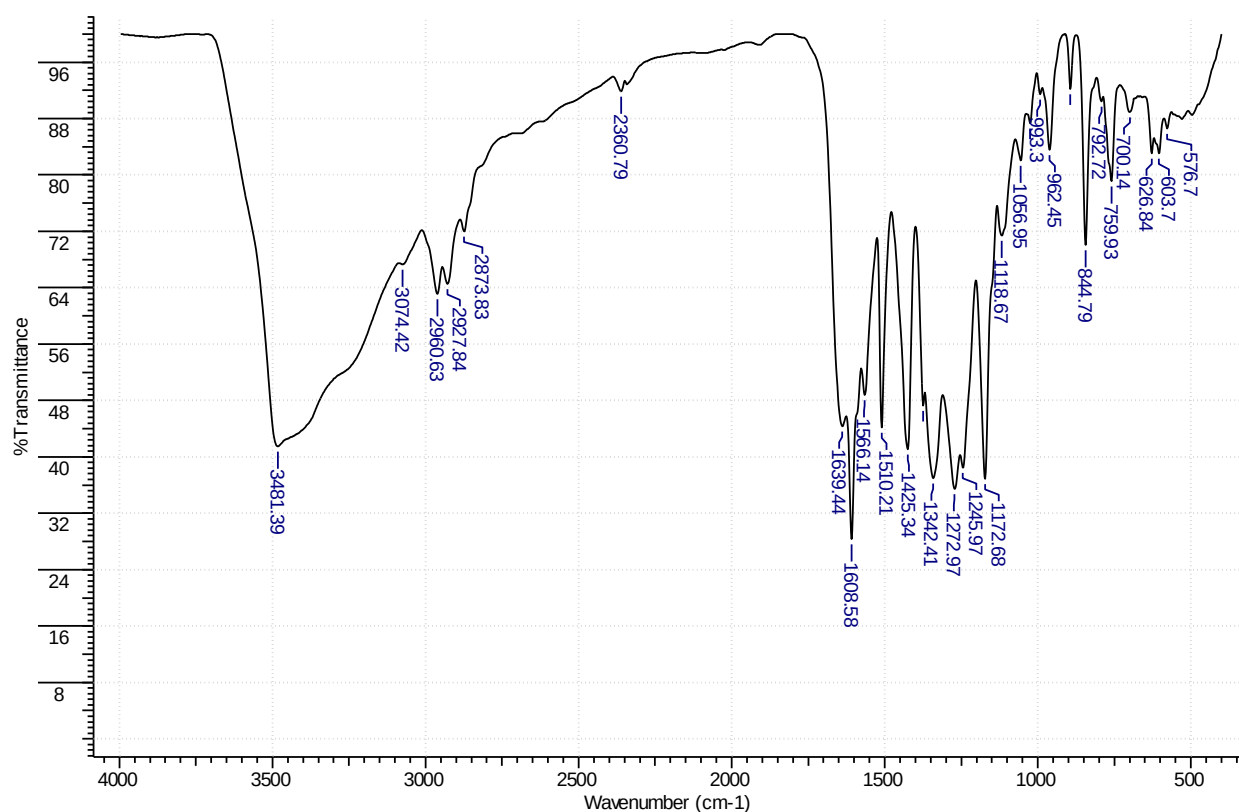


Fig. S20. FT-IR spectrum of compound **6** in KBr.

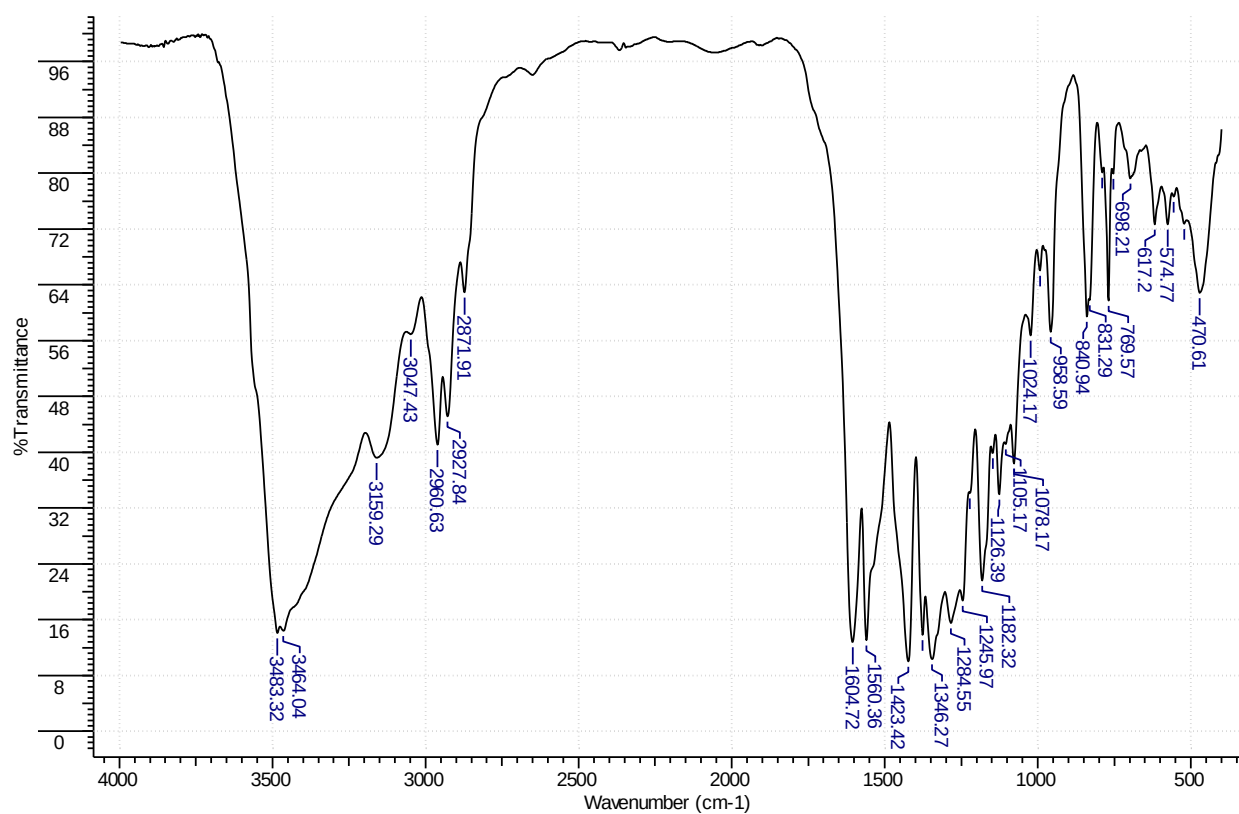


Fig. S21. FT-IR spectrum of compound 7 in KBr.

Reactions with DPPH

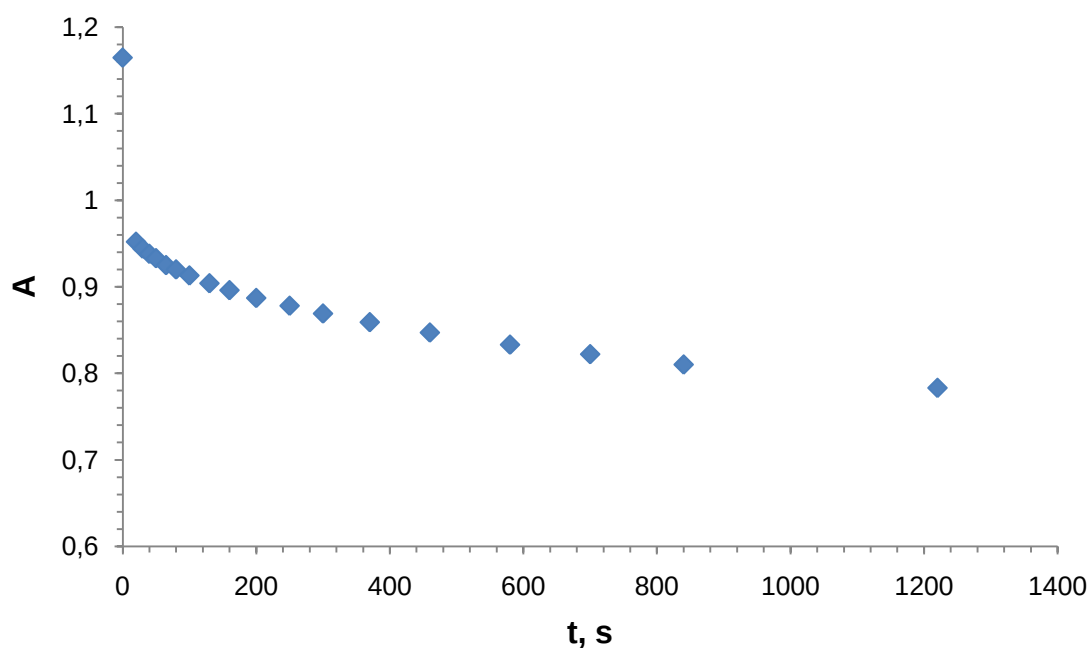


Fig. S22. Decay of the visible absorbance of DPPH solution (1.03×10^{-4} M) at 518 nm in ethanol after compound **1** (1.02×10^{-5} M) addition.

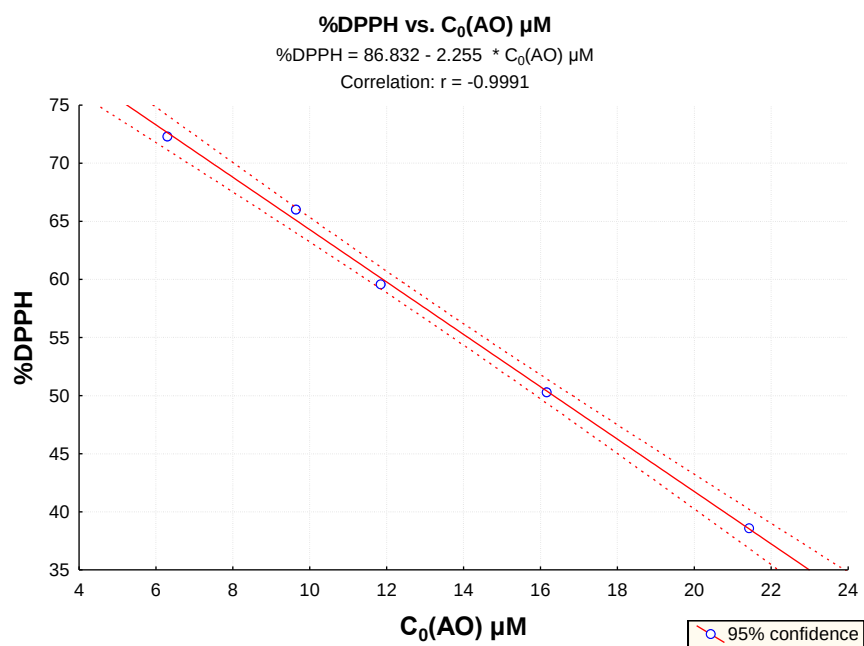


Fig. S23. The percentage of DPPH remaining (%) after 1200 s vs compound **1** initial concentration ($C_0(\text{AO})$).

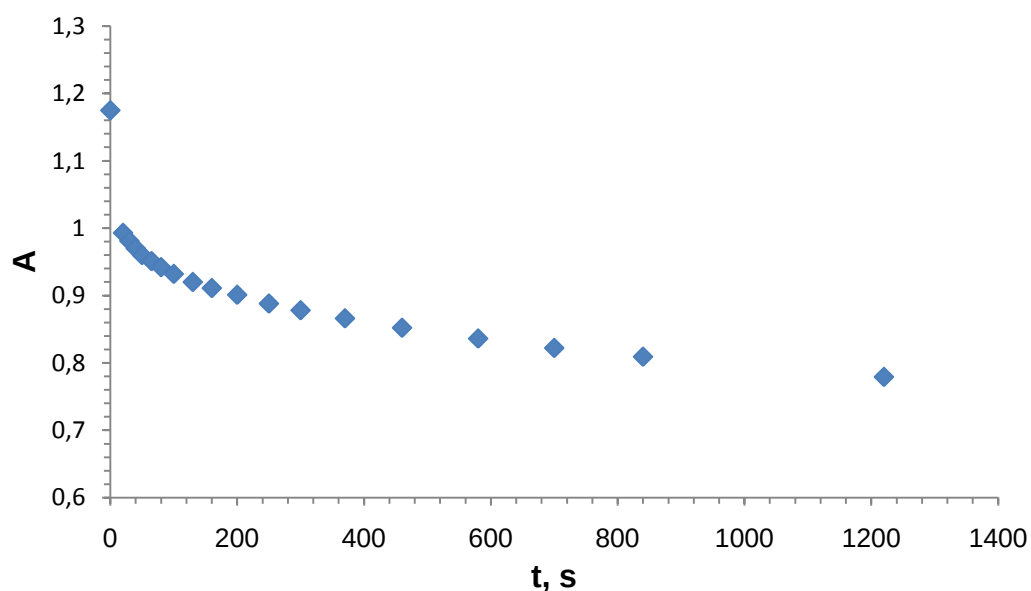


Fig. S24. Decay of the visible absorbance of DPPH solution (1.04×10^{-4} M) at 518 nm in ethanol after compound **2** (1.01×10^{-5} M) addition.

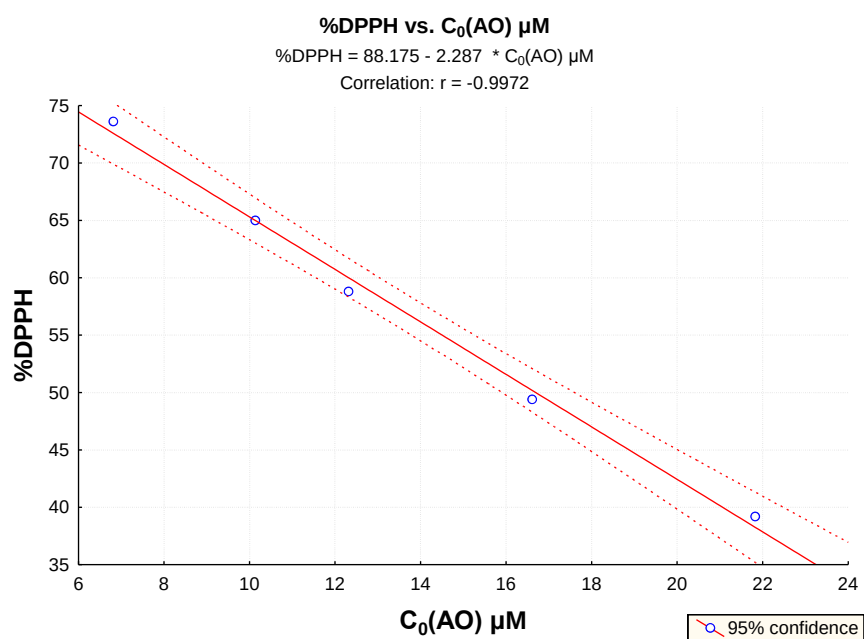


Fig. S25. The percentage of DPPH remaining (%) after 1200 s vs compound **2** initial concentration ($C_0(\text{AO})$).

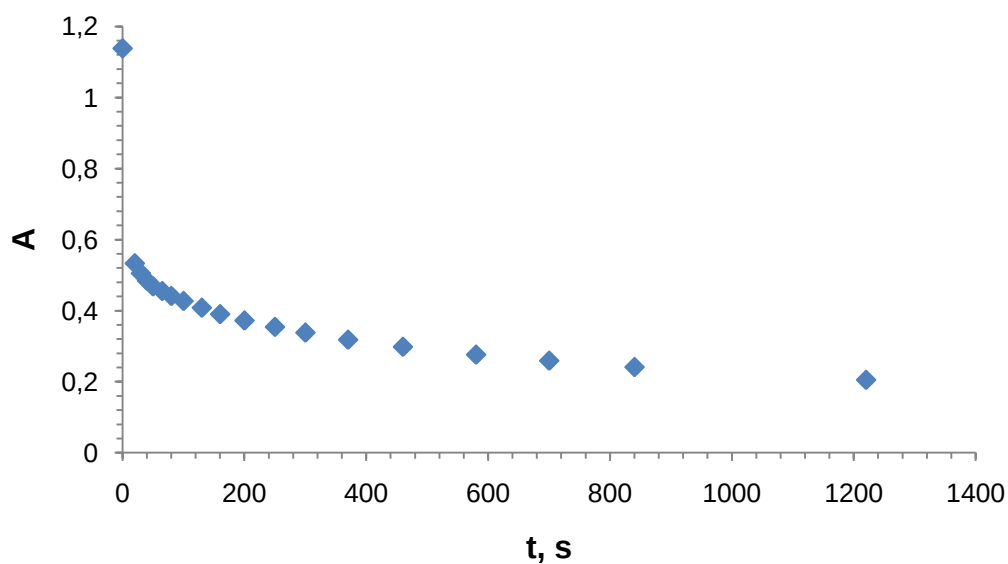


Fig. S26. Decay of the visible absorbance of DPPH solution (1.01×10^{-4} M) at 518 nm in ethanol after compound **3** (1.01×10^{-5} M) addition.

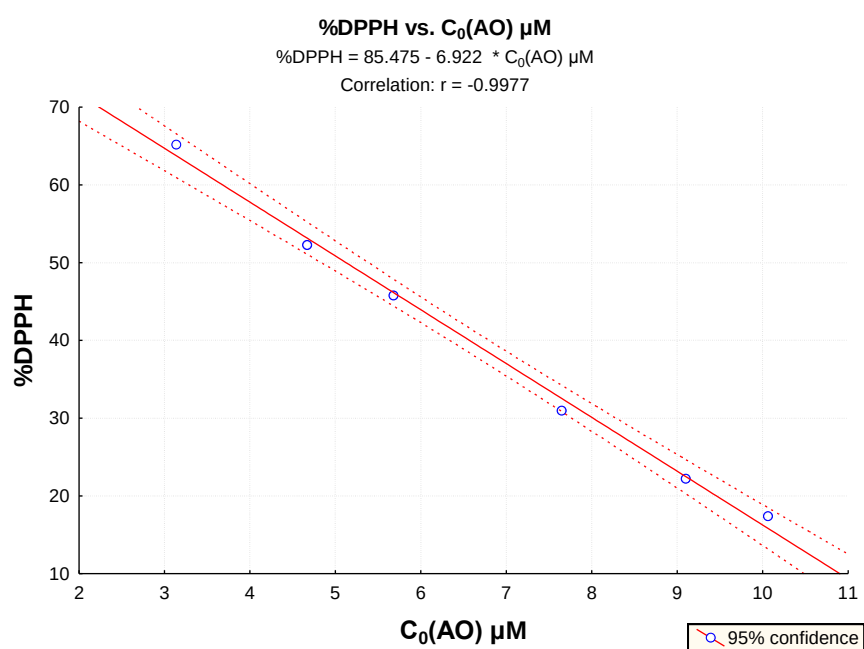


Fig. S27. The percentage of DPPH remaining (%) after 1200 s vs compound **3** initial concentration ($C_0(\text{AO})$).

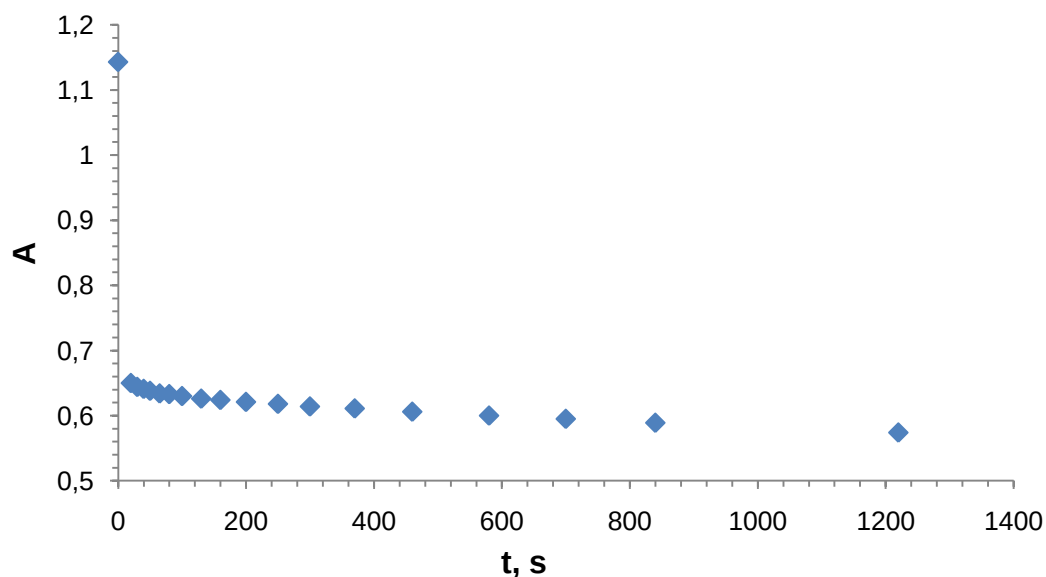


Fig. S28. Decay of the visible absorbance of DPPH solution (1.01×10^{-4} M) at 518 nm in ethanol after compound **4** (1.03×10^{-5} M) addition.

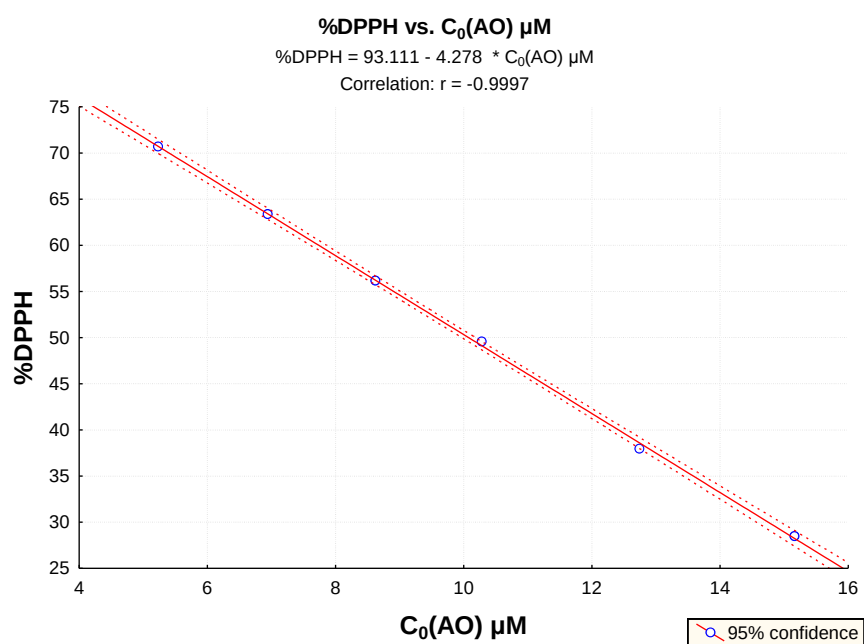


Fig. S29. The percentage of DPPH remaining (%) after 1200 s vs compound **4** initial concentration ($C_0(\text{AO})$).

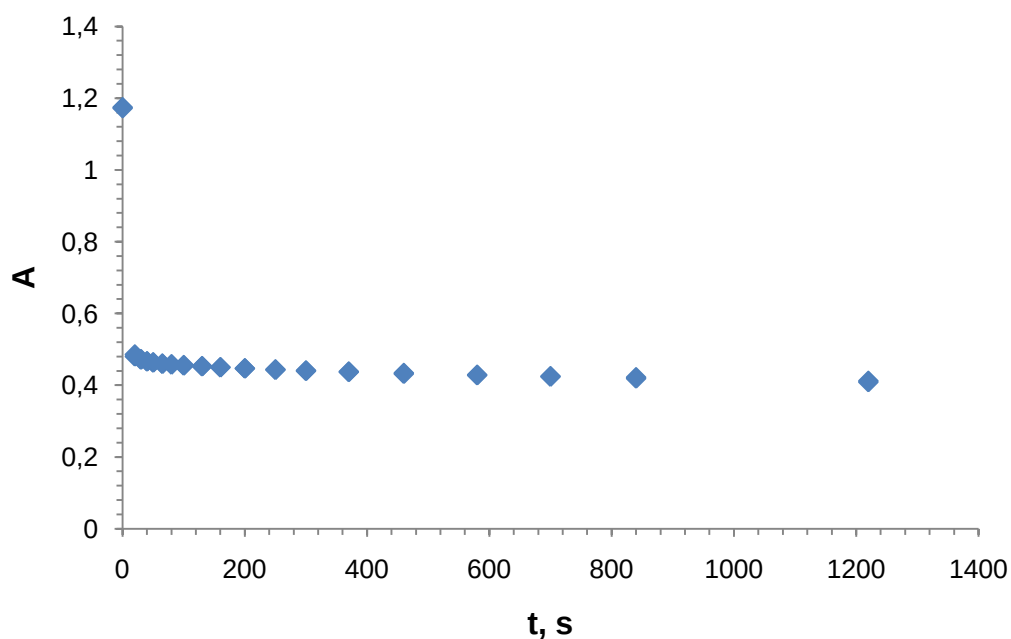


Fig. S30. Decay of the visible absorbance of DPPH solution (1.04×10^{-4} M) at 518 nm in ethanol after compound **5** (1.02×10^{-5} M) addition.

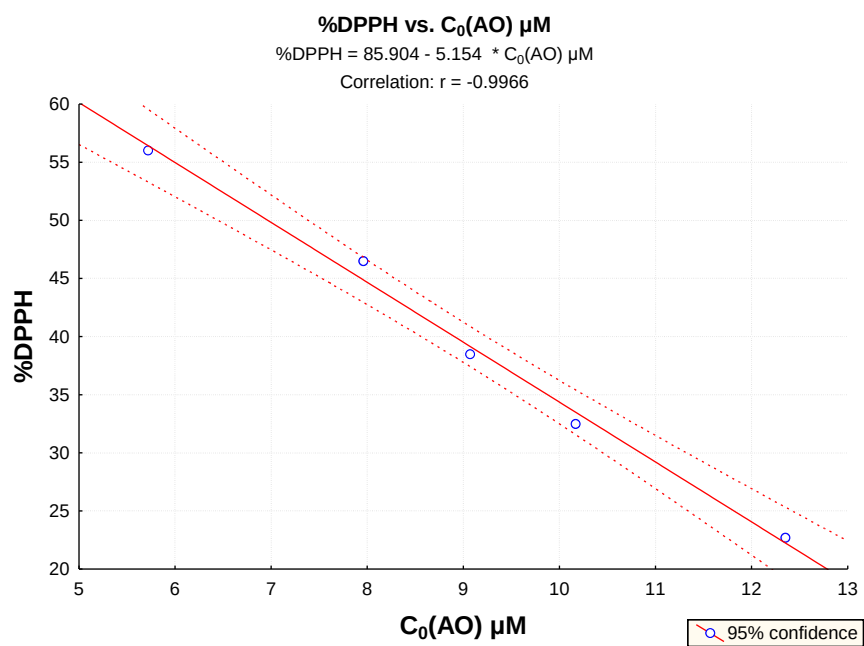


Fig. S31. The percentage of DPPH remaining (%) after 1200 s vs compound **5** initial concentration ($C_0(\text{AO})$).

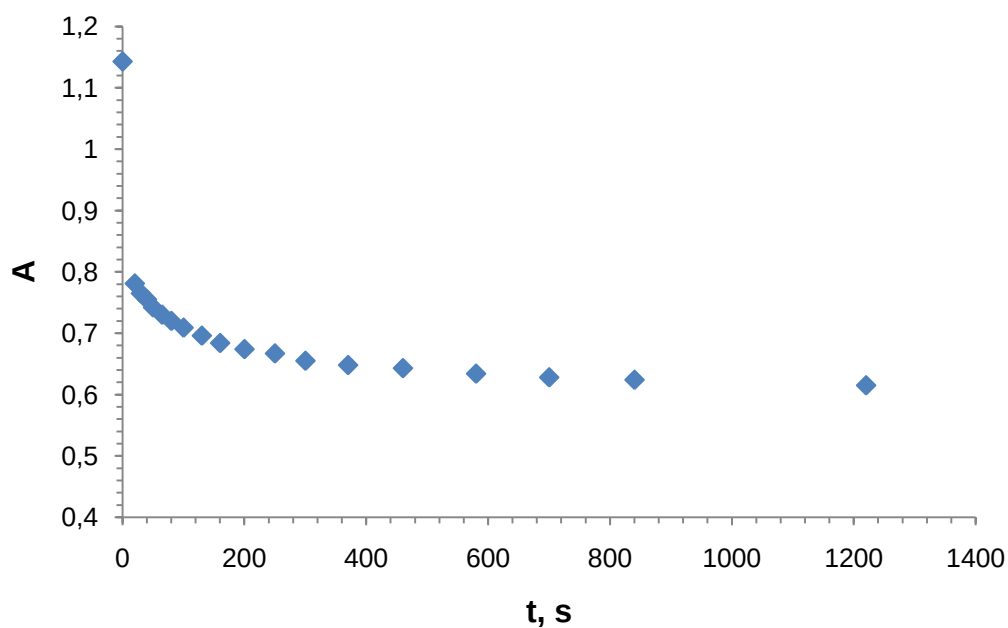


Fig. S32. Decay of the visible absorbance of DPPH solution (1.01×10^{-4} M) at 518 nm in ethanol after compound **6** (1.01×10^{-5} M) addition.

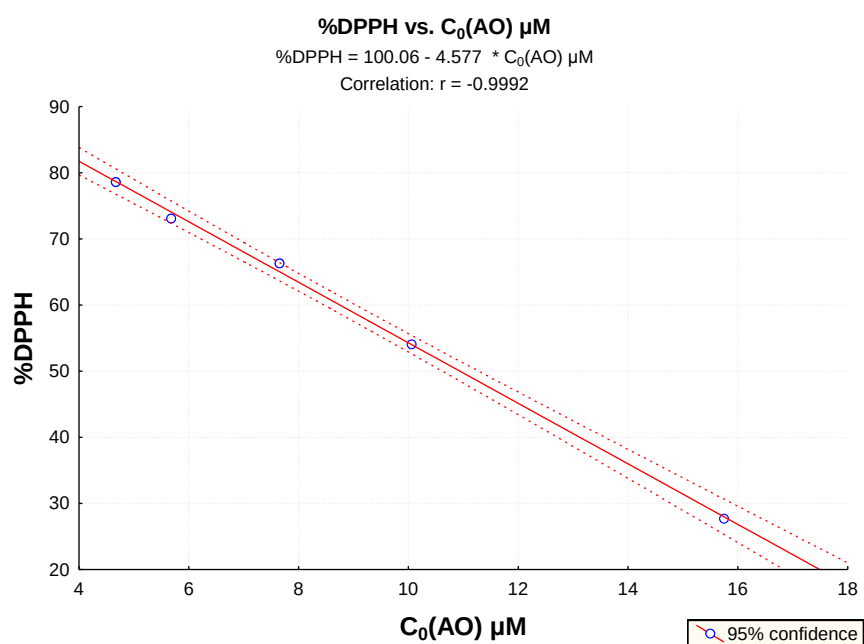


Fig. S33. The percentage of DPPH remaining (%) after 1200 s vs compound **6** initial concentration ($C_0(\text{AO})$).

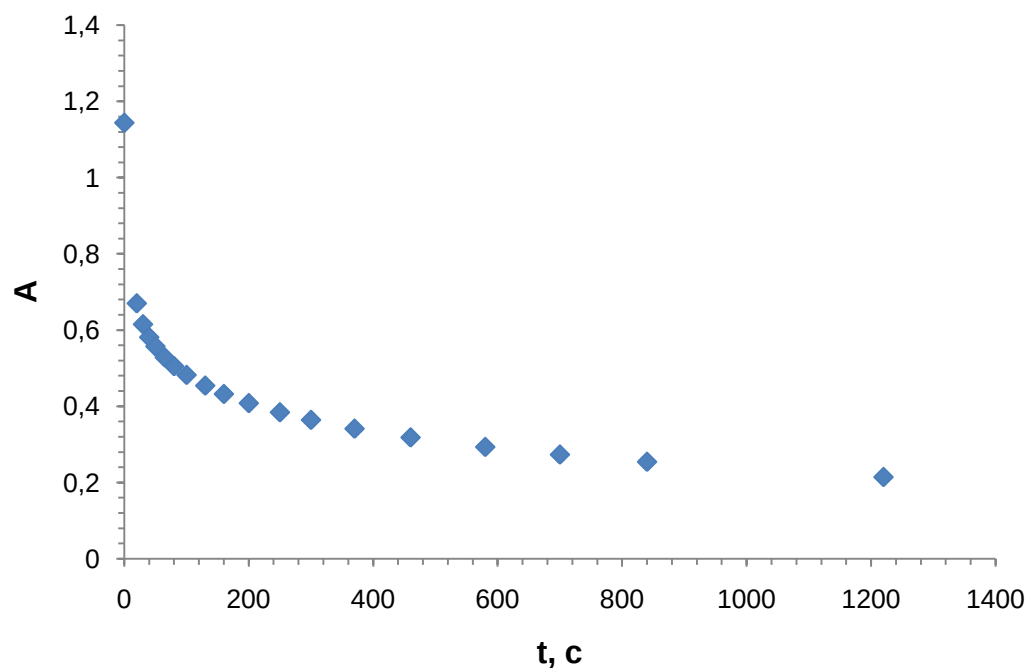


Fig. S34. Decay of the visible absorbance of DPPH solution (1.01×10^{-4} M) at 518 nm in ethanol after compound **7** (1.02×10^{-5} M) addition.

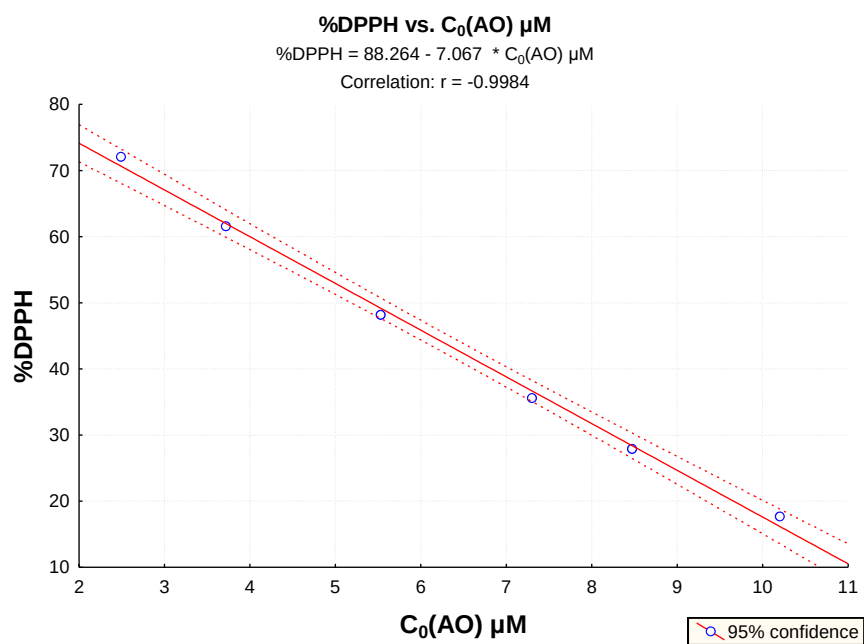


Fig. S35. The percentage of DPPH remaining (%) after 1200 s vs compound **7** initial concentration ($C_0(\text{AO})$).

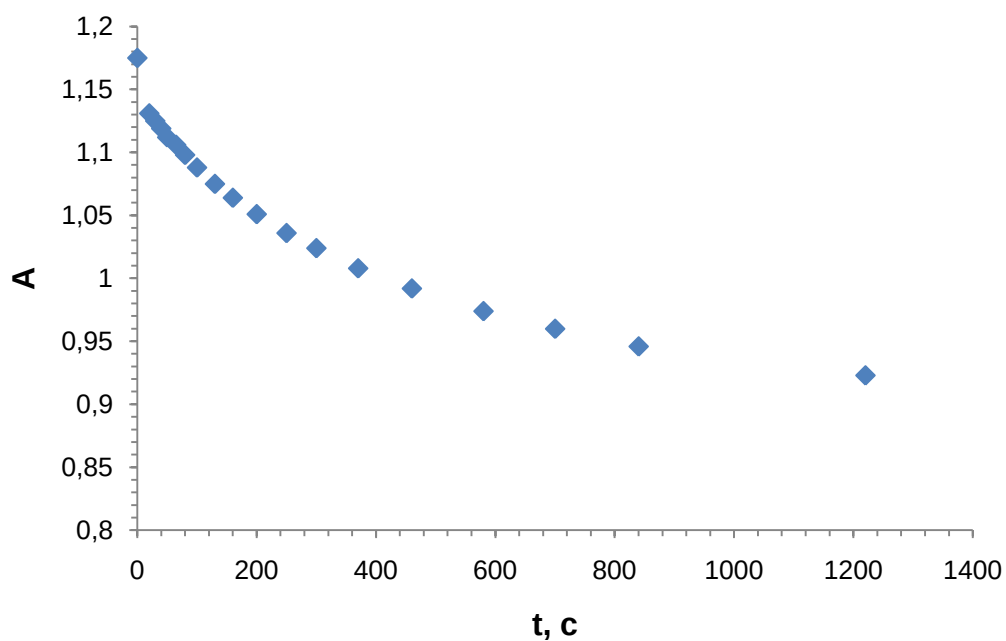


Fig. S36. Decay of the visible absorbance of DPPH solution (1.04×10^{-4} M) at 518 nm in ethanol after caffeic acid (1.04×10^{-5} M) addition.

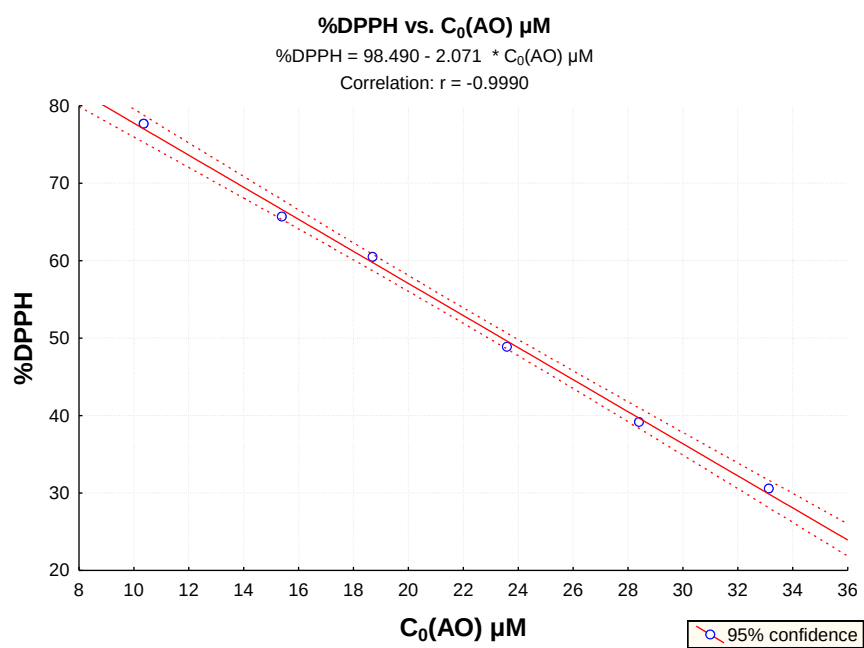


Fig. S37. The percentage of DPPH remaining (%) after 1200 s vs caffeic acid initial concentration ($C_0(\text{AO})$).