

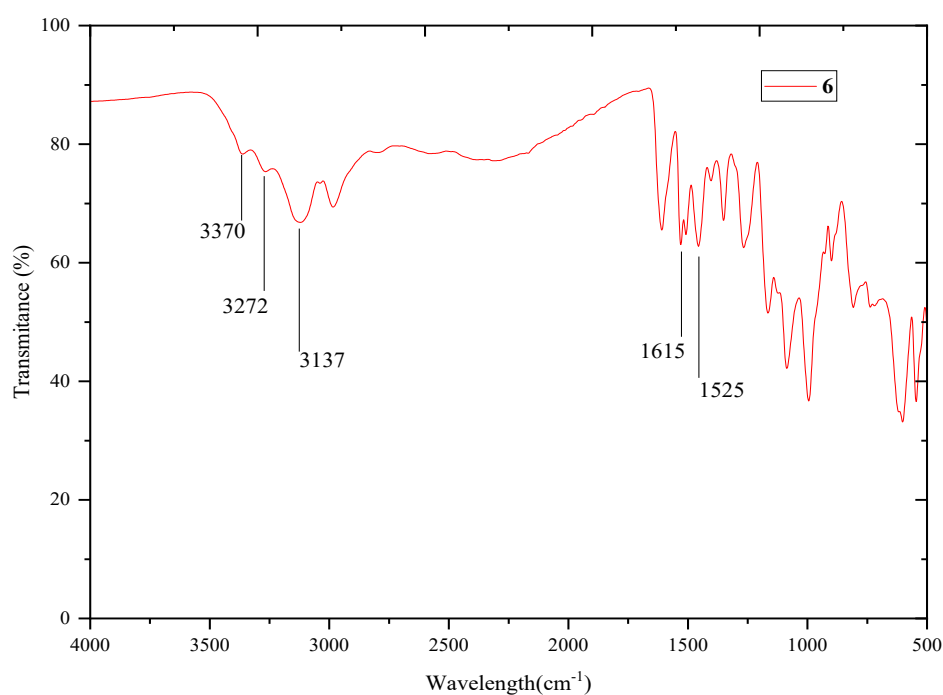
## Supporting Information

### Synthesis, Dyeing performance and Evaluation of Antimicrobial and Antioxidant Activities of Azo Dye derivatives Incorporated 1,3,4-thiadiazole combined with *in-silico* computational studies

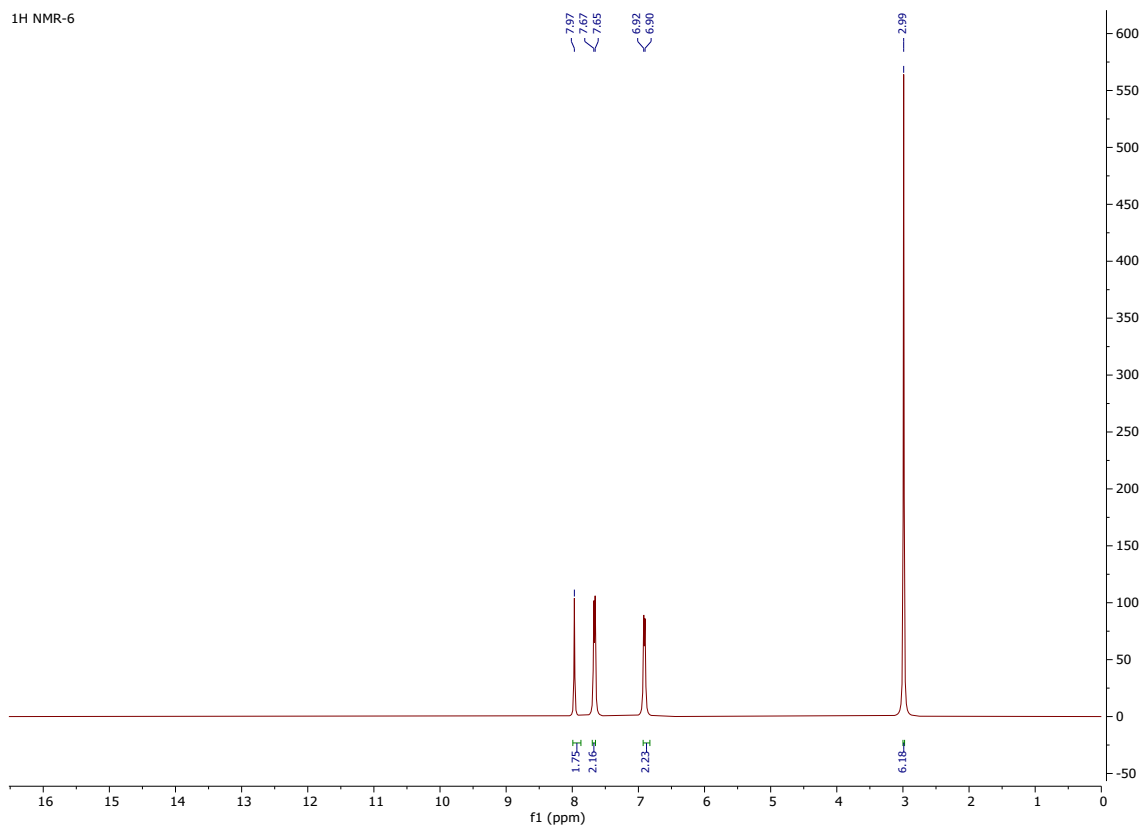
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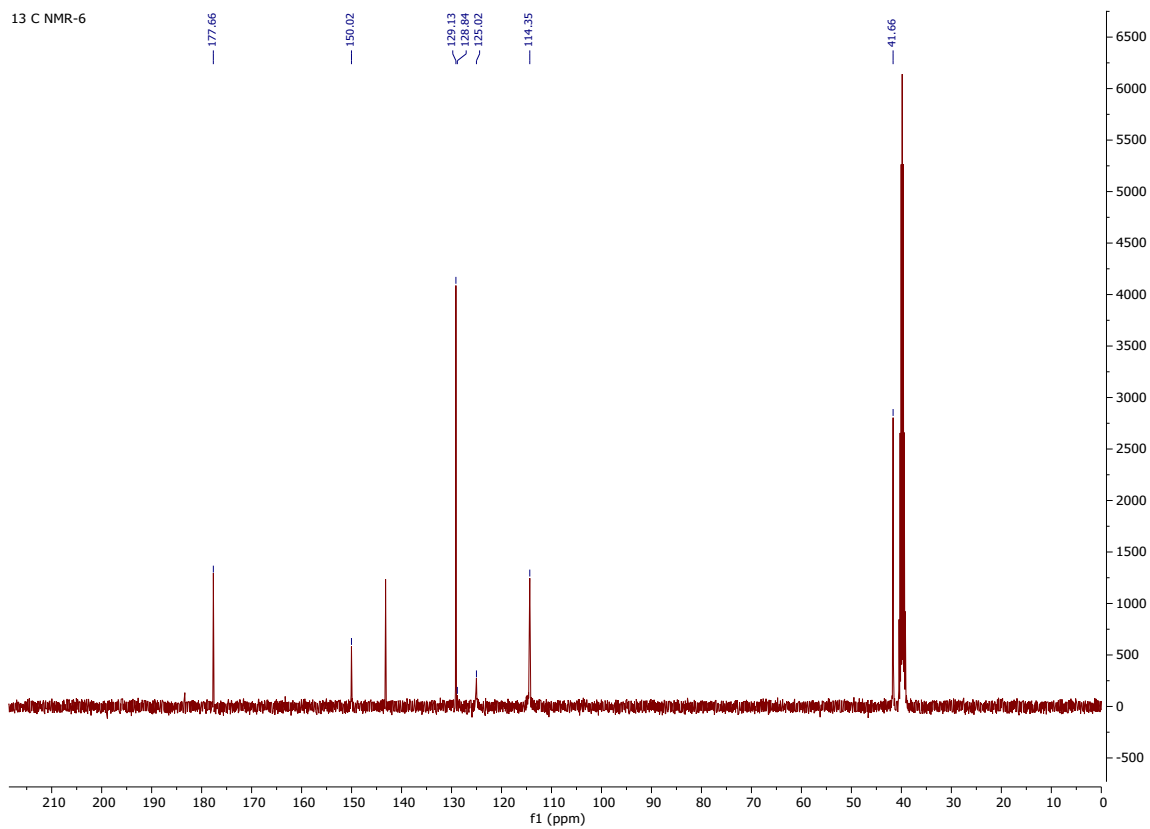
\* Correspondence: Endale Mulugeta (Phd) [endexindex05@gmail.com](mailto:endexindex05@gmail.com)



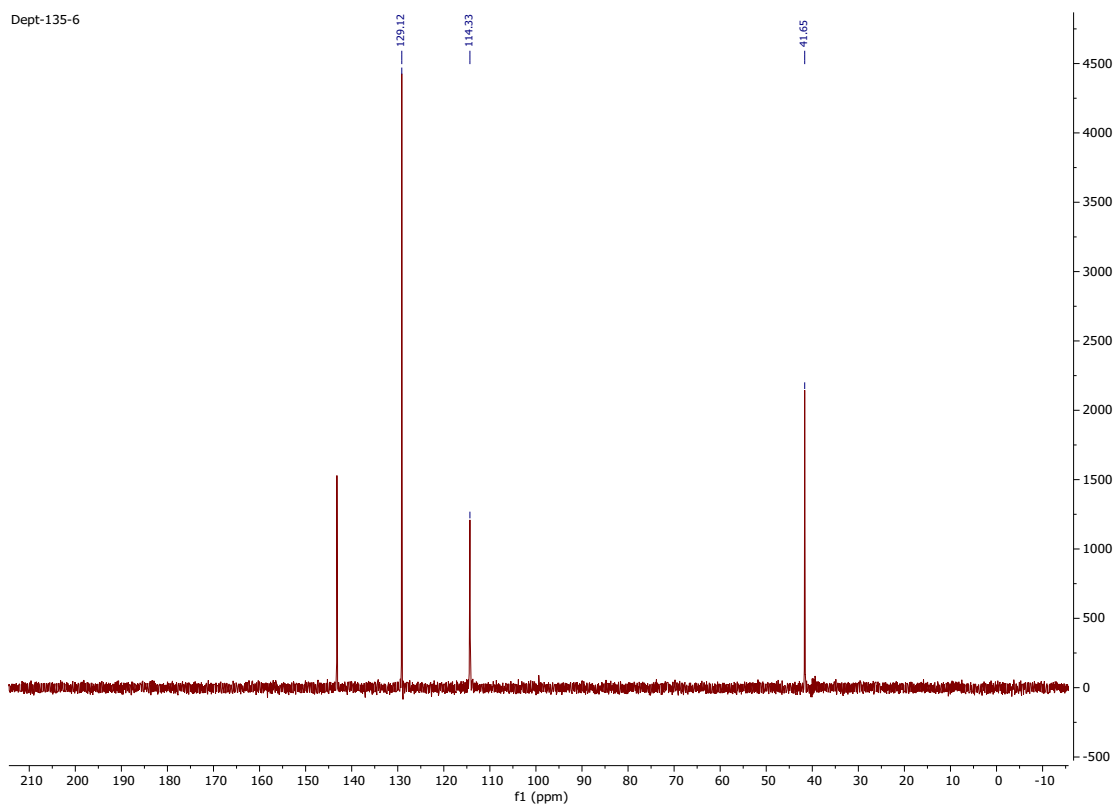
**Figure S1** : FTIR [(KBr)  $\nu_{\max}$ /cm<sup>-1</sup>] spectrum of compound **6**.



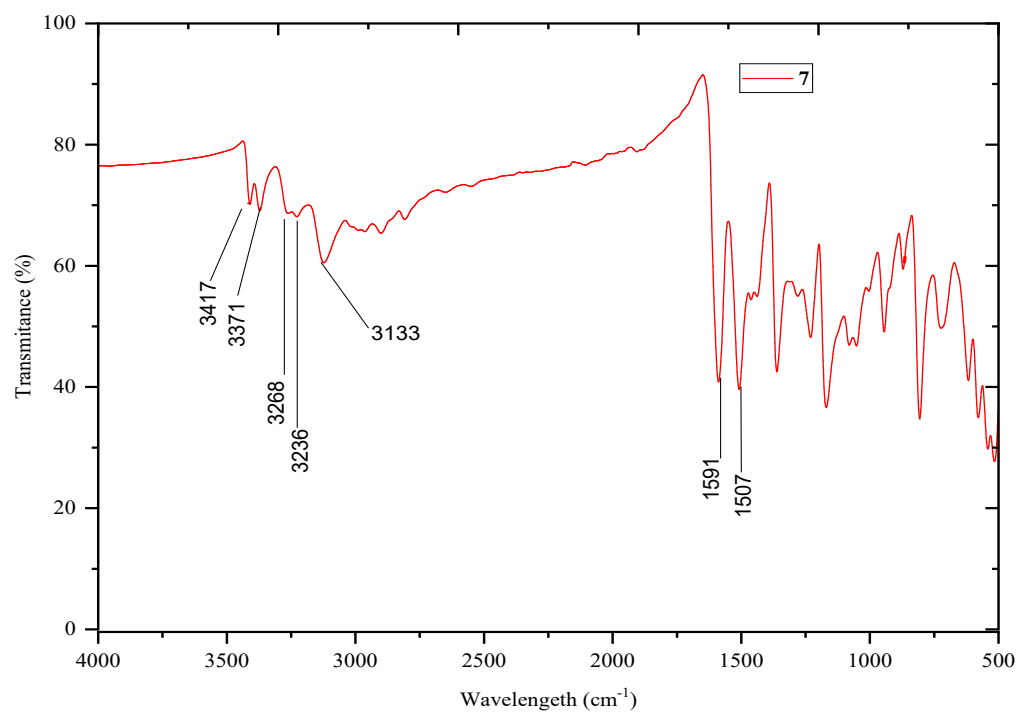
**Figure S2:** <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **6**.



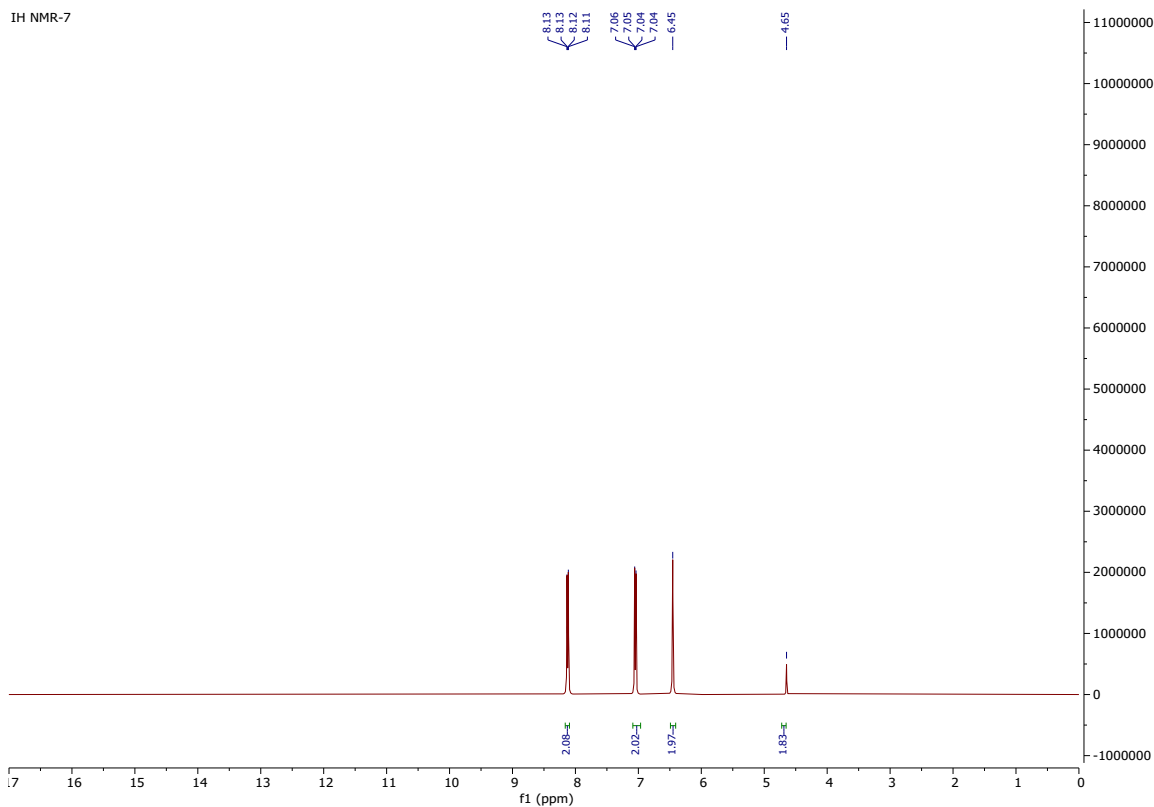
**Figure S3:** <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **6**.



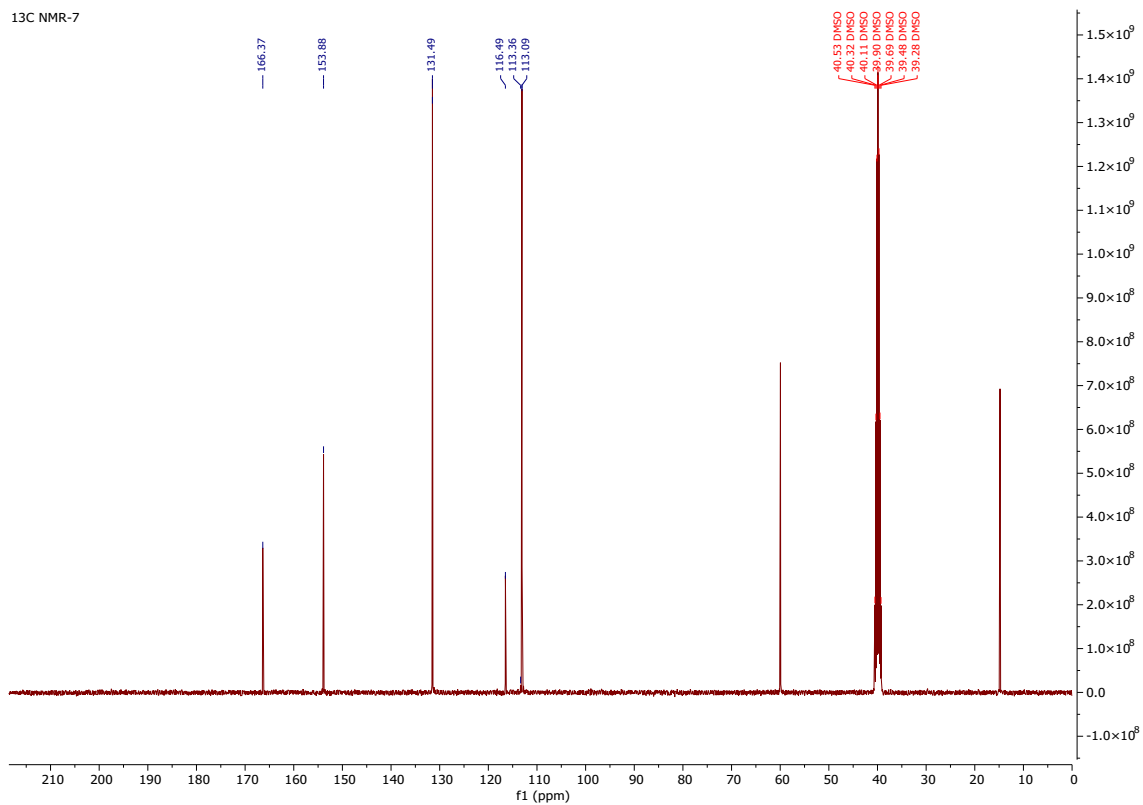
**Figure S4:** DEPT-135 (100 MHz, DMSO- $d_6$ ) spectrum of compound **6**.



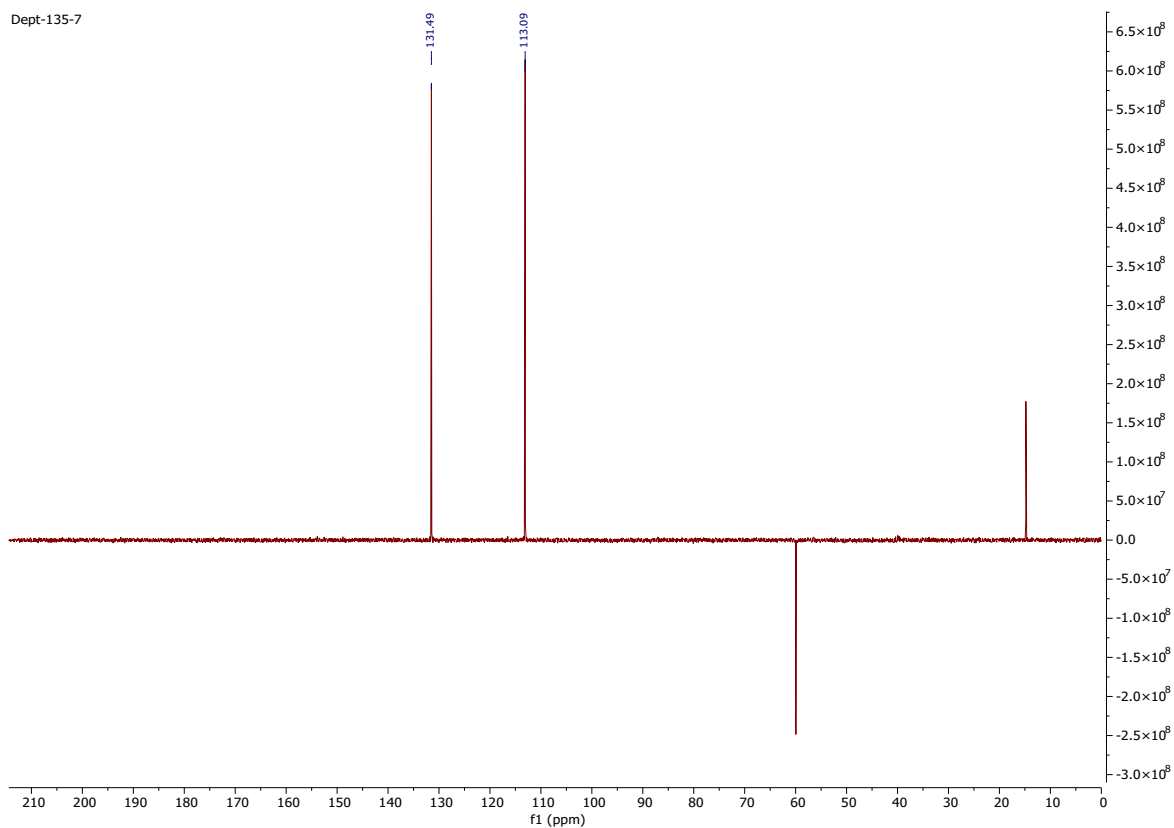
**Figure S5:** FTIR [(KBr)  $\nu_{\text{max}}/\text{cm}^{-1}$ ] spectrum of compound **7**.



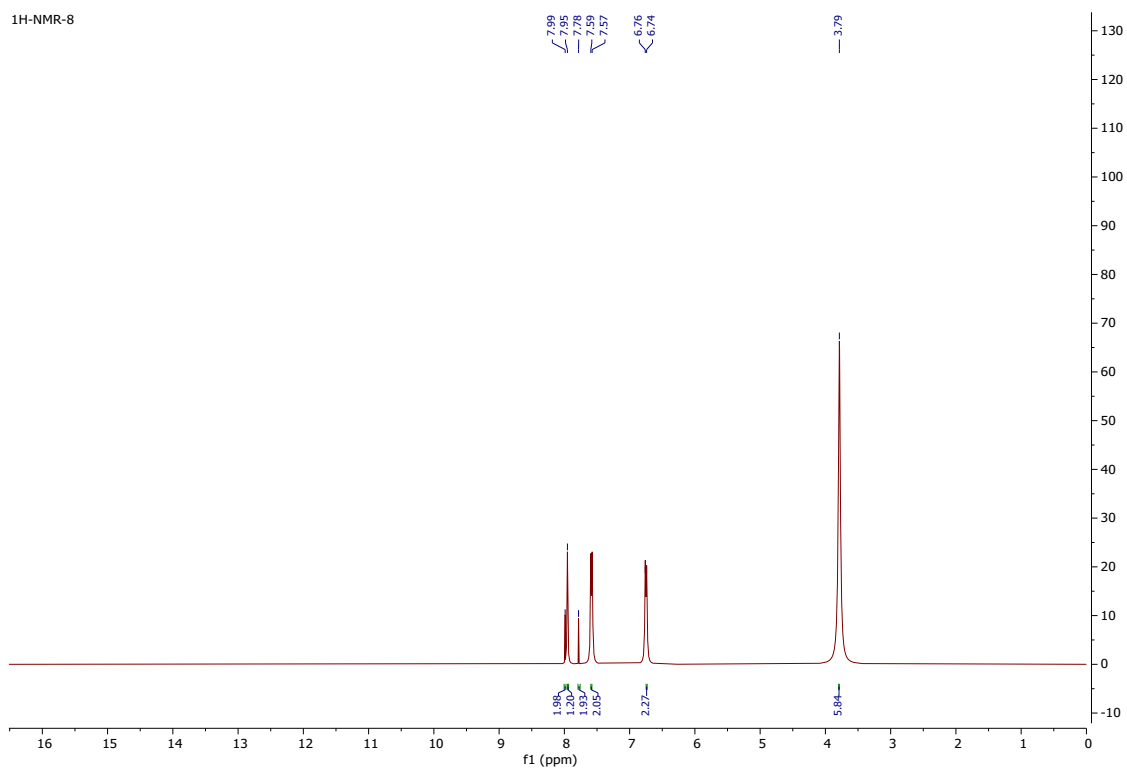
**Figure S6:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 7.



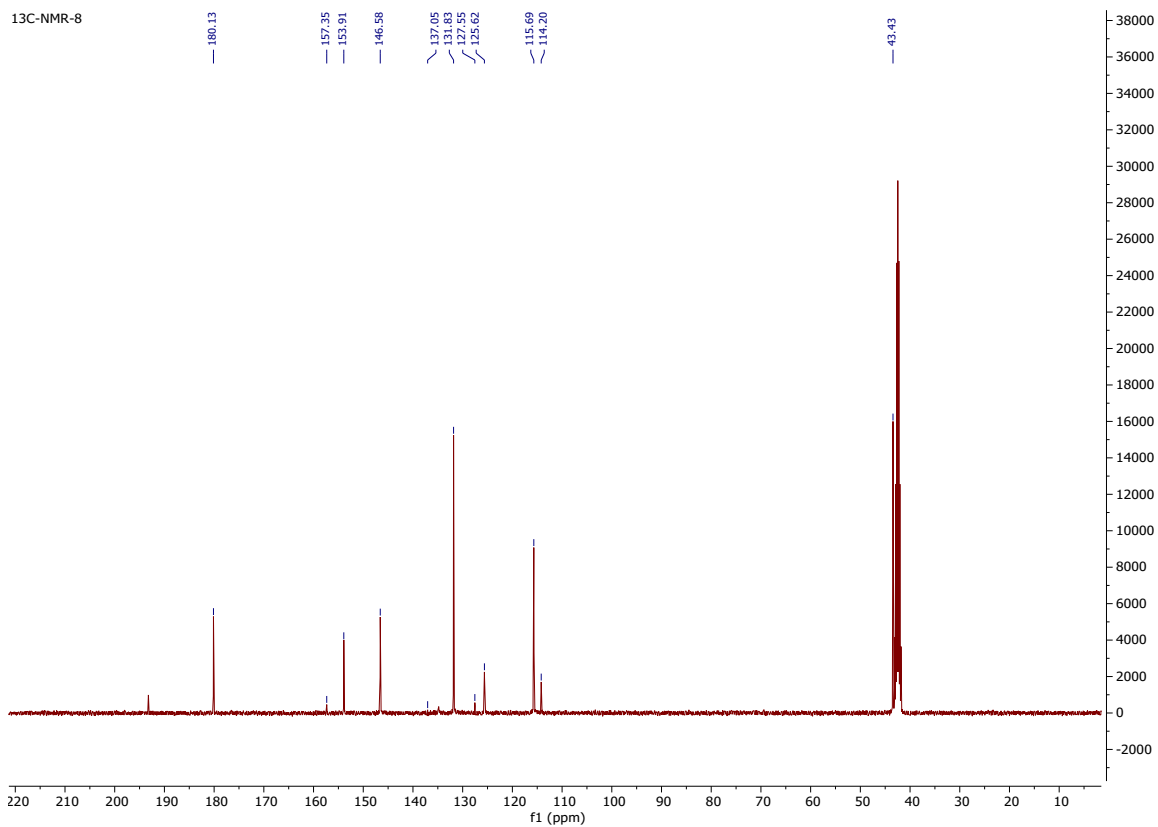
**Figure S7:**  $^{13}\text{C}$ -NMR (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 7.



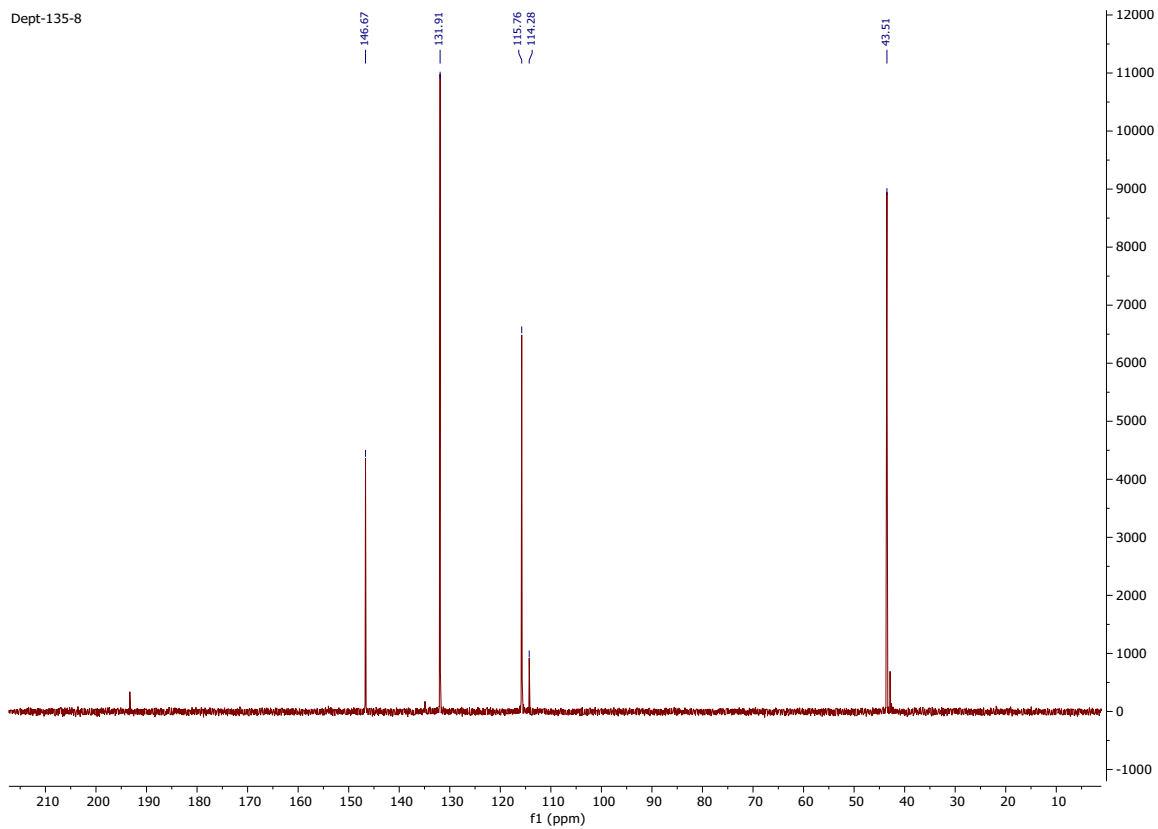
**Figure S8:** DEPT-135 (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **7**.



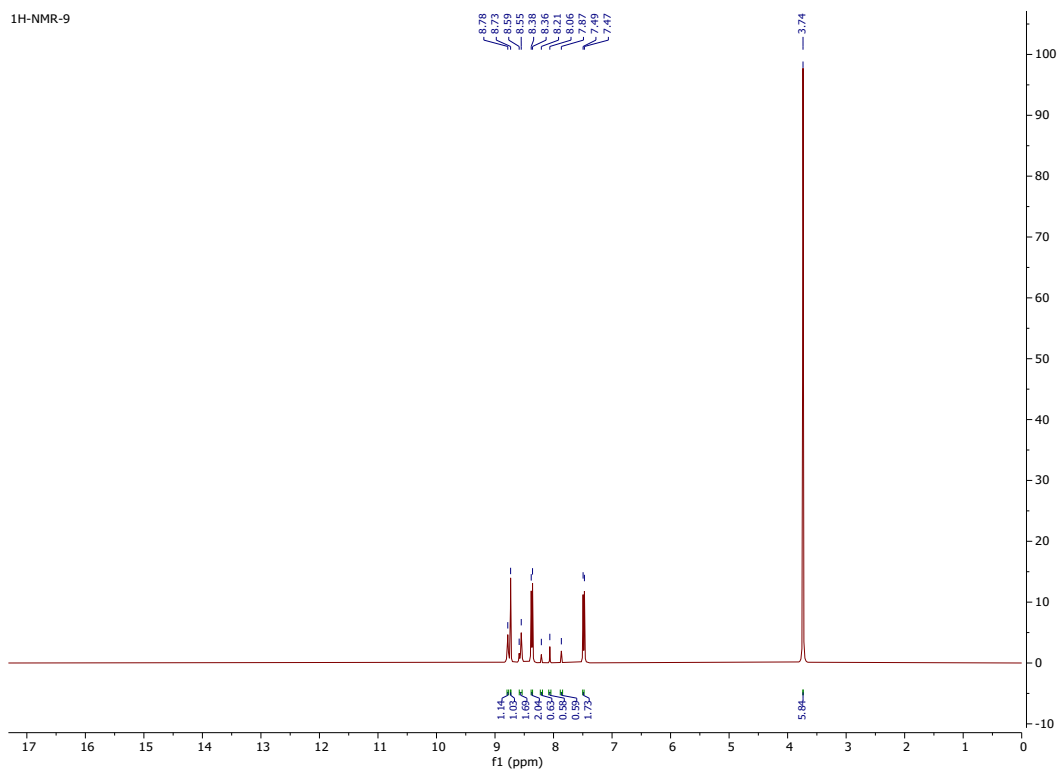
**Figure S9:** <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **8**.



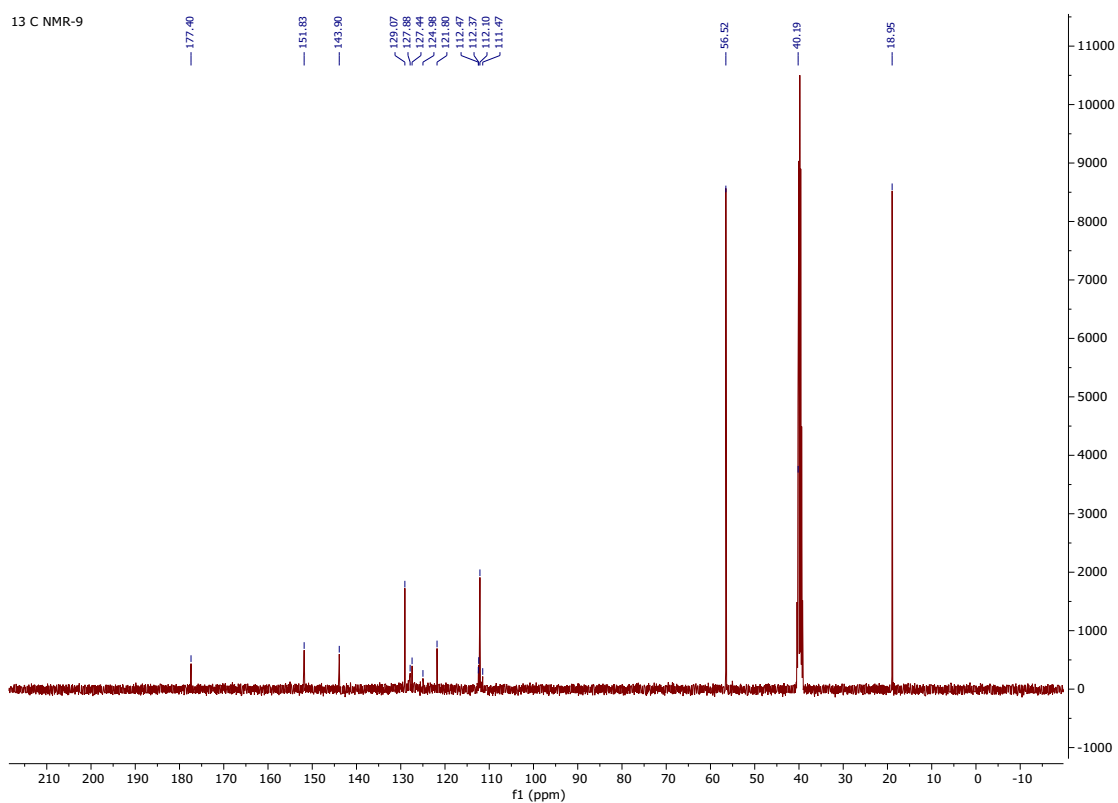
**Figure S10:**  $^{13}\text{C}$ -NMR (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **8**.



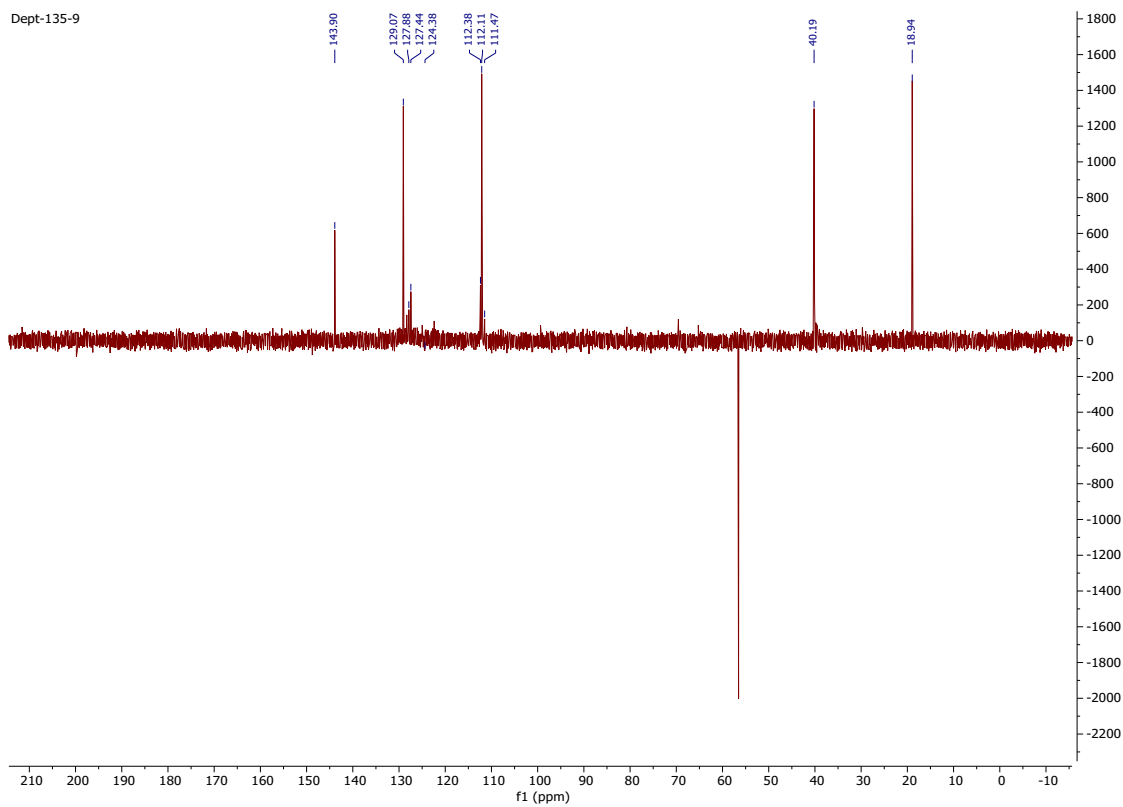
**Figure S11:** DEPT-135 (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **8**.



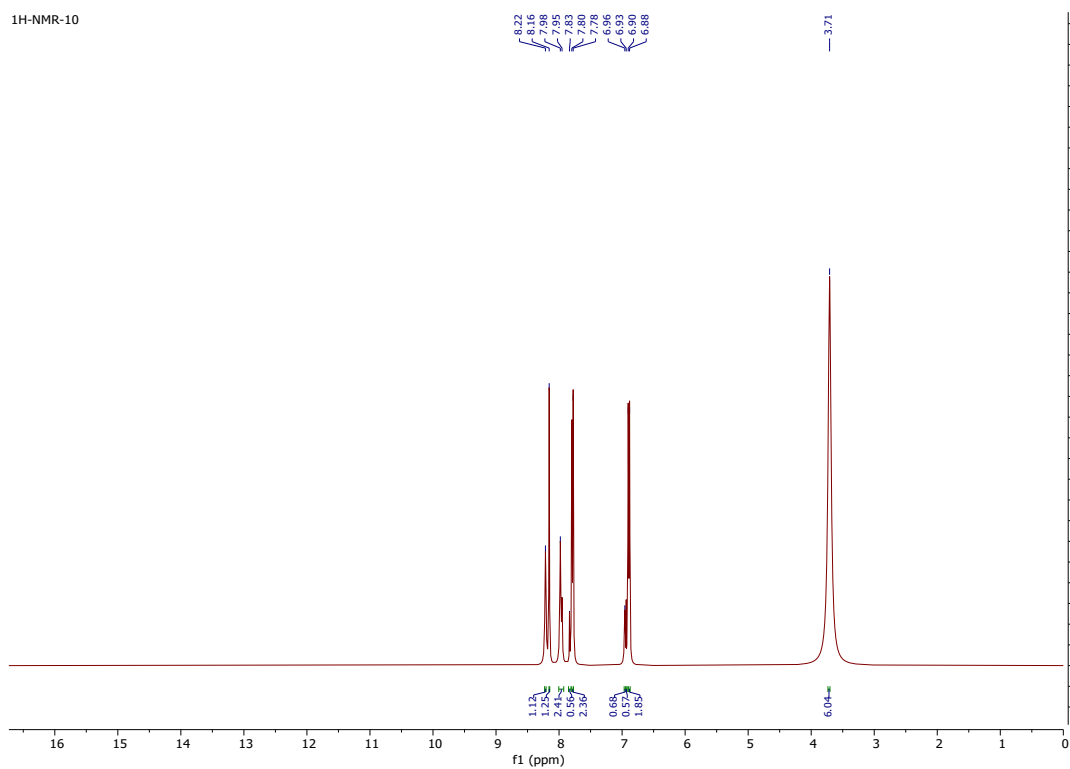
**Figure S12:**  $^1\text{H}$ -NMR (400 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **9**



**Figure S13:**  $^{13}\text{C}$ -NMR (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **9**.

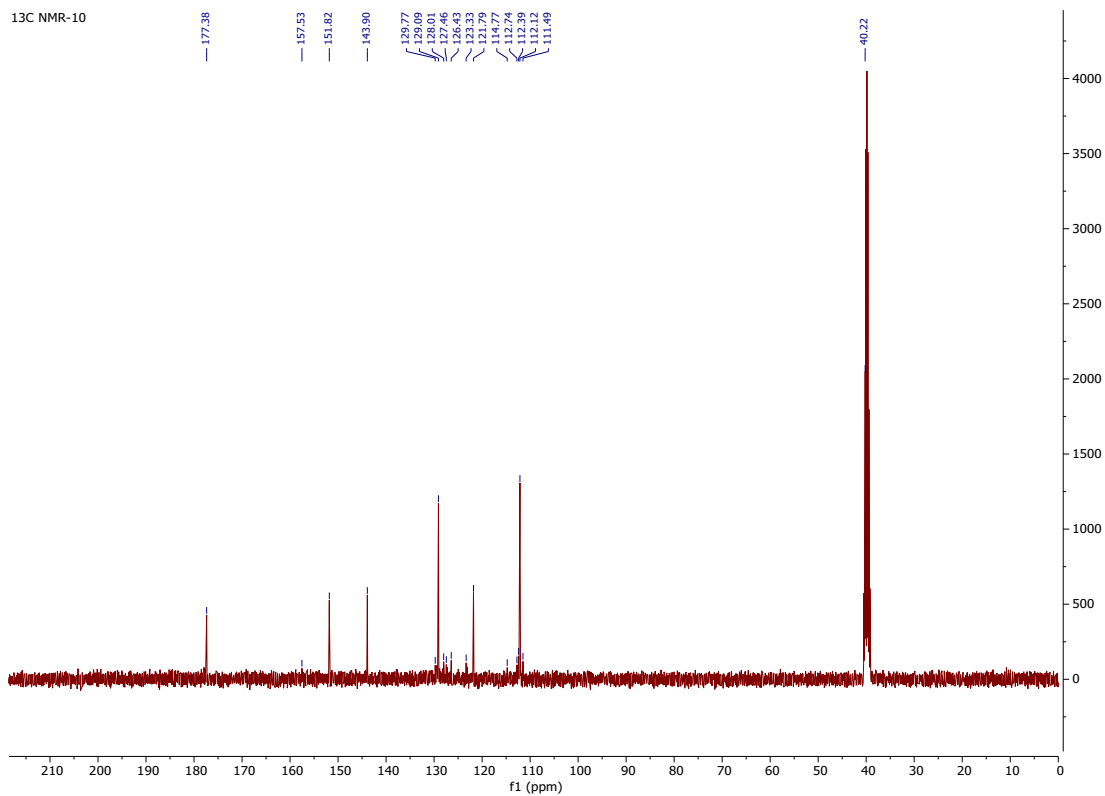


**Figure S14:** Dept-135 (100 MHz, DMSO- $d_6$ ) spectrum of compound **9**.

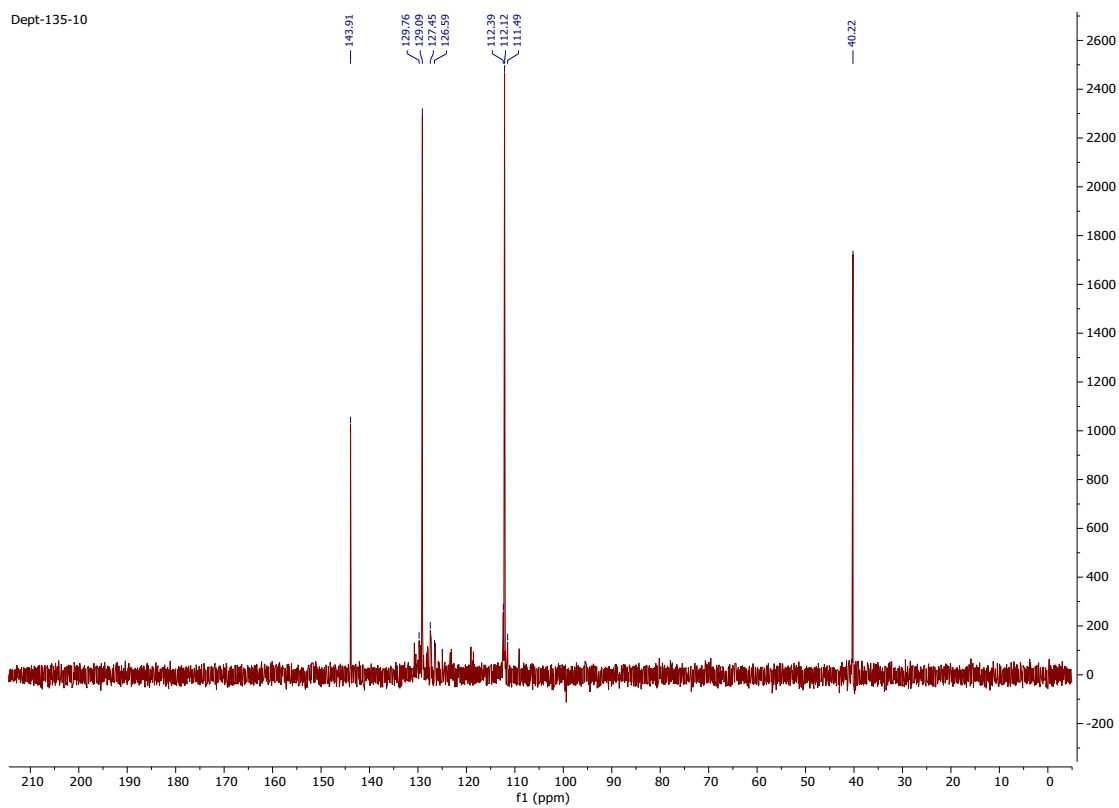


**Figure S15:**  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ ) spectrum of compound **10**.



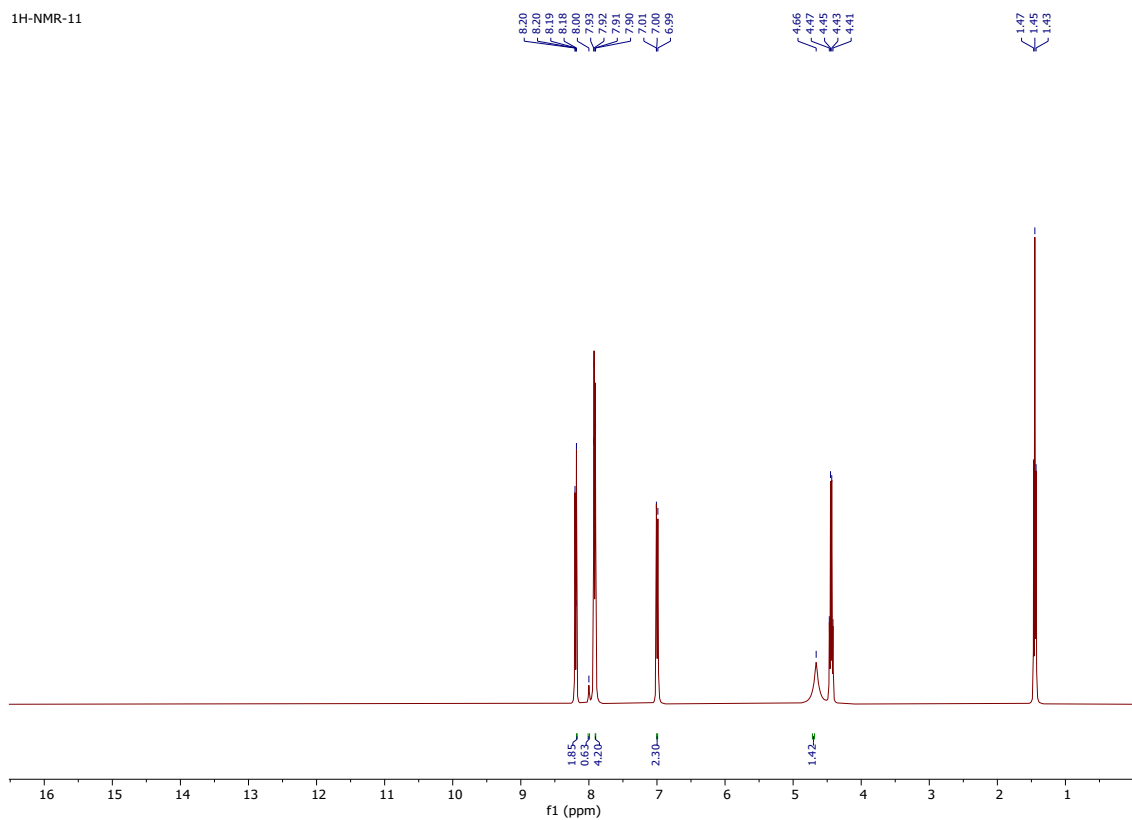


**Figure S16:**  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **10**.



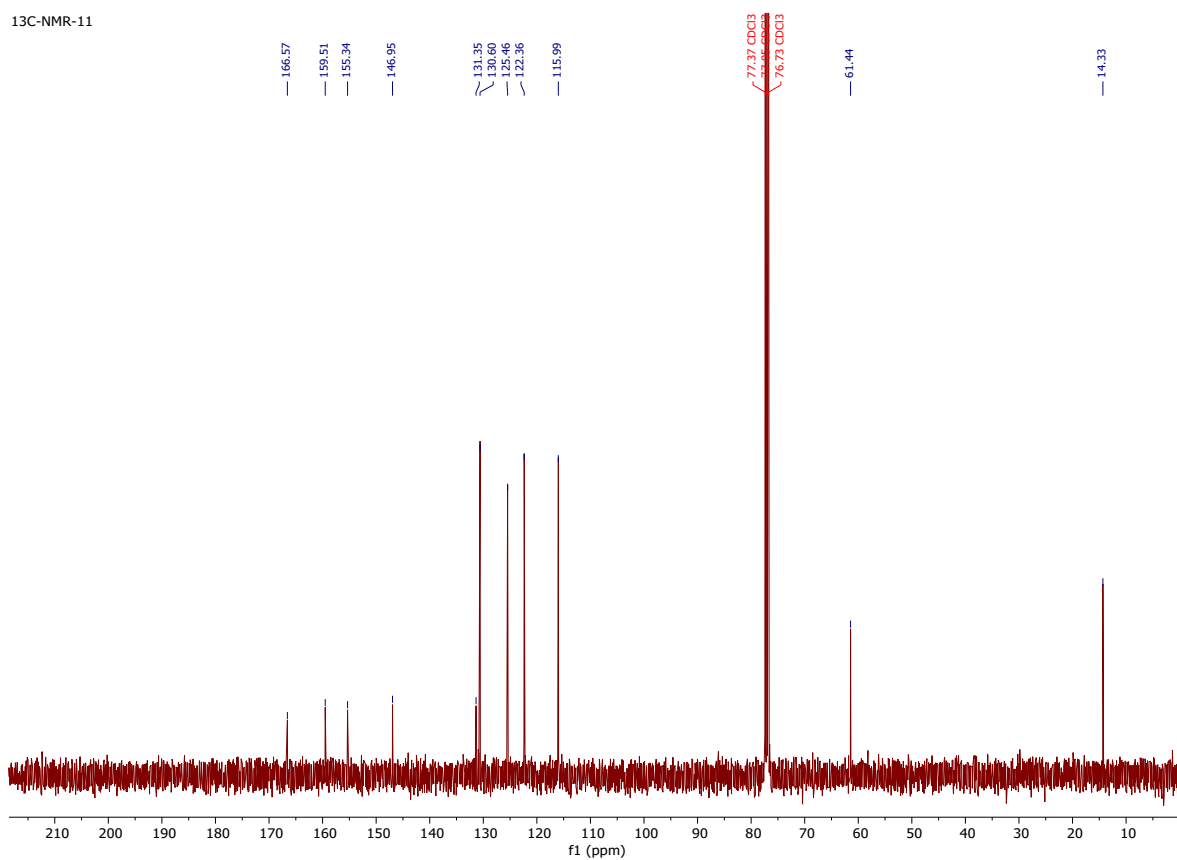
**Figure S17:** Dept-135 (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **10**.

1H-NMR-11

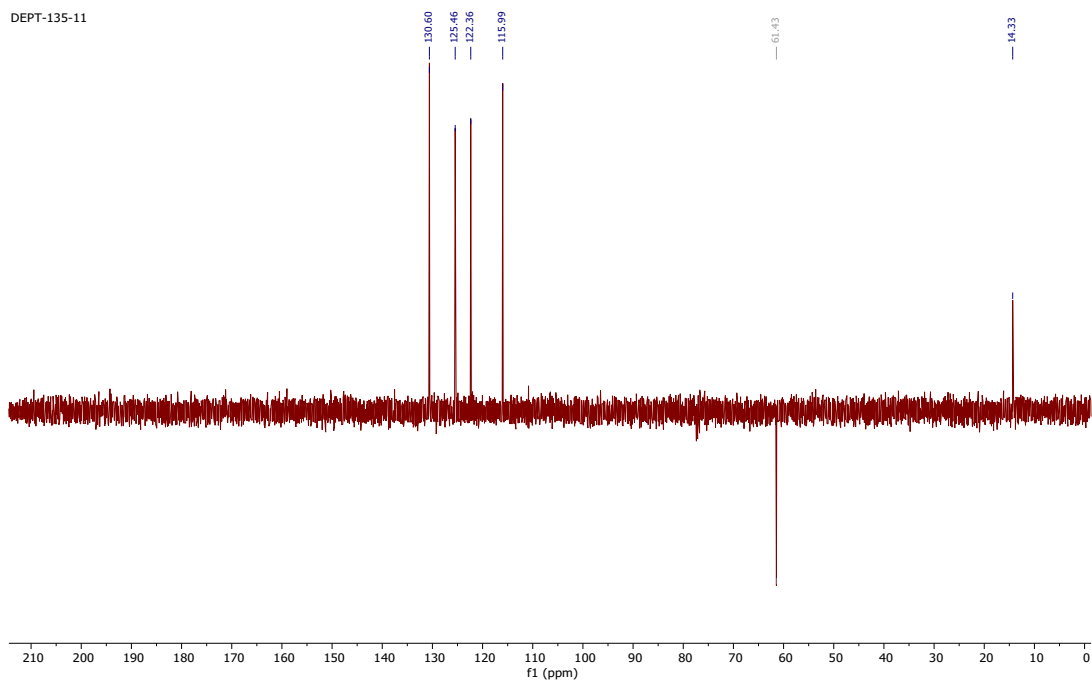


**Figure S18:**  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 400 MHz) spectrum of compound **11**.

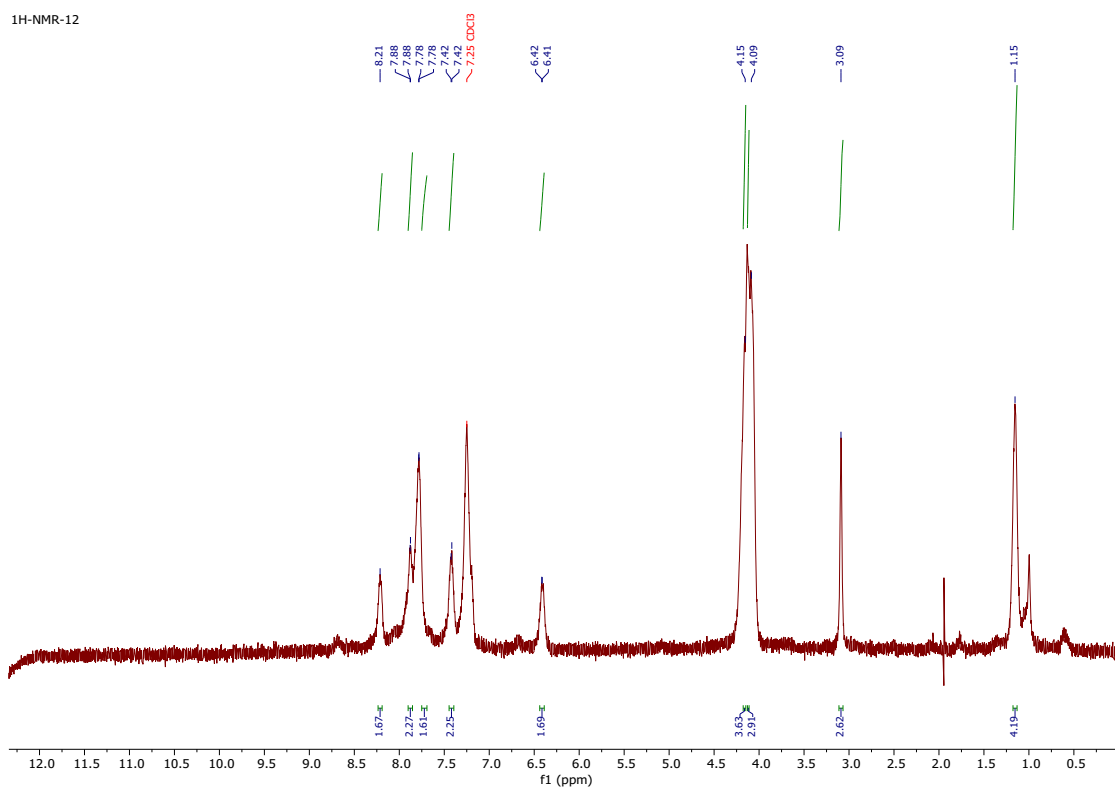
$^{13}\text{C-NMR-11}$



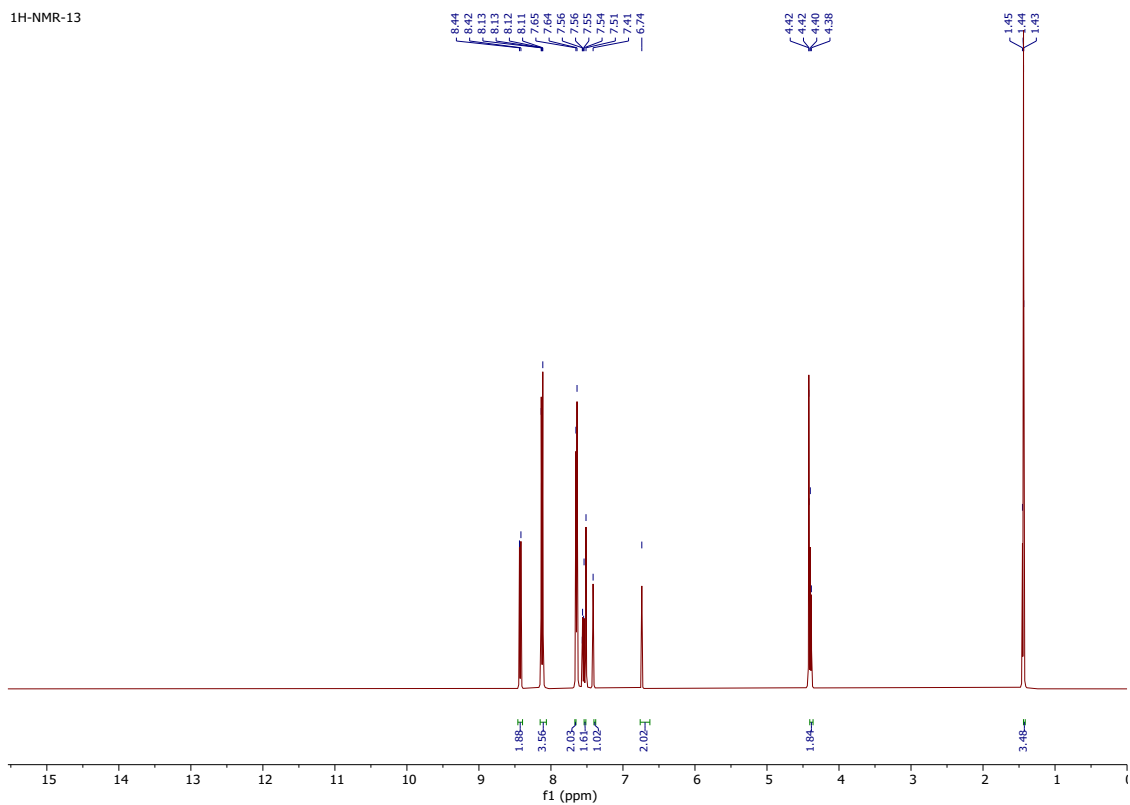
**Figure S19:**  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ , 101 MHz) spectrum of compound **11**.



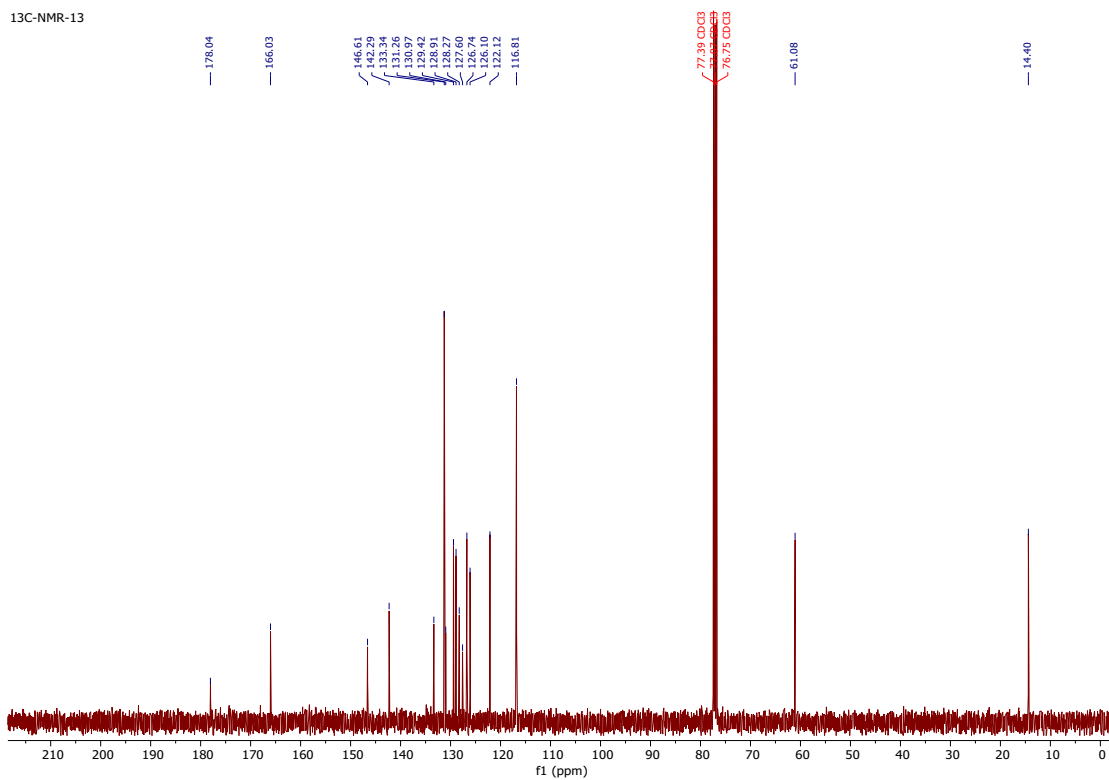
**Figure S20:** DEPT-135 (CDCl<sub>3</sub>, 101 MHz) spectrum of compound **11**.



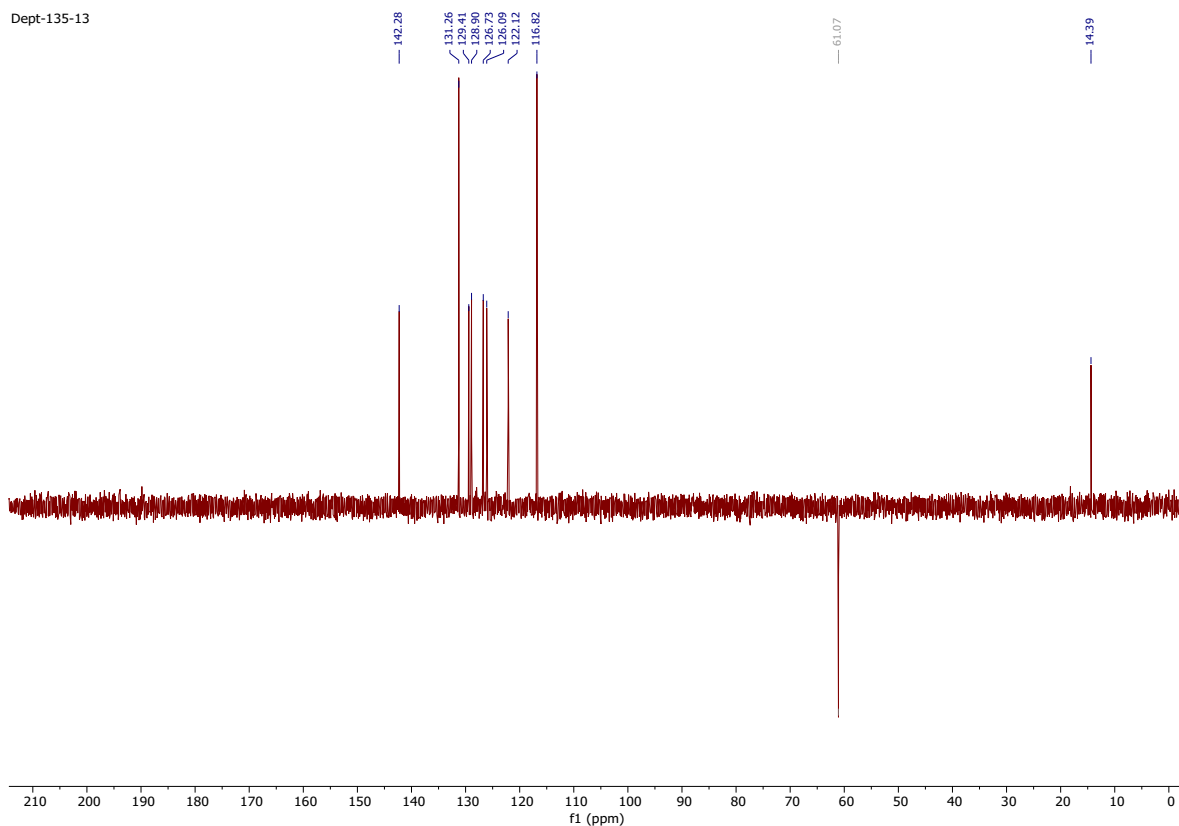
**Figure S21:** <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 400 MHz) spectrum of compound **12**.



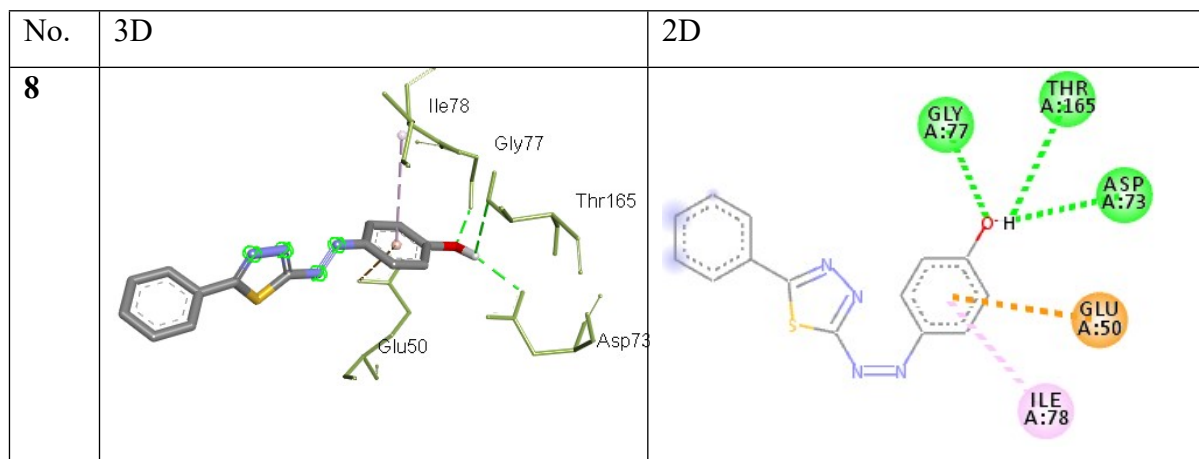
**Figure S22:**  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 400 MHz) spectra of compound **13**.

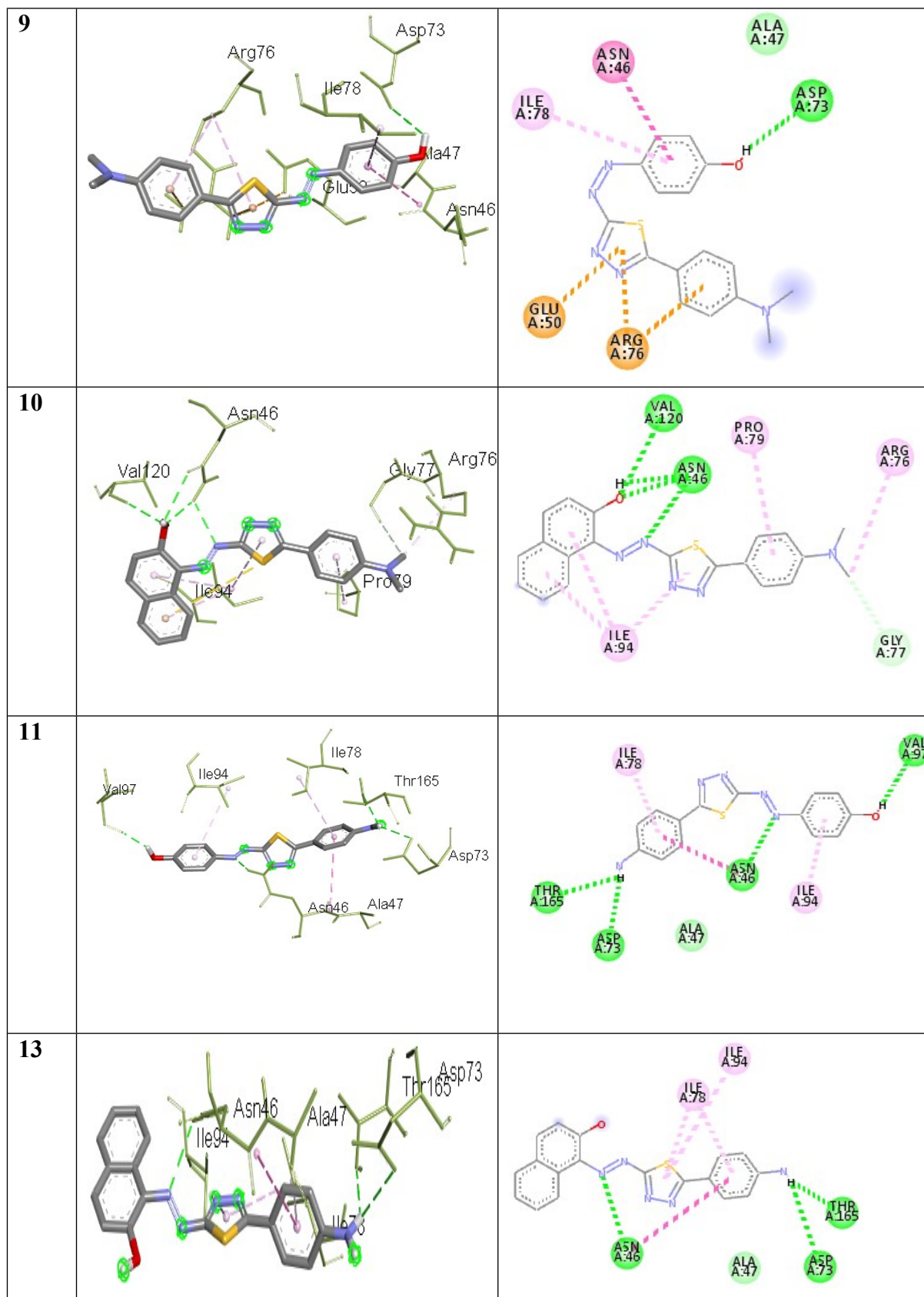


**Figure S23:**  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ , 101 MHz) spectrum of compound **13**.



**Figure S24:** DEPT-135 (CDCl<sub>3</sub>, 101 MHz) spectrum of compounds **13**.



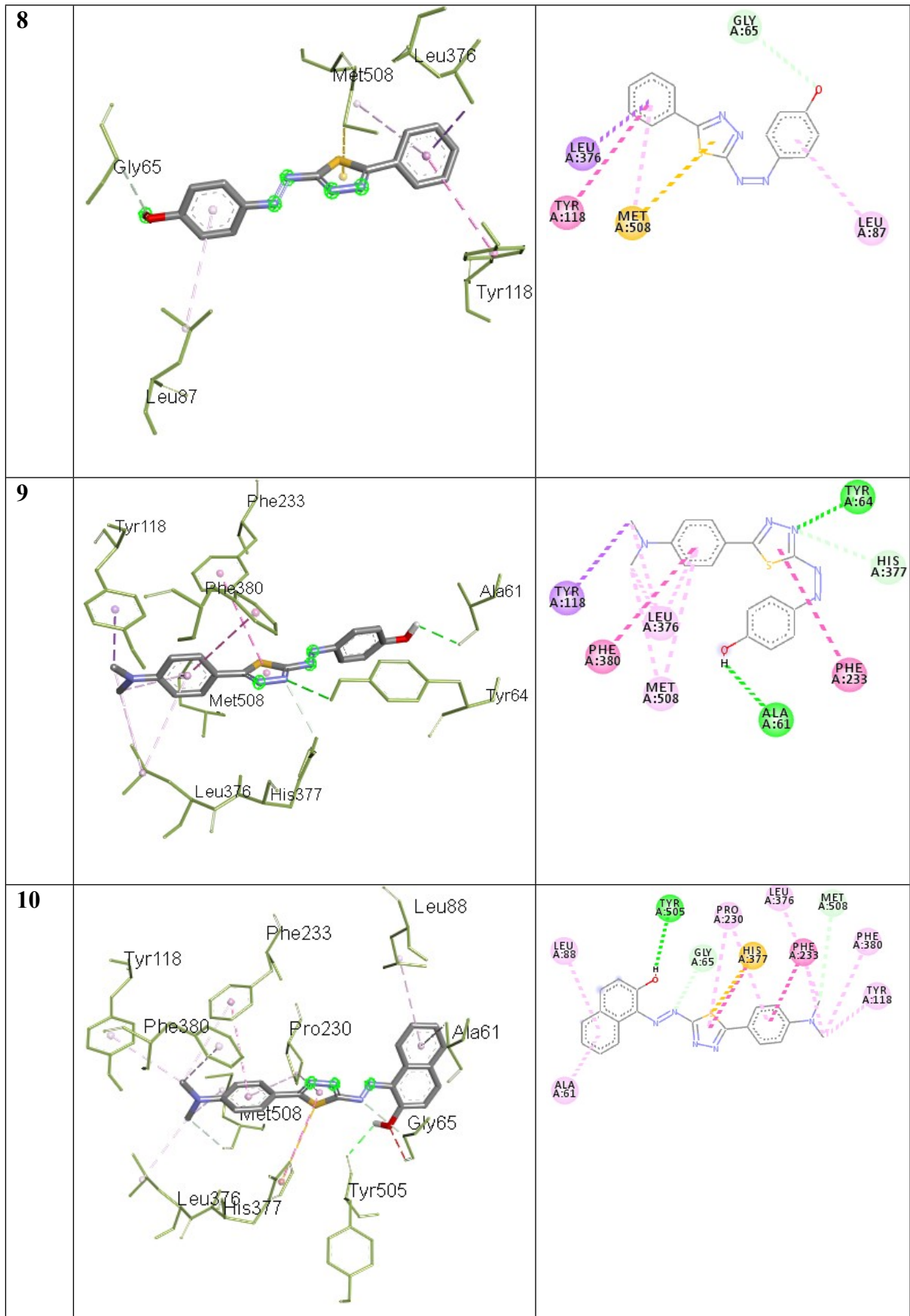


**Figure S25:** Binding interactions (3D & 2D) of the test compounds against *E. coli* DNA gyrase B.

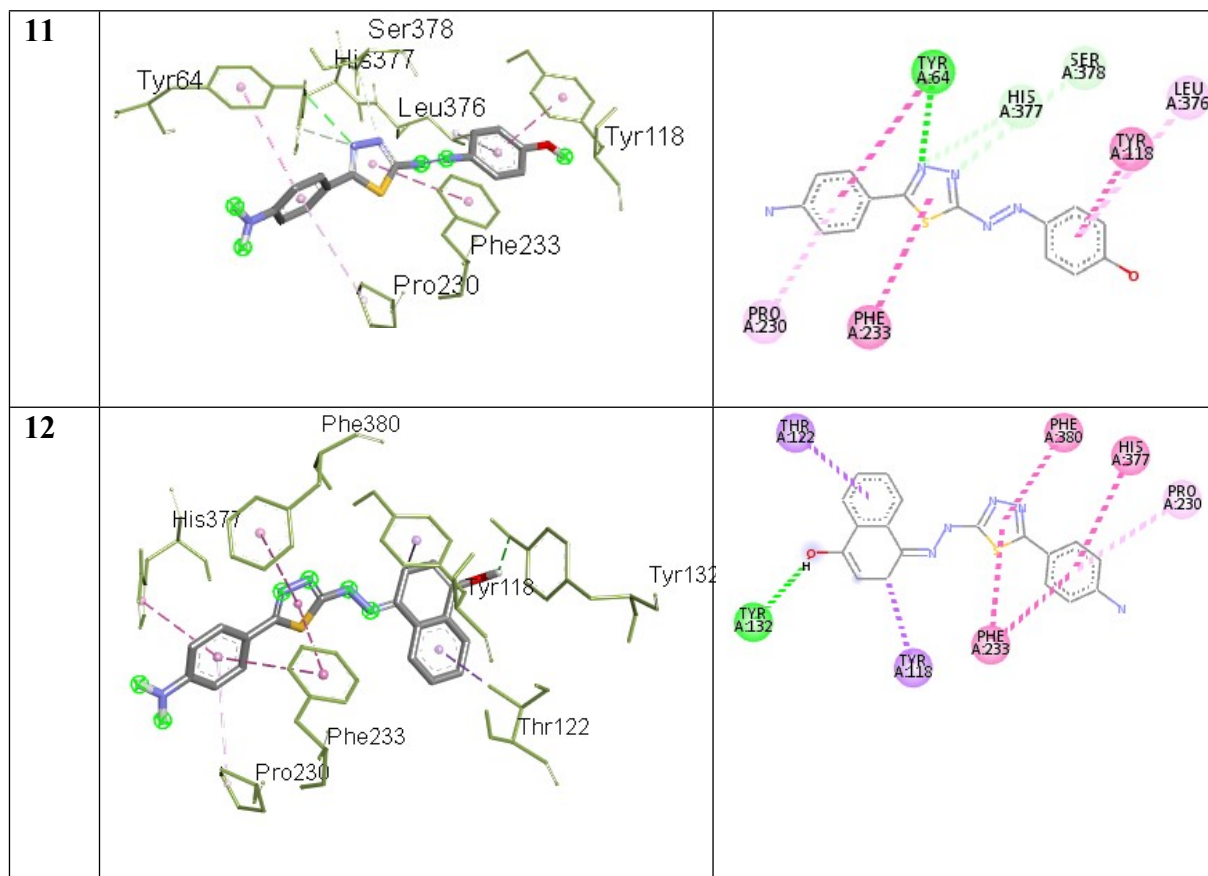
No.	3D	2D
8		
9		
11		
12		

**Figure S26:** Binding interactions (3D & 2D) of the test compounds against *S. aureus* PK

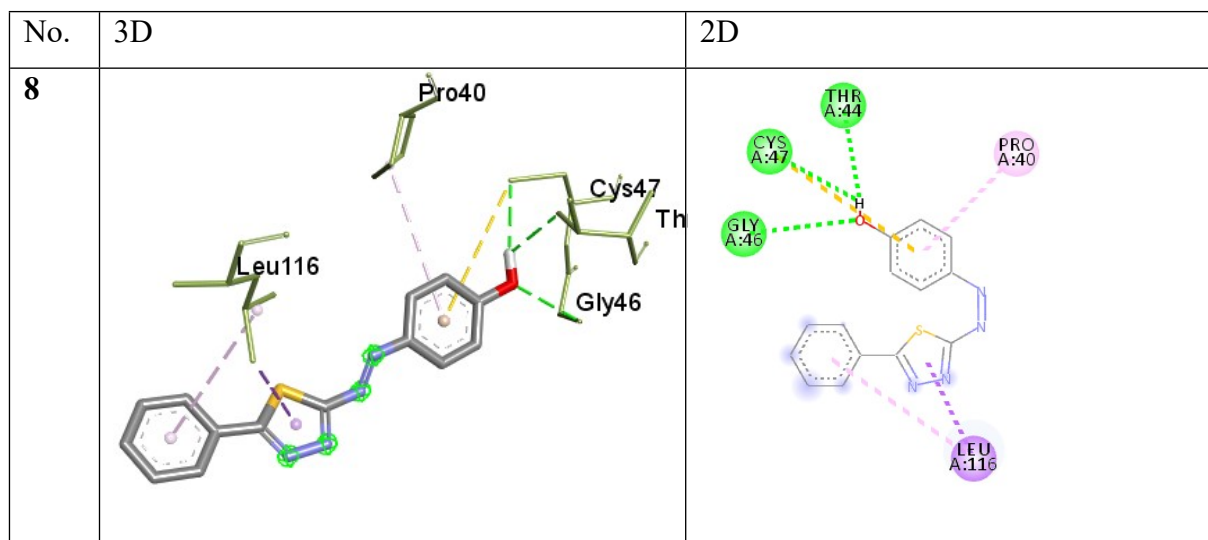
No.	3D	2D

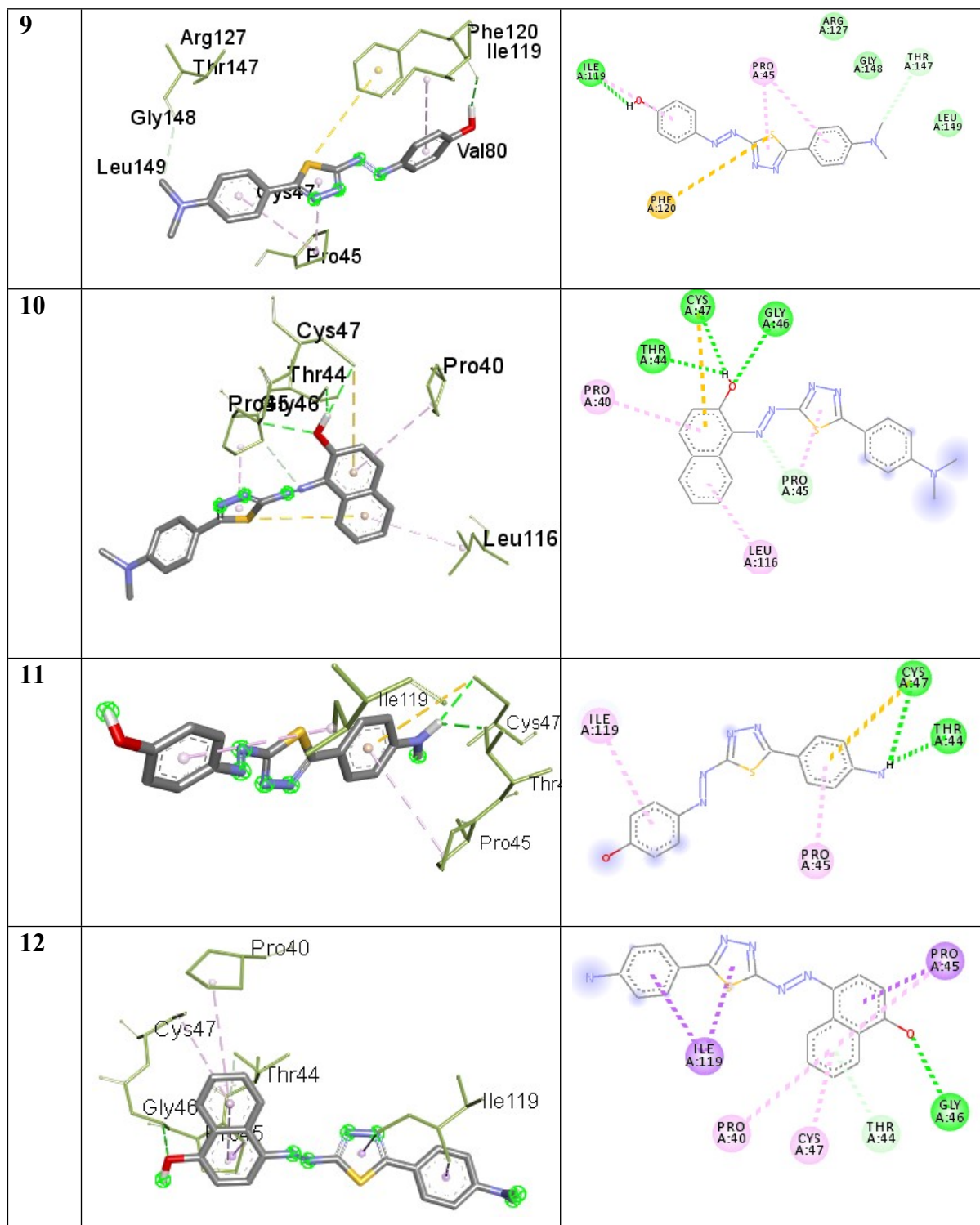






**Figure S27:** Binding interactions (3D & 2D) of the compounds (**8-13**) against *C. albicans* CYP51.





**Figure S28:** Binding interactions (3D & 2D) of the test compounds against human peroxidoxins 5