

## SUPPLEMENTARY MATERIAL

### Molecular docking reveals the potential of *Cleome amblyocarpa* isolated compounds to inhibit COVID-19 virus main protease

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#### Abstract

Nine flavonoids and one saponin were isolated from the aerial parts of *Cleome amblyocarpa*. Molecular Docking of isolated compounds on COVID-19 virus main protease showed variable binding affinities with scores ranging from (-8.63 to -6.08) compared to N3 inhibitor (-10.10) and binding modes better than N3 inhibitor in some of the isolated compounds. The descending order of binding affinity of the tested drugs was as follow; N3 inhibitor (**11**, docked) > kaempferitrin (**6**) > isorhamnetin 3,7-*O*- $\alpha$ -L-dirhamnoside (**3**) > kaempferol 3-*O*- $\beta$ -glucoside-7-*O*- $\alpha$ -rhamnoside (**2**) > soysaponin (**1**) > isorhamnetin 7-*O*- $\alpha$ -L-rhamnoside (**10**) > genistein-8-*C*-glucoside (**8**) > tamarixetin 7-*O*- $\beta$ -D-glucoside (**4**) > isoprunitin-7-glucoside (**9**) > genistin (**5**) > 5-*O*-methylgenistein (**7**). These results could be a good start for fast further examining the isolated compounds *in vitro* and *in vivo* either alone or in combinations for the treatment of COVID-19 virus. In addition, this work gives an explanation on the SAR required for targeting the newly emerged SARS-CoV-2 protease and facilitates the future design and synthesis of new drugs targeting it as well.

Key words: COVID-19; *Cleome amblyocarpa*; molecular docking; flavanoids

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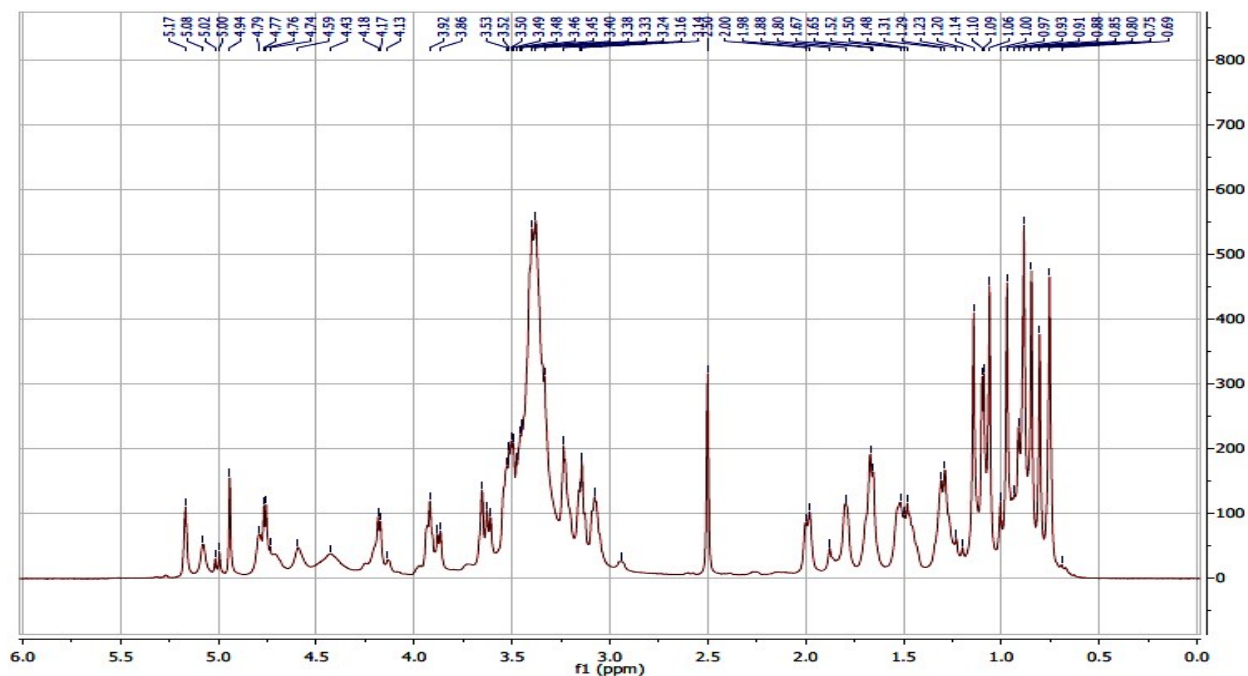


Figure S1:  $^1\text{H}$  - NMR spectrum (DMSO- $d_6$ , 400 MHz) of compound **1**

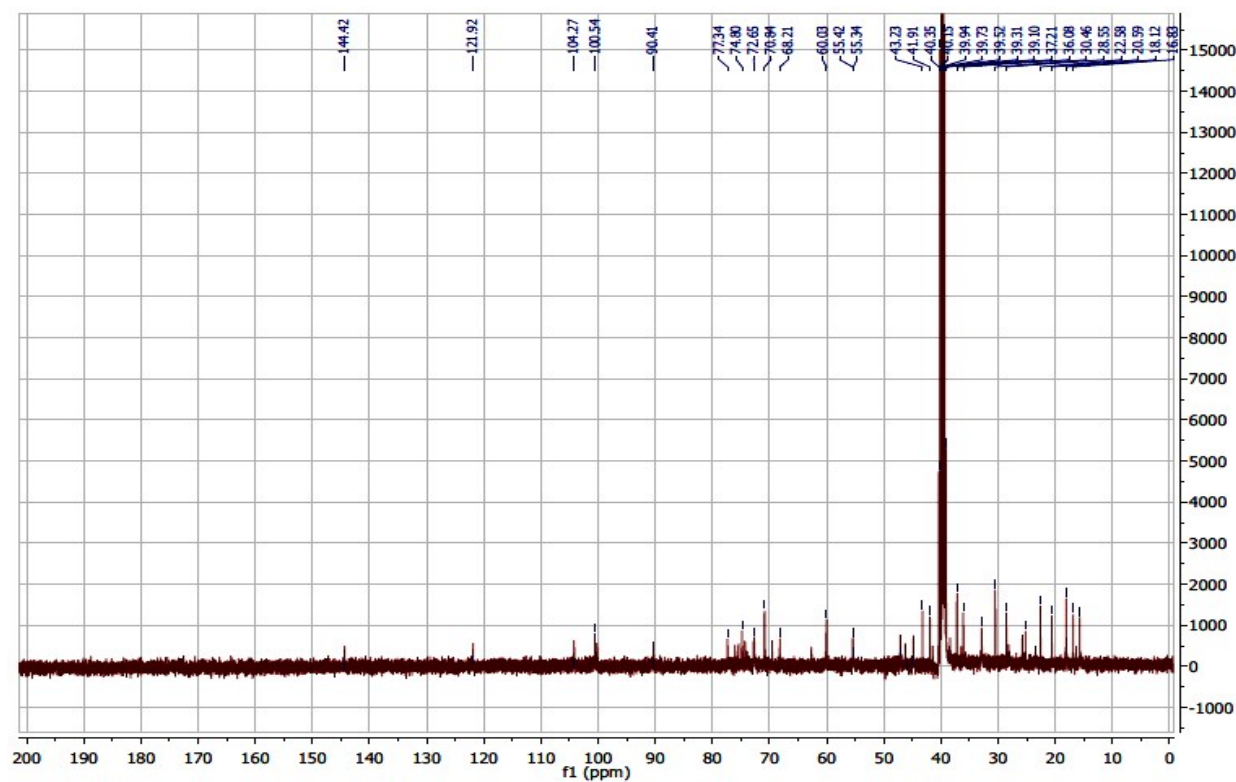


Figure S2:  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ , 100 MHz) of compound **1**

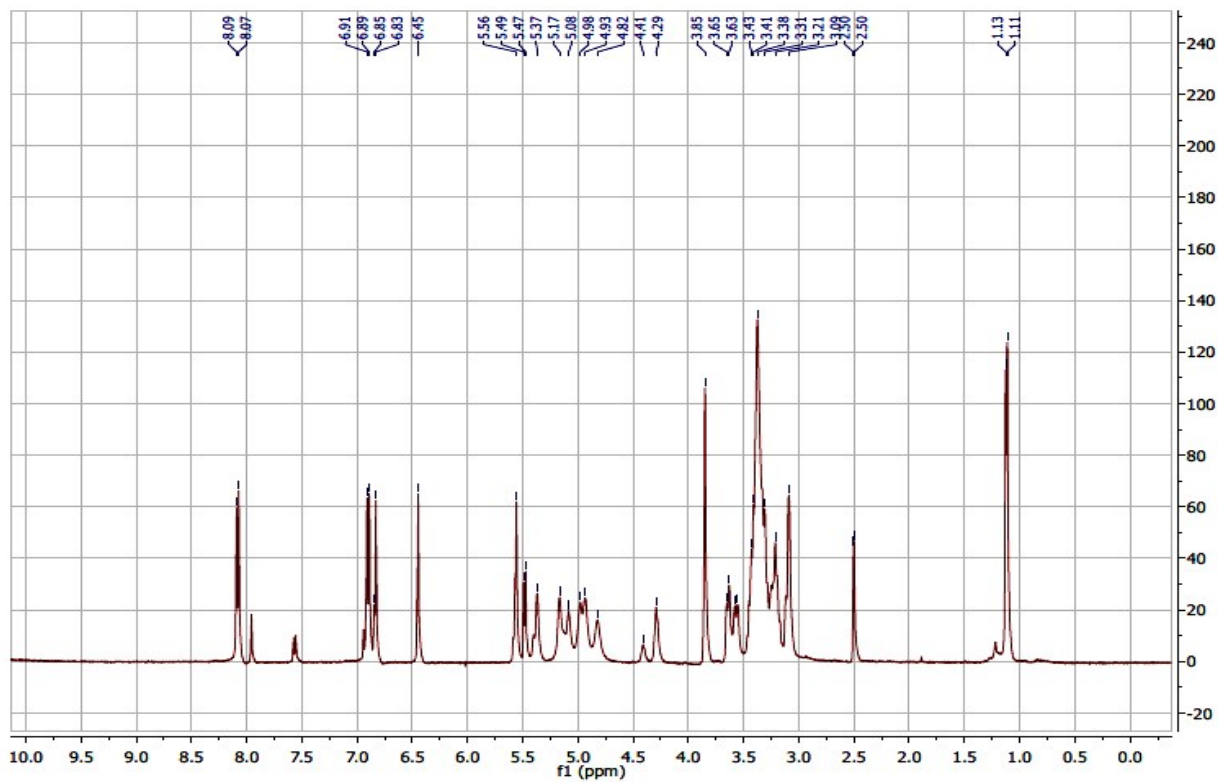


Figure S3:  $^1\text{H}$  - NMR spectrum (DMSO- $d_6$ , 400 MHz) of compound 2

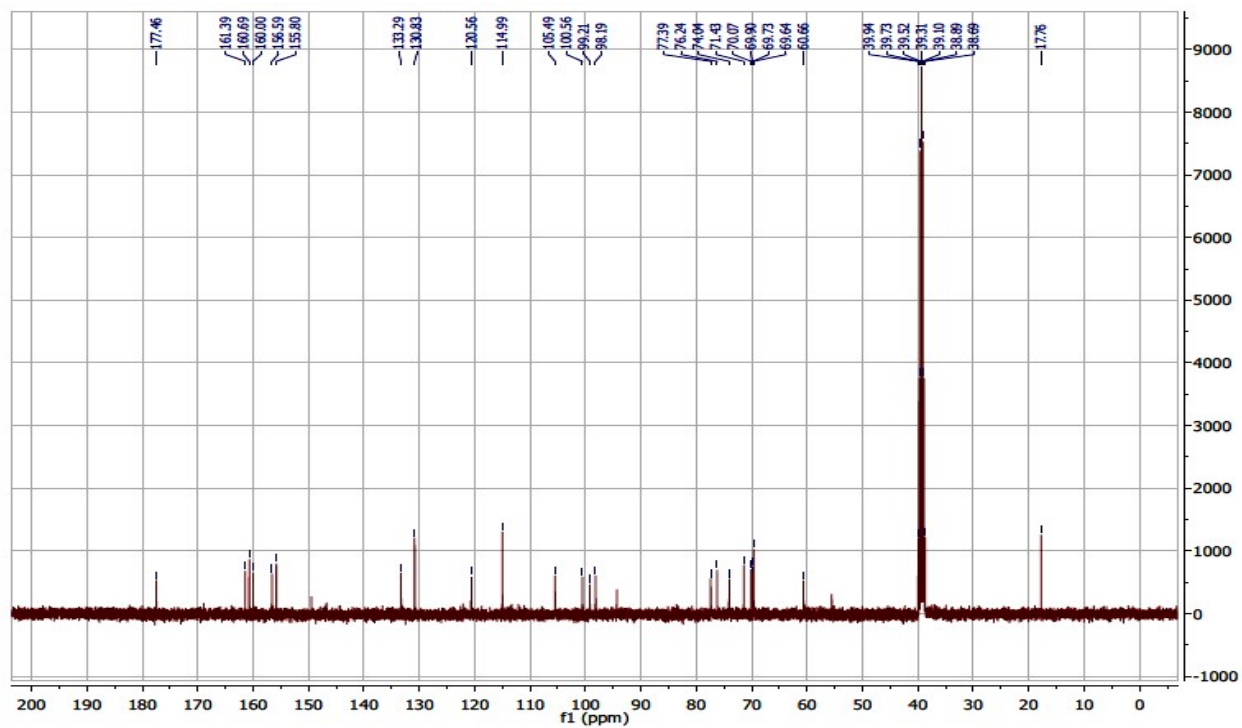


Figure S4:  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ , 100 MHz) of compound 2

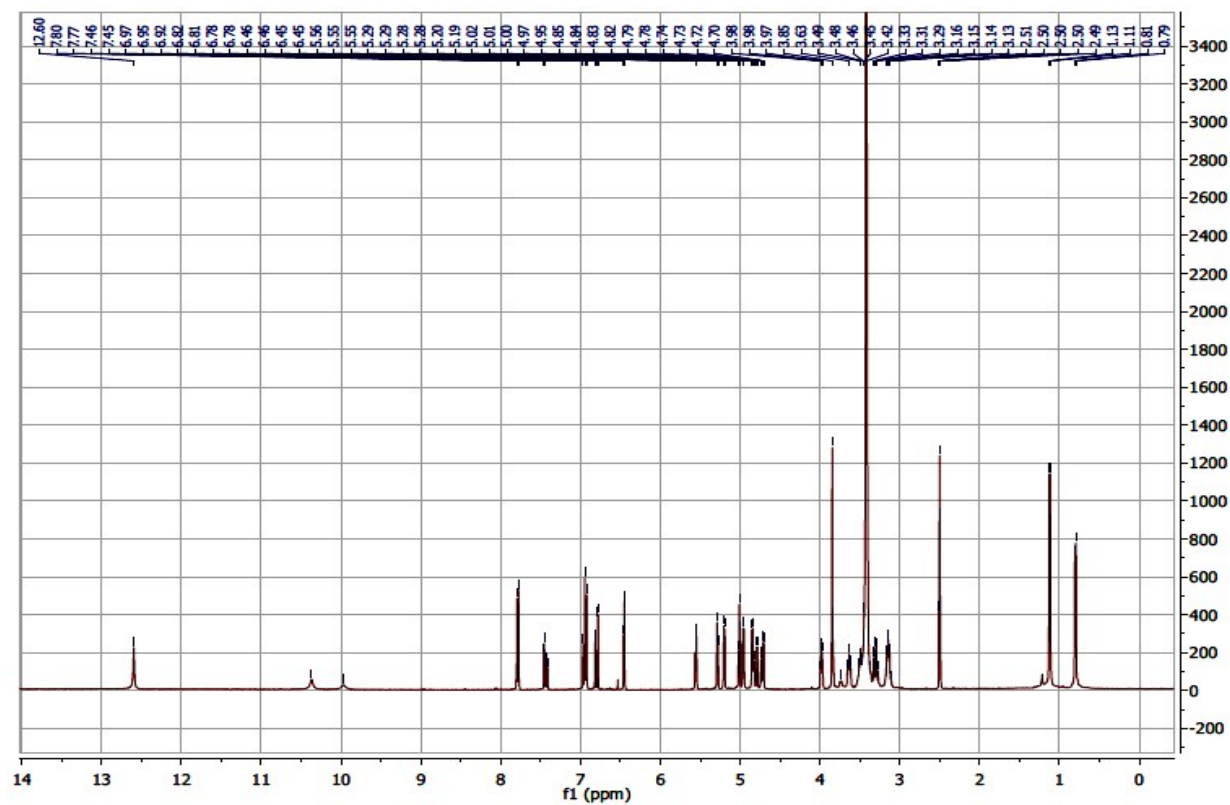


Figure S5:  $^1\text{H}$ -NMR spectrum ( $\text{DMSO-}d_6$ , 400 MHz) of compound 3

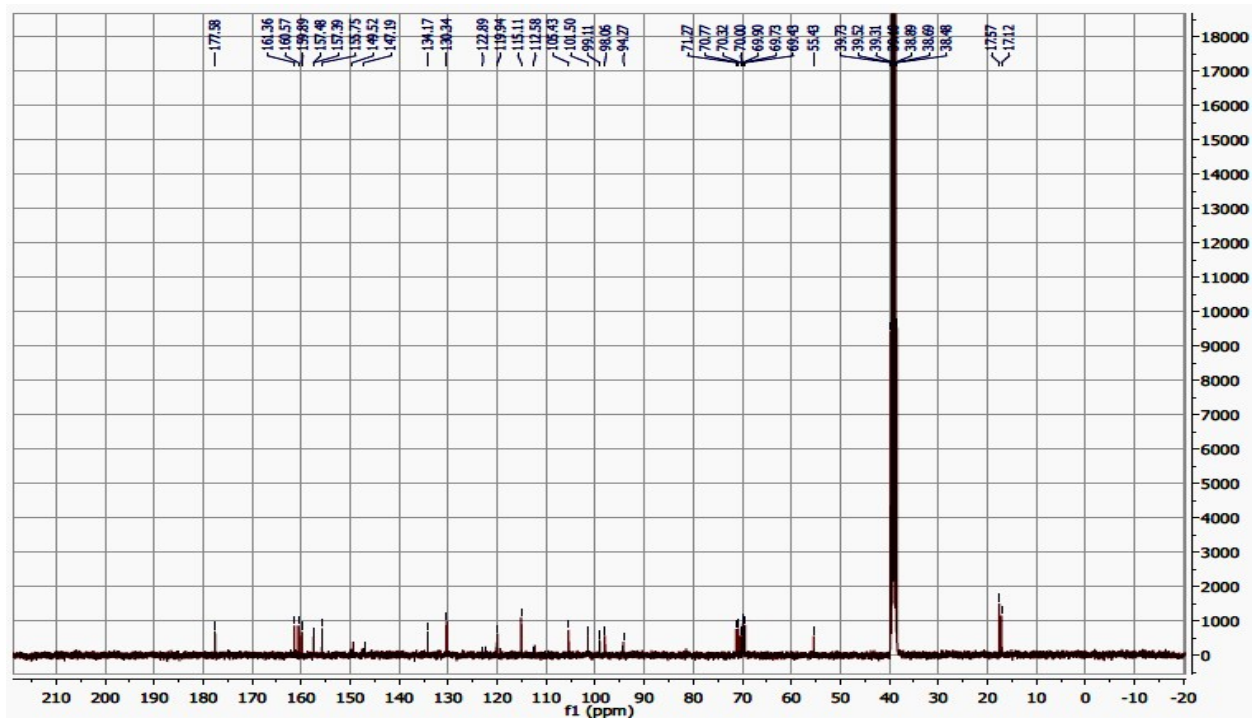


Figure S6:  $^{13}\text{C}$  NMR spectrum ( $\text{DMSO-}d_6$ , 100 MHz) of compound 3



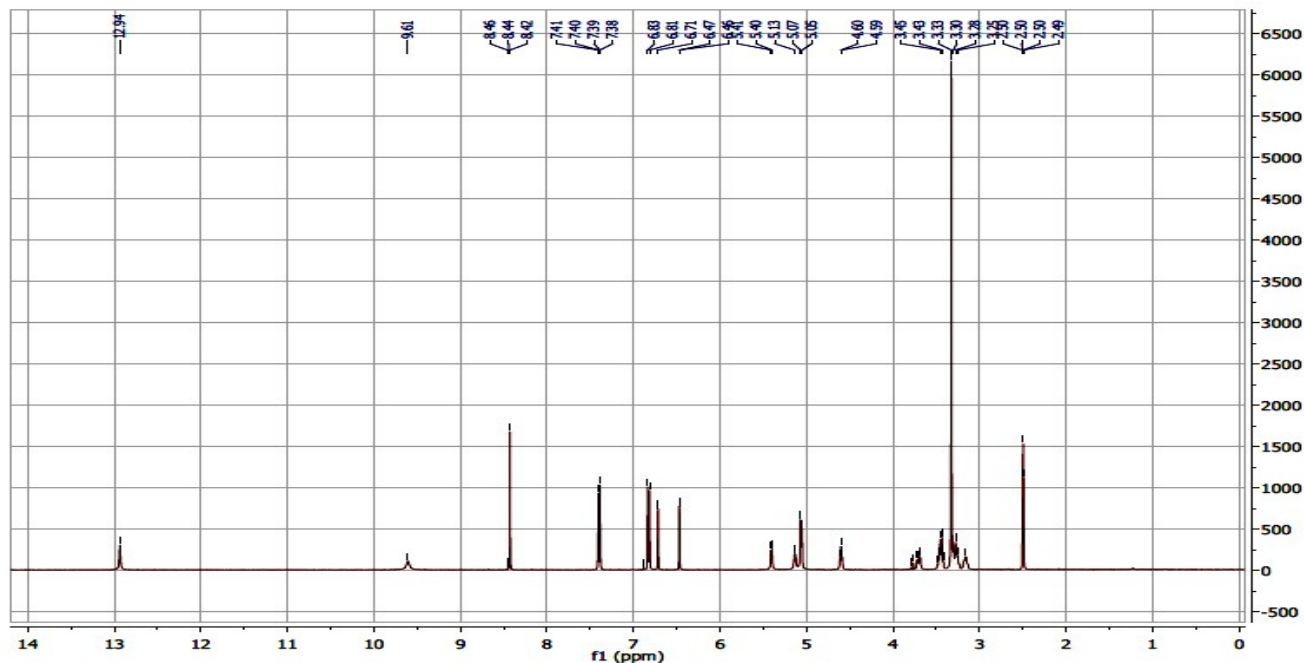


Figure S9:  $^1\text{H}$  - NMR spectrum (DMSO- $d_6$ , 400 MHz) of compound 5

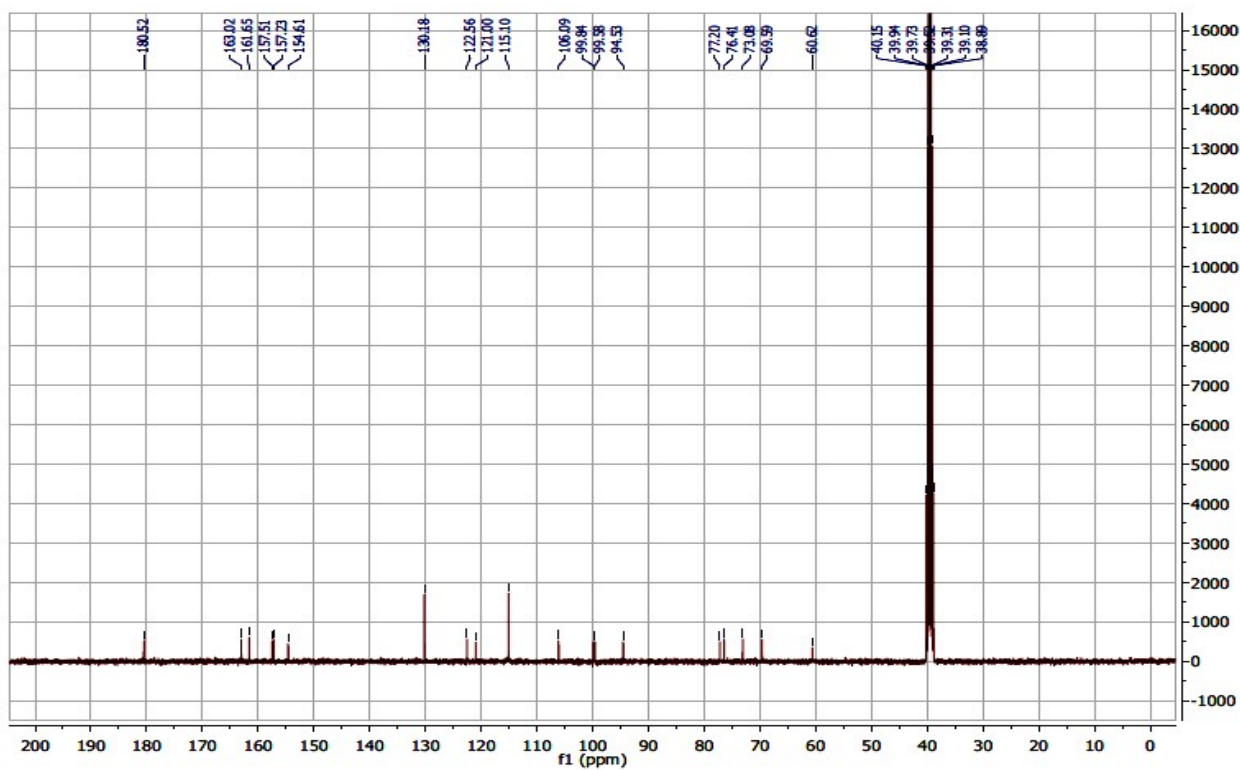


Figure S10:  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ , 100 MHz) of compound 5

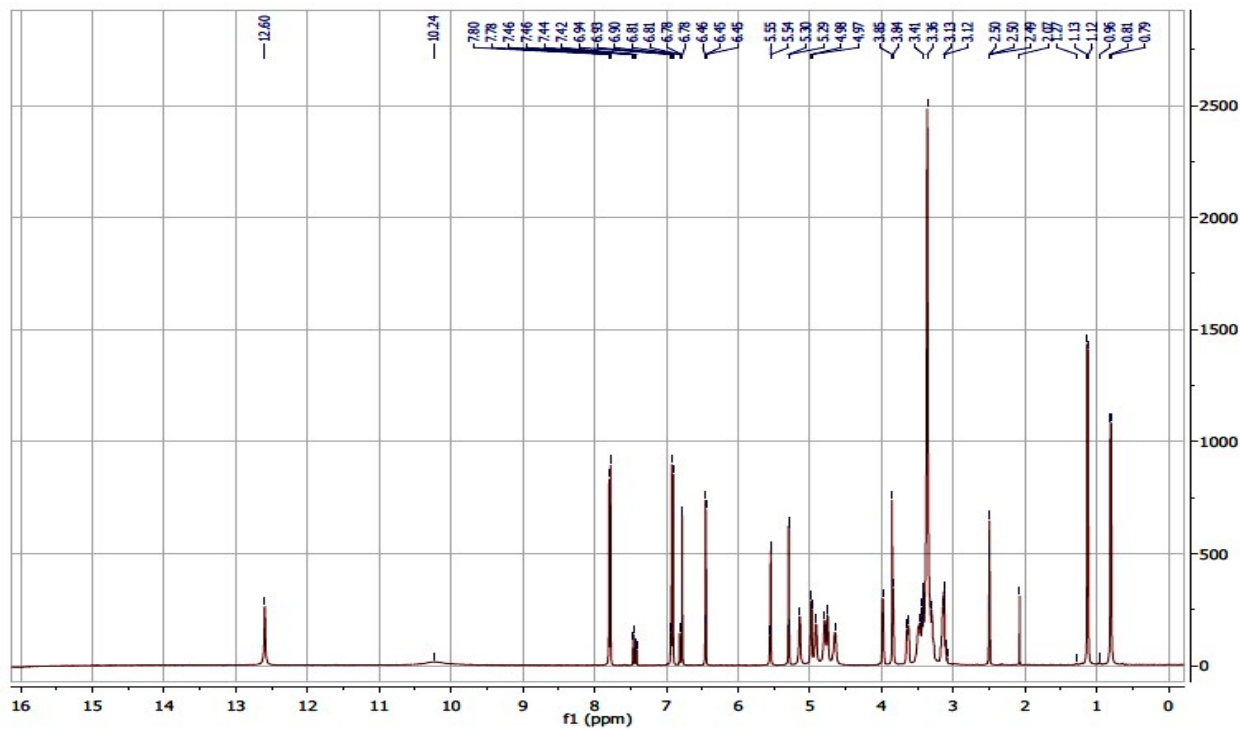


Figure S11:  $^1\text{H}$  - NMR spectrum (DMSO- $d_6$ , 400 MHz) of compound 6

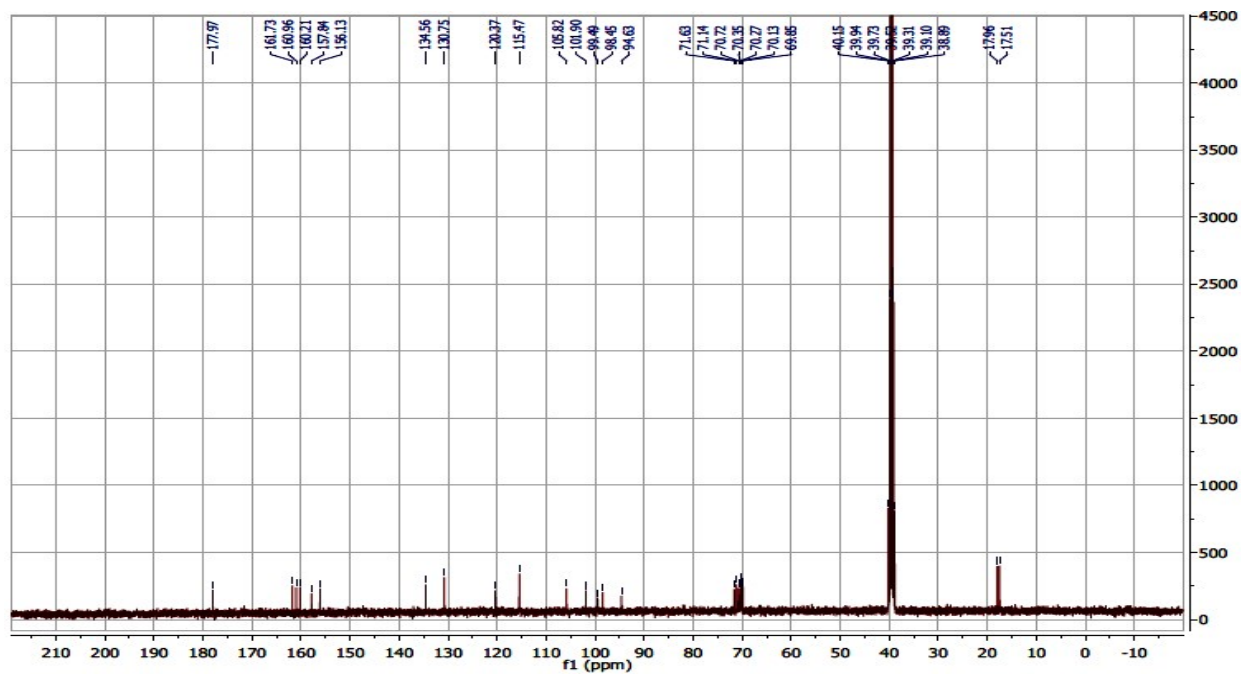


Figure S12:  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ , 100 MHz) of compound 6



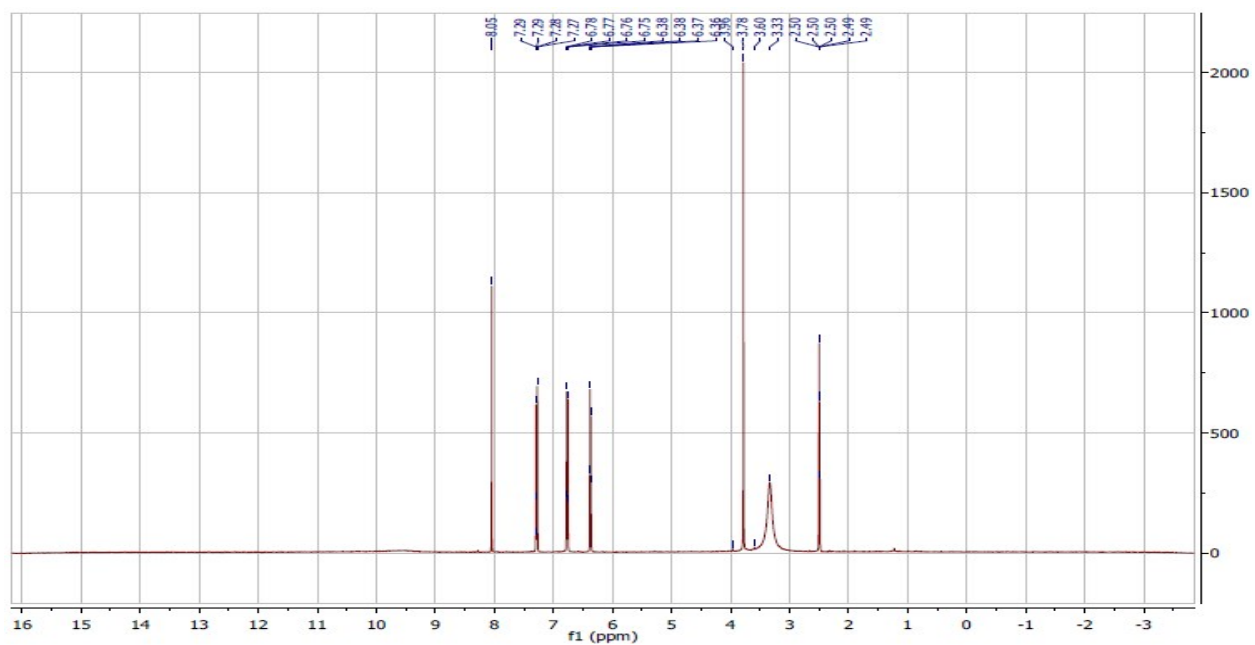


Figure S13:  $^1\text{H}$  - NMR spectrum (DMSO- $d_6$ , 400 MHz) of compound 7

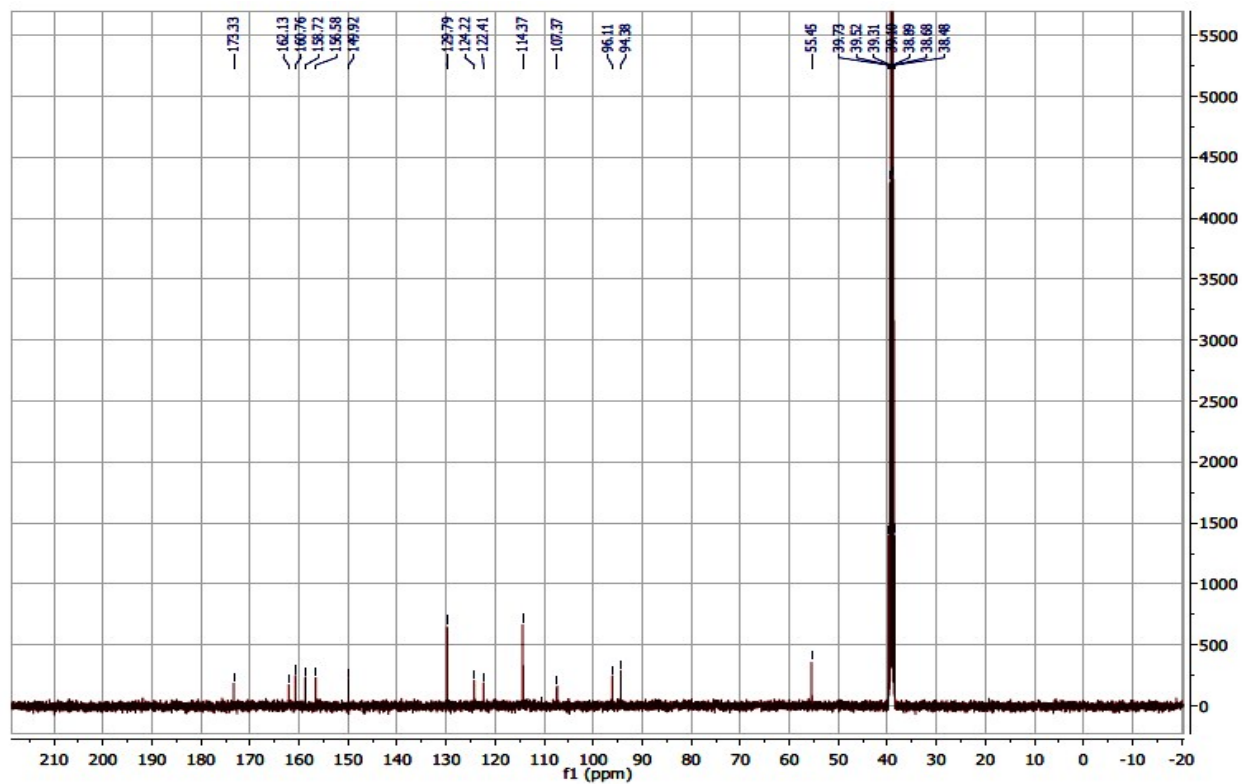


Figure S14:  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ , 100 MHz) of compound 7

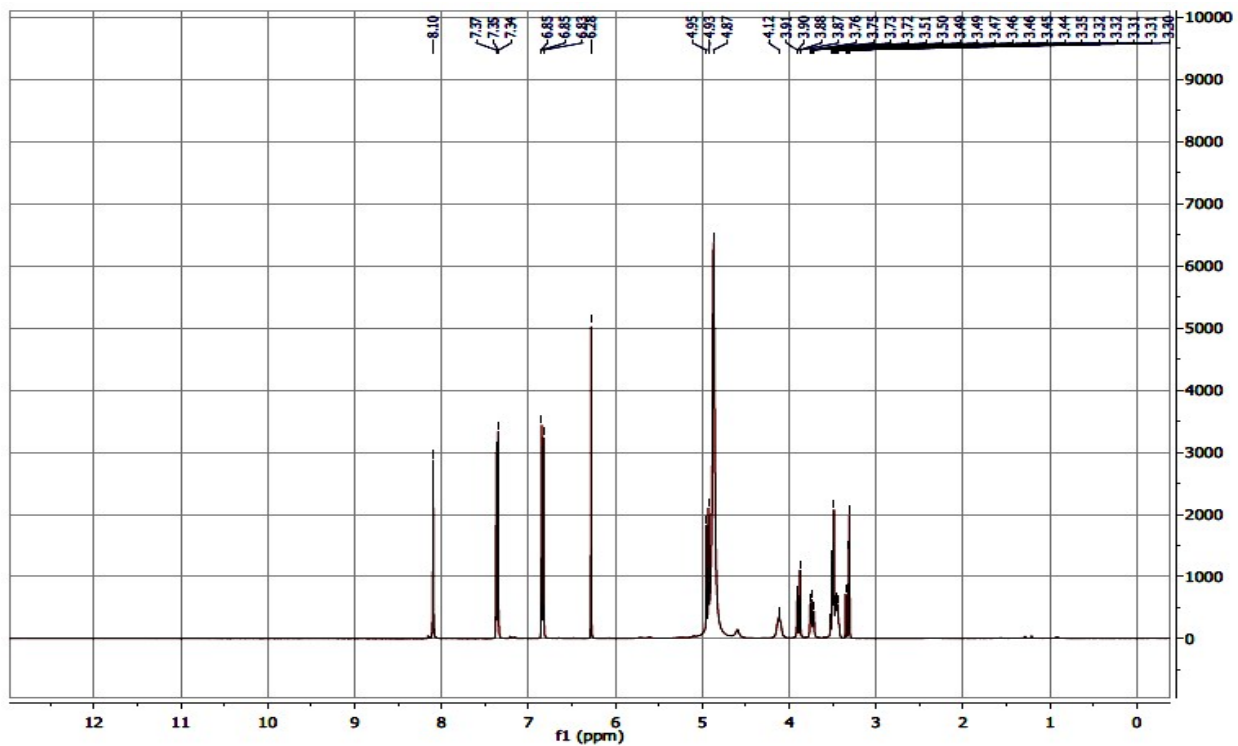


Figure S15:  $^1\text{H}$  - NMR spectrum ( $\text{CD}_3\text{OD}$ , 400 MHz) of compound **8**

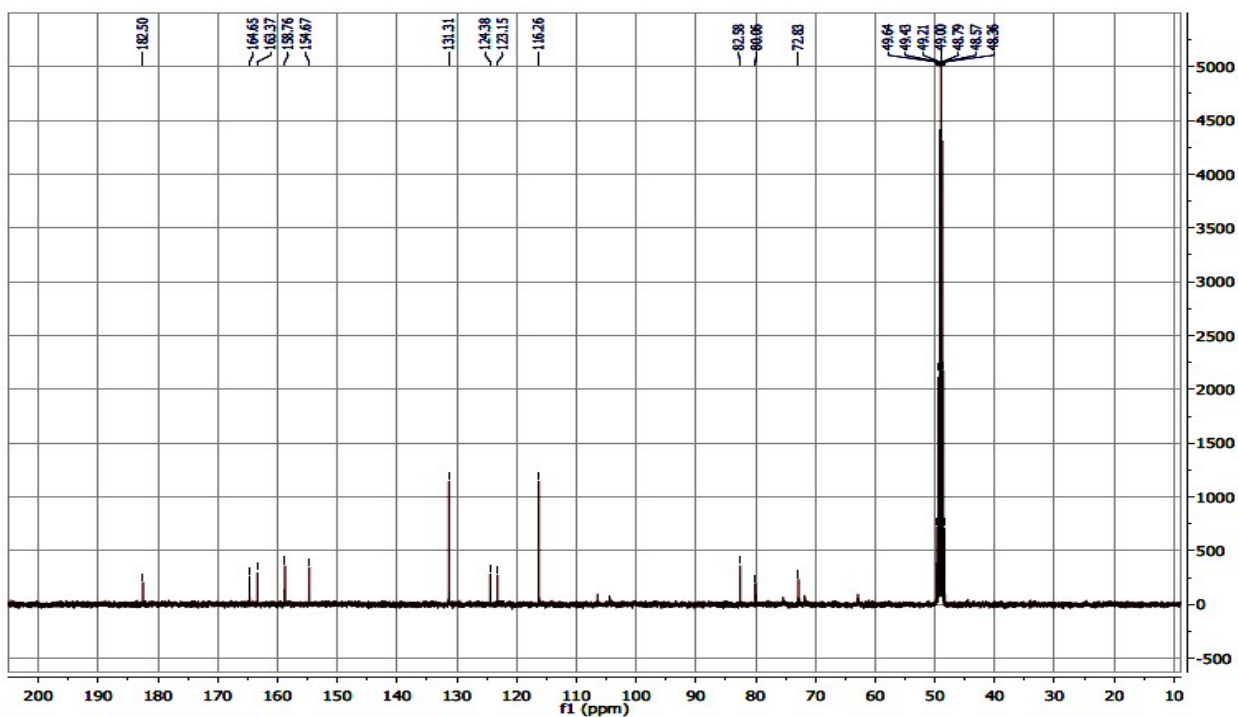


Figure S16:  $^{13}\text{C}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 100 MHz) of compound **8**

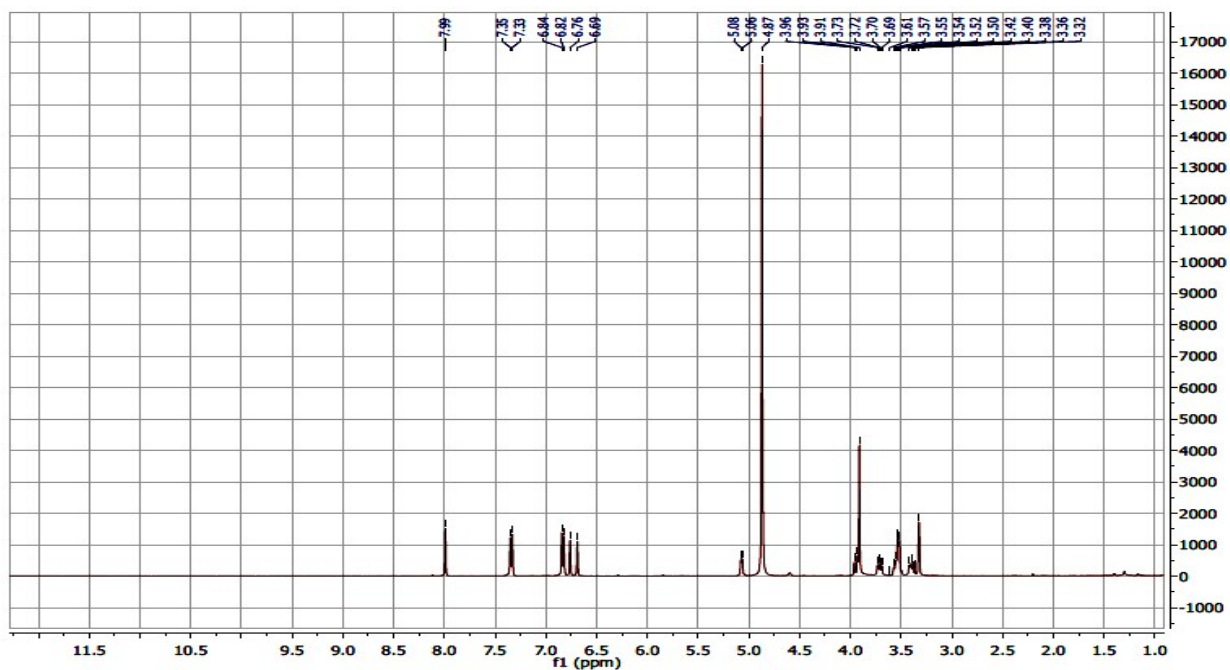


Figure S17: <sup>1</sup>H - NMR spectrum (CD<sub>3</sub>OD, 400 MHz) of compound 9

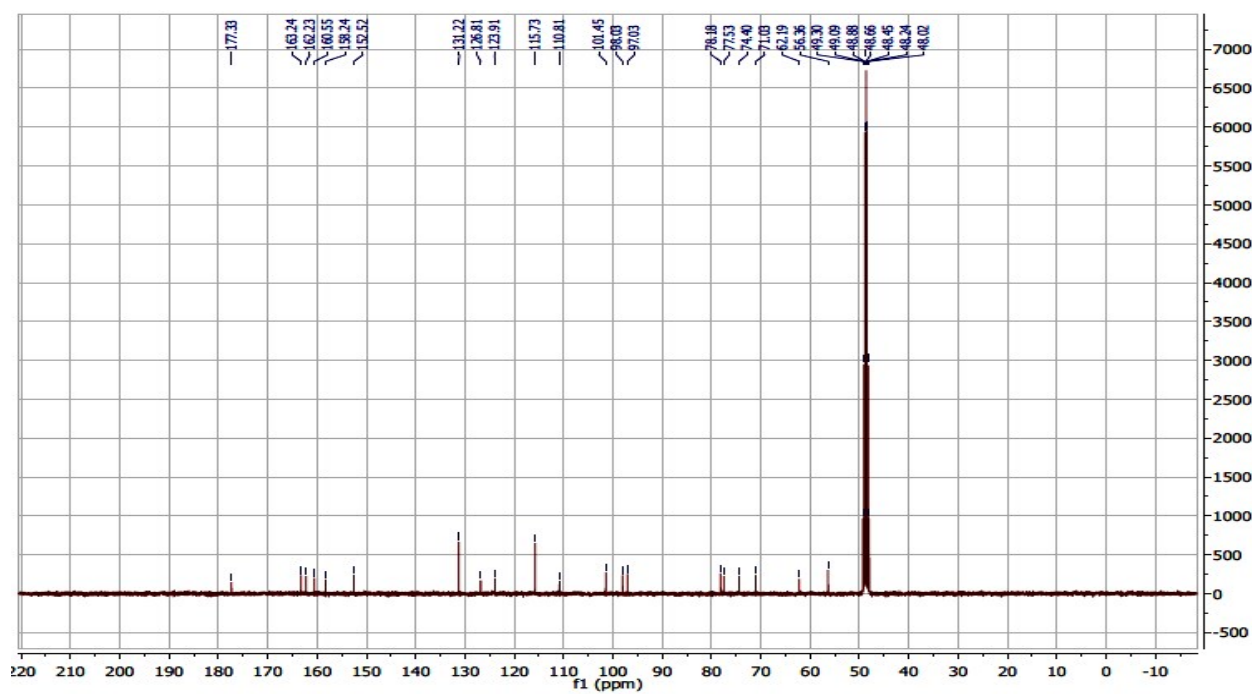


Figure S18: <sup>13</sup>C NMR spectrum (CD<sub>3</sub>OD, 100 MHz) of compound 9

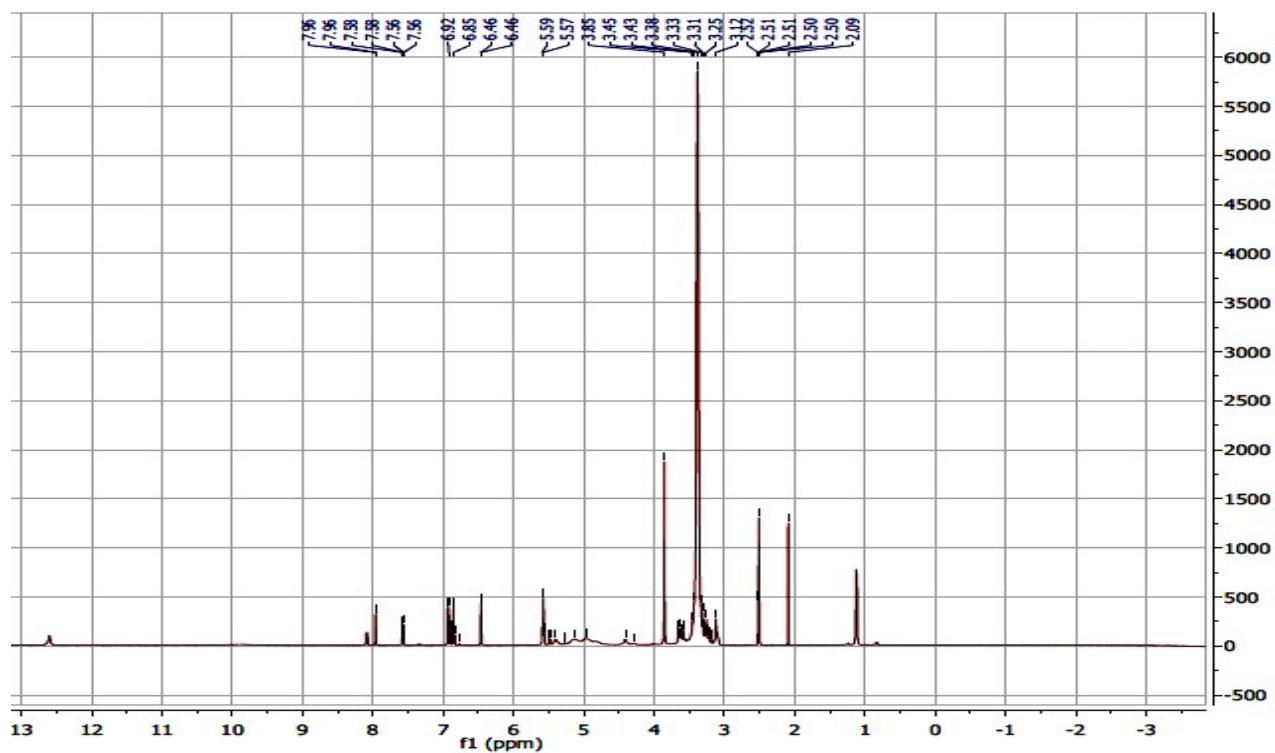


Figure S19:  $^1\text{H}$  - NMR spectrum (DMSO- $d_6$ , 400 MHz) of compound **10**

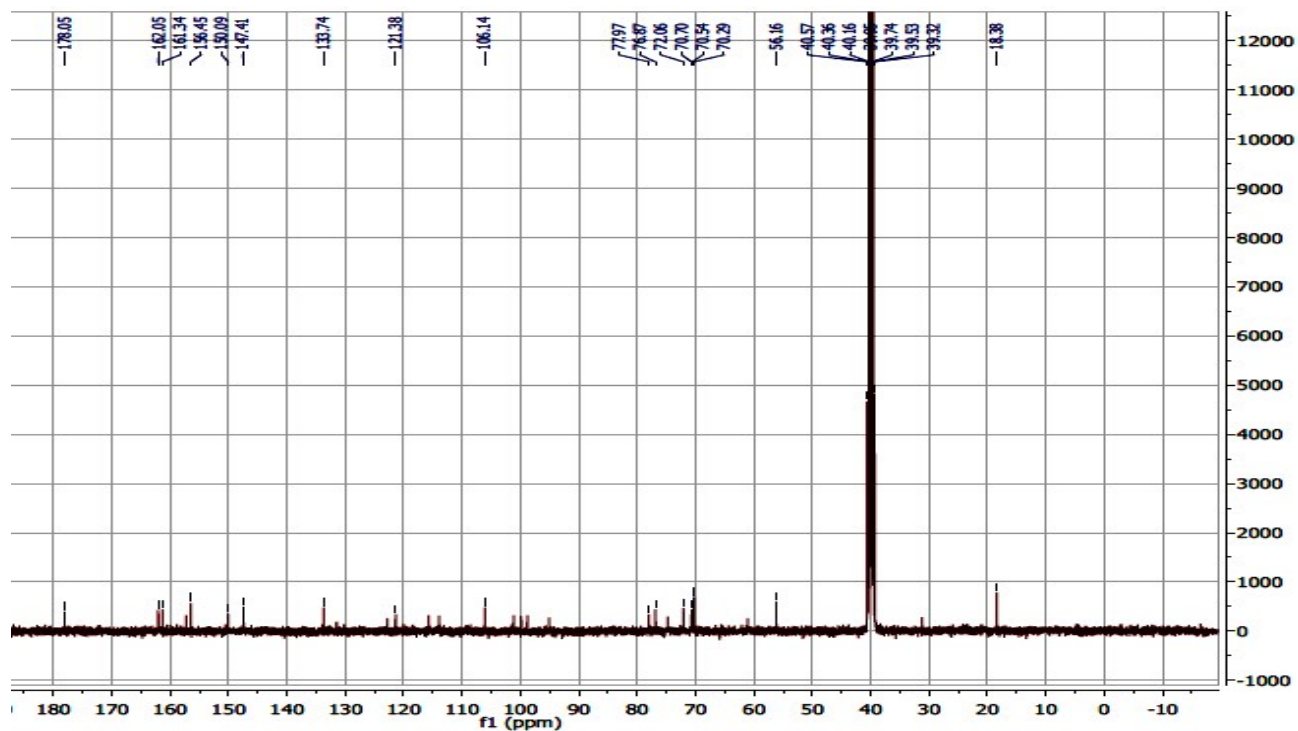


Figure S20:  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ , 400 MHz) of compound **10**