

# Supplementary material

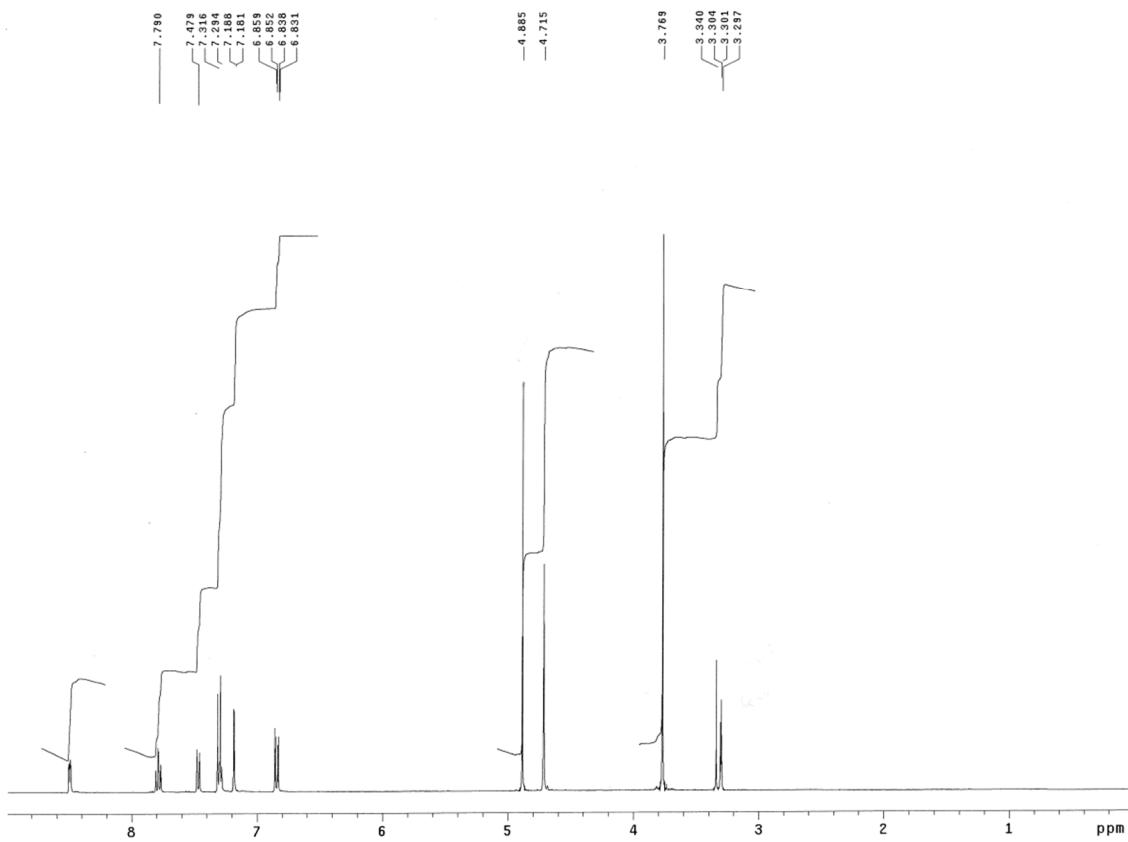
**Potent and selective benzothiazole-based antimitotics with improved water solubility:  
design, synthesis, and evaluation as novel anticancer agents**

Laura Gallego-Yerga <sup>1,2,3,\*</sup>, Valentín Ceña <sup>4,5</sup> and Rafael Peláez <sup>1,2,3,\*</sup>

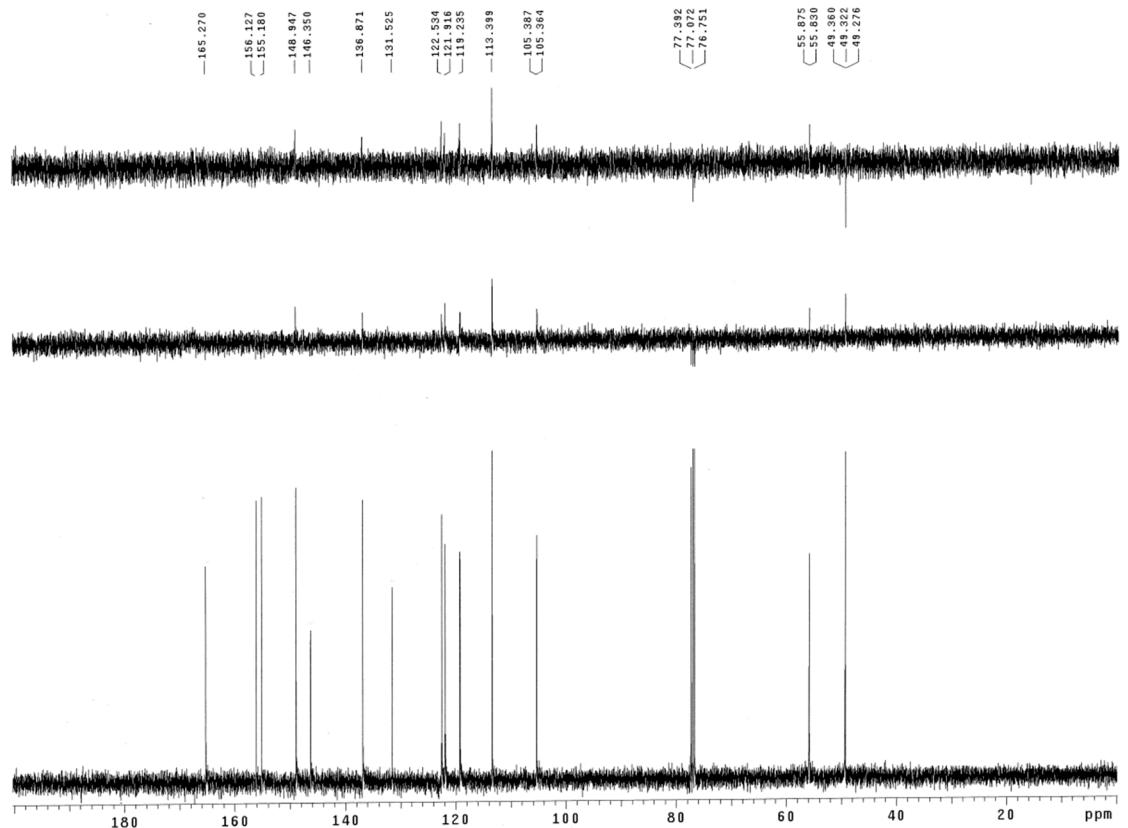
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**$^1\text{H}$  NMR**

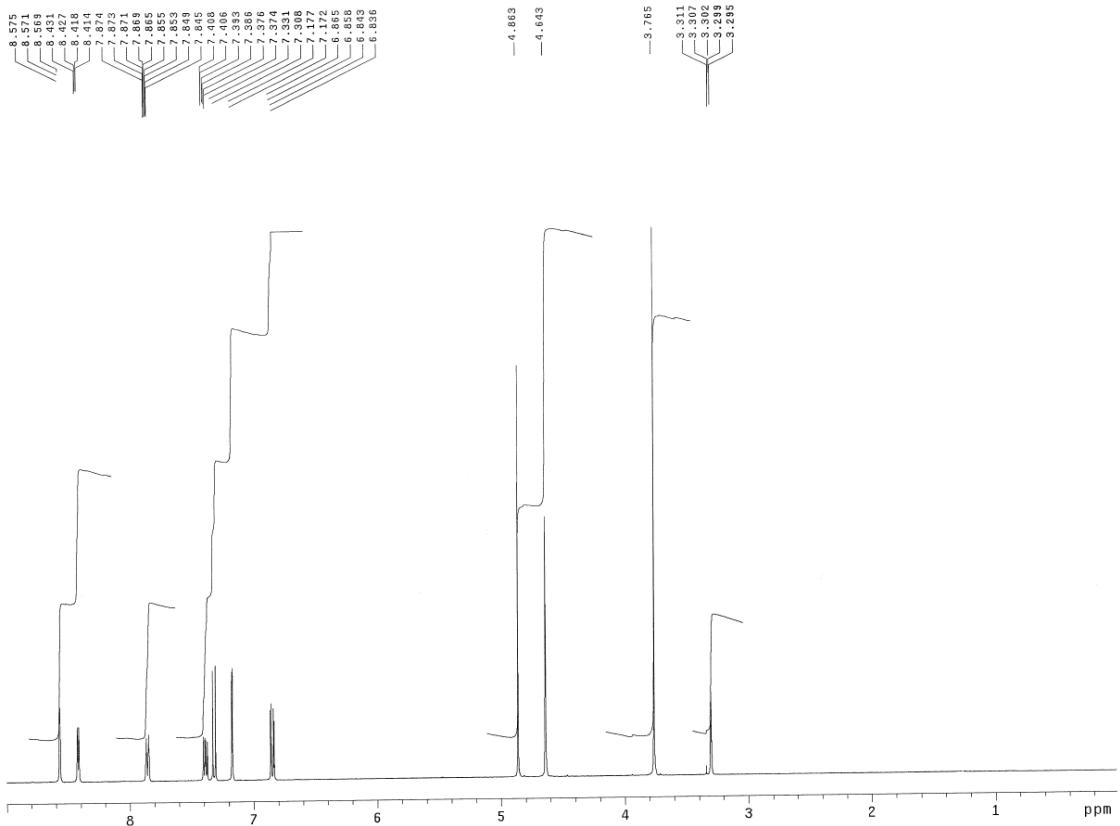
**$^{13}\text{C}$  NMR**



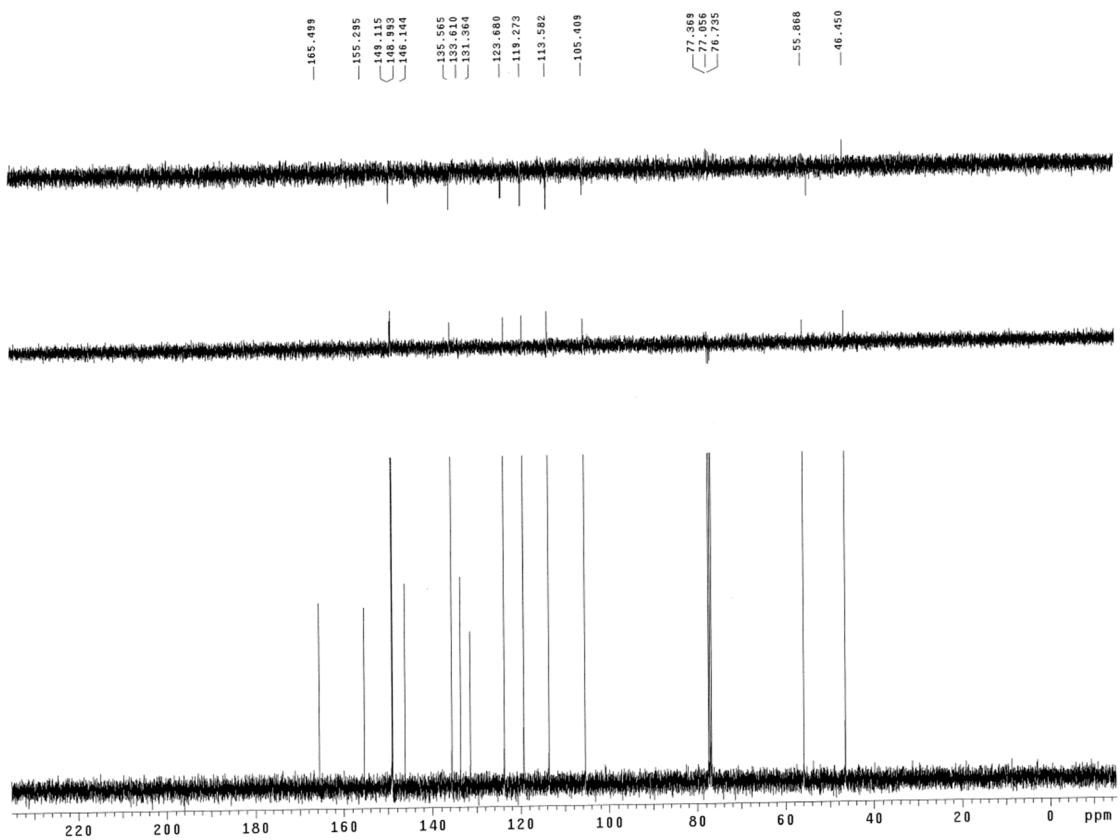
**Figure S1a.**  $^1\text{H}$  NMR (MeOD, 400 MHz) spectrum of compound **1**.



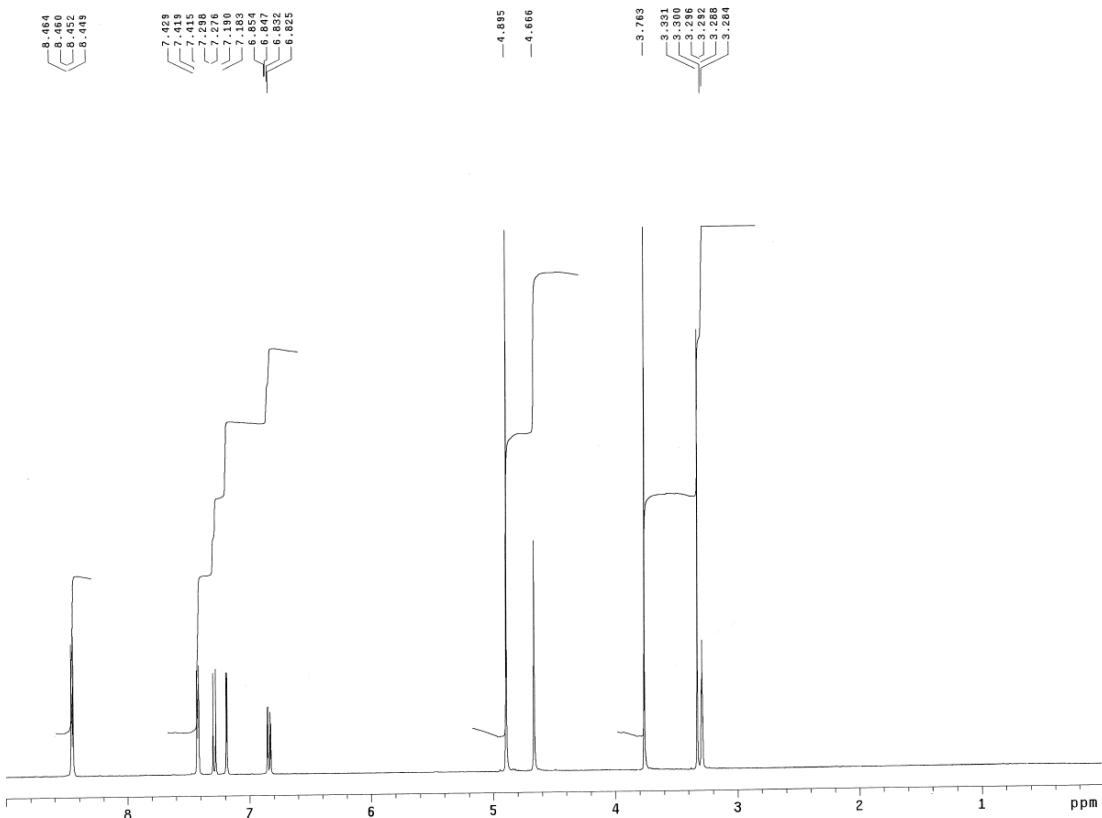
**Figure S1b.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectra of compound **1**.



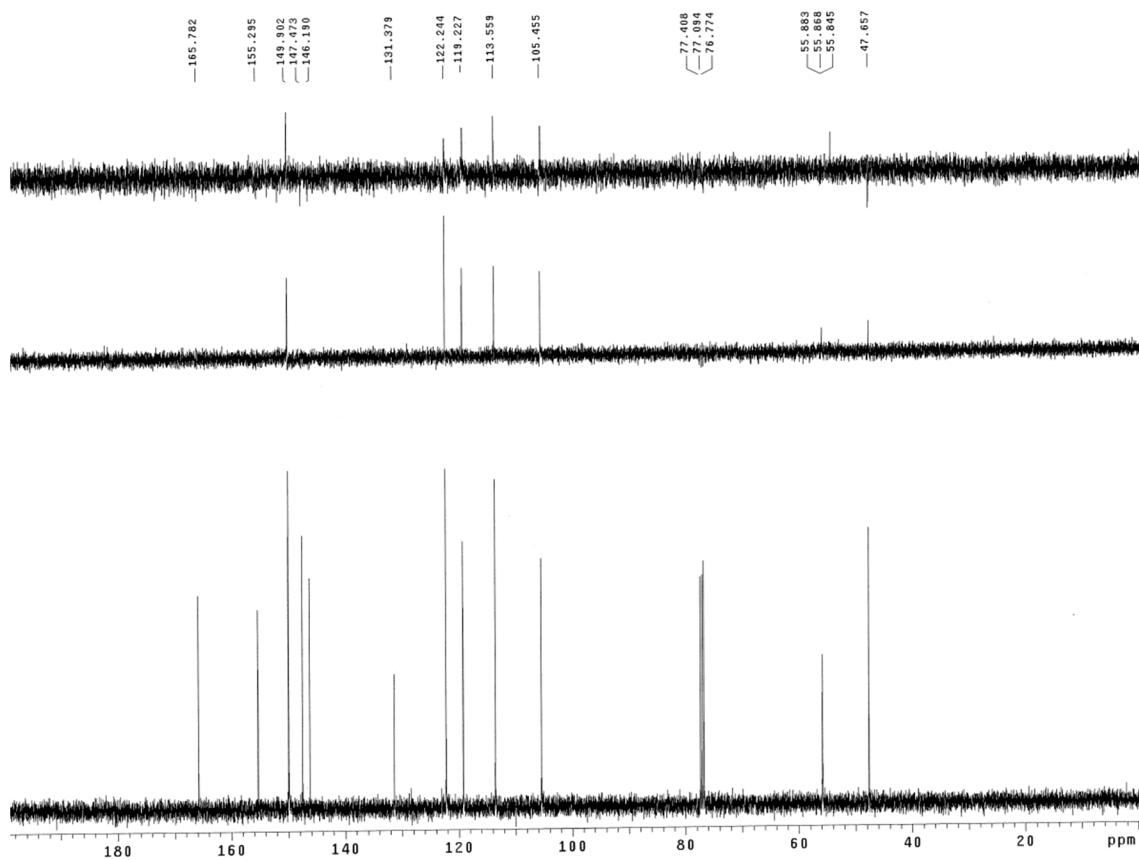
**Figure S2a.**  $^1\text{H}$  NMR (MeOD, 400 MHz) spectrum of compound 2.



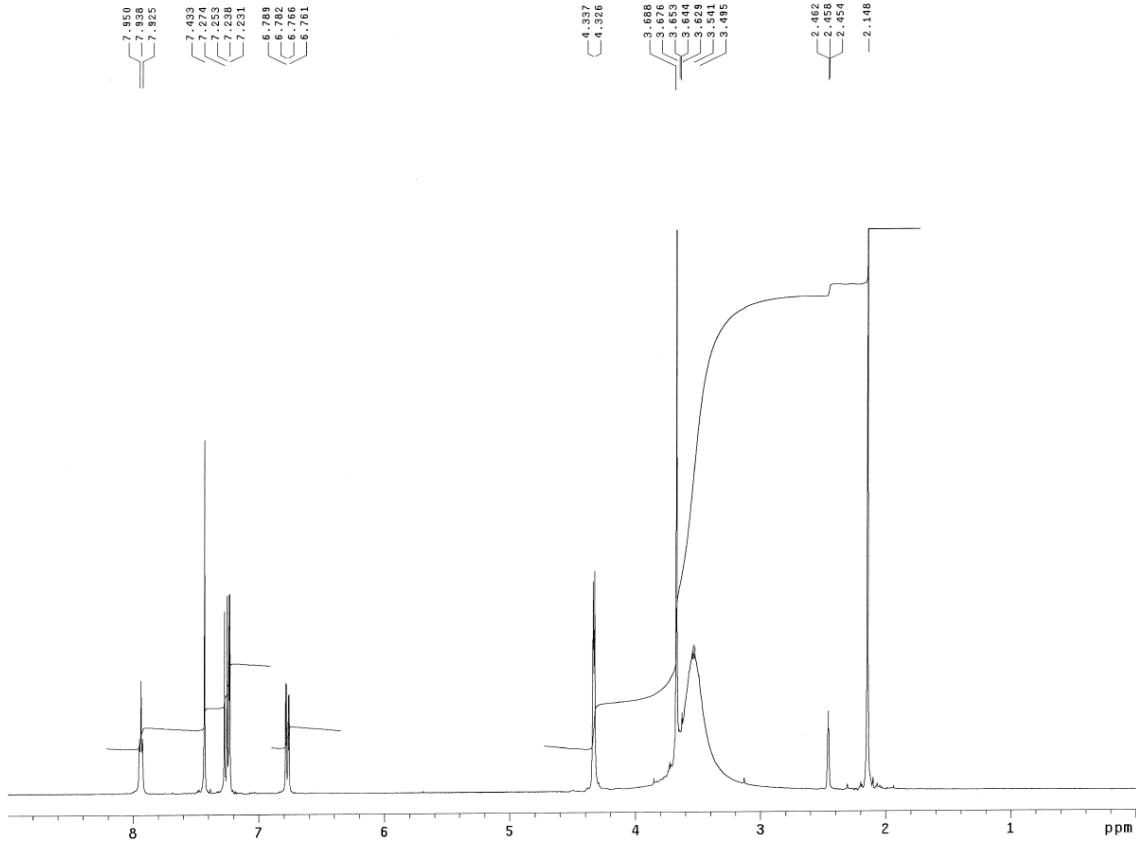
**Figure S2b.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectra of compound 2.



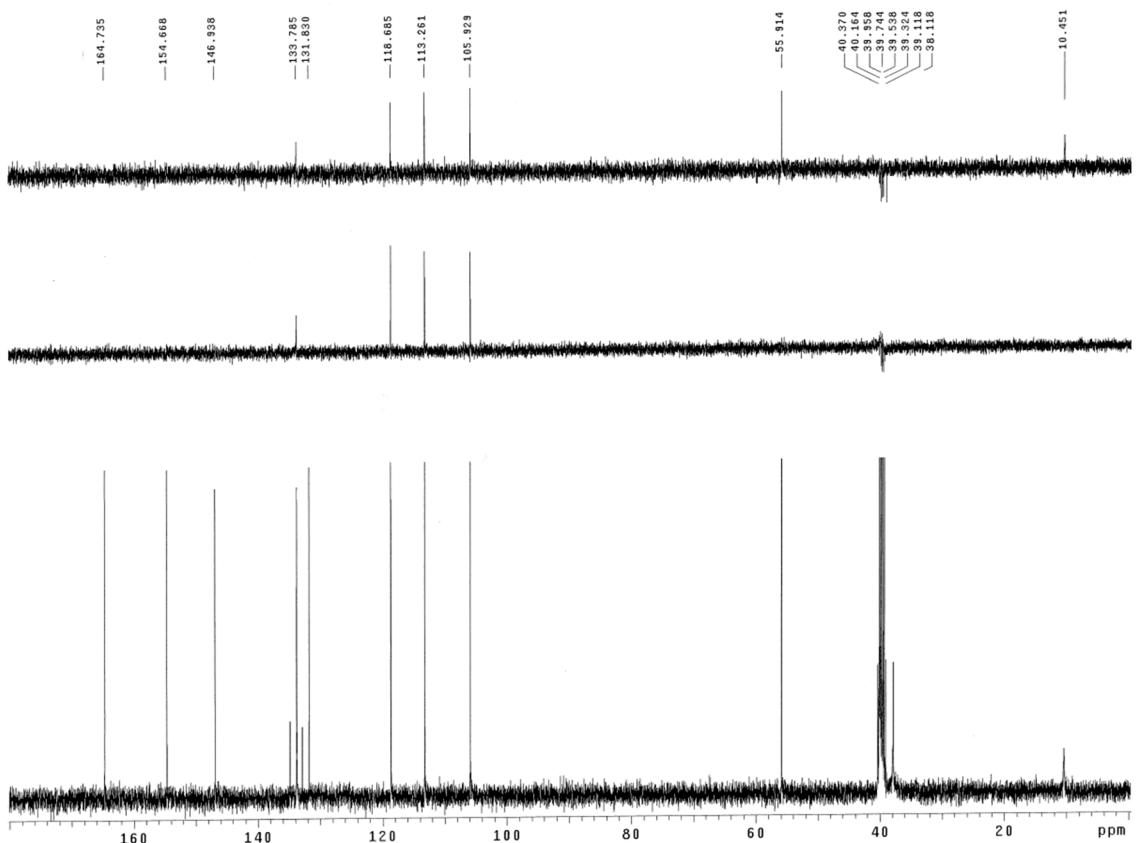
**Figure S3a.** <sup>1</sup>H NMR (MeOD, 400 MHz) spectrum of compound 3.



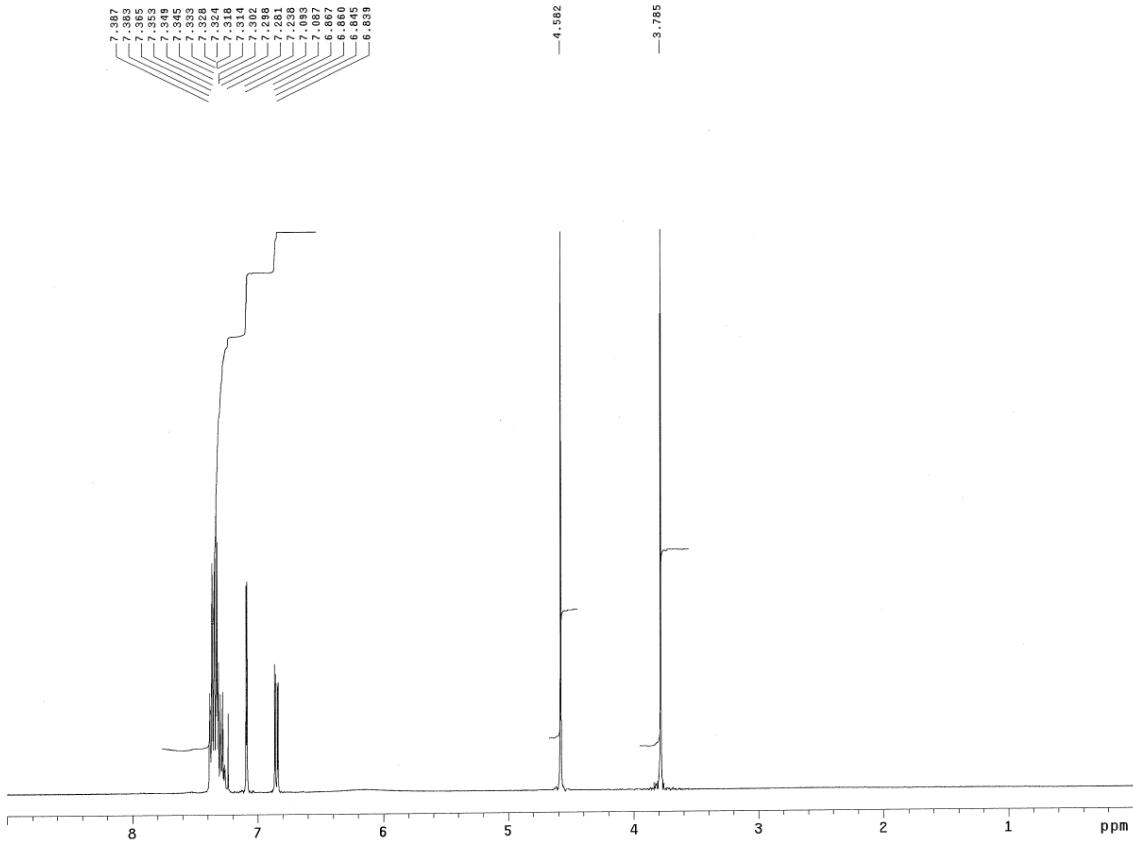
**Figure S3b.** <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) spectra of compound 3.



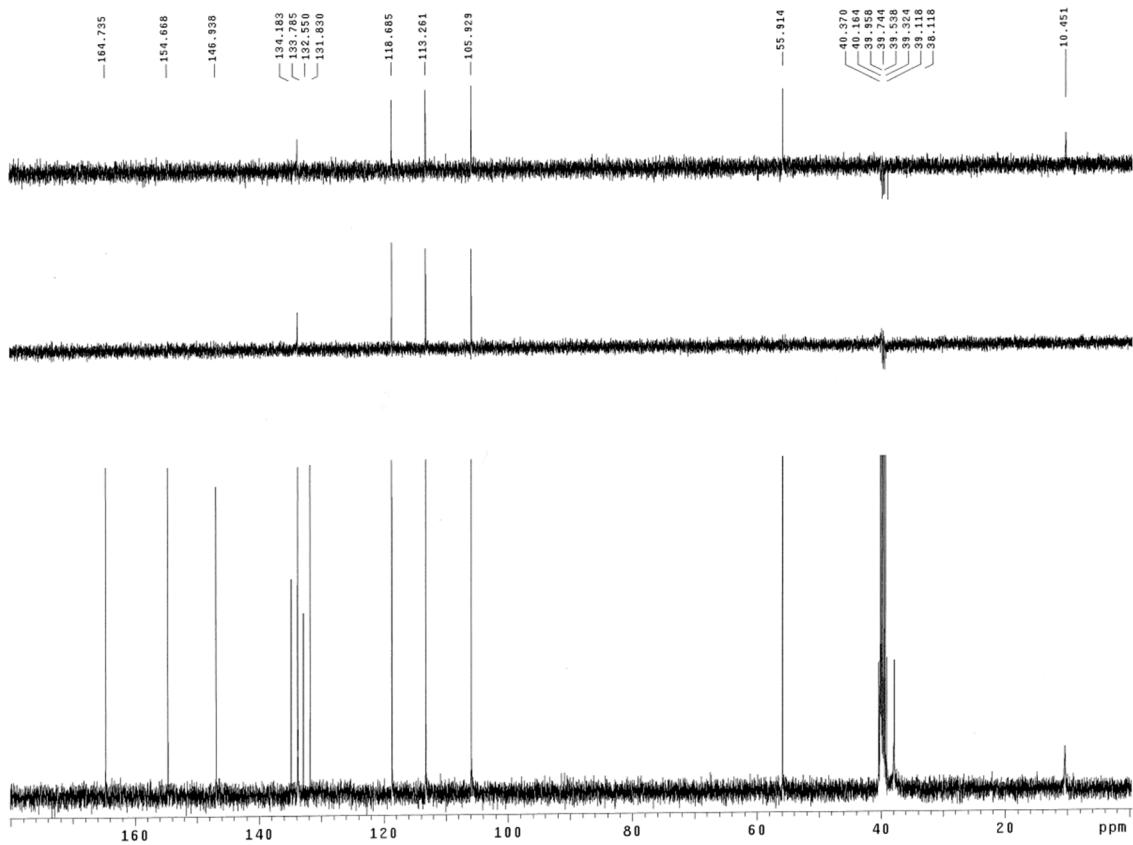
**Figure S4a.**  $^1\text{H}$  NMR (DMSO- $\text{d}_6$ , 400 MHz) spectrum of compound 4.



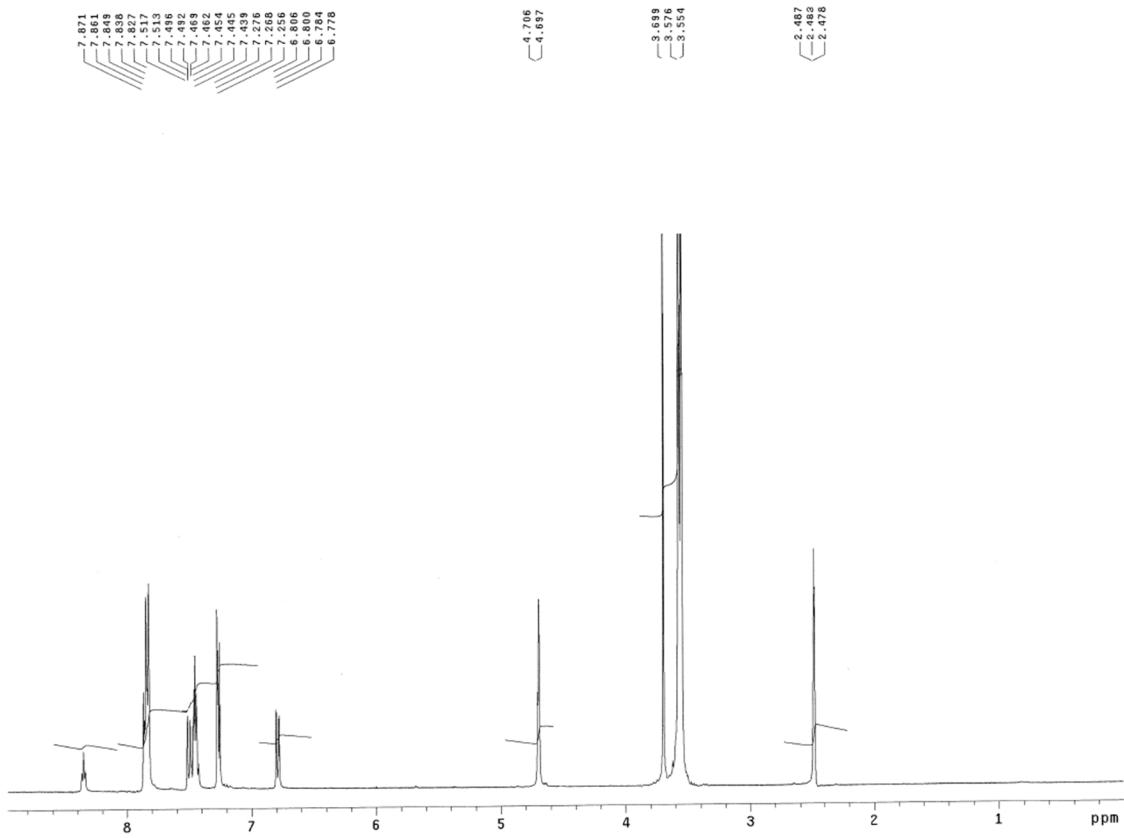
**Figure S4b.**  $^{13}\text{C}$  NMR (DMSO- $\text{d}_6$ , 100 MHz) spectra of compound 4.



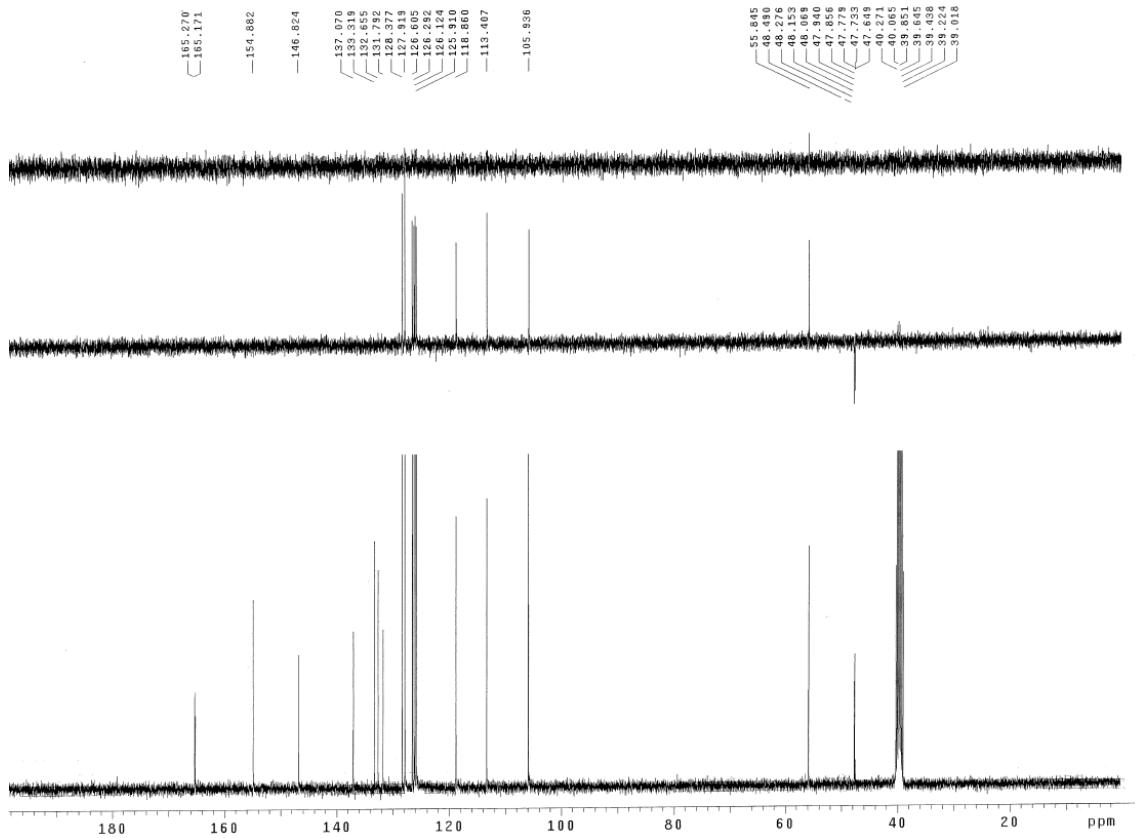
**Figure S5a.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) spectrum of compound 5.



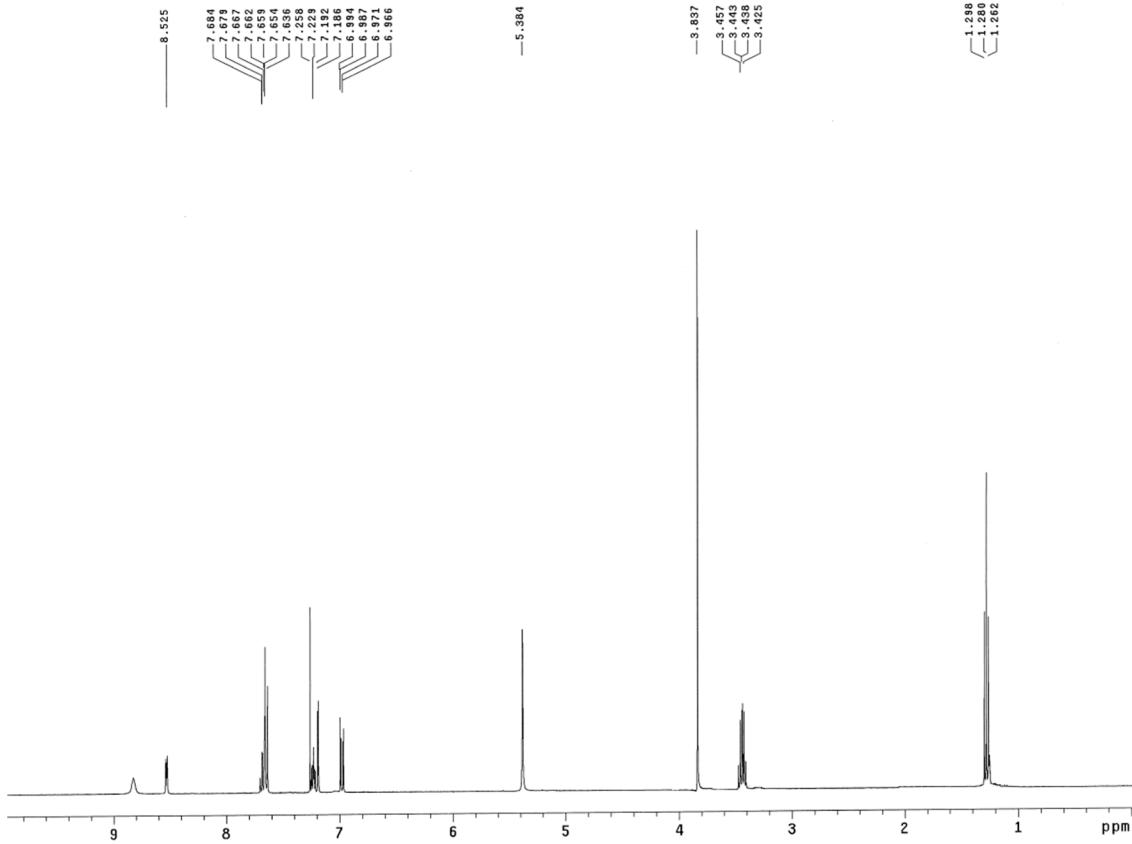
**Figure S5b.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectra of compound 5.



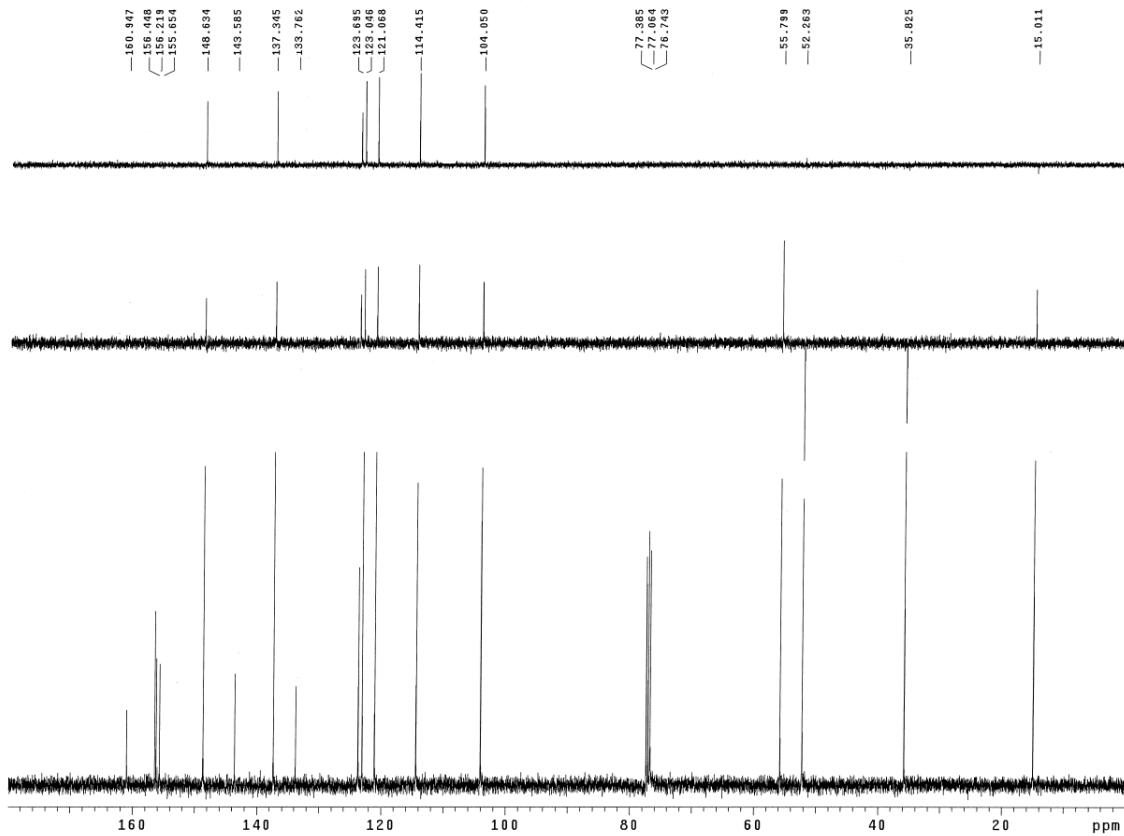
**Figure S6a.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) spectrum of compound 6.



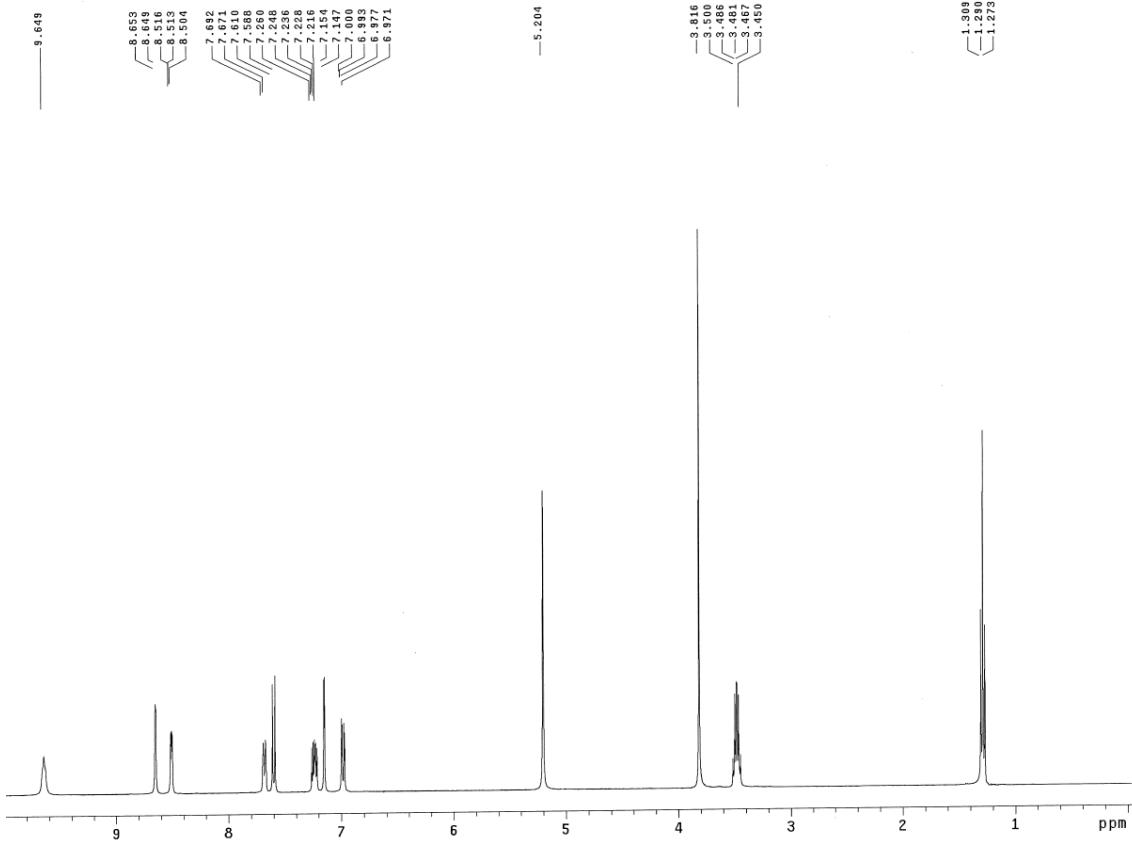
**Figure S6b.**  $^{13}\text{C}$  NMR ( $\text{DMSO-d}_6$ , 100 MHz) spectra of compound 6.



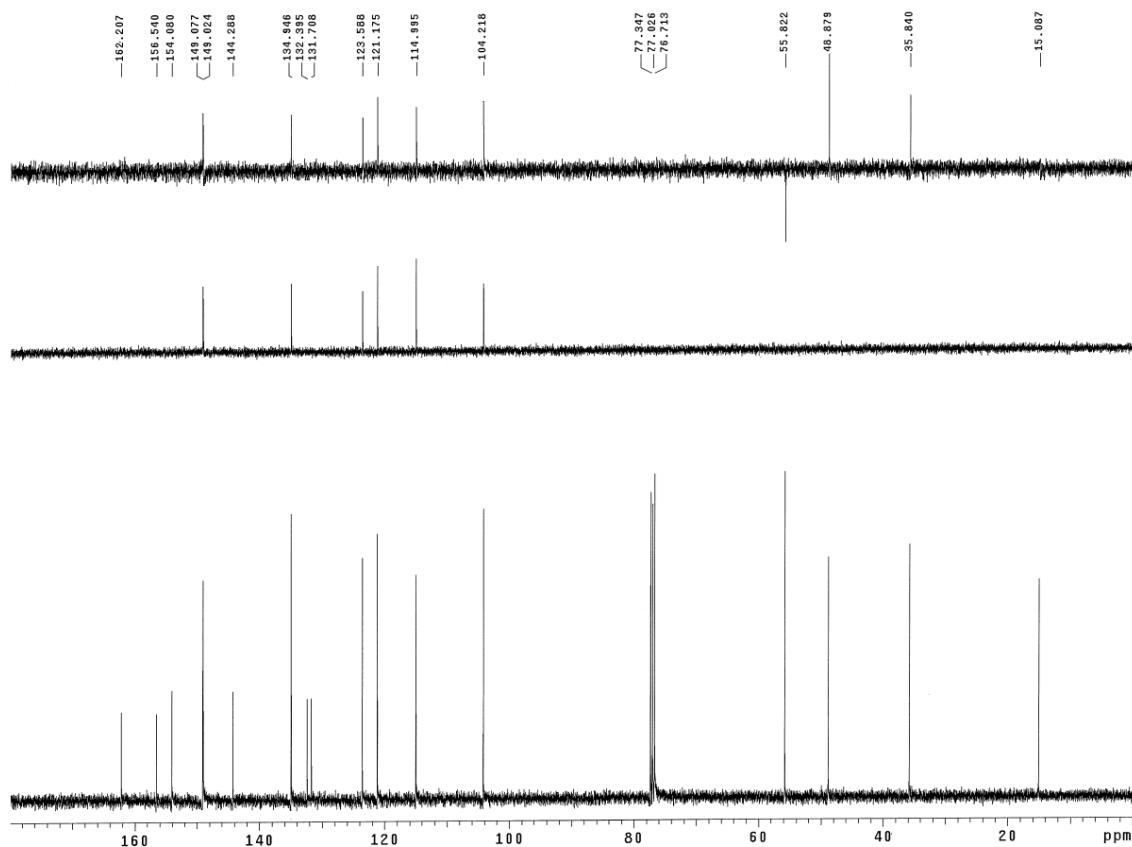
**Figure S7a.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) spectrum of compound 7.



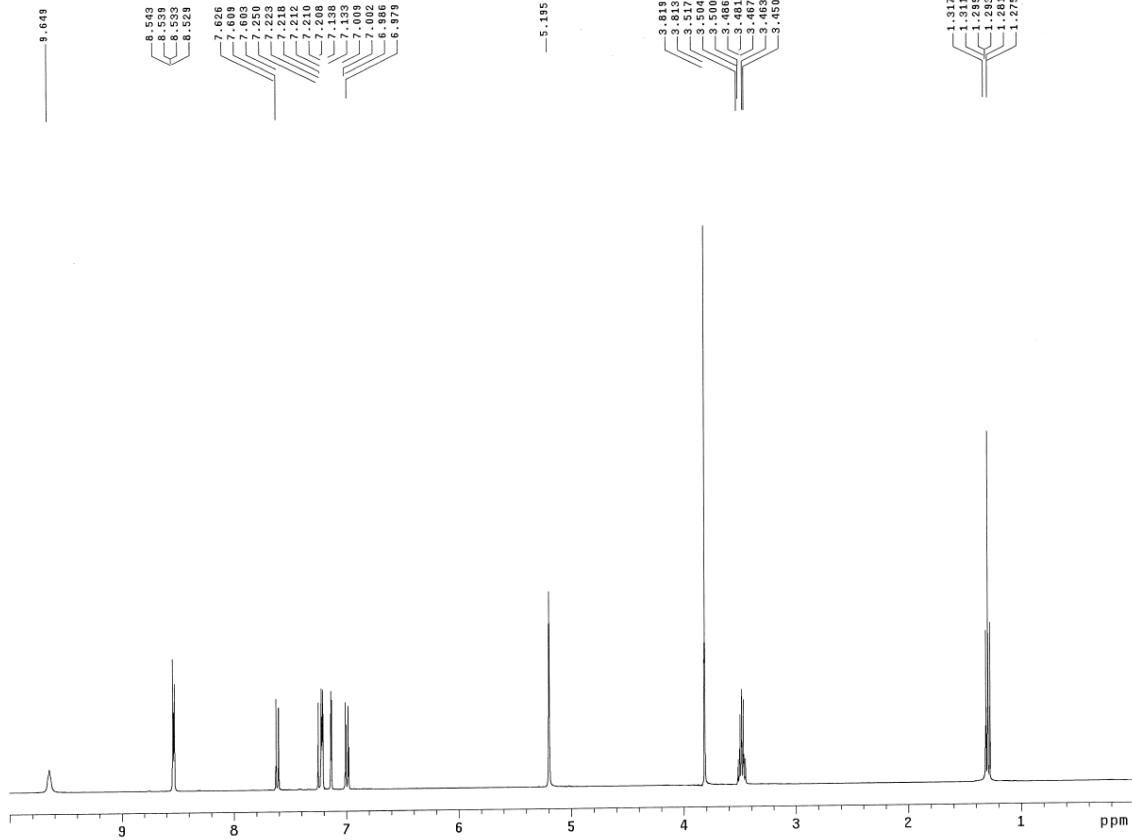
**Figure S7b.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectra of compound 7.



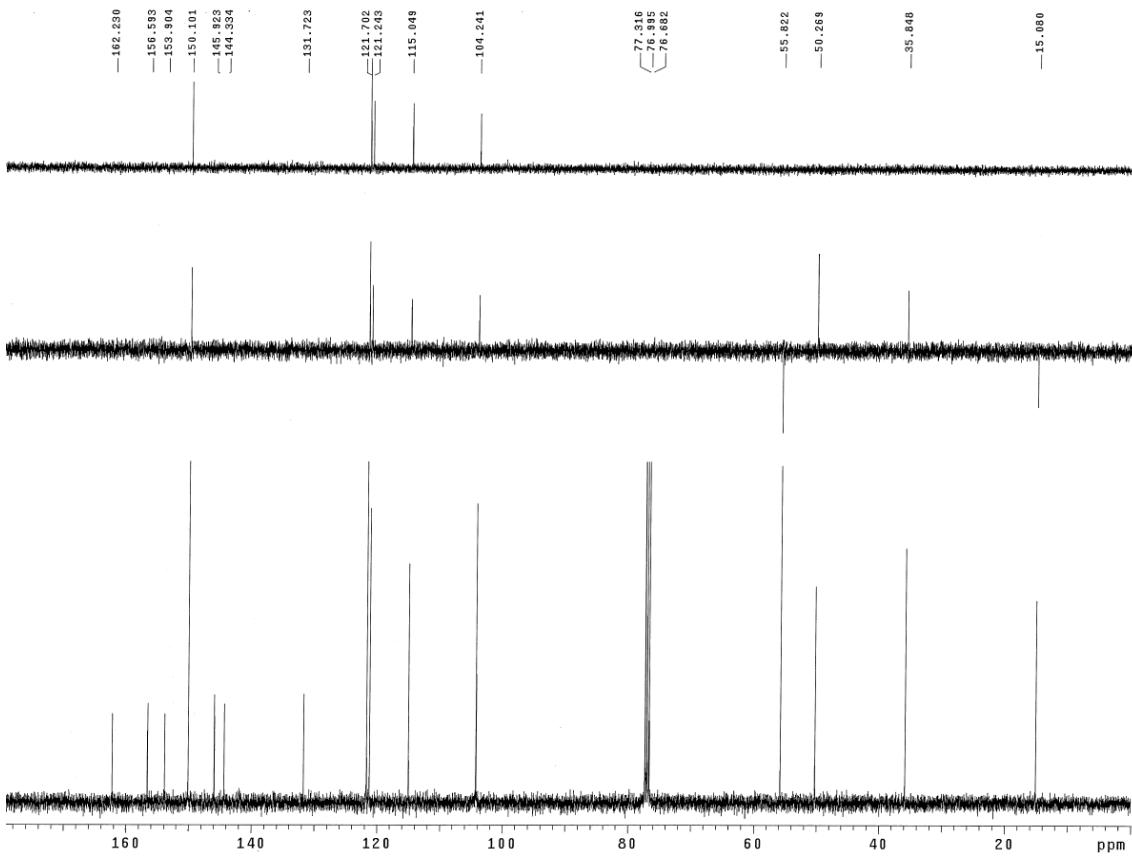
**Figure S8a.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) spectrum of compound 8.



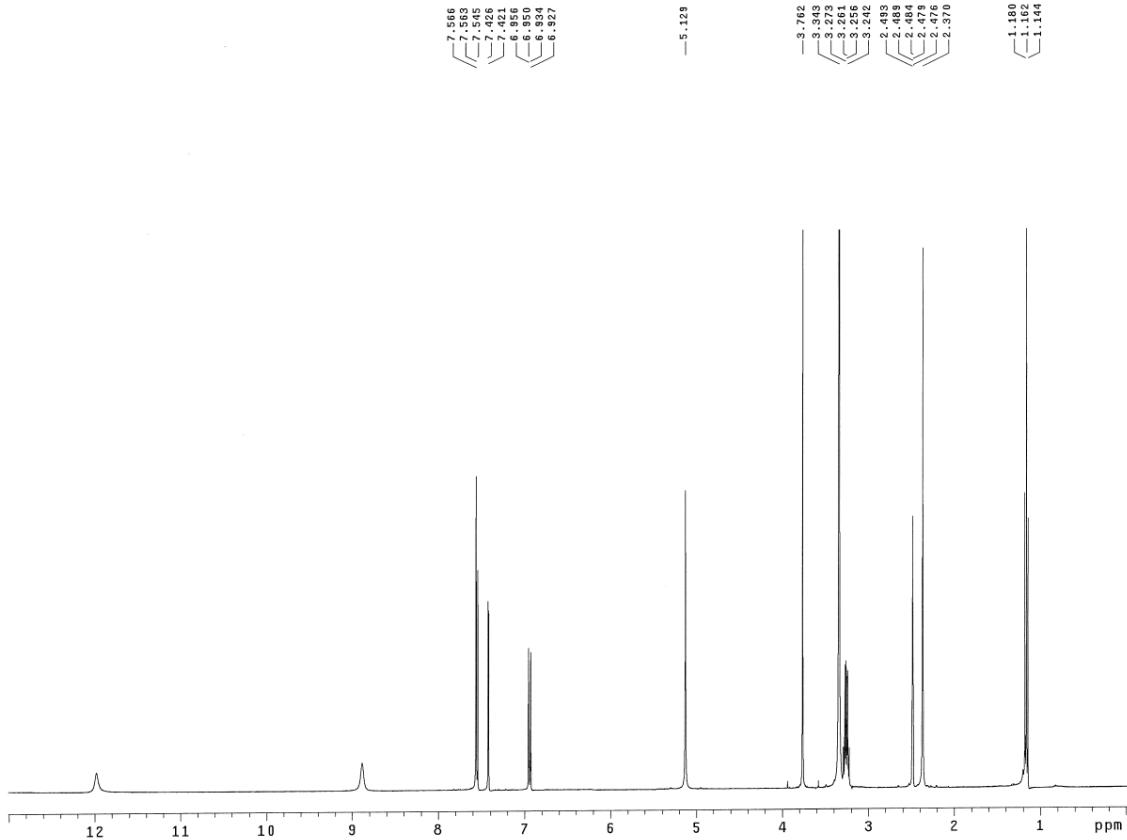
**Figure S8b.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectra of compound 8.



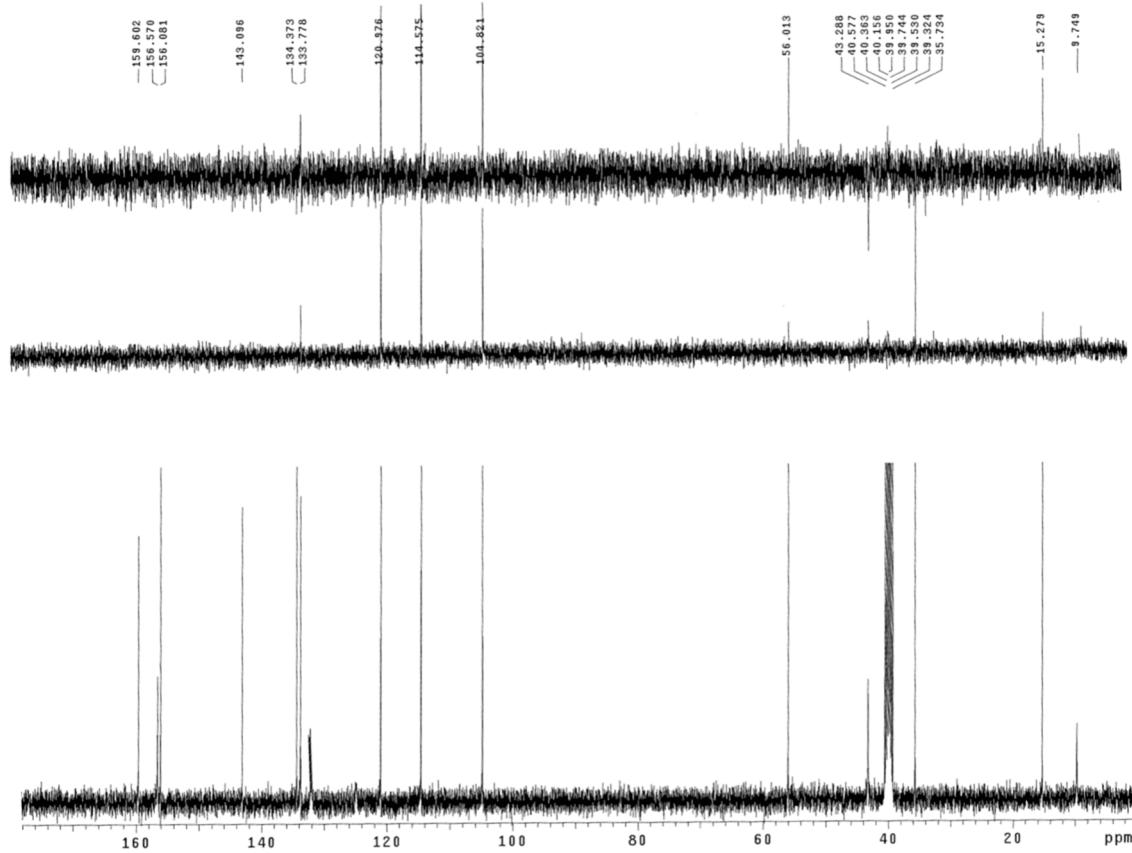
**Figure S9a.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) spectrum of compound 9.



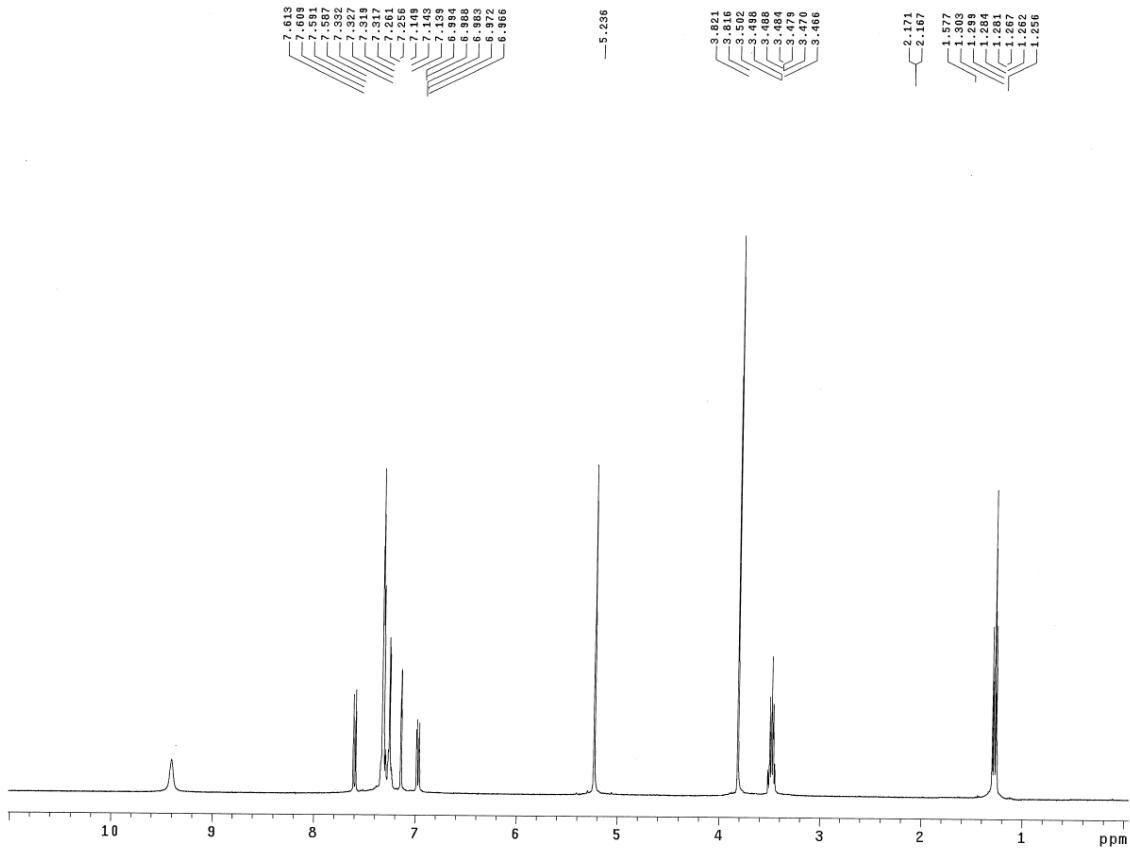
**Figure S9b.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectra of compound 9.



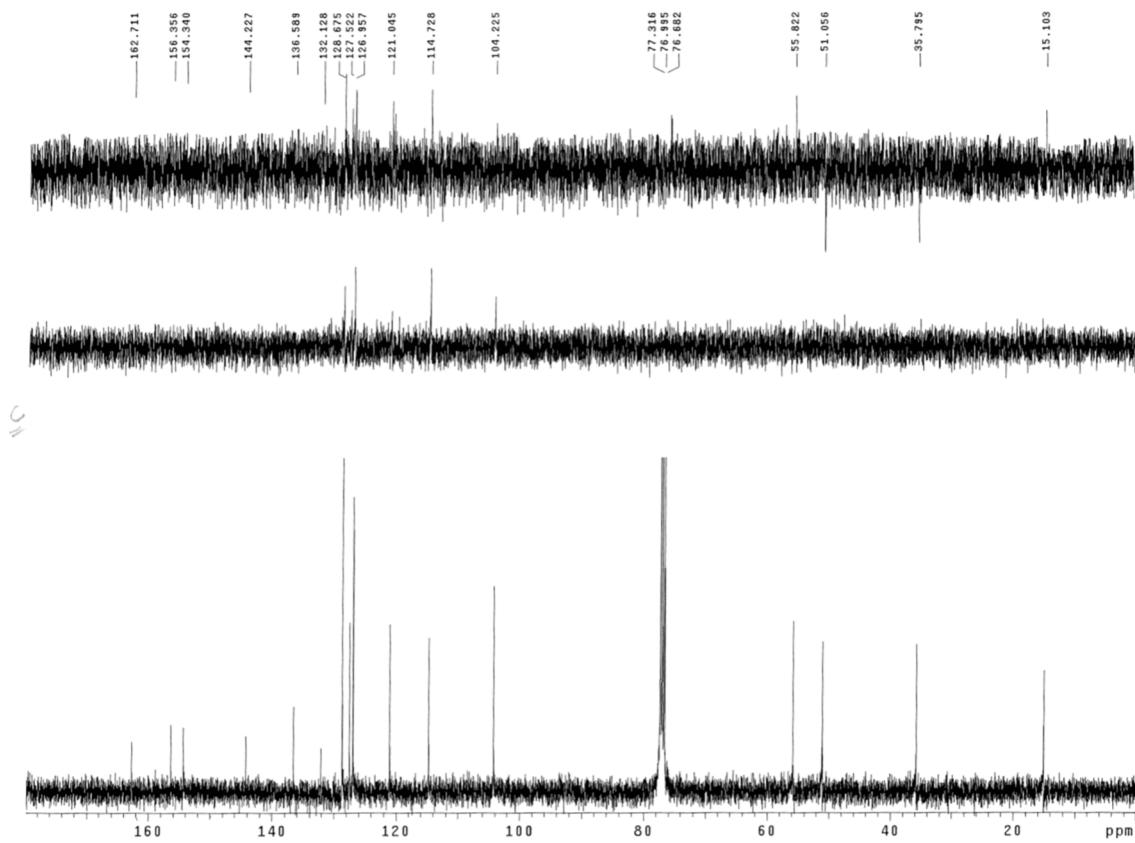
**Figure S10a.**  $^1\text{H}$  NMR (DMSO- $\text{d}_6$ , 400 MHz) spectrum of compound **10**.



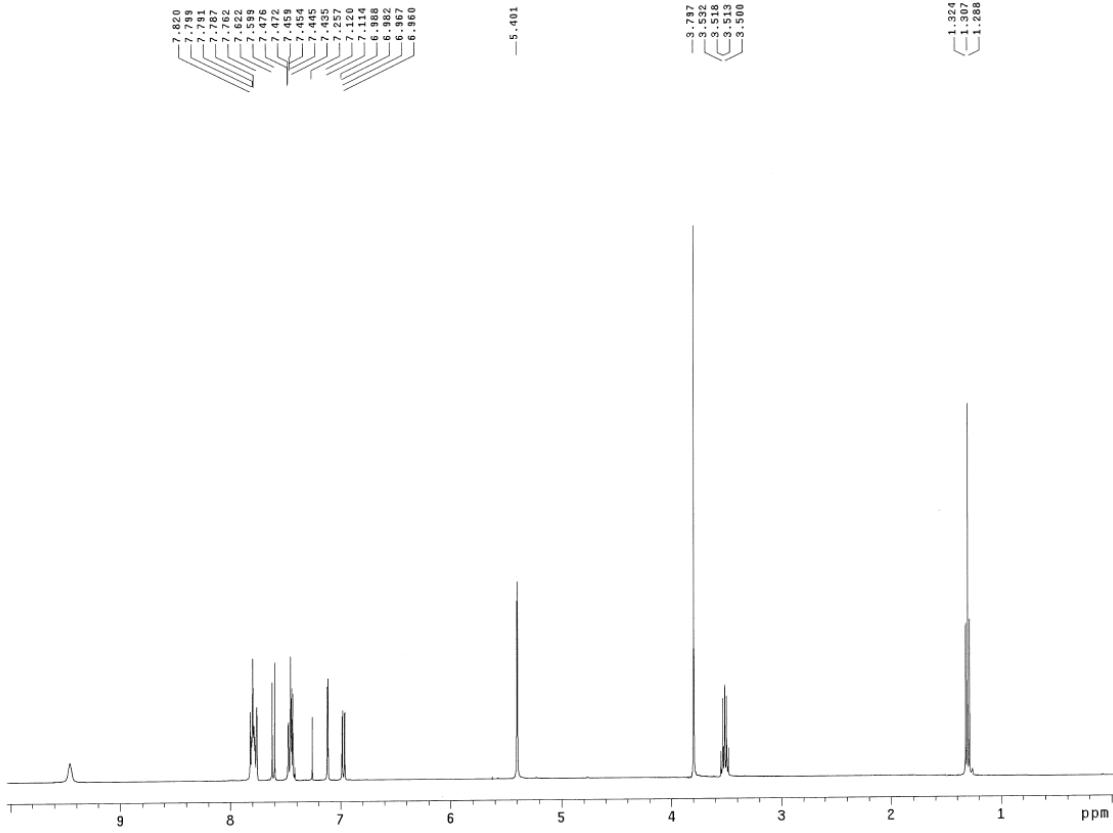
**Figure S10b.**  $^{13}\text{C}$  NMR (DMSO-d<sub>6</sub>, 100 MHz) spectra of compound **10**.



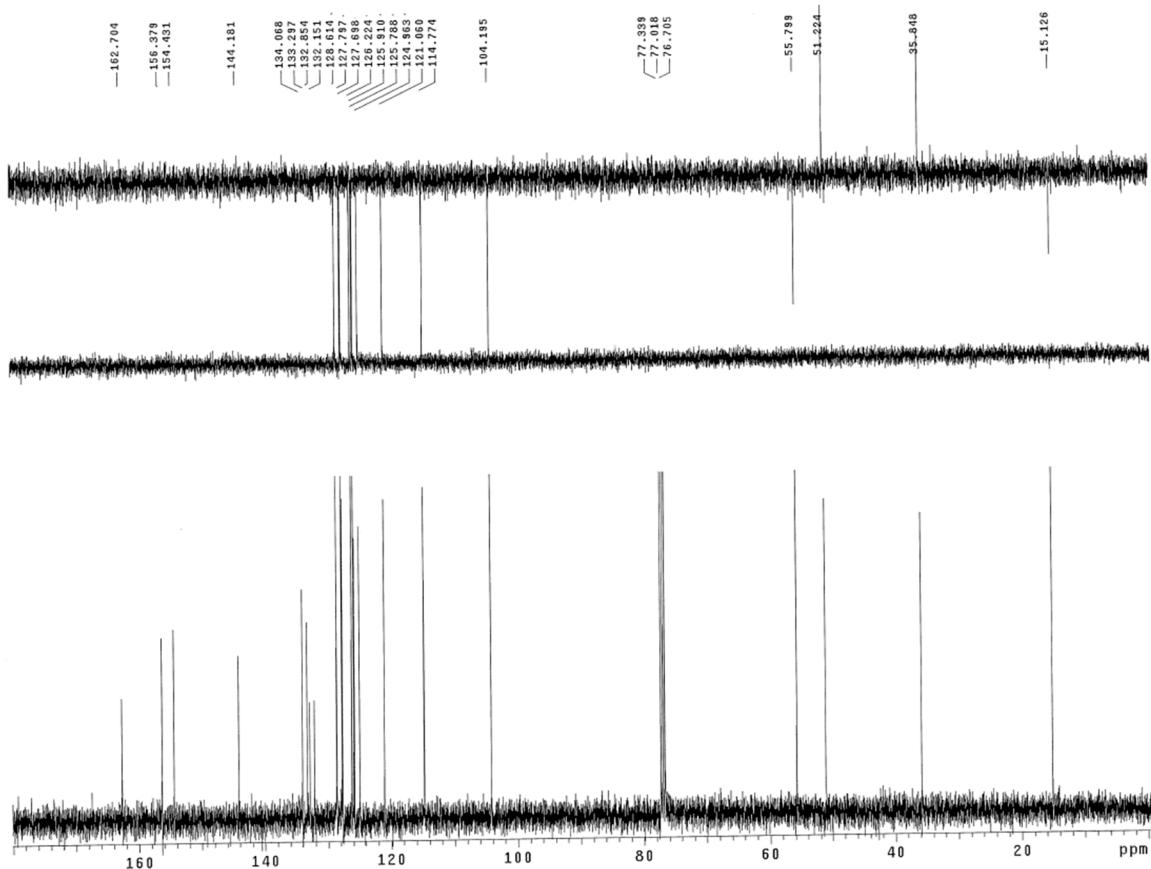
**Figure S11a.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) spectrum of compound **11**.



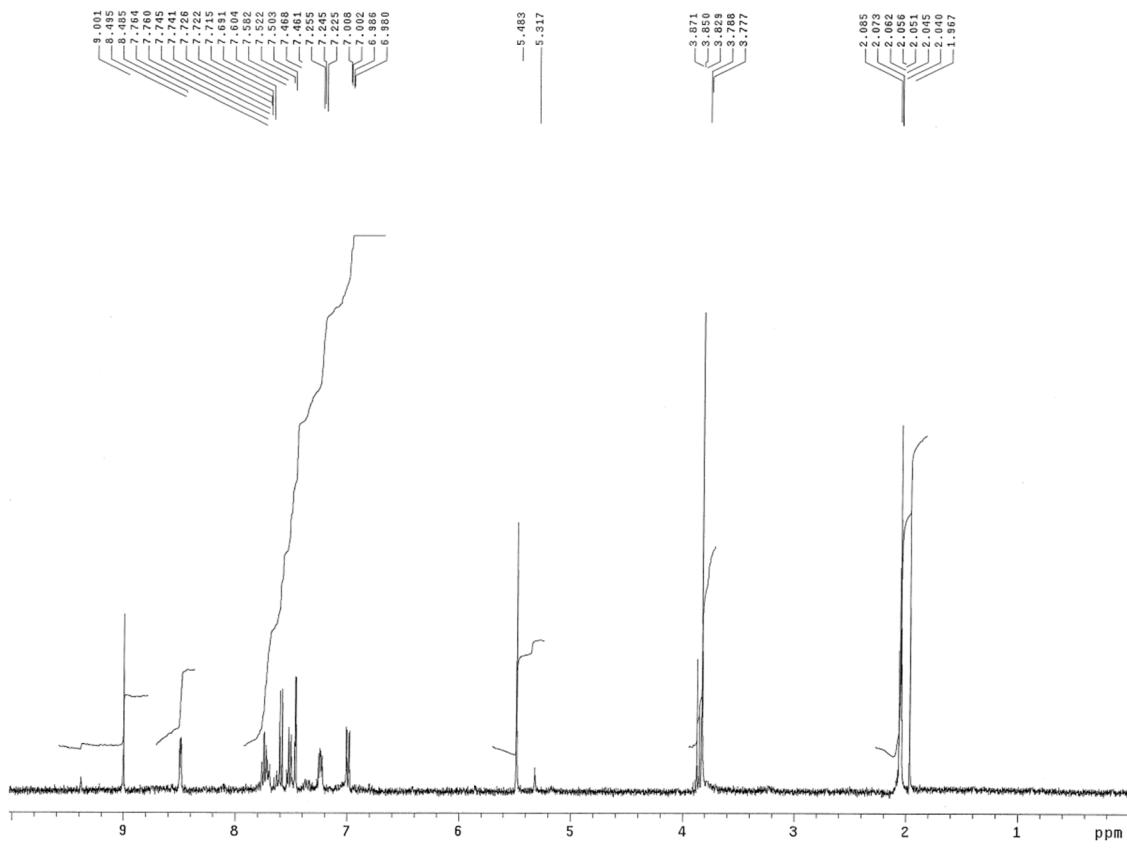
**Figure S11b.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectra of compound **11**.



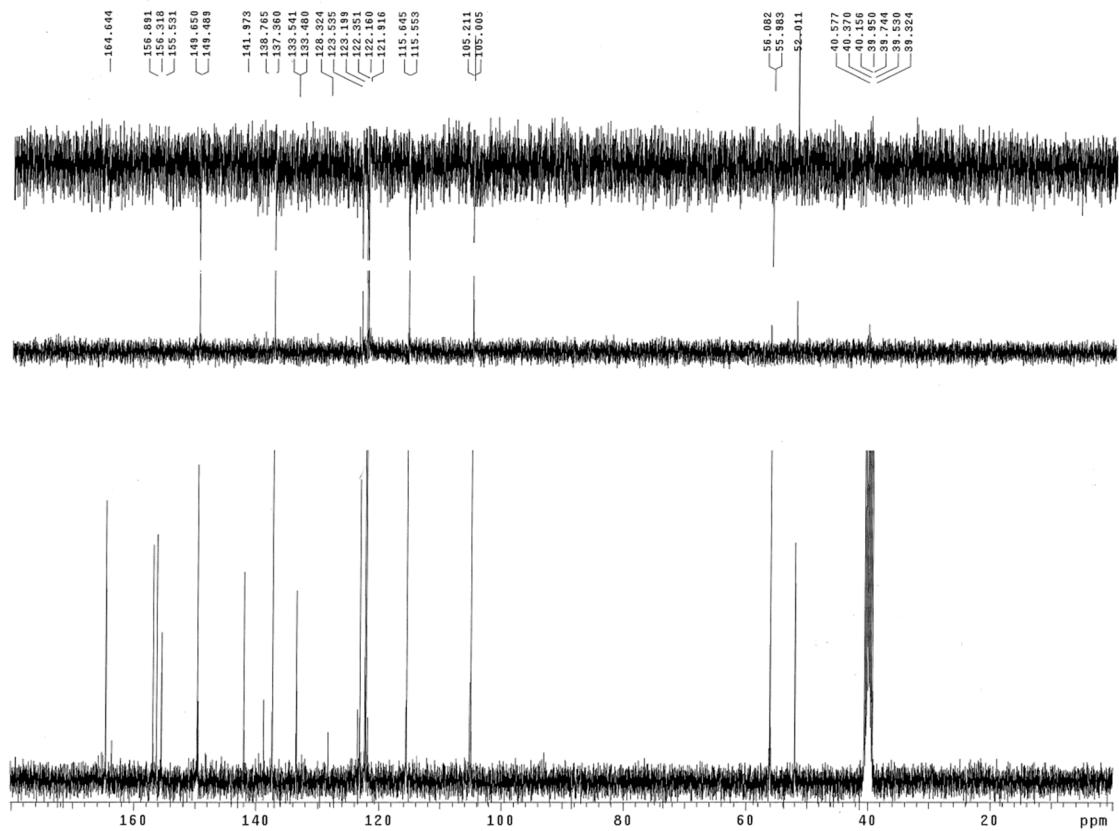
**Figure S12a.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) spectrum of compound **12**.



**Figure S12b.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectra of compound **12**.



**Figure S13a.**  $^1\text{H}$  NMR (acetone-d<sub>6</sub>, 400 MHz) spectrum of compound **13**.



**Figure S13b.**  $^{13}\text{C}$  NMR (DMSO-d<sub>6</sub>, 100 MHz) spectra of compound **13**.