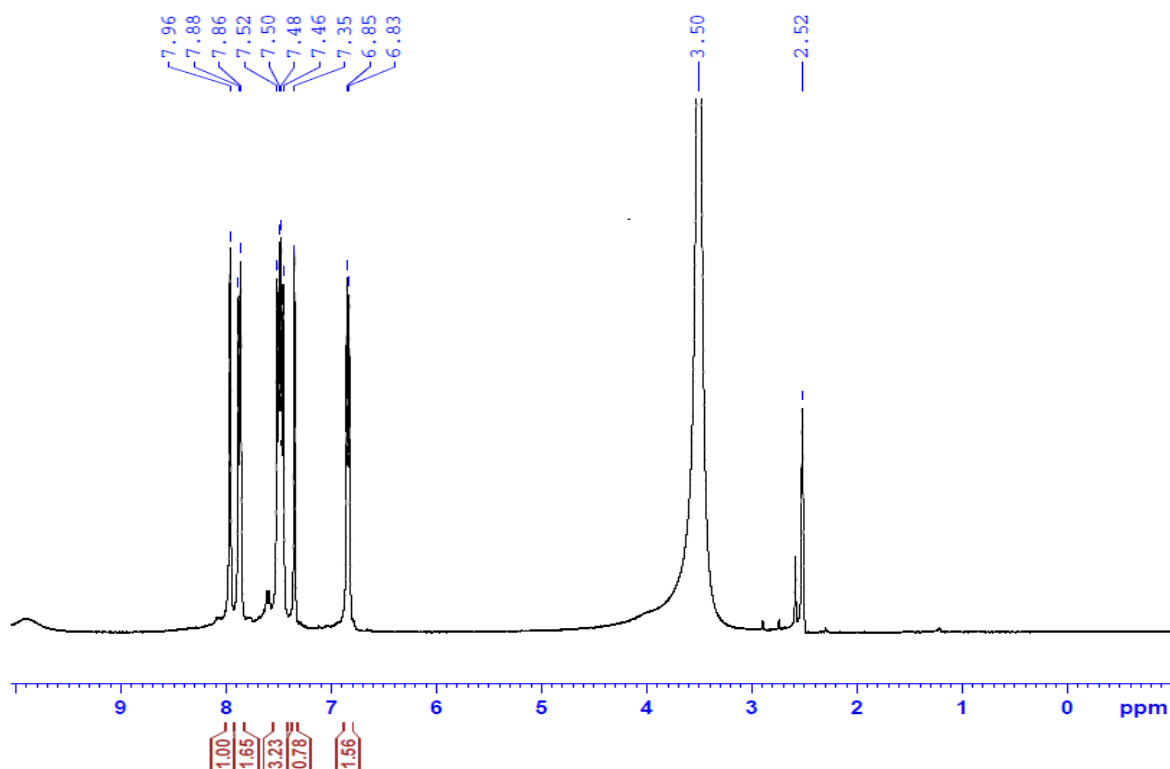
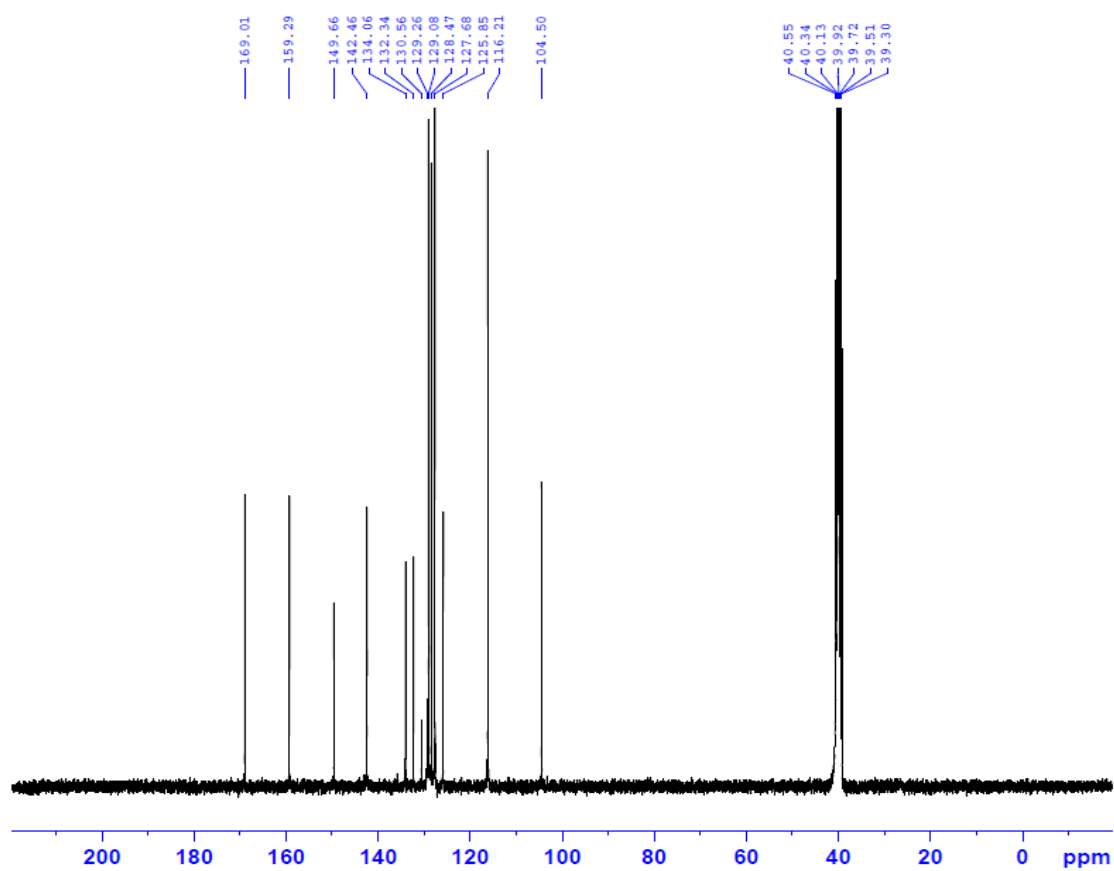


## **Supplementary Materials**

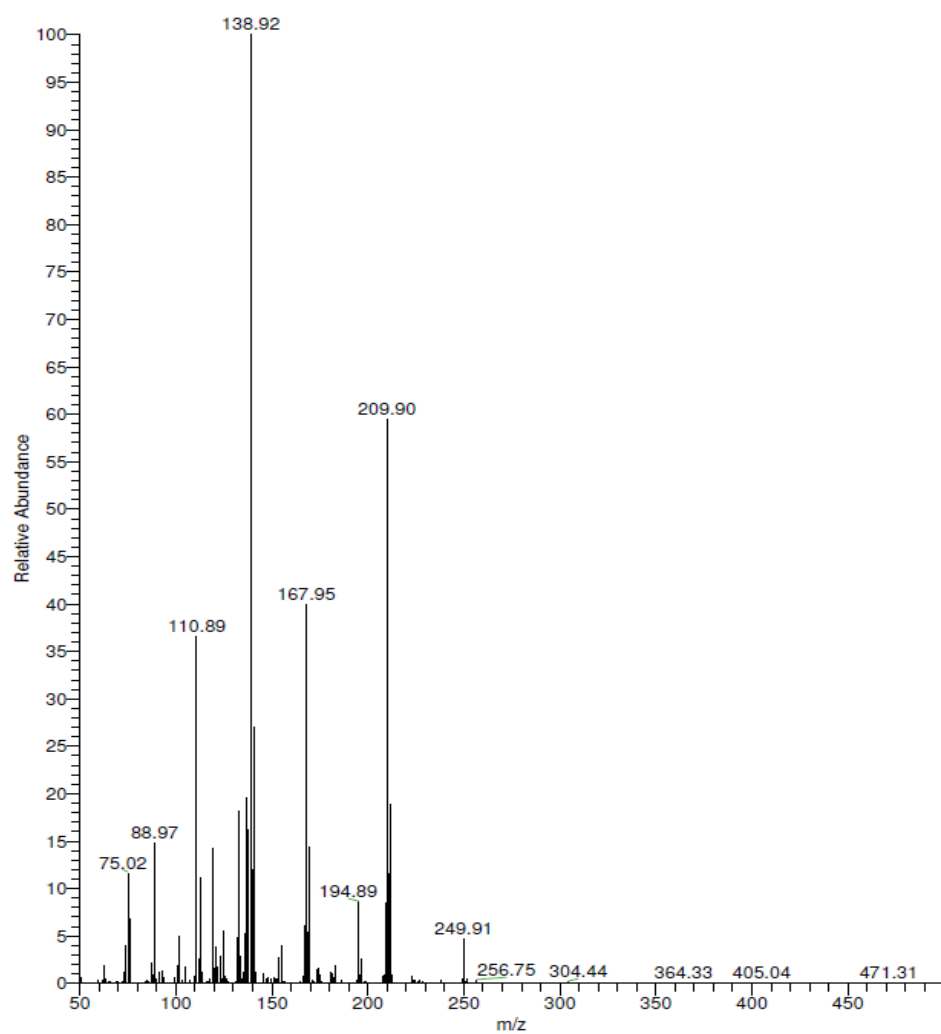
**Novel 1,3-Thiazole Analogues with Potent Activity against Breast Cancer: A Design, Synthesis, In Vitro, and In Silico Study**



**Figure S1a.** <sup>1</sup>H-NMR spectrum of compound **3a**



**Figure S1b.** <sup>13</sup>C-NMR spectrum of compound **3a**



**Figure S1c.** mass spectrum of compound **3a**

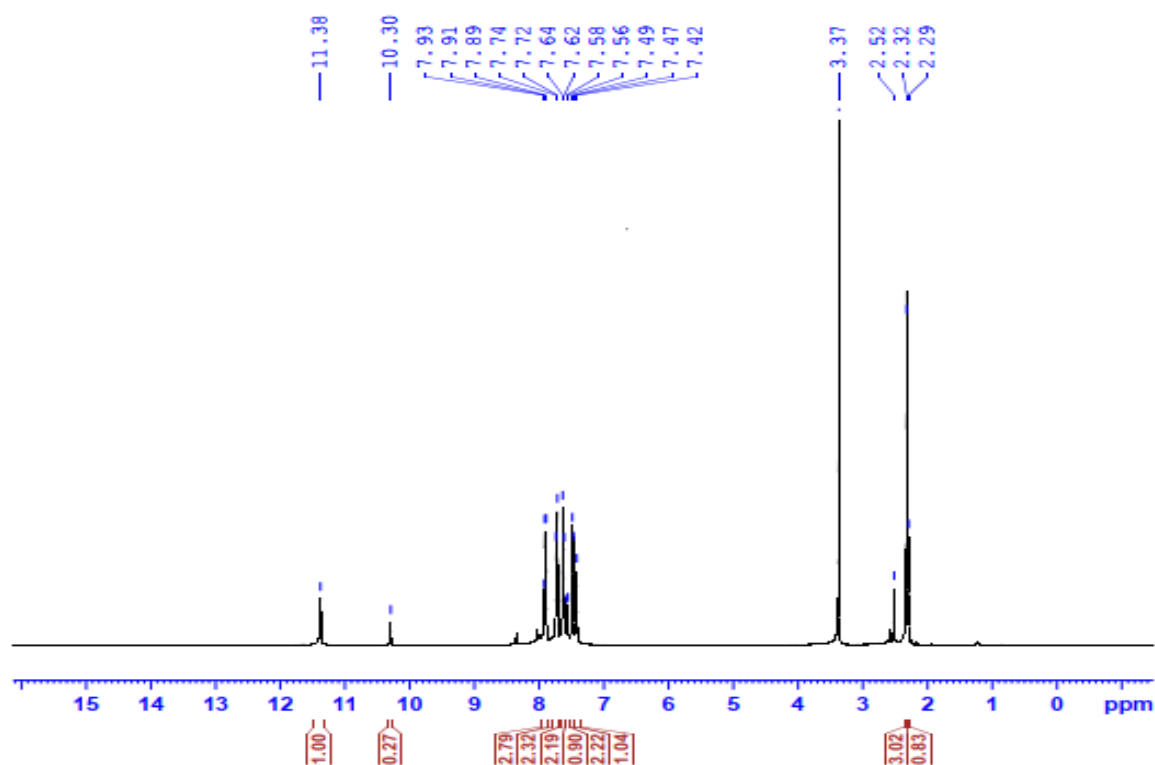


Figure S2a. <sup>1</sup>H-NMR spectrum of compound 3b

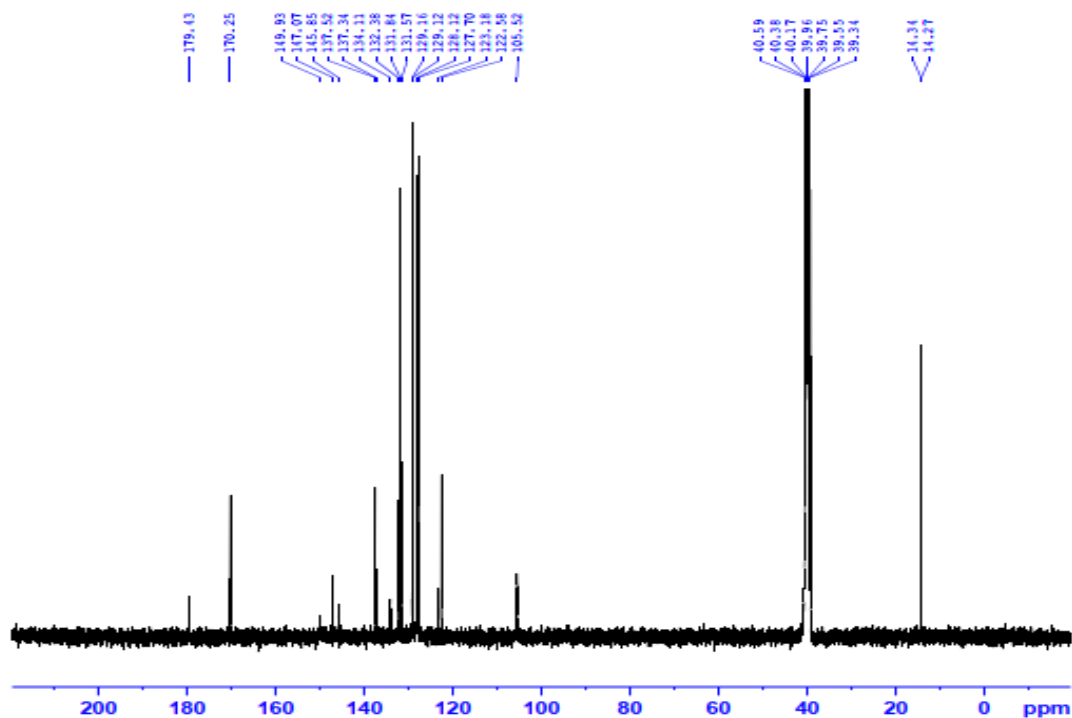
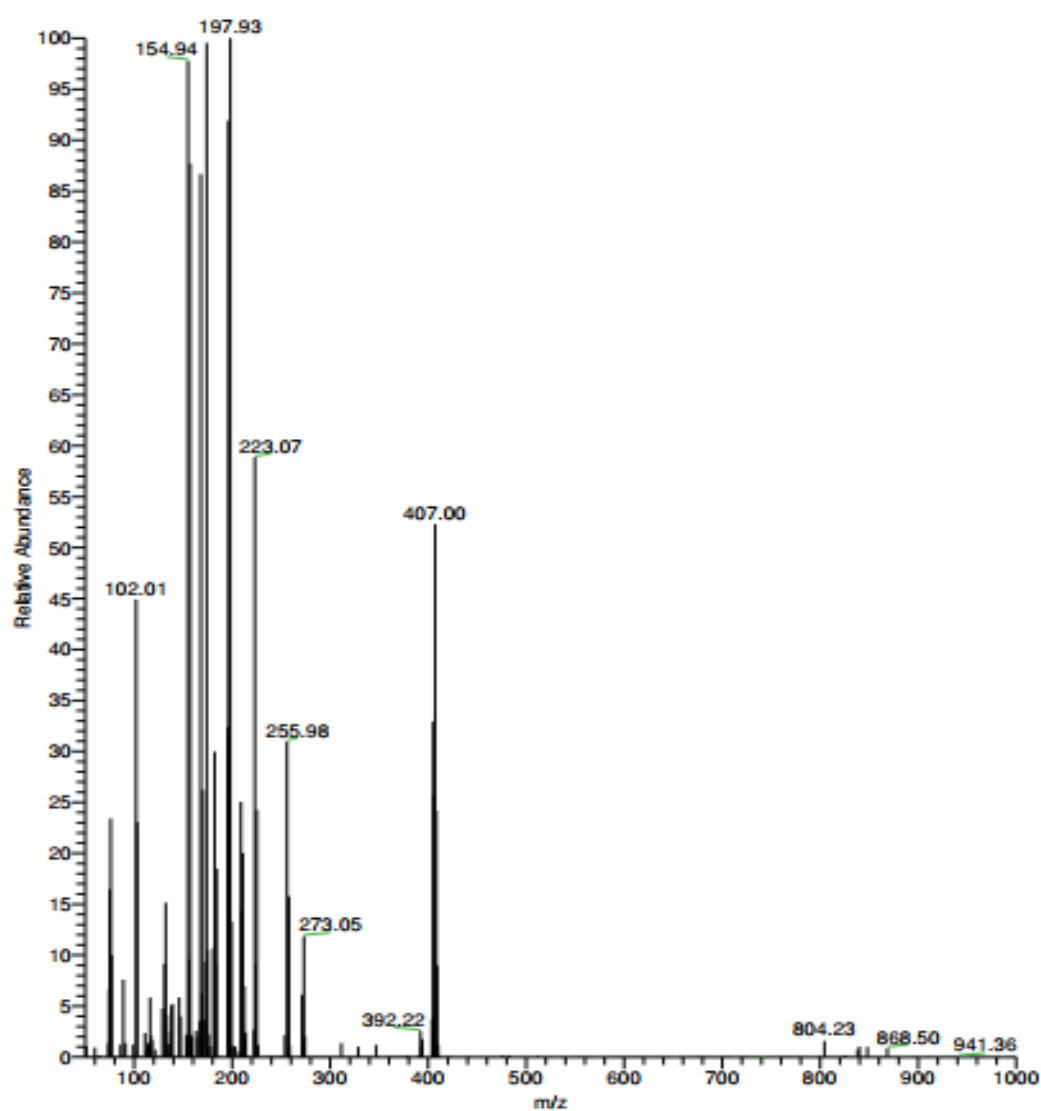
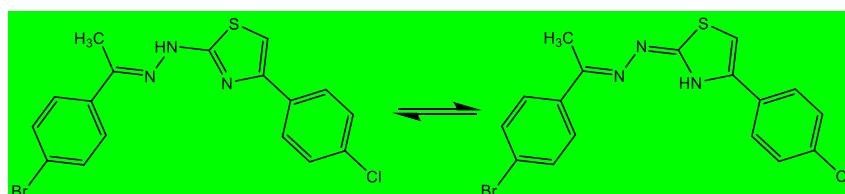


Figure S2b. <sup>13</sup>C-NMR spectrum of compound 3b



**Figure S2c.** Mass spectrum of compound **3b**



**Figure S2d:** Thiazole-thiazolidine tautomers of compound **3b**

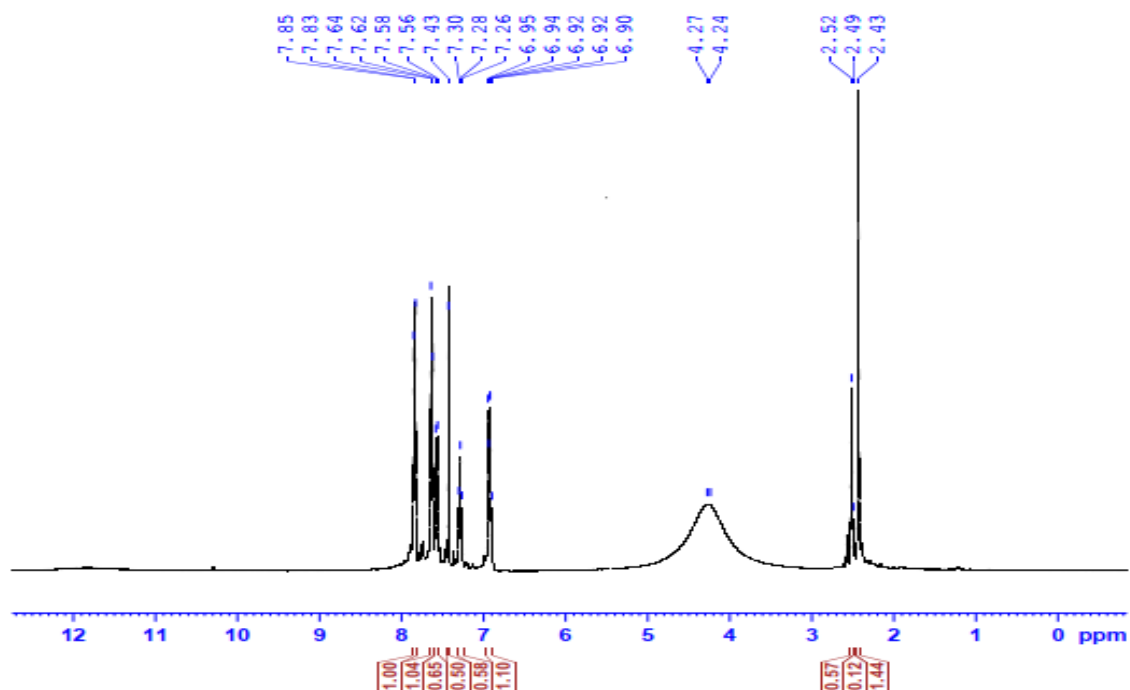


Figure S3a. <sup>1</sup>H-NMR spectrum of compound 3c

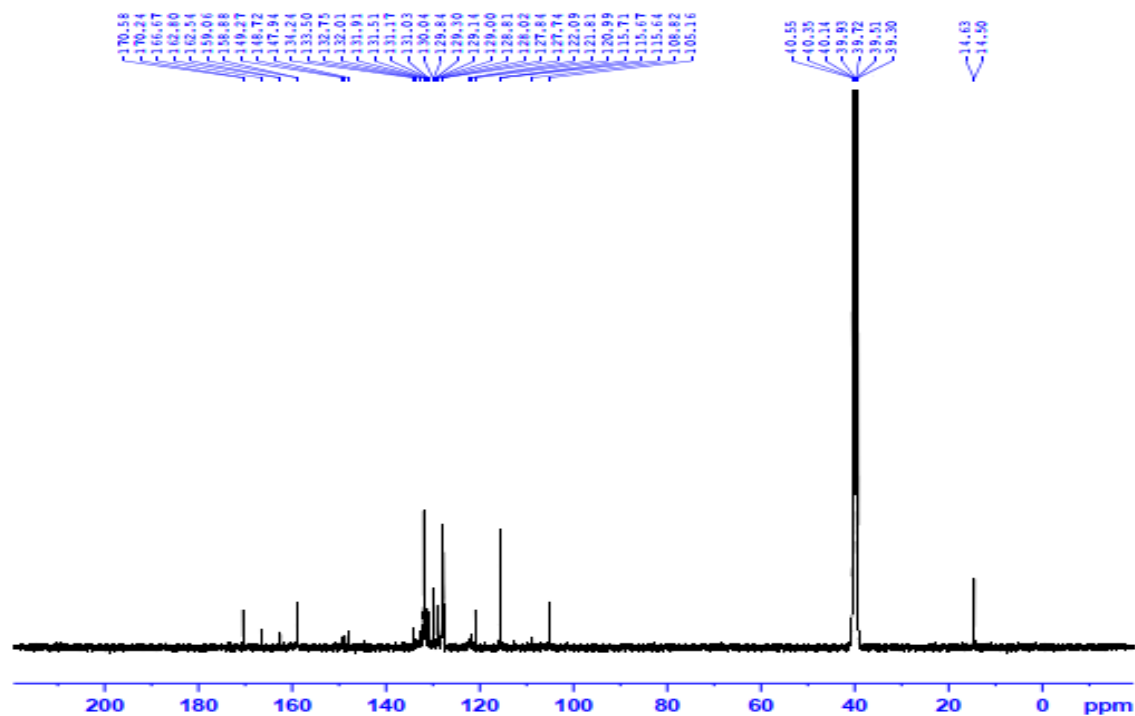
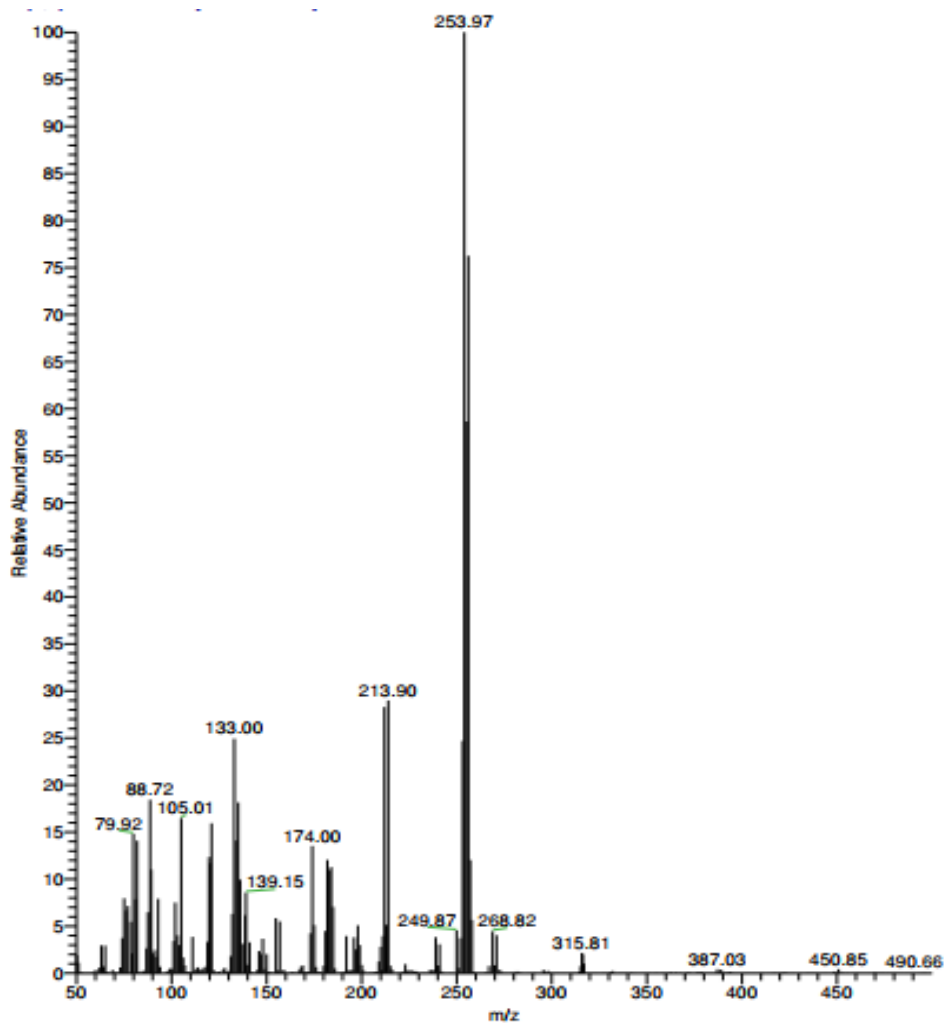
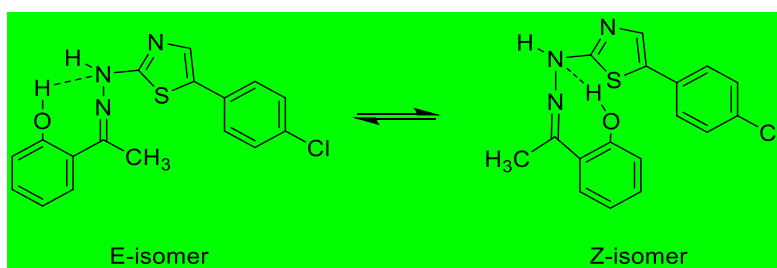


Figure S3b. <sup>13</sup>C-NMR spectrum of compound 3c



**Figure S3c.** Mass spectrum of compound **3c**



**Figure S3d:** The *E* and *Z* isomer of compound **3c**, and the formed hydrogen bond between phenolic hydroxyl with NH

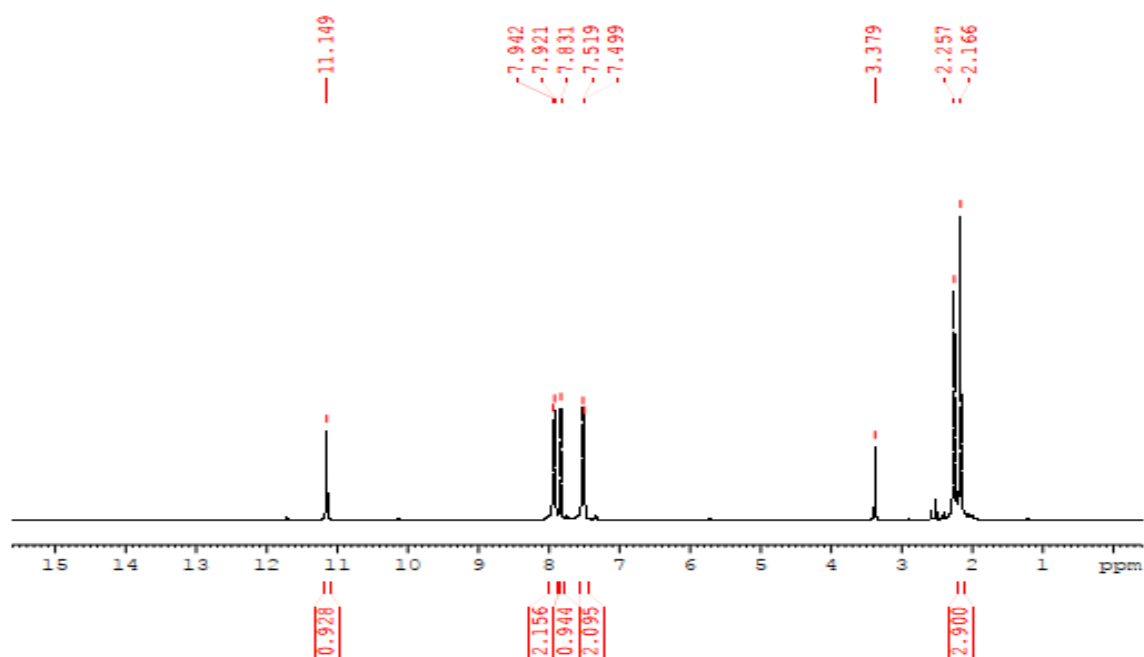


Figure S4a. <sup>1</sup>H-NMR spectrum of compound 4

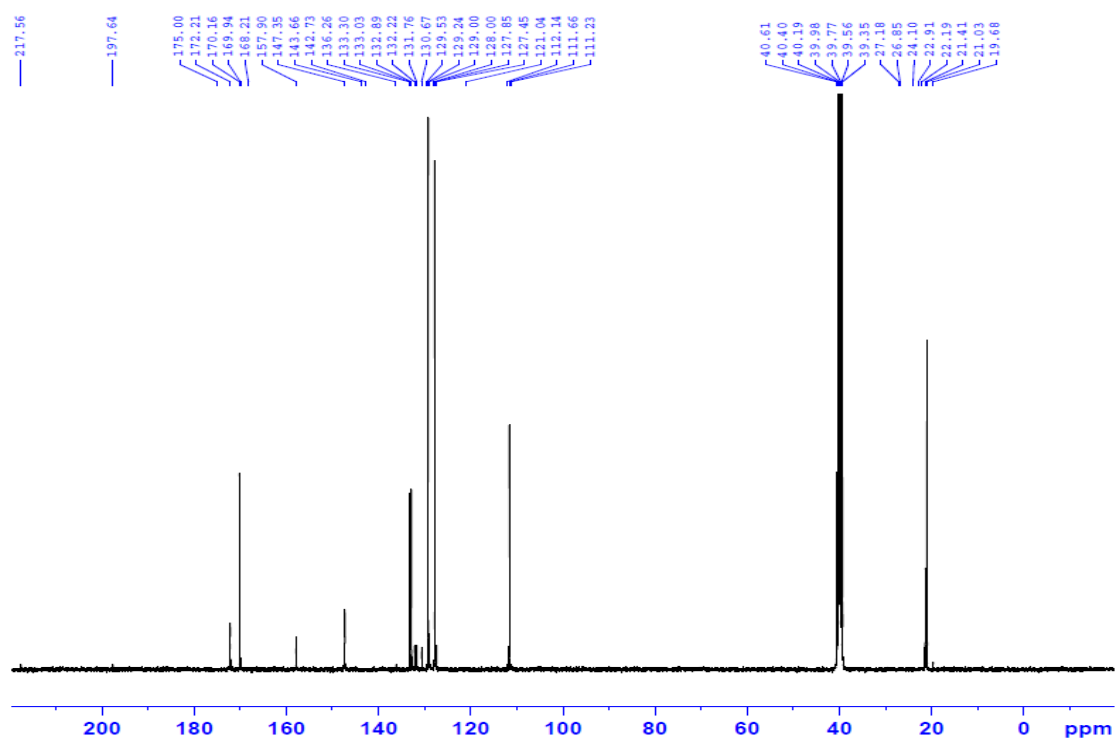
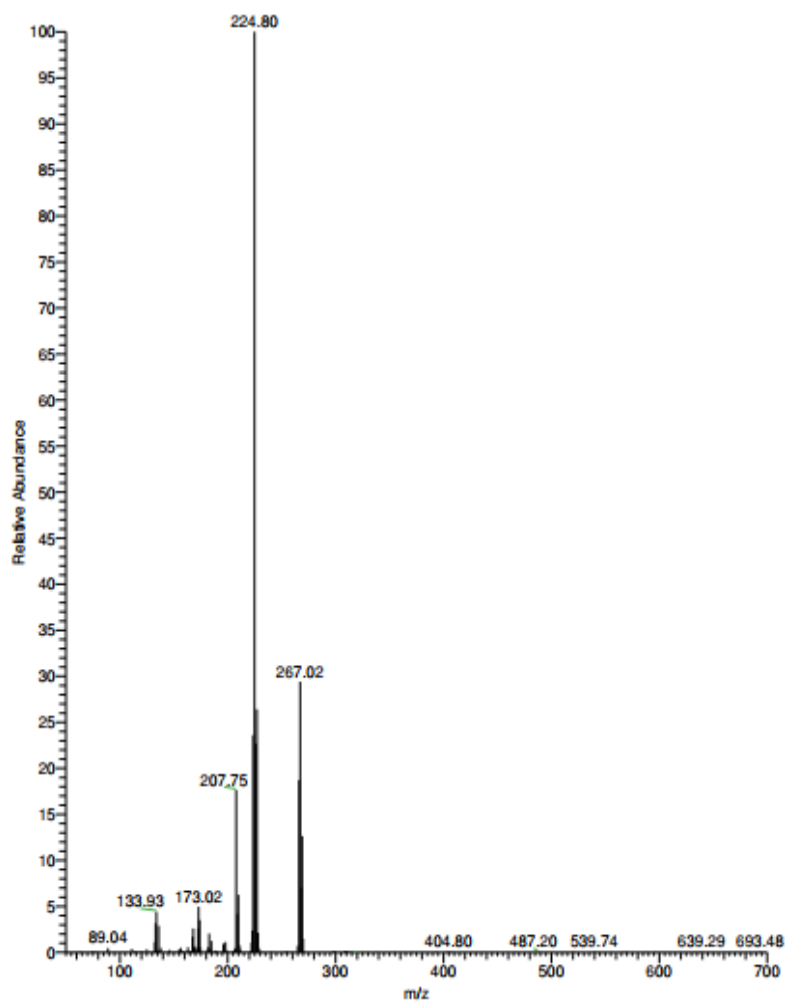
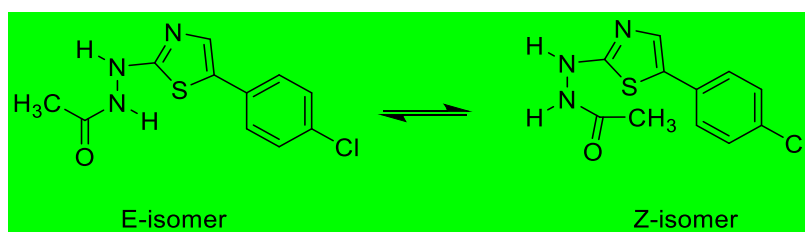


Figure S4b. <sup>13</sup>C-NMR spectrum of compound 4





**Figure S4c.** Mass spectrum of compound **4**



**Figure S4d.** Two isomers E and Z of compound (**4**)

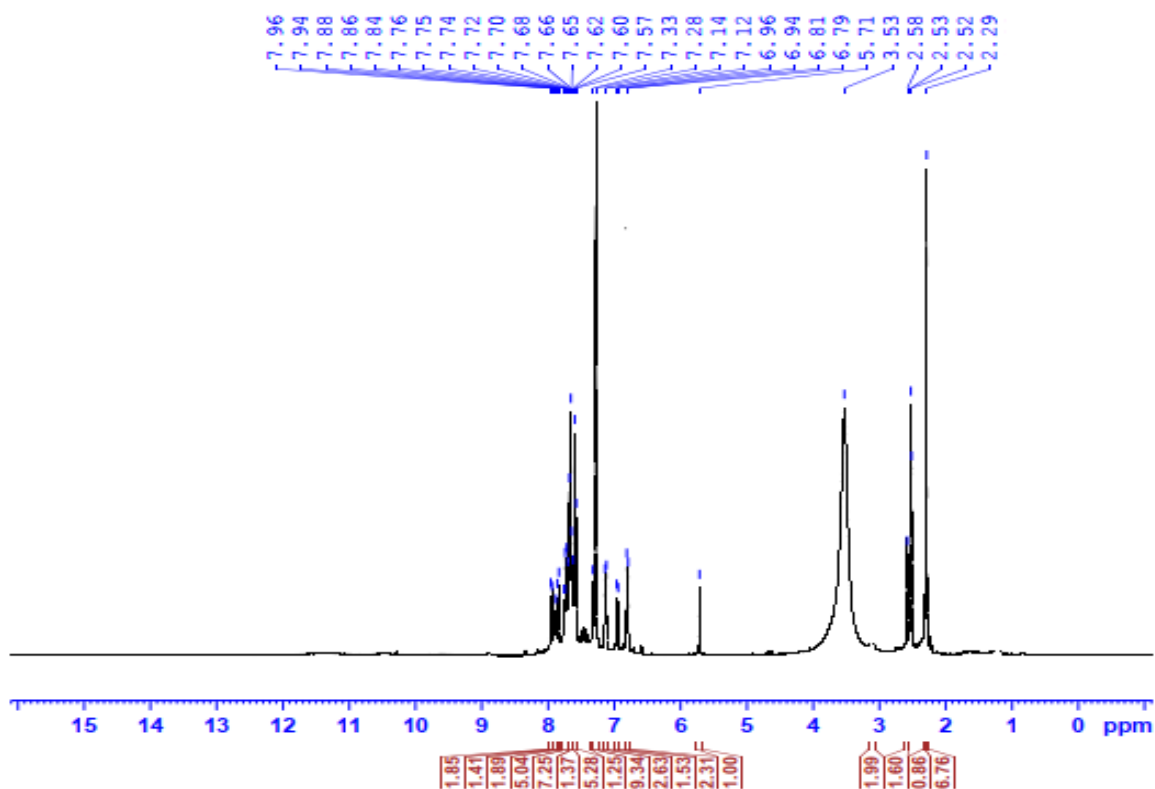


Figure S5a. <sup>1</sup>H-NMR spectrum of compound 5a

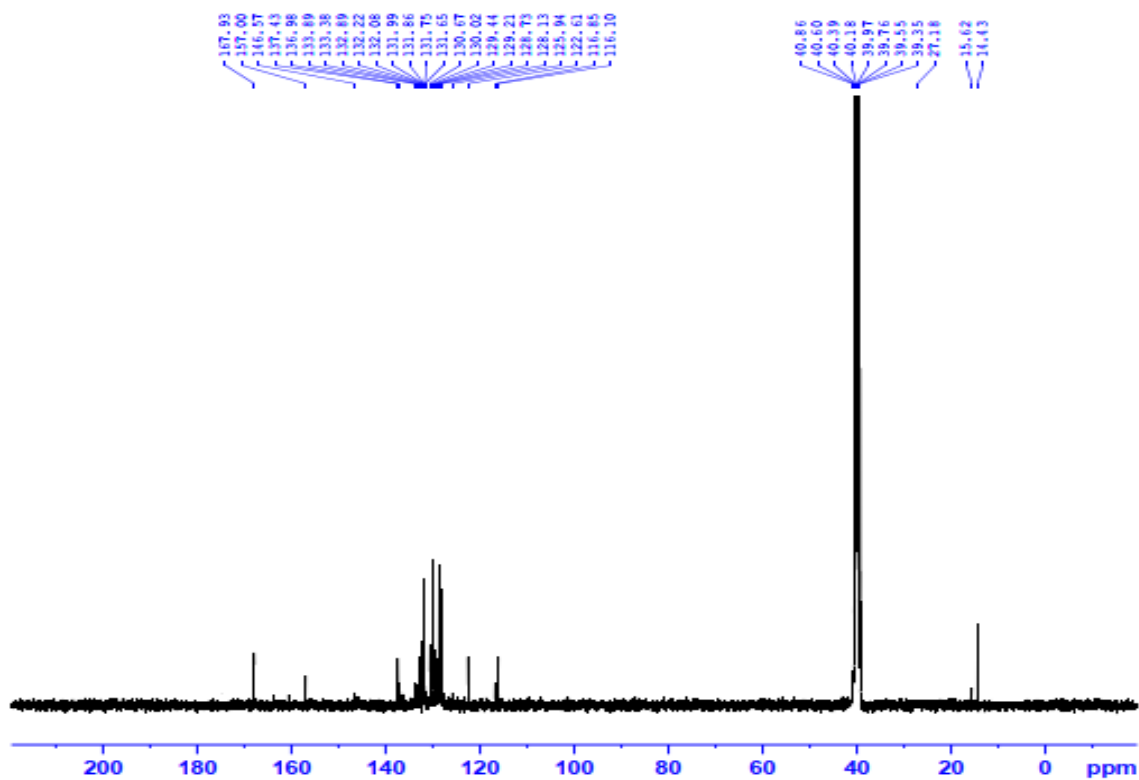
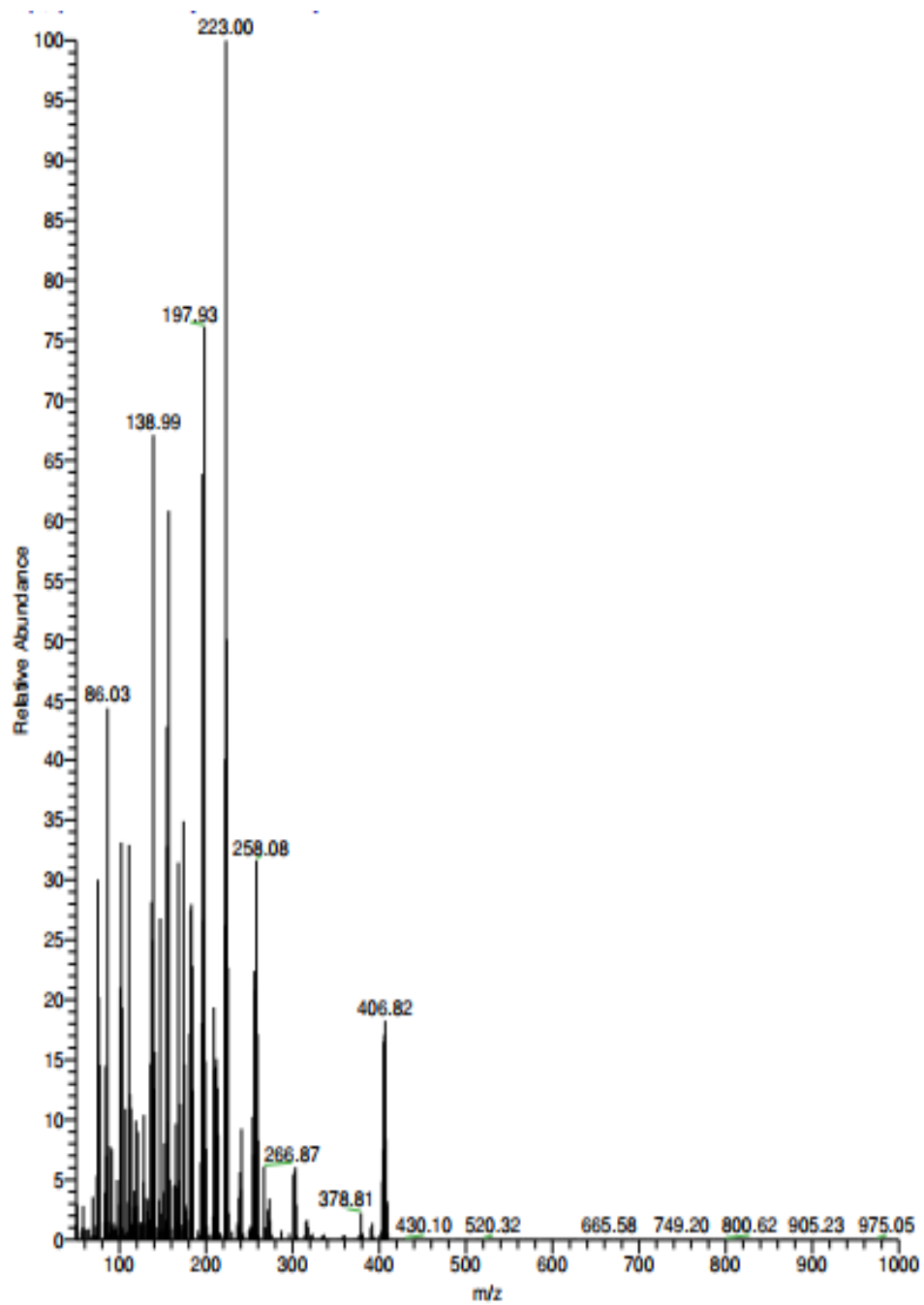


Figure S5b. <sup>13</sup>C-NMR spectrum of compound 5a



**Figure S5c.** Mass spectrum of compound 5a

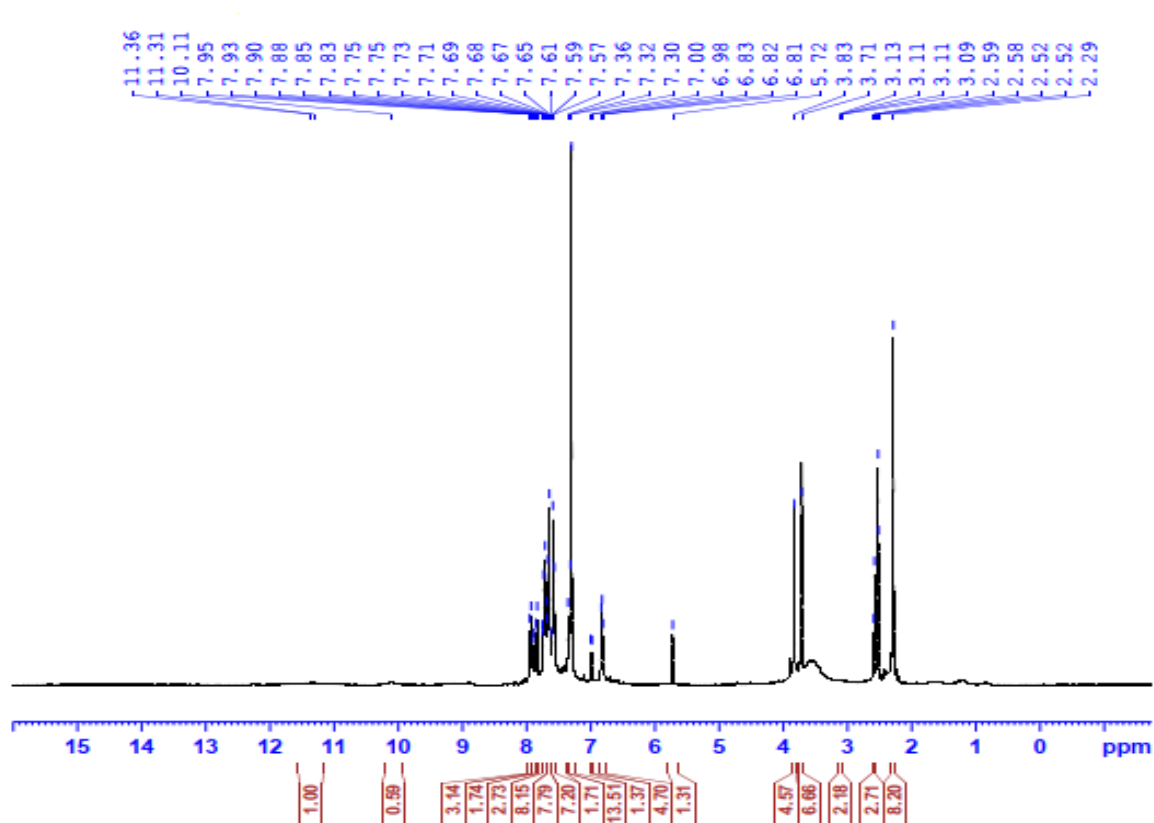


Figure S6a. <sup>1</sup>H-NMR spectrum of compound 5b

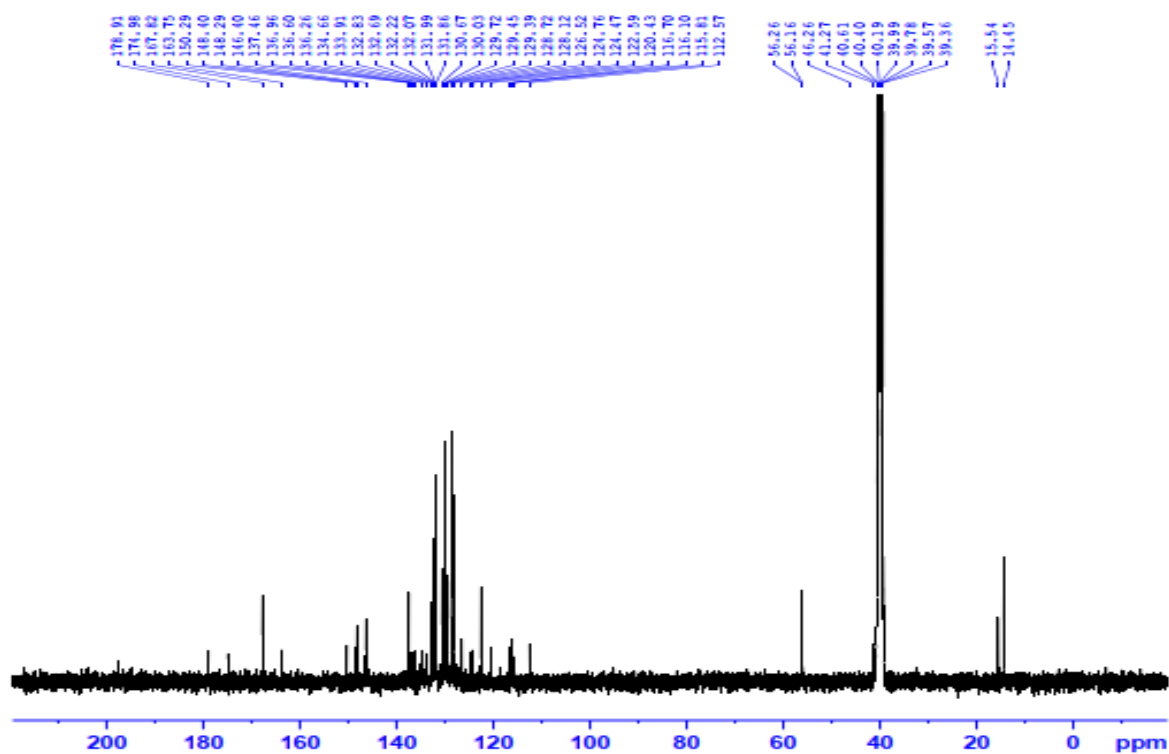


Figure S6b. <sup>13</sup>C-NMR spectrum of compound 5b.

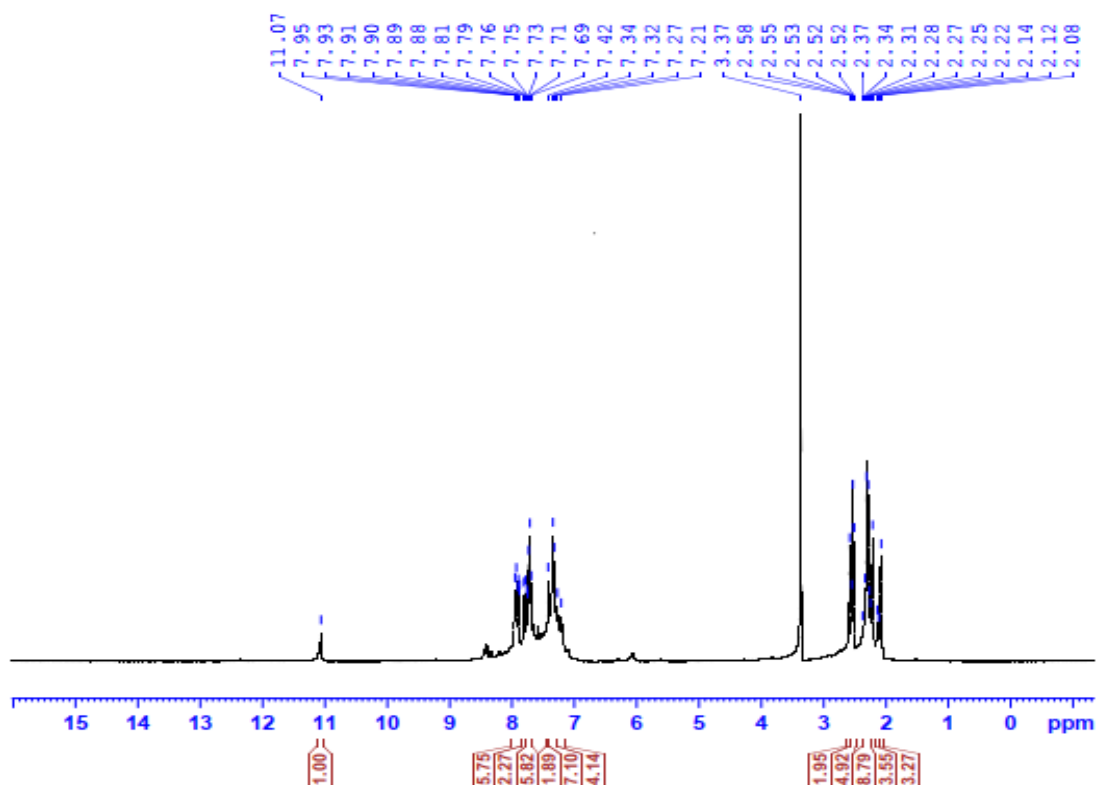


Figure S7a. <sup>1</sup>H-NMR spectrum of compound 6a

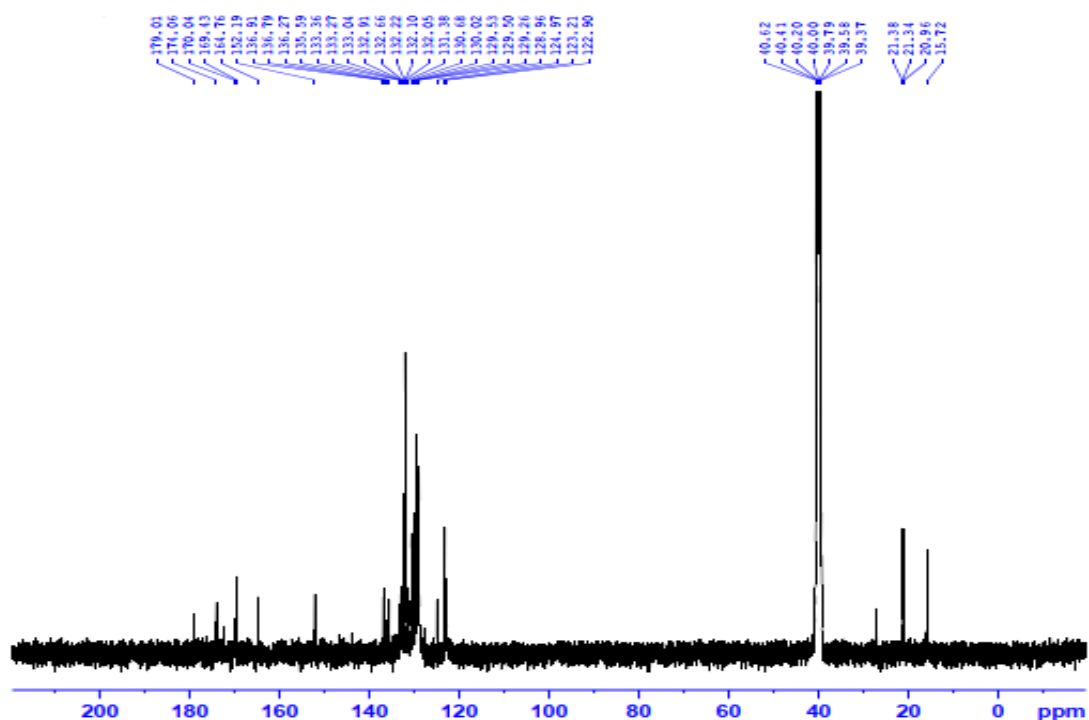
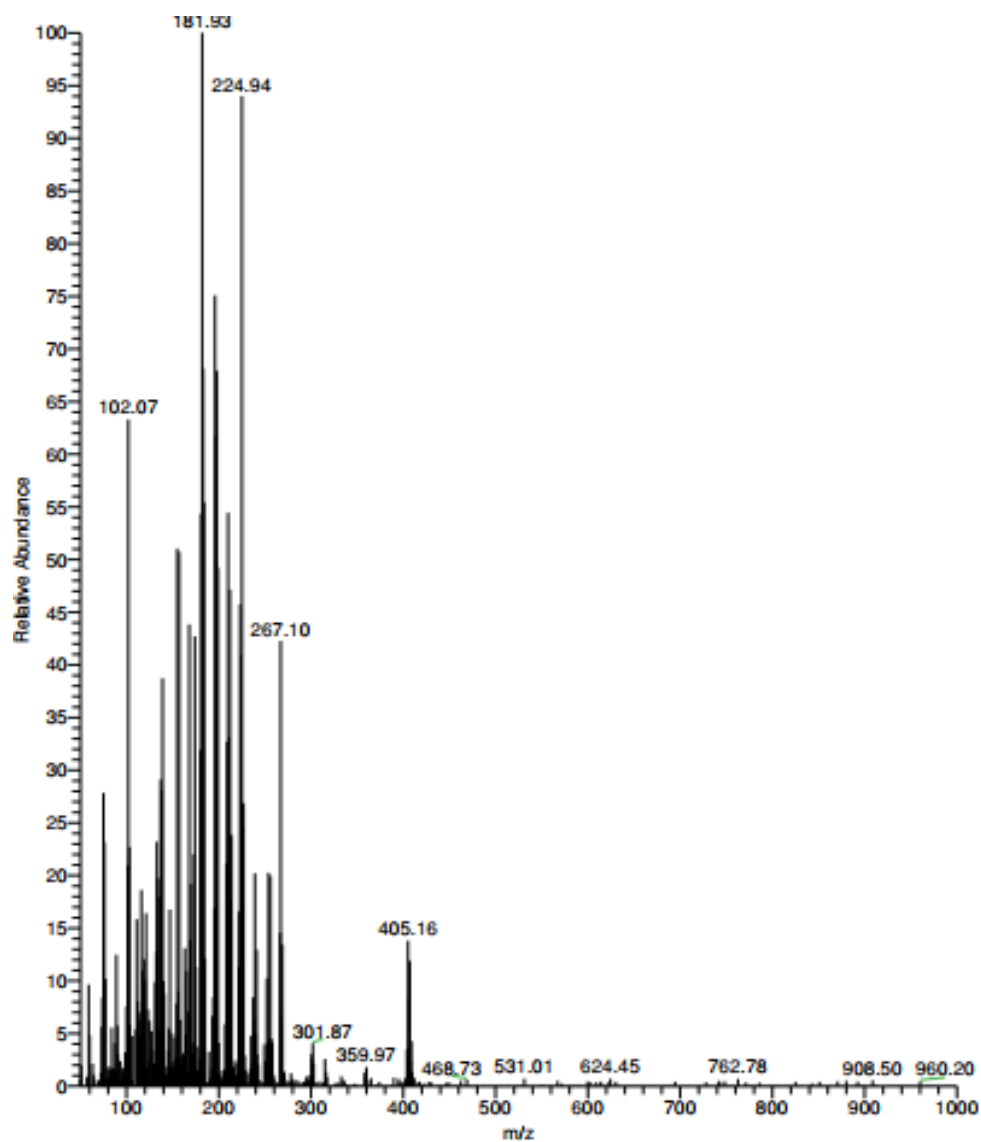
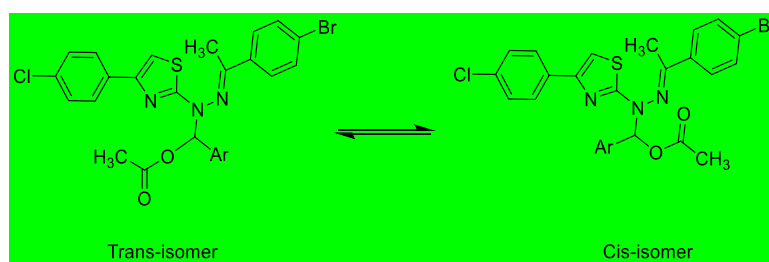


Figure S7b. <sup>13</sup>C-NMR spectrum of compound 6a



**Figure S7c.** Mass spectrum of compound **6a**



**Figure S7d.** Cis and Trans isomers of compounds **6a** and **6b**.

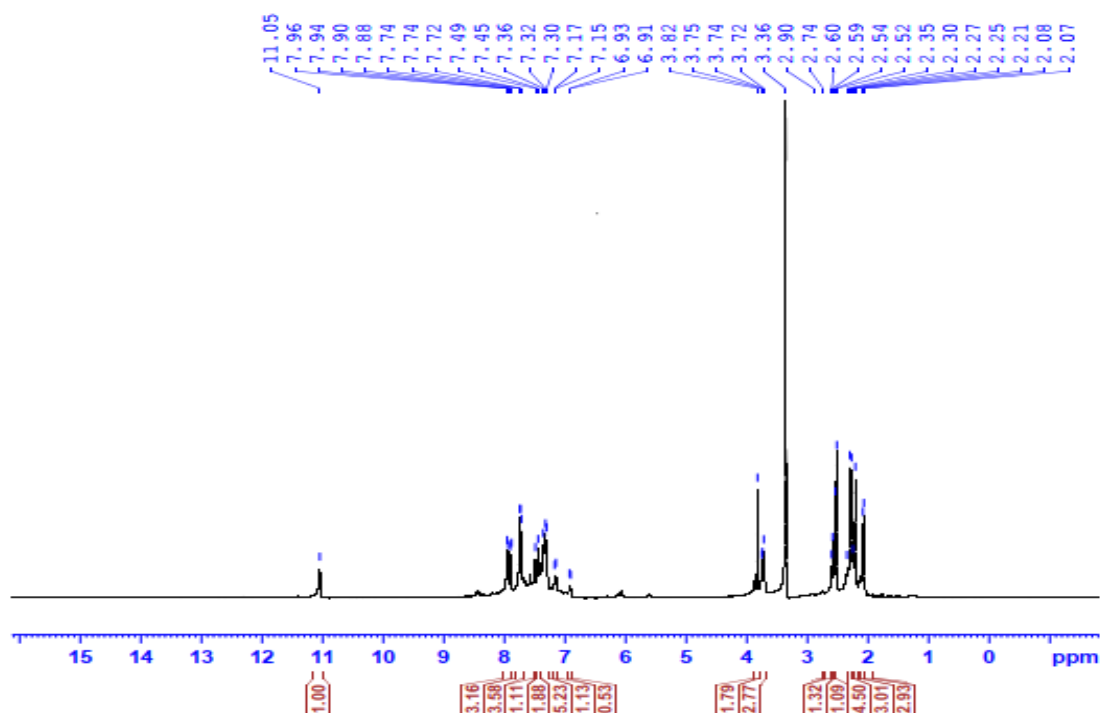


Figure S8a. <sup>1</sup>H-NMR spectrum of compound 6b

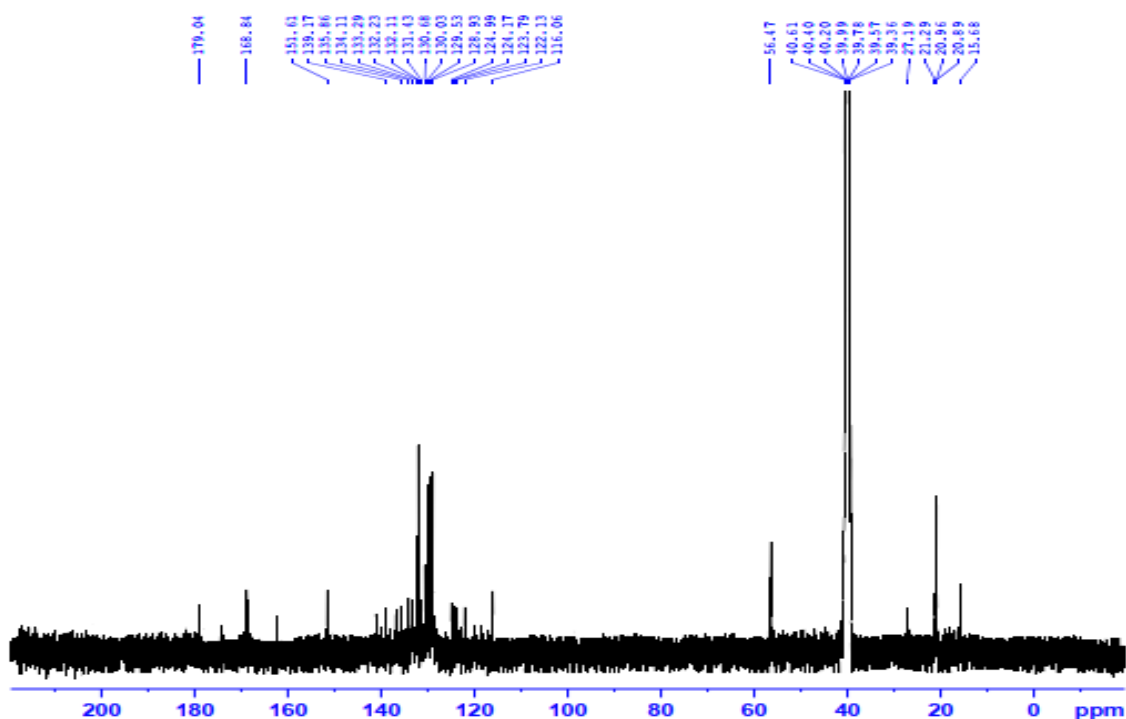
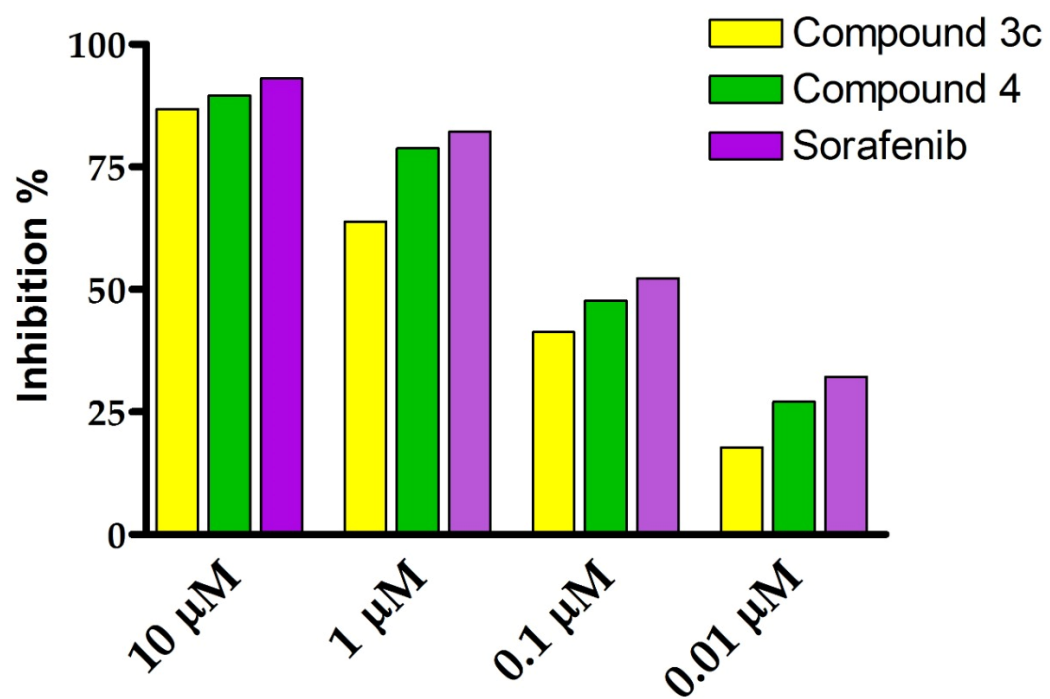


Figure S8b. <sup>13</sup>C-NMR spectrum of compound 6b



**Figure S9.** Inhibitory activity of compounds 3c, 4 and Sorafenib toward the VEGFR-2 kinase activity.