

Supplementary Materials

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

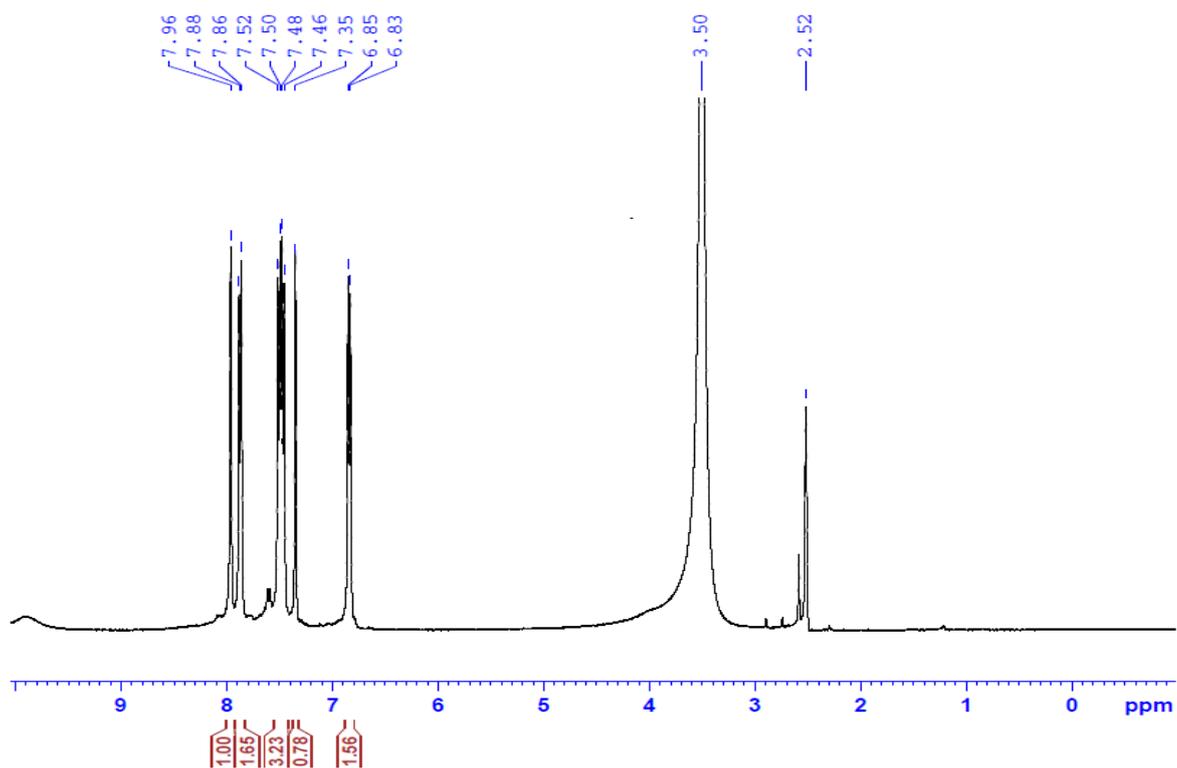


Figure S1a. ^1H -NMR spectrum of compound **3a**

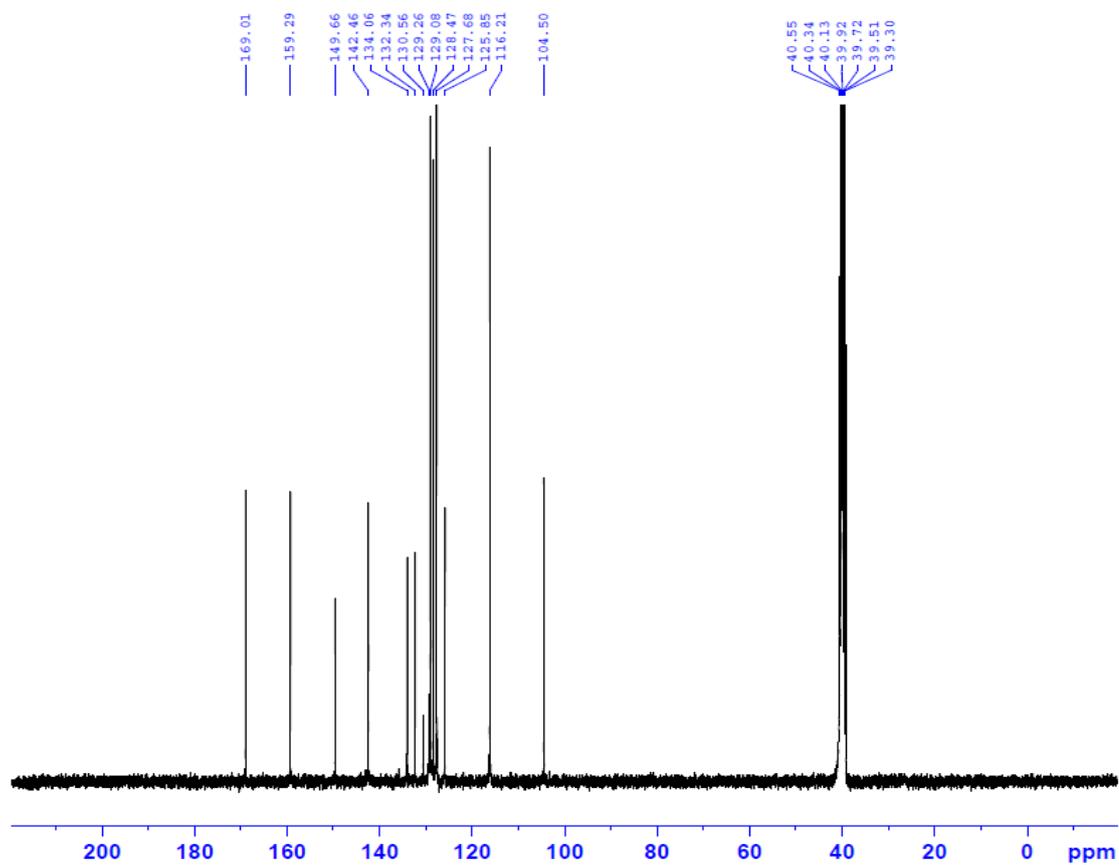


Figure S1b. ^{13}C -NMR spectrum of compound **3a**

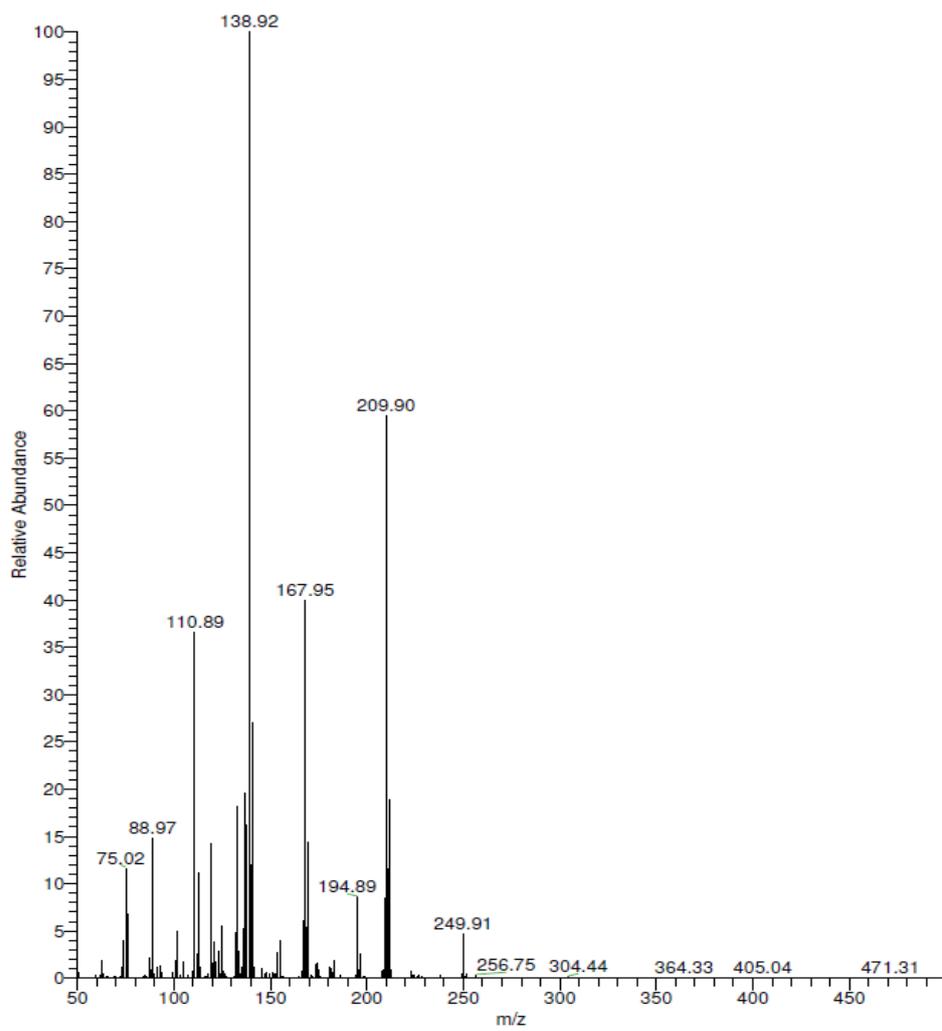


Figure S1c. mass spectrum of compound **3a**

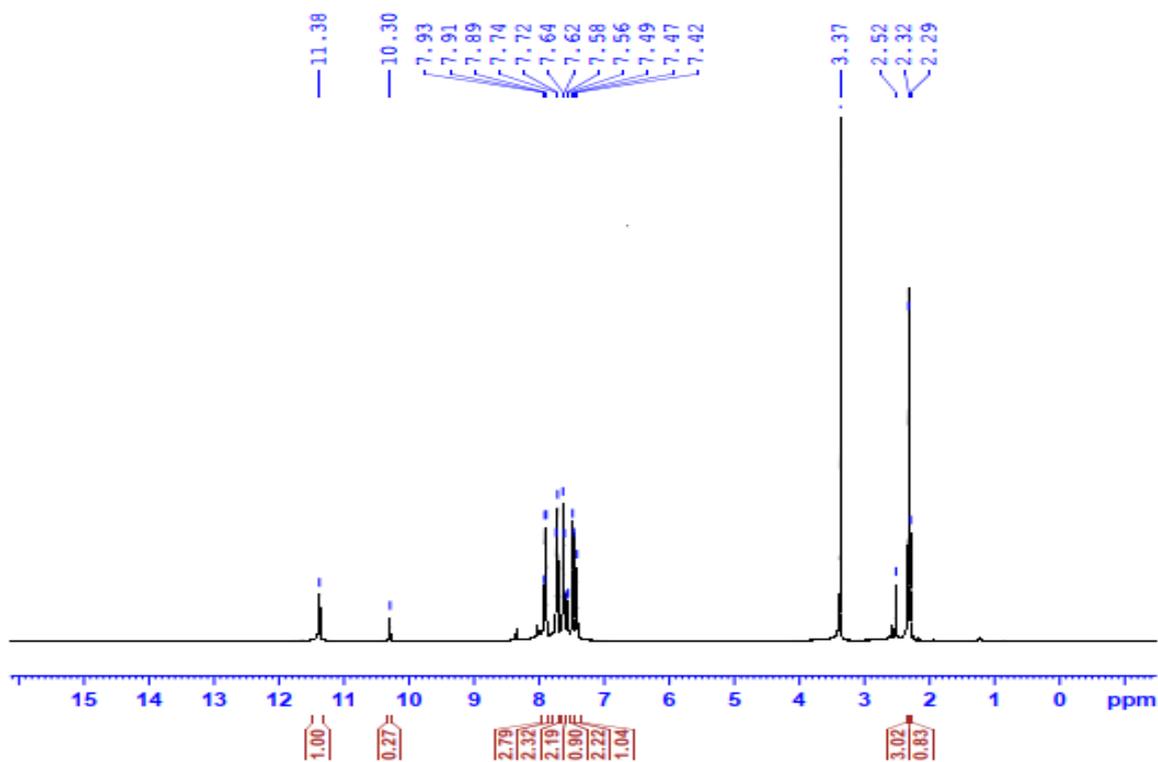


Figure S2a. ^1H -NMR spectrum of compound **3b**

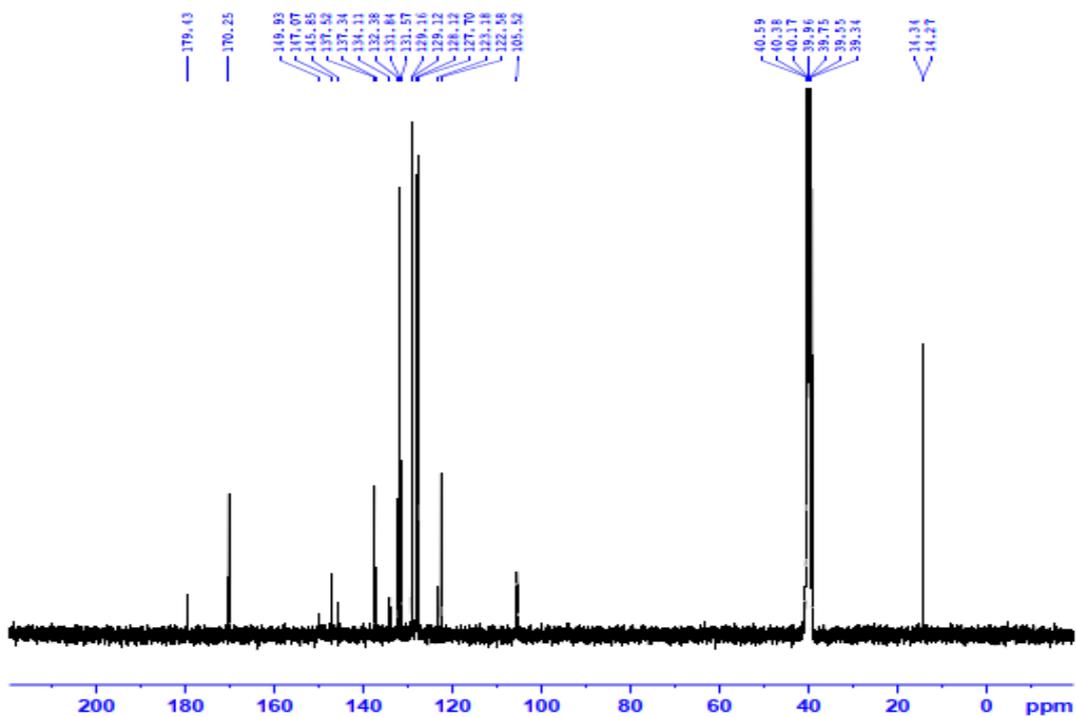


Figure S2b. ^{13}C -NMR spectrum of compound **3b**

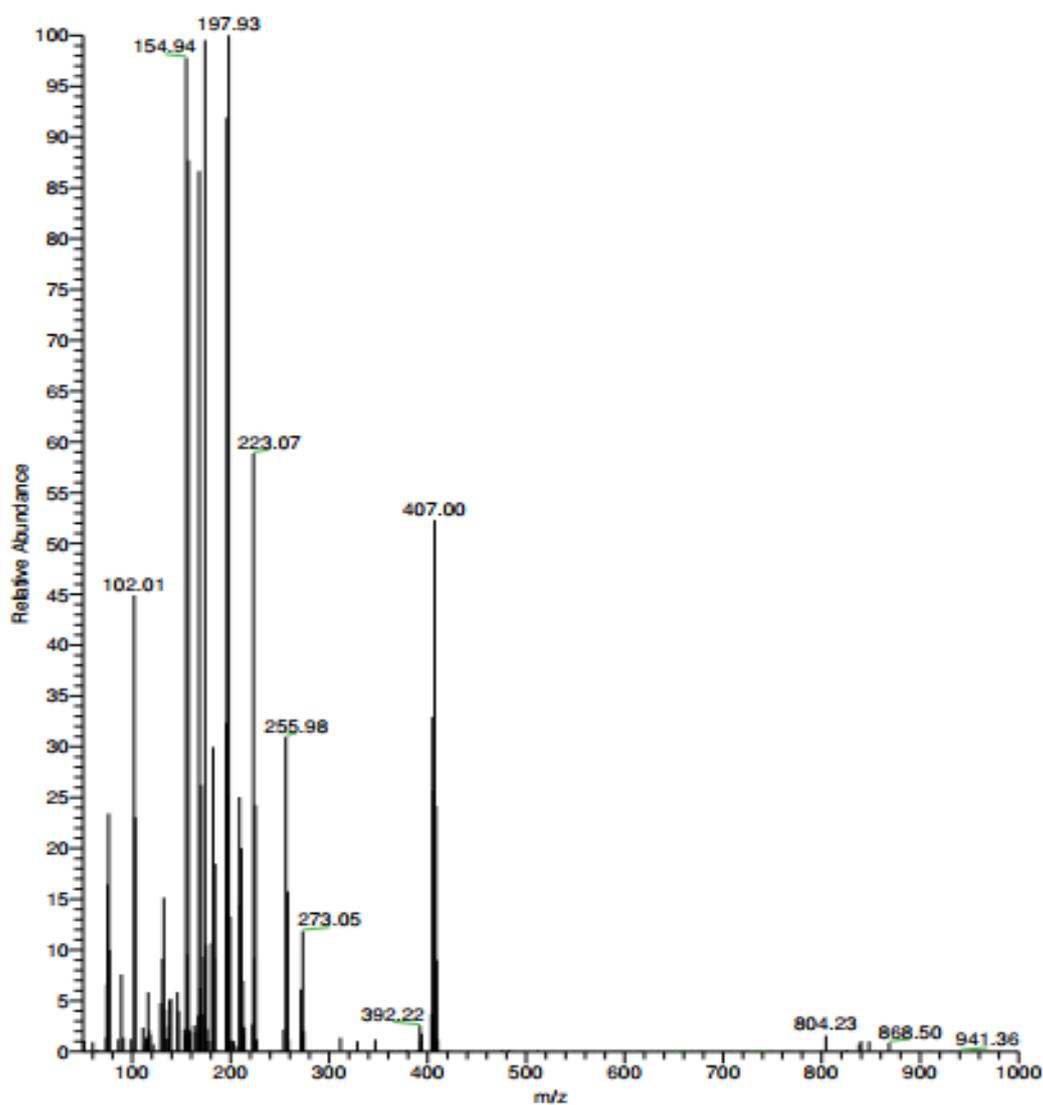


Figure S2c. Mass spectrum of compound **3b**

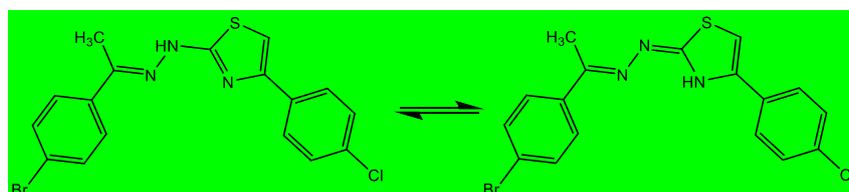


Figure S2d: Thiazole-thiazolidine tautomers of compound **3b**

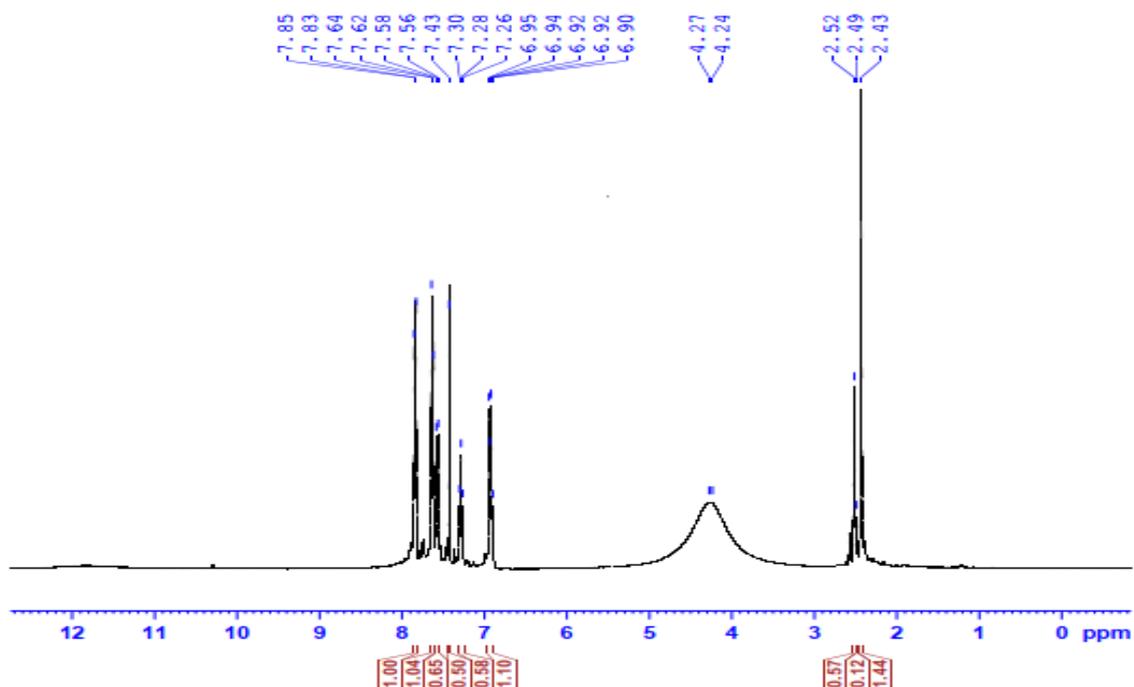


Figure S3a. ^1H -NMR spectrum of compound 3c

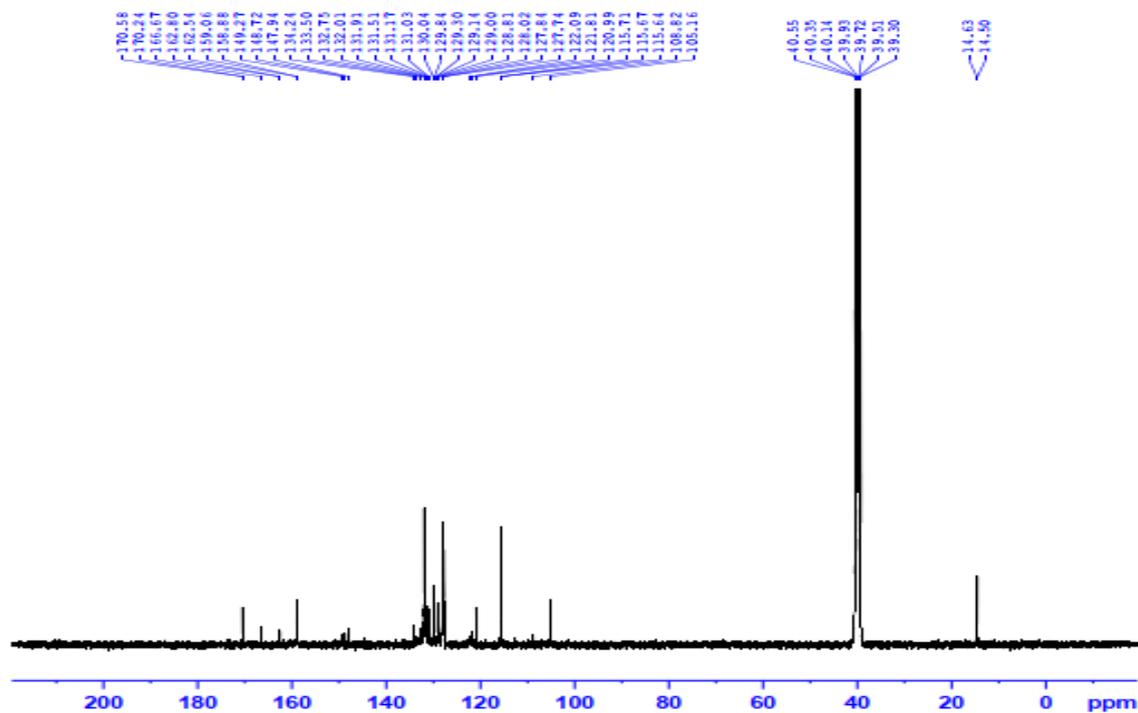


Figure S3b. ^{13}C -NMR spectrum of compound 3c

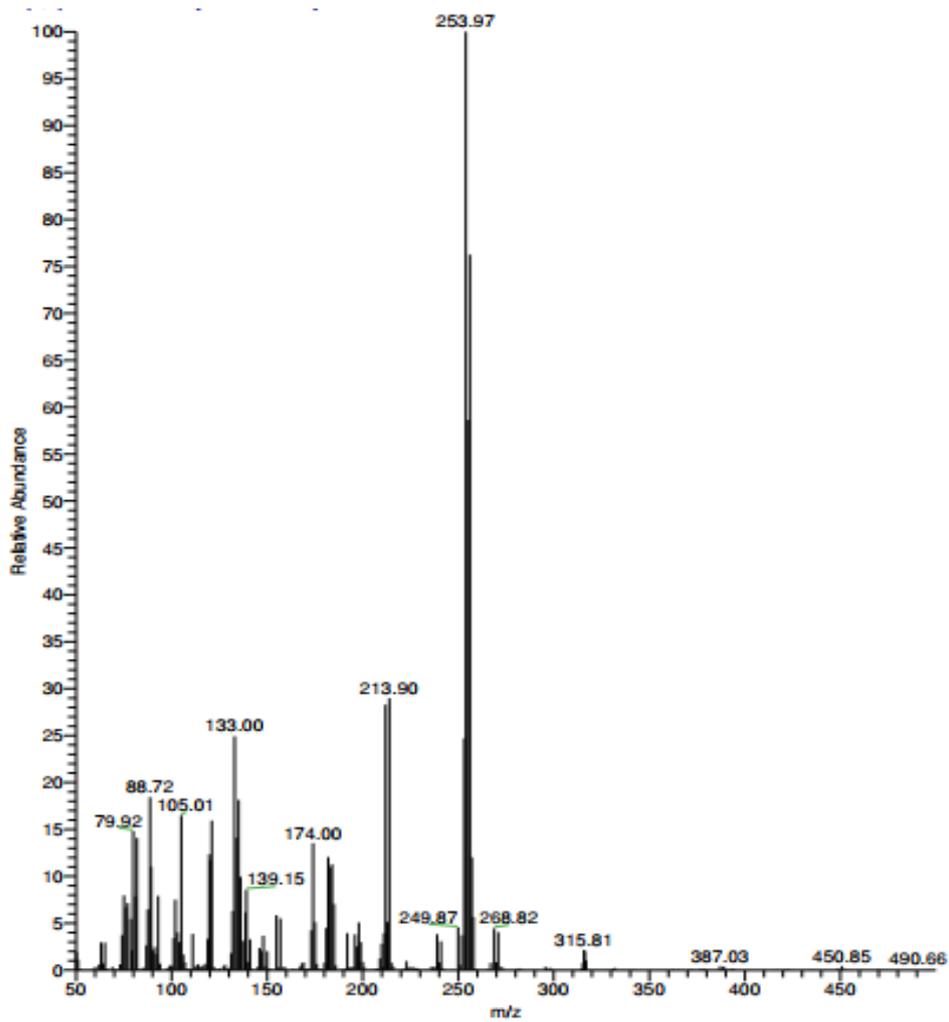


Figure S3c. Mass spectrum of compound 3c

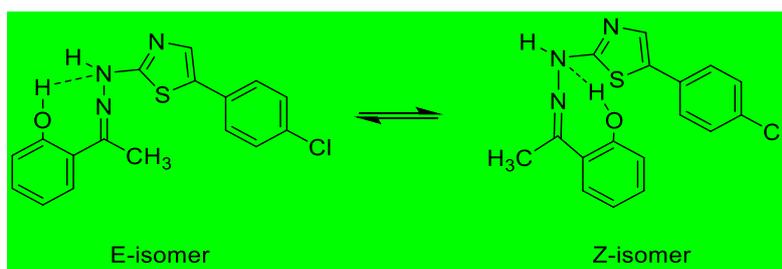


Figure S3d: The E and Z isomer of compound 3c, and the formed hydrogen bond between phenolic hydroxyl with NH

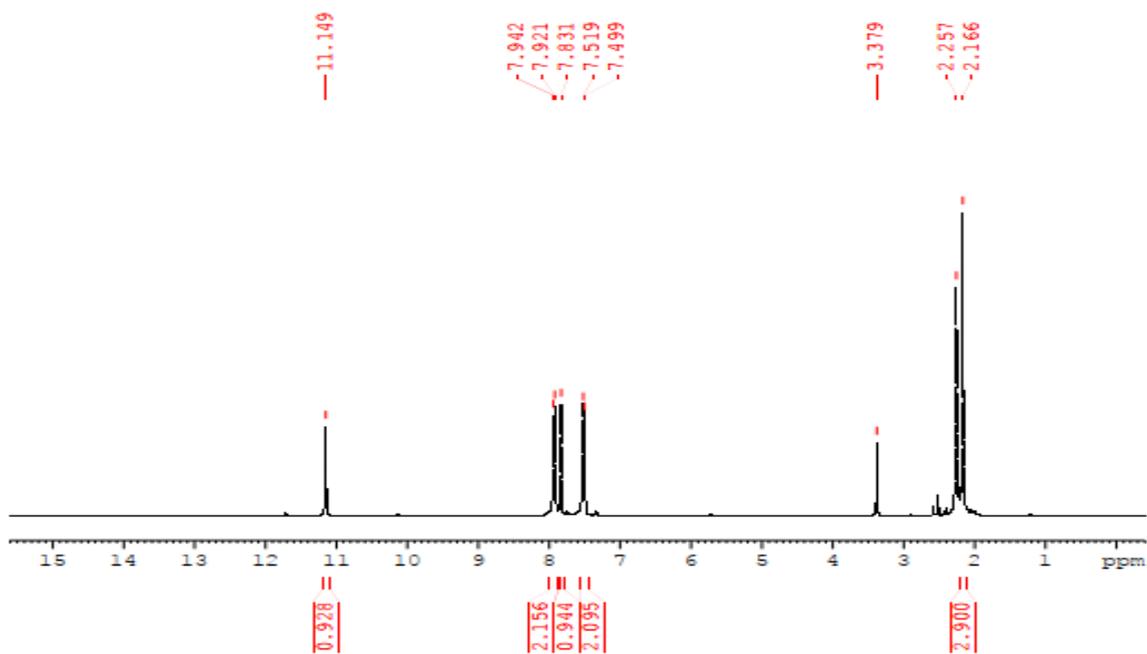


Figure S4a. ¹H-NMR spectrum of compound 4

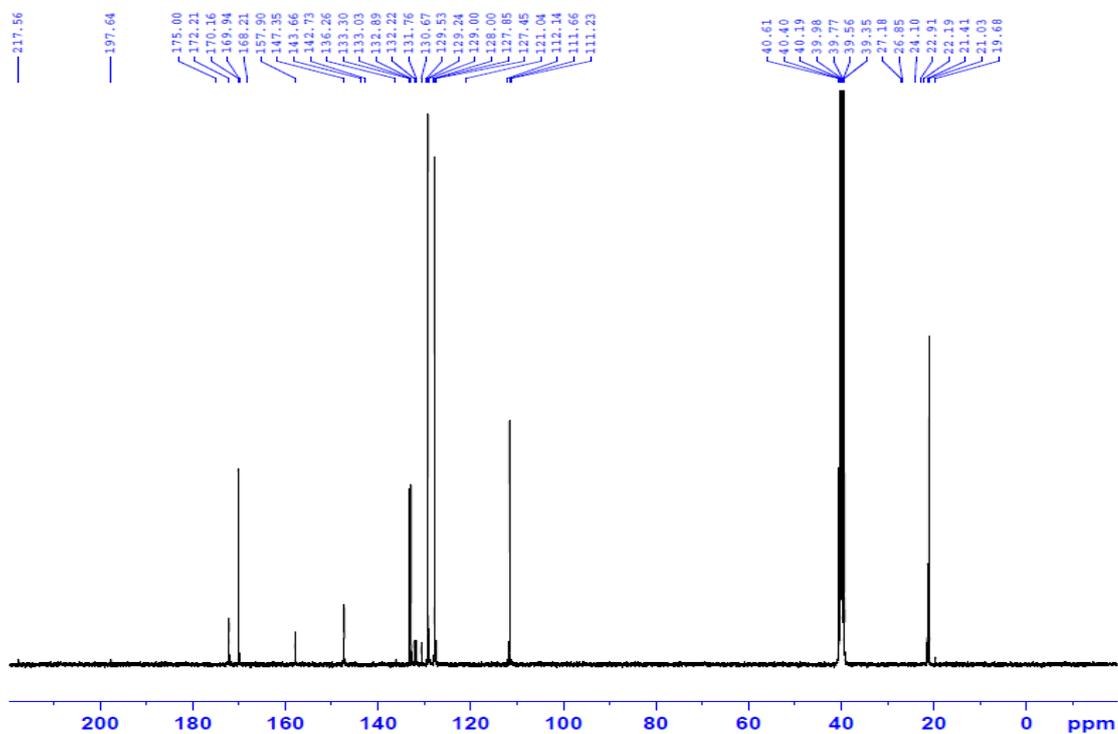


Figure S4b. ¹³C-NMR spectrum of compound 4

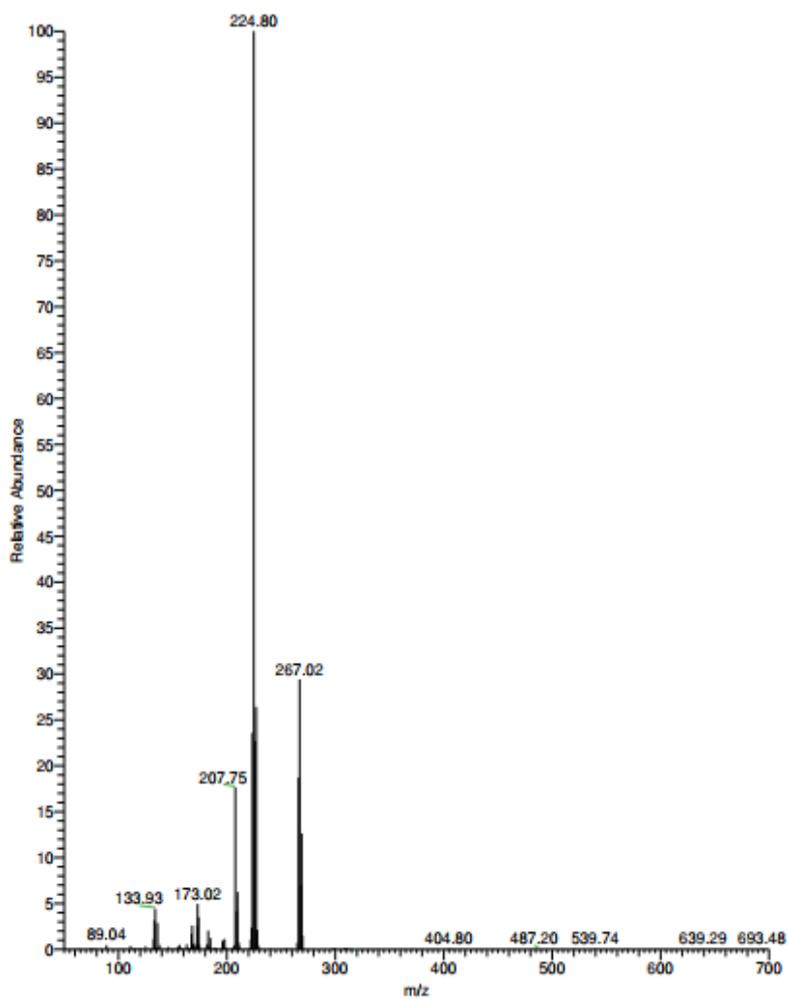


Figure S4c. Mass spectrum of compound 4

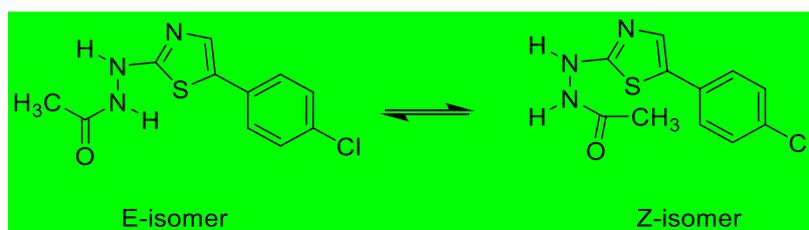


Figure S4d. Two isomers E and Z of compound (4)

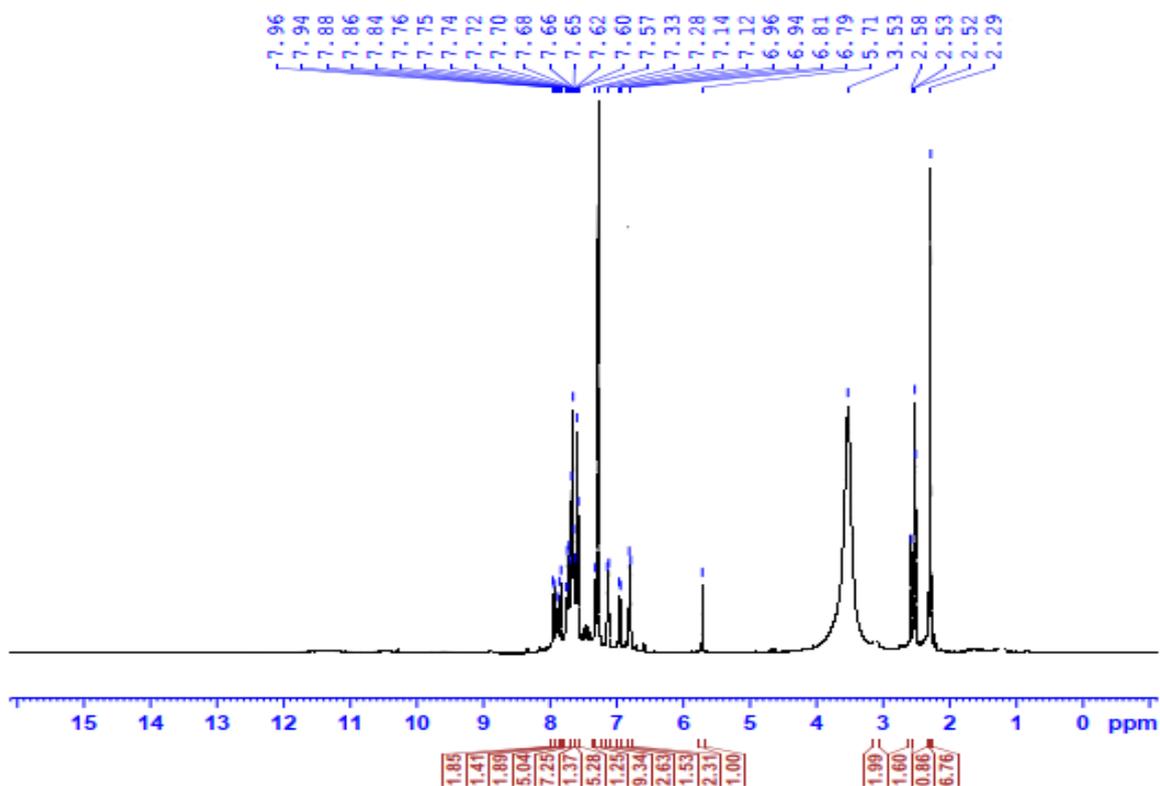


Figure S5a. ¹H-NMR spectrum of compound 5a

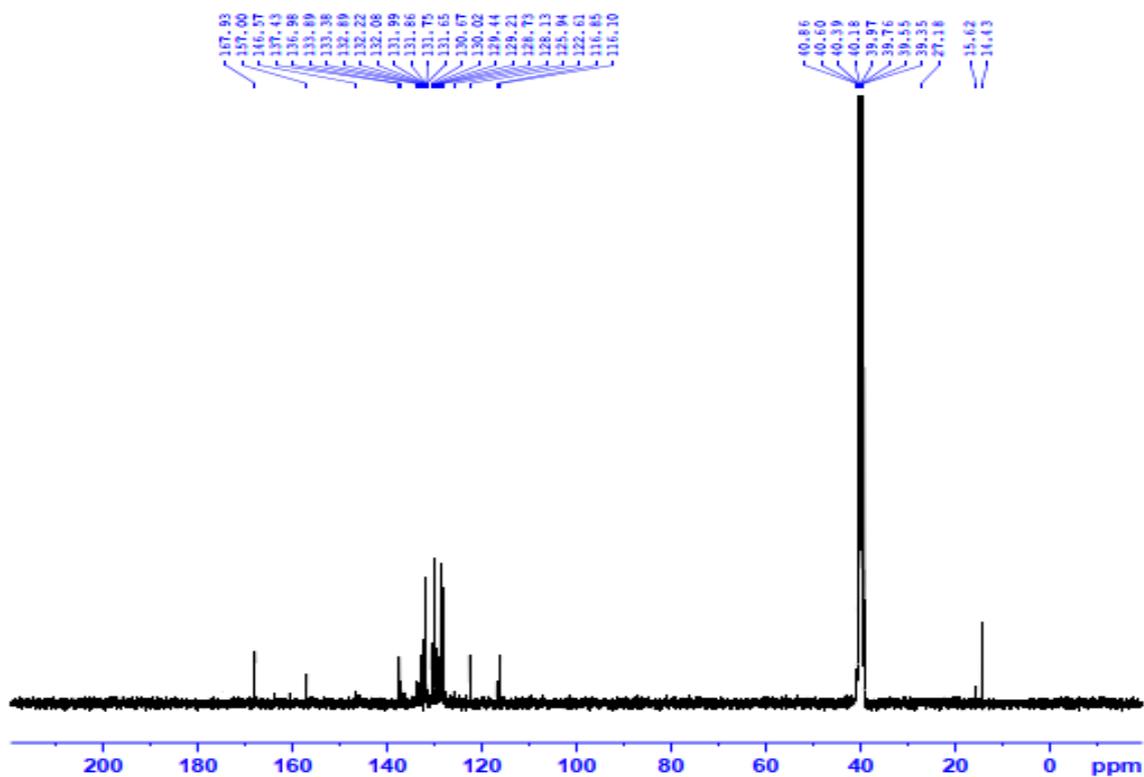


Figure S5b. ¹³C-NMR spectrum of compound 5a

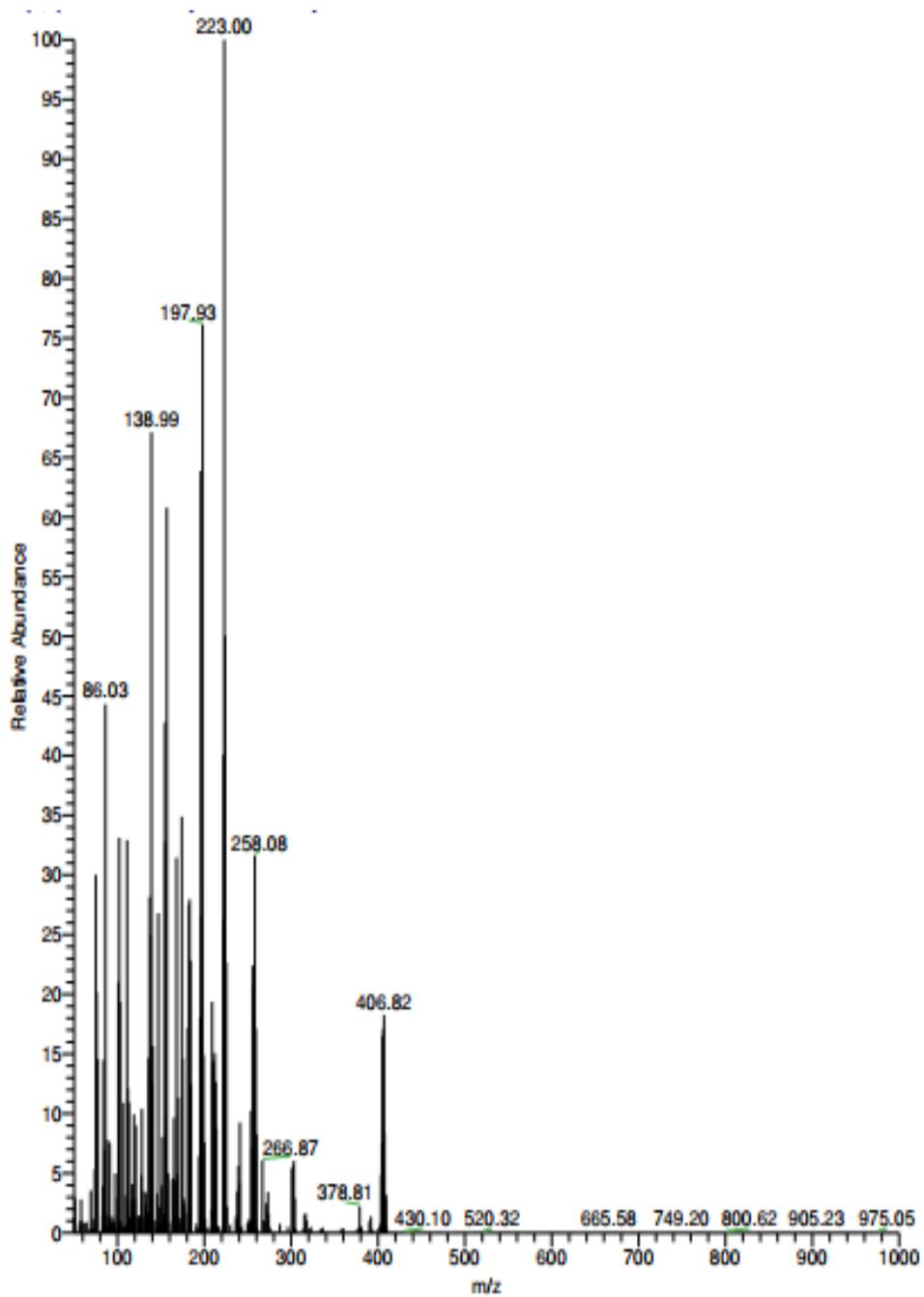


Figure S5c. Mass spectrum of compound 5a

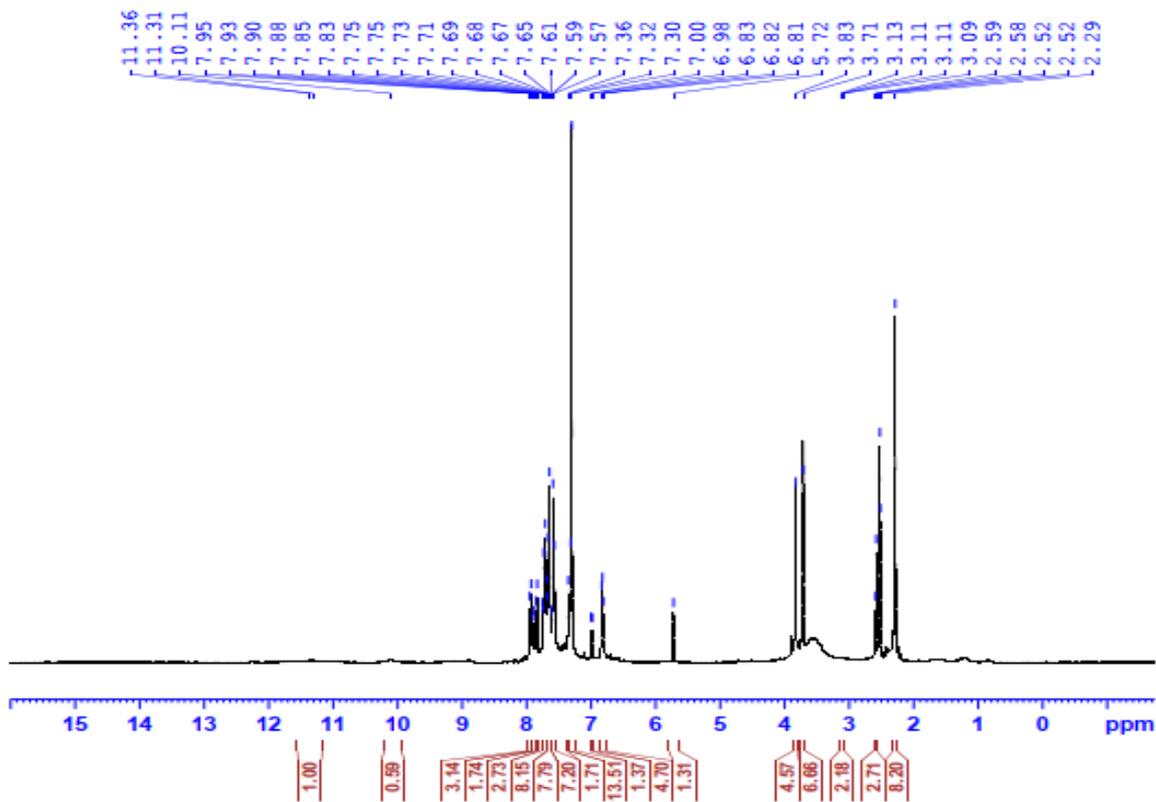


Figure S6a. ^1H -NMR spectrum of compound 5b

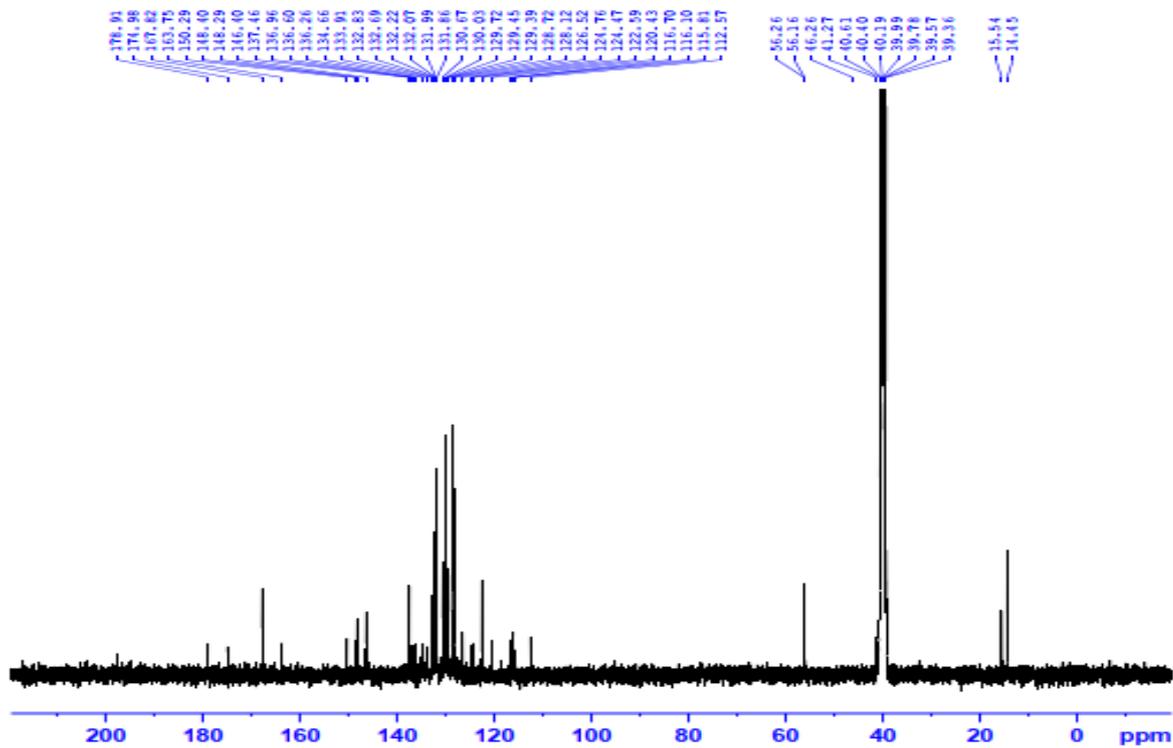


Figure S6b. ^{13}C -NMR spectrum of compound 5b.

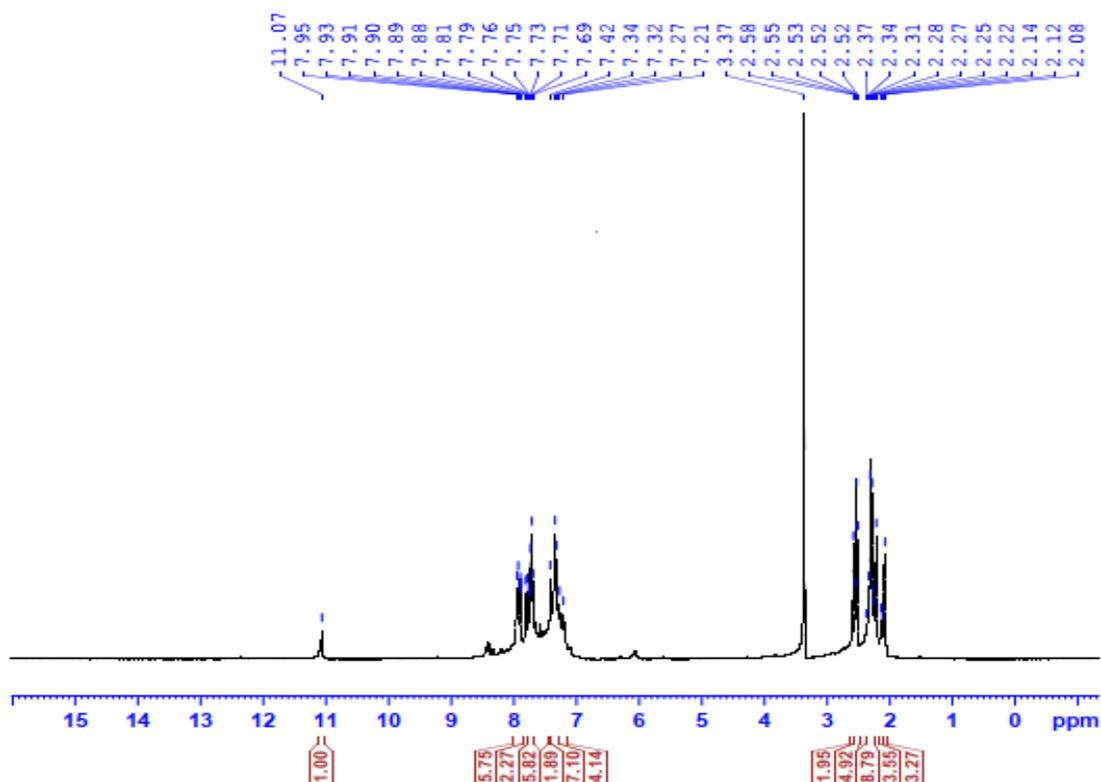


Figure S7a. $^1\text{H-NMR}$ spectrum of compound 6a

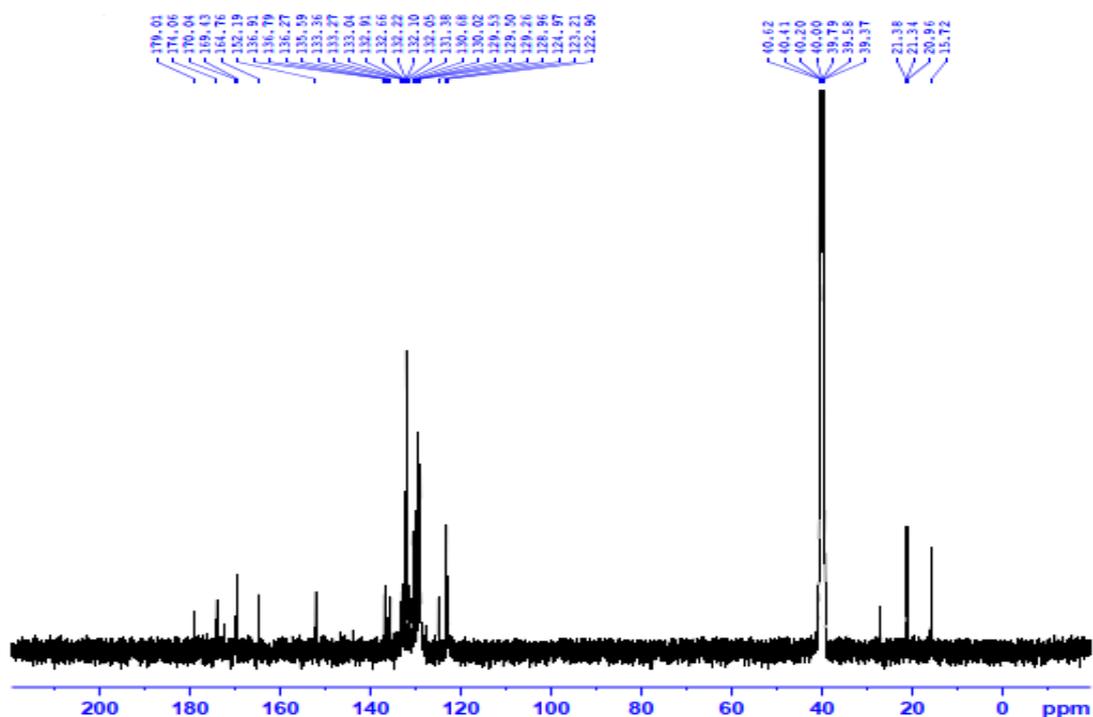


Figure S7b. $^{13}\text{C-NMR}$ spectrum of compound 6a

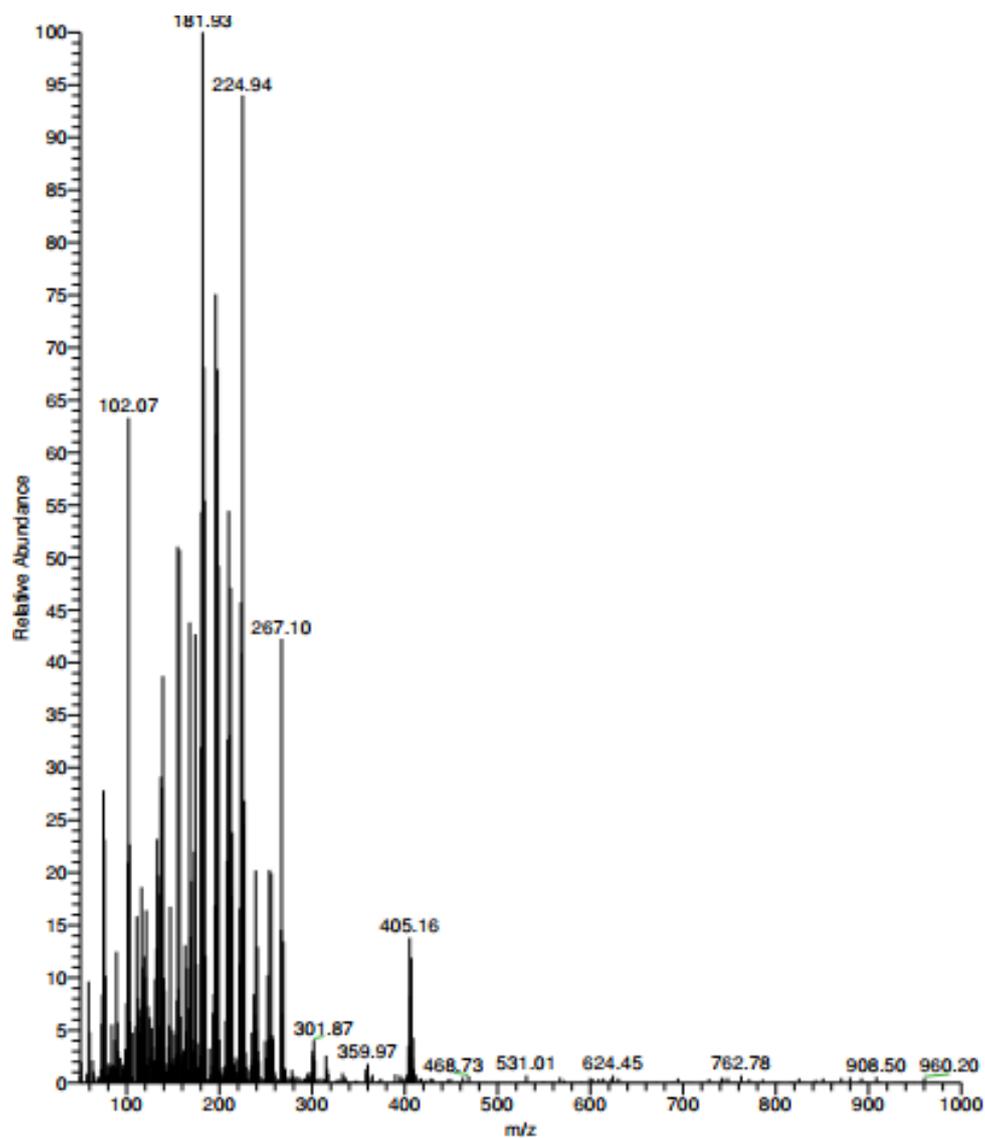


Figure S7c. Mass spectrum of compound 6a

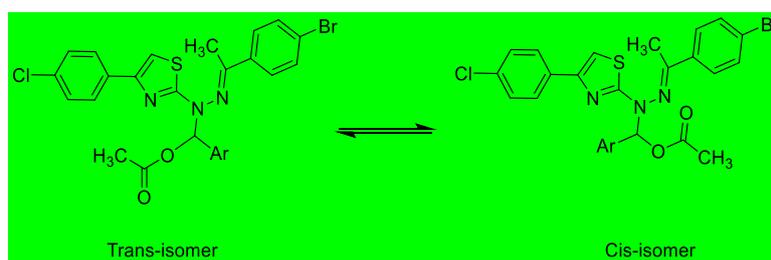


Figure S7d. Cis and Trans isomers of compounds 6a and 6b.

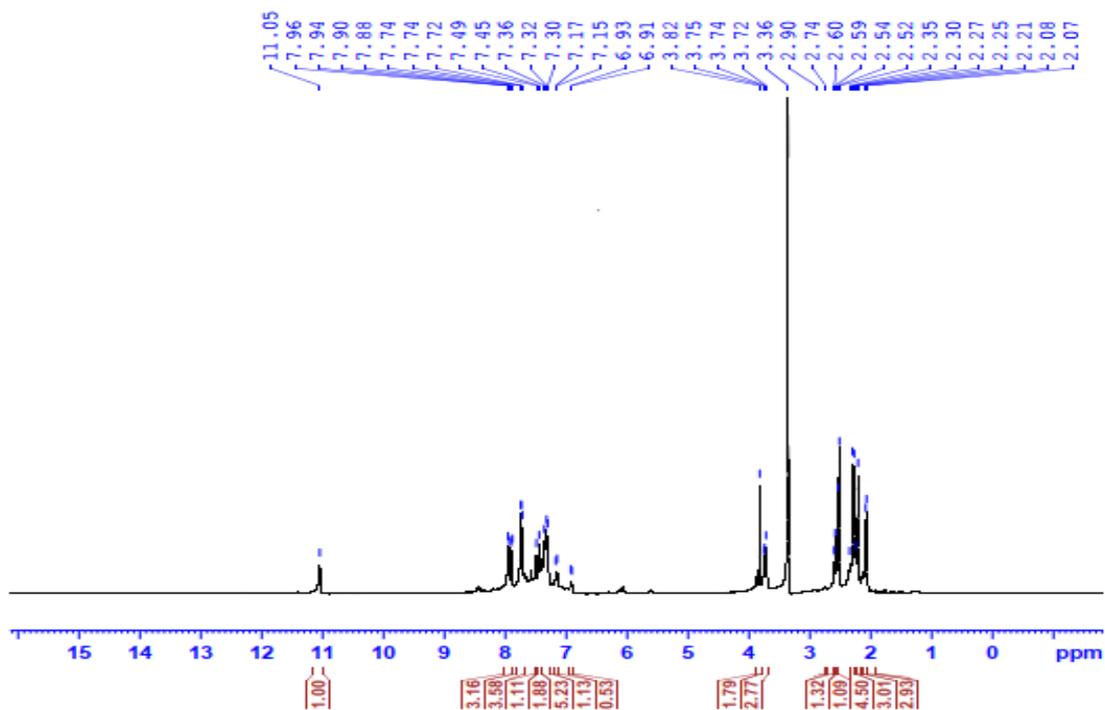


Figure S8a. ¹H-NMR spectrum of compound 6b

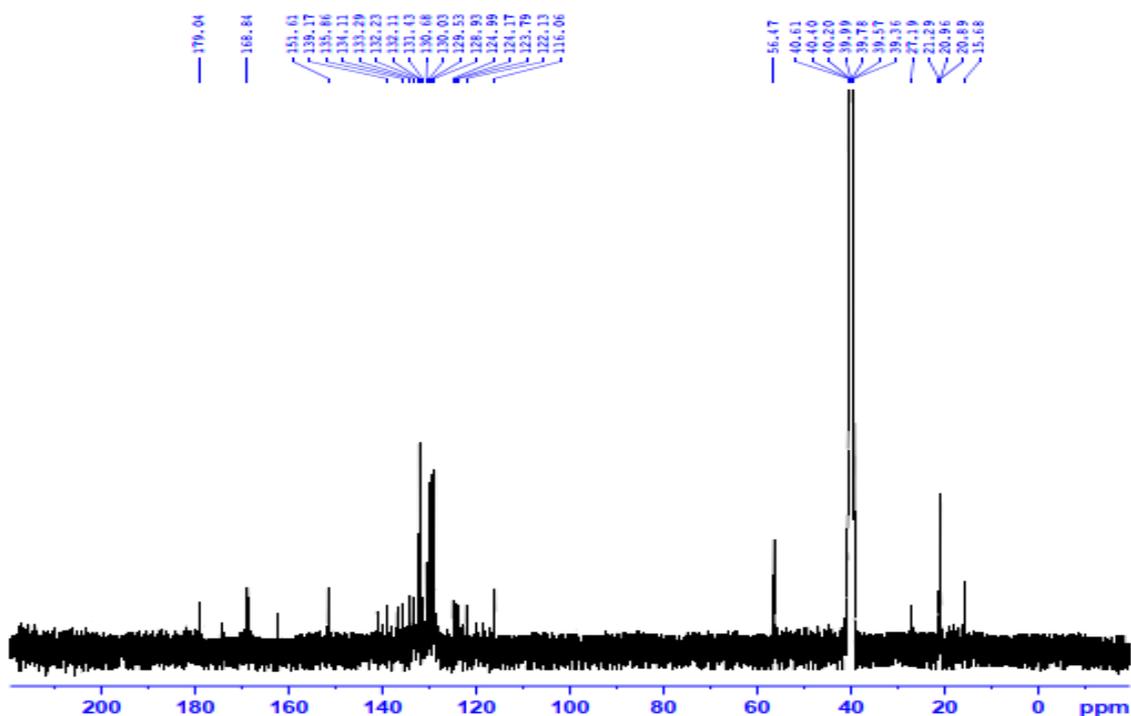


Figure S8b. ¹³C-NMR spectrum of compound 6b

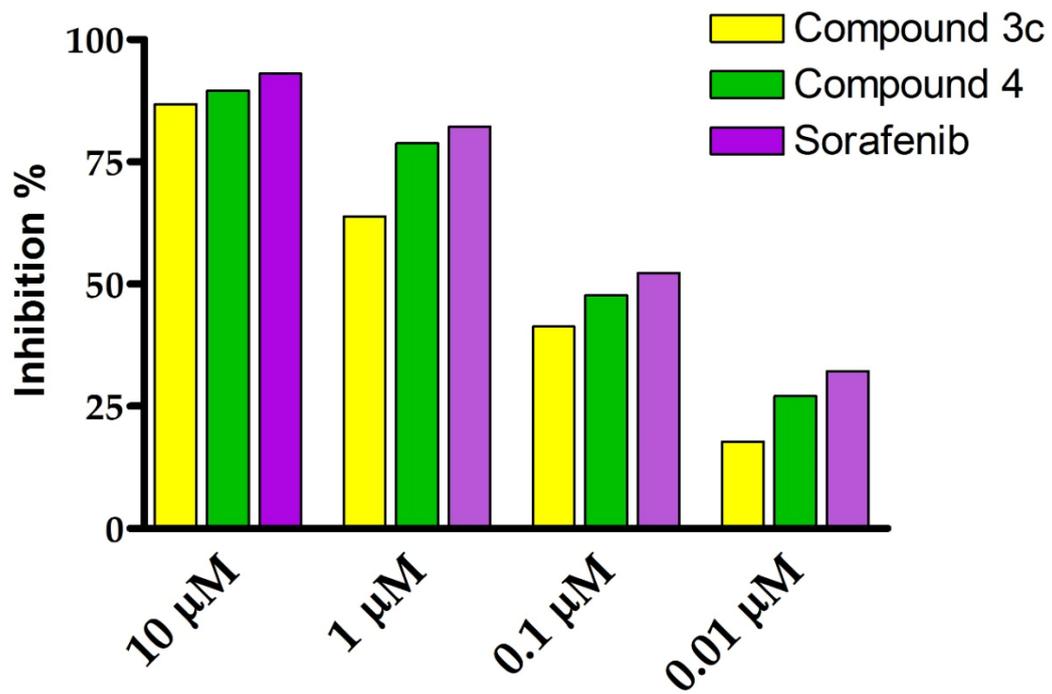


Figure S9. Inhibitory activity of compounds 3c, 4 and Sorafenib toward the VEGFR-2 kinase activity.