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Synthesis, characterization, and in silico studies of some thiazoles

Herein, we synthesized thiosemicarbazones using different aldehydes and thiosemicarbazide followed by hydrazinyl thiazole derivatives using different phenacyl bromide substituents. The synthesized thiosemicarbazones and hydrazinyl thiazole derivatives were confirmed through various spectroscopic techniques like FTIR, 1H NMR, and mass spectrometry. Molecular docking studies were performed using docking tools to assess the binding interactions of thiosemicarbazones and hydrazinyl thiazole derivatives with the target protein, Human Serum Albumin (HSA). The results obtained from docking studies elucidated the binding mechanism of thiosemicarbazones and hydrazinyl thiazole derivatives exhibited a binding constant range from -4.73 Kcal/mol to -9.50 Kcal/mol. Amongst them, (E)-2-((2-(4-(2-chlorophenyl) thiazol-2-yl) hydrazono) methyl)-5,6-dihydroimidazo[2,1-b] thiazole showed a maximum binding constant. Additionally, Density Functional Theory (DFT) calculations were carried out using Gaussian Software to investigate the electronic properties and ADMET analysis was carried out to evaluate the drug-like properties of the synthesized hydrazinyl thiazole derivatives.

Keywords: Thiosemicarbazones, Hydrazinyl thiazole derivatives, Molecular docking, DFT calculations, and ADMET analysis.

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