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Synthesis, characterization, and in silico studies of pyrrole-coupled with some phenacyl bromide derivatives

Pyrrole is an important nitrogen-containing aromatic heterocycle that can be found in numerous compounds of biological importance. Given its vast importance, pyrrole continues to be an attractive target for the development of new synthetic reactions. Hence, we synthesized pyrrole-coupled with some phenacyl bromide successfully and all the synthesized compounds were structurally elucidated using various spectroscopic tools including FTIR, 1H NMR and mass spectrometry techniques. In addition, the optimal structure of the produced molecules was determined by Density functional theory (DFT) computing. Molecular docking studies were performed to assess the binding energy and elucidated the interaction between the potential candidates and Human Serum Albumin (HSA) using the AutoDock tool. The binding constant range of the synthesized compounds was found to be in the range of -9.76 to -8.24 Kcal/mol, wherein the molecule (E)-2-(2-((1H-pyrrol-2-yl) methylene) hydrazinyl)-4-(4-methoxyphenyl) thiazole exhibited a strongest binding constant. ADMET analysis was carried out to assess the absorption, distribution, metabolism, excretion, and toxicity of the synthesized compounds. ADMET analysis was carried out using the Molinspiration tool. The toxicity was determined by pkCSM online software. The proposed research work helps to identify the potential drug candidates by predicting the binding affinity of small molecules to a protein and their ADMET parameters.

Key words: Pyrrole, phenacyl bromide, spectroscopic tools, DFT, molecular docking, ADMET.

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