World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:18, No:05, 2024

The Rational Design of Original Anticancer Agents Using Computational Approach

Authors : Majid Farsadrooh, Mehran Feizi-Dehnayebi

Abstract : Serum albumin is the most abundant protein that is present in the circulatory system of a wide variety of organisms. Although it is a significant macromolecule, it can contribute to osmotic blood pressure and also, plays a superior role in drug disposition and efficiency. Molecular docking simulation can improve in silico drug design and discovery procedures to propound a lead compound and develop it from the discovery step to the clinic. In this study, the molecular docking simulation was applied to select a lead molecule through an investigation of the interaction of the two anticancer drugs (Alitretinoin and Abemaciclib) with Human Serum Albumin (HSA). Then, a series of new compounds (a-e) were suggested using lead molecule modification. Density functional theory (DFT) including MEP map and HOMO-LUMO analysis were used for the newly proposed compounds to predict the reactivity zones on the molecules, stability, and chemical reactivity. DFT calculation illustrated that these new compounds were stable. The estimated binding free energy (ΔG) values for a-e compounds were obtained as -5.78, -5.81, -5.95, -5,98, and -6.11 kcal/mol, respectively. Finally, the pharmaceutical properties and toxicity of these new compounds were estimated through OSIRIS DataWarrior software. The results indicated no risk of tumorigenic, irritant, or reproductive effects and mutagenicity for compounds d and e. As a result, compounds d and e, could be selected for further study as potential therapeutic candidates. Moreover, employing molecular docking simulation with the prediction of pharmaceutical properties helps to discover new potential drug compounds.

Keywords : drug design, anticancer, computational studies, DFT analysis
Conference Title : ICMSN 2024 : International Conference on Materials Science and Nanoscience
Conference Location : Vancouver, Canada
Conference Dates : May 20-21, 2024