ORIGINAL RESEARCH ARTICLES

IN SILICO DESIGNING AND SCREENING OF CARBAZOLE DERIVATIVES AS TOPOISOMERASE II INHIBITORS

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ABSTRACT

Due to side effects and drug resistance, cancer treatment choices are limited despite continued attempts. Topoisomerases are essential for several cellular processes and human topoisomerase I and topoisomerase II alpha inhibitors have proven to be an effective chemotherapeutic alternative for a wide range of cancers, due to its fast proliferating cells and the higher level of these enzymes in solid tumors relative to normal tissue. In this study, around 30 carbazole derivatives were designed using Chem Draw Ultra and their ability to inhibit topoisomerase II was investigated using *in silico* docking studies and molecular dynamics. The results revealed ligand 10 and ligand 25 held good binding energy scores of -9.21 and -9.50, Kcal mol^{-1} respectively, with good interaction. ADMET analysis assured the drug likeness and better GI absorption than the parent drug and dexrazoxane. Desmond module of Schrödinger Suite was used and it demonstrated the stability in ligand receptor complexes.