Abstract

Cancer is a complex disease, characterized by an uncontrolled cell growth and spread with genetic mutation, normal cells follow strict regulation while cancer cells have an uncontrolled proliferation and metastatic, topoisomerase essential enzyme in the DNA regulation are classified into two families; TOPI and TOPII they play a vital role in the DNA process, topoisomerase inhibitors target these enzymes in cancer treatment to inhibit DNA supercoil relaxation and inducing cell death. Computer aided drug design utilizing docking and molecular dynamics helps in developing effective topoisomerase inhibitors. 113 β-lactam antibiotics database was used and docked against the active site of protein topoisomerase II (PDB ID: 3QX3); to assess the drug-protein interactions for antibiotics compared to EVP (the Co-Crystal inhibitor). Aspoxicillin, Amoxicillin, Cefalonium, Cefatrizine, Ceforanide, Ceftobiprole, Cyclacillin, Pivmecillinam, Sultamicillin, showed the best docking scores, Molecular dynamic simulations were performed for 300 nanoseconds, to analyze the movement of the compounds via: RMSDs, histograms, heatmaps, and according to the results Aspoxicillin was the most stable in the active site and could make a possible treatment for cancer.

Keywords: Cancer, β-lactam antibiotics, Topoisomerase II, TOP II, Docking, MD.