Docking Studies of Topoisomerase II Inhibitors

Tugba Taskin-Tok\textsuperscript{a}, Esin Aki\textsuperscript{b}, Ismail Yalcin\textsuperscript{b}, Ilkay Yildiz\textsuperscript{b}, Tugba Ertan-Bolelli\textsuperscript{b}, Kayhan Bolelli\textsuperscript{b}, Serap Yilmaz\textsuperscript{b}

\textit{a)} Gaziantep University, Faculty of Art and Science, Department of Chemistry, 27310, \c{S}ehitkâmil/Gaziantep, TURKEY

\textit{b)} Ankara University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, 06100, Tandogan/Ankara, TURKEY
ttaskin@gantep.edu.tr

Etoposide is an effective antitumor drug for Eukaryotic DNA-Topoisomerase II in a covalent complex with DNA. This drug is considered as one of the most important drugs in cancer chemotherapy. Unfortunately, its wide therapeutic application is often hindered by several limitations, including multidrug resistance (MDR), low water solubility and toxicity. In our previous study [1–8], benzoxazoles, benzimidazoles and related fused heterocyclic compounds, which exhibited significant in vitro antimicrobial and antiviral activities, were synthesized. In the present study, Molecular Docking method is used to sight and predict the possible structural motifs and interactions of these compounds as Eukaryotic Topoisomerase II inhibitors with Eukaryotic DNA-Topoisomerase II by using Discovery Studio (DS) 2.1 software [9].

REFERENCES