عنوان مقاله:

Design, Molecular Docking Studies of Enantiomers of New Warfarin Derivatives as Inhibitor Vitamin K Epoxide Reductase

محل انتشار:

دومین کنفرانس بین المللی در شیمی و مهندسی شیمی (سال: 1400)

تعداد صفحات اصل مقاله: 8

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خلاصه مقاله:

In this study, ۱۲ new warfarin enantiomers were evaluated for molecular docking studies and toxicity of designed ligands. Vitamin K epoxide reductase enzyme was selected as a drug-receptor with PDB ID: ۶WV۳. The proposed structures were designed in ChemDraw professional ۱۷.۱ software. The risk of toxicity, drug-likeness, solubility, TPSA, CLogP, drug score was reported by OSIRIS software for each structures. Then, the forms were transferred to MATERIAL STUDIO software to get geometric optimization. Next, molecular docking studies were performed using Molegro Virtual Docker software , and the results were analyzed by MMV and Discovery Studio software. Based on the results of docking studies, the most essential and effective bonds involved in drug-receptor binding were hydrogen bonds and hydrophobic bonds. Among the proposed compounds (۱۲ structures), the best results were related to R-۱ and S-۱ structures. The interaction energies of these two structures were -۱۸۴.۰۵ and -۱۸۲.۴۷۶, respectively. These, these two compounds had more ideal hydrogen bonds and much better interaction energy than the reference structures due to the reported validation. Finally, according to docking studies and toxicity risk assessment, the designed energy structures had a favorable interaction and have a much lower toxicity risk than the reference structures.

کلمات کلیدی:

Warfarin derivatives, Vitamin K epoxide reductase enzyme, Molecular docking, Toxicity risk assessment, Warfarin enantiomers