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Potential Anticancer Drug Candidate of Quinazoline Derivatives as EGFR Inhibitors: Docking and ADMET Studies

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ABSTRACT

Cancer is a fatal illness and the second most prevalent cause of mortality in the world, with a total of 9.6 million deaths in 2018. Molecular docking techniques and ADMET studies as a method to develop potential cancer drugs. The purpose of this study is to determine the interaction between quinazoline derivatives with the Epidermal Growth Factor Receptor (EGFR) and ADMET prediction. All compounds were docked with Molegro Virtual Docker (MVD) software. The rerank scores were determined by the smallest value. The 2D and 3D interaction images between the compound and amino acid residues of EGFR were analyzed. Druglikeness and pharmacokinetic parameter studies were performed with AdmetLab 2.0, and the results were analyzed. The molecular docking results showed that six quinazoline derivatives had a lower rerank score that was between 84.409 and -100.307 kcal/mol than quinazoline as the lead compound. All compounds fulfilled Lipinski's rule. Compounds Q1, Q2, and Q6 had good ADME properties, and all compounds have low toxicity. The six quinazoline derivatives had the potential to be synthesized based on their rerank score and ADMET properties as EGFR inhibitors.

Keywords: Quinazoline derivatives, Molecular docking, ADMET, EGFR