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Molecular Docking Studies of a Chalcone Derivative Compound *p*-hydroxy-*m*-methoxychalcone with Tyrosine Kinase Receptors

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Abstract

Chalcone compounds have been studied as therapeutic, especially as antitumor drugs. A chalcone derivate, *para*-hydroxy-*metha*-methoxychalcone (*p*H*m*MC) or 3-(4'-hydroxy-3'-methoxyphenyl)-1-phenyl-2propene-1-on, has been studied to explore its potential utilization as chemoprevention in several cancers cell lines. The main objective of the present work is to perform a docking analysis of *p*H*m*MC with tyrosine kinase receptors EGFR, HER2, and VEGFR comparing with ligand ATP. Docking studies were performed using PLANTS (Protein Ligand ANT System) software, while the preparations of protein and reference ligand was used YASARA, and visualizing amino acids was used Molecular Operating Environment (MOE) program. The docking studies indicated that the binding energy of *p*H*m*MC with EGFR (1XKK) and HER2 (3PPO) was higher than the ATP binding energy with the EGFR and HER2. However, the binding energy of *p*H*m*MC with VEGFR (2P2I) almost had the same energy binding compared with the ATP binding on VEGFR. VEGF is a protein that plays a role in angiogenesis. Data from the MOE program showed there were similarities in the amino acids involved in the interaction between *p*H*m*MC and ATP in binding to EGFR, HER2, and VEGFR. The results indicated that *p*H*m*MC has the potential to be developed as an anticancer which might through the mechanism of inhibiting the process of angiogenesis.

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Keywords

Molecular docking, pHmMC, EGFR, HER2, VEGFR.

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