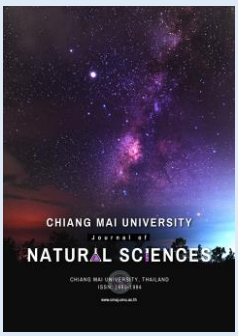

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Research article

Insight on the In Silico Study and Biological Activity Assay of Chalcone-Based 1, 5-Benzothiazepines as Potential Inhibitor for Breast Cancer MCF7

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Abstract In silico study was performed to twelve 1,5-benzothiazepine chalcone derivatives with the protein target from the crystallographic structure modeling of the enzyme tyrosine kinase. The objective of this study is to execute and to estimate the biological activity of chalcone-based 1,5-benzothiazepine derivatives as potential inhibitors for breast cancer MCF7. To get insight into potential anticancer activities, molecular docking, molecular dynamic and ADME prediction were performed. Docking results reported that compound MA9 with binding free energy of -11.2 kcal / mol can interact through hydrogen bonds with amino acids Cys788 on 1T46 protein active site. In addition, the lowest binding free energy conformation indicated its stability during molecular dynamic simulation. MA9 is also shown to have drug likeness properties based on ADME prediction. In order to evaluate the modeling outcomes, MTT assay were performed for some of the most and least promising benzologs (i.e., MA1, MA6, MA8 and MA9). As expected, compound MA9 with the best calculated anticancer properties revealed the best inhibition against MCF7cell line in vitro. Thus, this compound was chosen as the reference for the next stage in the drug design.

Keywords: ADME, Benzothiazepine, Docking, MCF7, Molecular Dynamic

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