ABSTRACT

MELINDA RAHMAT. 2024. ***POTENTIAL OF BIOACTIVE COMPOUNDS IN PALM SUGAR (Arenga pinnata) AS AN ANTIHYPERTENSIVE AGENT THROUGH IN SILICO MOLECULAR DOCKING TECHNIQUES FOR BIOLOGY SUPPLEMENT DEVELOPMENT.*** *Department of Biology Education, Faculty of Teacher Training and Education, Siliwangi University, Tasikmalaya.*

Hypertension is one of the leading causes of premature death globally and is largely associated with disruptions in the renin-angiotensin-aldosterone system (RAAS). In the RAAS, Angiotensin-Converting Enzyme (ACE) plays a critical role in converting angiotensin I to angiotensin II, which leads to elevated blood pressure. The purpose of this study is to analyze the potential of bioactive compounds in palm sugar (Arenga pinnata) as ACE inhibitors through an in silico approach. The research method used is a descriptive qualitative study conducted in silico. GC-MS (Gas Chromatography-Mass Spectrometry) analysis was performed to identify bioactive compounds in palm sugar. This study employed molecular docking techniques to predict the affinity and stability of compound interactions with ACE. The docking process involved several stages, including protein and ligand structure preparation, docking method validation, and interaction analysis. Physicochemical, pharmacokinetic, and toxicity predictions of the compounds were also conducted using SwissADME and ProTox-II software to assess their feasibility as potential antihypertensive drug candidates. The GC-MS analysis identified 22 compounds in palm sugar, with 8 of them showing potential antihypertensive properties: 9,10-Secocholesta-5,7,10(19)-triene, 10-Octadecenoic acid, methyl ester, Desulphosinigrin, d-Glycero-d-ido-heptose, d-Mannose, 16-Octadecenoic acid, 11-Octadecenoic acid and Dodecanoic acid, 2,3-bis (acetyloxy)propyl ester. Molecular docking result revealed that 9,10-Secocholesta-5,7,10(19)-triene exhibited the best binding affinity, with a score of -8.9 kcal/mol, outperforming captopril as a control ligand, which scored -5.9 kcal/mol. All tested compounds met Lipinski's rule of five, indicating favorable absorption and penetration through biological membranes. Pharmacokinetic analysis indicated that all test compounds exhibited suitable pharmacokinetic profiles as antihypertensive candidates. Toxicity profiling revealed that several compounds, notably d-Glycero-d-ido-heptose, and d-Mannose, displayed level 6 toxicity. Overall, these compounds demonstrate potential as safe candidates for an antihypertensive drug.

Keyword: *Palm sugar, bioactive compounds, antihypetensive, molecular docking, in silico, Angiotensin-Converting Enzyme (ACE)*