

ABSTRACT

JULIYA IRNANDIA 2024. ***The Analysis of Secondary Metabolites in Stinging Nettle (Urtica dioica L.) as an Anti-Aging Agent for Skin in Support of Biology Learning Materials*** (In silico Molecular Docking Method). Departement of Biology Education, Faculty of Teacher Training and Education, Siliwangi University, Tasikmalaya.

The nettle leaf (Urtica dioica L.) is commonly known as a weed; however, it contains various secondary metabolites with potential as an anti-premature skin aging agent, such as flavonoids, alkaloids, steroids, saponins, and tannins. This study aims to analyze the potential of secondary metabolites from nettle leaf extract as an anti-premature skin aging agent using an in silico approach with molecular docking methods. This research is qualitative in nature. The materials used include test ligands in the form of secondary metabolites from nettle leaves, a control ligand in the form of retinol, and a receptor in the form of Matrix Metalloproteinase-1 (MMP-1) with PDB ID 1HFC. The secondary metabolites were obtained through extraction using the maceration method and identified using Gas Chromatography-Mass Spectrometry (GC-MS). Data collection techniques included documentation studies in the form of literature reviews and computer simulations, while data analysis was conducted using molecular docking methods with Pyrx and Biovia Visualizer 2019 software to evaluate ligand interactions with the MMP-1 receptor. Binding affinity values were used to determine the strength of the interactions between test compounds and the receptor. Receptor validation was conducted using SAVESv6.1, while docking method validation was performed using PyMol. Physicochemical, pharmacokinetic, and Lipinski's rule of five analyses were conducted using SwissADME, and toxicity analysis was performed with ProTox and pkCSM. The results showed that the compound Propanoic acid, 2-(-3-acetoxy-4,4,14-trimethylandrosta-8-en-17-yl)- exhibited the best binding affinity of -6.8 kcal/mol, which was lower than the control compound retinol at -6.2 kcal/mol. Physicochemical, pharmacokinetic, and toxicity analyses confirmed that this compound meets Lipinski's rule of five, supporting its potential as a topical drug. In conclusion, secondary metabolites from nettle leaf extract have potential as an anti-premature skin aging agent, with the compound Propanoic acid, 2-(-3-acetoxy-4,4,14-trimethylandrosta-8-en-17-yl)- showing the strongest binding to MMP-1.

Key Words: *In silico, Molecular docking, Anti-aging, Urtica dioica L.*