

ABSTRACT

*Mohammad Imam Muzaki, 24020222130039. **Potential of Aloe vera (Aloe sp.) from Kalimantan and Semarang as an Anti-Aging Agent Using Molecular Docking**, under the guidance of Hermin Pancasakti Kusumaningrum and Rugayah.*

Aging is a process of gradual decline in skin function that can be caused by sun exposure (photoaging), which has a negative impact on aesthetics and health. The use of synthetic cosmetic products as a solution still has limitations, especially the irritating effect on sensitive skin, so the use of natural ingredients such as Aloe sp. as an alternative is considered safer. This study aims to examine the potential of Aloe sp. from Kalimantan as an anti-aging agent for the skin and compare it with local Aloe sp. cultivars from Semarang. This research method includes morphological characterization and molecular identification to determine the sequence differences between cultivars. In addition, bioactive compounds were also identified using gas chromatography-mass spectrometry (GC-MS) to determine the differences in compound profiles between Aloe sp. cultivars. The identified compounds were then selected using SwissTargetPrediction to select compounds that have interactions with MMP1 and MAPK receptors (ERK, P38 alpha, and JNK) that play a role in the skin aging process. The selected compounds were then molecularly docked with Molegro Virtual Docker to obtain rerank scores. Molecular analysis results showed significant differences in DNA sequences between the Semarang and Kalimantan cultivars of Aloe sp.. GC-MS results also showed differences in compound composition between cultivars. Based on the molecular docking conducted, it shows that the Kalimantan cultivar of Aloe sp. has better potential than the Semarang cultivar, especially in the MMP1, P38 alpha, and JNK1 receptors based on better rerank scores with inhibitor compounds as controls and the total abundance of potential compounds. Thus, Kalimantan Aloe sp. has superior potential as an anti-aging agent for skin.

Keywords: Photoaging, Molecular Characterization, Mitogen Activated Protein Kinase