ABSTRACT

Azka Emo, 24020222130047. ***Molecular Characterization and Analysis of Hepatoprotective Potential of Aloe sp. from Bogor and Semarang through Molecular Docking Against THR-β and SIRT1 in Non-Alcoholic Fatty Liver Disease*** (supervised by Hermin Pancasakti Kusumaningrum and Ria Cahyaningsih).

Non-Alcoholic Fatty Liver Disease (NAFLD) is a chronic liver disease with a prevalence rate of 51.04% in Indonesia. The limitations of current therapies have encouraged the exploration of natural product-based alternatives. This study aimed to analyze the molecular characterization, bioactive compound profiles, and hepatoprotective potential of Aloe sp. from Bogor and Semarang through molecular docking against the target proteins THR-β and SIRT1. Molecular docking was performed using PyRx, visualized with Discovery Studio Visualizer, and evaluated using SwissADME and pkCSM. BLASTn results showed percent identity values of 83.85% for the Bogor sample and 87.04% for the Semarang sample against Aloe vera isolates BPTPS102 and BPTPS162, respectively, with both samples clustering in the same clade as the reference Aloe vera sequences with a bootstrap value of 86%. GC-MS analysis detected 20 compounds in the Bogor sample, predominantly lactones, aliphatic alcohols, and cyclic ketones, and 40 compounds in the Semarang sample, predominantly fatty acids and fatty acid esters. The five compounds with the highest percentage area from each sample were selected as test ligands. Molecular docking results showed that di-tert-butyldiazene from Aloe sp. Bogor and 2,3-di(dodecanoyloxy)propyl dodecanoate from Aloe sp. Semarang exhibited binding affinity values ranging from -5.3 to -8.0 kcal/mol, which were more negative than the control ligand. A total of 9 out of 10 tested compounds fulfilled Lipinski's Rule of Five, were non-hepatotoxic, and demonstrated favorable ADMET profiles indicating their potential as hepatoprotective bioactive supplement candidates for supporting NAFLD management.

Keywords: binding affinity, GC-MS, hepatoprotective, ITS, molecular docking, bioactive compounds