ABSTRACT

Fani Rahmawati, 24020219130043. *In Silico Study of Benzoic Acid from Ramalina sp. as an Inhibitor of VEGF-A and EGFR in Triple-Negative Breast Cancer, Under the Guidance of* Dr. Dra. Arina Tri Lunggani, M.Si. *and* Puspa Hening, S.Pd.,M.Biotech.

Triple-negative breast cancer (TNBC) is an aggressive form of breast cancer that lacks specific targeted therapies because it does not express the ER, PR, and HER2 receptors, thus necessitating the development of new, more effective drug candidates. Potential targets in TNBC include the Vascular Endothelial Growth Factor (VEGF) and Epidermal Growth Factor Receptor (EGFR) proteins. This study aims to analyze the molecular interactions of benzoic acid from the lichen Ramalina sp. with VEGF-A and EGFR through molecular docking and to evaluate its pharmacokinetic and toxicity profiles (ADMET). The benzoic acid ligand structure was downloaded from PubChem with ID 243, while the VEGF-A and EGFR receptor protein structures were downloaded from RCSB PDB with IDs 6Z3F and 6LUD. Molecular docking was performed using AutoDock Vina on PyRx, interaction visualization using PyMol and BIOVIA Discovery Studio, ADME analysis via ADMET-AI, and toxicity analysis via GUSAR. The results of the study showed that the best binding affinity values for benzoic acid were −4,9 kcal/mol for VEGF-A and −5,6 kcal/mol for EGFR, and it was able to form important interactions with residues of both receptors in the form of hydrogen and hydrophobic bonds. Pharmacokinetic analysis indicates that benzoic acid meets all parameters of Lipinski's Rule of Five, and its toxicity prediction is classified as low (Class 5). Thus, benzoic acid has potential as an initial candidate inhibitor of VEGF-A and EGFR but requires further validation through in vitro and in vivo testing, as well as advanced ADMET analysis.

Keywords: TNBC, benzoic acid, VEGF, EGFR, molecular docking.