ABSTRACT

Cantika Melatiningtyas. 24020222130049. **Morphological Characterization, Molecular Identification and *Molecular Docking* of Bioactive Metabolites *Caulerpa* sp. As an anticancer candidate of breast against the caspase-3 protein (**under the guidance of Sri Pujianto and Nurina Tahta Afwi Maulina)

Caulerpa sp. is a green macroalgae that is known to contain various bioactive compounds with potential as antioxidants and anticancers. This study aims to identify *Caulerpa* sp. morphologically and molecularly, kinship relationships, determine the value of antioxidant activity, determine the metabolite profile of *Caulerpa* sp. methanol extract, and analyze candidates for breast anticancer compounds. This study includes morphological and molecular characterization based on the 18S rRNA gene as well as phylogenetic analysis, determination of antioxidant activity values through Total Phenolic Content (TPC) test and DPPH methods, and pharmacological potential evaluation through pharmacokinetic and molecular docking analysis of Caspase-3 protein (PDB ID: 1GFW). The results of morphological characterization through dichotomy locks and molecular identification showed C. *racemosa* species. Phylogenetic trees show *that Caulerpa* sp. is closely related to the clades consisting of *C. racemosa* var. corynephora and *C. veravalensis* with a bootstrap of 92%. Methanol extract *of Caulerpa* sp. has a total phenolic content of 54.889 ± 13.8728 mg GAE/g and shows very strong antioxidant activity with an IC_{50} value of 34.6 ppm. The results of molecular docking showed that the compounds 3,7,11,15-Tetramethyl-2-hexadecen-1-OL, Hexadecanoic acid methyl ester, and n-Hexadecanoic had a stable interaction with the Caspase-3 protein, characterized by binding affinity values lower than doxorubicin, RMSD value 0 Å, and similarity of amino acid residues at the active sites of proteins. Based on the results of the study, *Caulerpa* sp. has the potential to be a source of bioactive compounds that have antioxidant activity and anticancer candidates for breast cancer.

Keywords: *Anticancer, apoptosis, Caulerpa sp., DPPH, GC-MS, molecular identification*