

Keke Triananda NPM 220351100016. Skrining Senyawa Bioaktif *Padina* sp. sebagai Kandidat Antifungal melalui *Molecular Docking* terhadap Reseptor *Sterol 14alpha-Demethylase* (CYP51). Dibawah bimbingan **AB. Chandra, M. Si**

ABSTRAK

Alga coklat jenis *Padina* sp. tumbuh subur di pesisir Desa Nepa, Sampang dengan kondisi lingkungan perairan yang relatif stabil dan kaya nutrisi menjadikan *Padina australis* sebagai kandidat obat antifungal. Penelitian ini bertujuan untuk mengukur parameter kualitas air, kandungan proksimat, mengidentifikasi kandungan senyawa bioaktif dalam ekstrak *Padina australis* serta mengevaluasi potensinya sebagai kandidat antifungal melalui pendekatan *in silico*. Metode penelitian meliputi pengukuran parameter kualitas air (suhu, pH, salinitas, dan oksigen terlarut), analisis proksimat (air, abu, lemak, protein, dan karbohidrat), analisis kimia dengan *Gas Chromatography-Mass Spectrometry* (GC-MS) dan *molecular docking* terhadap protein target *Sterol 14alpha-Demethylase* (CYP51). Hasil identifikasi alga coklat Perairan Nepa termasuk spesies *Padina australis* dengan kondisi parameter perairan meliputi pH $7,91 \pm 0,10$, suhu $32,9 \pm 0,04^\circ\text{C}$, salinitas $34,33 \pm 0,09\%$, dan oksigen terlarut $8,6 \pm 0,06$ mg/L. Analisis proksimat menunjukkan hasil kadar air $6,54 \pm 0,13\%$, kadar abu $56,57 \pm 0,49\%$, kadar lemak $7,6 \pm 0,44\%$, kadar protein $0,26 \pm 0,13\%$, dan kadar karbohidrat $29,03 \pm 0,80\%$. Senyawa bioaktif yang ditemukan meliputi 7-Octen-2-ol, 2,6-dimethyl-, Linalool, Gentaminin a, Methyl 3-cis,9-cis,12-cis-octadecatrienoate, 4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, acetate, (R)-, Pterin-6-carboxylic acid, Tetraacetyl-d-xylonic nitrile, [1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester, E-10-Pentadecenol, 17-Octadecynoic acid, Pentadecanoic acid, 14-methyl-, methyl ester, Octadecanal, 2-bromo-, 10-Octadecenal, 1,4-Benzenediol, 2,6-bis(1,1-dimethylethyl)-. Analisis *molecular docking* menunjukkan bahwa seluruh 14 senyawa bioaktif berikatan stabil dengan CYP51 dengan nilai *binding affinity* antara -5,3 hingga -10,0 kkal/mol dan RMSD 0,0 Å. Senyawa dengan afinitas terbaik adalah Octadecanal, 2-bromo- dengan *binding affinity* -10,0 kkal/mol, diikuti oleh Gentamicin A -7,3 kkal/mol, dan [1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester -7,0 kkal/mol. Kontrol antifungal Isavuconazole sebagai pembanding menunjukkan *binding affinity* -9,2 kkal/mol.

Kata kunci: Antifungal, CYP51, *Molecular Docking*, *Padina australis*

Keke Triananda NPM 220351100016. Screening of Bioactive Compounds from *Padina* sp. as Antifungal Candidates through Molecular Docking against Sterol Receptor 14 α -Demethylase (CYP51). Under the guidance of **AB. Chandra, M. Si**

ABSTRACT

Brown algae of the Padina sp. species thrives on the coast of Nepa Village, Sampang with relatively stable and nutrient-rich water environmental conditions making Padina australis a candidate for antifungal drugs. This study aims to measure water quality parameters, proximate content, identify the content of bioactive compounds in Padina australis extract and evaluate its potential as an antifungal candidate through an in silico approach. The research methods include measuring water quality parameters (temperature, pH, salinity, and dissolved oxygen), proximate analysis (water, ash, fat, protein, and carbohydrates), chemical analysis with Gas Chromatography-Mass Spectrometry (GC-MS) and molecular docking against the target protein Sterol 14 α -Demethylase (CYP51). The results of the identification of brown algae in Nepa waters include the Padina australis species with water parameter conditions including pH was 7.91 ± 0.10 , temperature $32.9 \pm 0.04^\circ\text{C}$, salinity $34.33 \pm 0.09\%$, and dissolved oxygen 8.6 ± 0.06 mg/L. proximate analysis showed that the water content was $6.54 \pm 0.13\%$, ash content was $56.57 \pm 0.49\%$, fat content was $7.6 \pm 0.44\%$, protein content was $0.26 \pm 0.13\%$, and carbohydrate content was $29.03 \pm 0.80\%$. Bioactive compounds found include 7-Octen-2-ol, 2,6-dimethyl-, Linalool, Gentamicin A, Methyl 3-cis,9-cis,12-cis-octadecatrienoate, 4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, acetate, (R)-, Pterin-6-carboxylic acid, Tetraacetyl-d-xylonic nitrile, [1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester, E-10-Pentadecenol, 17-Octadecynoic acid, Pentadecanoic acid, 14-methyl-, methyl ester, Octadecanal, 2-bromo-, 10-Octadecenal, 1,4-Benzenediol, 2,6-bis(1,1-dimethylethyl)-. Molecular docking analysis showed that all 14 bioactive compounds bind stably to CYP51 with binding affinity values between -5.3 and -10.0 kcal/mol and a RMSD of 0.0 Å. The compound with the best affinity is Octadecanal, 2-bromo- with a binding affinity of -10.0 kcal/mol, followed by Gentamicin A -7.3 kcal/mol, and [1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester -7.0 kcal/mol. The antifungal control Isavuconazole as a comparison showed a binding affinity of -9.2 kcal/mol.

Keywords: Antifungal, CYP51, Molecular Docking, *Padina australis*