ABSTRAK

Nadya Imannia Syafirna, NIM 4213220044 (2025). Aktivitas Inhibisi Bakteriofag Hepatopankreas Udang Vaname sebagai Strategi Intervensi *Acute Hepatopancreatic Necrosis Disease* secara *Molecular Docking* dan *in Vitro*.

Penelitian ini bertujuan untuk mengidentifikasi senyawa aktif pada supernatan bakteriofag hepatopankreas udang vaname, menganalisis interaksi inhibisinya terhadap reseptor Pir-A dan Pir-B melalui *molecular docking*, serta terhadap *Vibrio parahaemolyticus* strain AHPND secara *in vitro*. Sampel hepatopankreas diisolasi menggunakan media TSB, kemudian disaring dengan membran filter 0,45 dan 0,22 µl, selanjutnya supernatan bakteriofag dianalisis menggunakan LC-HRMS. *Molecular docking* dilakukan dengan PyRx dan divisualisasi menggunakan BIOVIA Discovery Studio 2021, sedangkan uji antibakteri dilakukan melalui metode *spot test* menggunakan media TSA antara supernatan bakteriofag dengan *V. parahaemolyticus* strain AHPND. Analisis menggunakan LC-HRMS berhasil mengidentifikasi 450 senyawa aktif. Hasil *molecular docking* menunjukkan bahwa 3-Cyclohexanesulfonyl-heptanoic acid hydroxyamide, D-Tryptophan, dan Butabarbital memiliki afinitas kuat terhadap reseptor *PirA-like toxin* (3X0T) dan *PirB-like toxin* (3X0U) dengan nilai *binding affinity* berkisar ≤ –6,4 hingga –7,6 kcal/mol. Interaksi dominan berupa ikatan hidrogen dan hidrofobik pada residu kunci TRP57, ASN87, ALA88, PHE89, dan TYR90 (PirA), serta TYR201, THR209, ASP216, ARG236, PHE244, MET247, GLN251, GLU289, dan ASP290 (PirB). Uji *in vitro* menunjukkan terbentuknya zona bening yang menandakan kemampuan supernatan bakteriofag menghambat pertumbuhan *V. parahaemolyticus* strain AHPND secara signifikan. Hasil ini mengindikasikan potensi supernatan bakteriofag hepatopankreas udang vaname sebagai agen biokontrol alami yang efektif untuk pencegahan AHPND dalam budidaya udang

Kata kunci: Bakteriofag, *Litopenaeus vannamei*, *Vibrio parahaemolyticus*, *molecular docking*, AHPND

ABSTRACT

Nadya Imannia Syafirna, Student ID 4213220044 (2025). Inhibitory Activity of Hepatopancreatic Bacteriophage of Whiteleg Shrimp as an Intervention Strategy Against Acute Hepatopancreatic Necrosis Disease through Molecular Docking and In Vitro Testing.

This study aims to identify active compounds in the hepatopancreas bacteriophage supernatant of white shrimp, analyze its inhibitory interaction with the Pir-A and Pir-B receptors through molecular docking, and against *Vibrio parahaemolyticus* strain AHPND in vitro. Hepatopancreas samples were isolated using TSB media, then filtered with 0.45 and 0.22 µl membrane filters, then the bacteriophage supernatant was analyzed using LC-HRMS. Molecular docking was performed with PyRx and visualized using BIOVIA Discovery Studio 2021, while the antibacterial test was carried out using the spot test method using TSA media between the bacteriophage supernatant and *V. parahaemolyticus* strain AHPND. Analysis using LC-HRMS successfully identified 450 active compounds. Molecular docking results showed that 3-Cyclohexanesulfonyl-heptanoic acid hydroxyamide, D-Tryptophan, and Butabarbital have strong affinity for PirA-like toxin (3X0T) and PirB-like toxin (3X0U) receptors with binding affinity values ranging from ≤ –6.4 to –7.6 kcal/mol. The dominant interactions are hydrogen and hydrophobic bonds at key residues TRP57, ASN87, ALA88, PHE89, and TYR90 (PirA), as well as TYR201, THR209, ASP216, ARG236, PHE244, MET247, GLN251, GLU289, and ASP290 (PirB). In vitro tests showed the formation of a clear zone indicating the ability of bacteriophage supernatants to significantly inhibit the growth of *V. parahaemolyticus* strain AHPND. These results indicate the potential of vaname shrimp hepatopancreas bacteriophage supernatant as an effective natural biocontrol agent for the prevention of AHPND in shrimp farming.

Keywords: Bacteriophage, *Litopenaeus vannamei*, *Vibrio parahaemolyticus*, molecular docking, AHPND