ABSTRAK

STUDI *ONE-HEALTH* DENGAN PENDEKATAN *IN SILICO* FIBRINOGEN-BINDING PROTEIN A (FbsA) BAKTERI *Streptococcus agalactiae* ASAL IKAN DAN KASUS KLINIS MANUSIA

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Di Singapura dan Malaysia, Streptococcus Grup B (SGB) dengan *sequence type* (ST) 283 telah dilaporkan dapat menginfeksi manusia melalui konsumsi pangan asal hewan, seperti ikan mentah. Studi *one-health* terkait dengan protein faktor virulensi SGB belum dilakukan secara luas. Kasus SGB ST283 mendorong dilakukannya studi *one-health* terhadap *fibrinogen-binding protein* A (FbsA) dari SGB asal dari ikan dan kasus klinis manusia. Studi *one-health* secara *in silico* dilakukan untuk menguji kemiripan profil FbsA SGB yang berasal dari dua spesies inang yang berbeda dan untuk menyelidiki profil interaksi FbsA dengan fibrinogen (Fg) manusia. Dua sampel sekuen asam amino FbsA dari kasus klinis ikan dan manusia diperoleh dari *National Center of Biotechnology Information*, sementara struktur kristal protein fibrinogen manusia diperoleh dari *Protein Data Bank*. Penyejajaran dua sampel sekuen FbsA dari inang yang berbeda dilakukan menggunakan program MUSCLE untuk menilai kemiripan profil protein. Prediksi struktur tiga dimensi FbsA SGB dilakukan menggunakan ColabFold versi 1.5.5. Studi penambatan molekul dengan ClusPro versi 2.0 dilakukan untuk melihat interaksi antara FbsA SGB dan rantai Aα, Bβ, dan γ fibrinogen manusia. Hasil menunjukkan kedua sampel sekuen asam amino FbsA menunjukkan kemiripan urutan sebesar 100%. Interaksi menunjukkan residu-residu dalam wilayah berulang FbsA SGB berinteraksi dengan rantai α, β, γ rantai Fg manusia pada fragmen D Fg dan didominasi oleh kelompok residu kritis, residu yang dilaporkan memainkan peran penting dalam *Fg-binding*. Residu-residu kritis ini terutama terletak di wilayah berulang dari ke-45 hingga ke-60. Interaksi juga terjadi pada situs $\beta_{119\text{-}129}$, situs pembelahan protein fibrinolitik plasmin. Temuan ini diduga berkontribusi pada patogenesis penyakit, terutama dalam gejala klinis endokarditis dan septicemia, dan berpotensi sebagai penyakit zoonosis berasal dari ikan.

Kata Kunci: *One-health*, Zoonosis, *Streptococcus* Grup B, *Fibrinogen-binding protein* A, *In Silico*

ABSTRACT

IN SILICO ONE-HEALTH STUDIES OF FIBRINOGEN-BINDING PROTEIN A (FbsA) OF *Streptococcus agalactie* BACTERIA ORIGIN FISH AND HUMAN CLINICAL CASES

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In Singapore and Malaysia, Group B Streptococcus (GBS) with sequence type (ST) 283 has been reported to infect humans through the consumption of animal-derived food, such as raw fish. One-health studies related to the virulence factor proteins of GBS have not been extensively conducted. Cases of GBS ST283 prompted a one-health study of the fibrinogen-binding protein A (FbsA) of GBS originating from fish and human clinical cases. In silico one-health studies were conducted to examine the similarity of FbsA GBS profiles originating from two different host species and to investigate the interaction profiles of FbsA with human fibrinogen (Fg). Two samples of FbsA amino acid sequences from fish and human clinical cases were obtained from the National Center of Biotechnology Information, while the crystal structure of human fibrinogen protein was obtained from the Protein Data Bank. Alignment of the two FbsA sequence samples from different hosts was performed using the MUSCLE program to assess protein profile similarity. Three-dimensional structure prediction of fish FbsA GBS was conducted using ColabFold version 1.5.5. Molecular docking investigation with ClusPro version 2.0 was performed to examine the interaction between FbsA GBS and the Aα, Bβ, and γ chains of human fibrinogen. The results indicated that both samples of FbsA amino acid sequences exhibited a sequence similarity of 100%. The interaction showed residues in the repetitive regions of FbsA GBS interacting with human Fg chains at D fragment and was dominated by critical residue groups, residues reported to play crucial roles in fibrinogen binding. These critical residues are mainly located in the repetitive region from the 45th to the 60th. Interactions occurred at the $\beta_{119\text{-}129}$ site, the site of plasmin fibrinolytic protein cleavage. These findings are suspected to contribute to the pathogenesis of the disease, particularly in the clinical symptoms of endocarditis and septicemia, and potentially as a zoonotic disease of fish origin.

Keywords: One-health, zoonotic disease, Group B Streptococcus, Fibrinogen-binding protein A, In silico