KAJIAN POTENSI FIKOBILIPROTEIN DAN FIKOBILIN DARI *SPIRULINA PLATENSIS* SEBAGAI KANDIDAT ANTI-SARS-COV-2 BERDASARKAN STUDI *MOLECULAR DOCKING*

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diajukan untuk memenuhi salah satu syarat memperoleh Gelar Sarjana Sains
Program Studi Kimia

oleh

Riska Nur Pratiwi

NIM 1700436

PROGRAM STUDI KIMIA
DEPARTEMEN PENDIDIKAN KIMIA
FAKULTAS PENDIDIKAN MATEMATIKA DAN ILMU PENGETAHUAN ALAM
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Oleh

Riska Nur Pratiwi

Sebuah skripsi yang diajukan untuk memenuhi salah satu syarat memperoleh gelar Sarjana Sains pada Program Studi Kimia

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disetujui dan disahkan oleh pembimbing:

Pembimbing I

Gun Gun Gumilar, M.Si.

NIP. 197906262001121001

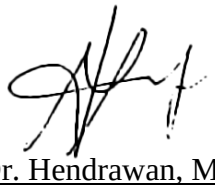
Pembimbing II

Dr. Heli Siti Halimatul Munawaroh, M.Si.

NIP. 197907302001122002

Mengetahui,

Ketua Departemen Pendidikan Kimia FPMIPA UPI



Dr. Hendrawan, M.Si.

NIP. 196309111989011001

ABSTRAK

Penelitian ini bertujuan untuk menganalisis potensi fikobiliprotein (C-fikosianin, alofikosianin, C-fikoeritrin) dan fikobilin (fikosianobilin dan fikoeritrobilin) dari *Spirulina platensis* sebagai anti-SARS-CoV-2, menggunakan simulasi *molecular docking*. *Docking* senyawa kandidat dilakukan terhadap reseptor M^{pro}, RBD, ACE2, dan RdRp dengan nelfinavir, klorokuin, hidroksiklorokuin, dan remdesivir sebagai pembanding. Tahapan penelitian meliputi preparasi protein dan ligan, validasi metode *docking*, simulasi *docking* protein-ligan maupun protein-protein, serta visualisasi dan analisis hasil *docking* menggunakan AutoDock Tools 1.5.6, AutoDock Vina 1.1.2, PyMOL 2.4.1, PRISM, dan BIOVIA Discovery Studio Visualizer 2021. Hasil penelitian menunjukkan adanya interaksi antara fikobiliprotein dan fikobilin dengan keempat protein target yang melibatkan ikatan hidrogen, hidrofobik, elektrostatik, van der Waals, π-sulfur, dan *unfavorable*. Fikobiliprotein yang memiliki afinitas pengikatan tertinggi dengan M^{pro}, RBD, ACE2, dan RdRp secara berturut-turut adalah C-fikosianin rantai F, C-fikosianin rantai B, C-fikoeritrin rantai B, dan alofikosianin. Fikobilin yang memiliki afinitas pengikatan tertinggi dengan keempat protein target adalah fikoeritrobilin. Afinitas pengikatan fikoeritrobilin-M^{pro} lebih tinggi dari klorokuin dan hidroksiklorokuin dengan selisih 2 dan 1,8 *kkal/mol*. Afinitas pengikatan fikoeritrobilin-RBD lebih tinggi dari klorokuin, hidroksiklorokuin, nelfinavir, dan remdesivir dengan selisih 2,5; 2,6; 1,0; dan 0,4 *kkal/mol*. Afinitas pengikatan fikoeritrobilin-ACE2 lebih tinggi dari klorokuin, hidroksiklorokuin, dan remdesivir dengan selisih 1,1; 1,2; dan 0,3 *kkal/mol*. Afinitas pengikatan fikoeritrobilin-RdRp lebih tinggi dari klorokuin, hidroksiklorokuin, dan remdesivir dengan selisih 2,8; 2,7; dan 0,8 *kkal/mol*. Sisi pengikatan fikobiliprotein bervariasi pada setiap protein target, sedangkan fikobilin memiliki sisi pengikatan yang sama dengan senyawa pembanding. Berdasarkan hasil simulasi, dapat disimpulkan bahwa fikobiliprotein dan fikobilin dari *Spirulina platensis* berpotensi sebagai kandidat anti-SARS-CoV-2.

Kata kunci: fikobilin, fikobiliprotein, *molecular docking*, SARS-CoV-2, *Spirulina platensis*

ABSTRACT

This study aims to evaluate the potential of phycobiliprotein (C-phycocyanin, allophycocyanin, C-phycoerythrin) and phycobilin (phycocyanobilin, phycoerythrobilin) from *Spirulina platensis* as anti-SARS-CoV-2, using molecular docking simulation. Docking of candidate compounds with M^{pro}, RBD, ACE2, and RdRp receptors was performed and comparing their potency toward nelfinavir, chloroquine, hydroxychloroquine, and remdesivir. The research stages include protein and ligand preparation, docking method validation, docking simulation of protein-ligand and protein-protein, visualization and analysis of docking results using AutoDock Tools 1.5.6, AutoDock Vina 1.1.2, PyMOL 2.4.1, PRISM, and BIOVIA Discovery Studio Visualizer 2021. An interaction among phycobiliprotein and phycobilin with the four target proteins were observed and involving in hydrogen bonding, hydrophobic, electrostatic, van der Waals, π-sulfur, and unfavorable. The order of binding affinity of phycobiliproteins with M^{pro}, RBD, ACE2, and RdRp were determined to be F-chain C-phycocyanin, B-chain C-phycocyanin, B-chain C-phycoerythrin, and allophycocyanin. Among phycobilin, the phycoerythrobilin showed the highest binding affinity with all target proteins. The binding affinity of phycoerythrobilin-M^{pro} was higher than those of chloroquine and hydroxychloroquine with free energy differences of 2 and 1.8 *kcal/mol*. The binding affinity of phycoerythrobilin-RBD was higher than chloroquine, hydroxychloroquine, nelfinavir, and remdesivir with free energy differences of 2.5; 2.6; 1.0; and 0.4 *kcal/mol*. The binding affinity of phycoerythrobilin-ACE2 was higher than chloroquine, hydroxychloroquine, and remdesivir with free energy differences of 1.1; 1,2; and 0.3 *kcal/mol*. The binding affinity of phycoerythrobilin-RdRp was higher than chloroquine, hydroxychloroquine, and remdesivir with free energy differences of 2.8; 2.7; and 0.8 *kcal/mol*. The binding site of phycobiliprotein varies with each target protein, while phycobilin was occupied the same binding site as the control compounds. Based on the simulation results, it can be concluded that phycobiliprotein and phycobilin from *Spirulina platensis* are potential to be used as candidates for anti-SARS-CoV-2.

Keywords: molecular docking, phycobilin, phycobiliprotein, SARS-CoV-2, *Spirulina platensis*

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