

KAJIAN POTENSI PIGMEN *Chlorella vulgaris* DAN *Spirulina platensis* SEBAGAI
INHIBITOR LIPASE DALAM APLIKASINYA SEBAGAI ANTI JERAWAT
BERDASARKAN STUDI MOLEKULER *DOCKING*

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Sebuah skripsi yang diajukan untuk memenuhi salah satu syarat
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ABSTRAK

Propionibacterium acnes merupakan bakteri yang paling banyak ditemui pada kulit berjerawat. Antibiotik yang biasa digunakan untuk mengatasi jerawat diantaranya eritromisin, klindamisin, dan tetrasiklin. Namun, resistensi bakteri menyebabkan kendala pada pengobatan jerawat. Pada penelitian ini dilakukan *screening* terhadap potensi pigmen mikroalga *Chlorella vulgaris* dan *Spirulina platensis* sebagai anti jerawat alami serta kajian interaksi molekulernya terhadap lipase menggunakan pendekatan *molekuler docking*. Simulasi dilakukan melalui *docking* pigmen astaxantin, β -karoten, cantaxantin, fukoxantin, kriptoxantin, lutein, violaxantin, zeaxantin, fikosianobilin, fikoeritrobin, dan feofitin a, serta fikosianin terhadap lipase. Sebagai pembanding digunakan eritromisin, klindamisin, dan tetrasiklin. Tahapan penelitian dilakukan sebagai berikut : 1) preparasi protein; 2) validasi metode *docking*; 3) optimasi dan preparasi ligan; 4) simulasi *docking*; 5) visualisasi interaksi molekuler. *Docking* dilakukan menggunakan program MOPAC; AutoDock Tools 1.5.1; AutoDock Vina 1.1.2; Biova *Discovery studio visualizer*; dan PyMoL. Hasil *docking* menunjukkan bahwa kompleks fikosianin-lipase memiliki afinitas 25,8 *kcal/mol* lebih rendah dibandingkan tetrasiklin-lipase. Afinitas yang lebih rendah juga ditunjukkan oleh kompleks astaxantin-lipase dengan energi afinitas lebih rendah 1,4 *kcal/mol* dari tetrasiklin-lipase. Ligan non protein membentuk kompleks dengan sisi pengikatan yang sama dengan pembanding. Interaksi yang terlibat pada pembentukan kompleks ialah ikatan hidrogen, ikatan hidrofobik, interaksi Van der Waals dan *unfavorable bump*. Cantaxantin, feofitin a, fikoeritrobin, fukoxantin, lutein, violaxantin, dan zeaxantin merupakan inhibitor kompetitif sedangkan astaxantin, β -karoten, fikosianobilin, dan kriptoxantin merupakan inhibitor bukan kompetitif. Berdasarkan hasil penelitian pigmen dari mikroalga *Chlorella vulgaris* dan *Spirulina platensis* berpotensi sebagai kandidat antibiotik untuk mengatasi jerawat.

Kata kunci: antijerawat, *docking*, mikroalga, lipase, pigmen

ABSTRACT

Propionibacterium acnes is the most common bacteria found on acne prone skin. Several antibiotics used to treat acne are erythromycin, clindamycin, and tetracyclines. However, bacterial resistance causes obstacles to acne treatment. In this study, we conducted a screening of the potential of microalgae pigments *Chlorella vulgaris* and *Spirulina platensis* as natural anti-acne and also studied their molekuler interactions with the lipase using a molekuler docking approach. Simulations were carried out by docking astaxanthin, β -carotene, canthaxanthin, fucoxanthin, cryptoxanthin, lutein, violaxanthin, zeaxanthin, phycocyanobilin, phycoerythrobilin, and pheophytin a, and phycocyanin pigments against lipase. Erythromycin, clindamycin, and tetracycline were used as comparison for the activity. The research stages were carried out as follows: 1) protein preparation; 2) validation of the docking method; 3) optimization and preparation of ligands; 4) docking simulation; 5) visualization of molekuler interactions. Docking is conducted using the MOPAC program; AutoDock Tools 1.5.1; AutoDock Vina 1.1.2; Biova Discovery studio visualizer; and PyMoL. The docking results showed that the phycocyanin-lipase complex had an affinity lower 25,8 kkal/mol than tetracyclines-lipase. A lower affinity was also shown by the astaxanthin-lipase complexes with an energy affinity of 1,4 kkal/mol lower than tetracyclines-lipase. The non-protein ligands form a complex with the same binding side as the comparison. The interactions involved in complex formation are hydrogen bonds, hydrophobic bonds, Van der Waals interactions and unfavorable bumps. Canthaxanthin, pheophytin a, phycoerythrobilin, fucoxanthin, lutein, violaxanthin, dan zeaxanthin are competitive inhibitors while astaxanthin, β -carotene, cryptoxanthin and, phycocyanobilin are non-competitive inhibitors. Based on the results of research, pigments from microalgae *Chlorella vulgaris* and *Spirulina platensis* have potential to be used as antibiotic candidates for treating acne.

Keywords: anti-acne, docking, microalgae, lipase, pigment

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KAJIAN POTENSI PIGMEN *Chlorella vulgaris* DAN *Spirulina platensis* SEBAGAI INHIBITOR LIPASE DALAM APLIKASINYA SEBAGAI ANTI JERAWAT BERDASARKAN STUDI MOLEKULER DOCKING
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