In-Vitro and In-Silico Study for Antioxidant Exploration Based on Pyocianin Pigment Isolated from Pseudomonas Aeruginosa Associated with Sea Sponges from Enggano Island

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Abstract

Sedentary behavior is a key factor contributing to the rise in various degenerative diseases. This condition is triggered by oxidative stress or high levels of oxidation. This study aims to characterize and explore the antioxidant potential of the pyocyanin pigment isolated from *Pseudomonas aeruginosa* SH-11 through in vitro and in silico studies. Pyocyanin pigment was extracted using acid-base extraction and maceration methods. The pigment was characterized using UV-visible spectrophotometry (UV-vis), nuclear magnetic resonance spectroscopy (NMR), and Fourier-transform infrared spectroscopy (FTIR). The DPPH assay was performed to obtain absorbance values, and then percentage inhibition and inhibitory concentration (IC_{50}) were calculated to determine antioxidant activity. Molecular docking techniques were used to analyze the interaction of pyocyanin compounds with the target protein, nuclear factor erythroid-2-related factor 2 (Nrf-2). The bacteria entered the stationary growth phase, reaching peak concentration at 72 hours. A thick blue-green pigment was produced after evaporation. Characterization of the pigment using UV-vis, NMR, and FTIR spectroscopy indicated the presence of pyocyanin pigment. Antioxidant activity testing showed that pyocyanin pigment has antioxidant activity against DPPH radicals with an IC_{50} value of 74.38 ± 0.68. Based on molecular docking analysis, the Gibbs free energy (ΔG) of the validation ligand (PDB ID: 7OFE) was -9.51 kcal/mol, with an RMSD of 0.869 Å and a Ki value of 106.31 nM. The P. aeruginosa SH-11 isolate produced pyocyanin pigment according to the three characterization methods, and the pigment demonstrated a strong ability to inhibit DPPH radicals and also showed strong binding with the Nrf-2 ligand.

Keywords

Antioxidant, Molecular Docking, *Pseudomonas aeruginosa*, Pyocyanin