SKRIPSI SARJANA FARMASI

PENGARUH *RUBRAXANTHONE* TERHADAP BEBERAPA ISOENZIM *CYTOCHROME P450* SECARA *IN SILICO*

OLEH:

HANIYATI NAILA

NIM: 2211012050

Pembimbing I: Dr. apt. Dira Hefni, S. Farm, M. Sc

Pembimbing II : Dr. apt. Meri Susanti, M.Farm

FAKULTAS FARMASI

UNIVERSITAS ANDALAS

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ABSTRAK

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Oleh:

HANIYATI NAILA

NIM: 2211012050

(Program Studi sarjana Farmasi)

Penggunaan obat herbal bersamaan dengan obat konvensional dapat menimbulkan interaksi obat-herbal melalui modulasi enzim Cytochrome P450 (CYP450). Rubraxanthone merupakan senyawa xanthone dari genus *Garcinia* yang memiliki berbagai aktivitas biologis, namun potensi interaksinya terhadap isoenzim CYP450 belum banyak diteliti. Penelitian ini bertujuan untuk menganalisis nilai skor docking dan pola interaksi rubraxanthone terhadap beberapa isoenzim CYP450 secara *in silico*. Metode penelitian meliputi preparasi protein dan ligan, validasi protokol docking menggunakan metode *re-docking* dengan parameter RMSD ≤ 2 Å, dan simulasi *molecular docking* menggunakan AutoDock Vina. Dari 39 protein yang diuji, 14 protein memenuhi kriteria validitas. Hasil docking menunjukkan rubraxanthone memiliki afinitas ikatan lebih tinggi dibandingkan *native ligand* pada enzim CYP2A6 (kode PDB: 4EJJ dengan skor -10,087 kcal/mol berbanding -6,084 kcal/mol; dan 1Z11 dengan skor -11,015 kcal/mol berbanding -7,668 kcal/mol). Visualisasi interaksi menunjukkan rubraxanthone berikatan pada *active site* CYP2A6 melalui ikatan hidrogen, interaksi hidrofobik, dan interaksi elektrostatik, dengan pola yang mirip *native ligand*. Sehingga rubraxanthone diprediksi berpotensi sebagai inhibitor kompetitif enzim CYP2A6 yang dapat menyebabkan interaksi obat-herbal.

Kata Kunci: Rubraxanthone, Cytochrome P450, CYP2A6, molecular docking, interaksi obat-herbal, *in silico*

ABSTRACT

THE EFFECT OF RUBRAXANTHONE ON SEVERAL CYTOCHROME P450 ISOENZYMES IN SILICO

By:

HANIYATI NAILA

Student ID Number: 2211012050

(Bachelor of Pharmacy Study Program)

The use of herbal medicines in combination with conventional medicines can cause drug-herbal interactions through the modulation of Cytochrome P450 (CYP450) enzymes. Rubraxanthone is a xanthone compound from the Garcinia genus that has various biological activities, but its potential interaction with CYP450 isoenzymes has not been widely studied. This study aims to analyze the docking scores and interaction patterns of rubraxanthone with several CYP450 isoenzymes in silico. The research methods included protein and ligand preparation, docking protocol validation using the re-docking method with RMSD ≤ 2 Å parameters, and molecular docking simulation using AutoDock Vina. Of the 39 proteins tested, 14 proteins met the validity criteria. Docking results show that rubraxanthone has a higher binding affinity than the native ligand for the CYP2A6 enzyme (PDB code: 4EJJ with a score of -10.087 kcal/mol compared to -6.084 kcal/mol; and 1Z11 with a score of -11.015 kcal/mol compared to -7.668 kcal/mol). Visualization of the interactions shows that rubraxanthone binds to the CYP2A6 active site via hydrogen bonds, hydrophobic interactions, and electrostatic interactions, with a pattern similar to that of the native ligand. Thus, rubraxanthone is predicted to have potential as a competitive inhibitor of the CYP2A6 enzyme, which could lead to drug-herb interactions.

Keywords: Rubraxanthone, Cytochrome P450, CYP2A6, molecular docking, herb-drug interaction, *in silico*