ANALISIS *IN SILICO* TOKSISITAS SENYAWA ANALOG KURKUMIN PADA ENZIM SITOKROM P450 3A4

Esti Mumpuni[1)*], Agus Purwanggana[2)] , Esti Mulatsari[3)], Wahyu Cahyono Rudi Saputro[4)]
[1] Fakultas Farmasi, Universitas Pancasila
Email: esti_mumpuni@yahoo.com
[2]Fakultas Farmasi, Universitas Pancasila
Email: agusp_12@gmail.com
[3]Fakultas Farmasi, Universitas Pancasila
Email: estimulatsari@gmail.com
[4]Fakultas Farmasi, Universitas Pancasila
*corresponding author

Abstrak

Penelitian mengenai sintesis senyawa analog kurkumin untuk memperbaiki bioavailabilitas kurkumin telah banyak dilakukan, akan tetapi tidak disertai dengan sifat toksisitasnya. Pada penelitian ini dilakukan uji toksisitas senyawa analog kurkumin secara *in silico* dengan metode *molecular docking* pada enzim sitokrom P450 3A4 yang berperan dalam proses detoksifikasi pada hati. Proses *docking* dilakukan dengan software PLANTS, preparasi protein dan ligand dengan YASARA dan ChemSketch, visualisasi interaksi ligand-protein dengan PyMOL. Uji toksisitas dilakukan pada 51 senyawa analog kurkumin alami dan senyawa analog kurkumin hasil sintesis beserta derivat – derivatnya. Berdasarkan hasil *nilai score docking* diperoleh sembilan senyawa analog kurkumin bersifat hepatotoksik yang dibandingkan dengan senyawa pembanding Allopurinol.

Kata kunci: *analog kurkumin, docking, toksisitas*

Abstract

Research on the synthesis of curcumin analog compounds to improve the bioavailability has been widely carried out, but it was not accompanied by its toxicity. In this study, the *in silico* toxicity test of curcumin analog compounds was carried out by molecular docking method on cytochrome P450 3A4 enzyme which plays a role in the detoxification process in the liver. The docking process was carried out with PLANTS software, protein and ligand preparation with YASARA and ChemSketch, visualization of ligand-protein interactions with PyMOL. *In silico* toxicity tests were carried out on 51 natural curcumin analog compounds and the synthesized curcumin analog compounds with theirs derivates. Based on the *docking score*, obtained nine curcumin analog compounds were hepatotoxic that compared with Allopurinol.

Keywords: *curcumin analog, docking, toxicity*