ABSTRAK

STUDI INTERAKSI SENYAWA AKTIF DARI *Curcuma xanthorrhiza* TERHADAP RESEPTOR *CAR* DAN *PXR* DENGAN METODE *MOLECULAR DOCKING*

Fadillah Resky Widiantoro[1], Muhamad Salman Fareza[2], Hanif Nasiatul Baroroh[2]

Latar Belakang : Senyawa aktif *Curcuma xanthorrhiza* dilaporkan dapat memodulasi enzim pemetabolisme obat sehingga dapat menyebabkan interaksi herbal-obat. Penelitian dilakukan untuk menganalisis interaksi senyawa aktif *Curcuma xanthorrhiza* dengan reseptor *CAR* dan *PXR*. Senyawa uji dikaji secara *in silico* menggunakan metode *molecular docking* untuk mengetahui energi dan jenis ikatannya terhadap reseptor *CAR* dan *PXR*.
Metodologi : Penelitian dilakukan dengan mengunduh struktur *CAR* dan *PXR* dari *PDB*, preparasi struktur protein menggunakan *AutoDock Tools*, validasi metode menggunakan *AutoDock Vina*, perhitungan *RMSD* menggunakan *PyMOL*, penambatan senyawa uji dengan protein target *CAR* dan *PXR*, dan visualisasi hasil penambatan menggunakan *BIOVIA Discovery Studio*.
Hasil Penelitian : Nilai energi ikatan (kkal/mol) yang diperoleh dari *molecular docking* terhadap protein target *CAR* yaitu fenitoin (-10,3), xanthorrhizol (-8,0), kurkumin (-9,2), zingiberene (-8,6), α-kurkumena (-8,8) dan β-kurkumena (-8,8); terhadap protein target *PXR* yaitu hiperforin (-8,3), xanthorrhizol (-7,5), kurkumin (-8,3), zingiberene (-6,8), α-kurkumena (-7,8) dan β-kurkumena (-7,6). Senyawa uji membentuk ikatan Van der Waals, Pi-sigma, Pi-Pi stacked, Alkil, dan Pi-alkil dengan protein target *CAR* dan *PXR*. Kurkumin membentuk ikatan hidrogen dengan protein target *CAR* dan *PXR* pada asam amino Asn165 dan Ser247.
Kesimpulan : Senyawa kurkumin pada *Curcuma xanthorrhiza* memiliki potensi yang kuat untuk berikatan dengan reseptor *CAR* dan *PXR*.

Kata Kunci : *Curcuma xanthorrhiza, CAR, PXR, Molecular Docking*

[1]Mahasiswa Jurusan Farmasi Fakultas Ilmu-Ilmu Kesehatan Universitas Jenderal Soedirman
[2]Jurusan Farmasi Fakultas Ilmu-Ilmu Kesehatan Universitas Jenderal Soedirman

ABSTRACT

STUDY OF INTERACTION ACTIVE COMPOUNDS FROM *Curcuma xanthorrhiza* WITH CAR AND PXR RECEPTOR USING MOLECULAR DOCKING METHOD

Fadillah Resky Widiantoro[1], Muhamad Salman Fareza[2], Hanif Nasiatul Baroroh[2]

Backgorund : The active compounds from *Curcuma xanthorrhiza* is reported to be able to modulate drug metabolizing enzymes, that can cause herbal-drug interactions. This study was conducted to analyze the interaction of the active compound from *Curcuma xanthorrhiza* with CAR and PXR receptors. The test compounds were studied in silico using the molecular docking method to determine the energy and type of binding to CAR and PXR receptors.
Methods : The research was conducted by downloading the CAR and PXR structures from PDB, preparation of protein structures using AutoDock Tools, method validation using AutoDock Vina, RMSD calculations using PyMOL, molecular docking of test compounds with CAR and PXR target proteins, and visualization of docking results using BIOVIA Discovery Studio.
Results : Energy binding (kcal/mol) obtained from molecular docking of the CAR target protein is phenytoin (-10,3), xanthorrhizol (-8,0), curcumin (-9,2), zingiberene (-8,6), α-curcumene (-8,8) and β-curcumene (-8,8); of the PXR target protein is hyperforin (-8,3), xanthorrhizol (-7,5), curcumin (-8,3), zingiberene (-6,8), α-curcumene (-7,8) and β-curcumene (-7,6). The test compounds have Van der Waals, Pi-sigma, Pi-Pi sacked, Alkyl, and Pi-alkyl bonds with CAR and PXR target proteins. Curcumin have hydrogen bonds with CAR and PXR target proteins at amino acids Asn165 and Ser247.
Conclusion : Curcumin in *Curcuma xanthorrhiza* has a strong potential to bind to CAR and PXR receptors.
Keywords : *Curcuma xanthorrhiza*, CAR, PXR, Molecular Docking

[1]Student of Pharmacy Department, Faculty of Health Sciences, Jenderal Soedirman University
[2]Pharmacy Department, Faculty of Health Sciences, Jenderal Soedirman University