Abstrak

STUDI INTERAKSI MOLEKULER SENYAWA BIOAKTIF BIJI JINTEN HITAM (*Nigella sativa*) TERHADAP CAR DAN PXR SECARA *MOLECULAR DOCKING*

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Latar Belakang : Jinten hitam (*Nigella sativa*) memiliki berbagai aktivitas farmakologis sehingga merupakan salah satu tanaman yang banyak digunakan sebagai obat herbal. Senyawa bioaktif dari jinten hitam yang berperan besar dalam aktivitas farmakologi diantaranya *thymoquinone*, *dithymoquinone*, *thymohydroquinone*, *carvacrol*, *p-Cymene* dan *4-terpineol.* Senyawa ini berpotensi dapat berinteraksi dengan reseptor CAR dan PXR yang dapat mempengaruhi ekspresi enzim pemetabolisme sehingga ketika terjadi perubahan ekspresi dari enzim pemetabolisme yang dimediasi oleh CAR dan PXR dapat berpotensi terjadinya interaksi herbal-obat. Sehingga, peneliti ingin meneliti mengenai interaksi senyawa aktif biji jinten hitam dengan reseptor CAR dan PXR menggunakan *molecular docking*.

Metodologi : Penelitian eksperimental dilakukan secara *in silico* dengan menambatkan molekul antara senyawa *thymoquinone*, *dithymoquinone*, *thymohydroquinone*, *carvacrol*, *p-Cymene* dan *4-terpineol* dengan reseptor CAR dan PXR dan kemudian dibandingkan dengan fenitoin dan hiperforin sebagai kontrol positif.

Hasil Penelitian : Nilai energi ikatan senyawa uji yang diperoleh secara *molecular docking* terhadap reseptor CAR yaitu *thymoquinone* (-6,9 kkal/mol), *dithymoquinone* (-8,0 kkal/mol), *thymohydroquinone* (-6,5 kkal/mol), *carvacrol* (-7,0 kkal/mol), *p-Cymene* (-6,8 kkal/mol), *4-terpineol* (-6,6 kkal/mol) dan nilai energi ikatan dari kontrol positif fenitoin adalah (-10,1 kkal/mol). Serta, nilai energi ikatan senyawa uji terhadap reseptor PXR yaitu *thymoquinone* (-6,6 kkal/mol), *dithymoquinone* (-8,5 kkal/mol), *thymohydroquinone* (-6,4 kkal/mol), *carvacrol* (-6,5 kkal/mol), *p-Cymene* (-6,5 kkal/mol), *4-terpineol* (-6,3 kkal/mol) dan nilai energi ikatan dari kontrol positif hiperforin (-8,3 kkal/mol).

Kesimpulan : Senyawa *dithymoquinone* dapat berpotensi berinteraksi dengan reseptor PXR karena memiliki nilai energi ikatan lebih rendah yaitu (-8,5 kkal/mol) jika dibandingkan dengan kontrol positif hiperforin yaitu (-8,3 kkal/mol).

Kata Kunci : *Nigella sativa; molecular docking;* CAR; PXR; 1XVP; 1SKX

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Abstract

STUDY OF MOLECULAR INTERACTIONS OF BIOACTIVE COMPOUNDS OF BLACK SEEDS (*Nigella sativa*) ON CAR AND PXR BY MOLECULAR DOCKING

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Background : Black cumin (*Nigella sativa*) has various pharmacological activities so that it is one of the plants that is widely used as herbal medicine. Bioactive compounds from black cumin that play a major role in pharmacological activity include thymoquinone, dithymoquinone, thymohydroquinone, carvacrol, p-Cymene and 4-terpineol. This compound has the potential to interact with CAR and PXR receptors which can affect the expression of metabolizing enzymes so that when there is a change in the expression of metabolizing enzymes mediated by CAR and PXR there can be potential herbal-drug interactions. Thus, researchers wanted to investigate the interaction of the active compounds of black cumin seeds with CAR and PXR receptors using molecular docking.

Methods : Experimental studies were carried out in silico by anchoring molecules between the compounds thymoquinone, dithymoquinone, thymohydroquinone, carvacrol, p-Cymene and 4-terpineol with CAR and PXR receptors and then compared with phenytoin and hyperforin as positive controls.

Results : The binding energy values of the test compounds obtained by molecular docking to the CAR receptor were thymoquinone (-6.9 kcal/mol), dithymoquinone (-8.0 kcal/mol), thymohydroquinone (-6.5 kcal/mol), carvacrol (- 7.0 kcal/mol), p-Cymene (-6.8 kcal/mol), 4-terpineol (-6.6 kcal/mol) and the binding energy value of the phenytoin positive control was (-10.1 kcal/mol). Also, the binding energy value of the test compound to the PXR receptor, namely thymoquinone (-6.6 kcal/mol), dithymoquinone (-8.5 kcal/mol), thymohydroquinone (-6.4 kcal/mol), carvacrol (-6.5 kcal/mol), p-Cymene (-6.5 kcal/mol), 4-terpineol (-6.3 kcal/mol) and the binding energy value of the hyperforin positive control (-8.3 kcal/mol).

Conclusion : The dithymoquinone compound has the potential to interact with the PXR receptor because it has a lower binding energy value (-8.5 kcal/mol) compared to the hyperforin positive control (-8.3 kcal/mol).

Keywords : *Nigella sativa; molecular docking;* CAR; PXR; 1XVP; 1SKX

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