

**KAJIAN INTERAKSI SENYAWA KURKUMIN DAN ANALOG KURKUMIN DENGAN
RESEPTOR DIPEPTIDYL PEPTIDASE-4 (DPP-4) MENGGUNAKAN
METODE DOCKING DAN DINAMIKA MOLEKULER**

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INTISARI

Kajian interaksi senyawa kurkumin dan analog kurkumin dengan reseptor dipeptidyl peptidase-4 menggunakan metode *docking* molekuler telah dilakukan. Tujuan dari penelitian ini adalah untuk menentukan senyawa analog kurkumin yang mempunyai potensi sebagai inhibitor dipeptidyl peptidase-4 secara *docking* molekuler dan dinamika molekuler. Penelitian ini diawali dengan *docking* senyawa kurkumin pada DPP-4 dan dilanjutkan dengan analog kurkumin. Berdasarkan *docking* molekuler, diperoleh nilai *binding site* dari masing-masing senyawa. Selanjutnya hasil *docking* dari analog kurkumin dibandingkan dengan hasil *docking* dari kurkumin untuk mengetahui senyawa terbaik. *Docking* molekuler kurkumin menghasilkan nilai energi bebas Gibbs ikatan -8,4 kkal/mol sedangkan analog kurkumin mempunyai nilai energi bebas Gibbs ikatan antara -7,5 kkal/mol sampai -8,4 kkal/mol. Salah satu analog kurkumin mempunyai nilai yang sama dengan kurkumin. Bahkan hasil uji aktivitas analog kurkumin tersebut lebih aktif dari kurkumin, sehingga analog tersebut sangat berpotensi untuk dijadikan senyawa obat antidiabetes baru.

Kata kunci: kurkumin, *docking* molekuler, analog kurkumin, DPP-4

**STUDY ON INTERACTION OF CURCUMIN AND CURCUMIN ANALOGUES WITH
DIPEPTIDYL PEPTIDASE-4 (DPP-4) RECEPTOR USING DOCKING
AND MOLECULAR DYNAMICS METHODS**

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ABSTRACT

Study on interaction of curcumin and curcumin analogues with dipeptidyl peptidase-4 receptor using molecular docking has been performed. The purpose of this study is to determine curcumin analog compounds that have potential as inhibitors of dipeptidyl peptidase-4 in docking and molecular dynamics. This work was started with docking of curcumin compound in dipeptidyl peptidase-4 and continued with curcumin analogues. Based on docking molecular, the value of binding affinity of each compound was obtained. The next procedure was to compare the result to find the best compound. The free energy Gibbs binding result from molecular docking of curcumin was -8.4 kcal/mol whereas curcumin analogues had free energy Gibbs binding with range values from -7.5 kcal/mol to 8.4 kcal/mol. One of the curcumin analogues had the same free energy Gibbs binding value as curcumin. In fact, it had better activity than curcumin hence it had potency to be the new precursor compound for drug development.

Key words: curcumin, molecular docking, curcumin analogues, DPP-4