ABSTRAK

STUDI POTENSI SENYAWA AKTIF ANTI KANKER SEBAGAI INHIBITOR EGFR

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Latar Belakang : *Epidermal Growth Factor* menjadi salah satu agen target molekuler dalam pengembangan obat antikanker. Senyawa pinosembrin, α-mangostin, γ-mangostin, galangin, pinostrobin, sinamaldehid, andrografolid, kukumin, xantorizol, etil p-metoksisinamat, alashanoid b dilaporkan memiliki aktivitas antikanker. Penelitian ini bertujuan melakukan uji aturan lipinski dan penambatan molekuler terhadap senyawa tersebut sehingga dapat dijadikan dasar untuk pengembangan obat baru.

Metodologi : Sebelas senyawa dilakukan pengujian aturan lipinski menggunakan web SCFBIO dilanjutkan dengan *moleculer docking*. *Moleculer docking* dilakukan dengan 5 cara yaitu mengunduh struktur EGFR dari PDB, Preparasi protein menggunakan *AutoDock Tools,* penambatan kembali dengan ligan natif menggunakan *AutoDock Vina*, perhitungan nilai RMSD menggunakan *PyMol* dan visualisasi hasil menggunakan *BIOVIA Discovery Studio.*

Hasil Penelitian : Semua senyawa uji memenuhi aturan lipinski. Energi ikatan (kkal/mol) pada senyawa pinosembrin (-8,7), α-mangostin (-8,6), γ-mangostin (-8,4), galangin (-8,4), pinostrobin (-8,3), dan kurkumin (-8,3) lebih rendah dibandingkan senyawa kontrol erlotinib (-7,9). Keenam senyawa tersebut membentuk ikatan hidrogen, hidrofobik, dan elektrostatik terhadap sisi aktif dari EGFR.

Kesimpulan : Senyawa pinosembrin, α-mangostin, γ-mangostin, galangin, pinostrobin, dan kurkumin memiliki fisikokimia yang baik dan berpotensi sebagai inhibitor EGFR.

Kata Kunci : Lipinski, EGFR, Penambatan molekuler

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ABSTRACT

STUDY OF POTENTIAL ANTI-CANCER ACTIVE COMPOUNDS AS EGFR INHIBITORS

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Backgrounds : The epidermal Growth Factor is one of the molecular target agents in the development of anticancer drugs. Pinocembrin, α-mangosteen, γ-mangosteen, galangin, pinostrobin, cinnamaldehyde, andrographolide, curcumin, xanthorrhizol, ethyl p-methoxycinnamate, alashanoid b were reported to have anticancer activity. This study aims to test the Lipinski rules and molecular docking of these compounds so that they can be used as the basis for the development of new drugs.

Methods : Eleven compounds were tested for Lipinski's rule using the SCFBIO web followed by molecular docking. Molecular docking was carried out in 5 ways, namely downloading the EGFR structure from PDB, protein preparation using AutoDock Tools, re-tethering with native ligands using AutoDock Vina, calculating RMSD values using PyMol, and visualizing the results using BIOVIA Discovery Studio.

Results : All test compounds complied with Lipinski's rules. Bond energy (kcal/mol) in pinocembrine (-8.7), α-mangostin (-8.6), γ-mangostin (-8.4), galangin (-8.4), pinostrobin (-8.3), and curcumin (-8.3) was lower than the control compound erlotinib (-7.9). The six compounds formed hydrogen, hydrophobic, and electrostatic bonds to the active site of EGFR.

Conclusion : Pinocembrin, α-mangostin, γ-mangostin, galangin, pinostrobin, and curcumin compounds have good physicochemical properties and have potential as EGFR inhibitors.

Keywords : Lipinski, EGFR, Molecular docking

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