ABSTRAK

STUDI POTENSI BEBERAPA SENYAWA AKTIF ANTIKANKER PARU-PARU SEBAGAI INHIBITOR ENZIM *INSULIN RECEPTOR (INSR)* SECARA *IN SILICO*

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Latar Belakang : Aktivasi InsR yang berlebihan berkorelasi dengan perkembangan kanker paru-paru. Obat yang telah dikembangkan diketahui memiliki resistensi. Diperlukan penemuan obat baru dari senyawa-senyawa alam seperti andrografolid, alfa mangostin, gamma mangostin, galangin, EPMS, pinostrobin, pinosembrin, xantorizol, sinamaldehid, dan alashanoid B sebagai penghambat InsR baru. Senyawa-senyawa tersebut dapat dikaji secara *in silico* untuk mengetahui potensinya sebagai penghambat InsR.

Metodologi : Penelitian eksperimental secara *molecular docking* untuk mengetahui energi serta jenis ikatan, lalu uji Lipinski untuk mengetahui sifat fisikokimia dilakukan terhadap sebelas senyawa. Satu senyawa terbaik kemudian diuji secara *molecular dynamic* untuk mengetahui interaksi pada kondisi fisiologis tubuh. Analisis data dilakukan dengan membandingkan hasil dengan linsitinib.

Hasil Penelitian : Nilai energi ikatan (kkal/mol) yang diperoleh secara *molecular docking* yaitu andrografolid (-7,8), alfa mangostin (-8,4), gamma mangostin (-8,4), pinostrobin (-8,2), pinosembrin (-8,2), sinamaldehid (-5,6), kurkumin (-7,6), galangin (-8,4), EPMS (-6,0), xantorizol (-7,5), alashanoid B (-6,2), ligan natif (-10,9), dan linsitinib (-9,8). Dari kesebelas senyawa, alfa mangostin diketahui tidak memenuhi syarat uji lipinski. Hasil *molecular dynamic* menunjukkan gamma mangostin dan linsitinib memiliki nilai RMSD *backbone* berturut-turut 1,541 Å dan 1,581 Å serta *energy binding* berturut-turut -9395,8 kkal/mol dan -9384,2 kkal/mol.

Kesimpulan : Gamma mangostin berpotensi sebagai inhibitor InsR.

Kata Kunci : Kanker Paru-Paru, Inhibitor *Insulin Receptor* (InsR), *Molecular Docking*, Uji Lipinski, *Molecular Dynamic*.

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ABSTRACT

STUDY OF THE POTENTIAL OF SOME ACTIVE ANTI-LUNG CANCER COMPOUNDS AS INSULIN RECEPTOR (INSR) ENZYME INHIBITOR WITH IN SILICO

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Background : Excessive InsR activation correlates to lung cancer development. Drugs that have been developed are known to have resistance. New drugs discovery is needed from natural compounds such as andrographolide, alpha mangosteen, gamma mangosteen, pinostrobin, pinocembrin, cinnamaldehyde, curcumin, galangin, EPMC, xanthorrizol, and alashanoid B as new InsR inhibitors. These compounds can be studied in silico to determine their potential as InsR inhibitors.

Methods : Experimental research using molecular docking to determine the energy and types of bond, then Lipinski's test to know the physicochemical of eleven compounds. One of the best compounds then tested by molecular dynamics. Data analysis was performed by comparing the results with linsitinib.

Results : Energy binding (kcal/mol) obtained by *molecular docking* of andrographolide (-7,8), alpha mangosteen (-8,4), gamma mangosteen (-8,4), pinostrobin (-8,2), pinocembrin (-8,2), cinnamaldehyde (-5,6), curcumin (-7,6), galangin (-8,4), EPMC (-6,0), xanthorrizol (-7,5), alashanoid B (-6,2), native ligan (-10,9), and linsitinib (-9,8). From eleven compounds, alpha mangosteen is known did not qualify for Lipinski test. Molecular dynamic results showed alpha mangosteen and linsitinib have backbone RMSD consecutive 1,541 Å and 1,581 Å as well as binding energy consecutive -9395,8 kcal/mol and -9384,2 kcal/mol.

Conclusion : Gamma mangosteen is potent as InsR inhibitors.

Keywords : Lung Cancer, Insulin receptor (InsR) Inhibitors, Molecular Docking, Lipinski Test, Molecular Dynamic.

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