

Study in Silico Luteolin as A Herbal Medicine to Prevent DILI in Depression Disorder

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Abstract

Depression is a serious mental illness that often affects the general public, characterized by impaired thinking, emotional processing and prolonged stress. Antidepressant drugs (ADs) can relieve symptoms of depression, but side effects such as hepatotoxicity and the risk of DILI (drug-induced liver injury) can be very dangerous. MMP-9 and Caspase-3 proteins play an important role in liver damage in DILI. Luteolin in celery (*Apium graveolens L*) as a natural compound is proven to effectively inhibit MMP-9 and promote Caspase-3 proteins, also determining the mechanism of Luteolin on DILI inhibition through molecular docking studies. Luteolin as a ligand in the docking process with MMP-9 protein with binding affinity value of -10.3 and Caspase-3 with the amount of -7.8. The docking study showed that Luteolin has high binding to MMP-9 protein, although it tends to bind to the surface area of the protein only. Potentially to reduce inflammation and can be consumed by individuals infected with DILI.

Keywords: Antidepressant, DILI, Luteolin, *Apium graveolens L*, MMP-9, Caspase-3, docking.

Study in Silico Luteolin sebagai Obat Herbal untuk Mencegah DILI pada Penderita Depresi

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Abstrak

Depresi merupakan penyakit gangguan mental serius yang kerap menjangkit khalayak umum, ditandai dengan gangguan berpikir, pengolahan emosi dan stres berkepanjangan. *Antidepressant Drug* (ADs) dapat meredakan gejala depresi, tetapi efek samping seperti hepatotoksisitas dan resiko DILI (*drug-induced liver injury*) dapat menjadi sangat berbahaya. Protein MMP-9 dan Caspase-3 memainkan peran penting dalam kerusakan hati pada DILI. Luteolin dalam seledri (*Apium graveolens L*) sebagai senyawa alami yang terbukti efektif menghambat protein MMP-9 dan mendorong Caspase-3 serta mengetahui mekanisme Luteolin pada penghambatan DILI melalui studi *molecular docking*. Luteolin sebagai ligan dalam proses *docking* dengan protein MMP-9 dengan nilai binding affinity -10,3 dan Caspase-3 dengan jumlah -7,8. Studi *docking* menunjukkan Luteolin memiliki pengikatan tinggi terhadap protein MMP-9, meskipun cenderung terikat di area permukaan protein saja. Berpotensi untuk meringankan peradangan dan dapat dikonsumsi oleh individu yang terinfeksi DILI.

Kata kunci: *Antidepressant*, DILI, Luteolin, *Apium graveolens L*, MMP-9, Caspase-3, *docking*.