Studi Molecular Docking Senyawa Aktif Propolis Indonesia terhadap -Site Amyloid Precursor Protein Cleaving Enzyme1 (BACE1) pada Penyakit Alzheimer = Molecular Docking Study of Indonesian Propolis Active Compounds on Î²-Site Amyloid Protein Precursor Cleaving Enzyme1 (BACE1) in Disease

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Abstrak

Alzheimer merupakan penyebab paling umum dari demensia dan penyakit dengan jumlah pasien yang terus meningkat setiap tahunnya. -Site Amyloid Precursor Protein Cleaving Enzyme1 (BACE1) diketahui sebagai protein yang sangat toksik dan dapat memicu penyakit Alzheimer. Propolis dengan flavonoid yang terkandung di dalamnya dilaporkan memiliki sifat pelindung saraf dalam studi in vitro dan in vivo melalui tindakan antioksidan, anti-inflamasi, dan imunomodulator. Pada penelitian ini, dilakukan studi in silico untuk mengetahui interaksi protein target BACE1 dan ligan pada senyawa propolis lokal Indonesia dengan melakukan molecular docking. Senyawa ligan yang digunakan pada penelitian ini yaitu, Sulawesin A, Broussoflanovol F, Sulawesin B, Glyasperin A, Deoxy-podophyllotoxin, Isorhamnetin, Xanthoxyletin, (--)-Isocalolongic acid, 2',3'-Dihydro-3'-hydroxypapuanic acid, Isopapuanic acid, (1's)-2-Cis,4 trans-abscisic acid, Curcumene, (1's)-2-Trans,4 trans-abscisic acid, Tetraline, P-coumaric acid, dan Thymol. Hasil menunjukkan bahwa molecular docking antara protein target BACE1 dengan native ligand memiliki nilai docking terbaik yaitu, -11 kkal/mol. Sedangkan, senyawa ligan yang memiliki nilai docking terbaik yaitu, Sulawesin A dengan nilai -9,3 kkal/mol.

.....Alzheimer's is the most common cause of dementia and disease with the number of patients increasing every year. -Site Amyloid Protein Precursor Cleaving Enzyme1 (BACE1) is known as a highly toxic protein and can trigger Alzheimer's disease. Propolis with flavonoids contained in it is reported to have neuroprotective properties in in-vitro and in-vivo studies through its antioxidant, anti-inflammatory, and immunomodulatory actions. In this study, an in-silico study was conducted to determine the interaction of the target protein BACE1 and its ligand on local Indonesian propolis compounds by molecular docking. The ligand compounds used in this study were Sulawesin A, Broussoflanovol F, Sulawesin B, Glyasperin A, Deoxy-podophyllotoxin, Isorhamnetin, Xanthoxyletin, (--)-Isocalolongic acid, 2',3'-Dihydro-3'-hydroxypapuanic acid., Isopapuanic acid, (1's)-2-Cis,4 trans-abscisic acid, Curcumene, (1's)-2-Trans,4 trans-abscisic acid, Tetraline, P-coumaric acid, and Thymol. The results showed that the molecular docking between BACE1 protein target and native ligand had the best docking value, namely -11 kcal/mol. Meanwhile, the ligand compound that has the best docking value is Sulawesin A with a value of -9.3 kcal/mol.