SKRINING SENYAWA AKTIF DARI BALIK ANGIN A. excels (Fenzl) Benth. TERHADAP RESEPTOR TNF-alpha convertase (TACE) DENGAN METODE DOCKING

ABSTRAK

Tumor necrosis factor-alpha (TNF-α) merupakan sitokin proinflamasi yang terlibat dalam berbagai penyakit seperti radang selaput otak, rematik, asma, tuberkolosiS, periontitis kronis, crohn desease, hepatitis dan sinusitis hidung. Sehingga ekspresinya perlu dikontrol untuk mengatasi penyakit ini. Penelitian ini bertujuan melakukan skrining inhibitor reseptor TNF-alpha convertase (TACE) sehingga menurunkan ekspersi TNF-α. Dengan menurunnya produksi TNF-α maka dapat sebagai antiinflamasi atau imunosupresan. Salah satu tanaman yang dapat dipergunakan untuk skrining ini adalah A.excels. Metode yang dipergunakan untuk skrining melalui PASSonline dan Docking dengan PLANTS serta dilihat prediksi memasuki peredaran darah dengan SWISSADME. Berdasarkan PASSonline Senyawa yang memiliki skor probability to be active imunosupreasant tinggi adalah batulinic acid (0,724), alphitolic acid (0,763), cis-coumaroyl alphitolic acid (0,771). Sedangkan yang memiliki probability to be active antiinflamasi adalah batulinic acid (0,741) dan cis-coumaroyl alphitolic acid (0,783). Berdasarkan stabilitas interaksi, senyawa yang memiliki kemampuan minimal 80% terhadap ligand referensi adalah alphitonin (98,25%), alphitexolide (92,33%), cis-coumaroyl alphitolic acid (98,31%). Kesimpulannya senyawa yang berpotensi yang memiliki stabilitas interaksi yang bagus adalah cis-coumaroyl alphitolic acid dan alphitonin

Kata kunci : TNF-α, A.excels, stabilitas interaksi

ABSTRACT

Tumor necrosis factor-alpha (TNF-α) is a proinflammatory cytokine that is involved in various diseases such as meningitis, rheumatism, asthma, tuberculosis, chronic periontitis, Crohn's disease, hepatitis and nasal sinusitis. So that its expression needs to be controlled to overcome this disease. The aim of this study was to screen for TNF-alpha convertase (TACE) receptor inhibitors to reduce TNF-α expression. By decreasing TNF- expression, it can act as an anti-inflammatory or immunosuppressant. One of the plants that can be used for this screening is A. excels. The method used for screening is through PASSonline and Docking with PLANTS and seen the prediction of entering the blood circulation with SWISSADME. Based on PASSonline Compounds that have a high probability of immunosuppressant activity score are batulinic acid (0.724), alphitolic acid (0.763), cis-coumaroyl alphitolic acid (0.771). Meanwhile, those with anti-inflammatory probability activity were batulinic acid (0.741) and cis-coumaroyl alphitolic acid (0.783). Based on the stability of the interaction, compounds that have a minimum ability of 80% against the reference ligand are alphitonin (98.25%), alphitexolide (92.33%), cis-coumaroyl alphitolic acid (98.31%). In conclusion, the compound that has the potential as an immunosuppressant, anti-inflammatory and has good interaction stability is cis-coumaroyl alphitolic acid and alphitonin.

Keywords: TNF-α, A.excels, interaction. interaction