AMINASI SENYAWA EUGENOL DAN AKTIVITAS INHIBISINYA TERHADAP *α*-AMILASE SEBAGAI KANDIDAT OBAT ANTIDIABETES

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INTISARI

Sintesis dan simulasi penambatan molekular senyawa turunan eugenol teraminasi dengan prekursor 2-((4-alil-2-metoksifenosi)metil)oksiran serta uji aktivitas inhibisinya terhadap enzim α-amilase telah dilakukan. Simulasi penambatan molekular dilakukan dengan menggunakan makromolekul enzim α-amilase dengan kode file PDB 4gqr. Nilai energi ikat senyawa prekursor, A, B dan C berturut-turut yaitu -4,24; -4,54; -5,39; dan -5,03 kkal/mol. Sintesis senyawa prekursor dilakukan dengan mereaksikan senyawa eugenol dan epiklorohidrin dengan katalis basa NaOH. Sintesis senyawa A (*1-(4-allyl-2-methoxyphenoxy)-3-(phenylamino), propan-2-ol*) dilakukan dengan mereaksikan senyawa prekursor dengan senyawa anilin. Sintesis senyawa B (*1-(4-allyl-2-methoxyphenoxy)-3-(m-tolylamino)propan-2-ol*) dilakukan dengan mereaksikan senyawa prekursor dengan senyawa m-toluidina dan sintesis senyawa C (*1-(4-allyl-2-methoxyphenoxy)-3-((4-chlorophenyl)amino)propan-2-ol*) dilakukan dengan mereaksikan senyawa prekursor dengan 4-kloroanilina. Ketiga senyawa A, B dan C disintesis dengan metode sonokimia dengan katalis basa K_2CO_3.

Produk hasil sintesis dianalisis strukturnya menggunakan spektrometer FTIR, GC/MS, DI/MS, LCMS/MS, TLC *Scanner*, ^{1}H-NMRdan ^{13}C-NMR. Sintesis senyawa prekursor, A, B dan C masing-masing menghasilkan rendemen sebesar 70,48; 88,35; 86,97 dan 93,02%. Uji aktivitas inhibisi menunjukkan empat senyawa turunan eugenol hasil sintesis memiliki aktivitas inhibisi lebih tinggi dari pada akarbosa, dimana senyawa B > C > Prekursor > A.

Kata kunci: turunan eugenol, enzim α-amilase, penambatan molekuler

AMINATION OF EUGENOL AND THEIR INHIBITORY ACTIVITY AGAINST α-AMYLASE AS ANTIDIABETIC DRUG CANDIDATE

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ABSTRACT

Synthesis and molecular docking simulation of the aminated eugenol derivative compounds from 2-((4-allyl-2-methoxyphenoxy)methyl)oxirane and inhibitory activity assay against α-amylase have been carried out. Molecular docking simulations were carried out using macromolecular enzyme α-amylase with 4gqr as the identity of the PDB file. The binding energy values of the basic precursor, compounds A, B, and C were -4.24, -4.54, -5.39, and -5.03 kcal/mol. Synthesis of precursor compound was carried out by reacting eugenol and epichlorohydrin with NaOH as a base catalyst. The synthesis of compound A 1-(4-allyl-2-methoxyphenoxy)-3-(phenylamino)propan-2-ol) was carried out by reacting precursor with aniline compound. Synthesis of compound B (1-(4-allyl-2-methoxyphenoxy)-3-(m-tolylamino)propan-2-ol) was conducted by reacting precursor with *m*-toluidine and synthesis of compound C (1-(4-allyl)-2-methoxyphenoxy)-3-((4-chlorophenyl)amino)propan-2-ol) was carried out by reacting the precursor compound with 4-chloroaniline. These compounds A, B, and C were synthesized through the sonochemical method using K_2CO_3 as a base catalyst.

The synthesized products were analyzed using FTIR, GC/MS, DI/MS, LCMS/MS, TLC Scanner, ^{1}H-NMR and ^{13}C-NMR spectrometers. Precursor, A, B, and C compunds produced 70.48, 88.35, 86.97, and 93.02% yield. Inhibition activity test showed that four compounds derived from eugenol had higher inhibitory activity than acarbose, where compound B > C > Precursor > A.

Key words: eugenol derivatives, α-amylase enzyme, molecular docking