SINTESIS SENYAWA KALKON DAN ISOKSAZOLA SERTA STUDI *IN SILICO*-NYA SEBAGAI KANDIDAT INHIBITOR PROTEIN HER2 DAN ALFA AMILASE

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INTISARI

Penelitian ini dilakukan untuk mensintesis senyawa kalkon dan isoksazola dari 4-dimetilamino benzaldehida dan 4-metoksiasetofen. Senyawa hasil sintesis kemudian dievaluasi sebagai kandidat inhibitor protein HER2 dan enzim α-amilase melalui penambatan molekul.

Senyawa kalkon disintesis melalui reaksi kondensasi *Claisen-Schmidt* dengan metode pengadukan dan sonikasi menggunakan 4-dimetilamino benzaldehida dan 4-metoksiasetofenon. Reaksi dilakukan dalam pelarut etanol dengan adanya katalis NaOH 30%, kemudian produk kalkon dielusidasi strukturnya dengan instrumentasi FT-IR, GC-MS, ^{1}H- dan ^{13}C-NMR. Selanjutnya kalkon disiklisasi menggunakan hidroksilamina hidroklorida dalam pelarut metanol menggunakan katalis CH_3COONa dan reaksi ini juga dilakukan dengan metode refluks dan sonikasi. Produk isoksazola dikarakterisasi menggunakan spektrometer FT-IR dan GC-MS. Tahap akhir dilakukan penambatan molekul kalkon dan isoksazola dengan protein HER2 dan enzim α-amilase untuk menguji aktivitasnya sebagai senyawa inhibitor.

Sintesis kalkon menghasilkan padatan kuning terang dengan persen hasil 71,17% dan titik leleh 123-126 °C untuk metode pengadukan, sedangkan metode sonikasi memberikan persen hasil 56,90% dengan titik leleh 125-128 °C. Sintesis isoksazola dengan metode refluks menghasilkan padatan kuning pucat dengan persen hasil 24,71% dan titik leleh 185 °C, sedangkan metode sonikasi memberikan padatan kuning terang dengan persen hasil 8,36% dan titik leleh 175-176,6 °C. Hasil penambatan molekul pada protein HER2, menunjukkan bahwa senyawa isoksazola lebih berpotensi dalam menghambat protein HER2. Sementara pada enzim α-amilase, senyawa kalkon lebih berpotensi menghambat enzim tersebut daripada senyawa isoksazola.

Kata kunci: α-amilase, HER2, isoksazola, kalkon, penambatan molekul.

SYNTHESIS OF CHALCONE AND ISOXAZOLE COMPOUNDS AND THEIR *IN SILICO* STUDIES AS CANDIDATES INHIBITORS OF PROTEIN HER2 AND ALPHA AMYLASE

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ABSTRACT

This study was conducted to synthesize chalcone and isoxazole from 4-dimethylamino benzaldehyde and 4-methoxyacetophenone. The synthesized compounds were then evaluated as inhibitor candidates for protein HER2 and α-amylase enzyme through molecular docking assays.

Chalcone was synthesized via Claisen-Schmidt condensation with stirring and sonication methods using 4-dimethylamino benzaldehyde and 4-methoxyacetophenone. The reaction was carried out in ethanol in the presence of 30% NaOH catalyst, and then the product was elucidated utilizing FT-IR, GC-MS, ^{1}H-, and ^{13}C-NMR instrumentation. Furthermore, the chalcone was cyclized using hydroxylamine hydrochloride in methanol with CH_3COONa as a catalyst, and this reaction was also carried out by reflux and sonication methods. Isoxazole products were characterized using FT-IR and GC-MS spectrometers. The final step is molecular dockings of chalcones and isoxazole with protein HER2 and α-amylase enzyme to test their activity as inhibitory compounds.

The chalcone synthesis produced a bright yellow solid with a yield of 71.17% and a melting point of 123-126 °C for the stirring method, while the sonication method gave a yield of 59.60% with a melting point of 125-128 °C. Synthesis of isoxazole under reflux yielded a pale-yellow solid in 24.71% and a melting point of 185 °C, while sonication method gave a bright yellow solid in 8.36% yield with a melting point of 175-176.6 °C. The molecular docking of HER2 protein showed that isoxazole is more potent in inhibiting the HER2 protein. Meanwhile, for α-amylase enzyme, the chalcone is more potential to inhibit the enzyme than the isoxazole compound.

Keywords: α-amylase, chalcone, HER2, isoxazole, molecular docking.