

Identifikasi Senyawa dengan Aktivitas Antidiabetes dari Fraksi Etil Asetat Ekstrak Etanol Daun Yakon (*Smallanthus sonchifolius*) secara *in vitro* dan *in silico*

INTISARI

Yakon (*Smallanthus sonchifolius*) secara empiris dimanfaatkan sebagai obat tradisional untuk penderita diabetes melitus. Tujuan dari penelitian ini adalah untuk melakukan isolasi serta identifikasi senyawa dari fraksi semipolar daun yakon, serta pengujian aktivitas secara *in vitro* dan *in silico*. Metode penelitian berdasarkan pendekatan fitokimia dimulai dari proses ekstraksi, fraksinasi, serta isolasi. Hasil isolat akan diidentifikasi dengan GC-MS dan spektrofotometri infrared. Molekul hasil identifikasi diuji secara *in silico* dan *in vitro* terhadap penghambatan enzim alfa glukosidase. Analisis statistik dengan uji T berpasangan untuk melihat perbedaan antara skor doking molekul dengan pembanding. Hasil isolasi memperoleh satu isolat dominan, yaitu isolat H. Hasil identifikasi dengan spektrofotometri inframerah dan GC-MS memperoleh senyawa paling dominan, yaitu *phthalic acid, di(2-propylpentyl) ester*. Pengujian kadar total fenolik dan flavonoid paling tinggi ditemukan pada fraksi etil asetat, yaitu 15,407 GAC/gram dan 18,447 QE/gram. Pengamatan interaksi ligand-reseptor dari molekul uji dengan *molecular docking* menunjukkan interaksi yang kurang stabil dengan reseptor alfa glukosidase dengan *score docking* -61,605 dibandingkan ligan asli -77,124. Namun, saat ditambahkan pada reseptor *dipeptidyl peptidase-4* memberikan interaksi yang lebih stabil dengan *score docking* -86,945 jika dibanding dengan ligan asli dengan skor -75,048. Pengujian hasil isolasi secara *in vitro* terhadap penghambatan enzim alfa glukosidase memperoleh nilai IC₅₀ sebesar 130,479 ppm. Hasil pengujian secara *in silico* dan *in vitro* menunjukkan bahwa senyawa hasil isolasi memiliki aktivitas kurang baik sebagai penghambat enzim alfa glukosidase.

Kata kunci : Yakon (*S. sonchifolius*), alfa glukosidase, *molecular docking*

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Identification Of Compounds With Antidiabetic Activity From The Ethyl Acetate Fraction Of Yacon (*Smallanthus Sonchifolius*) Leaves By In Vitro And In Silico Approach

ABSTRACT

Yacon (*Smallanthus sonchifolius*) is empirically used as a traditional medicine for people with diabetes mellitus. The purpose of this study was to isolate and identify compounds from the semipolar fraction of yacone leaves, as well as test their activity *in vitro* and *in silico*. The research method is based on a phytochemical approach starting from the process of extraction, fractionation, and isolation. The isolates will be identified by GC-MS and infrared spectrophotometry. The identified molecules were tested *in silico* and *in vitro* against the inhibition of the alpha-glucosidase enzyme. Statistical analysis with paired t test to see the difference between the molecular docking score and the comparison. Isolation results yielded one dominant isolate, namely isolate H. Identification results by infrared spectrophotometry and GC-MS obtained the most dominant compound, namely phthalic acid, di(2-propylpentyl) ester. The highest total phenolic and flavonoid levels were found in the ethyl acetate fraction, namely 15.407 GAC/gram and 18.447 QE/gram. Observation of the ligand-receptor interaction of the test molecule by molecular docking showed a less stable interaction with the alpha-glucosidase receptor with a docking score of -61.605 compared to the original ligand -77.124. However, when tethered to the dipeptidyl peptidase-4 receptor, it provides a more stable interaction with a docking score of -86.945 when compared to the original ligand with a score of -75.048. Testing the results of the isolation *in vitro* for the inhibition of the alpha-glucosidase enzyme obtained an IC₅₀ value of 130.479 ppm. The results of *in silico* and *in vitro* tests showed that the isolated compound had poor activity as an alpha-glucosidase enzyme inhibitor.

Keywords : Yacon (*S. sonchifolius*), alpha glucosidase, molecular docking