

STUDI PROFIL METABOLIT DAN UJI AKTIVITAS INHIBISI ENZIM α - GLUKOSIDASE FRAKSI HEMWAT DAUN JOMBANG (*Taraxacum officinale* F.H Wigg)

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ABSTRAK

Latar Belakang: Bahan alam menjadi alternatif terapi diabetes, salah satunya daun jombang (*Taraxacum officinale* F.H. Wigg.) yang diketahui mengandung flavonoid, fenol, terpenoid, dan alkaloid. Namun, studi mengenai profil metabolit dan aktivitas inhibisinya terhadap enzim α -glukosidase masih terbatas.

Tujuan: Mengetahui profil metabolit sekunder ekstrak dan fraksi daun jombang serta aktivitas inhibisi enzim α -glukosidase secara *in vitro* dan *in silico*.

Metode: Daun jombang diekstraksi menggunakan etanol dan difraksinasi dengan sistem pelarut HEMWat untuk memperoleh fraksi polar dan nonpolar. Kedua fraksi dianalisis menggunakan LC-HRMS untuk mengidentifikasi senyawa metabolit. Senyawa yang teridentifikasi diseleksi berdasarkan ketersediaan struktur 2D dan klasifikasi senyawa, kemudian dievaluasi secara *in silico* menggunakan Lipinski's Rule of Five, BOILED-Egg, molecular docking, dan visualisasi interaksi molekuler. Aktivitas penghambatan terhadap enzim α -glukosidase selanjutnya diuji secara *in vitro* melalui penentuan nilai IC_{50} .

Hasil: Analisis LC-HRMS menghasilkan 278 data metabolit dari fraksi polar dan non-polar. Setelah proses seleksi, 112 senyawa memenuhi kriteria untuk dilakukan analisis *in silico*. Hasil *molecular docking* menunjukkan bahwa 2-monolinolenin memiliki afinitas pengikatan terbaik terhadap enzim α -glukosidase. Fraksi polar dan non-polar menunjukkan aktivitas inhibisi terhadap enzim α -glukosidase dengan nilai IC_{50} masing-masing 5524 ppm dan 10533 ppm, sedangkan akar bosa sebesar 0,197 ppm. Fraksi polar menunjukkan aktivitas inhibisi yang lebih baik dibandingkan fraksi non-polar.

Kesimpulan: Fraksi polar dan non-polar HEMWat daun jombang berpotensi sebagai inhibitor enzim α -glukosidase, dengan fraksi polar menunjukkan aktivitas yang lebih baik.

Kata kunci: Diabetes melitus, *Taraxacum officinale*, enzim α -glukosidase.

**Study of Metabolite Profile and α -Glucosidase Enzyme Inhibition Activity
Test of HEMWAT Fraction from Dandelion (*Taraxacum officinale* F.H.
Wigg) Leaves**

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ABSTRACT

Background: Natural products have become an alternative therapy for diabetes mellitus, one of which is dandelion leaf (*Taraxacum officinale* F.H. Wigg.), which is known to contain flavonoids, phenols, terpenoids, and alkaloids. However, studies on the metabolite profile and its inhibitory activity against α -glucosidase enzyme remain limited.

Objective: To determine the secondary metabolite profile of dandelion leaf extract and fractions, and to evaluate their α -glucosidase enzyme inhibitory activity in vitro and in silico.

Methods: Dandelion leaves were extracted using ethanol and fractionated using the HEMWat solvent system to obtain polar and non-polar fractions. Both fractions were analyzed using LC-HRMS to identify metabolite compounds. The identified compounds were selected based on the availability of 2D structures and compound classification, then evaluated in silico using Lipinski's Rule of Five, BOILED-Egg, molecular docking, and molecular interaction visualization. The inhibitory activity against the α -glucosidase enzyme was subsequently tested in vitro by determining the IC₅₀ value.

Results: Results: LC-HRMS analysis yielded 278 metabolite data from the polar and non-polar fractions. Following a selection process, 112 compounds met the criteria for in silico analysis. Molecular docking results revealed that 2-monolinolenin exhibited the highest binding affinity toward α -glucosidase enzyme. The polar and non-polar fractions demonstrated inhibitory activity against α -glucosidase enzyme, with IC₅₀ values of 5524 ppm and 10533 ppm, respectively, while acarbose showed an IC₅₀ of 0,197 ppm. The polar fraction exhibited superior inhibitory activity compared to the non-polar fraction.

Conclusion: The HEMWat polar and non-polar fractions of dandelion leaf show potential as α -glucosidase enzyme inhibitors, with the polar fraction demonstrating superior activity.

Keyword: Diabetes mellitus, *Taraxacum officinale*, α -glucosidase enzyme