

STUDI PROFIL METABOLIT DAN UJI AKTIVITAS INHIBISI ENZIM α -GLUKOSIDASE FRAKSI HEMWAT DAUN SENDOK (*Plantago major* L.)

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ABSTRAK

Latar Belakang : Daun sendok (*Plantago major* L.) berpotensi sebagai antidiabetes melalui penghambatan enzim α -glukosidase, namun identifikasi senyawa aktif serta validasinya secara *in silico* dan *in vitro* masih terbatas.

Tujuan : Mengidentifikasi profil senyawa pada fraksi polar dan nonpolar hasil fraksinasi HEMWat daun sendok menggunakan LC-HRMS, mengkaji potensi senyawa tersebut sebagai inhibitor α -glukosidase secara *in silico*, serta mengevaluasi aktivitas penghambatannya secara *in vitro*.

Metode : Simplisia daun sendok diekstraksi dengan maserasi menggunakan etanol 96% dan difraksinasi menggunakan sistem pelarut HEMWat untuk memperoleh fraksi polar dan nonpolar. Kedua fraksi dianalisis menggunakan LC-HRMS, dilanjutkan dengan kajian *in silico* melalui analisis profil farmakokinetik dan *molecular docking*, serta pengujian aktivitas penghambatan enzim α -glukosidase secara *in vitro* dengan penentuan nilai IC_{50} .

Hasil : Analisis LC-HRMS mengidentifikasi 176 senyawa pada fraksi polar dan 112 senyawa pada fraksi nonpolar. Sebanyak 73 senyawa memenuhi kriteria untuk *molecular docking*. Tiga senyawa dengan afinitas terbaik, yaitu 1-Stearoylglycerol, (8E)-2-Amino-8-octadecene-1,3,4-triol, dan 2-Amino-1,3,4-octadecanetriol, memenuhi kriteria profil farmakokinetik. Fraksi polar menunjukkan aktivitas penghambatan α -glukosidase yang lebih baik (IC_{50} 11,865 ppm) dibandingkan fraksi nonpolar (IC_{50} 15,899 ppm).

Kesimpulan : Analisis LC-HRMS berhasil mengidentifikasi profil senyawa pada fraksi polar dan nonpolar daun sendok (*Plantago major* L.). Tiga senyawa menunjukkan potensi terbaik berdasarkan hasil *molecular docking* dan memenuhi kriteria profil farmakokinetik, sedangkan fraksi polar memiliki aktivitas penghambatan enzim α -glukosidase yang lebih baik berdasarkan nilai IC_{50} dibandingkan fraksi nonpolar.

Kata Kunci : *Plantago major* L., LC-HRMS, fraksinasi HEMWat, α -glukosidase, *molecular docking*, *in vitro*

METABOLITE PROFILING AND α -GLUCOSIDASE INHIBITORY ACTIVITY OF HEMWAT FRACTIONS FROM PLANTAIN LEAVES (*Plantago major* L.)

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ABSTRACT

Background: *Plantago major* L. has potential as an antidiabetic agent through α -glucosidase inhibition. However, information regarding its active compounds and their validation through *in silico* and *in vitro* approaches remains limited.

Objective: To identify the compound profile of the polar and nonpolar fractions obtained from HEMWat fractionation of *Plantago major* L. using LC-HRMS, evaluate the potential of the identified compounds as α -glucosidase inhibitors through *in silico* analysis, and assess their α -glucosidase inhibitory activity through *in vitro* assays.

Methods: *Plantago major* L. leaf simplicia was extracted by maceration using 96% ethanol and fractionated using the HEMWat solvent system to obtain polar and nonpolar fractions. Both fractions were analyzed using LC-HRMS, followed by *in silico* evaluation through pharmacokinetic profiling and molecular docking. The α -glucosidase inhibitory activity of each fraction was further evaluated *in vitro* by determining the IC₅₀ value.

Results: LC-HRMS analysis identified 176 compounds in the polar fraction and 112 compounds in the nonpolar fraction. A total of 73 compounds met the criteria for molecular docking analysis. Three compounds, namely 1-Stearoylglycerol, (8E)-2-Amino-8-octadecene-1,3,4-triol, and 2-Amino-1,3,4-octadecanetriol, showed the highest binding affinity and fulfilled the pharmacokinetic profile criteria. The polar fraction exhibited stronger α -glucosidase inhibitory activity (IC₅₀ = 11.865 ppm) than the nonpolar fraction (IC₅₀ = 15.899 ppm).

Conclusion: LC-HRMS successfully identified the compound profiles of the polar and nonpolar fractions of *Plantago major* L. Three compounds demonstrated the greatest potential as α -glucosidase inhibitors based on molecular docking and favorable pharmacokinetic profiles, while the polar fraction exhibited stronger α -glucosidase inhibitory activity than the nonpolar fraction based on the IC₅₀ value.

Keywords: *Plantago major* L., LC-HRMS, HEMWat fractionation, α -glucosidase, molecular docking, *in vitro*.