STUDI PROFIL METABOLIT DAN *VIRTUAL SCREENING* EKSUDAT TANAMAN MANGROVE (*Avicennia marina* (Forsk.) Vierh.) SEBAGAI AGEN PENGHAMBAT ENZIM α-AMILASE

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ABSTRAK

Latar Belakang: *Avicennia marina* diketahui berpotensi sebagai terapi diabetes, tetapi penelitian terdahulu berfokus pada bagian daun. Penelitian lain telah dilakukan terhadap kulit kayu spesies *Avicennia* lain (*A. officinalis*) yang berpotensi menghambat α-amilase. Namun, belum ada penelitian mengenai eksudat *A. marina* sebagai inhibitor α-amilase.
Tujuan: Mengetahui potensi fraksi HEMWat eksudat *Avicennia marina* sebagai inhibitor α-amilase secara *in vitro*, mengidentifikasi senyawa utamanya menggunakan LC-HRMS, serta mengetahui kandidat senyawa inhibitor α-amilase melalui *virtual screening.*
Metode: Eksudat *Avicennia marina* diekstraksi infundasi, difraksinasi 5 komposisi pelarut HEMWat (n-heksana, etil asetat, metanol, air). Fraksi dengan profil pemisahan KLT terbaik digunakan untuk uji inhibisi α-amilase dan analisis LC-HRMS. Senyawa teridentifikasi diuji farmakokinetik (Lipinski's *Rule of Five* dan BOILED-Egg Plot), dan dilanjutkan *molecular docking.*
Hasil: Fraksi HEMWat eksudat *Avicennia marina* menunjukkan inihibisi enzim α-amilase yang rendah (IC_{50} polar 7536,84 ppm; IC_{50} nonpolar 2001,11 ppm), sementara akarbosa 5,095 ppm. LC-HRMS mengidentifikasi 228 senyawa, didominasi senyawa fenolik. Senyawa utamanya 6-[(1E)-3,4-dihydroxy-3-methyl-1-buten-1-yl]-7-methoxy-2H-chromen-2-one (17,57%; polar) dan Karwinaphthol B (16,03%; nonpolar). *Virtual screening* menunjukkan L-α-Palmitin (-95,943) sebagai kandidat terbaik inhibitor α-amilase (berinteraksi dengan Asp197, Asp300, Glu233).
Kesimpulan: Fraksi HEMWat eksudat *Avicennia marina* berpotensi sebagai sumber senyawa kandidat inhibitor α-amilase.

Kata Kunci: α-amilase, diabetes melitus tipe 2, eksudat *Avicennia marina,* studi profil metabolit, *virtual screening*

METABOLITE PROFILING AND VIRTUAL SCREENING OF MANGROVE (*Avicennia marina* (Forsk.) Vierh.) EXUDATE AS AN α-AMYLASE INHIBITORY AGENT

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ABSTRACT

Background: *Avicennia marina* reported to have potential as diabetes therapy agent, but previous studies mainly focused on its leaves. *Avicennia officinalis* bark has shown α-amylase inhibitory activity. However, no study has investigated *A. marina* exudate as an α-amylase inhibitor.
Objective: To determine the potential of HEMWat fractions of *A. marina* exudate as α-amylase inhibitors in vitro, identify major compounds using LC-HRMS, and determine best candidates through virtual screening.
Methods: *A. marina* exudate extracted by infusion and fractionated with five HEMWat solvent compositions (n-hexane, ethyl acetate, methanol, water). Fraction with best TLC profiles underwent α-amylase inhibition assay and LC-HRMS analysis. Compounds were evaluated for pharmacokinetic (Lipinski's *Rule of Five* and BOILED-Egg Plot), followed by molecular docking.
Results: HEMWat fractions of *Avicennia marina* showed low α-amylase inhibitory activity, IC_{50} values of 7536.84 ppm (polar) and 2001.11 ppm (nonpolar), compared to 5.095 ppm for acarbose. LC-HRMS identified 228 compounds, predominantly phenolics. The major compound were 6-[(1E)-3,4-dihydroxy-3-methyl-1-buten-1-yl]-7-methoxy-2H-chromen-2-one (17.57%; polar) and Karwinaphthol B (16.03%; nonpolar). Virtual screening identified L-α-Palmitin as the best candidate (-95.943), interacting with Asp197, Asp300, Glu233.
Conclusion: HEMWat fractions of *Avicennia marina* exudate may serve as α-amylase inhibitor candidates.

Keywords: α-amylase, *Avicennia marina* exudate, metabolite profiling, type 2 diabetes mellitus, virtual screening