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In Vitro and In Silico Screening Analysis of Artabotrys sumatranus Leaf and Twig Extracts for α -Glucosidase Inhibition Activity and Its Relationship with Antioxidant Activity

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Abstract

Artabotrys sumatranus is one of the *Artabotrys* species, which lives in Sumatera, Java, and Borneo in Indonesia. No research has been found related to its activity. The objective of this study was to explore the potential of *A. sumatranus* leaf and twig extracts as the source of an anti-diabetic agent through the α -glucosidase inhibition mechanism, as well as the relationship between the antioxidant and the α -glucosidase inhibition activities in these extracts. Ethanol extracts from leaf and twig *A. sumatranus* were subjected to several assays: total phenolic content, total flavonoid content, antioxidant activity using DPPH (2,2-diphenyl-1-picrylhydrazyl), radical scavenging activity, and FRAP (ferric reducing antioxidant power) analysis, as well as α -glucosidase inhibition. Later, GC-MS (gas chromatography-mass spectrometer) and LC-MS/MS (liquid chromatography-mass spectrometer/mass spectrometer) analysis were conducted to identify the compounds inside the extracts. The identified compounds were tested for potential α -glucosidase inhibition activity using a molecular docking simulation. As a result, the *A. sumatranus* leaf extract showed more potential than the twig extract as α -glucosidase inhibitor and antioxidant agent. In addition, from the comparison between the measured quantities, it can be deduced that most of the α -glucosidase active compounds in the *A. sumatranus* are also antioxidant agents. Several active compounds with a high affinity to α -glucosidase inhibition were identified using the molecular docking simulation. It was concluded that *A. sumatranus* twig and leaf extracts seem to be potential sources of α -glucosidase inhibitors. © 2022 by the authors.

Author Keywords

antidiabetic; antioxidant; *Artabotrys sumatranus*; leaf extract; twig extract

Index Keywords

alpha glucosidase inhibitor, antidiabetic agent, antioxidant, *Artabotrys sumatranus* leaf extract, flavonoid, phenol derivative, plant extract, unclassified drug; antioxidant activity, *Artabotrys sumatranus*, Article, computer model, DPPH radical scavenging assay, enzyme inhibition assay, ferric reducing antioxidant power, in vitro study, inhibition constant, mass fragmentography, medicinal plant, molecular docking, molecular dynamics, simulation, twig

Tradenames

Agilent 7890B, Agilent

Manufacturers

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