Unraveling Potential Compounds of Uncaria gambir (W.Hunter) Roxb. as Antikeloid Agent: In Silico, In Vitro and Ex Vivo Experimental Validation

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Abstract

Background/Objectives: Keloid treatment remains challenging due to limited effectiveness and patient dissatisfaction. Herbal-based therapy offers promising alternatives that require further investigation. Uncaria gambir (W.Hunter) Roxb., an original plant from Indonesia, possesses an antifibrotic effect. However, its potential as an antifibrotic agent in keloid management remains unclear. This study aims to bridge this gap by evaluating the bioactive compound from gambir and its effects on keloid fibroblast primary culture. Methods: The bioactive compounds of gambir extract and fractions (ethanol, hexane, and ethyl acetate fractions) were identified by using liquid chromatography–mass spectrometry (LCMS/MS) analysis. The mechanism of gambir bioactive

compounds for keloid was predicted using the compound–protein interaction network and enrichment analysis, and validated using molecular docking and dynamic simulation. The experimental study results, including cytotoxic and bioactivity effects, were represented as IC_{50} and selectivity index (SI) values, and the ex vivo analysis of keloid tissue explants. Results: Uncariagambiriine was identified as the most potent compound with the lowest binding energy and high stability to the core protein targets: AKT1 and TGFB1. The ethanol fraction was determined to have the highest abundance of gambir's typical bioactive compounds, with the lowest IC_{50} (128.76 ± 0.24 µg/mL) and the highest SI (6.32) value. Furthermore, the results of the ex vivo analysis indicated the significant inhibition of keloid fibroblast proliferation and migration by the gambir ethanolic fraction. Conclusions: This study underlines the potential of the gambir ethanolic fraction as an antifibrotic agent in keloid, warranting further investigation and development for clinical applications. © 2025 by the authors.

Author keywords

bioactive compounds; bioactivity; gambir; keloid

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Abstract

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