Inflammatory Studies of Dehydroandrographolide: Isolation, Spectroscopy, Biological Activity, and Theoretical Modeling

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Abstract

Dehydroandrographolide (DA) was isolated and experimentally characterized utilizing FT-IR, UV-Vis, and NMR spectroscopy techniques along with detailed theoretical modelled at the DFT/B3LYP-D3BJ/6-311 + + G(d,p) level of theory. Substantially, molecular electronic property investigations in the gaseous phase alongside five different solvents (ethanol, methanol, water, acetonitrile and DMSO) were comprehensively reported and compared with the experimental results. The globally harmonized scale (GHS), which is used to identify and label chemicals, was also utilized to demonstrate that the lead compound predicted an LD50 of 1190 mg/kg. This finding implies that consumers can safely consume the lead molecule. Notable impacts on hepatotoxicity, cytotoxicity, mutagenicity, and carcinogenicity were likewise found to be minimal to nonexistent for the compound. Additionally, in order to account for the biological performance of the studied compound, *in-silico* molecular docking simulation analysis was examined against different anti-inflammatory target of enzymes (3PGH, 4COX, and 6COX). From the examination, it can be inferred that DA@3PGH, DA@4COX, and DA@6COX, respectively, showed significant negative binding affinities of -7.2 kcal/mol, -8.0 kcal/mol, and − 6.9 kcal/mol. Thus, the high mean binding affinity in contrast to conventional drugs further reinforces these results as an anti-inflammatory agent.

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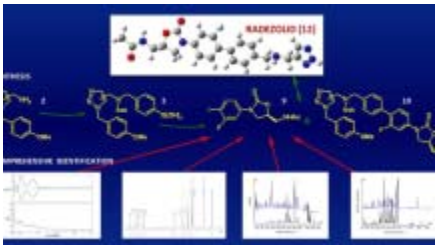

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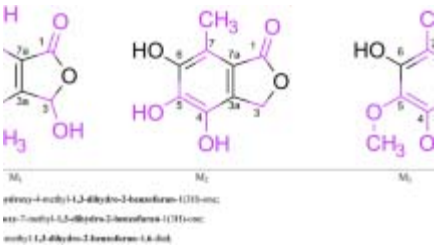

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Data Availability

All data generated or analyzed during this study are included within the article.

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Contributions

H.L. conceptualized, designed, and supervised the study. Resources validation and results analysis were performed by **L.L.**, **W.E.**, **C.C.** The first draft of the manuscript was written by **B.B.I.**, **I.B.**, **E.F.A.** and **A.E.M.;** and all authors commented on successive versions of the manuscript. All authors read and approved the final manuscript.

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Competing Interests

Authors declare no competing financial or interpersonal interests.

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Consent to Participate

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