

ABSTRACT 02

Network Pharmacology and Molecular Docking-Based Study on The Anti-Inflammatory and Antioxidant Mechanisms of Morindolide

Muhammad Amal Zulkipli¹, Yuslina Zakaria², Elhassane Anouar³, Mizaton Hazizul Hasan¹

Objective: Inflammation-related disorders, which cause much worldwide mortality, can be mitigated using network pharmacology. Network pharmacology may facilitate targeted therapy design and improve therapeutic results by finding drug- target interactions and signalling pathways. Previous studies suggest morindolide has anti-inflammatory and antioxidant properties. Thus, this study used network pharmacology and molecular docking to identify the mechanisms of these effects. **Methods:** Morindolide's target genes were identified using SymMap, Swiss Target Prediction and PharmMapper databases. Anti-inflammatory and antioxidant-related genes were retrieved from the GeneCards database. Common targets were identified through Venn analysis. A protein-protein interaction (PPI) network was constructed using STRING and Cytoscape to identify hub genes. GO function and KEGG pathway analyses were performed using DAVID and ShinyGO. Molecular docking between morindolide and hub proteins was conducted using AutoDock and visualised with LigPlot. **Results:** The analysis revealed 56 common targets between morindolide and anti-inflammatory/antioxidant effects. Seven hub genes were identified as PTGS2, IL1B, MMP2, HSP90AA1, NOS2, PLA2GA and CYP2E1. GO analysis showed morindolide's involvement in inflammatory response, nitric oxide biosynthesis and response to lipopolysaccharide. KEGG analysis highlighted pathways in cancer, arachidonic acid metabolism, IL-17 signalling and neurodegeneration. Molecular docking confirmed stable binding between morindolide and hub proteins, with binding energies ranging from -5.19 to -6.62 kcal/mol. The strongest interactions were observed with CYP2E1 (-6.62 kcal/mol), MMP2 (-6.6 kcal/mol) and NOS2 (-6.24 kcal/mol). **Conclusion:** This study utilised network pharmacology and molecular docking to predict the potential targets, biological processes and signalling pathways involved in morindolide's anti-inflammatory and antioxidant effects, providing a theoretical foundation for future experimental research and potential clinical applications of morindolide.

Keywords: Anti-Inflammatory; Antioxidant; Molecular Docking; Morindolide; Network Pharmacology

1. Department of Pharmacology and Life Sciences, Faculty of Pharmacy, University Teknologi MARA, Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor, Malaysia.
2. Department of Pharmacy Practice and Clinical Pharmacy, Faculty of Pharmacy, University Teknologi MARA, Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor, Malaysia.
3. Department of Chemistry, Alkharj College of Science and Humanity Studies, Prince Sattam bin Abdulaziz University, Al-kharj 11942, Saudi Arabia

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Correspondence to: Mizaton Hazizul Hasan, Professor and Pharmacology Lecturer, Department of Pharmacology and Life Sciences, Faculty of Pharmacy, University Teknologi MARA, Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor, Malaysia. Email: mizaton_hazizul@uitm.edu.my