Junior Science Communications
Faculty of Applied Sciences, UiTM Shah Alam
https://journal.uitm.edu.my/ojs/index.php/JSC

E-ISSN 2637-0689
Vol 51 2025

Colloquium on Applied Sciences 1 2025
20-24 January 2025, Faculty of Applied Sciences, UiTM Shah Alam, Malaysia

Computational Docking-Based Investigation of *Garcinia mangostana* Bioactive Compounds as H1N1 Influenza A Virus Neuraminidase

Muhammad Daniel Amani Azhar[a], Mohamad Zakkirun Abdullah[b], Latifah Munirah Bakar[a*]

Structured Abstract

Background: The H1N1 influenza virus, responsible for global pandemics, remains a significant public health challenge due to its high transmissibility and frequent mutations that render many antiviral drugs less effective. Current treatments, such as neuraminidase inhibitors, face limitations including drug resistance and adverse side effects. *Garcinia mangostana* (mangosteen), a tropical fruit traditionally valued for its medicinal properties, contains bioactive compounds with potential antiviral, antioxidant, and anti-inflammatory activities. This study explores the molecular docking of *G. mangostana* phytochemicals to identify potent inhibitors of the H1N1 neuraminidase enzyme, aiming to provide a foundation for the development of safer, plant-based antiviral therapies.

Methods: Bioactive compounds from *G. mangostana* were sourced from public databases and prepared for docking by converting them into Protein Data Bank format. The target protein, neuraminidase, was prepared similarly, and its active site was defined using grid box parameters derived from known inhibitors, oseltamivir. Docking simulations were conducted using AutoDock Vina, which provided binding affinity scores and predicted interaction profiles. The results were further analyzed using visualization tools such as PyMol and Discovery Studio to elucidate the types and strengths of interactions.

Results: Trapezifolixanthone exhibited the highest binding affinity (-8.9 kcal/mol) among the tested compounds, forming multiple electrostatic interactions and a hydrogen bond with the neuraminidase active site. Epicatechin (-8.3 kcal/mol) and rubraxanthone (-8.1 kcal/mol) also demonstrated strong binding stability, supported by robust interaction networks. The visualization of 3D binding structures confirmed that these compounds fit snugly within the active site, maximizing favorable interactions. These results highlight the potential of these compounds to serve as effective neuraminidase inhibitors.

Conclusion: In conclusion, the study identifies trapezifolixanthone as the most promising inhibitor, with epicatechin and rubraxanthone as strong alternatives. These compounds' interactions with neuraminidase suggest their ability to disrupt the viral replication cycle, making them suitable candidates for further experimental validation. By leveraging the bioactive potential of *G. mangostana*, this research bridges traditional medicinal knowledge and modern drug discovery, paving the way for the development of novel and safer antiviral treatments for influenza and similar viral threats.

Keywords: H1N1, *Garcinia mangostana*, Neuraminidase, Bioactive Compounds, Inhibitor

***Correspondence:** latifahmunirah@uitm.edu.my

[a] School of Biology, Faculty of Applied Sciences, Universiti Teknologi MARA, Shah Alam, Malaysia

[b] Department of Fundamental Dental and Medical Sciences, Kulliyyah of Dentistry, International Islamic University Malaysia Kuantan Campus, 25200 Kuantan, Pahang, Malaysia