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Computational Analysis of *Curcuma aeruginosa* Bioactive Compounds for Their Potential to Inhibit H1N1 Influenza A Virus Neuraminidase

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Structured Abstract

Background: The H1N1 virus presents a significant public health threat in Malaysia because of its high morbidity and mortality rates. High mutation rates of the virus have increased the drug-resistant strains, causing the existing medication to be ineffective. The influenza H1N1 virus possesses two glycoproteins, hemagglutinin and neuraminidase, which play crucial roles in viral replication, making them key targets for antiviral strategies. Additionally, *Curcuma aeruginosa* from a *Zingiberaceae* family is known to be rich in bioactive compounds, making it a suitable candidate. The purpose of this study is to investigate the potential bioactive compounds from *C. aeruginosa* that are able to act as H1N1 influenza A virus neuraminidase inhibitors using molecular docking.

Methods: In this study, a computational docking method was employed to investigate the binding affinity and binding interactions between bioactive compounds from *Curcuma aeruginosa* and neuraminidase enzymes. More than forty bioactive compounds were selected from the PubChem database to be investigated. The selection of compounds was based on their reported biological activities relevant to *C. aeruginosa*, as reported in previous literature. The molecular docking was done using software tools such as AutoDock Vina, AutoDock Tools, PyMol, and DS Biovia 2024. Binding affinities and interactions between the bioactive compounds and neuraminidase enzymes were analyzed to assess their inhibitory potential.

Results: This study shows that several bioactive compounds from *Curcuma aeruginosa* have demonstrated strong binding affinities and favourable interactions with the binding site of neuraminidase enzymes. Among all the bioactive compounds, curcumin, zederone, zedoarol, and aerugidiol have exhibited the strongest binding affinity. The results were validated by a redocking process, which involves redocking known inhibitors to confirm the accuracy of binding site prediction. These findings suggest the potential inhibitory activity of the bioactive compounds, indicating their suitability as promising drug candidates.

Conclusion: In conclusion, the findings of this study indicate that the bioactive compounds from *Curcuma aeruginosa* exhibit promising activity as neuraminidase inhibitors. The identified compounds have provided a foundation for future *in vitro* and *in vivo* studies, contributing to the development of new antiviral drugs for H1N1 virus neuraminidase.

Keywords: H1N1 influenza A virus, neuraminidase, *Curcuma aeruginosa*, bioactive compounds, molecular docking

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