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In Silico Screening of *Zingiber officinale* Bioactive Compound For Their Inhibitory Potential Against H1N1 Influenza A Virus Neuraminidase

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Structured Abstract

Background: The H1N1 influenza A virus remains a significant global health threat, necessitating the search for effective antiviral agents. Current antiviral drugs, such as oseltamivir face challenges due to the emergence of resistant strains. Natural products offer a promising alternative. *Zingiber officinale* (ginger) has been recognized for its medicinal properties, including its potential antiviral effects. This study aims to explore the bioactive compounds in ginger as potential inhibitors of the neuraminidase enzyme of the H1N1 influenza A virus, utilizing molecular docking techniques to predict their interactions.

Methods: The methodology employed in this study involved a comprehensive approach to molecular docking, utilizing AutoDock Vina as the primary software for simulating the interactions between bioactive compounds from *Zingiber officinale* and the neuraminidase enzyme of the H1N1 influenza A virus. Initially, the ligand structures were prepared in PDBQT format, and the grid box dimensions were defined based on the known position of the original inhibitor, ensuring accurate docking simulations. Following the docking process, binding affinities were calculated indicating the strength of ligand binding. Post-docking analyses were conducted using PyMOL and Discovery Studio to visualize the binding interactions, highlighting key amino acid residues involved in stabilizing the ligand-protein complexes. This method revealed the specific molecular interactions enhancing our understanding in antiviral drug discovery.

Results: The docking analysis revealed that quercetin exhibited the highest binding affinity (-8.8 kcal/mol), primarily through electrostatic interactions with key amino acid residues. [6]-gingerol and [6]-shogaol also demonstrated significant binding affinities (-6.4 kcal/mol and -6.3 kcal/mol, respectively), indicating their potential as effective neuraminidase inhibitors. The study highlighted the critical role of specific interactions in stabilizing ligand binding, providing insights into the mechanism of action of these compounds.

Conclusion: This study successfully identified several ginger-derived phytochemicals as potential neuraminidase inhibitors. The findings support further experimental validation of quercetin, [6]-gingerol, and [6]-shogaol as promising candidates for the development of novel antiviral therapies against the H1N1 influenza A virus.

Keywords: H1N1, Zingiber officinale, neuraminidase, antiviral, phytochemicals.

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