

IN SILICO MOLECULAR DOCKING REVEALS THE ANTIVIRAL POTENCY OF MORINGYNE FROM *Moringa oleifera* AGAINST INFLUENZA A VIRUS BY TARGETING NEURAMINIDASE

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Avian influenza A virus (IAV) is an RNA virus that causes a zoonotic infection and is responsible for periodic outbreaks of influenza (flu) in humans and livestock. The neuraminidase (NA) enzyme of IAV is currently targeted for treatment with available synthetic NA antagonists, such as Oseltamivir and Zanamivir. Due to the high mutation rate of RNA viruses, effective treatment of the disease with current antiviral drugs is challenging, necessitating the discovery of new potential antiviral drug candidates for effective treatment of IAV. *Moringa oleifera* is a perennial plant abundant in regions of South Asia, Africa, and Central America. *Moringa oleifera* plant body contains numerous bioactive compounds that exhibit important properties, including anti-tumor, anti-oxidant, anti-microbial, and anti-diabetic, that have been identified in previous studies. This study identified Moringyne (PubChem: 131751186), a hexose found in *M. oleifera*, as a potential IAV NA antagonist through *in silico* molecular docking. The IAV NA (PDB: 3TI6)-ligand docking of the active site was performed using AutoDock Vina, and the NA-ligand interactions were compared with Oseltamivir and Zanamivir. The results revealed that, except for the ARG118, SER246, and GLU276 residues, the remaining 14 amino acids involved in the interaction with NA are similar for both Oseltamivir and Moringyne. Additionally, ARG292, ARG371, and ASP151 of NA formed strong hydrogen bonds in all three drugs: Oseltamivir, Zanamivir, and Moringyne. Furthermore, Moringyne showed a binding affinity (-7.4 kcal mol⁻¹) with NA IAV, which is closer to Zanamivir (-7.9 kcal mol⁻¹) and greater than Oseltamivir (-6.7 kcal mol⁻¹). In conclusion, Moringyne may effectively inhibit IAV NA activity, affecting NA-mediated progeny virus escape and may indicate an effective IAV inhibitor. Further, pharmaceutical efficacy and safety need to be validated *in vitro* and *in vivo*.

Keywords: *In Silico*, Influenza, *Moringa oleifera*, Moringyne, Neuraminidase