# In Silico Screening of Variola Major H1 Phosphatase Inhibitors: Exploring Moringa oleifera-Derived Compounds for the Development of Novel Smallpox Antivirals

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## Abstract:

This study investigates the antiviral potential of Moringa Oleifera, known for its therapeutic properties, by specifically targeting the smallpox virus. Bioactive compounds extracted from its leaves are being evaluated for their ability to inhibit the viral enzyme phosphatase H1, which plays a critical role in regulating the replication and maturation of the virus through protein dephosphorylation. Inhibition of this enzyme could disrupt the viral life cycle and reduce the ability of the virus to infect host cells. Molecular docking simulations were performed using Maestro software to evaluate the interactions between Moringa Oleifera compounds and phosphatase H1. Two precision methods, Standard Precision (SP) and Extra Precision (XP), were used to measure the binding affinity of these compounds with the enzyme's active site. The study identified four compounds-epicatechin, kaempferol, myricetin, and quercetin- that exhibit strong affinity and stable molecular interactions with phosphatase H1. These findings suggest that Moringa oleifera compounds may act as specific inhibitors of phosphatase H1, paving the way for developing novel natural antiviral treatments against pathogens such as the smallpox virus.

## Keywords:

Moringa oleifera, phosphatase H1, Smallpox Antivirals, Docking, ADMET, Docking, MD Simulation