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Molecular docking studies of hydroxylated stilbenes as new neuraminidase inhibitors

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Influenza is a global pandemic that has caused severe loss in human life. The annual and unpredictable influenza outbreaks are significantly the human health concern, due to the quick viral antigenic shift and anti-viral drug resistance. To date, only two over-the-counter drugs, Tamiflu® (the phosphate salt of oseltamivir ethyl ester) and Relenza® (zanamivir) are prescribed to inhibit the activity of neuraminidase to control influenza infection in human. Thus, the discovery and development of neuraminidase inhibitors has been paying attention to all pharmaceutical agencies to invent a novel effective drug to prevent the next worldwide influenza outbreak. Searching for the new potential neuraminidase inhibitors, we are interested in hydroxylated stilbenes and bibenzyl analogs which generally found as plant secondary metabolites. The molecular docking experiments are performed to demonstrate the biding activity between the virus neuraminidase structure and the interesting hydroxylated stilbenes and bibenzyl compounds. The computational simulations provide the interesting results and suggest the potential use of hydroxylated stilbenes as the new neuraminidase inhibitors.

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