

## **In silico design of novel, high-affinity neuraminidase inhibitors for Influenza A/H1N1/2009 Virus**

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Since March 2009, an outbreak of H1N1 influenza in Mexico has led to hundreds of confirmed cases and a number of deaths. Neuraminidase is one of the major surface glycoproteins of the influenza virus. This viral enzyme cleaves the terminal sialic acid from the cellular receptor, to which newly formed virions are attached. This cleavage releases the progeny virions from the infected cell, enabling them to infect other cells. By blocking this releasing mechanism, the virus completes replication only once, preventing further infection. Therefore, neuraminidase has been considered a suitable target for designing anti-influenza drugs, and structure-based design of neuraminidase inhibitors has become an important area of research that could potentially yield promising drug candidates. The neuraminidase of the influenza virus is the target of antiviral drugs oseltamivir and zanamivir. Clinical practices have shown that zanamivir and oseltamivir are effective in treating the Influenza A/H1N1/2009 virus. However, drug resistance strains are also emerging. The complex structure of Influenza A/H1N1/2009 neuraminidase and these antiviral drugs is not available yet. In the present study, we have built the Influenza A/H1N1/2009 structure model by homology modeling. 523,366 compounds from ZINC database have been screened by docking study. Finally by using molecular dynamics simulation we aimed to figure out potent candidates for Influenza A/H1N1/2009 flu virus.

### **Biography**

Dr Shailendra Saxena is a Medical Microbiologist at Centre for Cellular and Molecular Biology (CCMB) in India. His main research interest is to elucidate the molecular mechanisms of host defense during human viral infections. He has received many awards and honors including the Fogarty International Center, NIH (USA) MERIT Award, and named as "Global Leader in Science" by The Scientist magazine (USA) and "International Opinion Leader / Expert" involved in the vaccination for JE by IPIC (UK).

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