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Novel inhibitor by modifying oseltamivir based on neuraminidase structure for treating drugresistant H5N1 virus using molecular docking, NMR and DSC methods

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National Facility for High Field NMR, Tata Institute of Fundamental Research, India The danger of H5N1 influenza virus is not only its high fatality but also its resistance to commercially available drugs. The virus contains two surface glycoproteins, haemagglutinin (HA) and neuraminidase (NA). HA is responsible for the binding of the virus to the target cells via the sialic acid residue. NA catalyzes the removal of the terminal sialic acid. NA plays essential role in virus replication. Inhibiting NA can delay the release of progeny virus from infected cells, thereby suppressing the viral population. Therefore, NA has become the main target for drug design against influenza viruses. Most commonly used NA inhibitors currently in the market are oseltamivir and zanamivir. Due to mutations in the active site region NA becomes resistant to oseltamivir.

As a part of our ongoing program of developing novel influenza virus inhibitors, derivatives of oseltamivir were prepared by modifying the amino group. The interactions of these derivatives with neuraminidase have been probed by molecular modeling techniques. Further, the interaction of these derivatives and the effect on the thermotropic behaviour and polymorphism of the lipid bilayers has been investigated. Results indicate that the glycyl derivative of oseltamivir has the most profound effects on the membrane, compared to the other derivatives and seems to be the most promising derivative for further pharmacological evaluation as a neuraminidase inhibitor.

Biography

Dr Sudha Srivastava has done PhD in chemistry from Tata Institute of Fundamental Research, Mumbai and is presently Manager, National Facility for High Field NMR, at TIFR, Mumbai. She is Fellow, National Academy of Sciences. Her major research areas are: NMR studies on intact cells, membrane architecture, drug-design, drug-DNA interactions, conformation and dynamics of bioactive peptides, proteins and hormones. She has more than 130 research publications in refereed journals and is serving as an editorial board member of repute.