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Mutation in Active Site: Majaor Problem for Designing New Inhibitors for Swine Flu

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Swine flu is a contagious and acute respiratory which cause morbidity and mortality worldwide. This is due to classical influenza virus H1N1 strains which have known for its ability to mutate.Currently there are two classes of antivirals medicine for swine flu, amantadine and neuraminidase inhibitors. Due to highly mutation till now there is no any appropriate drug and vaccine also.The swine flu virus, however, typically affects the younger population, i.e. from 5 to 65 years.

Present study deals the drug against mutant protein in H1N1 flu. We can target thee surface protein Neuraminidase (NA), Hemagglutinin (HA) and M2-protein channel which present on virus cell and are responsible for the penetration in host cells.Among this Neuraminidase (NA) is good target for inhibitor. Oseltamivir is the main target for Neuraminidase (NA), but due to mutation in NA at position H274Y, N294S, E11V etc. it change the binding site in neuraminidase protein so that no any inhibitors bind to the active site and it result fully resistance towards any drug including oseltamivir. We make virtual library of FDA approved drug, derivative of oseltamivir,paper reviewed potent neuraminidase inhibitorscompound.

By help of various computational studies like virtual screening, docking studyand verification score we developed the potent inhibitors as lead compound against resistant protein neuraminidase which could be future drug for swine flu. In this research we develop the virtual library, screen the all ligands of virtual library and analysis the structure of potent inhibitors by the help of Structure Activity Relationship (SAR). In this research Ideveloped the lead compounds which are analogous of oseltamivir for the binding to resistant neuraminidase structure which may be action as the potent neuraminidase inhibitors.

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