ABSTRACT

THESIS: Computational Antiviral Drugs Design

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DATE: July, 2010

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This study designed and computational docked a group of ligands intended to find potent inhibitors for Neuraminidase 4 which would have strong interactions with 8 conserved amino acids in the active site.

Several trials of ligands were designed based on derivatives of neuraminic acid and evaluated as inhibitors of influenza neuraminidase. Optimized geometries of those ligands were determined using HF/B3LYP/6-311++G** techniques. Binding energies of the ligands bound to the N4 subtype of the neuraminidase protein were determined using AutoDock 4.0. Currently used inhibitors for influenza viruses will also be analyzed in the exactly same way. Comparing the binding information of those candidates and current ligands can provide a useful data about the potential of these species as antiviral drugs.