COMPUTATIONAL ANTIVIRAL DRUG DESIGN

The goal of this research is to identify a compound or family of compounds that would allow effective treatment of the influenza virus without unnecessary risks and side-effects. Influenza is a substantial problem in today's society. Each year 36,000 people die in the United States due to influenza, or influenza related causes.

Influenza is caused by two types of the virus, Type-A and Type-B. There are currently four FDA approved drugs to treat influenza—two are proton channel blockers and two are neuraminidase inhibitors. The goal of my research was to design a new drug that would allow physicians to effectively treat Type-A and Type-B influenza virus without having their patients endure unnecessary risks and side-effects.

Density functional theory calculations were used to optimize the geometries of the ligands. Using sophisticated resources such as the Protein Data Bank and AutoDock, a library of twenty five ligands were docked into the N4 protein. Each docking was performed five times, resulting in one overall average docked energy. The averaged energies for each of the ligands were ranked from lowest to highest. Based upon a different study, one of my ligands were shown to have antiviral activity. From the docked energy for the ligand with confirmed antiviral activity, the results of the highest ranking ligand could be determined to have promising antiviral activity. The ligand shown below is the promising ligand, which will undergo further alterations and dockings to attempt to improve the antiviral activity.