



CALIFORNIA SCIENCE & ENGINEERING FAIR 2019 PROJECT SUMMARY

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| Name(s) Gordon Chen; Jacob Huang | Project Number J0503 |
| Project Title Inhibiting Rabies at the Molecular Level | |
| <p style="text-align: center;">Abstract</p> <p>Objectives The goal for our project was to find the best ligands to successfully inhibit the p75 neurotrophin receptor, which is one of the receptors that rabies uses to take over the cell. We wanted to find the docking scores of each docking simulation to the p75 neurotrophin receptor and see if the score is enough to ensure a successful bond. We hypothesized that a few ligands that could successfully dock.</p> <p>Methods We used Schrodinger Suites as our docking tool. First, we imported the structure of our receptor, p75 neurotrophin receptor, into Maestro, the interface for Schrodinger applications. We then prepared the cell receptor by passing it through Schrodinger Protein Preparation Wizard, which refines the structure by assigning formal charges, enumerating bond orders, adding hydrogens, etc. After using Schrodinger LigPrep to prepare a library of ligands, we docked the ligands into the cell membrane receptors using Schrodinger Glide. To get the final results, we used Epik state penalties and GlideScore to find the docking score, which ultimately determines the best ligand to dock to the cell receptor. Glide automatically created a spreadsheet of all the resulting data.</p> <p>Results In our data spreadsheet, we have the ligands listed in order from the best (lowest) docking score to the worst (highest). The ligands schrod_806203_1 and schrod_621088_3 have the lowest docking scores, -5.855 and -5.613 respectively. Thus, they have the highest binding affinity. Approximately 0.2% of our library of ligands satisfied our requirements of having a docking score less than -5.</p> <p>Conclusions Scientists can now create a new ligand based on the structure of the ligands with the highest binding affinity to the rabies virus receptor. With better ligands, better molecular treatments can be created and developed.</p> | |
| Summary Statement We used protein ligand binding to determine the best ligand to inhibit the rabies virus. | |
| Help Received Mrs. Peng helped us get the trial license for Schrodinger Suites. Online training videos by Schrodinger helped us with the project. We did everything else by ourselves. | |