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“Demonstration of interaction between Celecoxib and Sulindac Sulfide with COX-2 using docking approach”

Abstract

Background: Molecular docking is the mechanism of observing how certain molecules bind to one another. Through this approach, it is clear to see the precise location on the molecules where they attach to one another. Molecular docking can show the overall efficiency and strength of certain molecular bonds. There are numerous docking softwares that are available online, but they all have different advantages and drawbacks. AutoDock Vina is one docking software that has provided some of the best results. Docking methods have been used to observe the interaction between Celecoxib and COX-2, and Sulindac Sulfide and COX-2. It is shown that COX-2 is linked to tumor growth, but both Celecoxib and Sulindac Sulfide act as inhibitors against it. The two drugs act very similarly on COX-2, inhibiting the synthesis of prostaglandins, which COX-2 is responsible for. Furthermore, Clinical trials with celecoxib have shown that it can also greatly reduce the effect of rheumatoid arthritis and osteoarthritis.

Methods: I used AutoDock Vina for my study. Along with this software, I also used PyMOL, Raccoon, and AutoDockTools. I gathered the pdb files for Celecoxib, Sulindac Sulfide, and COX-2, and converted them into PDBQT format. I then proceeded to dock Celecoxib with COX-2 to view their binding interaction. I repeated this step with Sulindac Sulfide instead of Celecoxib.

Results: This study was to observe the docking mechanism between the drug celecoxib and the enzyme COX-2, and sulindac sulfide and COX-2 as well. Unfortunately, due to numerous technical problems with using the software, I was not able to dock these molecules with one another properly. However, I was able to see how the molecules bonded together. When I conducted this docking mechanism between Celecoxib and COX-2, I was able to see that they were both adjacent to one another. In the case of docking between Sulindac Sulfide and COX-2, I noticed that Sulindac Sulfide bonded at a single point on the COX-2 molecule. Although I was not able to receive the desired results, I was able to see how the two molecules interacted with one another prior to illustrating the proper docking mechanism.

Conclusion: The next steps will be to visualize and analyze my data through AutoDock Vina. I am currently exploring other options to get better data which will be presented. COX-2 was only recently discovered, so there is still a lot to study on this. The implications of these interactions can help inhibit and prevent tumor growth, finding a plausible treatment to cancer.

Special Instructions: The abstract is a summary of the project. Do not to exceed one page. Do not change margins, font style or font sizes on this page. **Use this format only- do not modify!!!**