[CASE STUDY ASSIGNMENT]

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Presented To:

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1. Introduction

Snakebite is classified by the world health organization as a neglected tropical disease. Acute neuromuscular weakness with respiratory involvement is the most clinically important neurotoxic effect. Symptom evolution and recovery, patterns of weakness, respiratory involvement, and response to antivenom and acetyl cholinesterase inhibitors are variable, and seem to depend on the snake species, type of neurotoxicity, and other variations. Furthermore, for preventing venom from binding to the acetylcholinesterase enzyme at the synaptic cleft (the area between two nerve cells), this enzyme breaks down the neurotransmitter acetylcholine, allowing future nerve impulses to be transmitted. The fatal toxin produced by the green mamba and other venomous snakes is an inhibitor of acetylcholinesterase. To block the interaction between the toxin in snake venom and acetylcholinesterase, so create a therapeutic target with pdb structure 1ACJ. In addition, following the steps for Molecular Docking with Autodock Vina and report the affinity of Tacrine to Acetylcholinesterase with finding out more inhibitors other than Tacrine that succeeded to inhibit the Acetylcholinesterase. Therefore, in our case study we are going to design a drug target to prevent the interaction between the toxin in snake venom and acetylcholinesterase.

2. Methodology

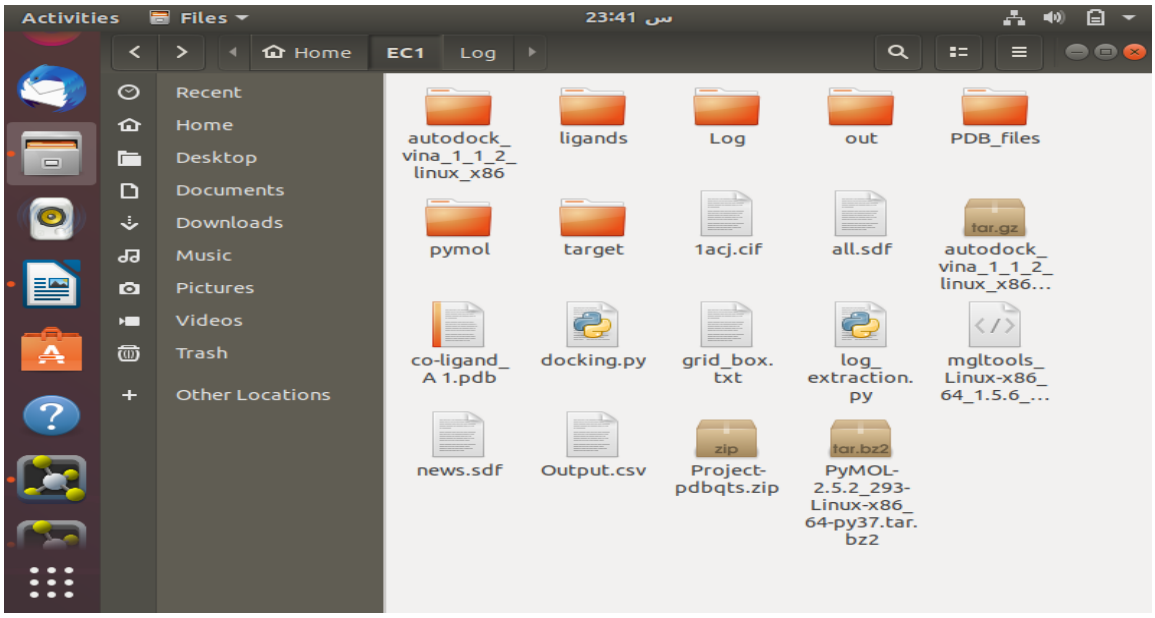
In our methods, we follow the steps for Molecular Docking with Autodock Vina to report the affinity of Tacrine to Acetylcholinesterase. Besides, finding out more inhibitors other than Tacrine that succeeded to inhibit the Acetylcholinesterase. So, we followed the steps to inhibit the Acetylcholinesterase as follows:

By Creating a new working directory for the Case study in the **Home** directory. Naming it by our enzyme class number, which is in our case was **EC1. Then**, Downloaded the required Python scripts from Moodle and the virtual screening library. Afterwards, we determine our Grid box dimensions and converting the protein to PDBQT format. Then, we run MGLTools (ADT), perform Virtual Screening and selecting the Best Hits. Finally, we visualize our structure using PyMOL so we can design our drug target.

3. Results

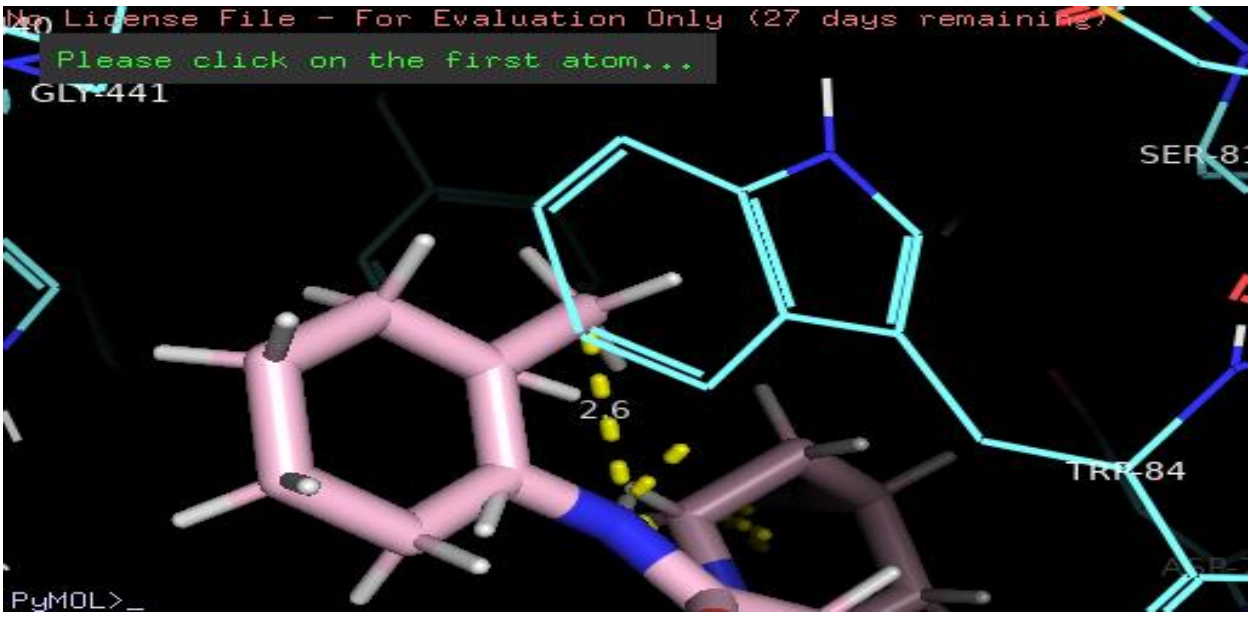
Our results showed that:

(Fig 1): Shows the files of our class enzyme EC1 in Home directory that all was worked in.

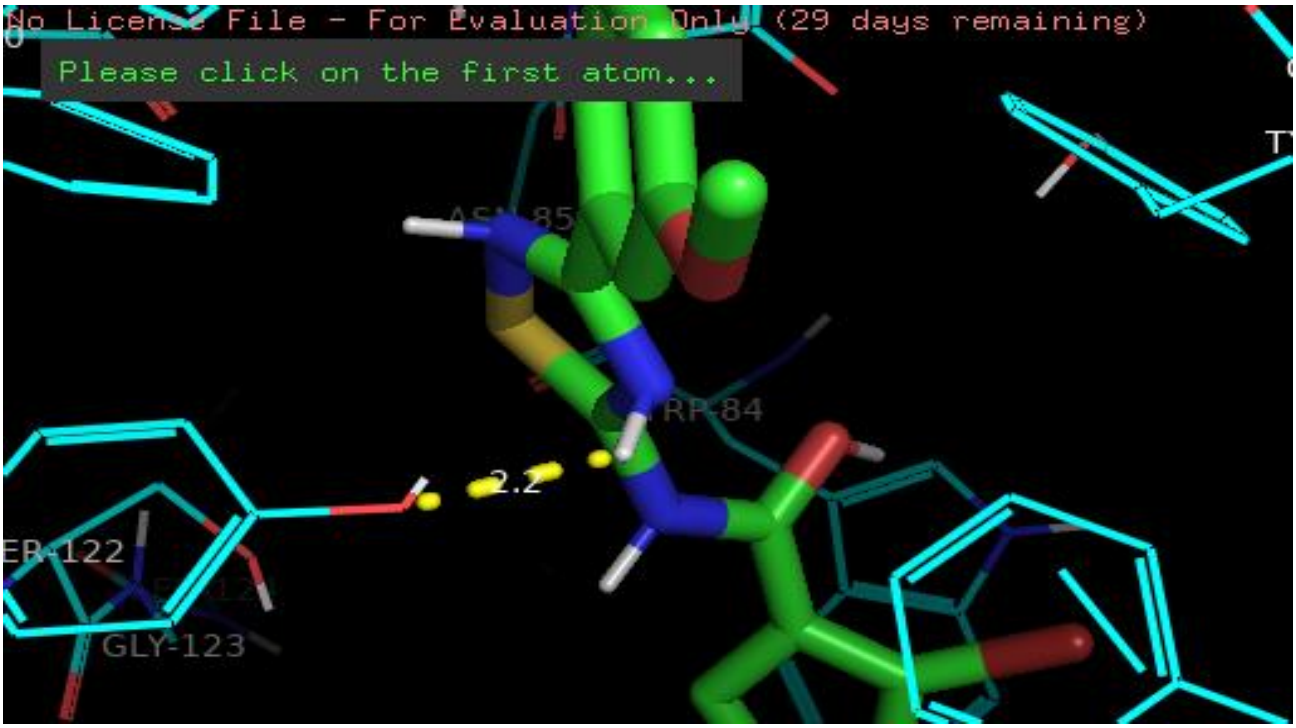


✓ **Now, let's get our visualization of our top 3 compounds**

(Fig 2): shows the visualization of the best 1st compound with higher affinity with the measurement of the hydrogen bond length with the protein.



(Fig 3): shows the visualization of the best 2nd compound with higher affinity.



(Fig 3): shows the visualization of the best 3rd compound with higher affinity.

4. Discussion & Conclusion

In our case study we concluded that, a therapeutic target with pdb structure 1ACJ to prevent the interaction between the toxin in snake venom and acetylcholinesterase. In addition, using Autodock Vina, follow the instructions for Molecular Docking as well as reporting the affinity of Tacrine for Acetylcholinesterase, as well as finding more inhibitors other than Tacrine that were successful in inhibiting Acetylcholinesterase. As a conclusion, in our case study, we designed a pharmacological target to prevent the poison in snake venom from interacting with acetylcholinesterase.

5. Future Work & Suggestions

In our future work, more research into these fascinating molecules and their diverse actions would not only help us improve management of neurotoxic envenoming but may also enable their use as potential treatments for infections, cancer, and various neurological disorders.