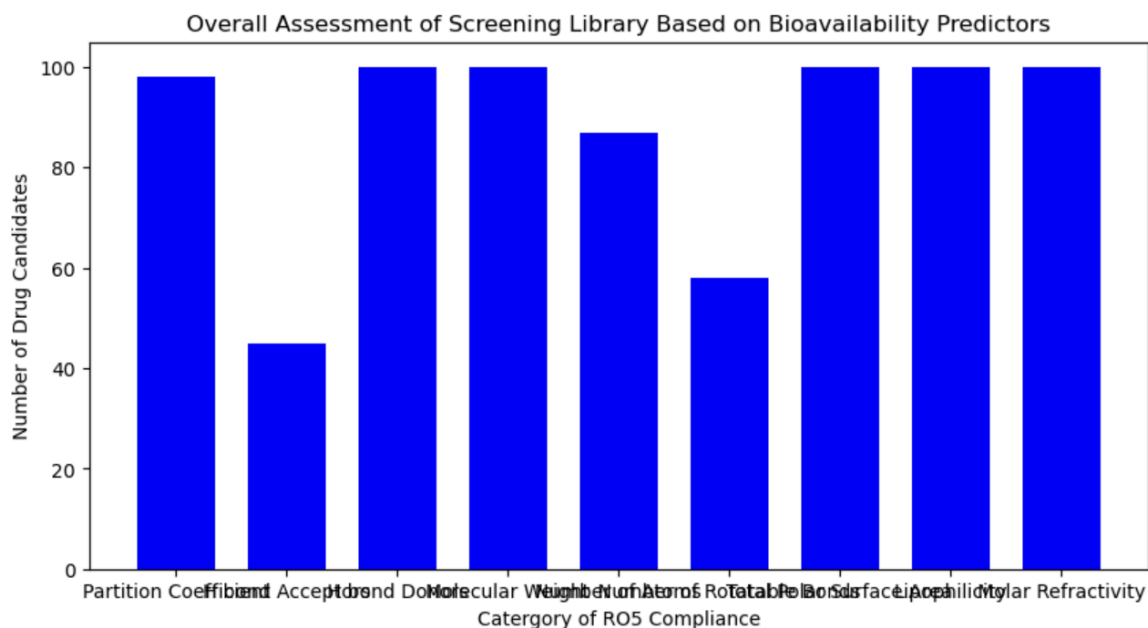
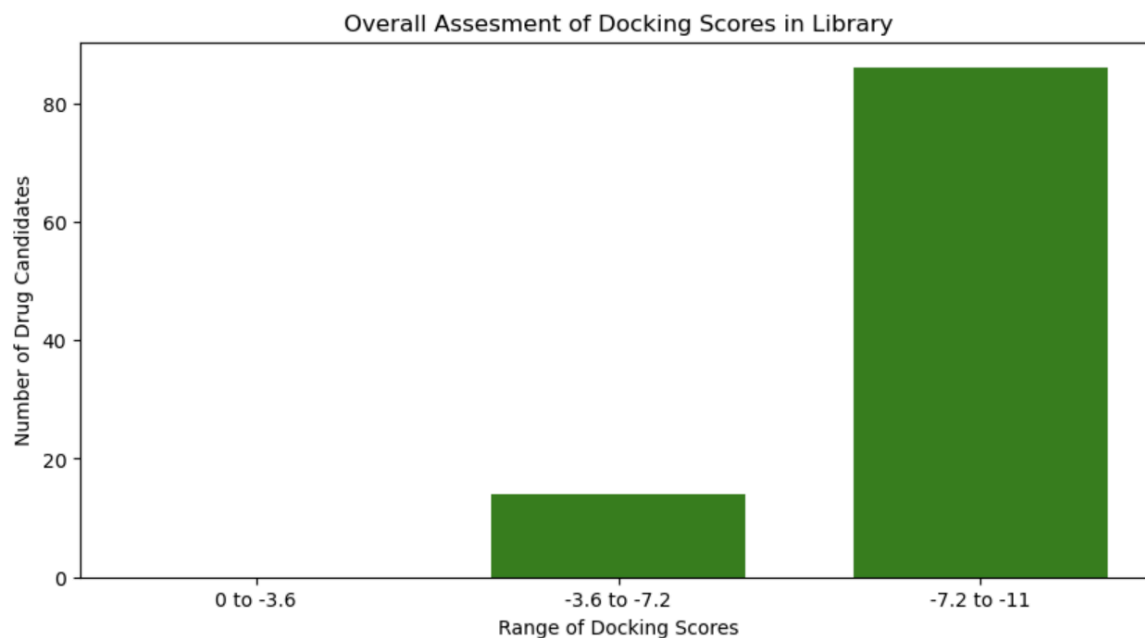


Example charts from tuberculosis drug candidate screening

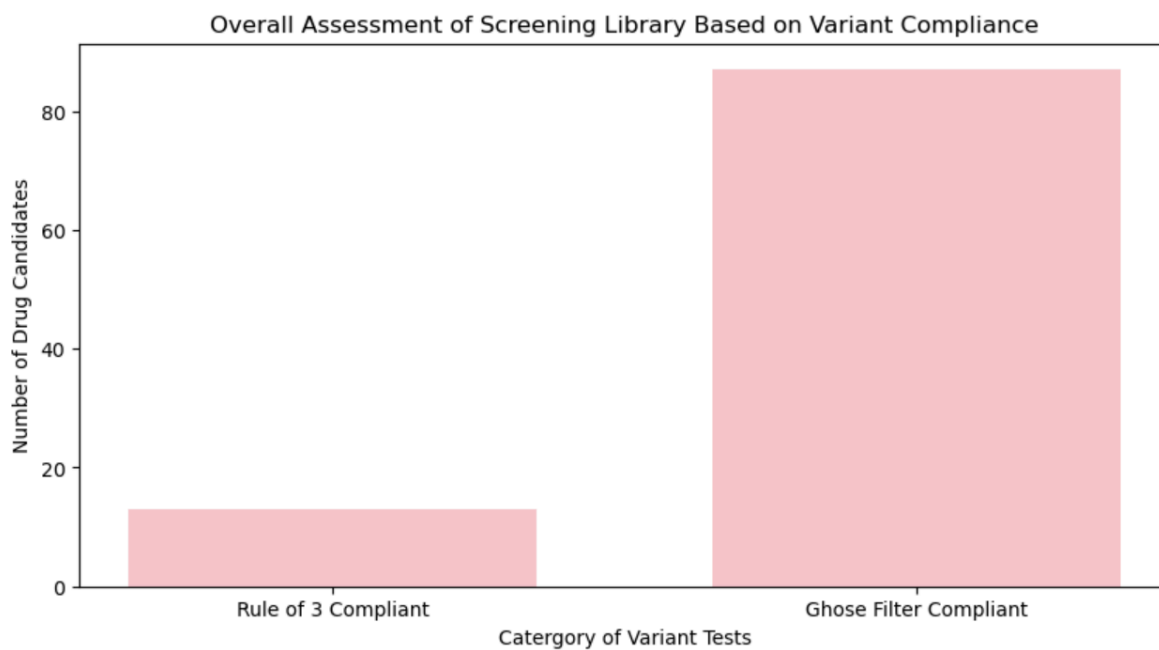
I unfortunately did not have time before turning this in to clean these charts up properly but they demonstrate the softwares capability to read and rank and sort the chemical properties of a large list of drug candidates.



This chart shows the number of drugs which are in the accepted range of values for Lipinski's rule of 5 compliance for each of these categories.



This chart shows the portion of the candidates that fall into one of 3 ranges of docking scores, -11 is the highest score possible and below -7.2 is considered strong affinity



This chart shows the number of drug candidates compliant with two variants on the rule of 5 the rule of 3 and the ghose filter.

Sample Docking Photos

Here are some photos taken through molecular modeling softwares showing ligands docked in the enzyme

