Week 4 - - add your stuff here Michael- Dr. B

Week 4

Date: 6/26/20

Figure 11: Covid-19 main protease structure 6M03 shown as a green cartoon with attached ligands O6K and DMS after aligning with structure 6Y2F in PyMol.

Analysis: This method allows for the 6M03 structure to be able to be used in GOLD docking due to defining the active site and making the process much easier. The file is now ready for the next step in the research process.

Date: 6/24/20

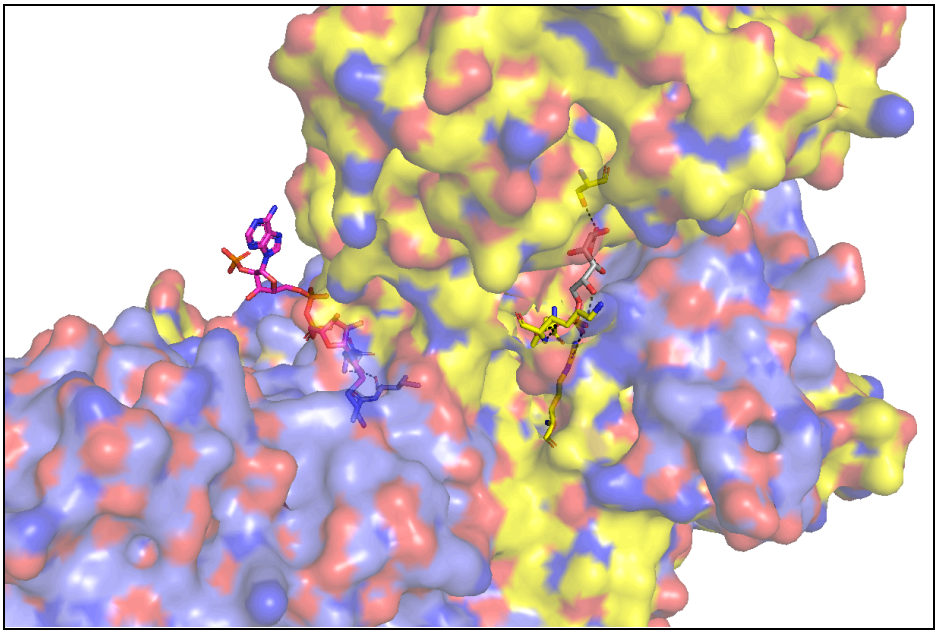

Figure 10: The two active sites of both ligands 6PG, shown as sticks with gray carbons, and NADP, shown as sticks with magenta carbons. The homology model protein 1pgj is shown as a transparent

surface with chain A carbons yellow and chain B carbons periwinkle. The interacting residues with the ligands are shown as sticks and the polar bonds are shown as black dashes.

Analysis: This portion of the Lm6PGDH medium steps helped visualize what the active sites that were created with the homology model looked like. By showing the interactions, it helps show how the molecules interact and why it is a good part of the protein to bind to. This will be crucial for later labs when understanding how the active site affects the protein of interest.

Date: 6/23/20

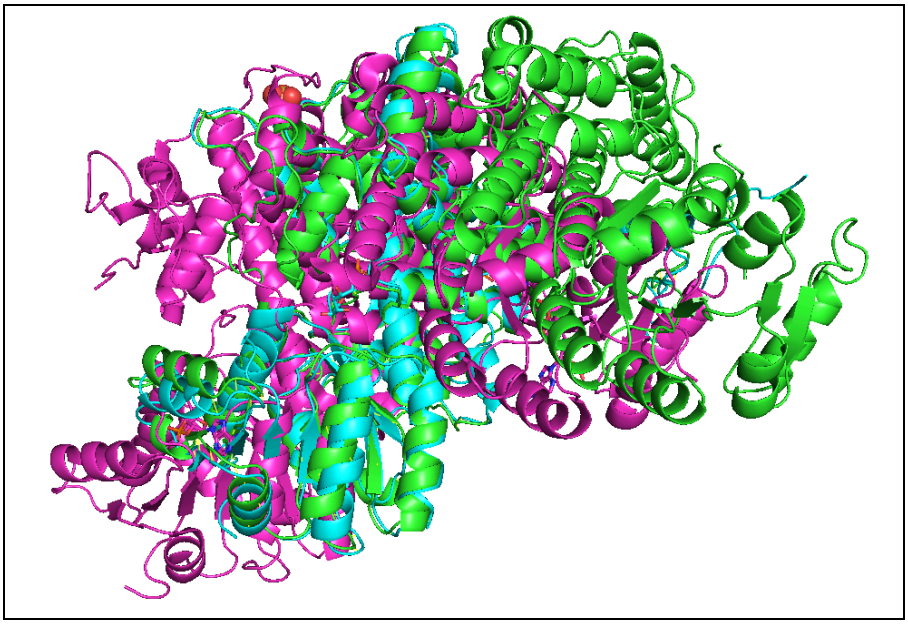

Figure 9: Alignment of 1pgj homology model, shown as a green cartoon, with both known PDB structures 1pgp, shown as a cyan cartoon, and 2iyp, shown as a magenta cartoon.

Analysis: In the Lm6PGDH medium steps, it was important to align known structures with ligands to the homology model created earlier in the lab in order to make sure that the homology model will have its active site defined. The methods to conduct these steps are important in understanding how to use structures without known active sites in virtual screening later.

Week 3- add your stuff here Michael- Dr. B

Week 3

Date: 6/19/20

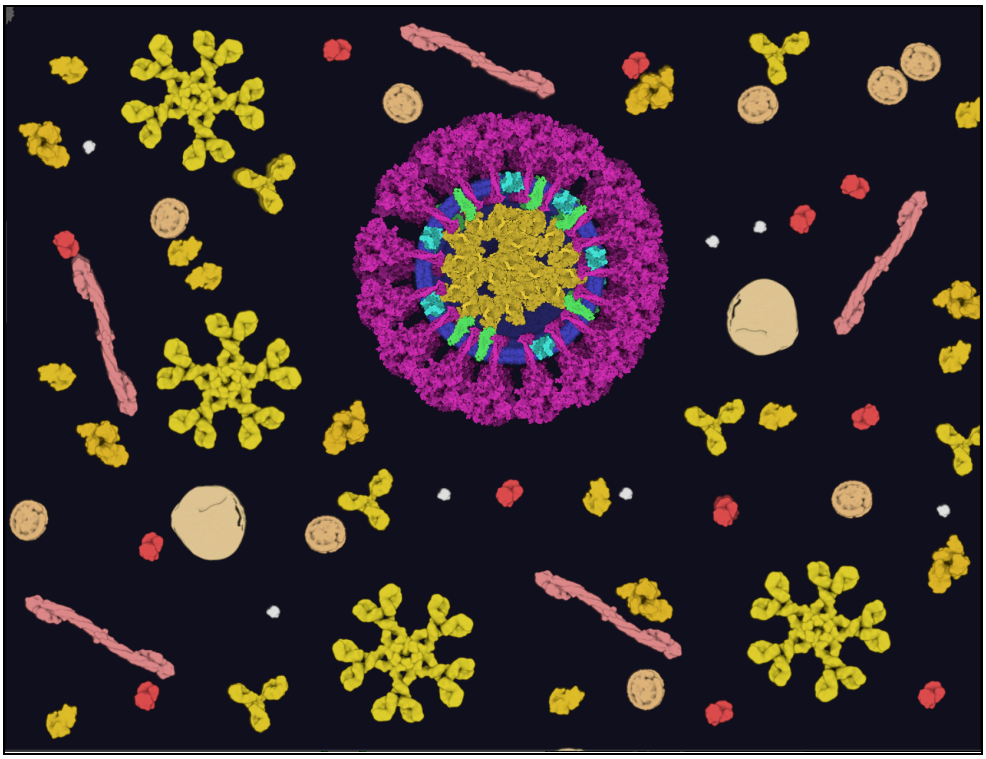

Figure 8: Image taken through CellPaint of a Coronavirus drawing with a navy background.

Analysis: Although it was a little difficult to understand how to work the site in the beginning, an image was made after a few attempts. This was a nice visualizer for what the class is researching in the lab now.

Date: 6/18/20

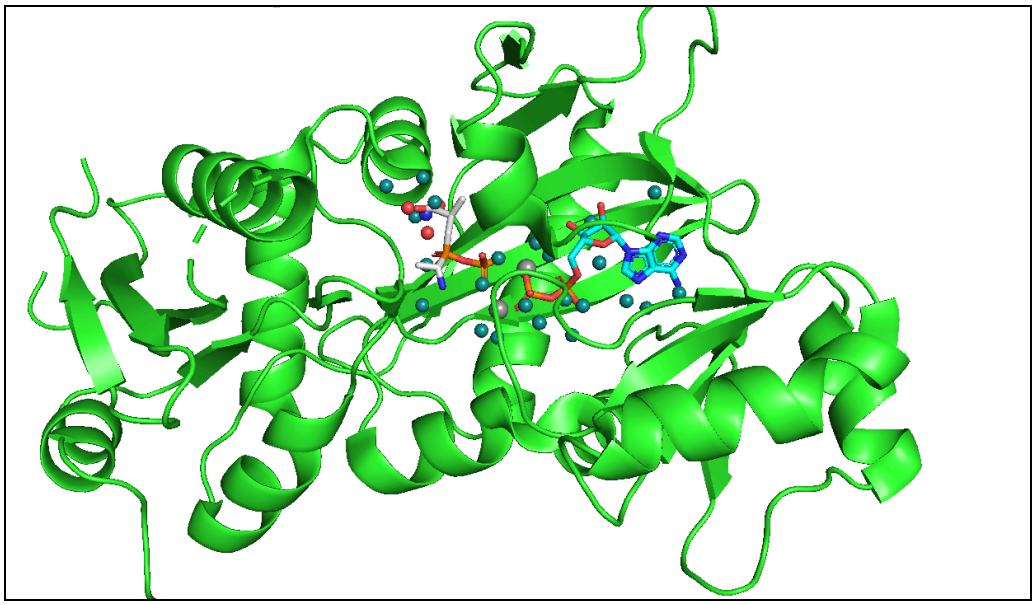

Figure 7: Structure 3lwb shown as a green cartoon with the ligands from structure 1iow aligned and shown as sticks with ADP with cyan carbons and phosphonic acid with white carbons. Waters in the active site are shown as teal spheres and the two magnesiums are shown as grey spheres.

Analysis: In the MtDalaDala medium steps, it was made possible to understand how to use PyMol to align different structures in order to find the active site of an apo or non ligand structure. This will be essential for my COVID-19 target project later, as my structure 6M03 is an apo form of the main protease.

Date: 6/18/20

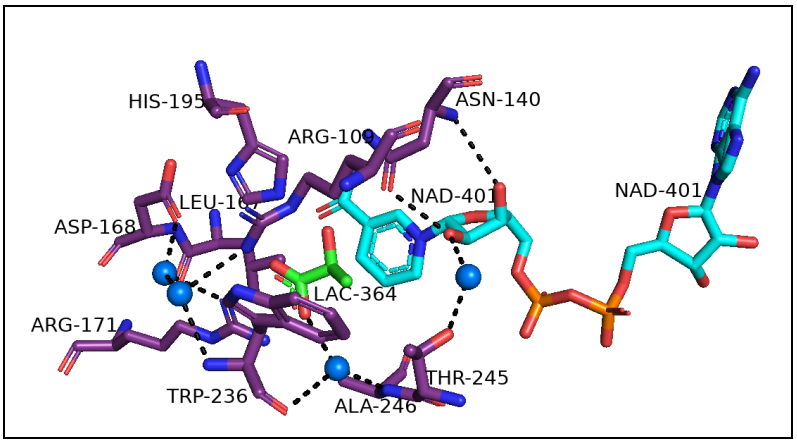

Figure 6: Structure 2fn7's residues that interact with ligands shown as sticks with carbons colored purple. The ligand NAD has carbons colored cyan and ligand LAC has carbons colored green. Water molecules are shown as blue spheres and polar bonds are shown as black dashes. Residues are labelled.

Analysis: This image was created using the LDH medium steps protocol. This feature of PyMol allows us to fully understand the polar interactions of a crystal protein structure with other ligands and water molecules. This can be helpful when going into virtual screening and finding where the active site of the protein is.

Date: 6/16/20

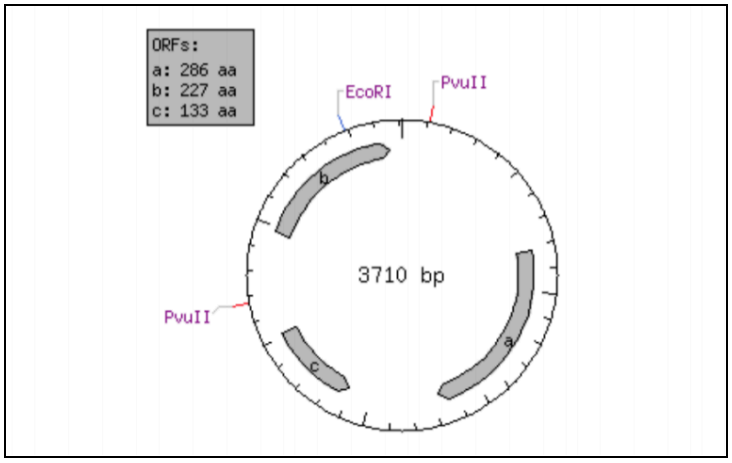

Figure 5: Plasmid pGBR22 cut with both restriction enzymes EcoRI and PvuII shown as a circular sequence. ORFs are shown as gray areas of the plasmid.

Analysis: Understanding how plasmids are made with the DNA sequence can greatly help for future labs. This data shown also helps show where on the sequence the restriction enzymes are.

Week 2

Week 2 - great work Michael- Dr. B

Date: 6/12/20

Figure 4: Image of 6M03 covid main protease molecule in apo form after running through molprobity. Chain A is shown as a green cartoon.

Analysis: This hydrolase structure is very important in the covid-19 structure and will help for future processing and docking for the project. Hopefully by looking more into the crystal structure of this virus will help understand how to choose potential inhibitors.

Date: 6/11/20

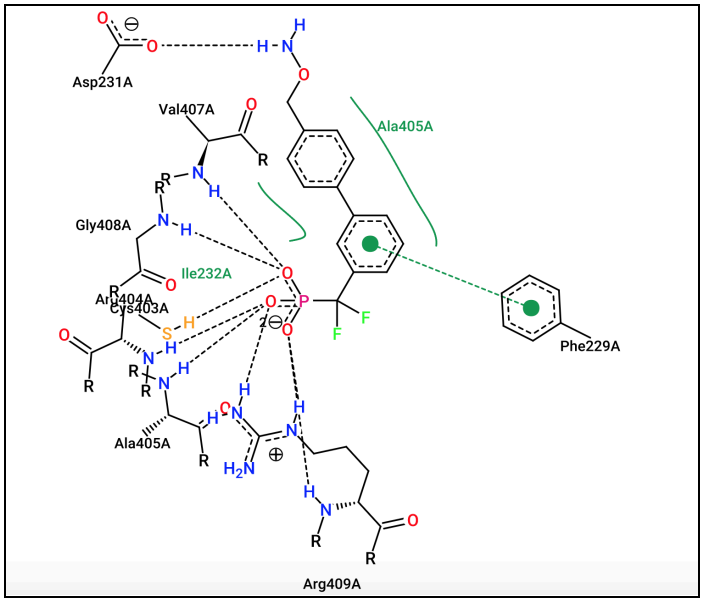

Figure 3. Poseview of crystallized ligand YI1 2D interactions present in YopH protein 2y2f. Hydrogen bonds are shown as black dashes, hydrophobic interactions shown as green lines, and pi-pi interactions are shown as green dots connected by dashes.

Analysis: Understanding binding interactions between ligands and their protein are critical in realizing the function of the ligand. A structure with both hydrophobic and polar bonding is a good potential target.

Date 6/9/20

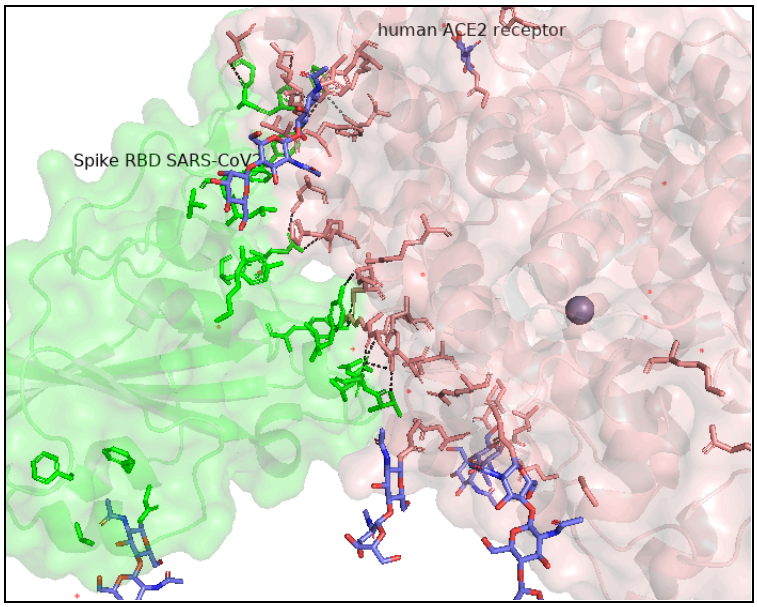

Figure 2: The PDB structure of 6vw1. Spike RBD SARS-coV2 protein is shown in green and the human ACE2 receptor is shown in salmon. Both proteins are shown as transparent surfaces and cartoons. The sugar molecules are shown as sticks and colored by element with carbons a blue-purple. Interacting molecules in the two proteins are displayed as sticks with polar contacts shown as dashed lines.

Analysis: Understanding the interactions between the sugars and ligands as well as the receptor and spike protein will further help researchers in developing a drug/vaccine. Further virtual screening and research will add more critical information essential to understanding the binding relationships.

Week 1

Michael - well done - put in Reverse Chronological order (newest stuff at top) - Thx, Dr. B
Date 6/7/20

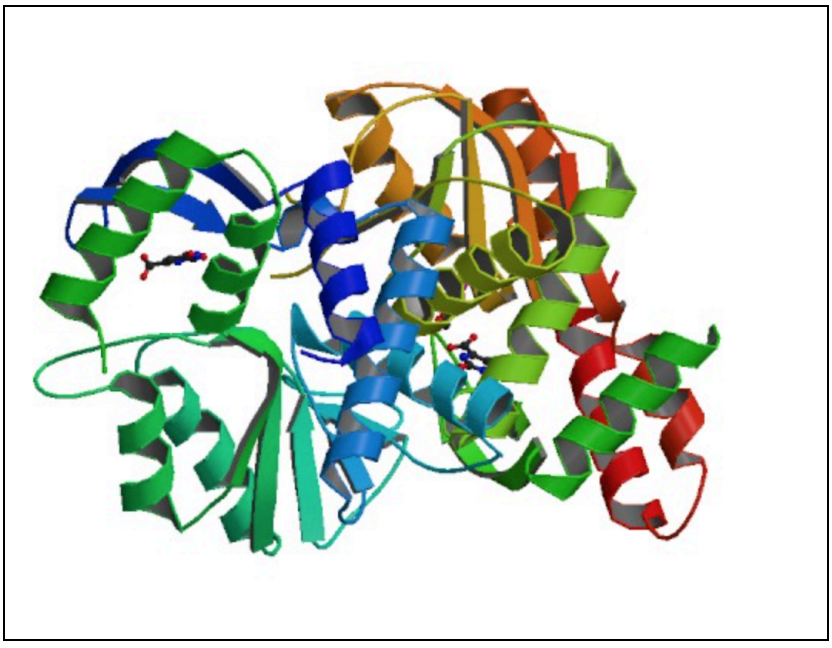

Figure 1. PDB entry 1LH0 Omp Synthase [Salmonella enterica subsp. enterica serovar Typhimurium] as the homology model for Orotate Phosphoribosyltransferase in *Toxoplasma Gondii*. Shown as a cartoon with rainbow colors.

Analysis: For this first week of summer research, the main focus was on part 2 of the target discovery protocol, in which a potential target is found for an organism that can cause diseases. The target chosen was protein Orotate Phosphoribosyltransferase of organism *Toxoplasma Gondii*. After finding different sources for essentiality, assayability, and purification, the one source not present was a structure. However, after performing a BLASTP search for a potential homology model, PDB entry 1LH0 was found. With positives of 61%, and maximum percent identities of 42%, this model had enough in common to be a potential homology model for this target.