Week 5

7/3/2020

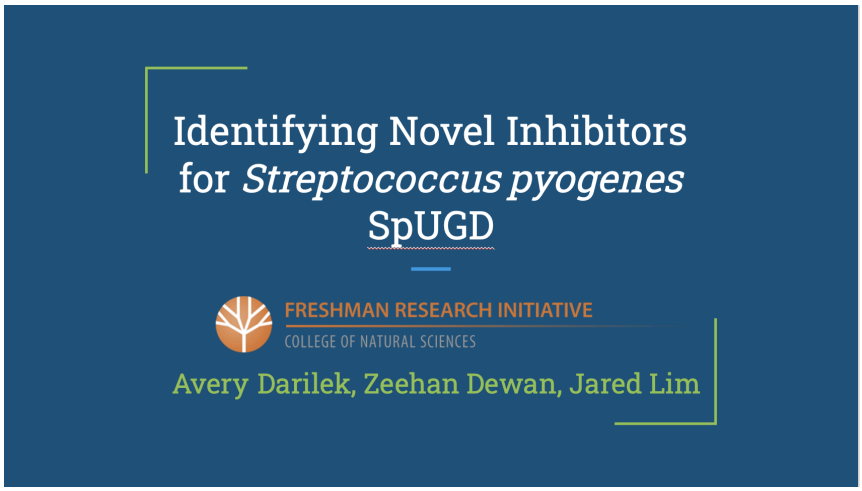


Figure 14: Image shows the target project that was done this summer for the target UDP glucose 6 dehydrogenase.

Analysis: This project included virtual screening and making a presentation for the rest of the class. It was interesting to see that our negative controls outscored our positive controls. After the presentation, comments were given to us so that we can improve our presentation and powerpoint in the future.

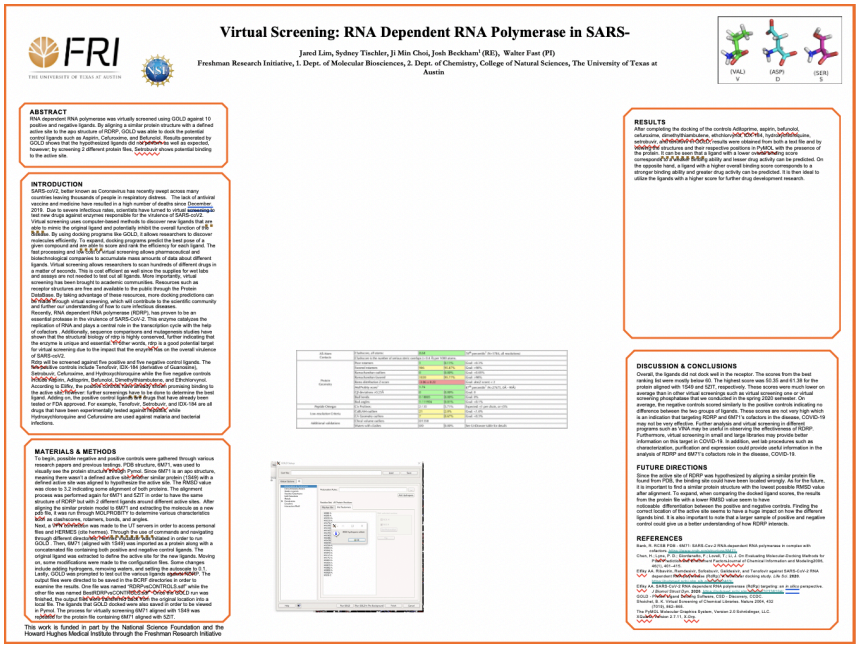


Figure 15: Image shows the poster for the COVID-19 project with elements of the poster currently being filled out.

Analysis: This project included virtual screening as well as making a scientific research poster to display our results and analysis.

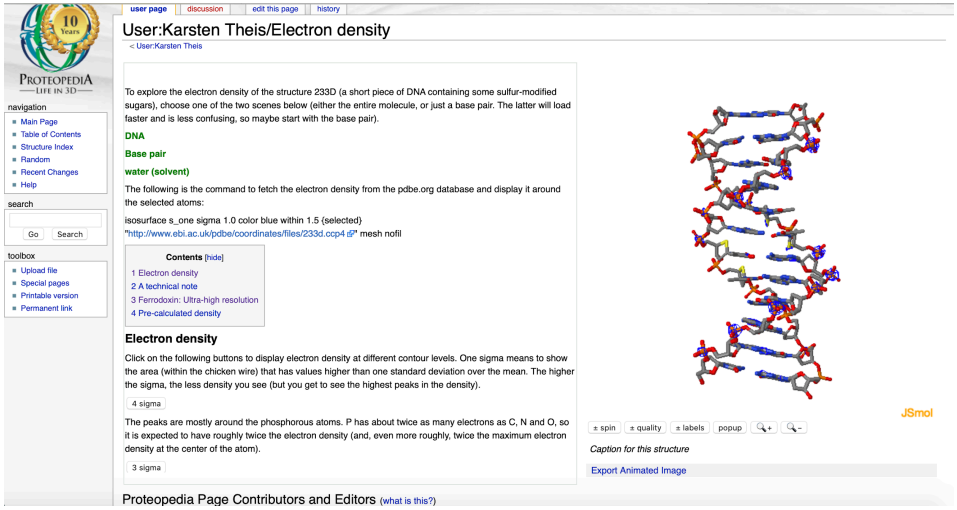


Figure 16: Image shows the proteopedia page with information about electron density on it.
Analysis: By selecting the number of sigmas, the diagram on the right changes to see all the various interactions in the structure.

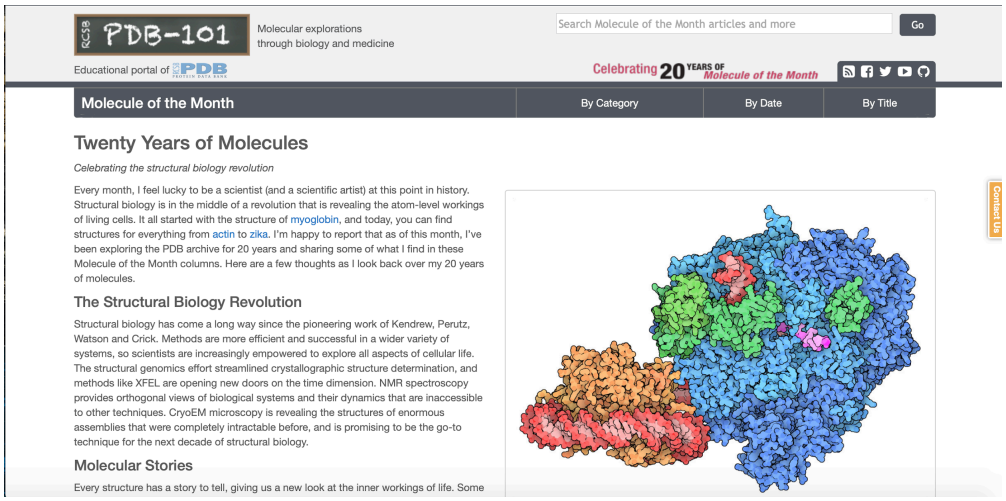


Figure 17: Image shows the website on PDB about twenty years of molecules and various diagrams to show different molecules and structures.
Analysis: Structures in biology are very different and unique. Some can be symmetrical while some can contain many various elements. Overall, as time continues, our understanding of these biological structures expands.

Week 4

Good work Jared. Dr. B

6/23/2020

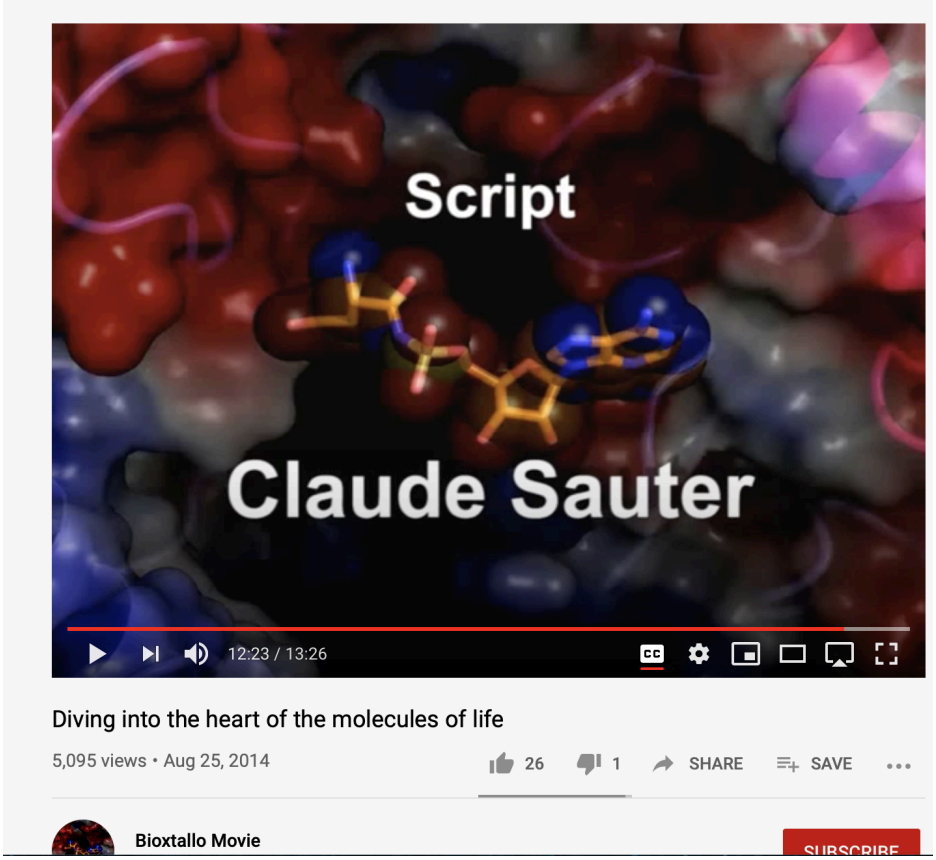


Figure 11: Image shows the video on determining protein structures.
Analysis: This video highlighted the importance of X-ray crystallography in order to photograph molecules at an atomic level.

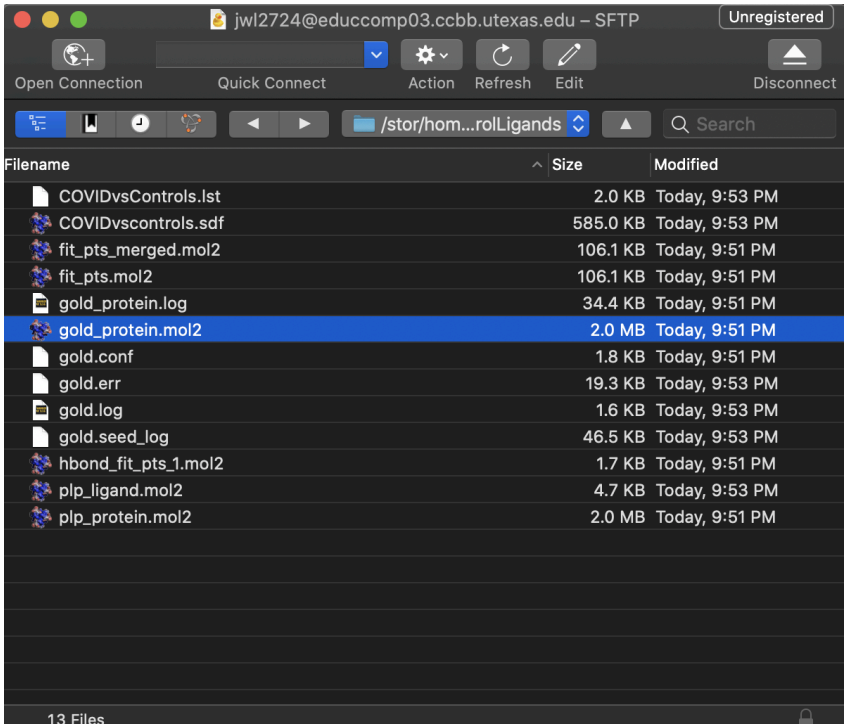


Figure 12: Image shows the run in Cyberduck from GOLD for the COVID-19 screening project.
Analysis: The virtual screening of the target for COVID-19 was done and the poster is being worked on. The result gave me a list of scores.

```
# Download 1DLJ to your computer and open with the file menu or fetch
it.
fetch 1DLJ, type=pdb

# Color the background white
bg white

# Hide the water molecules in the structure
hide non

# Display the structure sequence ligand
set seq_view, 1

# Create a separate object for each (NAI & UGA)
sele NAI, resn NAI
sele UGA, resn UGA

# color ligands, NAI by element as magenta, UGA by element as cyan
util.cbac UGA
util.cbam NAI

# Make a selection of all of the ligands to represent the active site
```

Figure 13: Image shows the pymol script for the target UDP glucose 6 dehydrogenase.
Analysis: The pymol script for the target UDP glucose 6 dehydrogenase was written. The file was then converted to .pml and can show the various angles and scenes of the structure in Pymol.

Week 3

Excellent work Jared. - Thx, Dr. B

6/17/2020

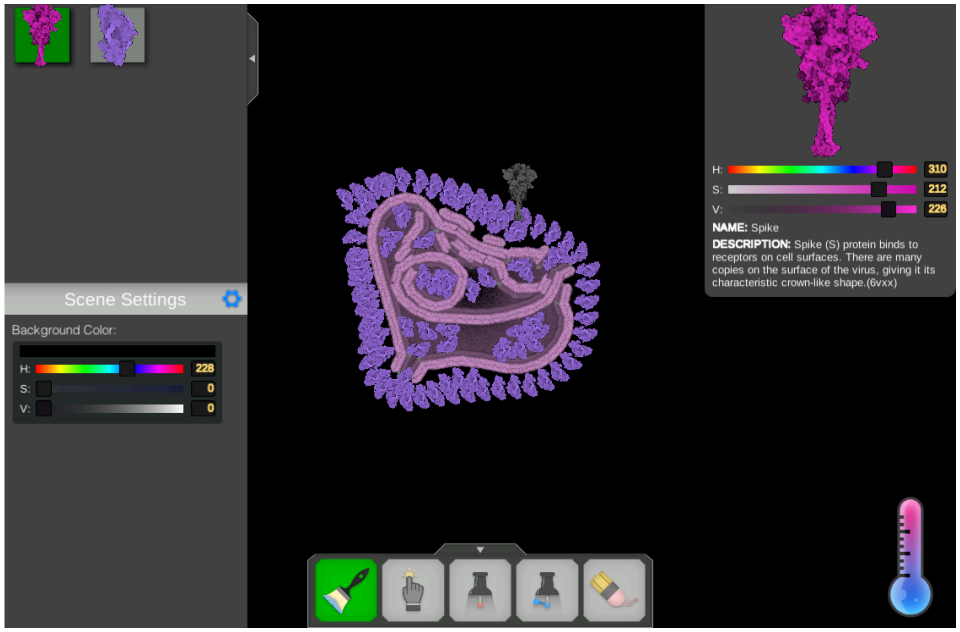
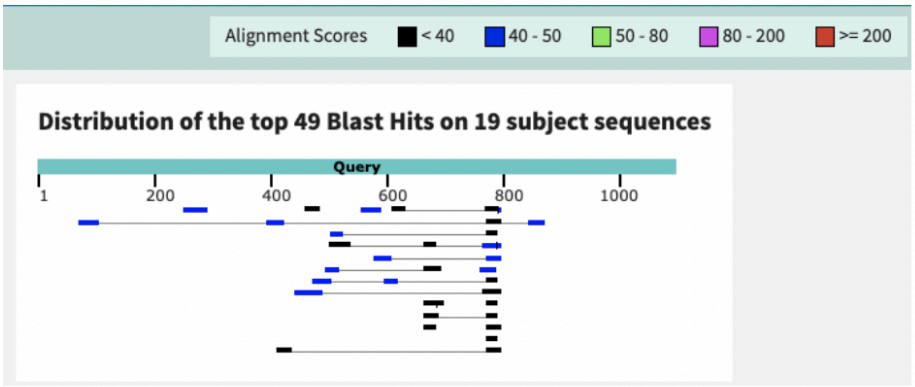


Figure 6: Image shows Cell Paint website showing viruses in blood plasma along with human cells

Analysis: Cell Paint was explored for about 10 minutes to see how the application can display different varieties of viruses in blood plasma along with simple human cells.

Figure 7: Image shows the presentation watched from the ASBMB virtual meeting website. This presentation and poster is about bacteria populations and plastic in Southern California waters.

Analysis: This virtual presentation of a poster describes how microbial populations such as antibiotic production affect potential plastic degradation. More specifically, the genus Vibrio is prevalent in these Southern California waters. Bacteria were placed on two different types of Agar in order to observe growth. At first, there was no clear pattern of colonization; however, with longer incubation times, there was an increase in unknown/uncultured bacteria. In conclusion, this poster shows that there are differences in the microbial communities growing on coastal marine plastic debris. This could then have a negative effect on humans affecting our health and environment.



Graphic Summary of BLAST of Sequence compared to Human Genome

Do another BLAST to see if your sequence is found in other genomes.
Under 'Database' choose 'Nucleotide collection (nr/nt)'
Select 'Somewhat similar sequences (blastn)'
Begin Search.

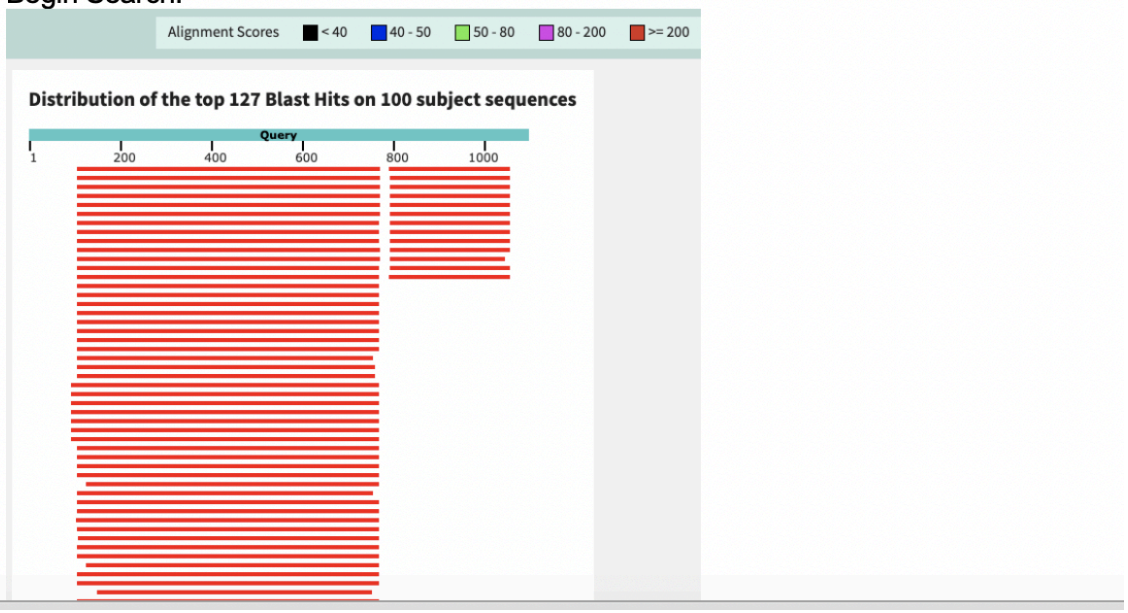


Figure 8: Image shows the alignment scores of two different sequences.

Analysis: This image was gathered for the assignment, Analyze DNA Sequencing. This assignment included editing DNA sequences and identifying the start and stop codons. This assignment will be useful in the future because it allows us to learn about DNA sequences.

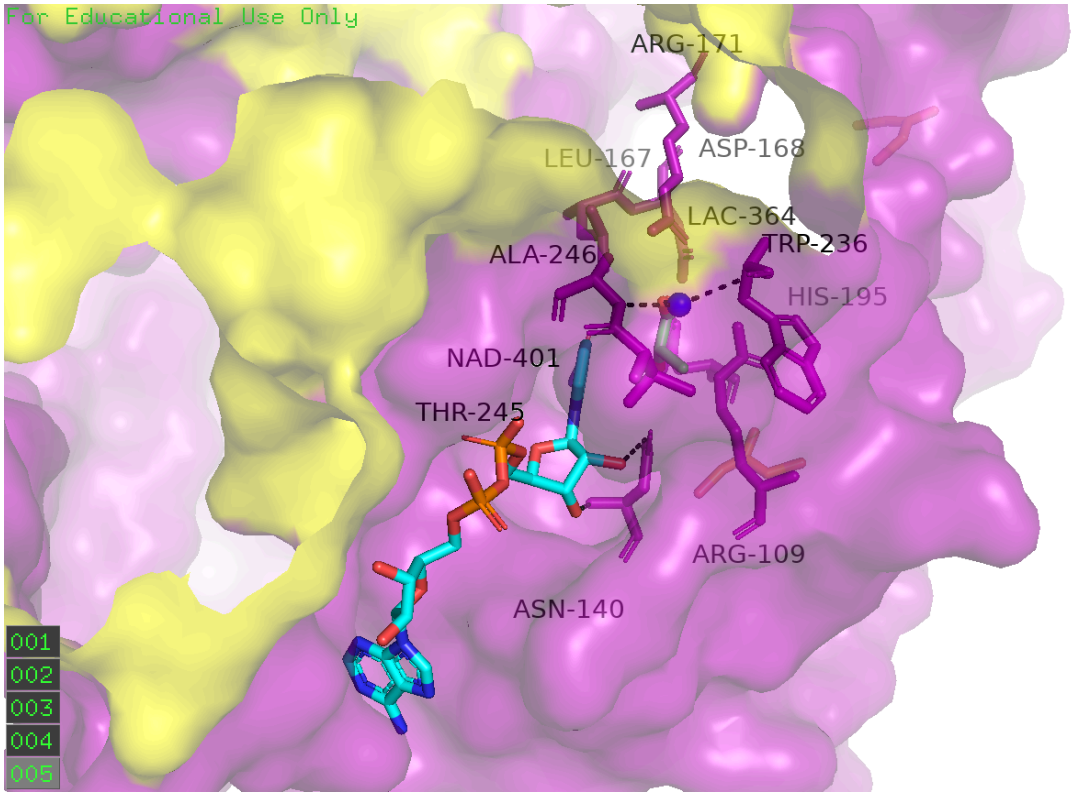


Figure 9: Pymol representation shows the 5th scene in the LDF Pymol scripting assignment. The image shows the polar contacts and residues labeled. There is a pocket in the active site and the rest of the protein is shown as a surface.

Analysis: This assignment was done using only the medium steps. This made it more difficult than when we had the granular steps. The assignment was done to improve on Pymol skills and analyze further how active sites and proteins interact.

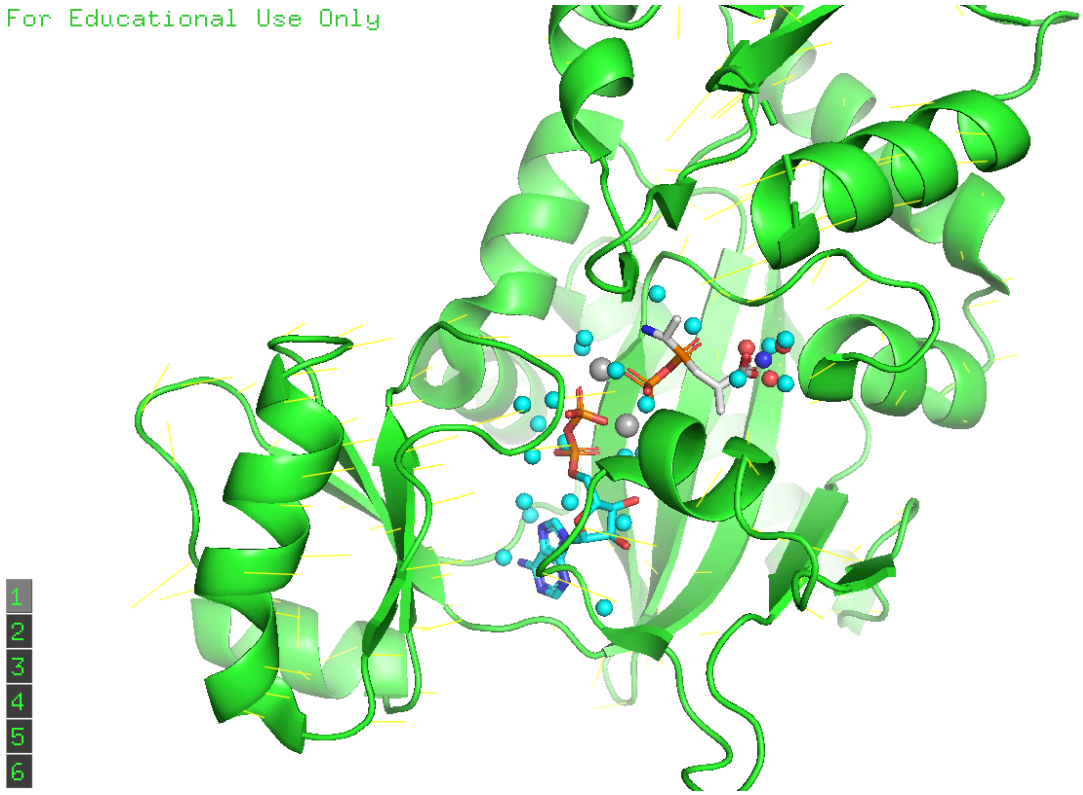


Figure 10: Pymol representation shows chain A as a cartoon and the ligand as sticks with some NO3, magnesium, and others as spheres.

Analysis: This assignment was done using only the medium steps. This made it more difficult than when we had the granular steps. The assignment was done to improve on Pymol skills and analyze further how active sites and proteins interact.

Week 2

Week 2 - great work Jared- Dr. B

6/11/20

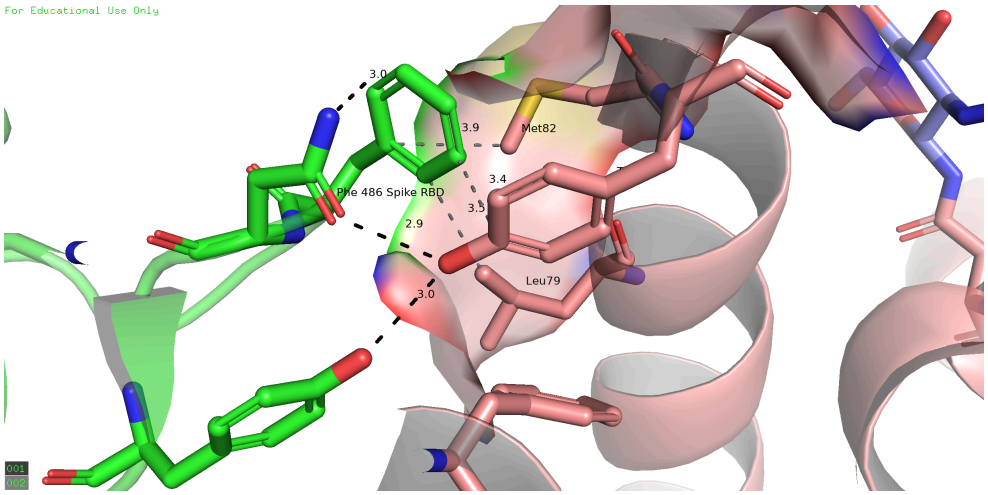


Figure 2: Pymol representation shows a scene of 6VW1 and the polar interactions between molecules in the structure. The structure was colored by element and some amino acids were labeled.

Analysis: Pymol scripting was done in this activity. A set of detailed instructions were followed in order to get the correct pictures and scenes. Only line commands were used instead of using the mouse to influence and change the structure in Pymol. This activity was done to learn new line commands for future use.

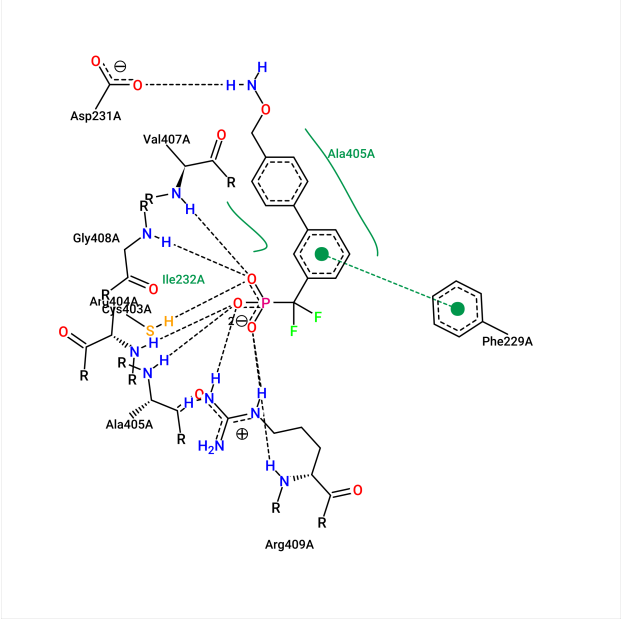


Figure 3: Diagram shows poseview of YopH generated from the PDB file and ZBH University Hamburg website.

Analysis: A poseview diagram of YopH was generated. This was done to visualize how YopH looks in two dimensions.

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	8.7		97th percentile* (N=97, 2.90Å ± 0.25Å)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.11%	Goal: <0.3%
	Favored rotamers	906	95.87%	Goal: >98%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	1020	95.77%	Goal: >98%
	Rama distribution Z-score	-3.06 ± 0.22		Goal: abs(Z score) < 2
	MolProbity score^	1.76		100th percentile* (N=3760, 2.90Å ± 0.25Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	0 / 8805	0.00%	Goal: 0%
	Bad angles:	1 / 11956	0.01%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	2 / 35	5.71%	Expected: ≤1 per chain, or ≤5%
Low-resolution Criteria	CaBLAM outliers	21	2.0%	Goal: <1.0%
	CA Geometry outliers	7	0.67%	Goal: <0.5%
Additional validations	Chiral volume outliers	0/1354		
	Waters with clashes	0/0	0.00%	See UnDowser table for details

Figure 4: Image shows traffic light table generated in Molprobity of 6M71.

Analysis: The target 6M71 was put through Molprobity and this traffic light table was generated. Asn/Gln/His flips and hydrogens were added. In addition, Flips were made. In the picture, the summary statistics were overall very good. The only red line in the summary statistics was the Rama distribution Z-score.

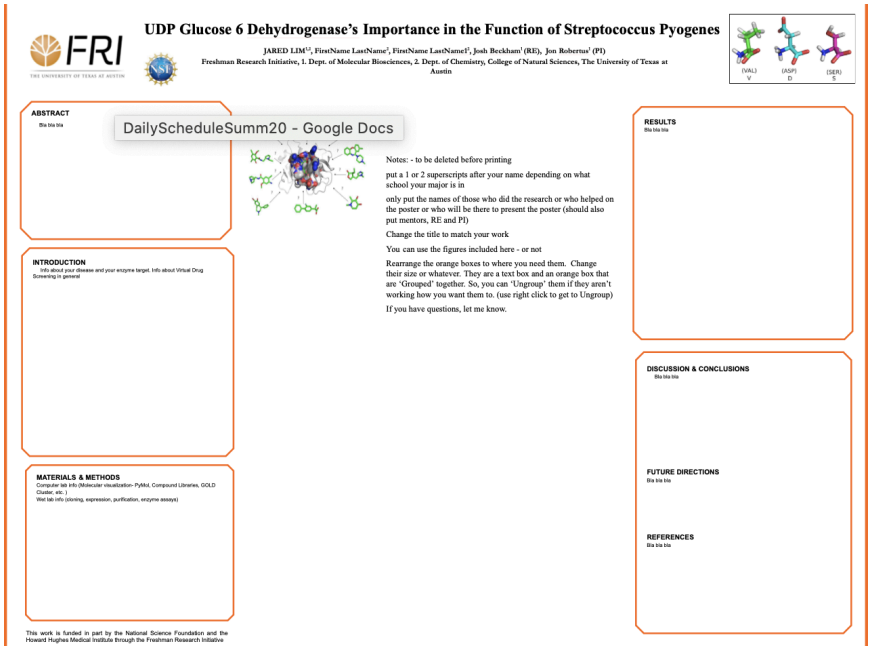


Figure 5: Image shows edited template for poster with my name and title for my target and organism.

Analysis: The template for the poster was edited with my name and title for my target and organism. This poster will be edited throughout the summer and fall until it is completely filled out and is ready for a presentation.

Week 1

Jared- good work - put in Reverse Chronological order (newest stuff at top) - Thx, Dr. B

6/5/2020

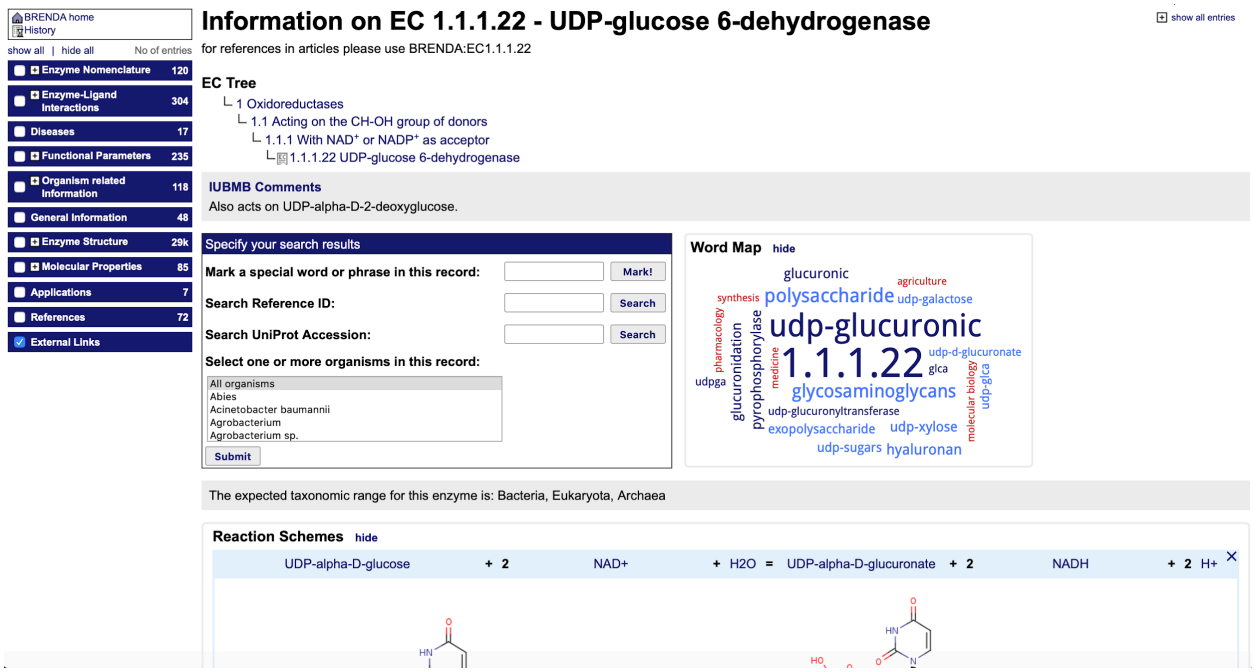


Figure 1: Image shows the Brenda site for the enzyme chosen, UDP-glucose 6-dehydrogenase. There is a reaction scheme diagram shown in the image. From this website, many components of the target discovery page were filled out.

Analysis: A specific disease was chosen and from that, an enzyme or target was chosen to do a target discovery page on. The target that was chosen was UDP-glucose 6-dehydrogenase in Streptococcus pyogenes. Most of the information found for this target was found from the Brenda website shown in Figure 1. The target met most of the criteria. For example, the target had a resolution less than 3. Also, another example is that the target is crucial for the survival of the infectious organism. The target is essential for formation of the antiphagocytic capsule that protects many virulent bacteria from the host's immune system.