**10.12 Weekly Report**

Caiya Zhang

**What you have done in the past week:**

1. This week, I mainly focused on completing the draft proposal. During the process of writing proposal, I sorted out several goals that I need to achieve in order to complete the project, and I’m a little bit clearer about the overall time schedule.

2. I have quickly read over the two articles on Plos Computational Biology and Nature Methods. So far, I think GeoPPI can be an alternative to the baseline method or project for comparison, and the SKEMPI 2.0 dataset mentioned in several papers may also be an alternative to the baseline dataset.

**What are major challenges/issues you need to discuss in the meeting:**

I wrote my draft based on structure of the sample given by the instructor, combined with the proposal I received, and I found there is no module that requires me to describe the method and data sets in the given outline, which was what I might need to show from my perspective. So far, I have only mentioned them in the Abstract and Objectives, which are relatively brief and general, so I was wondering if I need to explain more about methods and datasets I may use in this project.

**What you want to accomplish in the next week/weeks:**

1. Continue to modify and improve my proposal.
2. Continue doing literature review and collect some ideas about choosing specific graph neural network structure in my work.
3. Carefully understand the feature extraction methods in the two key papers, as well as learn more about the use of AlphaFold database.

**Reference**

Jankauskaitė, J., Jiménez-García, B., Dapkūnas, J., Fernández-Recio, J., & Moal, I. H. (2018). SKEMPI 2.0: An updated benchmark of changes in protein–protein binding energy, kinetics and thermodynamics upon mutation. *Bioinformatics*, *35*(3), 462–469. https://doi.org/10.1093/bioinformatics/bty635

Liu, X., Luo, Y., Li, P., Song, S., & Peng, J. (2021). Deep geometric representations for modeling effects of mutations on protein-protein binding affinity. *PLOS Computational Biology*, *17*(8). <https://doi.org/10.1371/journal.pcbi.1009284>

Tubiana, J., Schneidman-Duhovny, D., & Wolfson, H. J. (2022). Scannet: An interpretable geometric deep learning model for structure-based protein binding site prediction. *Nature Methods*, *19*(6), 730–739. <https://doi.org/10.1038/s41592-022-01490-7>