Predicting Possible Oligomerization States of Protein Sequences

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▶ **Idea:** We attempt to develop an ML algorithm that predicts possible oligomerization states given a FASTA sequence of a particular protein chain.

▶ **Dataset:** We curate our own dataset by scraping the RCSB Protein Data Bank

▶ **Relevant Papers:**

1. Jumper, J, Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., Tunyasuvunakool, K., Bates, R., Žídek, A., Potapenko, A., Bridgland, A., Meyer, C., Kohl, S. a. A., Ballard, A. J., Cowie, A., Romera-Paredes, B., Nikolov, S., Jain, R., Adler, J., . . . Hassabis, D. (2021). Highly accurate protein structure prediction with AlphaFold. Nature, 596(7873), 583–589. https://doi.org/10.1038/s41586-021-03819-2

2. Shen, H., & Chou, K. (2009). QuatIdent: a web server for identifying protein quaternary structural attribute by fusing functional domain and sequential evolution information. Journal of Proteome Research, 8(3), 1577–1584. https://doi.org/10.1021/pr800957q

3. Simeon, S., Shoombuatong, W., Anuwongcharoen, N., Preeyanon, L., Prachayasittikul, V., Wikberg, J. E. S., & Nantasenamat, C. (2016). osFP: a web server for predicting the oligomeric states of fluorescent proteins. Journal of Cheminformatics, 8(1). https://doi.org/10.1186/s13321-016-0185-8

▶ **<u>Work Divison:</u>**
- ▶ Agney K Rajeev: Literature review on various ML implementation, preprocessing of data, database cleaning
- ▶ Joel Joseph KB: Literature review on Protein oligomerization, feature extraction, and identifying important features in training data
- ▶ Both: Database curation, Slides, Reports, and Implementation of Algorithms

▶ **Algorithms to be implemented:**
- ▶ k-Nearest Neighbour, Random Forest and Neural Network

▶ **Midway Targets:**
- ▶ Data curation and organization
- ▶ Research about possible embedding and preprocessing of data
- ▶ Implementation of 1 or 2 above-mentioned algorithms

▶ **<u>Expected Results:</u>**
- ▶ We expect improved results compared to the existing models in the literature due to our extensive database($\sim$150,000) and advanced algorithms implemented.