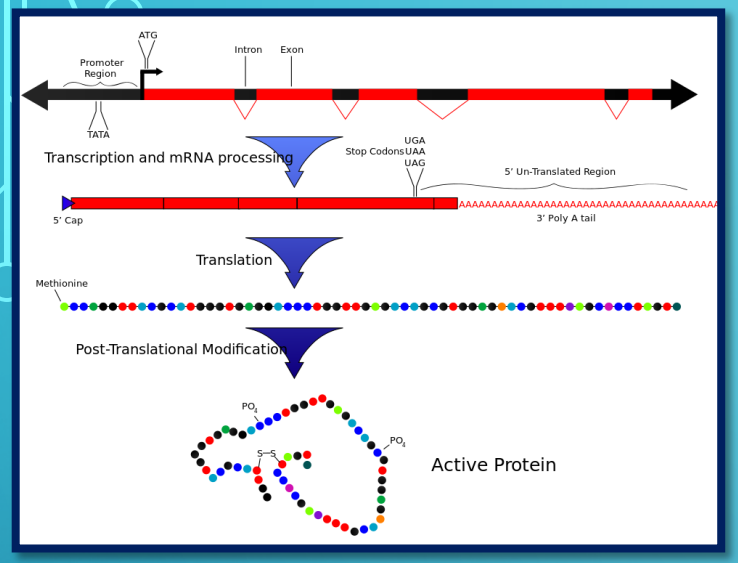
# MODULE 5 CAPSTONE

SEETA RAJPARA

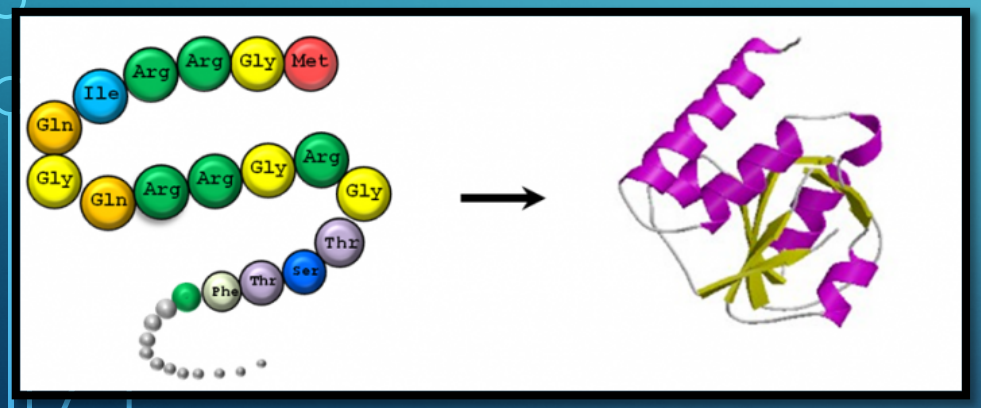
SELF-PACED DATA SCIENCE BOOTCAMP

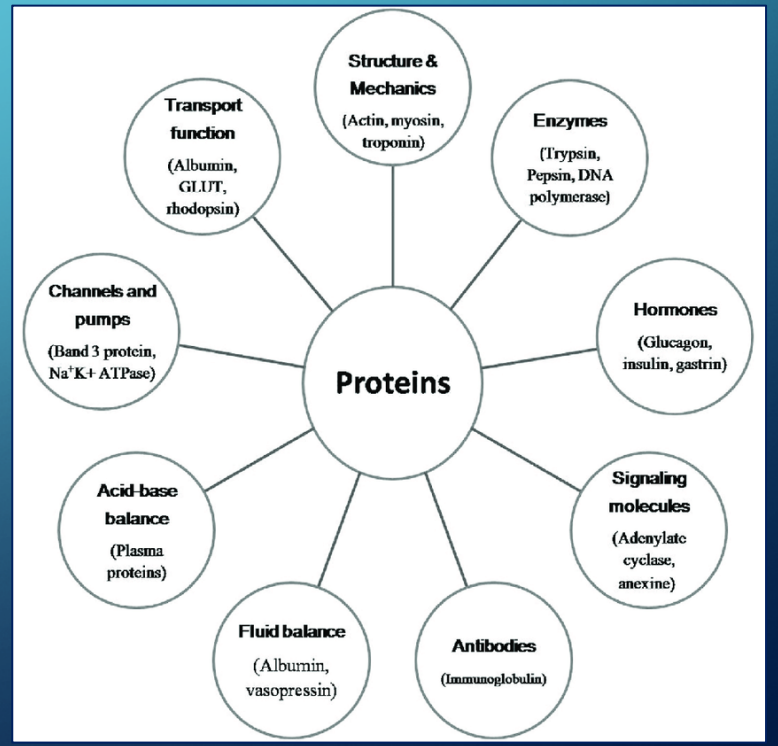
SEPTEMBER 19TH, 2021

# BACKGROUND AND PURPOSE




- DNA encodes the instructions for making proteins
- Proteins carry out all the functions of our cells
  - Made up of amino acid chains
  - 20 amino acids make up proteins found in the human body
- The sequence of amino acids influence how the proteins fold, which dictates the function of the protein
- Protein function is a vast area of research in biotechnology, and understanding this further is critical for developing therapeutics and precision diagnostics
- Dataset:
  - We have 2 .csv files
    - Physical properties
    - Amino acid sequences
    - Focusing on only top 20 classifications

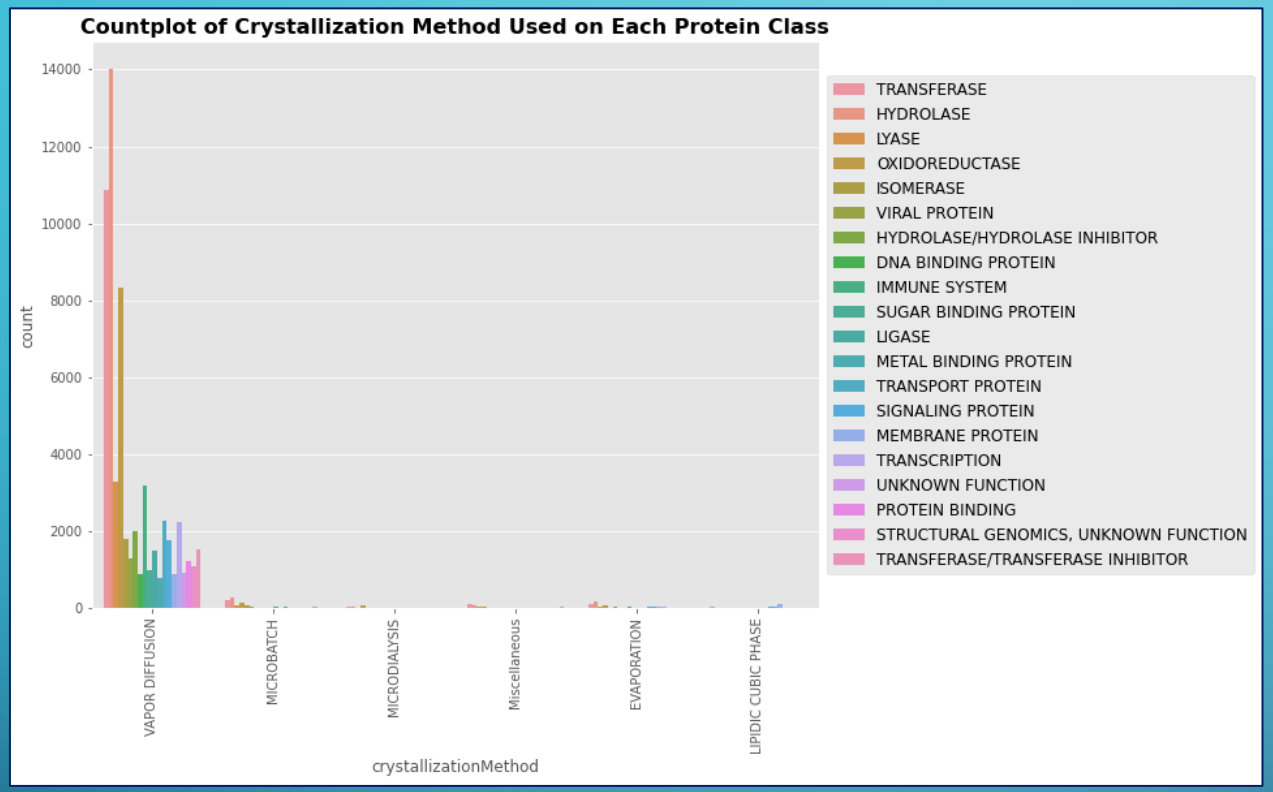



https://www.ncbi.nlm.nih.gov/books/NBK557845/

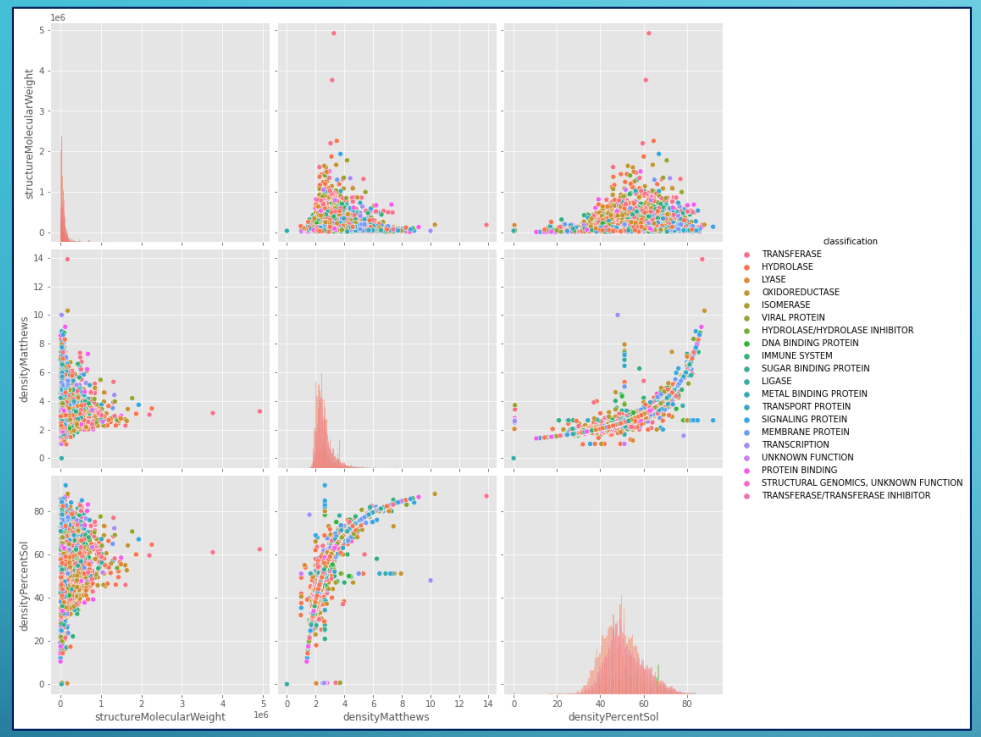
https://www.ebi.ac.uk/training/online/courses/protein-classification-intro-ebi-resources/protein-classification/

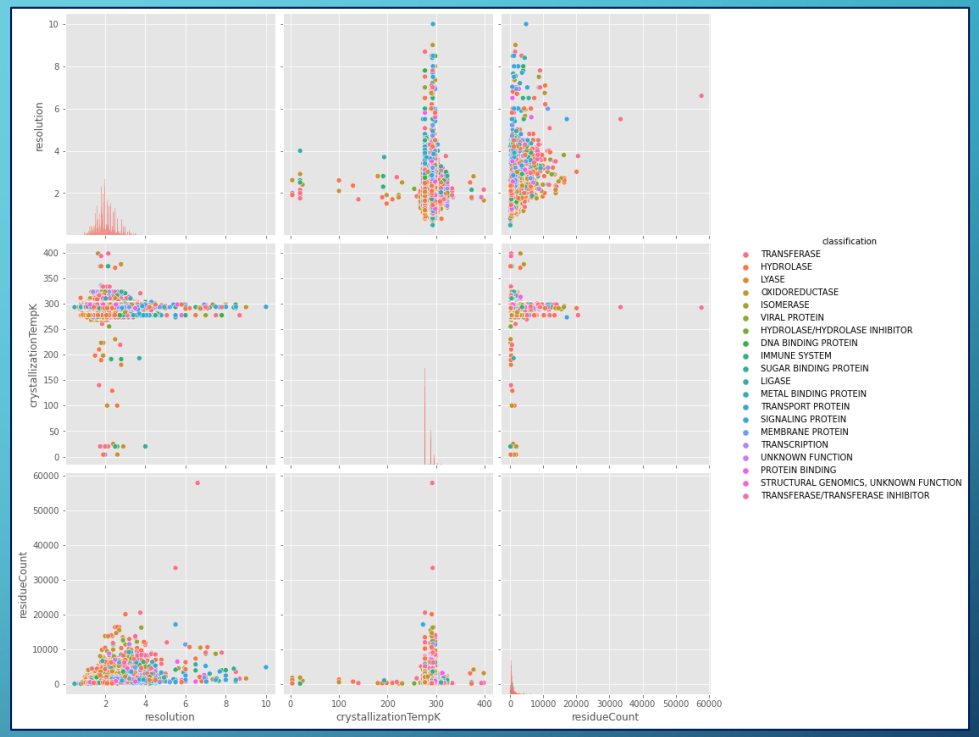
# EXPLORATORY ANALYSIS
## CATEGORICAL VARIABLE




- Various crystallization methods were used for purifying proteins from their aqueous media
- As demonstrated by this count plot, however, methods related to vapor diffusion were primarily used to generate the data in this study
- This won't be critical for us in classifying protein type

# EXPLORATORY ANALYSIS
## NUMERICAL VARIABLES

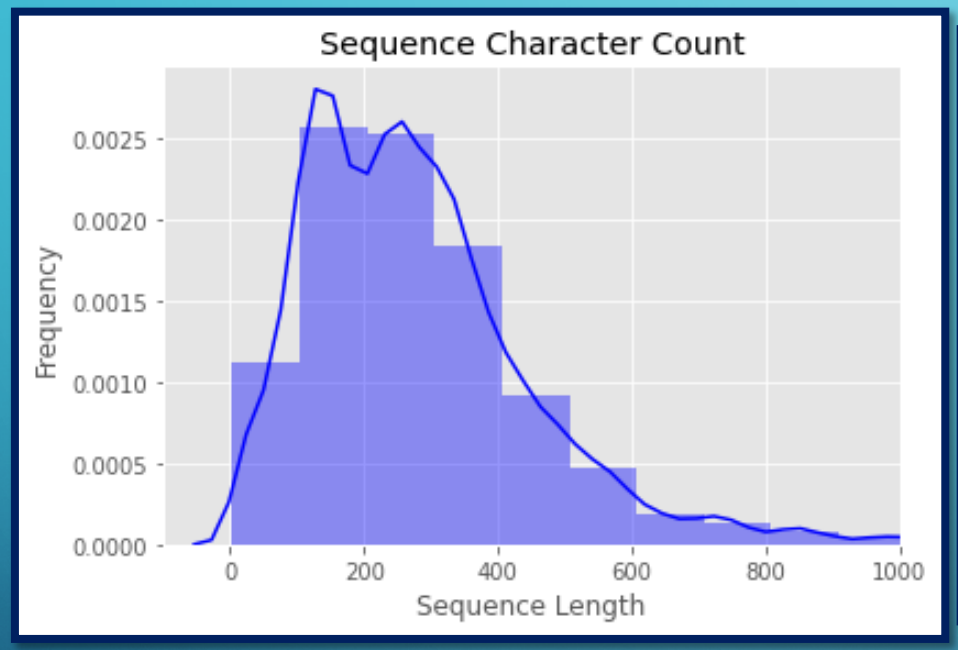


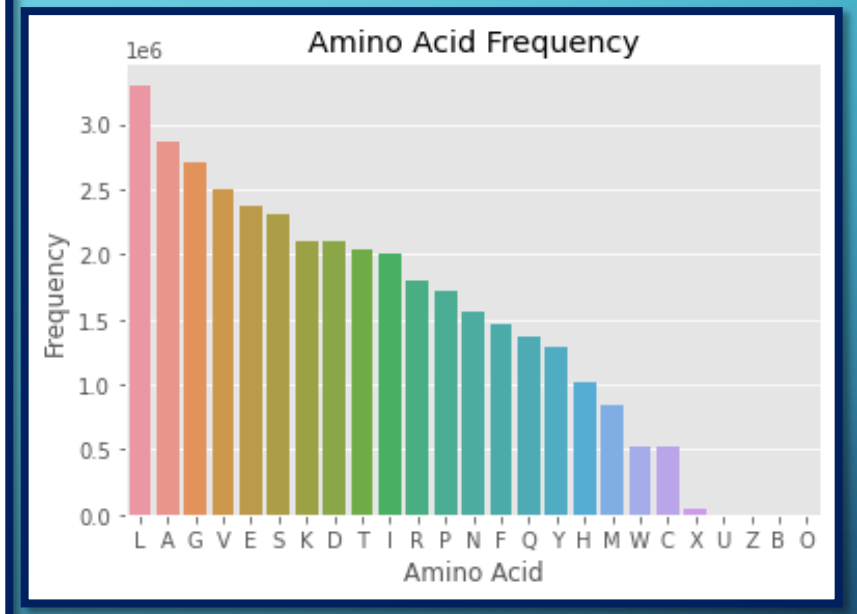




- These numerical variables don’t seem to

# SEQUENCE ANALYSIS

| | sequence | classification |
|---|---|---|
| 4 | MVLSEGEWQLVLHVWAKVEADVAGHGQDILIRLFKSHPETLEKFDR... | OXYGEN TRANSPORT |
| 7 | MNIFEMLRIDEGLRLKIYKDTEGYYTIGIGHLLTKSPSLNAAAKSE... | HYDROLASE(O-GLYCOSYL) |
| 8 | MVLSEGEWQLVLHVWAKVEADVAGHGQDILIRLFKSHPETLEKFDR... | OXYGEN TRANSPORT |
| 11 | MNIFEMLRIDEGLRLKIYKDTEGYYTIGIGHLLTKSPSLNSLDAAK... | HYDROLASE(O-GLYCOSYL) |
| 12 | MVLSEGEWQLVLHVWAKVEADVAGHGQDILIRLFKSHPETLEKFDR... | OXYGEN TRANSPORT |

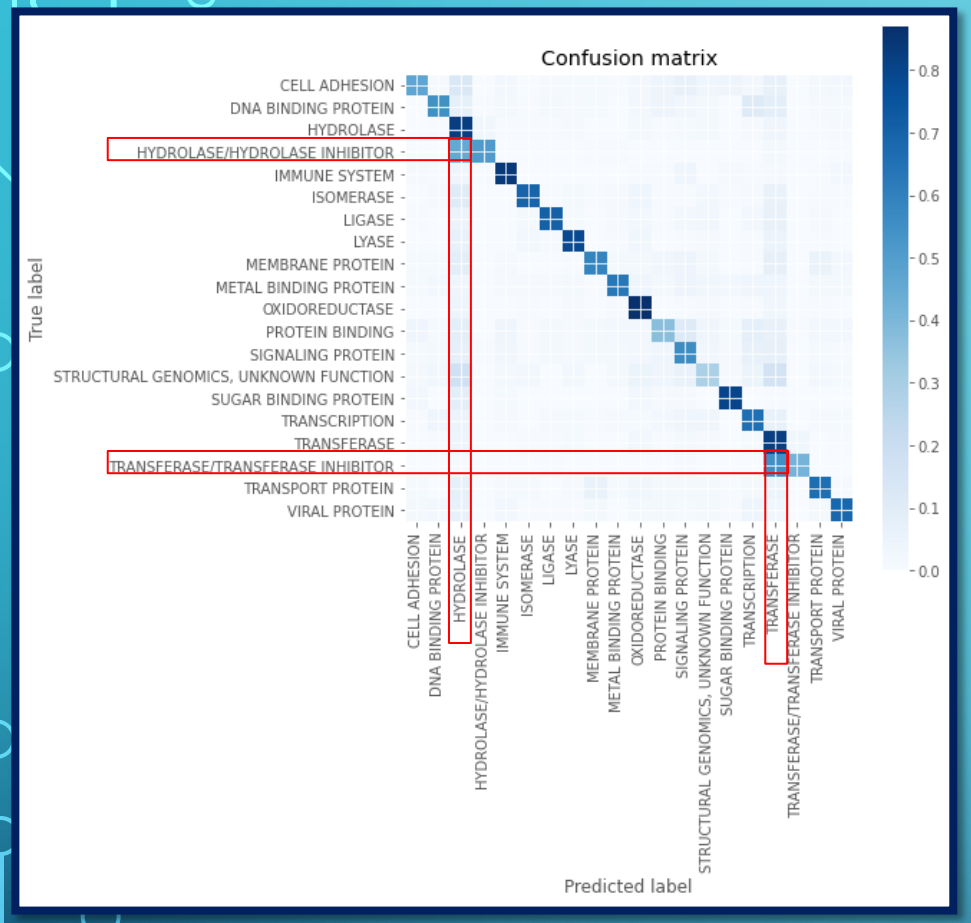


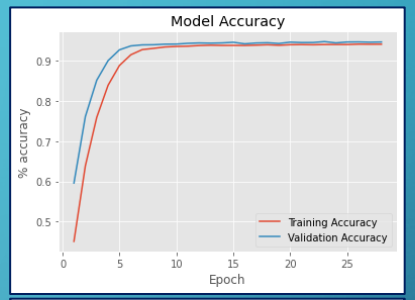

- Average length of each sequence ~285.9 AA's
- Most frequent AA is Leucine (L) which is involved in the biosynthesis of proteins
- A good model for classification using character sequences would be a recurrent neural network (RNN)

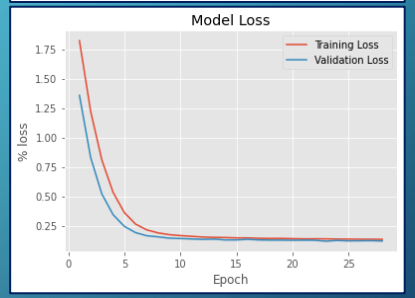
https://en.wikipedia.org/wiki/Leucine

# MODEL PERFORMANCE




| | precision | recall | f1-score | support |
|---|---|---|---|---|
| CELL ADHESION | 0.56 | 0.47 | 0.51 | 259 |
| DNA BINDING PROTEIN | 0.56 | 0.55 | 0.55 | 278 |
| HYDROLASE | 0.77 | 0.82 | 0.80 | 4025 |
| HYDROLASE/HYDROLASE INHIBITOR | 0.64 | 0.51 | 0.57 | 497 |
| IMMUNE SYSTEM | 0.86 | 0.84 | 0.85 | 786 |
| ISOMERASE | 0.76 | 0.70 | 0.73 | 519 |
| LIGASE | 0.75 | 0.71 | 0.73 | 401 |
| LYASE | 0.81 | 0.79 | 0.80 | 852 |
| MEMBRANE PROTEIN | 0.66 | 0.59 | 0.62 | 324 |
| METAL BINDING PROTEIN | 0.66 | 0.63 | 0.65 | 274 |
| OXIDOREDUCTASE | 0.88 | 0.87 | 0.87 | 2477 |
| PROTEIN BINDING | 0.50 | 0.37 | 0.43 | 408 |
| SIGNALING PROTEIN | 0.49 | 0.56 | 0.52 | 538 |
| STRUCTURAL GENOMICS, UNKNOWN FUNCTION | 0.27 | 0.29 | 0.28 | 318 |
| SUGAR BINDING PROTEIN | 0.80 | 0.80 | 0.80 | 296 |
| TRANSCRIPTION | 0.65 | 0.66 | 0.65 | 711 |
| TRANSFERASE | 0.75 | 0.82 | 0.79 | 3015 |
| TRANSFERASE/TRANSFERASE INHIBITOR | 0.58 | 0.41 | 0.48 | 332 |
| TRANSPORT PROTEIN | 0.79 | 0.66 | 0.72 | 680 |
| VIRAL PROTEIN | 0.72 | 0.69 | 0.70 | 488 |
| accuracy | | | 0.74 | 17478 |
| macro avg | 0.67 | 0.64 | 0.65 | 17478 |
| weighted avg | 0.74 | 0.74 | 0.74 | 17478 |

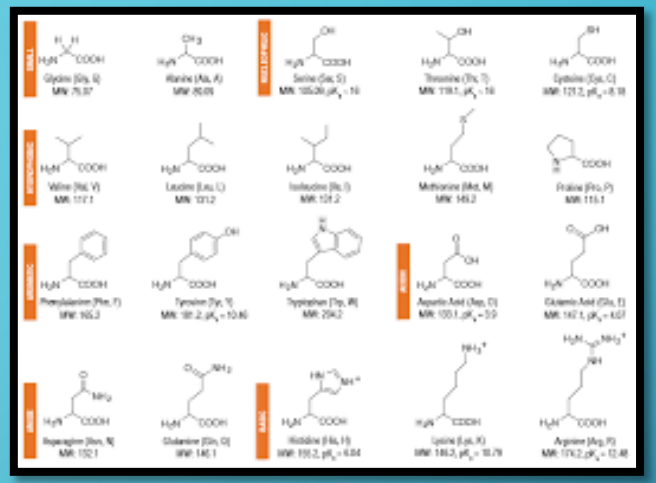


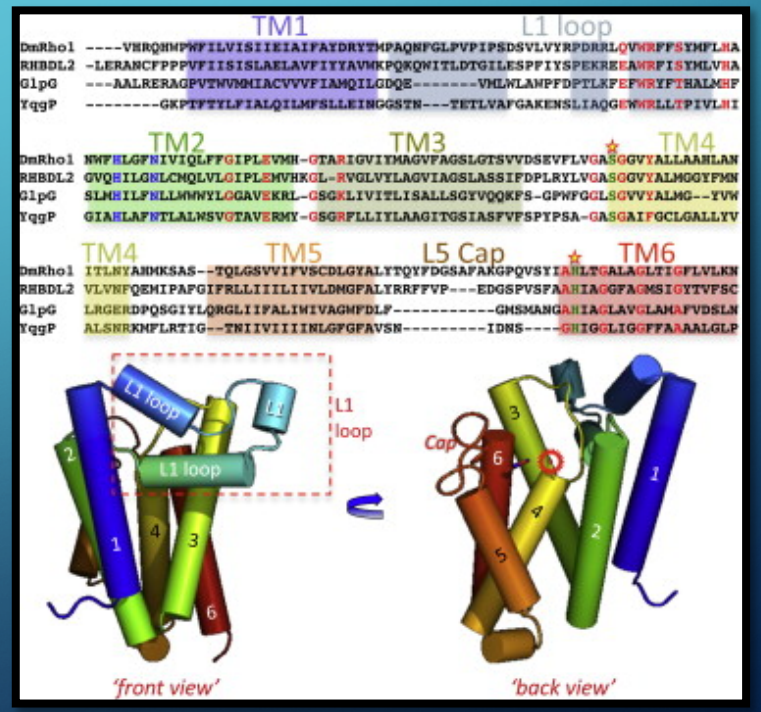




- With a specific type of RNN model (long short term memory, LSTM), we are able to predict protein classification with relatively high precision as plotted above
- This shows that the sequence of amino acids inform protein function to a high degree and this can be used as key to understanding protein function

# CONCLUSIONS AND FUTURE STEPS

1) Protein classification is influenced by amino acid sequence
2) Many physical properties are shared by proteins of all classes, but granular data can be extracted from these features
3) Experimental techniques applied to each protein classification are often the same, but building more general classes for each protein type specified in the dataset could help mitigate the issues with data notation



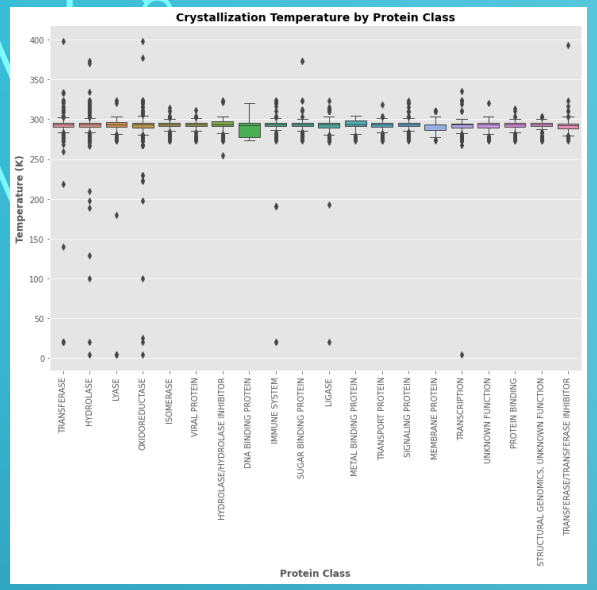


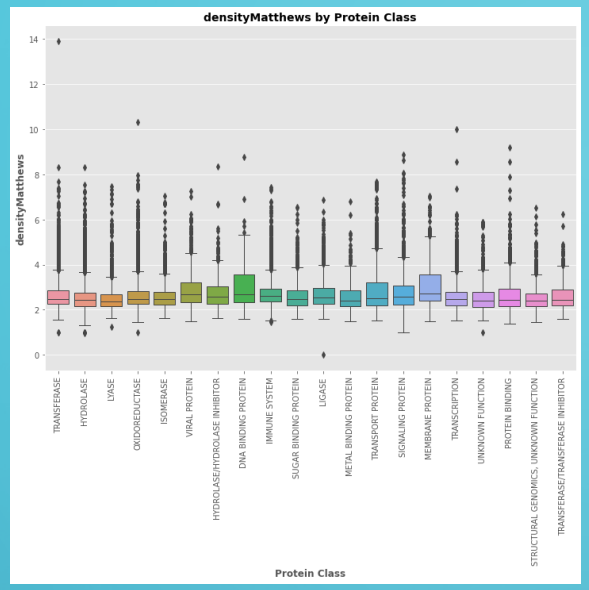

Next Steps

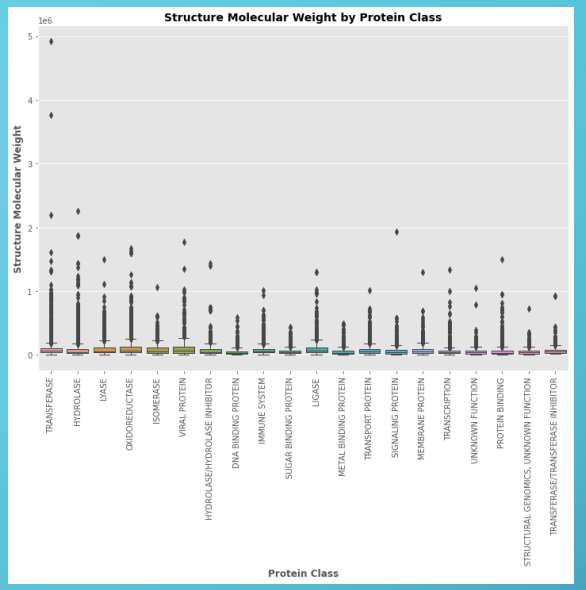
- Try focusing only on the top 10 protein classifications instead of top 20, might get better results with fewer labels
- Include numerical variables into a mixed model, somehow incorporating regression and RNN models to predict with high precision

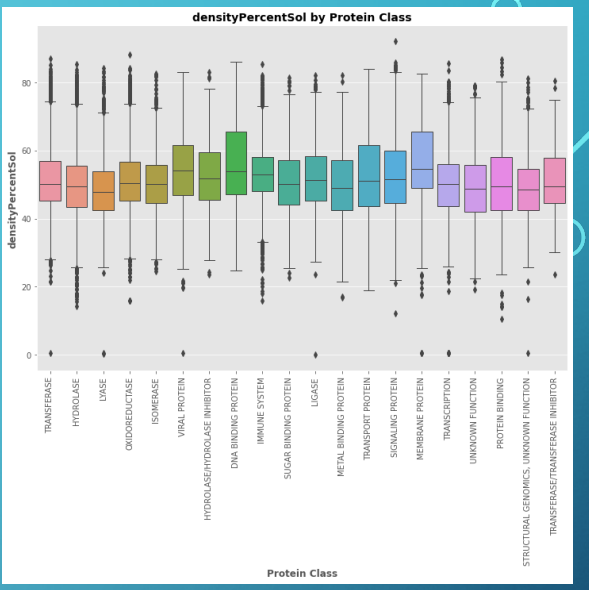
# THANK YOU!

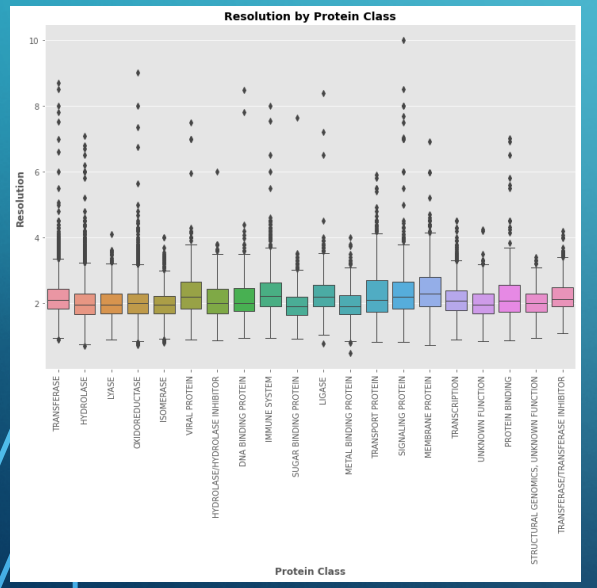
# APPENDIX

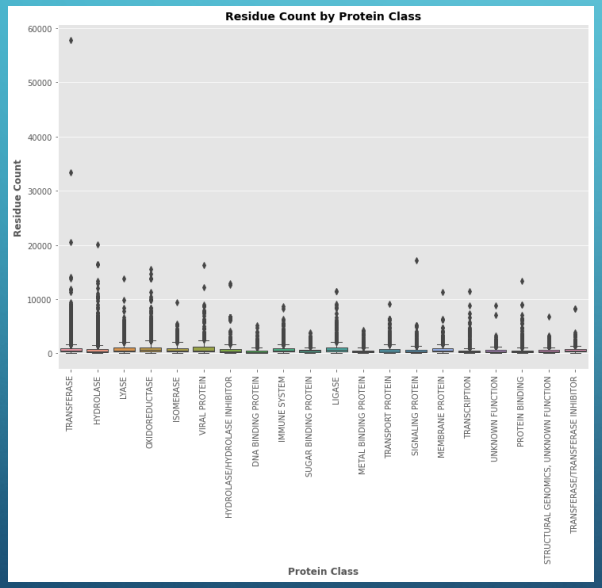

Crystallization Temperature by Protein Class
Temperature (K)
Protein Class
TRANSFERASE
HYDROLASE
LYASE
OXIDOREDUCTASE
ISOMERASE
VIRAL PROTEIN
HYDROLASE/HYDROLASE INHIBITOR
DNA BINDING PROTEIN
IMMUNE SYSTEM
SUGAR BINDING PROTEIN
LIGASE
METAL BINDING PROTEIN
TRANSPORT PROTEIN
SIGNALING PROTEIN
MEMBRANE PROTEIN
TRANSCRIPTION
UNKNOWN FUNCTION
PROTEIN BINDING
STRUCTURAL GENOMICS, UNKNOWN FUNCTION
TRANSFERASE/TRANSFERASE INHIBITOR

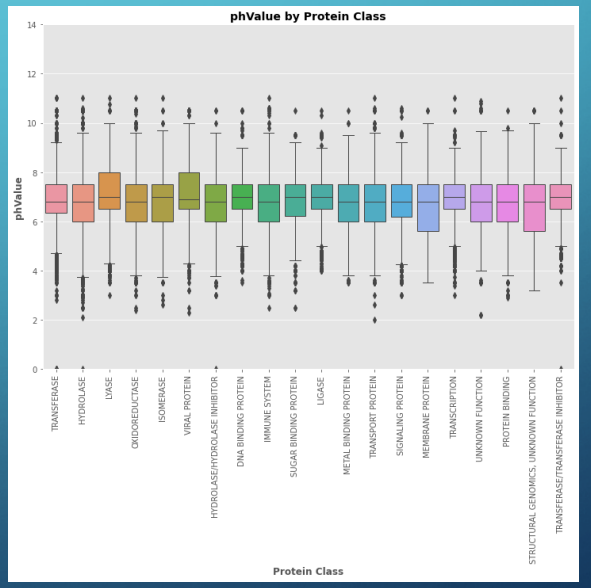

densityMatthews by Protein Class
densityMatthews
Protein Class
TRANSFERASE
HYDROLASE
LYASE
OXIDOREDUCTASE
ISOMERASE
VIRAL PROTEIN
HYDROLASE/HYDROLASE INHIBITOR
DNA BINDING PROTEIN
IMMUNE SYSTEM
SUGAR BINDING PROTEIN
LIGASE
METAL BINDING PROTEIN
TRANSPORT PROTEIN
SIGNALING PROTEIN
MEMBRANE PROTEIN
TRANSCRIPTION
UNKNOWN FUNCTION
PROTEIN BINDING
STRUCTURAL GENOMICS, UNKNOWN FUNCTION
TRANSFERASE/TRANSFERASE INHIBITOR

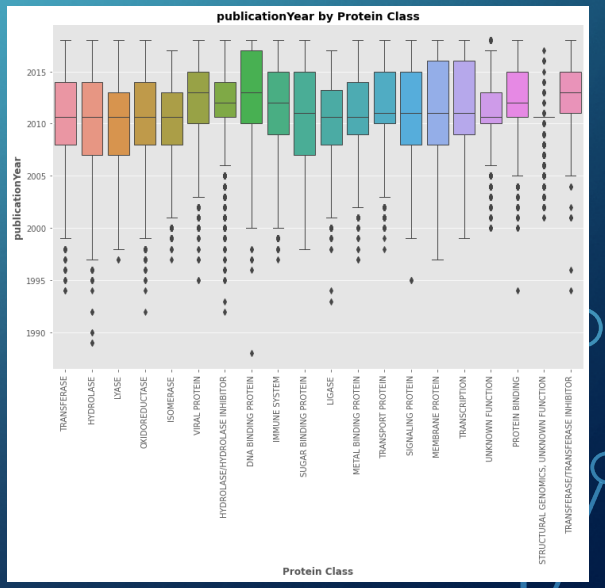

Structure Molecular Weight by Protein Class
1e6
Structure Molecular Weight
Protein Class
TRANSFERASE
HYDROLASE
LYASE
OXIDOREDUCTASE
ISOMERASE
VIRAL PROTEIN
HYDROLASE/HYDROLASE INHIBITOR
DNA BINDING PROTEIN
IMMUNE SYSTEM
SUGAR BINDING PROTEIN
LIGASE
METAL BINDING PROTEIN
TRANSPORT PROTEIN
SIGNALING PROTEIN
MEMBRANE PROTEIN
TRANSCRIPTION
UNKNOWN FUNCTION
PROTEIN BINDING
STRUCTURAL GENOMICS, UNKNOWN FUNCTION
TRANSFERASE/TRANSFERASE INHIBITOR


densityPercentSol by Protein Class
densityPercentSol
Protein Class
TRANSFERASE
HYDROLASE
LYASE
OXIDOREDUCTASE
ISOMERASE
VIRAL PROTEIN
HYDROLASE/HYDROLASE INHIBITOR
DNA BINDING PROTEIN
IMMUNE SYSTEM
SUGAR BINDING PROTEIN
LIGASE
METAL BINDING PROTEIN
TRANSPORT PROTEIN
SIGNALING PROTEIN
MEMBRANE PROTEIN
TRANSCRIPTION
UNKNOWN FUNCTION
PROTEIN BINDING
STRUCTURAL GENOMICS, UNKNOWN FUNCTION
TRANSFERASE/TRANSFERASE INHIBITOR


Resolution by Protein Class
Resolution
Protein Class
TRANSFERASE
HYDROLASE
LYASE
OXIDOREDUCTASE
ISOMERASE
VIRAL PROTEIN
HYDROLASE/HYDROLASE INHIBITOR
DNA BINDING PROTEIN
IMMUNE SYSTEM
SUGAR BINDING PROTEIN
LIGASE
METAL BINDING PROTEIN
TRANSPORT PROTEIN
SIGNALING PROTEIN
MEMBRANE PROTEIN
TRANSCRIPTION
UNKNOWN FUNCTION
PROTEIN BINDING
STRUCTURAL GENOMICS, UNKNOWN FUNCTION
TRANSFERASE/TRANSFERASE INHIBITOR


Residue Count by Protein Class
Residue Count
Protein Class
TRANSFERASE
HYDROLASE
LYASE
OXIDOREDUCTASE
ISOMERASE
VIRAL PROTEIN
HYDROLASE/HYDROLASE INHIBITOR
DNA BINDING PROTEIN
IMMUNE SYSTEM
SUGAR BINDING PROTEIN
LIGASE
METAL BINDING PROTEIN
TRANSPORT PROTEIN
SIGNALING PROTEIN
MEMBRANE PROTEIN
TRANSCRIPTION
UNKNOWN FUNCTION
PROTEIN BINDING
STRUCTURAL GENOMICS, UNKNOWN FUNCTION
TRANSFERASE/TRANSFERASE INHIBITOR


phValue by Protein Class
phValue
Protein Class
TRANSFERASE
HYDROLASE
LYASE
OXIDOREDUCTASE
ISOMERASE
VIRAL PROTEIN
HYDROLASE/HYDROLASE INHIBITOR
DNA BINDING PROTEIN
IMMUNE SYSTEM
SUGAR BINDING PROTEIN
LIGASE
METAL BINDING PROTEIN
TRANSPORT PROTEIN
SIGNALING PROTEIN
MEMBRANE PROTEIN
TRANSCRIPTION
UNKNOWN FUNCTION
PROTEIN BINDING
STRUCTURAL GENOMICS, UNKNOWN FUNCTION
TRANSFERASE/TRANSFERASE INHIBITOR


publicationYear by Protein Class
publicationYear
Protein Class
TRANSFERASE
HYDROLASE
LYASE
OXIDOREDUCTASE
ISOMERASE
VIRAL PROTEIN
HYDROLASE/HYDROLASE INHIBITOR
DNA BINDING PROTEIN
IMMUNE SYSTEM
SUGAR BINDING PROTEIN
LIGASE
METAL BINDING PROTEIN
TRANSPORT PROTEIN
SIGNALING PROTEIN
MEMBRANE PROTEIN
TRANSCRIPTION
UNKNOWN FUNCTION
PROTEIN BINDING
STRUCTURAL GENOMICS, UNKNOWN FUNCTION
TRANSFERASE/TRANSFERASE INHIBITOR