Protein Classification

Functional & Cellular Location Prediction

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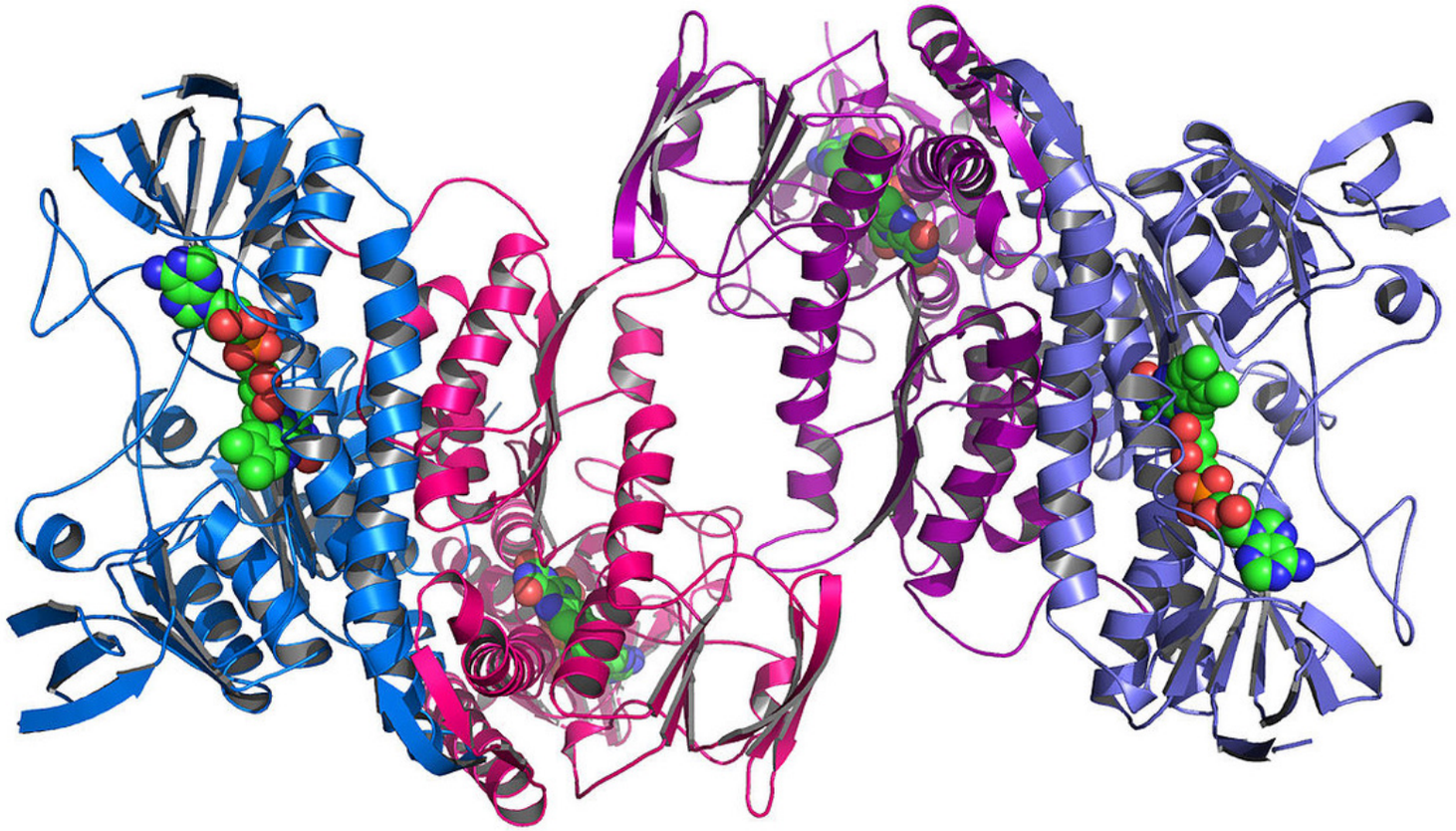
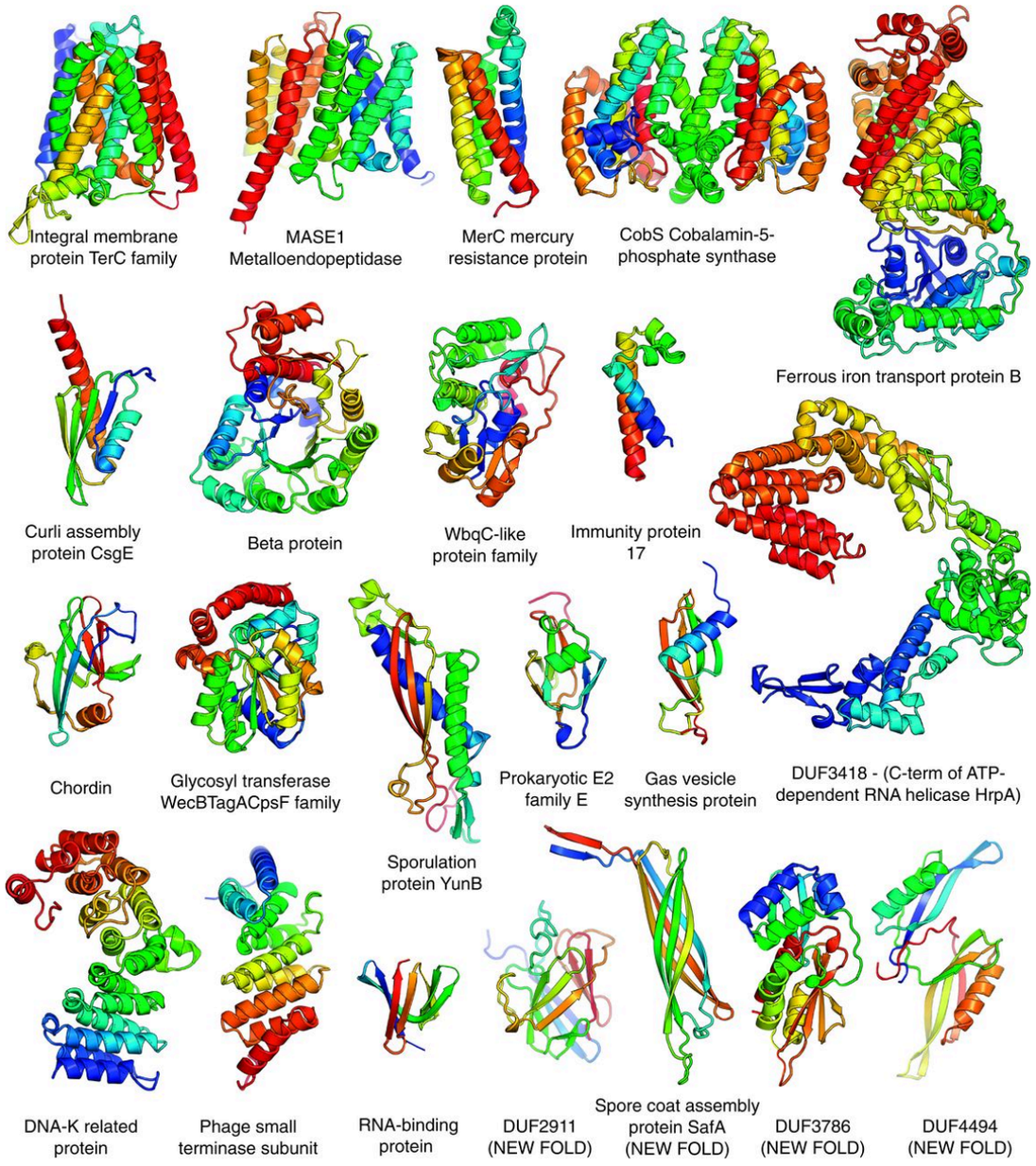


Proteins

- **Biological Polymers**
- **Made of 20 naturally occurring amino acids**
- **Essential for life: enzymes, immune system defenders, necessary for thought, sensation, digestion, breathing, …..**



Outline

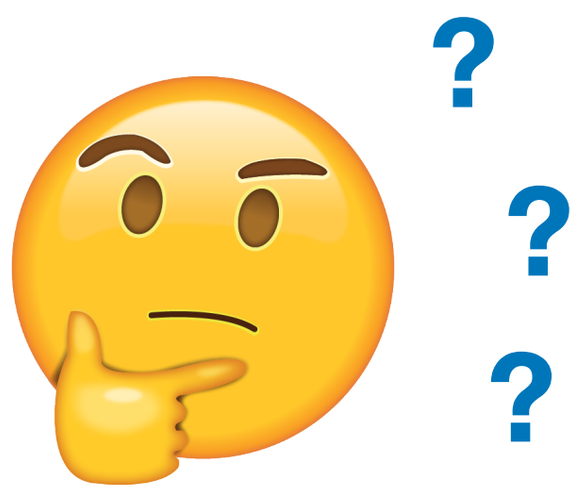
- **Supervised Machine Learning Classification *using only the Protein Amino Acid Sequence***

- **Predict the function: *what does the protein do?***

- **Predict the cellular location: *where is the protein inside the cell?***

Motivation

- *A scientist in biotech industry or academia discovers a novel Protein that plays a vital role in some disease*



- *How to determine what it does? Or where it is located?*

- *One solution: apply Machine Learning Methods to predict the function and location ….Save time & energy*

Functional Class

What does the protein do?

Some Functions:

Hydrolase (a type of enzyme)

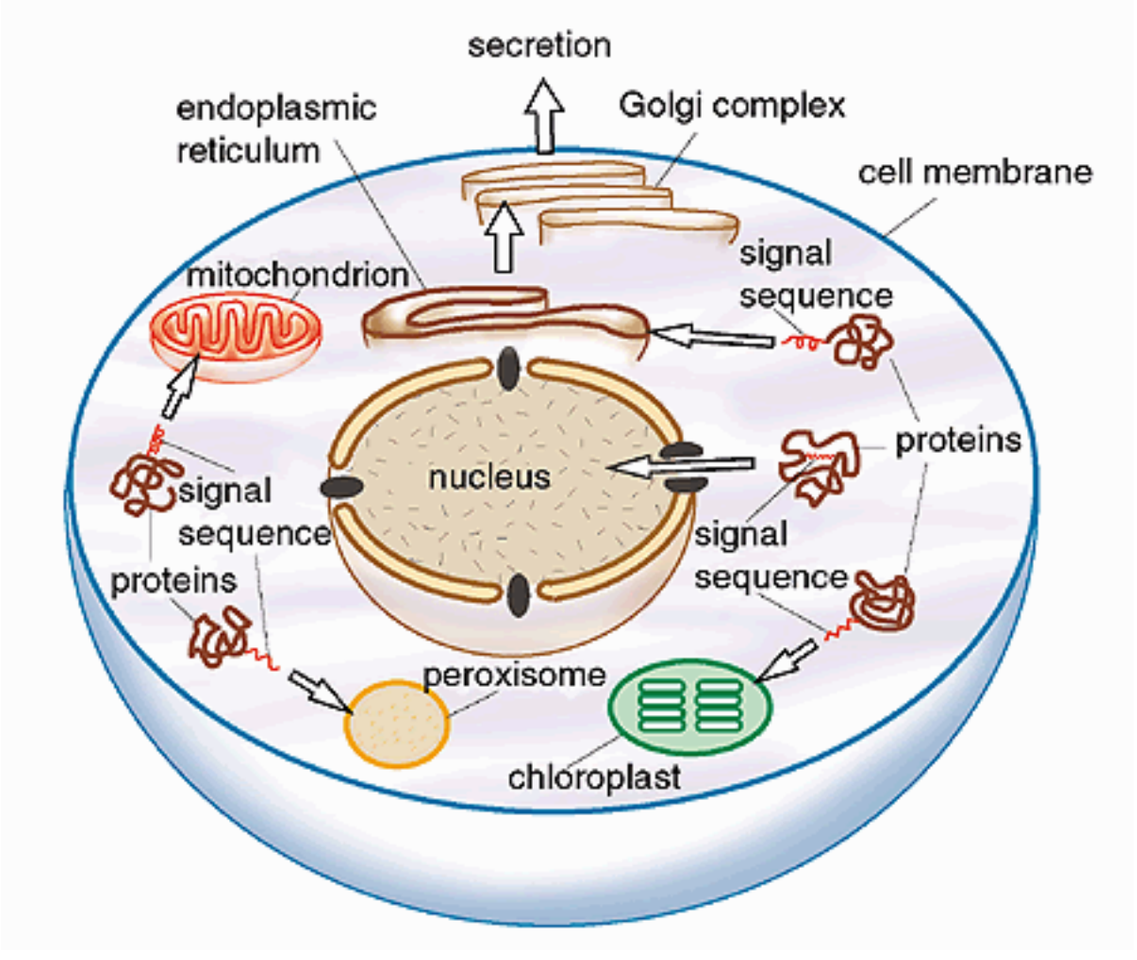
DNA binding

Transporter

Immune system

Cellular Location

- Cell is divided into compartments
- Each protein has it's own location inside the cell
- Predict where the protein is: Nucleus? ER? mitochondrion?….etc, etc



Peptide Count:

Sliding Window

WALALEU

WALALEU

WALALEU

WALALEU

WALALEU

WAL	ALA	LAL	ALE	LEU	PAW
1	1	1	1	1	0

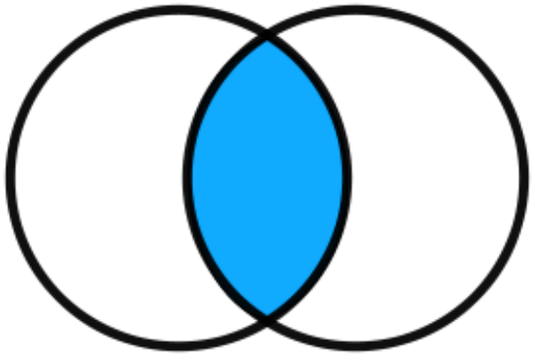
One-Hot Encoding

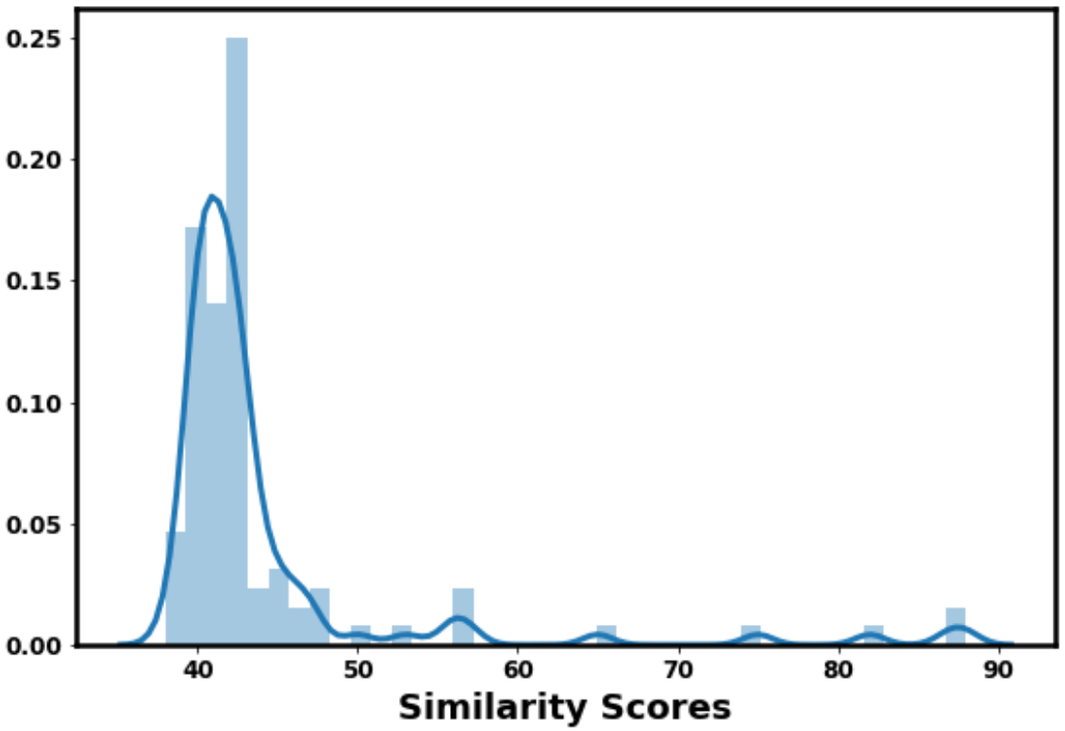
Count Vectorizer

String is converted into a Vector

Using Peptide (Substring) Count with Sliding Window

“all models are flawed, but some are useful”





Fuzzy Wuzzy Analysis for String Comparison

100 Hydrolase sequences were compared with Transporter Sequences using Fuzzy Wuzzy

Most Hydrolases have < 50% similarity with Transporter sequences.

But,some have more than 70% similarity……
Overlapping categories

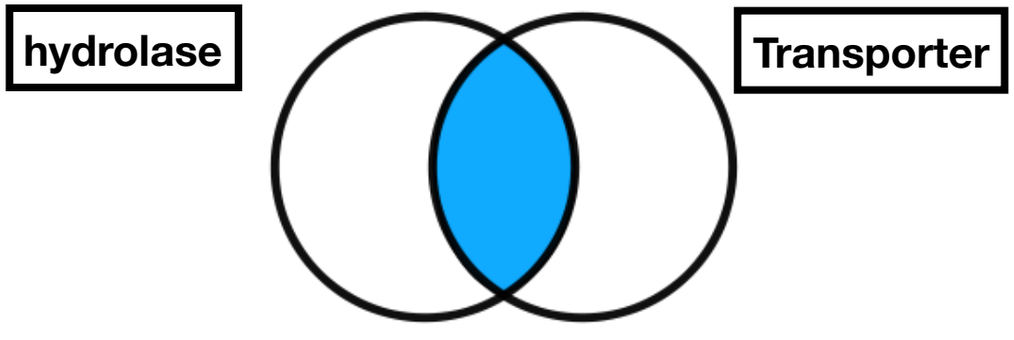
ABC Transporters

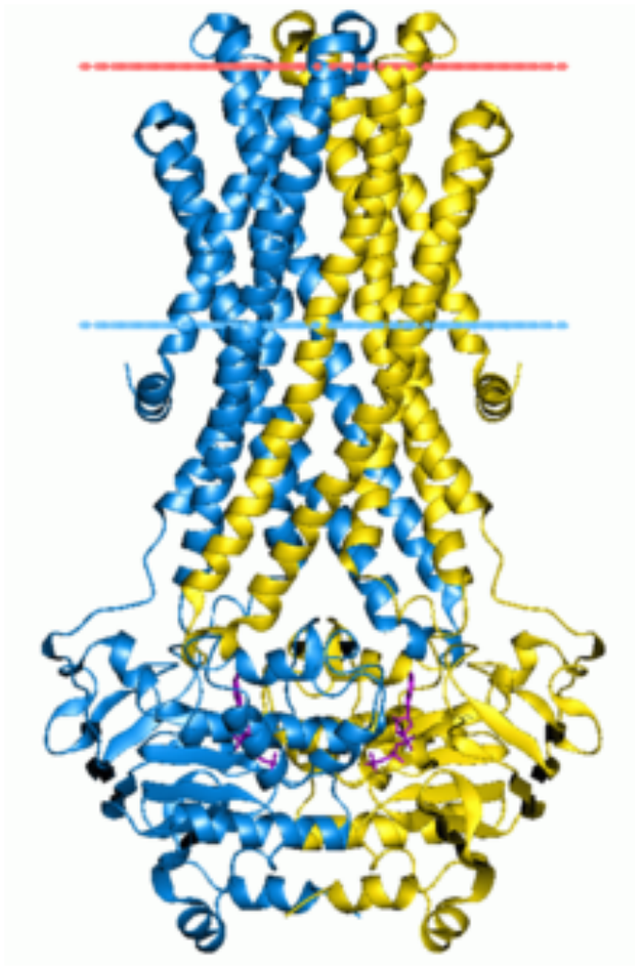
ABC Transporters are proteins that can be classified as <u>BOTH</u>:

a hydrolase (an enzyme)!

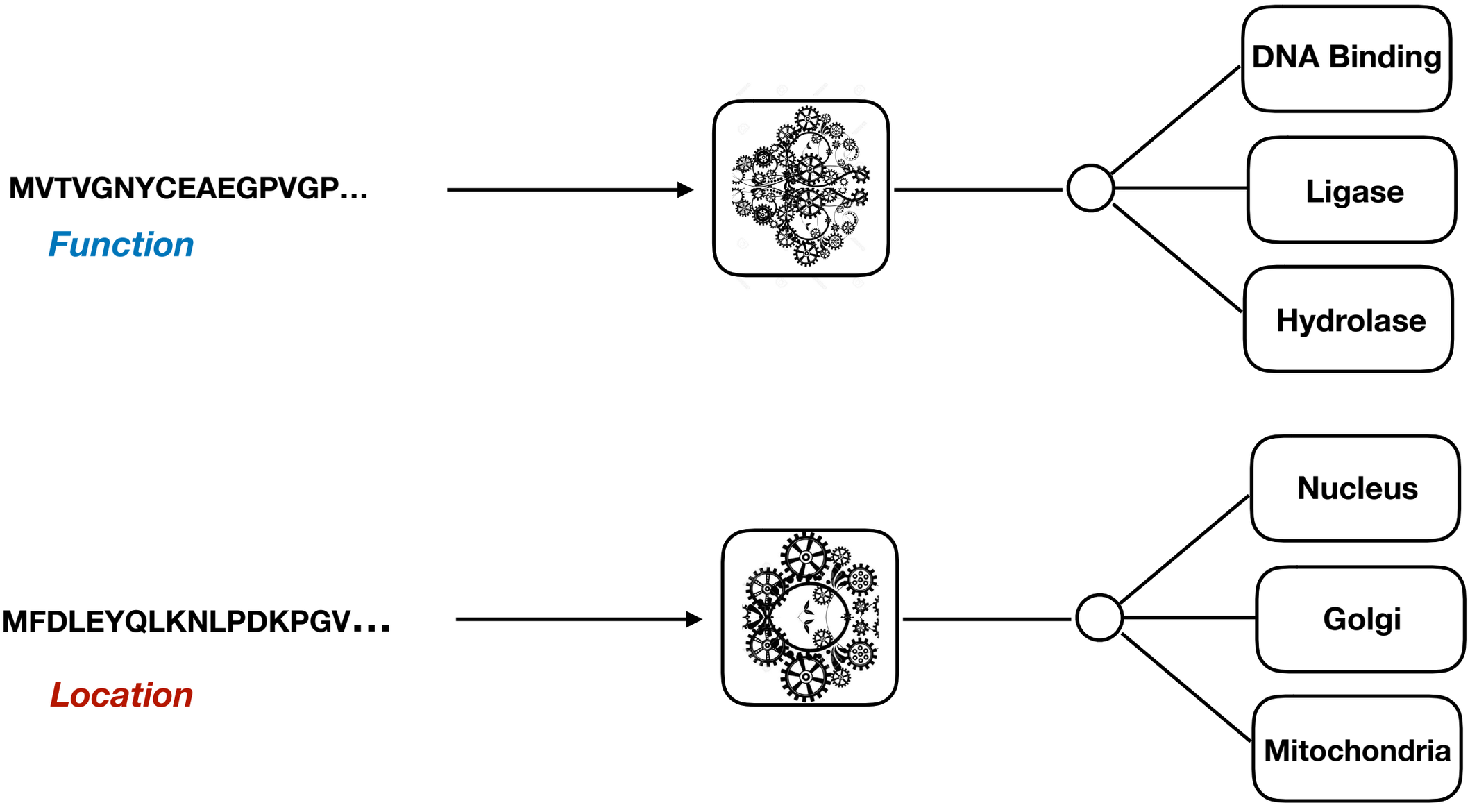
<u>AND</u> a Transporter!

Belong to 2 Functional Classes!





Machine Learning Classification



Classifiers

- **Function Prediction:** **Majority Voting Classifer** **made of *Linear Model SGD*, *Passive Aggressive Classifier*, & *Multinomial Naive Bayes***

- **Location Prediction:** **Majority Voting Classifer** **made of *Linear Model SGD*, *Passive Aggressive Classifier*, *Perceptron*, & *Multinomial Naive Bayes***

Accuracy & F1 Scores

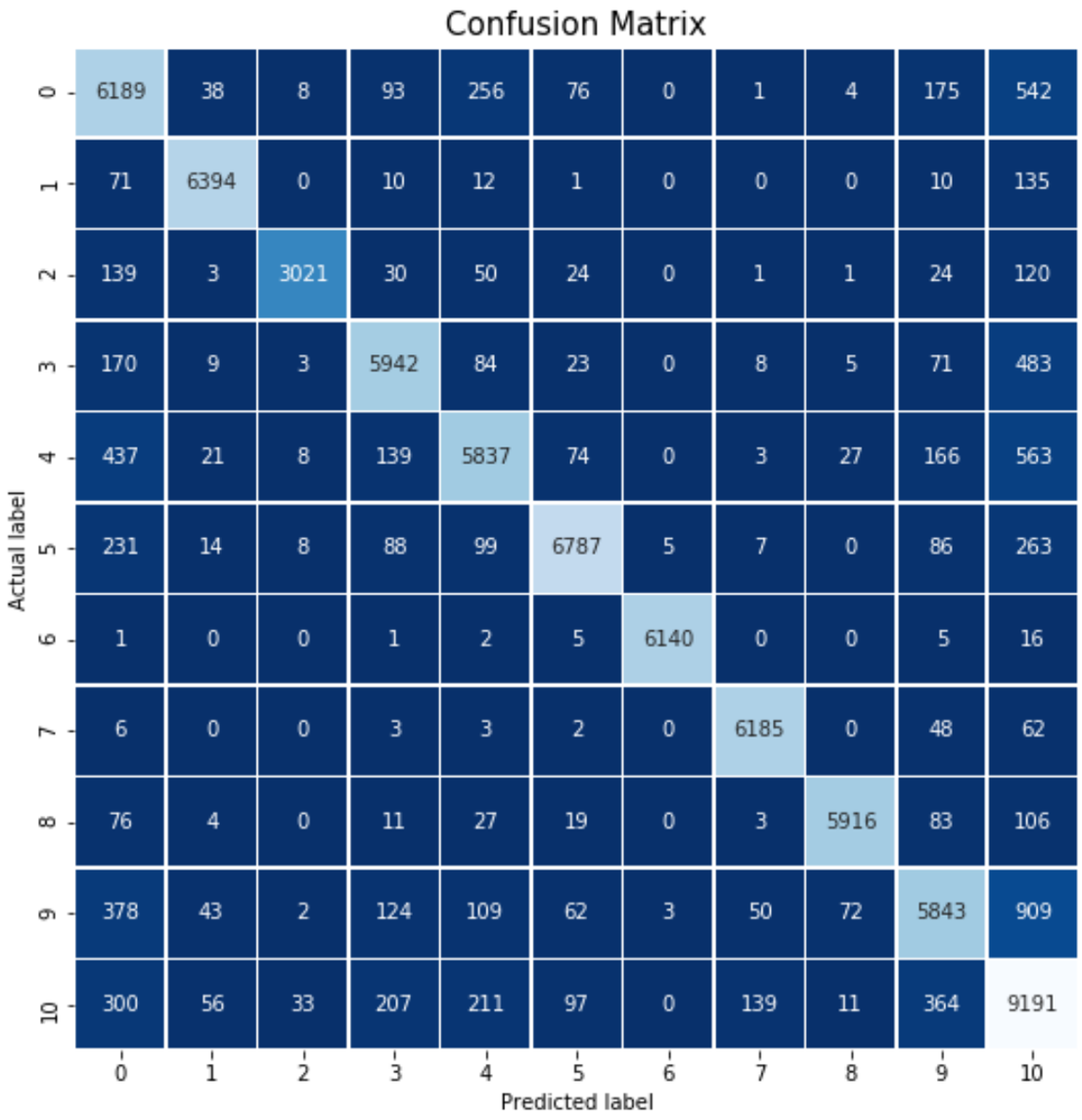
- ***Accuracy on Test Data For Function Classification Model: 89%***

- ***F1 Score Range for Function Classification Model: 0.81-1.0***

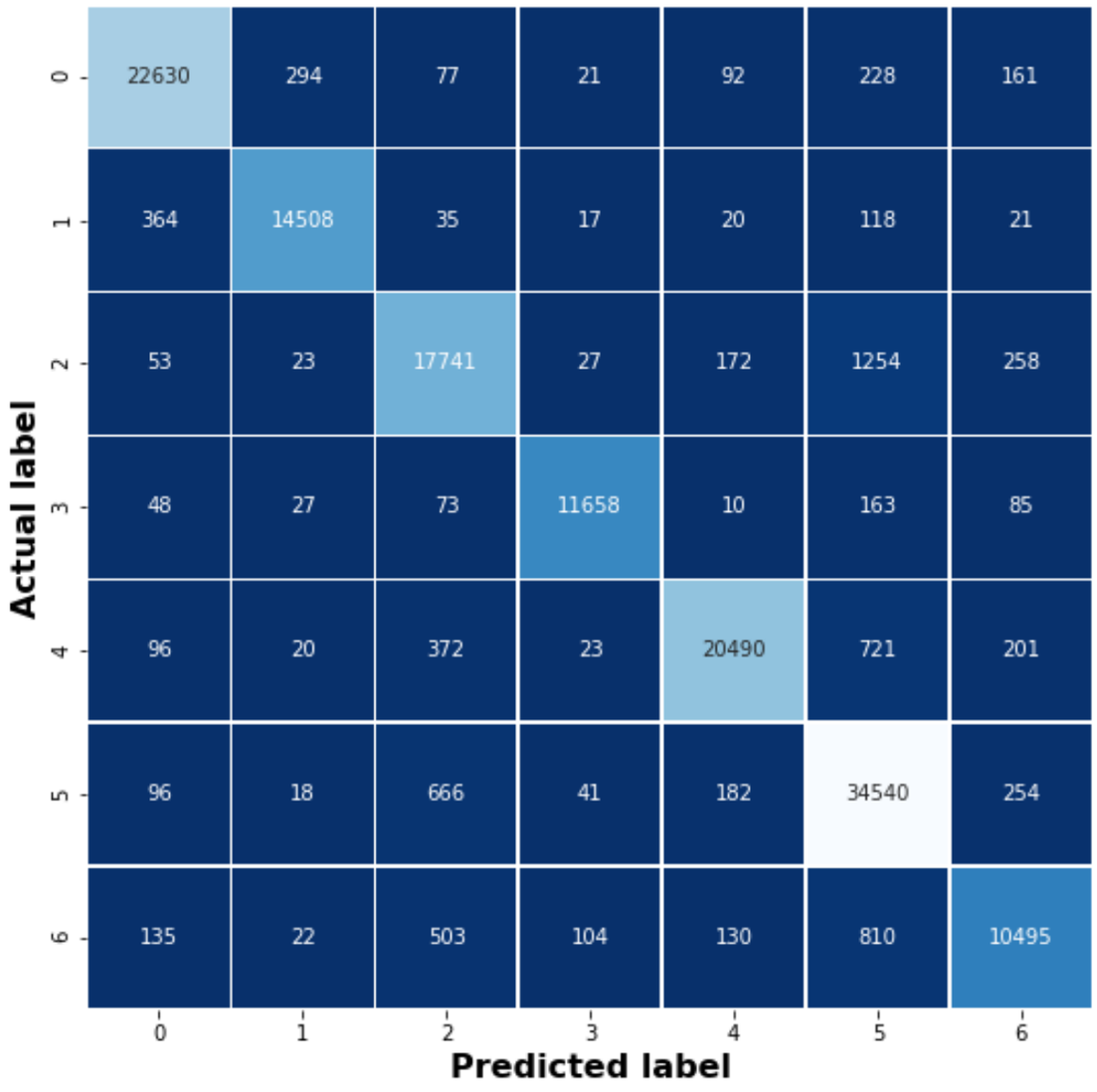
- ***Accuracy on Test Data For Location Classification Model: 94%***

- ***F1 Score Range for Location Classification Model: 0.89-0.97***

Confusion Matrices



Function Prediction



Location Prediction

Conclusions

- ***Machine Learning can predict both the function & location of a novel protein***

- ***ML Models can predict 11 Functions & 7 Cellular Locations***

- ***Overlapping protein classes can be tricky to predict***