

Title:

3D Structure Prediction from Protein Sequences Using Computational Methods

Problem Statement:

Calculate protein aggregation in a given protein sequence.

Algorithm:

1. **Data Collection:** Collect protein sequences and structural data from datasets like Protein Data Bank (PDB) and UniProt.
2. **Sequence Analysis:**
 - Predict secondary structure using tools like PSIPRED.
3. **Model Refinement:** Use energy minimization techniques (e.g., PyRosetta) to refine and stabilize the predicted 3D model.
4. **Validation:** Validate the predicted structure using quality assessment tools like PROCHECK.

Dataset Authentication:

1. Protein Data Bank (PDB):
2. Kaggle Protein Datasets

Expected Output:

The project aims to generate accurate 3D models of proteins from their sequences and calculate protein aggregation in a given protein sequence.

Team members:

Mahalaya – 2320040027, Divya Sri - 2320040141

