

Parkinson's Disease Prediction in AI

ABSTRACT:

Parkinson's Disease (PD) is a progressive neurodegenerative disorder characterized by the loss of dopaminergic neurons in the brain. A significant factor in the disease's pathogenesis is the misfolding and aggregation of alpha-synuclein protein, leading to the formation of insoluble Lewy bodies. Understanding the 3D structure of these proteins and their pathological variants is critical for uncovering disease mechanisms and designing targeted therapeutics.

This project aims to leverage Artificial Intelligence (AI) and bioinformatics to predict and analyze the 3D structures of proteins associated with Parkinson's Disease. By utilizing amino acid sequence data from the Protein Data Bank (PDB) and advanced computational techniques, the project seeks to identify structural features linked to protein misfolding and aggregation, aiding in drug discovery and therapeutic advancements.

DATASET:

Title: Protein Data Bank (PDB)

Source: RCSB Protein Data Bank

Content: Protein structures associated with Parkinson's Disease, including alpha-synuclein and related proteins.

ALGORITHM:

1. Data Collection

- Extract protein sequences and structural data for alpha-synuclein and other PD-associated proteins from the PDB.

2. Sequence Analysis

- **Secondary Structure Prediction:** Use AI-powered tools like AlphaFold or PSIPRED to predict structural motifs such as alpha-helices and beta-sheets.
- **Homology Modeling:** Employ AI-assisted homology modeling techniques using MODELLER to generate 3D structural models based on templates from the PDB.

3. Aggregation Prediction

- **Machine Learning:** Develop and train an AI model using protein aggregation datasets to identify aggregation-prone regions in alpha-synuclein sequences.

4. Model Refinement

- Refine the predicted 3D structures using energy minimization techniques such as PyRosetta, ensuring stability and accuracy.

5. Validation

- Validate the structural models using tools like PROCHECK and AI-based validation systems for higher accuracy in quality assessment.

6. Visualization

- Visualize the 3D structures and identified aggregation-prone regions using molecular visualization tools like PyMOL or Chimera.

POSTER:

PARKINSON'S DISEASE PREDICTION IN AI

PROBLEM STATEMENT:

PARKINSON'S DISEASE ANALYSIS USING ARTIFICIAL INTELLIGENCE

Algorithm:

Extract protein sequences and structure data from PDB. Predict secondary with AlphaFold; generate 3D models with MODELLER.

Use AI to identify aggregation-prone regions in sequences. Refine models using PyRosetta for stability.

Dataset:

Title: Protein Data Bank(PDB)

Source: RCSB Protein Data Bank

Expected Output:

→ Identify misfolding and aggregation Patterns using AI

→ Predict binding sites for therapeutic Molecules

→ Enhance understanding of Parkinson's Disease mechanisms



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