International Journal of Scientific Research in Engineering and Management (IJSREM)
Volume: 09 Issue: 12 | Dec - 2025 SJIF Rating: 8.586 ISSN: 2582-3930

Protein Structure Prediction Using AI

Divya Tyagi [1]
Dept of Information Science and
Engineering (ISE) AMCEC
divyatyagi@amceducation.in

Meghana S R[2], Arun Kumar K S[3], Swathi Reddy K A[4] , Ashwini Ishwar Naik [5]

Dept of information Science and
Engineering (ISE)AMCEC
1am22is062@amceducation.in , 1am22is016@amceducation.in, 1am22is115@amceducation.in ,
1am22is017@amceducation.in

Abstract – Understanding Protein Structure is crucial a as a protein's three dimension (3D) configuration. Traditional laboratory methods, including x-ray crystallography and Nuclear Magnetic Resonance (NMR), provide precise structural details bit are expensive, labor-intensive, and time consuming.
With exponential growth of protein sequence data, computational methods have become essential for bridging the gap between sequence availability and structural knowledge.

This paper introduces a web-based platform that leverages Artificial Intelligence (AI) and Deep Learning to predict protein structure from Amino acid Sequences. The system integrates a secure backend with modern web technologies to deliver accurate predictions and interactive 3D visualization. Users can put input amino acid sequence, Obtain predicted 3D structures, and explore them within browser environment. The platform demonstrates hoe AI-enabled protein structure prediction can be made accessible for educational, research, and computational biology applications.

Key words: Protein Structure Prediction, Artificial Intelligence, Deep Learning, Bioinformatics, 3D Visualization, Web Application.

1. INTRODUCTION

Proteins essential molecules that perform a variety of biological functions, such as enzymatic activity, cellular signaling, molecular transport, and structural support. The functionality of a protein is largely determined by its 3D structure, which results from the folding of its amino acid sequence. Understanding protein structure is therefore crucial in molecular biology, medicine, and drug discovery.

Experimental methods for protein structure determination, including X-ray crystallography, NMR spectroscopy, and cryo-electron microscopy, high-resolution results bit are limited by high cost, long processing time, and technical complexity. As genome sequencing technologies continue to generate vast amounts of protein sequence data, the gap between known sequences and known structures has increased significantly.

Artificial Intelligence, particularly deep learning, offers a promising solution. AI models can learn complex folding patterns from large datasets and predict protein 3D structures directly from amino acid sequences. Despite the development of several AI tools, many lack user-friendly interfaces, interactive visualization, and secure data management. This integrates AI to prediction with an interactive 3D visualization platform to address these limitations.

2. Problem Statement

The growing platform volume of protein sequence data presents a challenge in determining their corresponding 3D structures using traditional experimental techniques. Laboratory- based methods are resource-intensive and cannot scale to meet the demand. While AI-based computational methods exist, many require complex setups, high performance computing, and lacking intuitive interfaces.

Moreover, most existing platforms do not provide secure autentication , efficient data storage, or web accessibilty. An intergarted solution that combines AI-driven prediction

interactive visualization, data security, and ease of use is necessary . The projects aims to create such a system, allowing researches and students to predict and explore protein structures convinently.

3. Methodology

The system adopts a modular approach intergarting the frontend intergrating the fontend, backend and AI prediction services :

1. Sequence Input
   - Users submit amino acid sequences through a web- baesd interface.
2. AI-Based prediction
   - The sequence is processed by an AI model through an AI Gateway . The model uses deep learning techniques to predict the protein's 3D structure.
3. Data Processing
   - The predicted structural data is formatted and stored securely in the backend database.
4. 3D Visualization
   - The predicted protein structured is rendered using web-based 3D visualization libraries, allowing user interaction.
   - Structures are displayed interactively, enabling rotation, zoom, and structural analysis.
5. Result Storage and export
   - Prediction results can be saved and exported for further analysis.
   - Users can save prediction for further offline analysis or reporting.

4. Implementation

The frontend is implemented using React and TypeScript, ensuring responsive user interactions.Tailwind CSS and componenet libraries maintain consistent styling. React Three Fiber and Three.js render predicted protein structures in 3D within browser.

For 3D visualization, the system employs WebGL-based rendering through specilasied libraries that enable real-time intercation with predicted protein structures. Users can rotate, zoom, and inspect the structures to understand folding patterns and spatial arrangements.

The back end supabase, offering secure authentication , database services, and row-level security.Edge functions handle communication with AI prediction models, providing a scalable and efficient system architectre. This design ensures secure, high performance processing of user requests.

AI component is accessed through an AI Gateway, whoch abstracts model communication and ensures scalability. This design allows the system to adapt to future model uprgrades without major architectural changes.

5. Result and Discussion

The implemented system succesfully predicts protein structures from sequences input and provides interactive visualization. Users can inspect protein structures, explore domains and analyze conformational feutures in 3D. The AI predictions offer accurate structural approximations and significantly reduce the time compared to conventional experimental methods.

The interactive visualization feauture enabled users to analyze protein structures effectively. Users cold observe folding patterns, structural domains, and overall molecular geometry in a user friendly environment. The web based nature of the system eliminated the need for specialised software installation,enhancing accessibility.

The web-based interface enhances accessibility, making the system suitable for both educational and research purposes . While predictions are computational models, they align closely with know protein structures reported in literature.

From a performance perspective, the system demonstarted reliable handling of multiple prediction requestes due to its serverless backend architecture. Secure data storage and access control ensured user privacy and data integrity.

Although the predicted structures are computational approximations, the results showed strong consistency with known structural characteristics reported in existinng biological literature. This confirms the effectiveness of AI-based approaches for protein structure prediction.

6. Conculsion

This study presens a web based AI system for protein structure prediction that combines deep learning with interactive visualization. The platform addresses limitations of traditional methods by providing a user friendly ,scalable , and secure environment for predicting and exploring protein structures. It is suitable for researches, students, and educators, demonstrating the practical applications of AI in bioinformatics.

Future work many include advanced feautures such as protein-ligand interaction prediction, mutation impact analysis, and dynamic simulations of protein conformational changes.

The project demonstrates the pratical application of Artificial Intelligence in bioinformatics and highlights its potential in bridging the gap between protein sequence data and structural knowledge . future enhancements may include advanced biological analyses such as mutation impact prediction, protein -ligand interaction studies, and dynamic simulations, further expanding the scope and applicability of the system.

REFERENCES

- *Jumper, J., et al., "Highly Accurate Protein Structure Prediction with AlphaFold," Nature, 2021*
- *Baek, M.,et al., "Accurate Prediction of Protein Structures using RoseTTaFold,"Science,2021.*
- *Chen, l.,et al., "Protein Structure Prediction via Deep Learning ," Frontiers in Pharmacology, 2025.*
- *Meng,Y., et al., "Protein Structure Prediction via Deep Learning." Frontiers in Pharmocolgy,2025.*
- *Paracha, H.A.,et al., "Recent Advances in Protein Structure Prediction ." 2024.*
- *Ille, A.M.,et al., "AI for Protein Structure and Conformational Dynamics." 2025.*