



# AI for Protein Structure Prediction: Accelerating Discovery Through Cross-Disciplinary Collaboration

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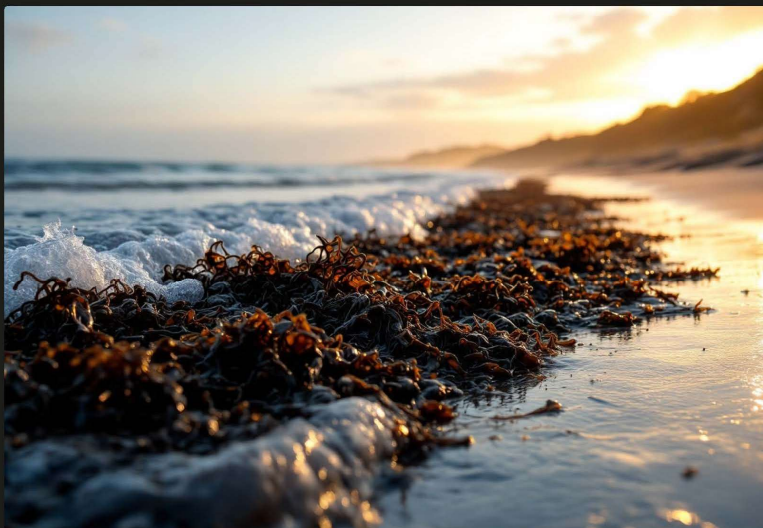
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# An AI Assistant for Biologists Tackling Sargassum Overpopulation

## Why This Matters

- Environmental Challenge: Sargassum blooms disrupt marine ecosystems but hold potential as bioresource
- Scientific Barrier: Marine protein sequences are poorly annotated — slows enzyme discovery



## AI-Driven Solution

An intelligent agent that acts as a **research assistant for biologists**, helping them rapidly analyze, validate, and act by:

### Predict Structures

Converts protein sequences to 3D structures using **AlphaFold2**

### Find 3D Homologs

Identifies similar structures using **FoldSeek** and **RCSB PDB**

### Suggest Function

Proposes potential functions via **CAZy** database

# How Collaboration Made This Possible



## AlphaFold2

Structure prediction algorithm developed by DeepMind, revolutionising protein structure determination



## FoldSeek

Structural similarity search tool from MPI Bioinformatics that rapidly identifies related protein structures



## RCSB PDB & CAZy

Validated 3D protein structures and functional annotation for carbohydrate-active enzymes

## Faculty Mentors:

- Prof. **Sagar Khare**, Dept. of Chemistry and Chemical Biology



## Advice for Students

- Use programs like **RAD SURF** to explore interdisciplinary ideas
- Don't wait for permission — **email professors with clear goals**
- Think: Where can your skills fill a gap in someone else's field?