Sehoon Park (박세훈)

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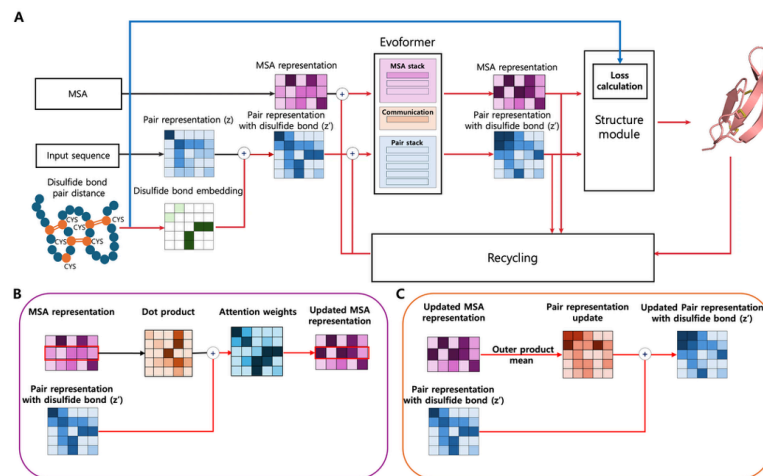- **Contact**: +82 10-9881-3664

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1. Summary

Dedicated AI researcher and developer specializing in **protein structure prediction**. Proficient in **deep learning**, particularly in **AlphaFold2**, **biophysical modeling**, and **computational biology**. Experienced in AI-driven research projects and competitions, with a track record of innovation and technical excellence.

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2. Major AI Projects

2.1. Bio & AI Projects

2.1.1. AlphaSS: Protein Structure Prediction with Disulfide Bond Information

- **Objective**: Enhance AlphaFold2 by integrating **disulfide bond embeddings** and **disulfide loss** to improve prediction accuracy, especially in low-MSA scenarios.
- **Approach**:
  - Conducted in-depth protein structure data analysis and feature extraction.
  - Developed and optimized a modified AlphaFold2 pipeline.
  - Benchmarked performance improvements against standard datasets.
- **Results**:
  - Findings presented at **BIOINFO2024**.

- ○ Based on TM-score, we observed a performance improvement of **2–3%** under sufficient MSA conditions and **5–10%** under insufficient MSA conditions.
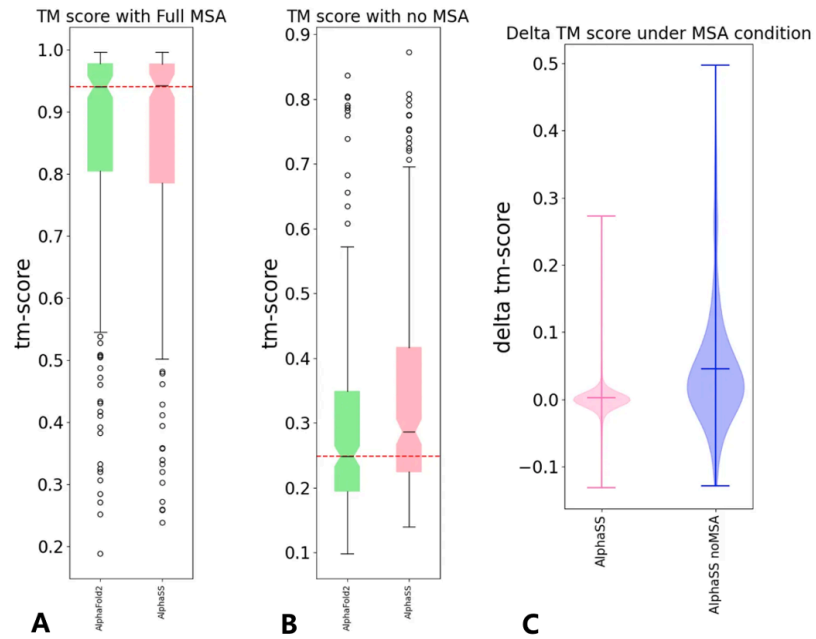

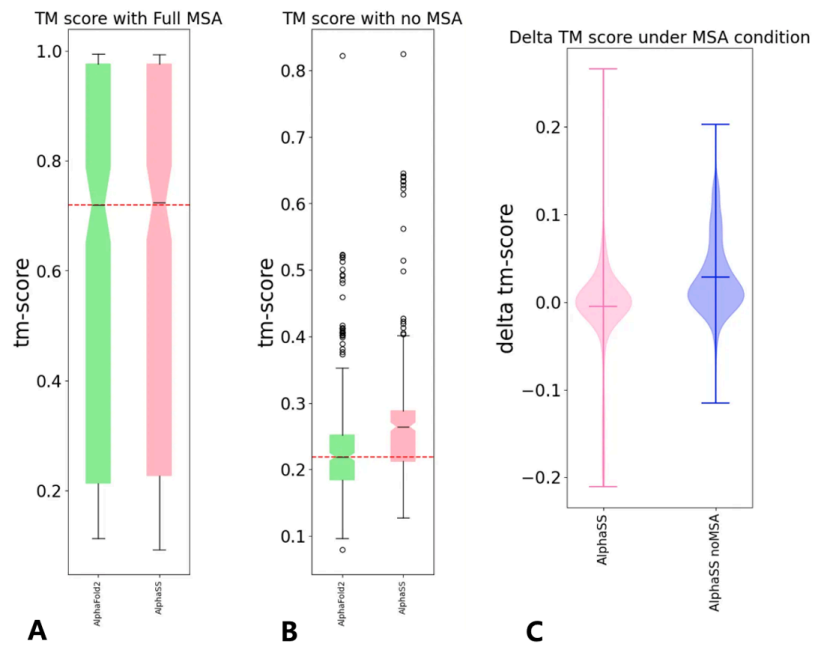**Figure 10.** AlphaSS performance comparison against AlphaFold2 on intra-SS bond test dataset.

Figure 14. AlphaSS performance comparison against AlphaFold2 on inter-SS bond test dataset.

- ○ Additionally, **disulfide bond prediction recall** improved by **50–100%** with sufficient MSA, and by **60–100%** when MSA was limited.
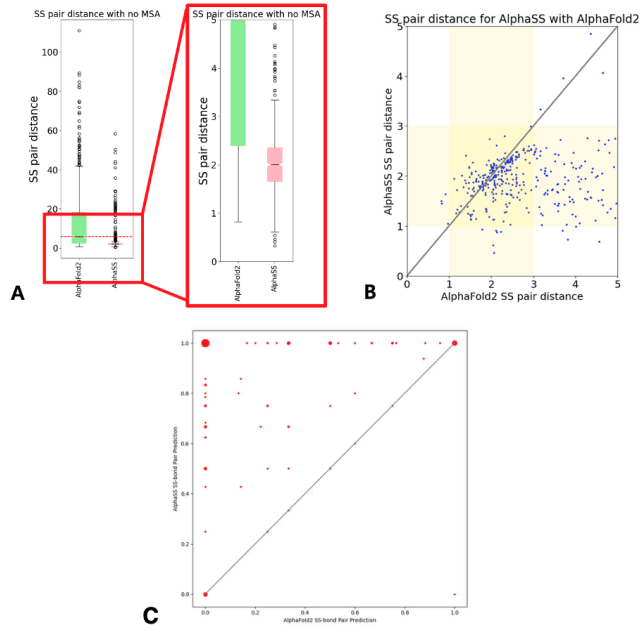
Figure 13. Comparison the SS bond pair distance (A,B) & SS-bond pair prediction performance (C) between AlphaFold2 and AlphaSS under **no MSA conditions** in intra-SS test data.

Figure 12. Comparison the SS bond pair distance (A,B) & SS-bond pair prediction performance (C) between AlphaFold2 and AlphaSS under **full MSA conditions** in intra-SS test data.
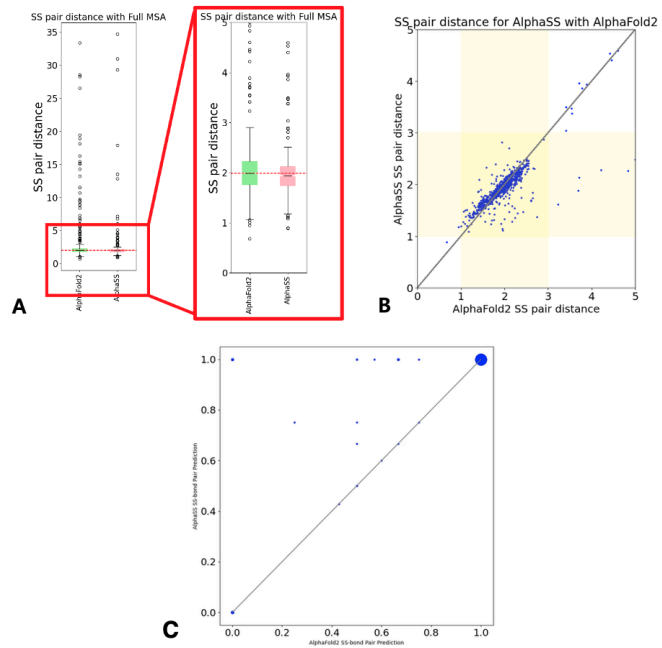
Figure 16. Comparison the SS bond pair distance (A,B) & SS-bond pair prediction performance (C) between AlphaFold2 and AlphaSS under **full MSA conditions** in inter-SS test data.
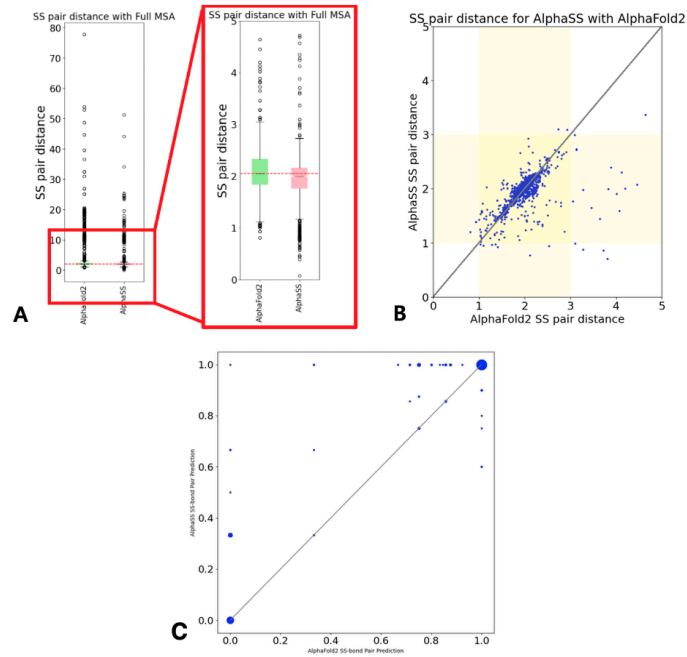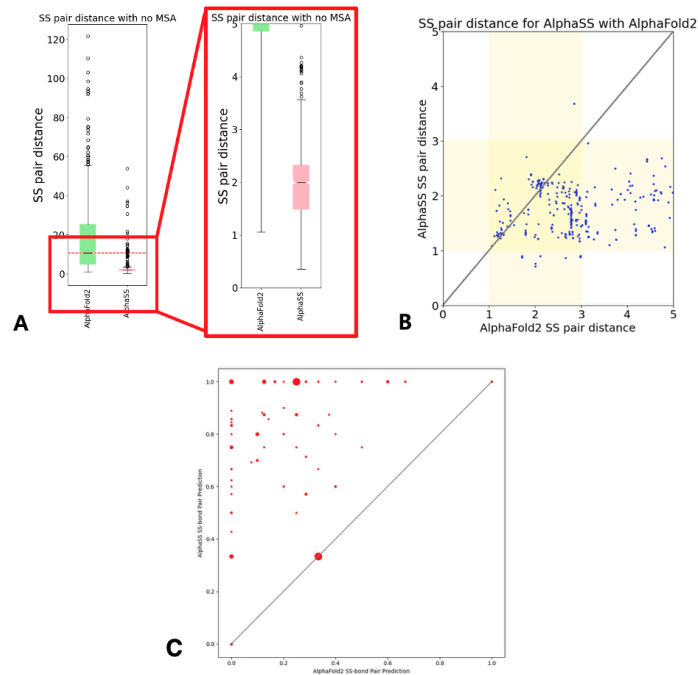

Figure 17. Comparison the SS bond pair distance (A,B) & SS-bond pair prediction performance (C) between AlphaFold2 and AlphaSS under **no MSA conditions** in inter-SS test data.

- ○ This study demonstrates that incorporating **disulfide bond information** contributes to improved protein structure prediction performance, with particularly notable benefits under low-MSA conditions.
- ○ git : https://github.com/iitp-ppi/AlphaSS.git
- ○ paper: 📄 박세훈_AlphaSS-Improving_protein_structure_prediction_with_d…
- **Technologies**: Python, PyTorch, AlphaFold2, Deep Learning, Protein Structure Prediction

2.1.2. CASP16 Competition (DeepFold Team Member)

- **Objective**: Compete in **CASP16**, leveraging advanced AI models for protein structure prediction.
- **Approach**:
  - Collaborated with the **DeepFold** team on state-of-the-art prediction methodologies.
  - Developed strategies focusing on **antibody and peptide structure prediction**.
- **Results**:
  - **Achieved 3rd place** in the **Antibody/Peptide category**.
  - Presented results at **CASP16 Conference**.
  - paper : 📄 DeepFold_TS.pdf
  - poster : 📄 casp16 poster_final (2).pdf

2.1.3. PSM Rescoring: Improving Percolator Performance with Feature Enhancement (April 2023 - July 2023)

- **Objective**: Enhance **PSM (Peptide-Spectrum Match) scoring** in proteomics by improving Percolator's feature extraction capabilities.
- **Approach**:
  - Analyzed the impact of **Spectral Contrast Angle (SA), Shared Peak Counts (SPC), and Delta Retention Time (ΔRT)**.
  - Implemented feature engineering techniques to refine Percolator's scoring mechanism.
  - Conducted **False Discovery Rate (FDR) optimization** to maximize peptide identification accuracy.
- **Results**:
  - **PSM identification improved by 9.57% (K562 dataset) and 4.33% (HEK293 dataset)**.
  - Results validated through benchmarking and statistical analysis.
- **Technologies**: Python, Machine Learning, Percolator, Mass Spectrometry Data Processing

2.2. AI Projects

2.2.1. AI Pharmacist Chatbot Service

- **Objective**: Develop an **AI-driven chatbot** to assist with supplement and medication intake.
- **Approach**:
  - Designed and implemented chatbot functionality using **LLMs, Langchain, RAG, and Gradio**.
  - Optimized responses through **retrieval-augmented generation (RAG)**.
- **Results**:
  - Finalist in **Global AI Week Hackathon (Upstage AI Hackathon)**.
  - git : https://github.com/sehooni/NutriPharmAI.git

2.2.2. AI-based Menu Demand Forecasting using N-HiTS model

- **Objective**: Develop an **AI model** to forecast the real-world menu demand.
- **Approach**:
  - Based on **N-HiTS**, combining **calendar-derived covariate** information with a **masked SMAPE loss** to enhance predictive robustness and real-world applicability.
- **Results**:
  - Finalist in **Menu Demand Forecasting AI Hackathon for F&B Establishments (LG Aimers 7th AI Hackathon)**.

2.2.3. AI-driven Game Scenario Generator

- **Objective**: Create an **AI-based game scenario generator** for dynamic content creation.
- **Approach**:
  - Applied **GPT fine-tuning, prompt engineering, and DALL·E**.
  - Developed an interactive UI using Gradio.
- **Results**:
  - **1st place winner at Smilegate AI Service Weeklython**.
  - git : https://github.com/sehooni/AIStoryWeaver.git