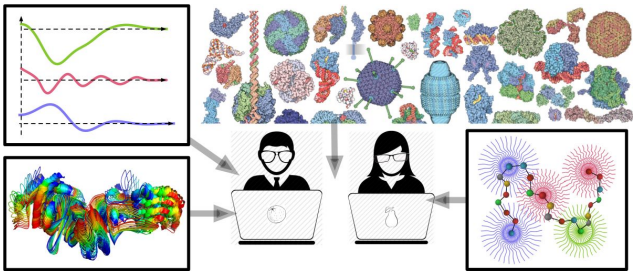

Contribution ID: **55** Type: **Talk**

Integrated pipeline for protein docking with extended and enhanced Alphafold-based modeling methods

Wednesday, 14 February 2024 15:00 (30 minutes)

Our group, Kiharalab, participated in both the prediction and scoring stages for complex targets. We combined three components in our pipeline, DistPepFold [1], AFSample [2], and a consensus-based score called ranksum we developed for our LZerD protein docking program [3]. For peptide docking, we used our new approach, DistPepFold. DistPepFold improves protein-peptide complex docking using an Alphafold-Multimer (AFM) based architecture through a privileged knowledge distillation approach. DistPepFold leverages a teacher model that uses native interaction information during training and transfers its knowledge to a student model through a teacher-student distillation process. Benchmark study showed that DistPepFold outperforms AFM on peptide docking. AFSample is a protocol to run Alphafold2 with combinations of several settings, and thereby generating many more models, thousands of models per target. In our pipeline, we ran DistPepFold and an in-house implementation of AFSample. Then generated models were clustered and scored mainly based on the ranksum score. The ranksum uses three scoring functions and identifies models that are ranked consistently high by the three scoring functions. For human submission, we also refer to literature when available.

Reference:
1. Zhang Z, Verburgt J, Kagaya Y, Christoffer C, & Kihara D. Improved Peptide Docking with Privileged Knowledge Distillation using Deep Learning. bioRxiv, DOI: 10.1101/2023.12.01.569671 (2023)
2. Wallner B, AFsample: improving multimer prediction with AlphaFold using massive sampling. Bioinformatics, btad573, (2023)
3. Christoffer C, Terashi G et al., Performance and enhancement of the LZerD protein assembly pipeline in CAPRI 38–46, Proteins, 88: 948-961 (2020)

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