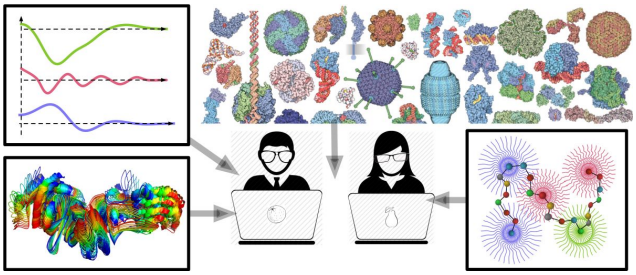

Contribution ID: **35** Type: **Talk**

Prediction and refinement of protein assemblies with ClusPro, Alphafold and Molecular Dynamics.

Wednesday, 14 February 2024 16:45 (30 minutes)

In the latest CAPRI round our group used a combination of Alphafold-Multimer (AFM), the ClusPro webserver for docking, and Molecular Dynamics based sampling to refine models for small targets. Assembly prediction was based on a two-stage methodology, in which we first generate an ensemble of initial models using AlphaFold-Multimer using standard protocol for MSA generation. We stop the search if the model is of sufficiently high confidence, otherwise we perform template based search using ClusProTBM and free docking using ClusPro. The resulting structures are transferred to Alphafold-Multimer (AFM) as starting templates for generating "refined" structures of the target complex. For smaller targets such as T231 we have explored an additional refinement step based on constrained MD based sampling, where we constrained the high confidence protein and peptide regions and performed additional sampling in the other regions, followed by template based refinement.

Submitting to:

8th CAPRI assessment meeting

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Session Classification: CAPRI