# Integrated Modelling of PROTEIN Complexes VIA Single Shot Registration using DREAM (IMPROVISeD)

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## 1. Integrative Modelling Platform (IMP)

- 1. The IMP provides a computational approach designed to model the structure of macromolecular assemblies.
- 2. It models large macromolecular complexes by integrating data from experiments, statistical analyses, physical principles, and prior models.

### 2. Drawbacks of IMP

- 1. Computationally expensive.
- 2. Uses Markov Chain Monte Carlo (MCMC) sampling.

## 3. Proposed Method

- 1. We propose to replace the MCMC sampling with a bottom-up approach.
- 2. We will use DREAM algorithm to replace the MCMC sampling.

# 4. Distance Restraints and Energy Assisted Modelling (DREAM)

This algorithm takes distance restraints data and models the structure of proteins which includes 3 steps:

- 1. Constructing the substrucutres.
- 2. One shot registration of all the substrucutres.
- 3. Gap filling using hybrid approached.

# Sub Topic 2

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#### Graphical Overview Data and Measurements from Structure Modelling Using a **Different Sources** Bottom-Up Approach Cryo-EM Maps Random Initial Configurations Residue specific cross-One-shot registration using DREAM Processing Generation of approximate Distance Restraints inal Combined Structure **Extracted Constraints** Excluded volume Density cross-correlation restraints Post-processing for Refinements Starting models

#### Conclusions and Future Work

Final conclusions

### QR Code for Recording

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