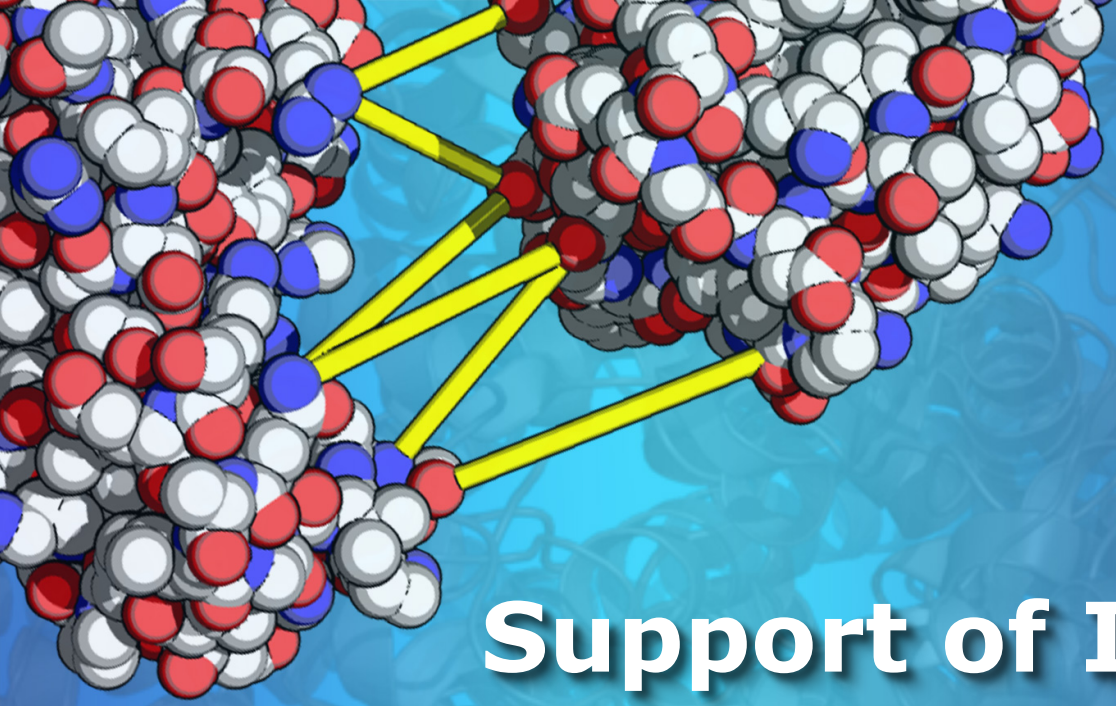
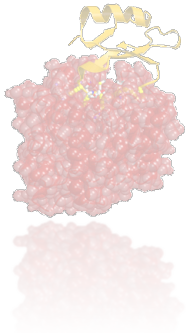


Support of IHM mmCIF format in HADDOCK 2.4

Dr. Mikael Trellet
Bijvoet Center for Biomolecular Research
Faculty of Science, Utrecht University
the Netherlands
m.e.trellet@uu.nl

Utrecht Bioinformatics Center

Objectives

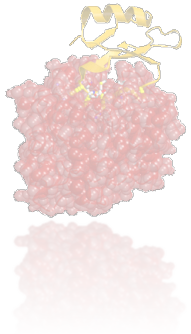


- **IHM PDBx/mmCIF files accepted as input…**
  - Read/convert atom_site information (coordinates, segid, etc.)
  - Read/convert experimental data as parameters (EM map, Xlinks, etc.)
- **… and output - generation of IHM PDBx/mmCIF from the results page**
  - Generate atom coordinates only
  - Generate atom coordinates + interface (ihm_model_representation)
  - Generate atom coordinates + interface + restraints

  → 1) Single model

  → 2) Ensemble of models (cluster)
- **Use mmCIF as internal format for pre- and post-processing**
  - Feasibility to be discussed, involves significant efforts

Conclusion



- Different read/write modules rely on python-ihm (https://github.com/ihmwg/python-ihm)
- Preview of beta-version: