FAIR IMPLEMENTATION FOR NI4OS-EUROPE SERVICE PROVIDERS

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Drug discovery tools onboarded on NI4OS-Europe

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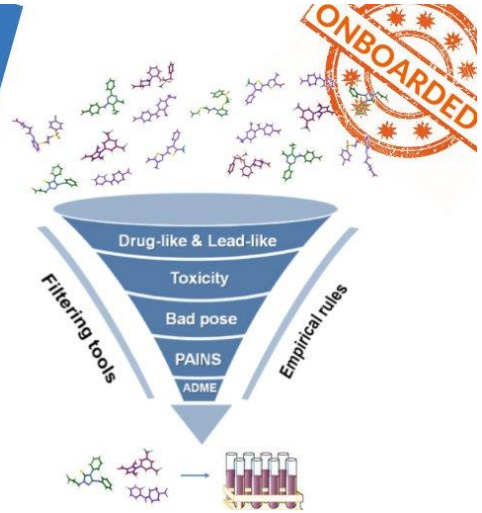
NI4OS-Europe Catalogue

Thematic services

ChemBioServer is a publicly available web application for effectively **filtering and clustering chemical compounds** used in drug discovery.

http://chembioserver.vi-seem.eu/



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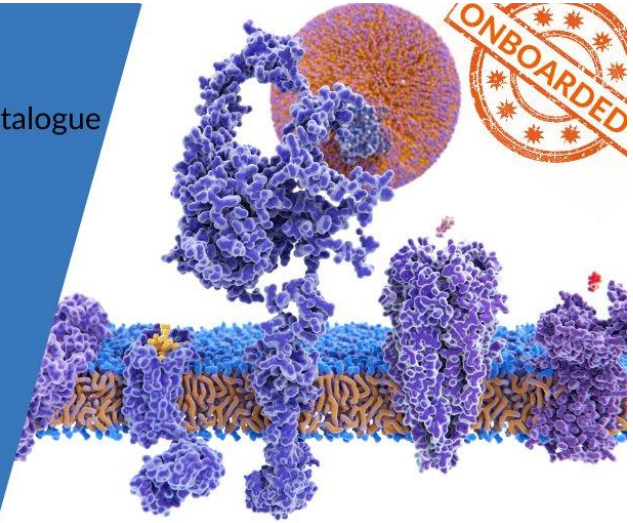
DREAMM is a novel web-based tool that **predicts the protein-membrane interfaces of peripheral membrane proteins** using ensemble machine learning.

http://dreamm-ni4os.eu/



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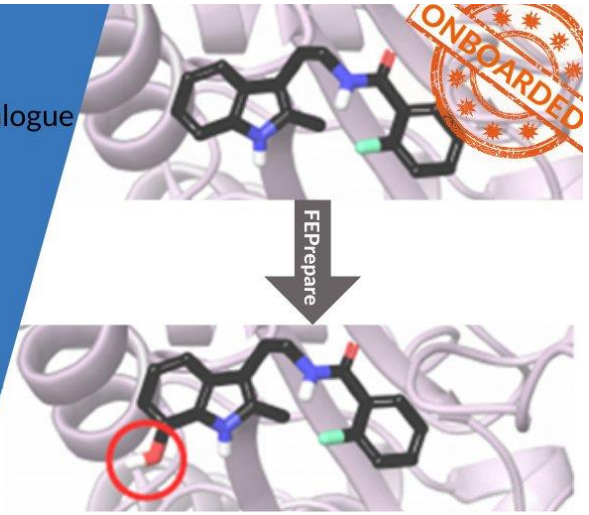
FEPrepare is a webserver, which automates the set-up procedure for performing **NAMD/FEP simulations**.

http://feprepare.vi-seem.eu



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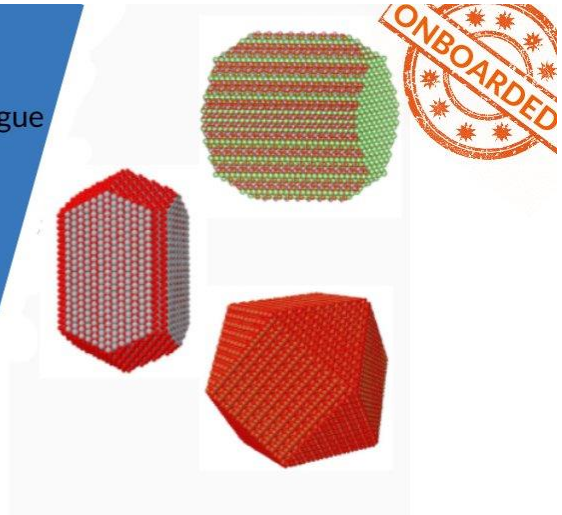
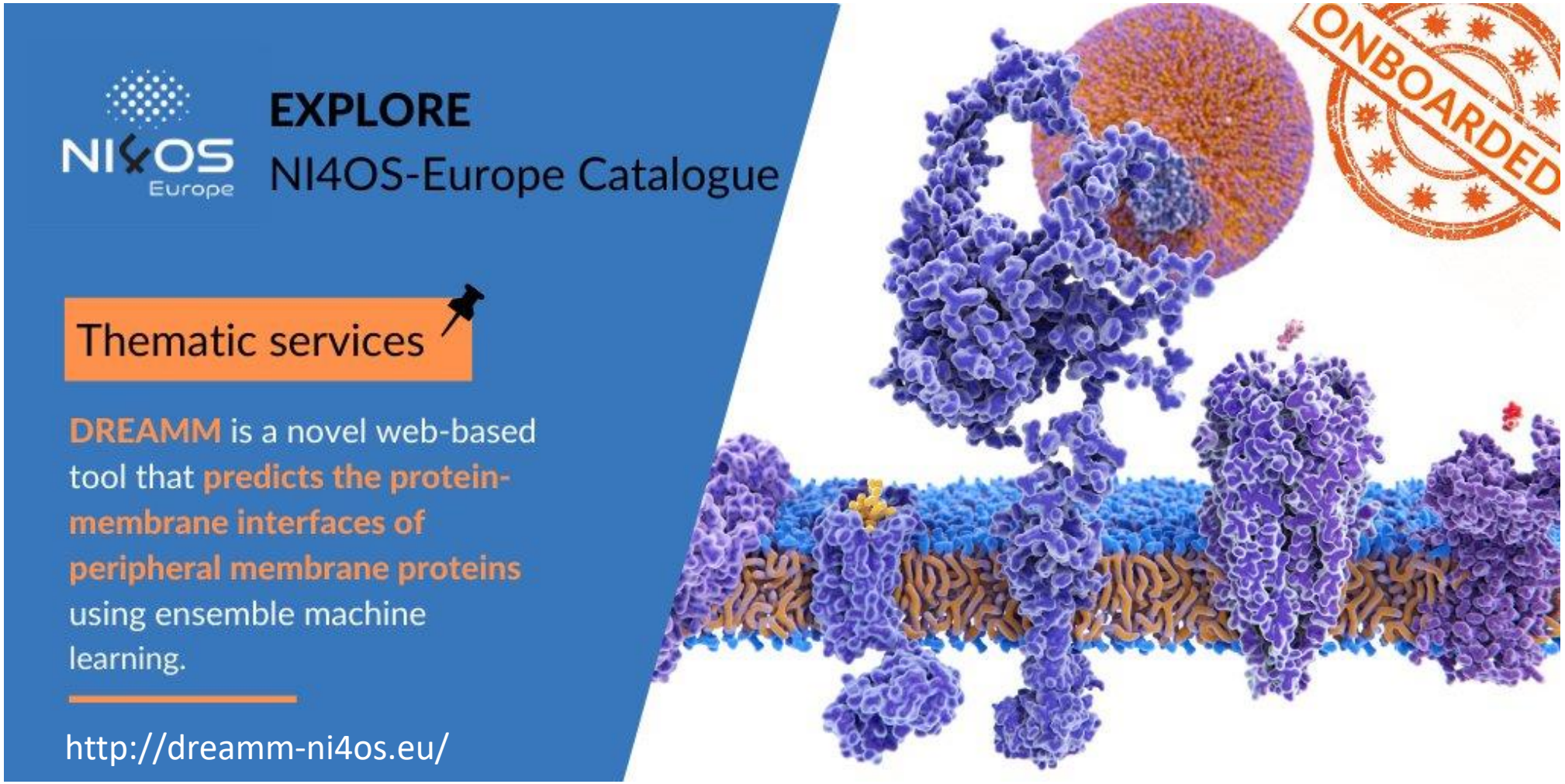
Thematic services

NanoCrystal is a novel web-based **crystallographic tool** for the construction of nanoparticles from any material crystal structure.

http://nanocrystal-seem.eu

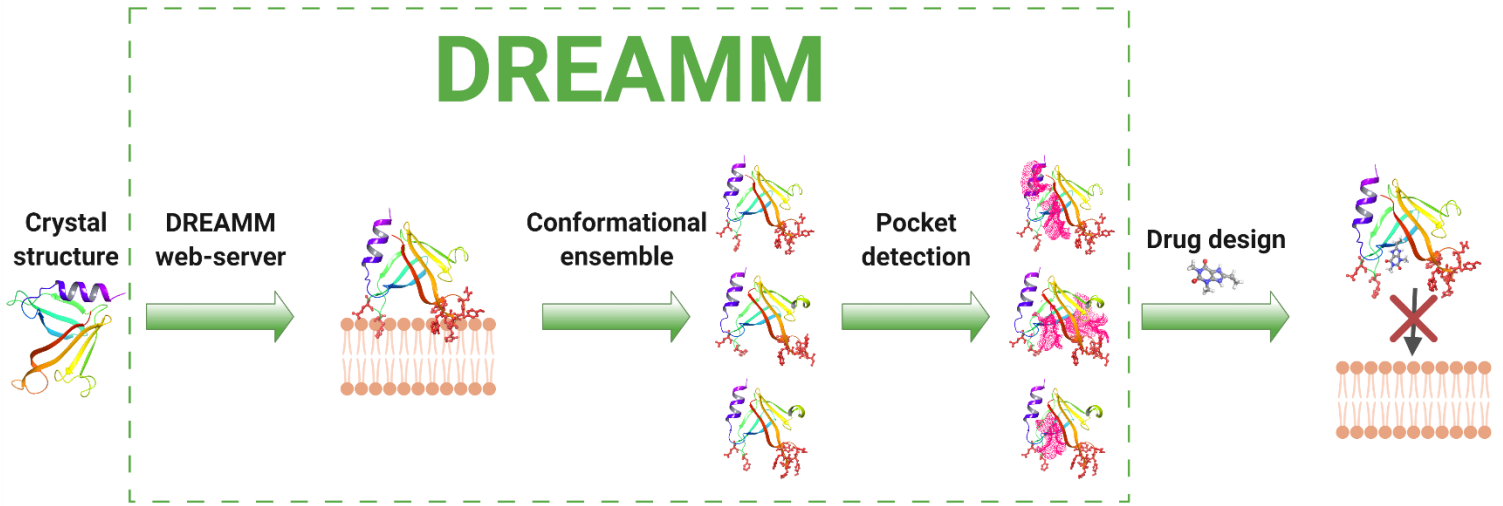


DREAMM: Predicting cavities at protein-membrane interfaces

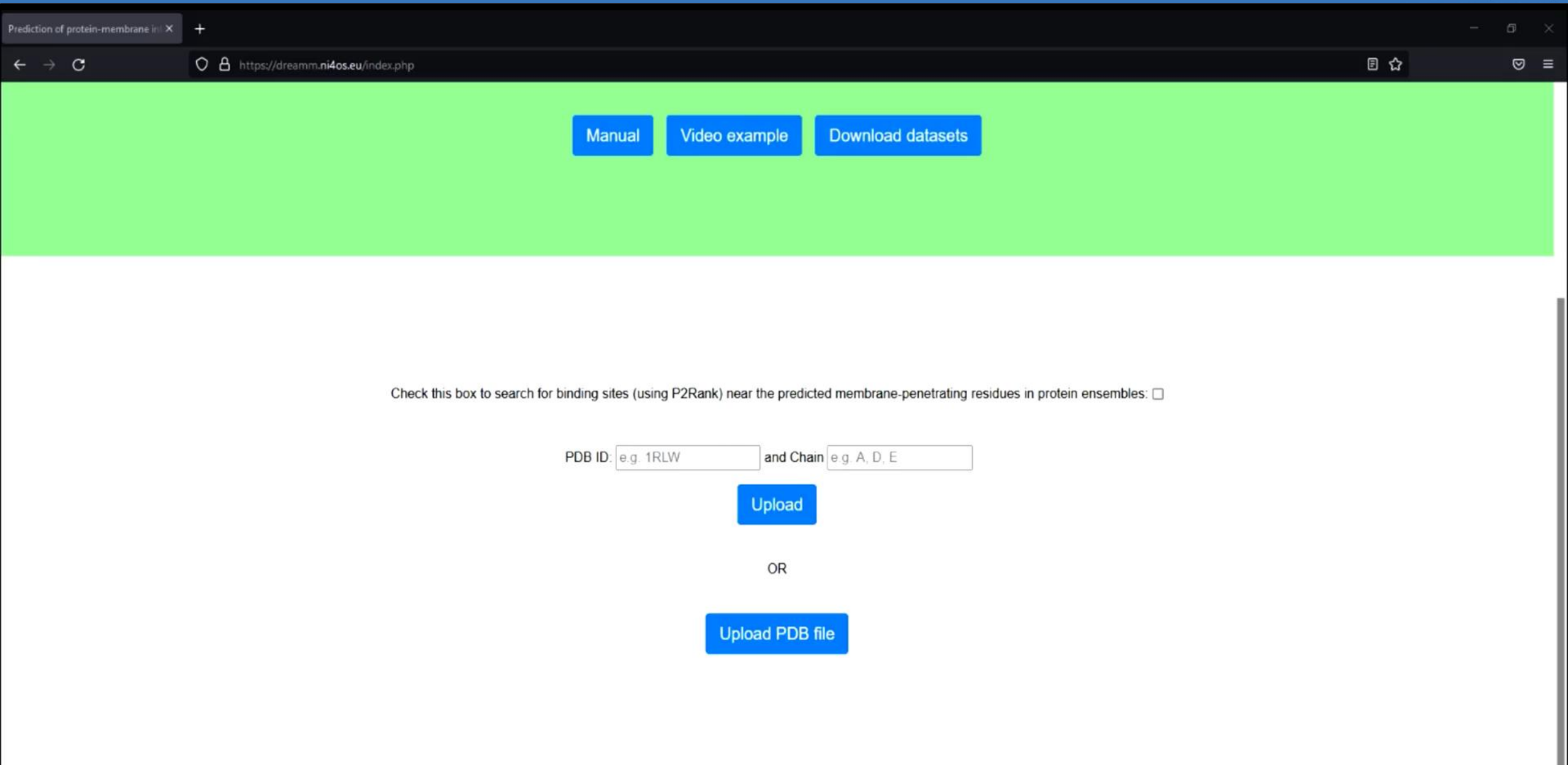


DREAMM Main Features

- Use an ensemble machine learning model that predicts the protein-membrane interfaces of peripheral membrane proteins
- Predict binding sites in the predicted protein-membrane regions in conformational ensembles using P2Rank
- Cluster the predicted binding sites for all protein conformations based on the binding sites center coordinates
- Create a novel web-based tool for predicting and drugging protein-membrane interfaces



DREAMM Video Example



DREAMM: Predicting cavities at protein-membrane interfaces

- Information in NI4OS-Europe Agora: https://catalogue.ni4os.eu/?_=/resources/bc445004-2869-43c9-9ef3-e5aa6b44d2e3
- Access: https://dreamm.ni4os.eu/
- Training Material: https://training.ni4os.eu/mod/scorm/view.php?id=1187

DREAMM FAIR demands

- **Findability:** Onboarded to NI4OS-Europe
- **Accessibility**:
- Persistent identifier (PID) assigned to each job and URL of the results
- Results are only findable and accessible by the user who ran the prediction and deleted after 2 days
  - **Possible Solution**: Create a web-database storing the results, enabling search for relevant information through their metadata, by linking them
- **Interoperability**: Only PDB structures are interoperable.
- PyMOL visualizations and csv, txt, xlsx containing clustering results are not.
  - Onboarded
  - **Solution**: Add the binding site spheres as dummy atoms in the PDB structure and export clustering results in JSON or XML format
- **Reusable**: A detailed video example and a well-documented manual is available containing:
  - A short description of what data it includes
  - Definitions of column headings and row labels for tabular data
  - Whom to contact with questions
  - Data are released with a clear and accessible data usage license: https://wiki.ni4os.eu/images/7/77/DREAMM-Terms_of_use.pdf

Thanks for your attention!