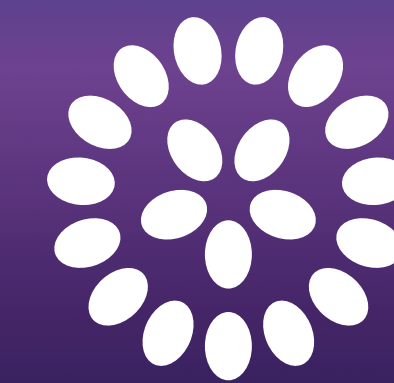


FAIRMD – Disorder to Order: Streamlining Biomolecule Simulation Re-Use with FAIR NMRIpids database



OSCAR

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The FAIRMD project builds on the success of the NMRIpids Databank, which provides open access to molecular dynamics (MD) simulations of lipid bilayers. By expanding the database to include MD simulations of disordered proteins, and by improving its interoperability with existing public databases, FAIRMD will offer high-quality, FAIR data to support AI model development.



LSRI
Life Sciences

Challenge

Disordered biomolecules, such as lipids and intrinsically disordered proteins (IDPs), are crucial to understanding cellular membranes and protein behaviours, yet standardised and accessible training data is lacking. This creates a barrier for AI-driven research and limits advancements in areas, such as drug development and biomaterial design.

Solution

FAIRMD aims to expand the NMRIpids Databank, a collaborative resource for MD simulations of lipid bilayers, to include disordered proteins. This advancement will enable the development of AI models to predict structural and dynamical properties of disordered biomolecular complexes from atomistic details.

Scientific Impact

By addressing practical challenges in data distribution with open collaboration and overlay-databank approaches, the project promotes FAIR data sharing and supports the development of AI-based tools.

<https://www.oscars-project.eu/projects/fairmd-disorder-order-streamlining-biomolecule-simulation-re-use-fair-nmrlipids-database>

Partners

University of Bergen, VTT
Technical Research Centre
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