OSCARS
Open Science Clusters' Action for Research & Society

Funded Project

FAIRMD - Disorder to Order

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What problem(s) did you plan to solve?

1. Extending the existing NMRlipids Databank to include molecular dynamics (MD) simulations of a new molecule class: IDPs (intrinsically disordered proteins).

2. Improving the interoperability of NMRlipids Databank with existing public databases and enhancing the metadata on molecules and the data catalogue.

What have you done to solve the problem?

- Created metadata schema for IDPs in line with ELIXIR IDP community guidelines.
- Developed quality-evaluation metrics of MD of IDPs based on experimental data.
- Developed the core of the FAIRMD IDP Databank.
- Refactored the code base to accommodate different types of data.
- Created strong continuous integration (CI) routines and support functions for data submission and processing.
- Implemented molecular metadata and crosslinks to other DBs (lipidmaps, swisslipids, ChEBI, ChEMBL, PubChem) with ‘autocomplete’ from InChIKeys.
- Exposure of bioschema.org.

What are the key results achieved to date and how have you made them available to the broader community?

- Workshops on Databank development and Workflow FAIRification.

- Code improvements on quality evaluation and restructuring to allow different data/molecule types.
- IDP quality evaluation used in a submitted manuscript
- Python module released.

- More reference data included.
- Metadata for quality control experiments.
- Standard metadata and crosslinking for molecules for enhanced findability.

- Ready-to-use data on LUMI.

How will make your results sustainable over time - How will the scientific community/-ies further exploit them?

- FAIRMD has applied to become an ELIXIR-NO service.
- In discussion with other repositories to enhance data exchange & crosslinking.
- All results open source.
- Directly usable data with python module on LUMI.

TEAM: Who has been doing it?

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Project leads

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Community

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