

A FAIR unified research infrastructure aiming to enhance interoperability, streamline workflows, and foster interdisciplinary collaboration.

CALL FOR FAIR UNIFIED DATABASE

MDDDB aspires to establish a research infrastructure tailored for communities engaged in biomolecular simulation, structural biology, biophysics, medicinal chemistry, biotechnology, bioinformatics, genomics, and personalized medicine, and unify these communities under a common platform using FAIR (Findable, Accessible, Interoperable, Reusable) data principles, ultimately, breaking down barriers between scientific domains and drive collaborative advancements in research and innovation

ALIGNMENT WITH EXISTING INITIATIVES

To leverage existing resources, avoid duplication of efforts, and foster a cohesive scientific ecosystem, MDDDB aims to align with establish initiatives and complement existing biomolecular data repositories by addressing the unmet needs of biomolecular dynamics simulations. Through its consortium members and active participation in initiatives like EOSC-life and BioExcel CoE, MDDDB ensures collaboration with prominent Life Science data repositories, building upon their experiences to discern the most suitable strategies and offer best practices guidelines in the field.

NATIONAL ROADMAPS TO ESFRI ROADMAP

In line with national and European strategic priorities, MDDDB is engaged with national roadmaps as essential steps towards integration with the broader ESFRI roadmap. This strategic alignment enables MDDDB to significantly contribute to pan-European scientific research and innovation, leveraging European funding and resources while affirming its contribution to the scientific community.

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KEY STRATEGIES

Implementing good practices: Establishing clear guidelines and stringent quality checks for collection of simulation data to ensure reliability and integrity of data available in MDDB.

Defining standards of interoperability: Interoperable data formats and seamless integration of MD data into the Life Science Data ecosystem foster collaboration across communities.

Ensuring access guidelines: Implementing transparent procedures for fair access to MDDB, including data deposition, access, post-analysis, training and new federated node deployment.

Addressing data storage and analysis capacity: Developing a distributed database policy and securing commitment from computing centres and funding agencies to sustain MDDB's data storage and analysis capacity.

Engaging stakeholders: Collaborating with academia, industry, and government agencies to ensure MDDB meets stakeholder needs, maximising its impact and relevance.

Involving national communities and HPC centres: Engaging national communities connected to HPC centres to build and maintain local infrastructures in coordination with MDDB.

Monitoring and evaluation: Regularly assessing MDDB's impact and effectiveness through user feedback to enhance functionality and responsiveness to community needs.