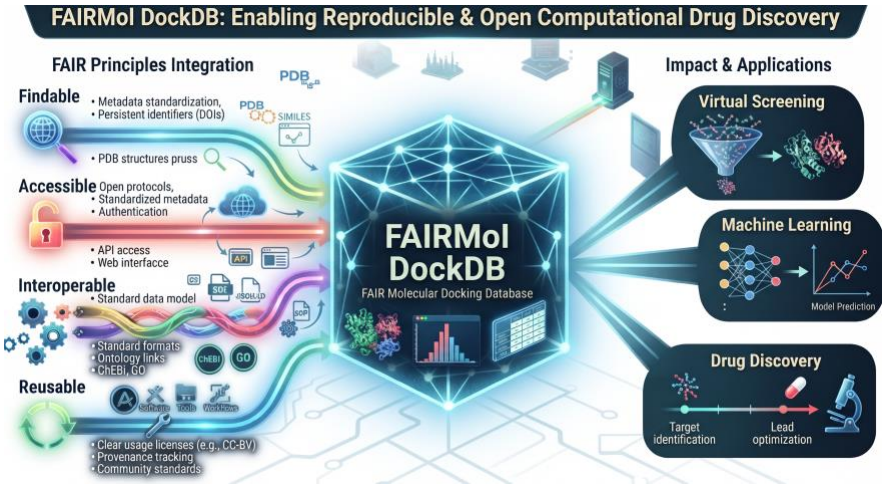
OHD Project Report – October 2026

Project: OneHealthdrugs (COST Action CA21111) acronym: OHD:LUB project
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1. Introduction

The OHD project is a collaborative initiative within the OneHealthdrugs COST Action, focusing on the application of computational methods for the discovery of new antiparasitic compounds.
The project combines large-scale structure-based virtual screening with the development of FAIRMol DockDB (https://fairmoldockdb.molekule.net), an interactive database platform for storing, visualizing and analyzing molecular docking results.
The main scientific objective is to identify promising compounds from available chemical libraries and facilitate their further experimental evaluation through collaboration between computational researchers, compound owners and laboratories capable of biological testing.



2. Objectives

The main objective was to perform virtual screening of a collected chemical library containing more than 30,000 compounds against 22 selected protein target configurations relevant to parasitic diseases.
Specific objectives included:
Preparation of protein targets and chemical structures for molecular docking.
Large-scale virtual screening and identification of promising ligand–target interactions.
Development of a prioritization protocol to select the most relevant docking results.
Development of FAIRMol DockDB as an interactive database for visualization, analysis and sharing of screening results.
Establishment of a framework for connecting compound owners with researchers performing experimental biological assays.

3. Activities Completed

Target preparation and virtual screening

A collection of 22 target configurations (T01–T22) was prepared for virtual screening. These targets represent proteins from six organisms: *Homo sapiens*, *Leishmania major*, *Leishmania infantum*, *Leishmania donovani*, *Trypanosoma brucei* and *Trypanosoma cruzi*.

The target collection includes DHFR, DHFR-TS, PTR1, R5P, SIR2, ODC, TR and Rab5a proteins. Several proteins are represented by multiple target configurations corresponding to different binding sites or receptor preparations with and without selected water molecules.
Examples of target configurations include PTR1 from *L. major* (T04–T05), SIR2 from *L. infantum* (T11), R5P from *T. brucei* (T12), four binding sites of TR from *T. brucei* (T17–T20), R5P from *T. cruzi* (T21) and Rab5a from *L. donovani* (T22).
Each compound from the library of more than 30,000 compounds was docked against all 22 targets, resulting in more than 660,000 docking calculations.

Prioritization of docking results

Following virtual screening, a prioritization protocol was applied to remove geometrically unsuitable docking poses, computational artifacts and poorly ranked results. The best retained pose for each chemical structure and target was selected for database storage.
The resulting prioritized database contains:
14,918 selected docking poses, approximately 680 per target.
5,571 distinct compounds represented in at least one target-specific selection.
Between 428 and 661 different compounds per individual target.
The selected compounds differ between targets because each target has its own ranking and filtering results. Importantly, the database already contains a curated and prioritized collection of virtual-screening results, rather than the complete set of docking calculations. Storing and providing interactive access to all calculated complexes would require substantially greater computational, database and storage resources.

Development of FAIRMol DockDB

The FAIRMol DockDB platform has been established to provide interactive access to molecular docking results.
The platform supports browsing docking experiments, visualization of protein–ligand complexes, inspection of docking poses, comparison of molecular interactions, compound prioritization and exploration of chemical properties, including ADMET and ecotoxicological predictions.
The public demonstration database currently contains 10 targets, 147 docking poses and 144 compounds. This is a limited demonstration subset and should not be confused with the larger prioritized collection.
Platform: https://fairmoldockdb.molekule.net/ui

4. Ongoing Work

Current activities are focused on further analysis of prioritized docking results and identification of the most promising compounds for experimental validation.
Additional analysis includes evaluation of protein–ligand interactions, chemical diversity, predicted ADMET properties and ecotoxicological characteristics. These results will help identify suitable candidates for biological testing.
Further development of FAIRMol DockDB focuses on improving data organization, search functionality, integration of molecular information and efficient access to screening results.
A particularly important task is the integration of the docking-results database with the existing compound database. This would make it possible to search compounds not only by chemical structure and predicted activity but also by compound owner, research group, project, compound collection and other relevant metadata.
Work is also directed toward establishing stronger links between laboratories providing chemical compounds and laboratories capable of performing experimental assays.

5. Perspectives and Future Development

The next stage of the OHD initiative will focus on expanding both the scientific scope and collaborative capabilities of FAIRMol DockDB.

Expansion of the target collection

New protein targets associated with parasitic and other relevant diseases could be included, allowing previously screened compounds and new libraries to be evaluated against a broader panel of biological targets.

Integration of compound and docking databases

The platform should connect the compound database (OHD database + any other database) with virtual-screening results through common compound identifiers. This would enable searches based on chemical structure, molecular properties, docking results, compound ownership, associated projects and other metadata.

Connecting compound owners with experimental laboratories

An especially interesting future direction is to develop FAIRMol Dock into a collaborative platform connecting compound providers with researchers performing biological assays.

A researcher owning a compound or compound collection could submit molecular structures for virtual screening against available protein targets. If promising interactions are identified, the platform could help establish contact with laboratories capable of experimentally testing the compounds.

Such functionality could facilitate compound sharing, scientific collaboration, selection of appropriate biological assays and collection of experimental results. Open access platform and project summary.

Appropriate access permissions and ownership information would protect the interests of participating researchers.

Experimental results could subsequently be linked to the original docking predictions, providing valuable feedback for improving computational prioritization methods.

Infrastructure and sustainability

Further expansion will require additional computational and storage infrastructure, particularly if the complete virtual-screening results are to be retained and made accessible.

An improved database architecture, standardized metadata, user management and controlled data sharing would support long-term sustainability and future scientific collaborations.

The long-term vision is to transform FAIRMol Dock from an interactive molecular docking database into a collaborative drug-discovery platform that connects computational screening, compound collections, compound owners and experimental laboratories.

6. Conclusion and perspective

The OHD initiative has successfully completed virtual screening of more than 30,000 compounds against 22 protein target configurations, generating more than 660,000 docking calculations.

A prioritized collection containing 14,918 docking poses representing 5,571 distinct compounds has been established, together with the FAIRMol Dock interactive database platform.

These achievements provide a foundation for identifying promising antiparasitic compounds and supporting their experimental evaluation.

Future efforts will focus on expanding the target collection, improving database integration and developing collaborative functionality to connect compound owners with laboratories performing biological testing.

The project therefore provides a foundation for a sustainable, FAIR-oriented computational and experimental drug-discovery environment within and beyond the OneHealthdrugs network.

Project websites:

https://www.onehealthdrugs.com/

https://fairmoldockdb.molekule.net/ui

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