

Implementing FAIRness in structure-based drug design through Fragalysis Cloud



The project aims to enhance the transparency and accessibility of structure-based drug design (SBDD) data by making it fully open and compliant with FAIR principles. Leveraging Diamond's XChem service and the Fragalysis Cloud platform, the project will streamline data deposition and establish a first-of-its-kind tool for sharing, exploring, and evolving SBDD experiments.



Challenge

Existing datasets for exploring and improving structure-based drug design (SBDD) are highly inadequate. Moreover, data is often fragmented across various tools and hidden in unstructured formats, making it difficult for researchers to access and build upon existing datasets.

Solution

The project will enhance the Fragalysis Cloud platform used for curating, sharing and disseminating views of 3D data, to facilitate open and FAIR-compliant sharing of SBDD data. By integrating data from 50–150 experiments, the project will create an accessible mechanism for depositing and querying large-scale datasets.

Scientific Impact

The project will enable researchers to explore SBDD projects with comprehensive data on context, provenance, design rationales and inspection of computational analyses. It will revolutionise accessibility and reuse of SBDD data, providing an innovative tool for examining collective datasets in a FAIR manner.

<https://www.oscars-project.eu/projects/implementing-fairness-structure-based-drug-design-through-fragalysis-cloud>

Partners

Diamond Light Source, Informatic Matters, M2M Solutions