



OSCARS

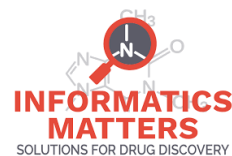
Open Science Clusters' Action
for Research & Society

Funded Project

Implementing FAIRness in structure-based drug design through Fragalysis Cloud

Presenter: Warren Thompson, Diamond Light Source, 0000-0003-1474-7810

Implemented by



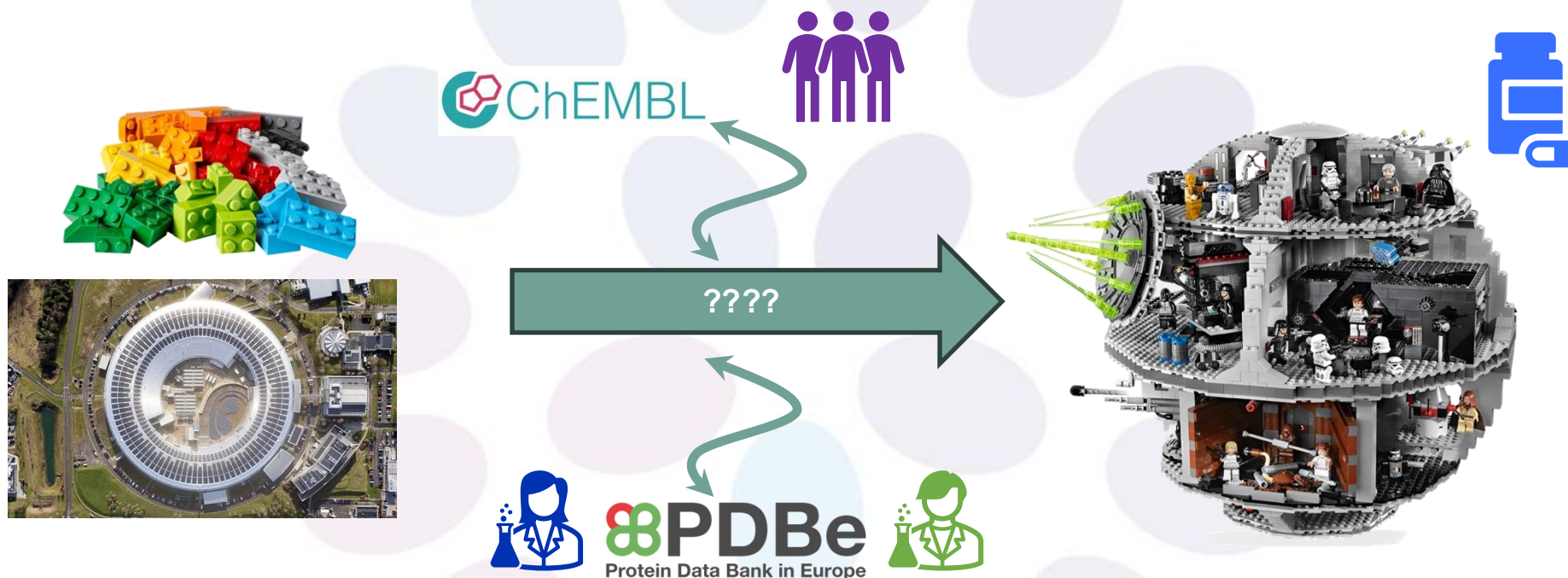
Research Complex
at Harwell



Funded by
the European Union

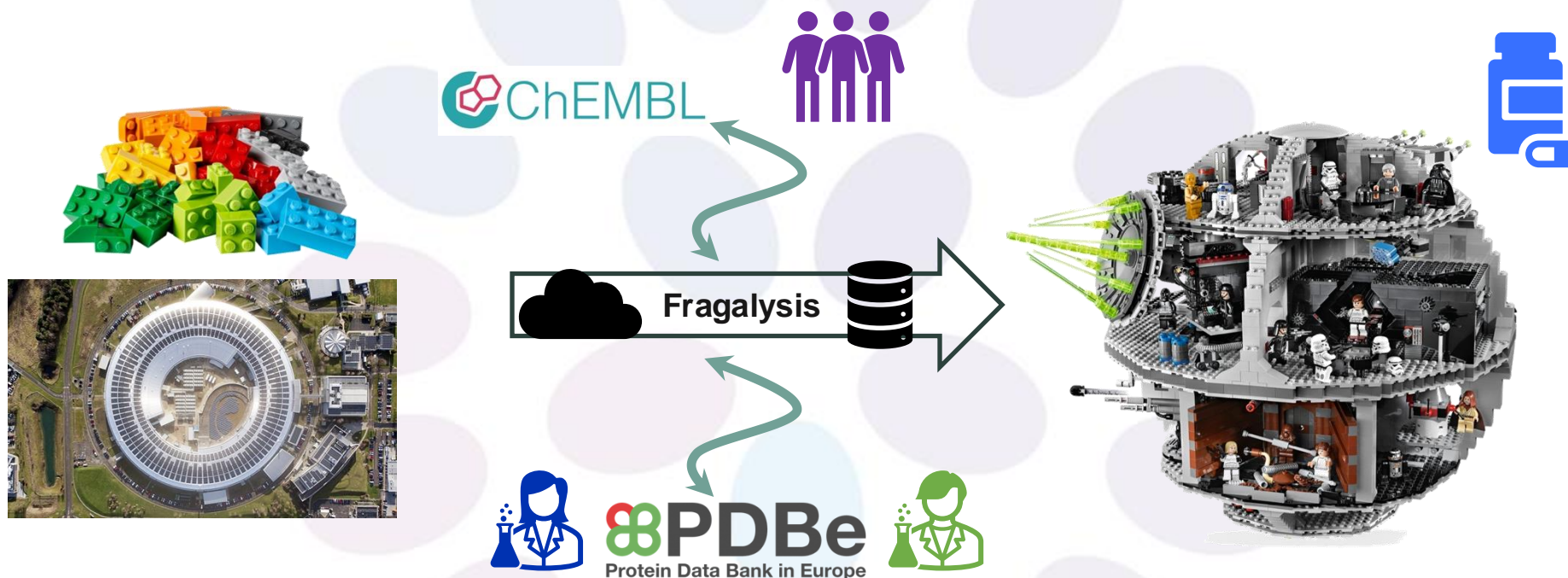
CHALLENGE ADDRESSED

- Existing datasets for exploring and improving structure-based drug design (**SBDD**) are highly inadequate.
- Data is fragmented across various tools and hidden in unstructured formats, making it difficult for researchers to **access and contextualise**

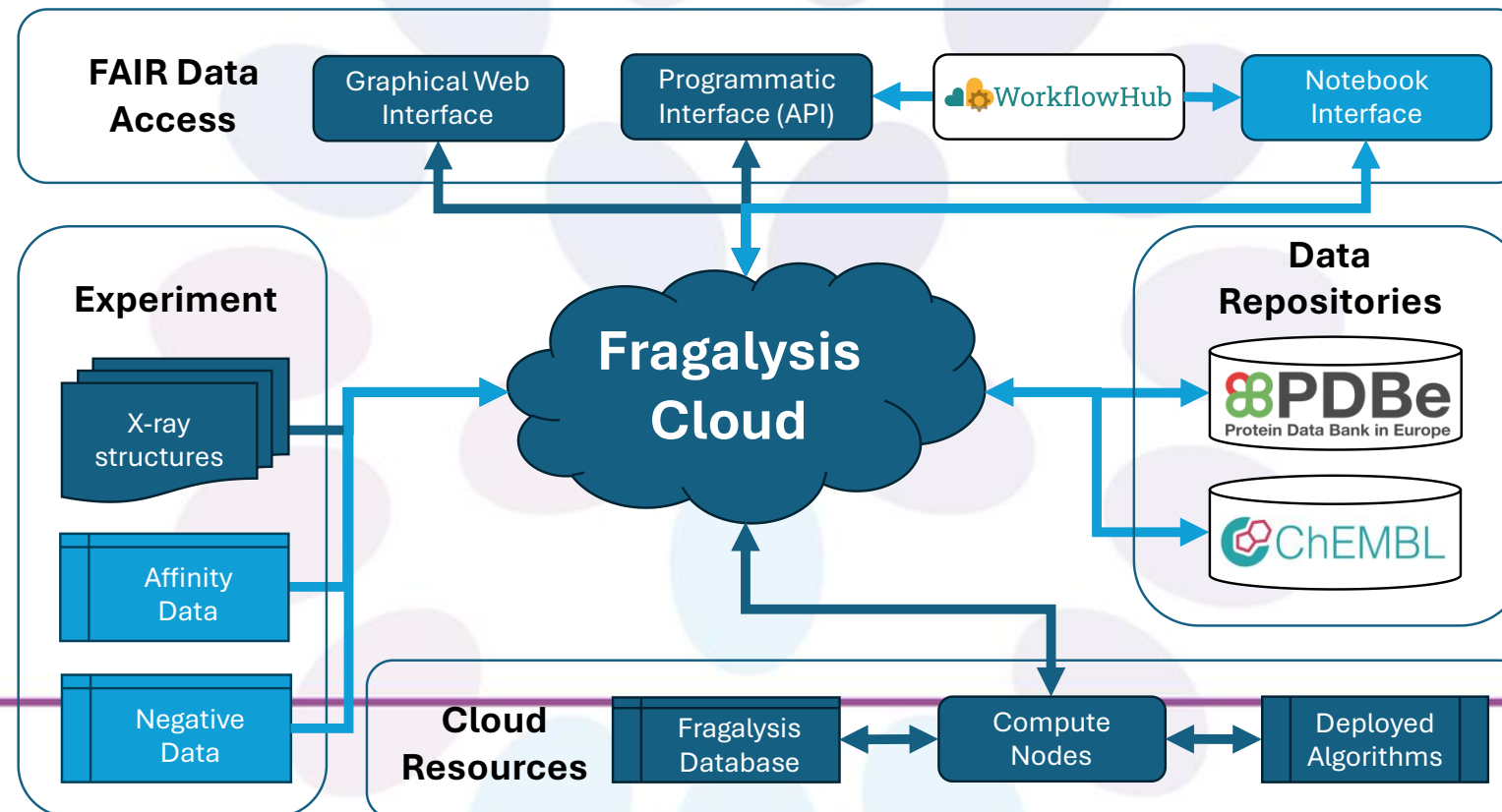


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- The project aims to enhance the **Fragalysis Cloud** platform to facilitate open and FAIR-compliant sharing of SBDD data.
- The project will enable researchers to explore SBDD projects with comprehensive data on **context, provenance, design rationales** and inspection of **computational analyses**.



Fragalysis-Cloud is publicly available:

- <https://fragalysis.diamond.ac.uk/viewer/react/landing>

Workshops:

- User workshop scheduled to host algorithmic developers to deploy data analysis tools to Fragalysis-Cloud

Workflows:

- Data analysis and compound design workflows will be published to WorkflowHub

Documentation published to Read the Docs:

- <https://fragalysis.readthedocs.io/en/latest/index.html>
- <https://fragalysis-backend.readthedocs.io/en/latest/index.html>
- <https://xchem-align.readthedocs.io/en/latest/ALGORITHM-GUIDE.html>
- <https://fragalysis-stack-kubernetes.readthedocs.io/en/stable/>

All code is Open-Source and published to repositories:

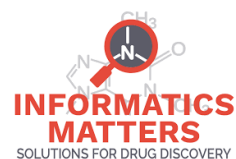
- <https://github.com/PDBEurope/Investigations>
- <https://github.com/m2ms/fragalysis-frontend>
- <https://github.com/xchem/fragalysis-stack>
- <https://github.com/xchem/fragalysis>
- <https://github.com/xchem/fragalysis-api>
- <https://github.com/xchem/xchem-align>

Scope:

- The rapid dissemination, specifically curation and annotation **capturing context**, of structural and affinity data is an ambitious challenge.
- This project will generate many opportunities for the curation, annotation and analysis of drug-discovery data.

Budget & Time:

- Estimating the development time needed to **fully-deploy** backend and frontend code that captures the scientific use-case is non-trivial.
 - Opportunities will be documented, as GitHub tickets, and prioritised, with help from Fragalysis-Cloud **users** and **active** drug-discovery projects, for roll-out.
 - This **OSCARS** supported project will generate further opportunities to apply for follow-up funding.
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Frank von Delft



Tim Dudgeon



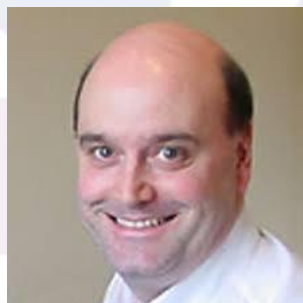
Boris Kovar



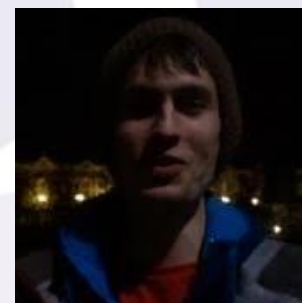
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