DataFAIRy BioAssay Annotation & *In Vitro* Pharmacology

The Pistoia Alliance DataFAIRy and IVP Teams

Key Information

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Project websites:

Sponsors/ Steering

Public Private Partnership between FDA and Pistoia Alliance for the IVP project

Contributors

Thanks to our funders who are making this project possible.
Thanks for all the in-kind contributions for their time and expertise.

Publications

D. Vanderwall, V.A. Makarov, "Bioassays have an integration problem: collaboration will be key to making them FAIR", BioIT World, February 10th 2023

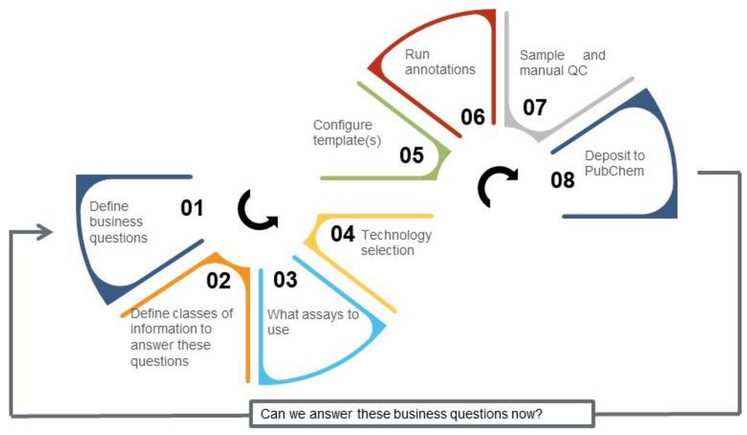
R. Balakrishnan, E.L. Berg, C.C. Butler, A.M. Clark, S.P. Denker, I.Feierberg, J. Harris, T.P. Ikeda, S. Jeschonek, V.A. Makarov, C. Southan, D. Vanderwall, Peter Winstanley, "Bioassay Protocol Metadata Annotation: Proposed Standards Adoption", https://doi.org/10.31219/osf.io/pz8u7, submitted to SLAS Discovery

Project Summary and History

- In 2020 – 2024 we developed and published a minimal information model for assay metadata.
- Over 2300 assay protocols were annotated according to this new metadata model.
- The data model and its applications are described in the 2024 paper recently submitted to SLAS Discovery (please see Publications)
- PA and US FDA use a modified DataFAIRy annotation template for In-Vitro Pharmacology standards in the private-public partnership between the Pistoia Alliance and the US FDA – see below

How We Did It

1. Business analysis
2. Minimal information model development
3. Annotation using NLP and expert review ("AI in the Loop")
4. Test that we can answer the desired questions



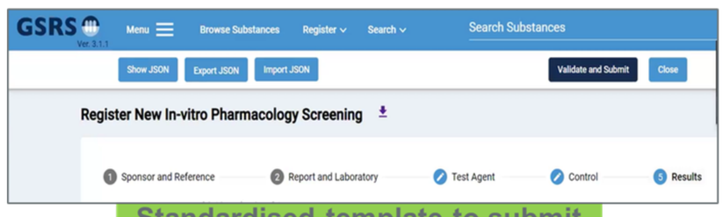
Future DataFAIRy Assay Annotation Scope

- Now we are aiming to create data models for the entire bioassay life cycle: (1) Register a protocol → (2) Instantiate → (3) Capture experimental data → (4) Report to regulators. Applicable to experiments and results of in-silico models
  - FAIR standards for scientific data across the board
  - Ideally, all information published in a paper should be accompanied by the ready-to-use publicly accessible digital content
- We will use ELISA assays as the initial use case
- We are also considering expansion of the BioAssay Ontology (BAO) according to current needs

In-Vitro Pharmacology Work Cycle: An Application of the Assay Annotation Template

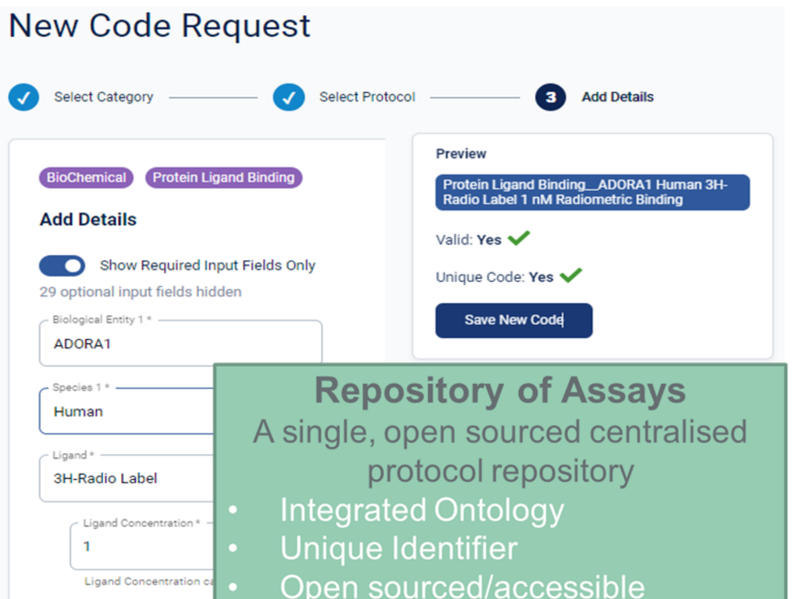
A unique platform allowing:

- The establishment of a **common** and **standardized** data structure utilizing existing or amended **ontologies** for the description of commons assays (repository of assays) and for result submission.
- An **output** that will be **human** and **computer readable**, increasing capacity for provenance and attribute connection for insight and analysis.



Standardised template to submit *In Vitro* secondary and safety pharmacology to regulatory bodies

- Agreed set of information which will comprise of the critical sections required for review by regulatory bodies
  - Screening assays
  - Quantitative data
- A controlled vocabulary & a well-curated ontology



Repository of Assays
A single, open sourced centralised protocol repository
- Integrated Ontology
- Unique Identifier
- Open sourced/accessible

Global Substance Registration System – GSRS

Assist agencies in registering and documenting information about substances found in medicines.
- A common identifier for all of the substances used in medicinal products
- Utilizing a consistent definition of substances globally, including active substances under clinical investigation
- consistent with the ISO 11238 standard.

Pistoia Alliance: Collaborating to lower barriers to R&D innovation

The Pistoia Alliance is a global, not-for-profit alliance of life science companies, vendors, publishers, and academic groups that work together to lower barriers to innovation in R&D.

Our members collaborate as equals on open projects that generate significant value for the worldwide life science community.

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