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Open PHACTS Data

With Acknowledgment to the Open PHACTS project consortium

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- Data sources presently in Open PHACTS selected by:
- Choosing data sources to answer business questions
- Selecting appropriate data sources based on licensing
- Filtering criteria of judged data quality
- **Chemistry Data**: ChEBI, ChEMBL, Drugbank aggregated through ChemSpider – initial focus on pharmacology
- **Biology Data**: SwissProt, GO/GOA and ENZYME
- Data underpins public version plus all related exemplars
- Data are intended to be updated quarterly for the near future
- Curation/annotation flow intended to be continuous

Data in Open PHACTS

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The process:

- Chemicals imported to ChemSpider and registered with CSIDs
- Registered compounds passed to ConceptWiki
- ConceptWiki passes data to Identifier Mapping Service
- RDF generated from ChemSpider for deposition to cache
- Linked Data Cache receives RDF from various original data sources – RDF is provided by data source provider, or is sourced from alternate provider, or is generated by Open PHACTS team

The Process

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RDF is well suited to describing complex data

- Open and supported by a growing body of tools and scientists
- Critical data sources are published as RDF
- Producers of RDF can enhance their RDF with information required to create Nanopublications
- We will support data providers to generate RDF as necessary

RDF

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- We will publish guidelines for producing RDF. These are community-endorsed best practices. For instance:
  - "Good URIs" (stable, opaque, dereferencable)
  - Attention to quantitative data
  - The use of semantic models for the dataset
- RDF will be used to produce and integrate nanopublications

- How many of your organizations already have skills and experience in generating RDF?

Making the RDF

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- Data licensing is hard! Licenses are commonly obscure…

- Open PHACTS hopes to accommodate both **open** and **license-restricted** data
- We will go live in September with data sets that have well-defined licensing
- We will develop a licensing strategy around public data to ensure OPS complies with the terms for use and distribution
- We will support restricted datasets within the platform in the future - licensed or private content.
- We are contracting expertise in data licensing to navigate…

Data Licencing

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- ChemSpider registers compounds and provides services to perform structure/substructure/similarity searches
- Each data source providing chemistry is “registered”
  - This process assigns them a unique CSID
  - CSIDs, preferred name, synonyms, Inchi string & key and SMILES are published back into the cache
  - Chemical structure standardization rules are in development using FDA SRS standards. Validation included
  - ChemSpider provides validated synonyms to ConceptWiki for text-based searching/look-up

Chemistry Representation

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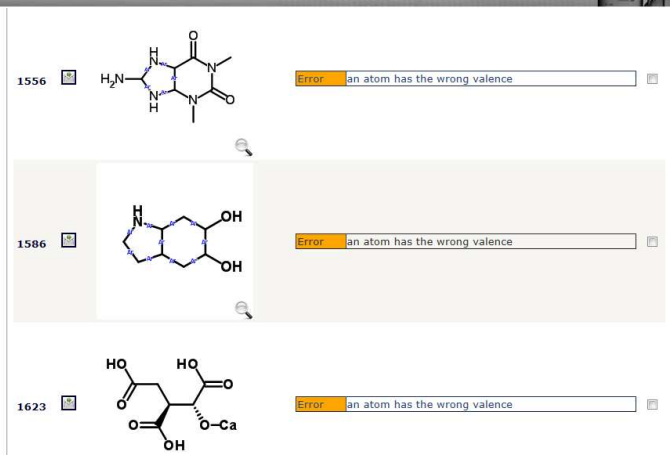

Curation and Annotation

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- Develop **systems** to validate and standardize data – our preference is to be proactive in data quality when possible
- Provide interactive ability to curate and annotate data from data sources
- Existing systems to be integrated and enhanced – ConceptWiki and ChemSpider **already** provides curation/annotation features
- Provide feedback to data suppliers regarding identified issues and help clean up existing data to contribute back to providers

- Our primary concern is participation – not the systems.

Curation and Annotation

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- Additional data sources will be identified based on project needs, data licensing, partner provisions

- What do you see as possibilities for integrating **YOUR** data?

- How might you want to use Open PHACTS data/technologies (recall that there will be Open APIs into the system)?

Future