Collaborative Ontology Design and Implementation for the OpenTox Toxicity Prediction Framework

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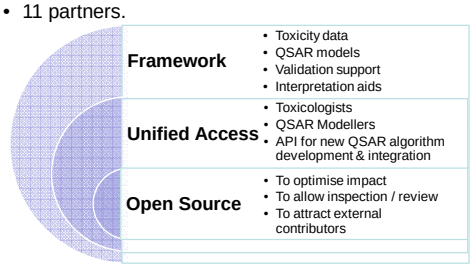
The OpenTox Project http://www.opentox.org

OpenTox Objectives

- European Commision Framework Programme 7, HEALTH-2007-1.3.3 Promotion, development, acceptance and implementation of QSARs (quantitative structure-activity relationship) for toxicology;
- The overall objective of the OpenTox project is to develop a framework that provides a unified access to toxicity data, predictive models, procedures supporting validation and additional information that helps with the interpretation of predicted results;
- 11 partners.

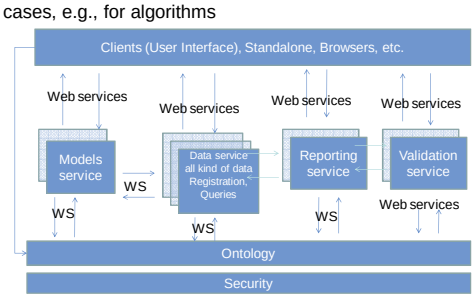


Distributed Web Services for Predictive Toxicology

- Distributed Web services for predictive toxicology
- **REST** technology - Every object has an unique URI; URIs are dereferentiable; Multiple representation of an object is encouraged (e.g. RDF, but also others); Fixed operations – GET, PUT, POST, DELETE
- Every object has **RDF** representation – Compounds; Datasets; Compound; Properties; Prediction algorithms; Models; Validation statistics; Reports.
- **Ontologies**: Opentox.owl, Blue Obelisk algorithm ontology, OpenTox algorithm types ontology, OpenTox endpoints ontology, based on ECHA endpoints classification; specific Toxicologycal endpoints ontology.
- **WEB Applications**:
  - o **ToxPredict** supports the case of a user providing an input chemical structure, to then predict a toxicity endpoint;
  - o **ToxCreate** supports the case of creating a predictive toxicology model.

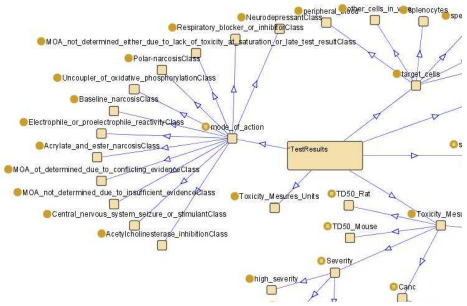
The Role of the Ontologies

- **What**? - Formal, shared conceptualization of a domain.
- **Why**? - Distributed services need to be able to „talk to each other", i.e. have a common understanding of endpoints, any type of property, methods, etc.
- Our **strategy**: use existing work and standards wherever possible, however we also build new ones as needed for tox use cases, e.g., for algorithms



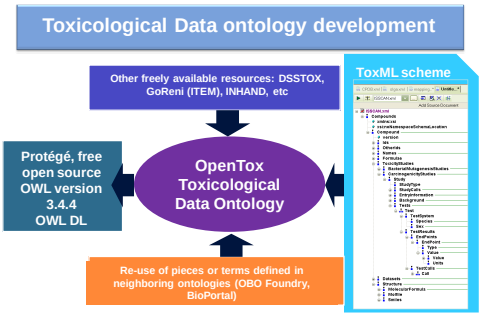
Information exchange based on standardized ontologies and REST web services. All the information from different services might be used separately or via an ontology repository with reasoning capabilities

Ontologies



Toxicological Endpoints Ontology

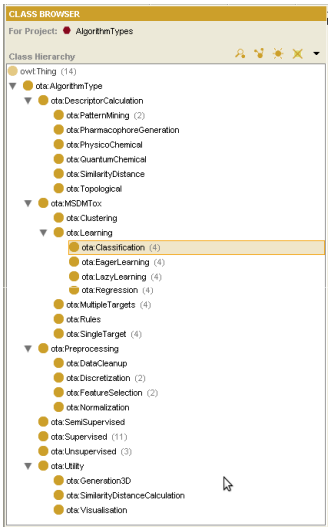
Overlapping biomedical ontologies:
- Chemical Entities of Biological Interest (ChEBI)
- Ontology for Biomedical Investigations OBI
- NCI Thesaurus
- Foundational Model of Anatomy (FMA)
- Mouse Adult Gross Anatomy (MA)
- Mouse Gross Anatomy and Development (EMAP)
- Units of Measurement UO Ontology
- Chemical Information Ontology
- CARO – Common Anatomy Reference Ontology
- Ontology of Scientific Experiments (EXPO)



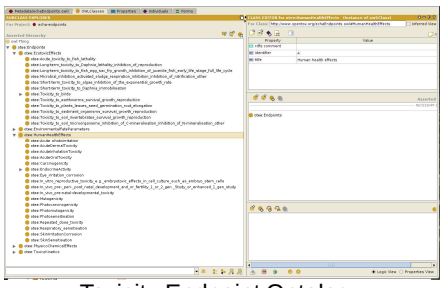
Ontology For Target Organs

INHAND (International Harmonization of Nomenclature ad Diagnostic Criteria for Lesions in Rates and Mice)

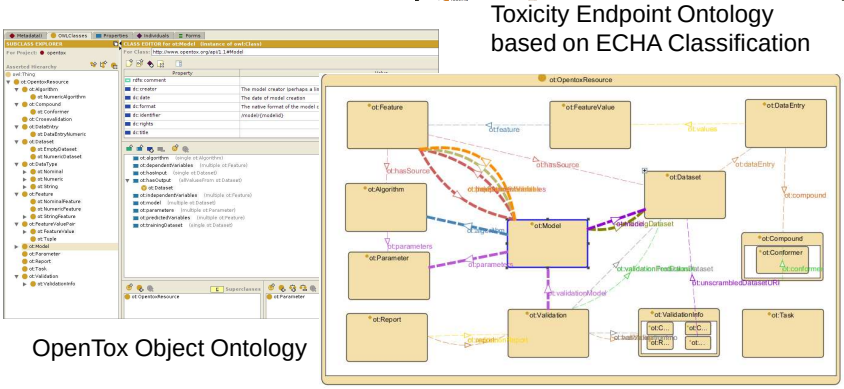
New developments in the ontology:
- more synonyms regarding organs systems, target organs and their subclasses;
- organs are more detailed, up to histological components;
- reviewed by pathologists, who have been involved in the INHAND process;
- linking of the organ systems and their components with pathologic effects.



Algorithm Types Ontology



Toxicity Endpoint Ontology based on ECHA Classification



OpenTox Object Ontology