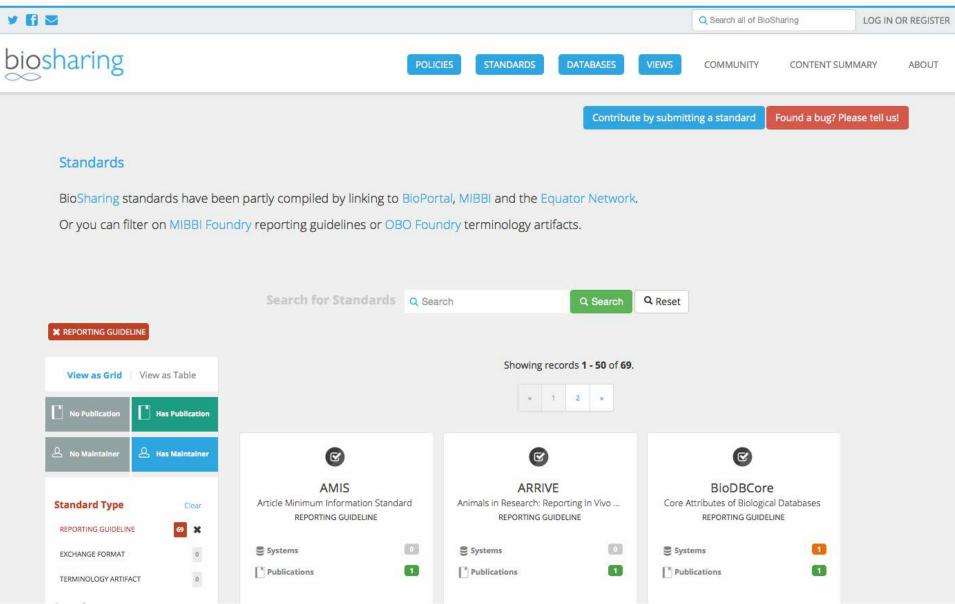


#### Types of data standards

- Reporting guideline (checklist) specifies what information need to be captured about an experiment for a particular purpose
- (Controlled) vocabulary terminological resource that provides the identification and definition of entities
- **Data exchange format** is a specification how data are encoded to be computer-readable / -processable

• **Data structure** refers to organization of data, data schema, entity relations

#### BioSharing Standards (http://www.biosharing.org)



#### **Checklists – Minimum Information Guidelines**

#### mibbi Bioscience reporting guidelines and tools

#### Portal

- Foundry
- About

#### Minimum Information guidelines from diverse bioscience communities

- If you want to register your checklist to MIBBI, please contact the BioSharing team
- Excel spreadsheet and XML document (schema) describing all registered projects

#### Bioscience projects registered with MIBBI

CIMR	Core Information for Metabolomics Reporting	I	L	X
GIATE	Guidelines for Information About Therapy Experiments			
MIABE	Minimal Information About a Bioactive Entity	I	L	X
MIABIE	Minimum Information About a Biofilm Experiment			
MIACA	Minimal Information About a Cellular Assay			
MIAME	Minimum Information About a Microarray Experiment	I	L	X
MIAPA	Minimum Information About a Phylogenetic Analysis			
MIAPAR	Minimum Information About a Protein Affinity Reagent			
MIAPE	Minimum Information About a Proteomics Experiment			
MIAPepAE	Minimum Information About a Peptide Array Experiment			
MIARE	Minimum Information About a RNAi Experiment	I	Ŀ	X
MIASE	Minimum Information About a Simulation Experiment	I	L	X
MIASPPE	Minimum Information About Sample Preparation for a Phosphoproteomics Experiment			
MIATA	Minimum Information About T Cell Assays			
MICEE	Minimum Information about a Cardiac Electrophysiology Experiment			
MIDE	Minimum Information required for a DMET Experiment			
MIFlowCyt	Minimum Information for a Flow Cytometry Experiment	I	L	X

#### Minimum Information Standard may not exist

Journal of Neurotrauma					
About Thi	is Journal				
Minimum Information about a Spinal Cord Injury Experiment: A Proposed Reporting Standard for Spinal Cord Injury Experiments					
Beattie Christin	<b>rticle:</b> e P., Ferguson Adam R., Popovich Phillip G., Xu Xiao-Ming, Snow Diane M., Igarashi Michihiro, ne E., Bixby John L., and the MIASCI Consortium. Journal of Neurotrauma. August 1, 2014, 31(15): ii:10.1089/neu.2014.3400.				
	Volume: 31 Issue 15: August 4, 2014				
	of Print: July 11, 2014				

Regenbase: Integration of diverse data related to nerve regeneration in the context of spinal cord injury

http://regenbase.org

# Vocabulary vs. ontology

- Controlled vocabularies / thesauri
  - describe what things mean (link terms to human description)
  - Entities with identity criteria
  - Share knowledge in a common language
  - Natural language synonyms for search and text mining

# Vocabulary vs. ontology

- Ontologies
  - Contains entities (classes) and their relationships (object properties)
  - Capture / abstract knowledge using logical axioms
  - Explicit specification (OWL-DL)
    - Building formal (computable) models
    - Computing with knowledge (reasoning engines)
    - Foundation of Semantic Web information systems

### **Ontology resources**

#### **NCBO Bioportal**

#### **EBI Ontology Lookup Service OLS**

search all ontologies	Find an ontology  Poid  Poid  Explore  Explore Explore  Explore  Explore  Explore  Explore  E	Search resources	Project Publications Developer Resources Download Implementation Overview Javadoc Webservice documentation Y Contact Us Acknowledgements	Enter Ontology Term — Search Ontology: Chemical Entities of Biological Interest Term Name: (include obsolete terms ) pyridine Pyridine pyridine ning pyridine rings Benzo[c]pyridine benzo[b]pyridine benzo[b]pyridine pyridine-N-oxide pyridine N-oxides pyridine alkaloid pyridine alkaloid pyridine alkaloid pyridine nucleoside pyridine nucleoside pyridine nucleoside pyridine nucleosides pyridine nucleosides pyridine nucleosides pyridine nucleosides pyridine nucleosides	t [CHEBI] + Browse Term ID: d terms that match what are b corresponding ID will be d values, you can select this As an example, enter mitor in xxample, if you are looking for 4 <sup>1</sup> . to the ontology selector. To me has been selected, it will be Search' button to quickly obtain	Introduction The Ontology Lookup Service is a spin-off of the PHIDE project, which required a centralized query interface for ontology and controlled vocabulary lookup. The OLS provides a web service interface to query multiple ontologies from a single location with a unified output format. The OLS can integrate any ontology available in the Open Biomedical Ontology (OBO) format. OLS Statistics Version 1.21 Ontologies 83 Terms 2577564 Last Thu Feb 19 17:08:15 GMT updated 2015 See the full breakdown of loaded
Resources Indexed 48 Indexed Records 39,464,136	New Term Proposal-Attestation (Radiology Lexicon) over 1 year ago by rboden			all pertinent information for this term. Searches are case-sensition ontology prefix is used (GO:, rather than go: or Go:).	ve, so ensure that the proper	ontologies here and load statistics here.

Ontologies	Resources	Participate	About			
development with the g who have expressed ar In addition to a listing of services to facilitate ont	oal of creating a suite interest in this goal i OBO ontologies, this plogy development. V	of orthogonal interop are listed below, follow site also provides a s We welcome feedback that column. The Ss	erable reference ont wed by other relevant statement of the OBO s and encourage part link to the term reque	Foundry principles, discussion fora, technical icipation.	developing ontologies	Cutck Links Cutck Links Council a strength formats Council and alternate formats Cutrent events Cutrent events Cutrent events To obin
			O Foundry onto			OBO Foundry paper in Nature
I	itle	Domain	Prefix	Eile	Last changed	Biotechnology, November 2007
Biological process		biological process	GO	<u>ao.obo</u> 🍯		
Cellular component		anatomy	GO	<u>ao.obo</u> 眷		Other Ontology Lists
Chemical entities of b	iological interest	biochemistry	CHEBI	chebi.obo 👙		
Molecular function		biological function	GO	ga.aba 眷		OntoBee
Ontology for biomedia	al investigations	experiments	OBI	obi.owl 🍣		Ontology Lookup Service (OLS) (O Foundry term lookup)
Phenotypic quality		phenotype	PATO	quality.obo 🍅		· · · · · · · · · · · · · · · · · · ·
Plant Ontology		anatomy and development	PO	plant_ontology.obo?view=co 👙		
PRotein Ontology (PR	0)	proteins	PR	pro.obo 🍯		
Xenopus anatomy an	d development	anatomy	XAO	xenopus_anatomy.obo		
Zebrafish anatomy ar	nd development	anatomy	ZFA	zfa.obo 🍯		
	OBO For	undry candidate	ontologies and	other ontologies of interest		
Т	itle	Domain	Prefix	File	Last changed	
Adverse Event Report	ting Ontology	health	AERO	aero.owl		
Anatomical Entity Ont	ology	anatomy	AEO	aeo.obo	2012/06/01	
Ascomycete phenotyp	e ontology	phenotype	APO	ascomycete_phenotype.obo	2014/06/30	
			BFO	1.1		

bcgo.owl 🍣

bco.owl 🗳

Beta Cell Genomics Ontology

**Biological Collections Ontology** 

experiments

BCGO

BCO

## Metadata specifications

Metadata: Data not directly measured in an experiment (or obtained in a study)

Why metadata:

- Facilitate data replicability, reproducibility, reuse
- Interpret results, perform data analysis, hypotheses
- Repurpose data for other projects
- Information systems (search, query, data integration and exchange)

What metadata to capture in a standardized format with controlled vocabularies (and formal descriptions)?

## A useful distinction of metadata

#### Model metadata:

- Required to understand, interpret, and meaningfully integrate experimental results
- Typically queryable in software systems
- Important parameters to describe conclusions (data visualizations)

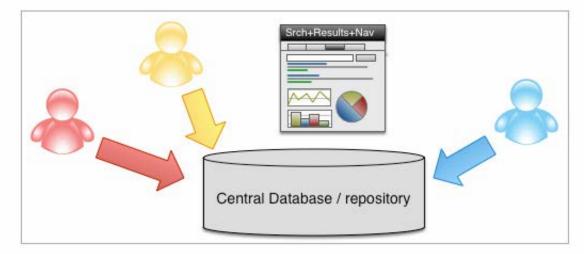
#### Confounder metadata:

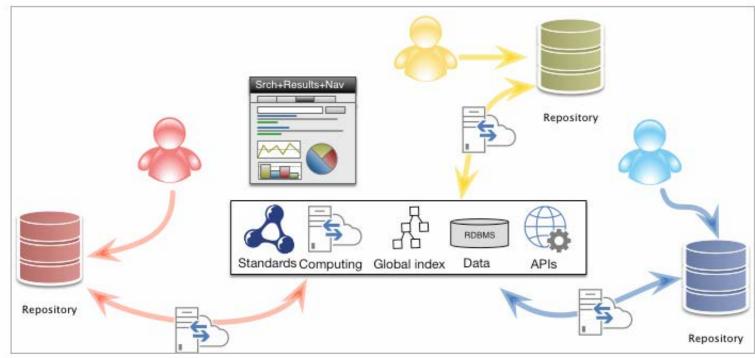
- Non model metadata required to replicate and reproduce experimental results
- Needed for "data forensics" (e.g. batches of reagents, maintenance of experimental equipment, etc.)

## Standardized metadata

- **Capture all** (detailed descriptions, SOP) **Make model metadata explicit** (controlled vocabulary, standard format)
- But what's really model metadata?
- Data and informatics use cases
  - Types of queries and analyses
  - Integration with other data sources
  - Information systems / UI components
  - Consider re-use of data for other projects

#### **Data Coordination**





### Data set IDs and provenance

Permanent ID via (authoritaitve) repository or data publication

- DOI
- PURL

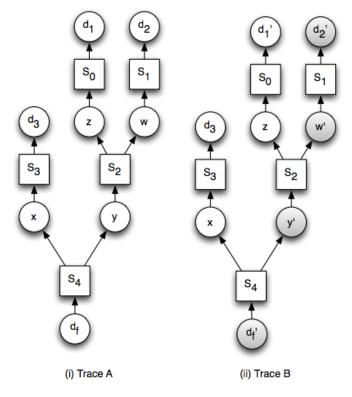
Capture data provenance

- PROV-O: The PROV Ontology (W3C)
   http://www.w3.org/TR/prov-o/
- PAV (Provenance, Authoring Versioning) Ontology http://purl.org/pav/

#### Provenance

The link between source data, computation / processing and derived data / results

- static verifiable record
- track changes
- compare / discrepancies
- repeat / reproduce
- Citation
- version
- data release



PDIFF, Woodman 2011

### **RDBMS vs Semantic Web technologies**

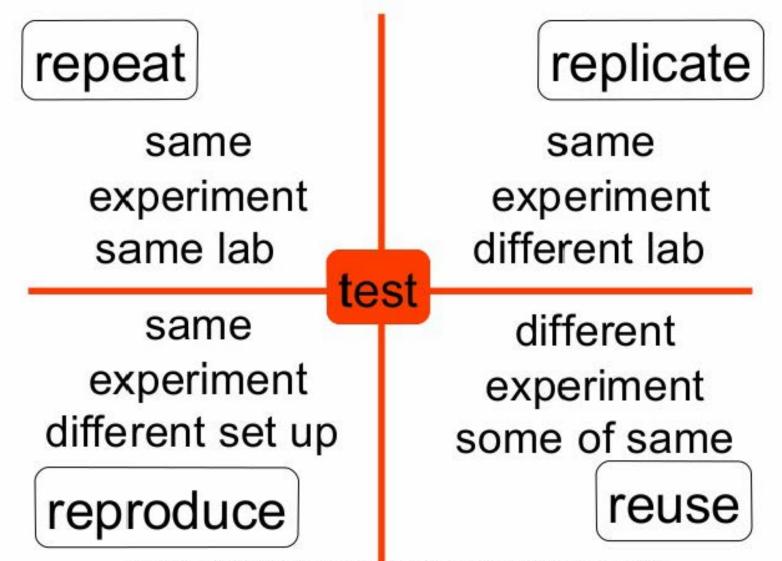
# RDBMS

- Closed world assumption
- No reasoning support
- Need to know schema for highly specialized queries
- Data sharing not easy, no semantics
- Efficient RDBMS access
- Established technology
- Industry standard

# Ontologies

- Open world assumption
- Reasoning support
- Provide restriction-free framework (formal semantics)
- Easy data/knowledge sharing
- Triple store access
- Relatively early stage
- Standards emerging

## **Replicability vs Reproducibility**



Drummond C Replicability is not Reproducibility: Nor is it Good Science, online Peng RD, Reproducible Research in Computational Science Science 2 Dec 2011: 1226-1227.