



Metadata for Interoperable Bioscience

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DDI Metadata Sprint

October 19-23 2015



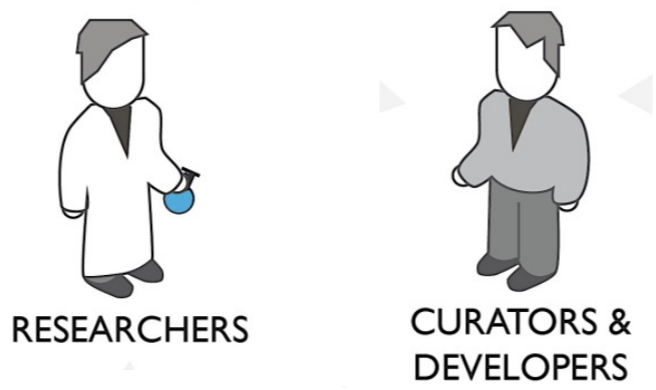
LIFE, NATURAL & BIOMEDICAL SCIENCES



Our areas of activity:

- Data capture and curation
- Data (nano)publication
- Data provenance
- Open, community ontologies and standards
- Semantic web
- Software development
- Training

Communities we work with/for:

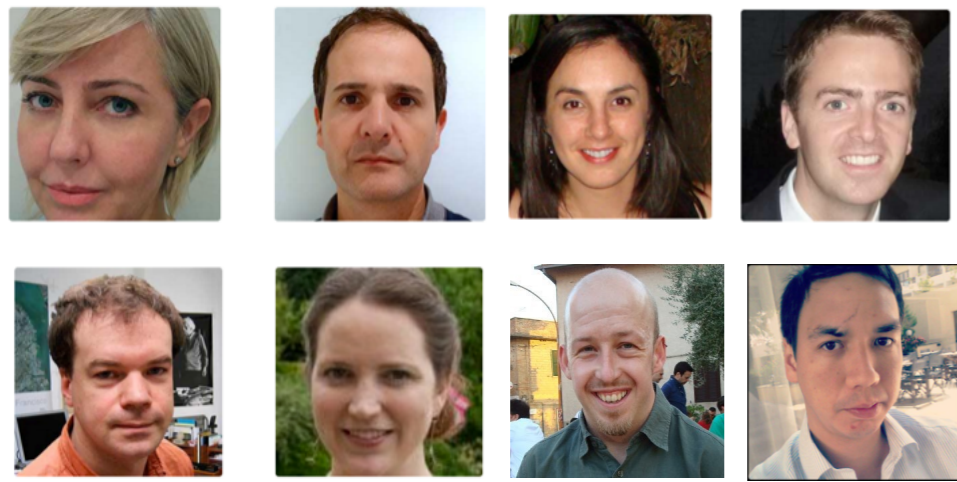


FUNDERS, JOURNAL EDITORS & LIBRARIANS

As part of:

- UK, European and international consortia
- Pre-competitive informatics public-private partnerships
- Standardization initiatives

Some of the groups we engage with incl.:



Overview

biosharing.org

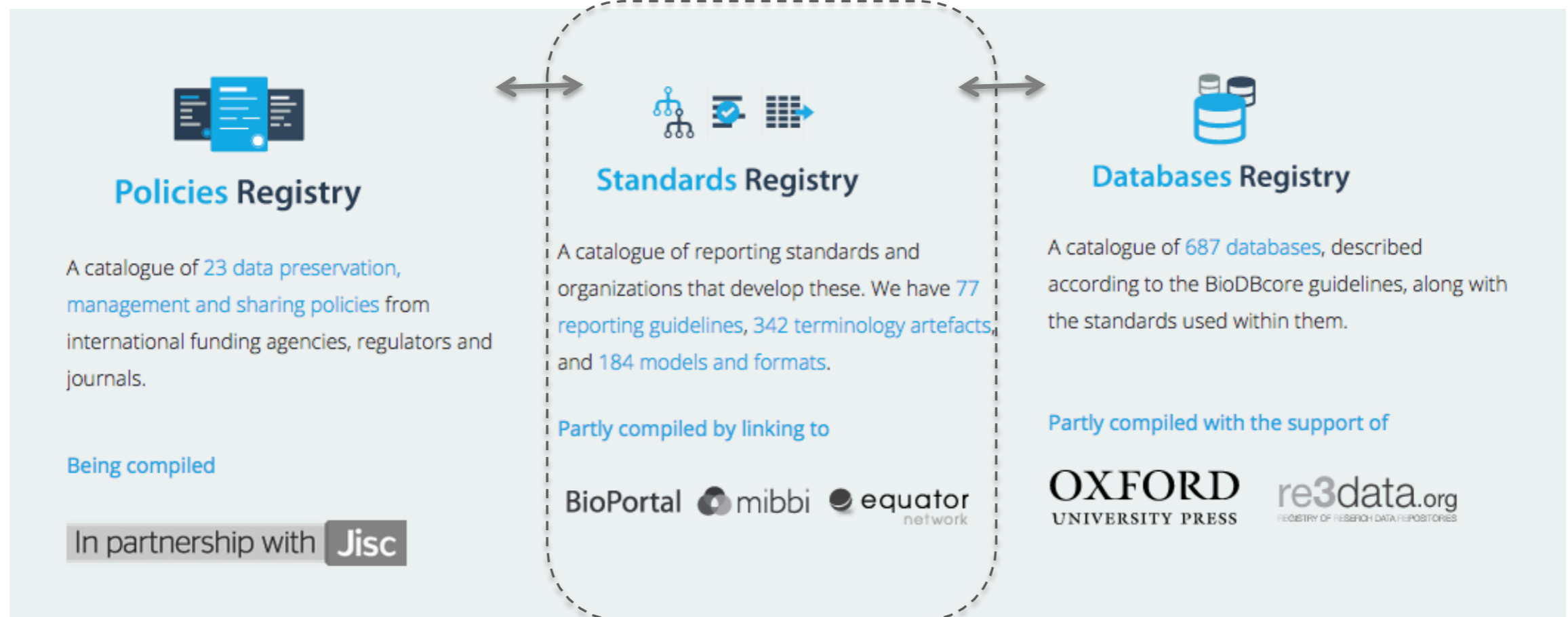
isa-tools.org
isacreator configurator isacreator bii converter Risa linkedisa

NIH
NIH Big Data to Knowledge (BD2K)

 CEDAR
CENTER FOR EXPANDED DATA ANNOTATION AND RETRIEVAL

bio
CADDIE

stat@-ontology.org
statistics ontology



A web-based, curated and searchable registry ensuring that **biological standards** and **databases** are *registered, informative and discoverable*; also monitoring the **development and evolution** of standards, their **usage** in databases and the **adoption** of both in data **policies**.

Search filter, refine

Core functionalities:

- search and filtering, e.g. by funder, domain, type of standard
- Refine by publication, maintainer etc.
- add new records, edit existing records
- “claim” records
- person’s profile (as maintainer of records) associated to the ORCID profile (for credit)
- visualization and views of content and linking

Annotation Sources:

- 4 axes: (material, process, quality, information)
- NIF,OBI,CL,GO,IAO,EDAM

The screenshot displays a search results interface with a left sidebar for filters and a main grid of record cards. The top right indicates 'Showing records 1 - 50 of 585.' The sidebar filters include:

- View as Grid** | View as Table
- No Publication** | **Has Publication**
- No Maintainer** | **Has Maintainer**
- Deprecated** | **Current**
- Standard Type**: TERMINOLOGY ARTIFACT (337), EXCHANGE FORMAT (178), REPORTING GUIDELINE (70)
- Domains**: DNA (54), ANATOMY (44), PROTEIN (35), HOMO SAPIENS (31)
- Taxonomies**: ALL (18), HOMO SAPIENS (16), HOMO SAPIENS (5), ARCHAEA (3)
- Countries**: USA (28), CANADA (9), UK (9), GERMANY (8)
- Maintainers**: NIF (35)

The main grid shows detailed views for:

- AAO** (Amphibian gross Anatomy Ontology): 2 Data types (ANATOMY, AMPHIBA)
- ABA** (ABA Adult Mouse Brain): 2 Data types (BRAIN, MUSCULUS)
- ABCD** (Access to Biological Collection Data EXCHANGE FORMAT): No data types defined.
- ABCDDNA** (Access to Biological Collection Data DN... EXCHANGE FORMAT): 4 Data types (DNA, BIOLOGICAL DIVERSITY, DNA SEQUENCE DATA, SEQUENCE)
- .ACE format** (.ACE format EXCHANGE FORMAT): 5 Data types (CONTIG ASSEMBLY, DNA SEQUENCE DATA, CONTIG, GENOME, DNA)
- ACGT** (Cancer Research and Management ACGT Mas...): No data types defined.

Collections

EDITORIAL

Open Access



Better reporting for better research: a checklist for reproducibility

Amye Kenall^{1*}, Scott Edmunds², Laurie Goodman², Liz Bal¹, Louisa Flintoft³, Daniel R Shanahan¹ and Tim Shipley⁴

BioMed Central The Open Access Publisher BioMed Central journal guidelines and checklist

This collection houses all the databases and standards mentioned in the submission checklist for the BioMed Central stable of journals. The checklist itself is listed as a policy document in this collection.

[Homepage](#)

Search within this collection

Search Policies, Standards, Databases Search

Showing records 1 - 50 of 56.

< 1 2 >

View as Grid | View as Table

Best Match Sort Descending Sort Ascending

No Publication Has Publication

No Maintainer Has Maintainer

Deprecated Current

Standard Type

REPORTING GUIDELINE 13
MODEL AND FORMAT 2
TERMINOLOGY ARTIFACT 0

Domains

HOMO SAPIENS 6
PROTEIN 5
DNA 4
CLINICAL TRIAL 4

SHOW MORE

<p>Addgene</p> <ul style="list-style-type: none"> Standards: 2 Publications: 3 In Collections: 2 <p>No taxa defined.</p> <p>5 Data types, including: PLASMID, REPOSITORY, REFERENCES, DNA, NON-PROFIT</p>	<p>ArrayExpress</p> <ul style="list-style-type: none"> Standards: 6 Publications: 2 In Collections: 2 <p>1 Taxa types, including: ANY</p> <p>7 Data types, including: HIGH THROUGHPUT GENOMICS (RNA-SEQ), NUCLEOTIDE, CHIP-SEQ</p>	<p>ARRIVE REPORTING GUIDELINE</p> <ul style="list-style-type: none"> Systems: 0 Publications: 2 In Collections: 1 <p>No taxa defined.</p> <p>4 Data types, including: IN-VIVO STUDY, METAZOA, LIVING ANIMAL, ANIMAL RESEARCH</p>	<p>BioMed Central Journal Submission Check... 2015</p> <ul style="list-style-type: none"> Publications: 0 In Collections: 1 <p>1 Taxa types, including: ANY</p> <p>No data types defined.</p>	<p>NCBI BioSample</p> <ul style="list-style-type: none"> Standards: 1 Publications: 1 In Collections: 1 <p>No taxa defined.</p> <p>7 Data types, including: ASSAY, SEQUENCE DATA, EXPRESSION STUDIES</p>
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The  **isa** infrastructure

 **isa** model

generic model for experimental
description and data exchange
(tab, RDF, JSON, ...)



community engagement



open source software tools



Towards interoperable bioscience data: Presenting the ISA Commons, authored by more than 50 collaborators at over 30 scientific organizations around the globe.

Sansone et al, 2012
Nature Genetics



ISA software suite: Overview of ISA-Tab and first set of tools

Rocca-Serra et al, 2010
Bioinformatics

Formats & Database Fragmentation



MAGE-TAB



PRIDE ML



SRA XML



Sample-Tab



ISA-Tab



ARRAYEXPRESS



PRIDE



ENA
European Nucleotide Archive



BioSamples



EMBL-EBI
MetaboLights

Transcriptomics data files & relevant experimental descriptors

Proteomics data files & relevant experimental descriptors

Sequence data files & relevant experimental descriptors

Biological sample information

Metabolomics data



MAGE-TAB



PRIDE ML



SRA XML

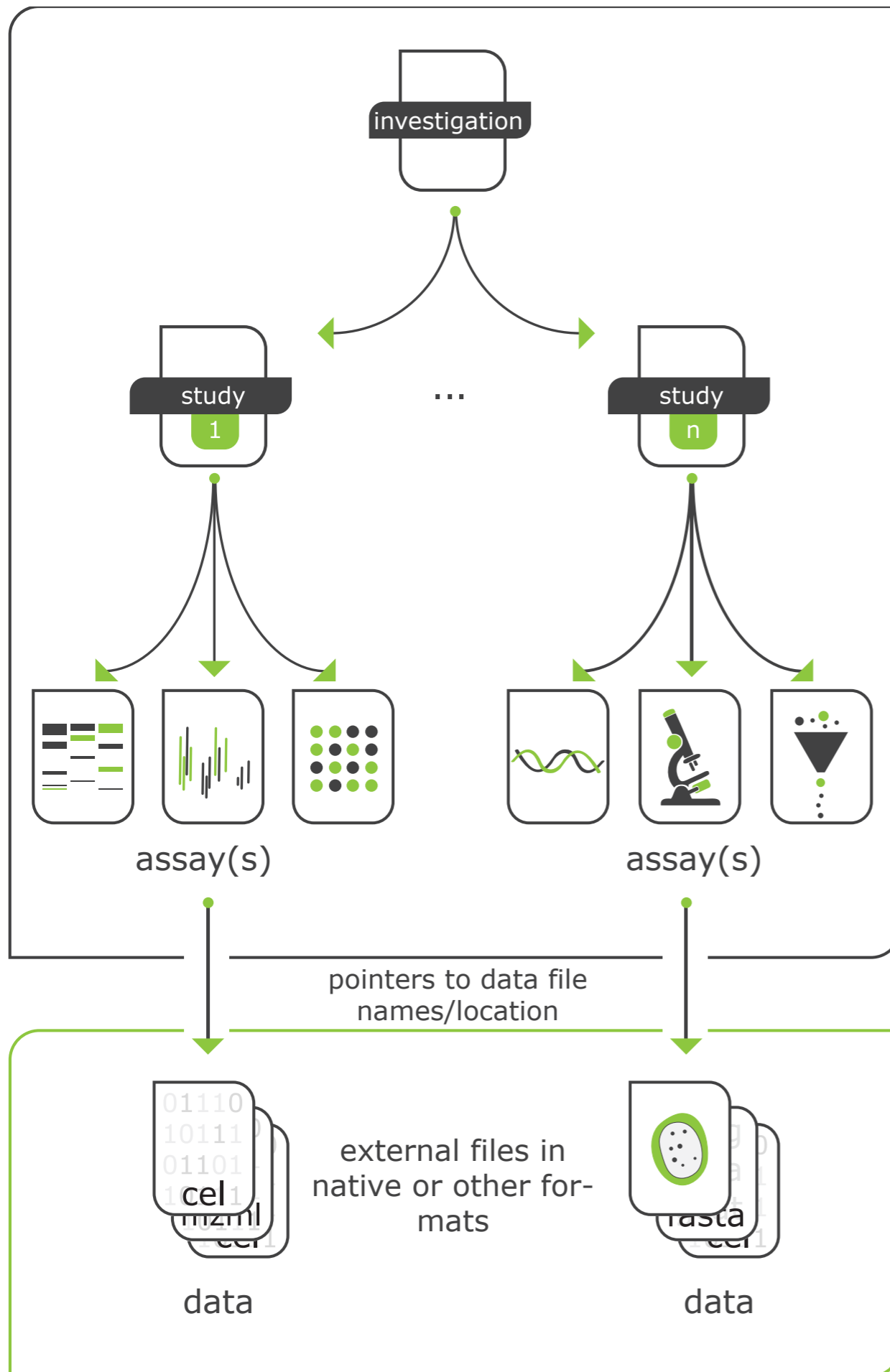


Sample-Tab



ISA-Tab





investigation

high level concept to link related studies

study

the central unit, containing information on the subject under study, its characteristics and any treatments applied.

a study has associated assays

assay

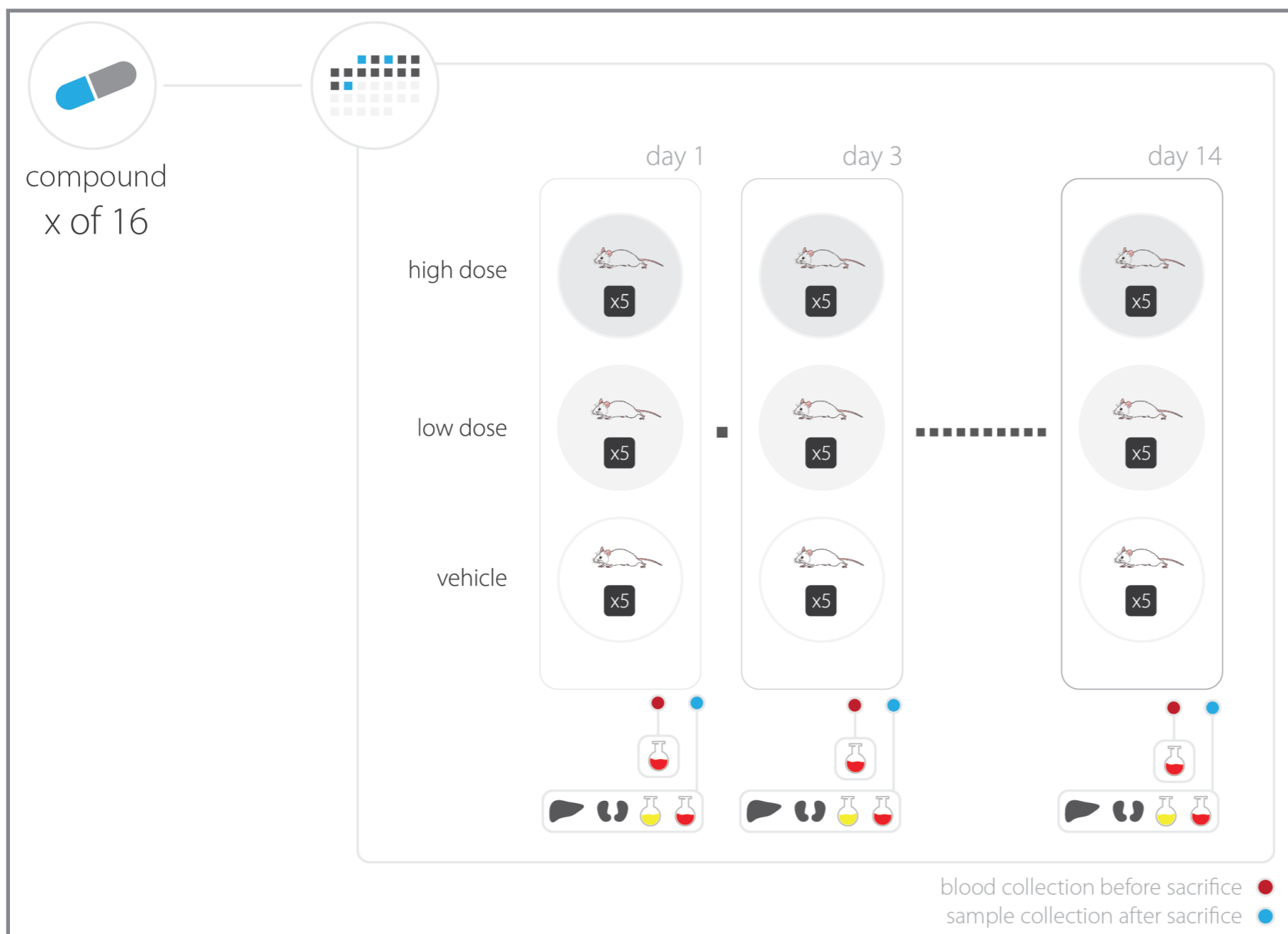
test performed either on material taken from the subject or on the whole initial subject, which produce qualitative or quantitative measurements (data)



isacommmons
isacommmons.org

- environmental health
- environmental genomics
- metabolomics
- metagenomics
- nanotechnology
- proteomics
- stem cell discovery
- system biology
- transcriptomics
- toxicogenomics
- communities working to build a library of cellular signatures

The experimental plan



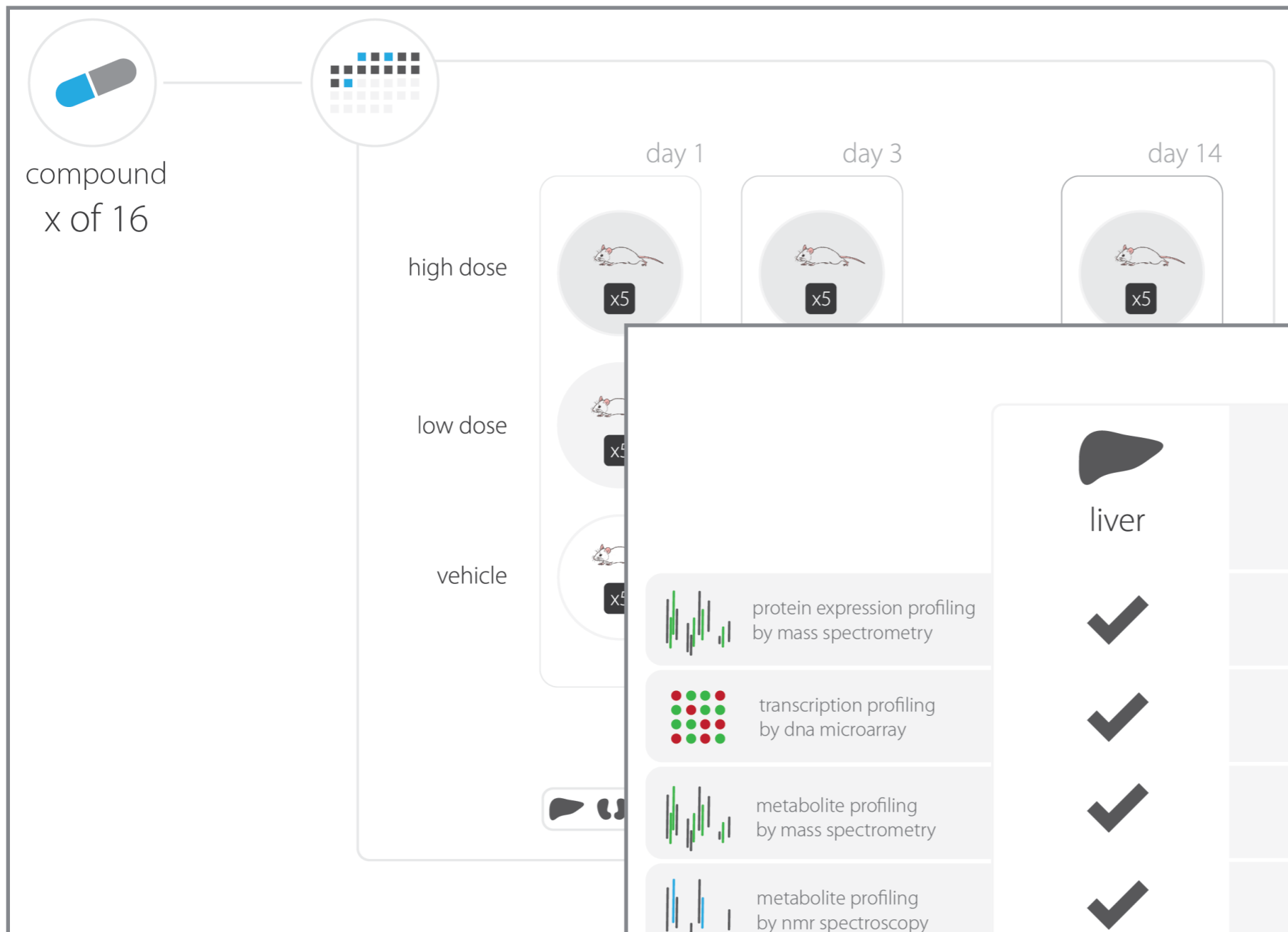
experimental design
sample characteristic(s)
experimental variable(s)

InnoMed PredTox Project

2-week systemic rat study using male Wistar rats (N=15 per dose group)

14 proprietary drug candidates from participating companies and
2 reference toxic compounds

The experimental plan



experimental design
 sample characteristic(s)
 experimental variable(s)

technology(s)
 measurement(s)
 protocols(s)
 data file(s)
 ...

	liver	kidney	blood serum plasma		urine
protein expression profiling by mass spectrometry	✓	✓	✓		✓
transcription profiling by dna microarray	✓	✓	✓	✓	
metabolite profiling by mass spectrometry	✓	✓	✓		✓
metabolite profiling by nmr spectroscopy	✓	✓	✓		✓
histology	✓	✓	✓	✓	✓
clinical chemistry			✓	✓	✓
hematology			✓	✓	

Purple Non-sulfur Jan Rhee

Notes

the TA took the anaerobic jars of the 305 plates out of the lighted incubator, & examined it a bit. the smell is fresh - like a dead animal. My plate is pretty damp, but not really very bad, like vomit.

plate

It has a variety of clear, white & yellowish colonies

lots of big dark red colonies - too small to make out clearly - appear round & maybe raised?

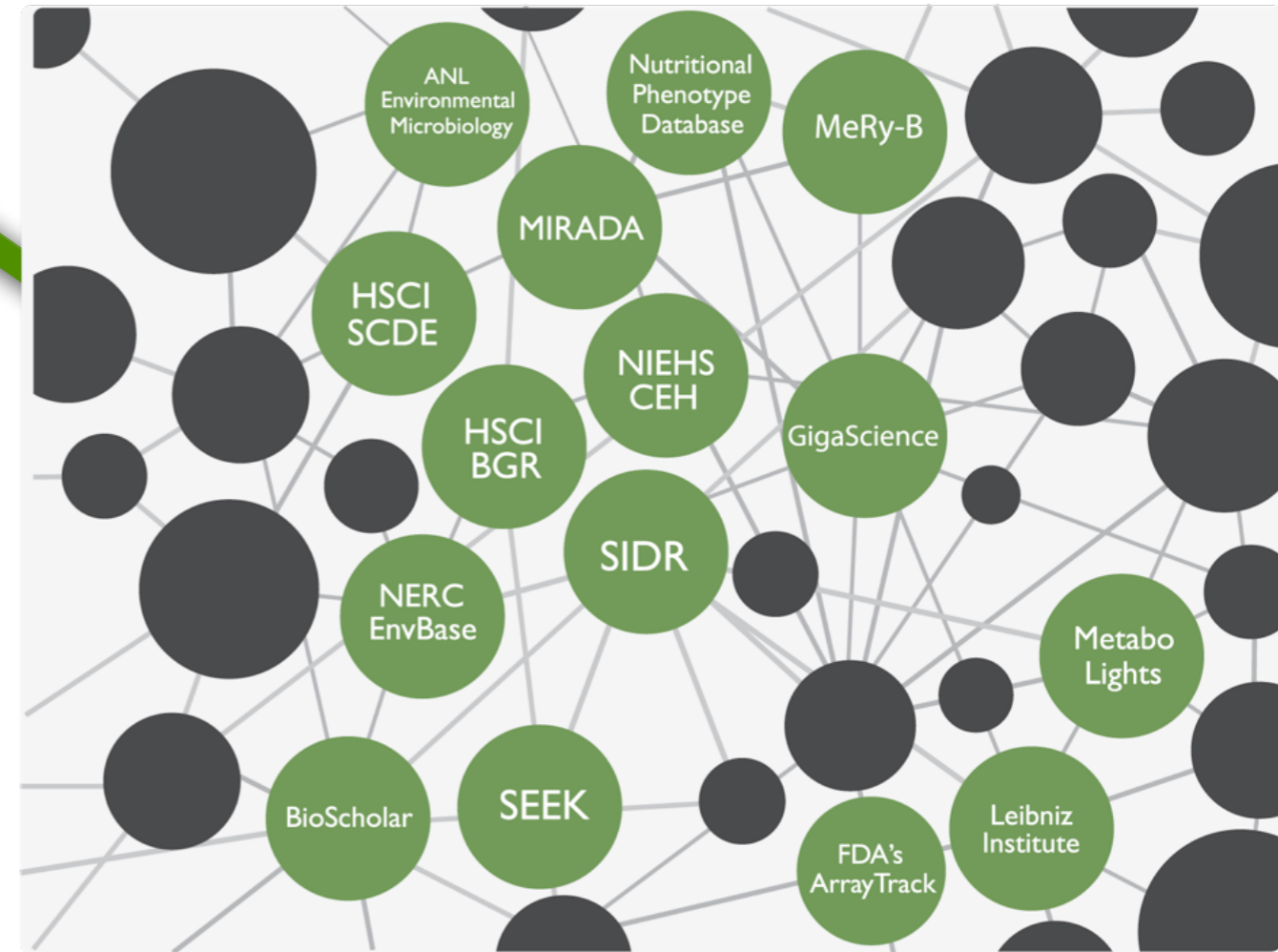
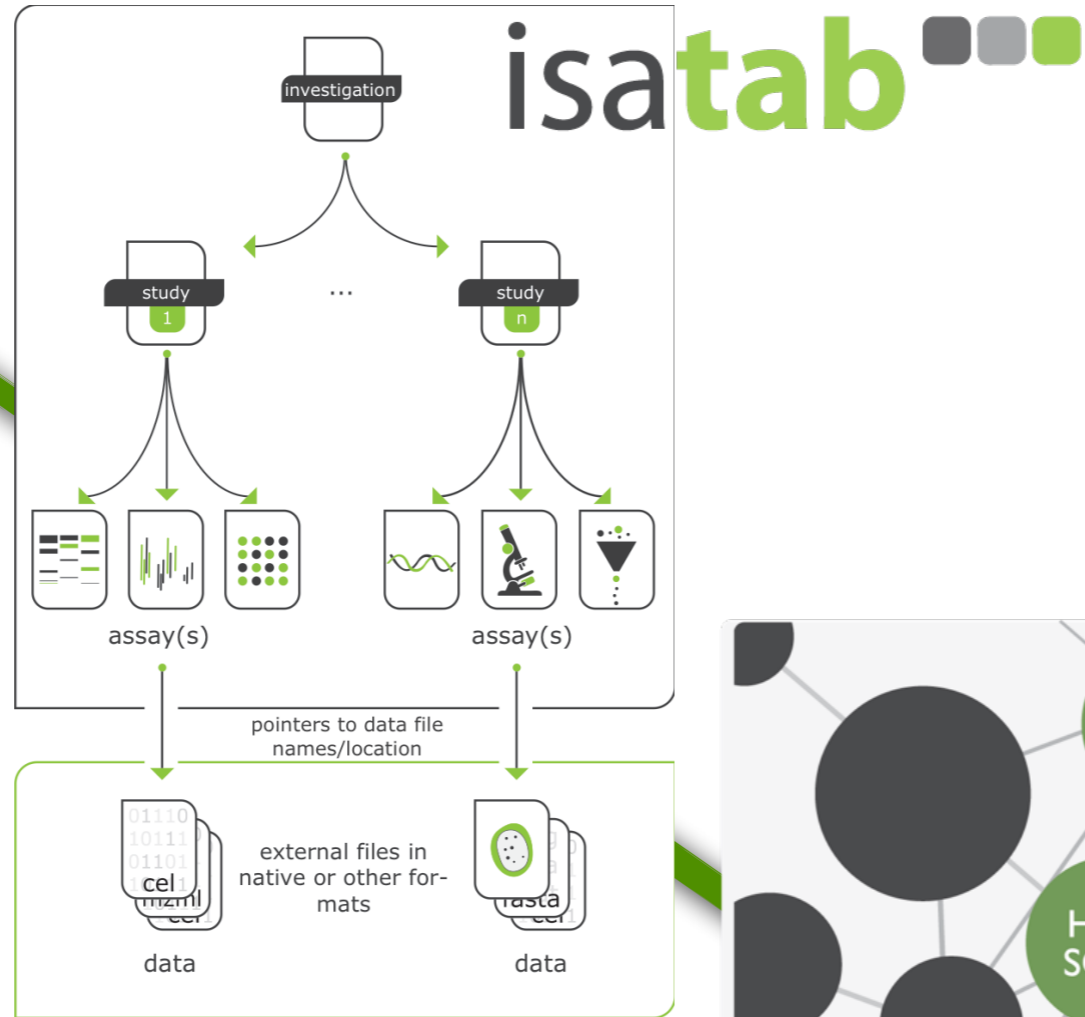
1000x image of a red colony (next board)

maybe 100s many red colonies are there, but they're small

← still R. rubrum?

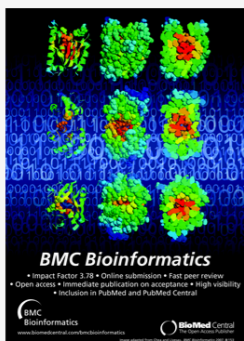
(2 other red colonies had cells of the same microscopic morphology)

A well-isolated red colony was picked & streaked onto a fresh 305 plate & incubated into an anaerobic jar for incubation at 30°C in the light anaerobically.



linkedISA: semantic representation of ISA-Tab experimental metadata

Alejandra González-Beltrán*, Eamonn Maguire, Susanna-Assunta Sansone and Philippe Rocca-Serra

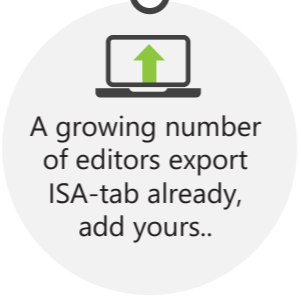


BMC Bioinformatics, Issue 15(Suppl 14):S4, 2014. [10.1186/1471-2105-15-S14-S4](https://doi.org/10.1186/1471-2105-15-S14-S4).

Describe & curate your experiment with geographically distributed collaborators



Describe & curate your experiment using a desktop-based, platform independent tool



A growing number of editors export ISA-tab already, add yours..

Create your own repository



Perform data analysis



Submit your experiments to public repositories



ARRAYEXPRESS

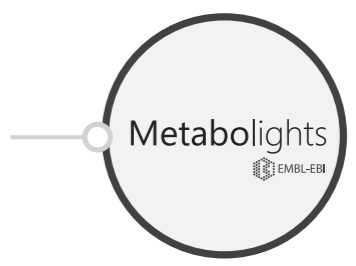
ENA European Nucleotide Archive



PRIDE



Direct submission



Share, link and reason over experiments with linked data



Publish, along with your research articles

BioMed Central The Open Access Publisher

(GIGA)ⁿ SCIENCE

npg SCIENTIFIC DATA

(GIGA)ⁿ DB

The Dataverse Network Project

DRYAD

figshare

& specialised community repositories

Core ISA tools Powered by ISA tools Externally Developed Tools

Biodiversity research in the "big data" era: *GigaScience* and Pensoft work together to publish the most data-rich species description

Scott C Edmunds^{1*}, Chris I Hunter¹, Vincent Smith², Pavel Stoev^{3,4} and Lyubomir Penev^{3,5}

<http://dx.doi.org/10.5524/100063>

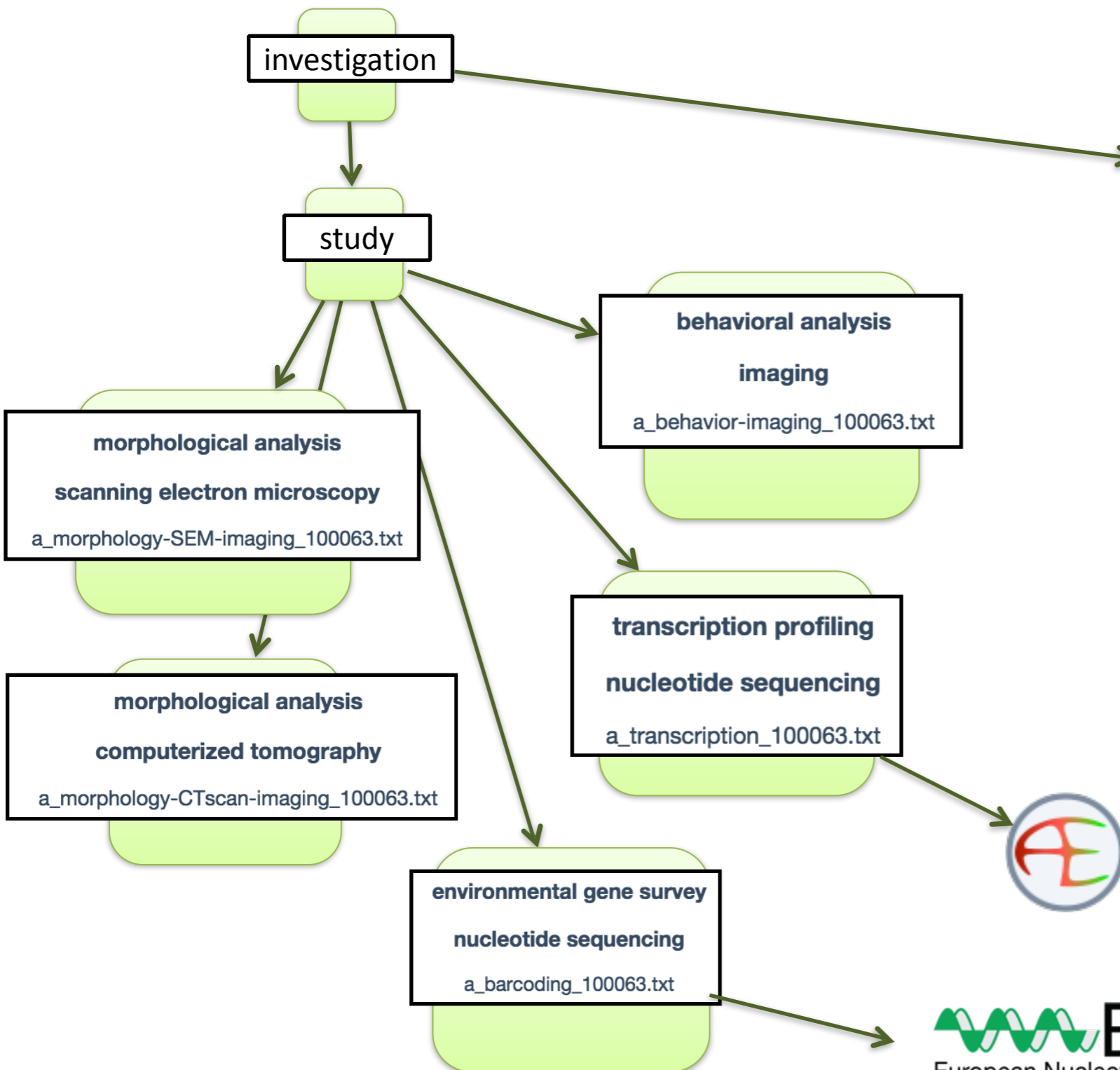



Biodiversity Data Journal 1: e1013 (28 Oct 2013)
doi: 10.3897/BDJ.1.e1013



Taxonomic paper

Eupolybothrus cavernicolus Komerički & Stoev sp. n. (Chilopoda: Lithobiomorpha: Lithobiidae): the first eukaryotic species description combining transcriptomic, DNA barcoding and micro-CT imaging data



ecology | advanced 

<http://www.nature.com/search?journal=sdata&q=ecology>

Research | 31 March 2015 | OPEN

A summary of eight traits of Coleoptera, Hemiptera, Orthoptera and Araneae, occurring in grasslands in Germany

Martin M Gossner, Nadja K Simons [...] Wolfgang W Weisser

Scientific Data 2, 150013

[Rights & permissions »](#)

Research | 03 March 2015 | OPEN

Allometry and growth of eight tree taxa in United Kingdom woodlands

Matthew R Evans, Aristides Moustakas [...] Stefanie Schäfer

Scientific Data 2, 150006

[Rights & permissions »](#)

Research | 17 March 2015 | OPEN

A global database of lake surface temperatures collected by *in situ* and satellite methods from 1985–2009

Sapna Sharma, Derek K Gray [...] Kara H Woo

Scientific Data 2, 150008

[Rights & permissions »](#)

Research | 30 September 2014 | OPEN

Genomes of diverse isolates of the marine cyanobacterium *Prochlorococcus*

Steven J. Biller, Paul M. Berube [...] Sallie W. Chisholm

Scientific Data 1, 140034

[Rights & permissions »](#)

Ecology

Ecology is the study of how organisms interact with each other and their environment. It considers processes that occur at the population, community and ecosystem ...

[Latest research & reviews on Ecology](#)

DISCOVER MORE SUBJECTS

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Subject areas keep you updated on key developments in a field of interest with content from across nature.com in a single place.

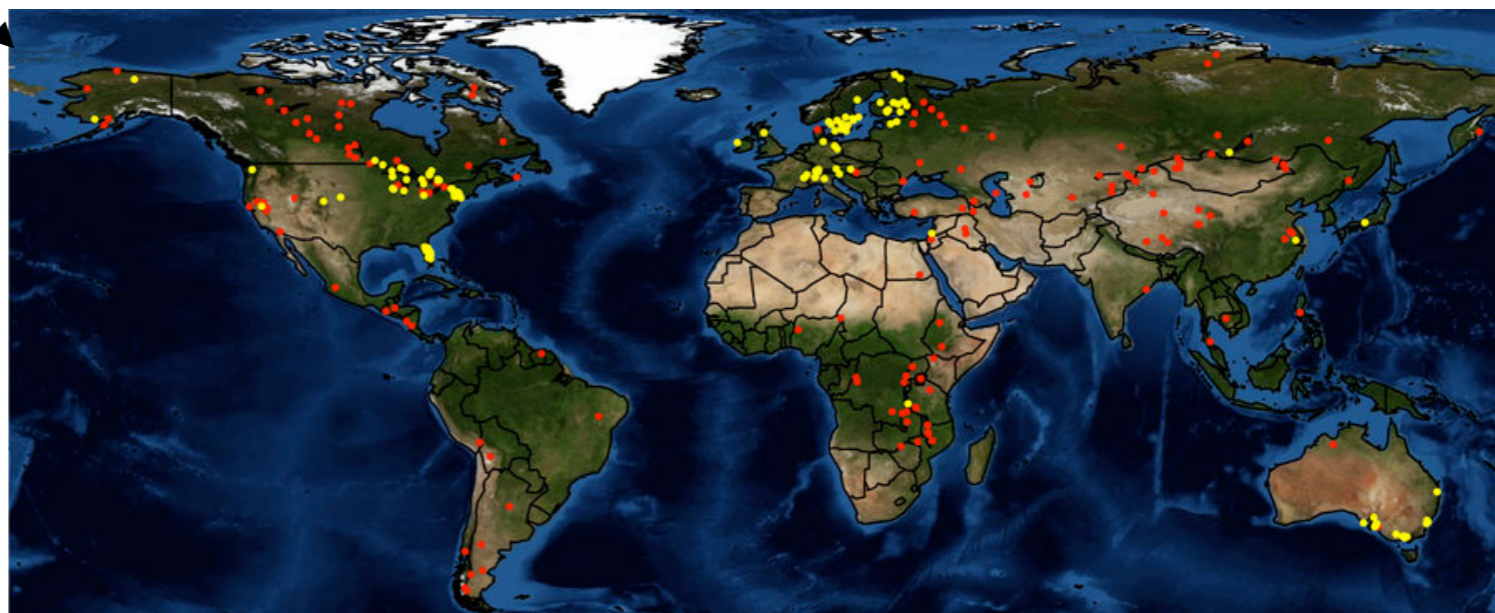
[Browse all subjects »](#)

<http://www.nature.com/articles/sdata201513>

Subject terms: [Biodiversity](#) • [Community ecology](#) • [Entomology](#) • [Grassland ecology](#)

Design Type(s)	observation design • time series design • species comparison design
Measurement Type(s)	phenotype
Technology Type(s)	phenotype characterization
Factor Type(s)	
Sample Characteristic(s)	Coleoptera • Hemiptera • Orthoptera • Araneae • multicellular organism • Germany • grassland

<http://www.nature.com/articles/sdata20158>



1 **Map** the landscape of content standards via [biosharing.org](https://www.biosharing.org)

2 Structure

Develop methods for creating templates.



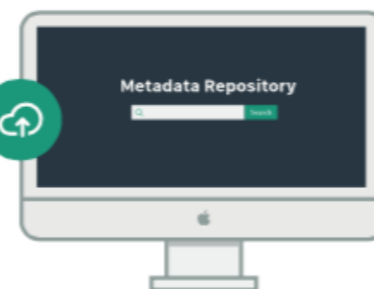
3 Annotate

Develop methods to ease the use of templates.

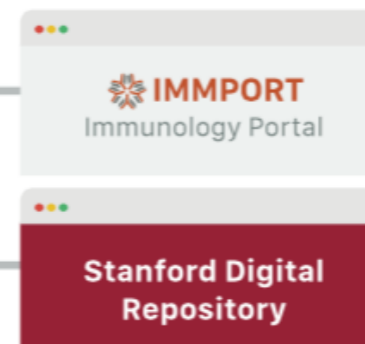


4 Explore

Create a repository of populated templates.



5 Case Studies



Authoring of metadata templates.

Annotation of data with metadata.

Exploration and reuse of datasets through metadata.

Facilitate submission of datasets to our two case study repositories and progressively to others.

Create and use 'elements' from content standards [biosharing.org](https://www.biosharing.org)

Create a language to represent relations among 'elements' **W3C** HCLS WGs

Use existing examples of templates **isatools** **IMMPORT** **HIPC**

Contribute

Fill in template


Submit, Search, & Reuse




Scientists




CEDAR
CENTER FOR EXPANDED DATA ANNOTATION AND RETRIEVAL

6  Analyze the CEDAR repository of populated templates to reveal patterns in the metadata that will enable the metadata tools to use predictive data entry to ease the task of filling out the templates.

 Augment those metadata with links to the published literature (including secondary analyses and retractions).

 Augment those metadata with links to follow-up experiments (in online databases and in the literature).

 Allow the scientific community to comment on the experiment through structured metadata.

WG3 Metadata - work to date

Home / Workgroup 3 Group Links

GROUP MENU

- Group Home
- Members
- Group Files**
- Calendar

WORKGROUP 3 GROUP LINKS

- WG3 Working files** (in Google Drive; no login required)
- WG3 Telecon minutes, presentations and recordings.

- ① Standard Operating Procedure (SOP)
- ② Selected Competency Questions
- ③ Metadata Mapping
- ④ Core Metadata Elements

Done by:

Alejandra Gonzalez-Beltran - Oxford e-Research Centre, University of Oxford
Philippe Rocca-Serra - Oxford e-Research Centre, University of Oxford
Mary Vardigan - ICPSR, University of Michigan
Susanna-Assunta Sansone - University of Oxford

with contributions, comments from several WG 3 members and colleagues, in particular: Joan Starr, George Alter, Ian Fore, Kevin Read, Stian Soyland-Reyes, Muhammad Amith, Michel Dumontier...

- ① Standard Operating Procedure (SOP) document:
 - ✦ contains lists of material reviewed
 - data discovery initiatives and metadata initiatives
 - existing meta-models for representing metadata elements
 - ✦ outlines the approach used to identify metadata descriptors
 - Via *use cases* and *competency questions* (top-down approach)
 - *Mapping* generic and life science-specific *metadata schemas* (bottom-up approach)
 - Listed in the [BioSharing collection for bioCADDIE](#)
 - ✦ The results of both approaches has been compared and converged on the core set of metadata

② Selected Competency Questions:

- ✧ representative set from use cases workshop, white paper, submitted by the community and from Phil Bourne
- ✧ questions have been abstracted and key metadata elements have been highlighted and color-coded and categorized
- ✧ as the set of core and extended metadata elements are defined, it will become clearer which questions the Data Discovery Index will not be able to answer if full and which only in part.

BGUC2	Search for organism x in biological process y (apoptosis) at scale z with an estimate of the reliability of the annotations
BGUC3-1	Search for new drug x to predict and track biological process x (cardiotoxicity)
BGUC3-2	Search for data type x ('omics correlates) of biological process for drugs related to drug x
BGUC3-3	Search for data types a, b, and c (EHR data, self-report, sensor) to determine natural history of patients given drugs similar to drug x
BGUC3-4	Track responses to treatment to ensure detection of biological process x
BGUC3-5	Find patient data "like these" with similar treatments, responses to treatment, genetics
	Search for studies a-z with patient data with biological process x (e.g. obesity as

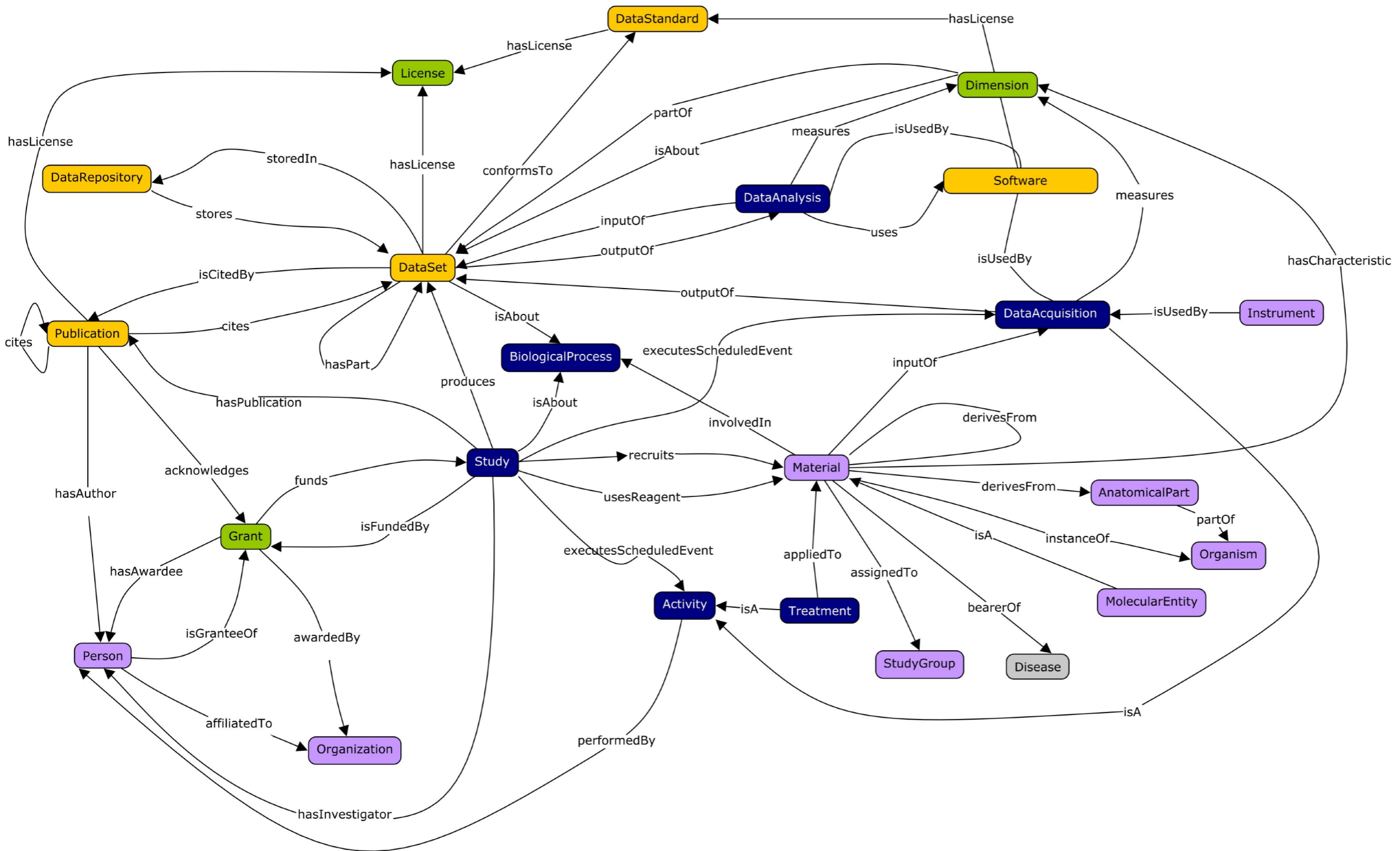
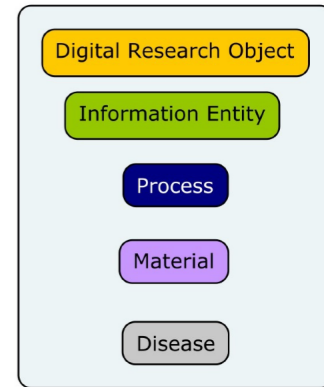
③ Metadata Mapping:

- ✧ both *generic* and (progressively more) *life science-specific* metadata schemas are being mapped to identify common metadata elements
 - ✧ if available, formal representations such XML schema document (XSD) and semantic model (RDF/OWL representations) will be used as input material to the mapping process
 - provenance information each metadata schema/model is described and made available in the BioSharing collection, including: version; source of metadata elements (e.g. XSD), the URL where the model or schema has been sourced; documentation, including URL where the documentation is located
-

④ Core Metadata Elements:

- ✧ the result of the combined approaches, as outlined documents 1-3, is delivering a set of core metadata elements and progressively these will be extended to domain specific ones
 - ✧ we aim to have maximum coverage of use cases with minimal number of data elements, but we do foresee that not all questions can be answered in full
-

JSON-schemas
JSON examples





Open Biological and biomedical Ontologies (OBO) Foundry

- origins related to Gene Ontology (GO)
- collection of orthogonal reference ontologies in the biological and biomedical domain
 - e.g GO, chemical entities (ChEBI), investigations (OBI), phenotypes (PATO, MP), ...
- agreed set of principles; best practices on ontology development
 - open
 - well-defined format, e.g. **obo** or **owl**
 - uses identifiers according to **obo** id policy
 - ontology life-cycle/versioning
 - clearly specified and delineated content
 - unambiguous definitions
 - uses or extends relations in the **obo** relations ontology
 - well-documented
 - plurality of users (mailing list, issue tracker)
 - developed collaboratively
 - orthogonal, modular



- General-purpose statistics ontology (formal logic-based representation)
- Coverage for processes (e.g. statistical tests and their condition of application) and information needed or resulting from statistical methods (e.g. probability distributions, variable, spread and variation metrics)
- STATO also benefits from: (i) **extensive documentation** with the provision of textual and formal definitions; (ii) an **associated R code snippets** using the dedicated R-command metadata tag, aiming at facilitating teaching and learning while relying of the popular R language; (iii) **query examples** documentation, highlighting how the ontology can be harnessed for reviewers/tutors/student alike.

1

Which **statistical tests** may be used to test **association between categorical variables**?

Ask STATO

2

Which **statistical tests** evaluate **group difference**?

Ask STATO

3

Which **statistical tests** evaluate **goodness of fit**?

Ask STATO

4

What are the **statistical tests** which can be used to test **within subject variation**?

Ask STATO

5

Which **statistical tests** evaluate **homogeneity hypothesis**?

Ask STATO

6

Which **statistical tests** evaluate if **sphericity hypothesis** holds?

Ask STATO

7

Which **statistical tests** evaluate **variance equality**?

Ask STATO

8

Which **statistical tests** require the **variance equality hypothesis** to be true?

Ask STATO

9

Which **statistical tests** may be applied for group comparison if both **normality and equivariance hypotheses** are met?

Ask STATO

10

Which **statistical tests** use a **contingency table**?

Ask STATO

11

Which **statistical tests** make use of **variable ranking**?

Ask STATO

12

Which **statistical tests** relies on an **F-distribution**?

Ask STATO

13

Which **plots** may be used to represent the results of a **genetic association study**?

14

Which **plots** may be used to represent the results of a **meta-analysis**?

15

Which **plots** use **effect size estimate**?

16

Which **plots** may be used to render a **differential expression analysis**?

Which **stat** be used to **betwee** **va**

istical used to **ject**

STATO results

exact binomial test

A

Kolmogorov-Smirnov test

Pearson's Chi square test of goodness of fit

Pearson's Chi square test of goodness of fit

Pearson's Chi-Squared test for goodnes of fit is a statistical null hypothesis test which is used to either evaluate goodness of fit of dataset to a Chi-Squared distribution

Which **s** evaluate **hyp**

tests **ance** **is** to be

F-test

Barlett's test

A

Levene's test

Likelihood-ratio test

Which **stat** be app **comp** **non** **equivaria** **a**

tests **ubution**?

Anderson-Darling test

Hardy-Weinberg equilibrium testing

A

Shapiro-Wilk test

one sample Hotelling T2 test

Which **plot** represent **genetic**

e used to **ntial** **ysis**?

hypergeometric test

STATO returned 12 results.

Which **stat**
be used to
betwee
va

istical
used to
ject

STATO results

exact binomial test

Kolmogorov-Smirnov test

Pearson's Chi square test of goodness of fit

Pearson's Chi square test of goodness of fit

Jump To:



Details Visualization Notes (0) Class Mappings (0) [🔗](#)

- one way ANOVA
- paired t-test
- permutation numbering
- ranking
- + regression analysis method
- repeated measure ANOVA
- Scheffe test
- Shapiro-Wilk test
- statistical hypothesis test
 - + between group comparison statistical test
 - chi square test
 - Pearson's Chi square test of goodness of fit**
 - + Pearson's Chi square test of independence between categor
 - Fisher's exact test
 - + goodness of fit statistical test
 - + homoskedasticity test
 - + non-parametric test
 - + odds ratio homogeneity test
 - one tailed test
 - + sphericity test
 - + Student's t-test
 - + test of association between categorical variables
 - + two tailed test
 - + within subject comparison statistical test
- statistical test power analysis
- survival analysis data transformation
- Tarone's test for homogeneity of odds ratio
- transmission disequilibrium test
- Tukey HSD for Post-Hoc Analysis
- two sample Hotelling T2 test
- two sample t-test with equal variance
- two sample t-test with unequal variance

Preferred Name	Pearson's Chi square test of goodness of fit
Synonyms	
Definitions	Pearson's Chi-Squared test for goodnes of fit is a statistical null hypothesis test which is used to either evaluate goodness of fit of dataset to a Chi-Squared distribution
ID	http://purl.obolibrary.org/obo/STATO_0000309
achieves_planned_objective	goodness of fit testing objective
alternative term	Chi2 test for goodness of fit
definition source	adapted from: http://stat.ethz.ch/R-manual/R-patched/library/stats/html/chisq.test.html and http://en.wikipedia.org/wiki/Pearson's_chi-squared_test
has curation status	http://purl.obolibrary.org/obo/IAO_0000125
has_specified_input	Chi-square probability distribution false positive rate contingency table number of degrees of freedom
has_specified_output	p-value
label	Pearson's Chi square test of goodness of fit
prefLabel	Pearson's Chi square test of goodness of fit
R command	http://stat.ethz.ch/R-manual/R-patched/library/stats/html/chisq.test.html chisq.test(x = NULL, correct = FALSE, p = rep(1 / length(x), length(x)), rescale.p = FALSE, simulate.p.value = FALSE, B = 2000)
STATO alternative term	
term editor	Orlaith Burke Alejandra Gonzalez-Beltran

Thanks for your attention!

Questions?

You can email us...
isatools@googlegroups.com

View our websites

 isa-tools.org
     

stato-ontology.org

biosharing.org

View our Git repo & contribute
<http://github.com/ISA-tools>

View our blog
<http://isatools.wordpress.com>

Follow us on Twitter
[@isatools](https://twitter.com/isatools)

