



OXFORD
e-Research
CENTRE



The open source ISA software suite and its international user community: Knowledge management of experimental data

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Outline

- Knowledge management of experimental data
 - Setting the scene
 - The  isa ecosystem: ISA-tab, tools, community
 - Use case
- Latest additions



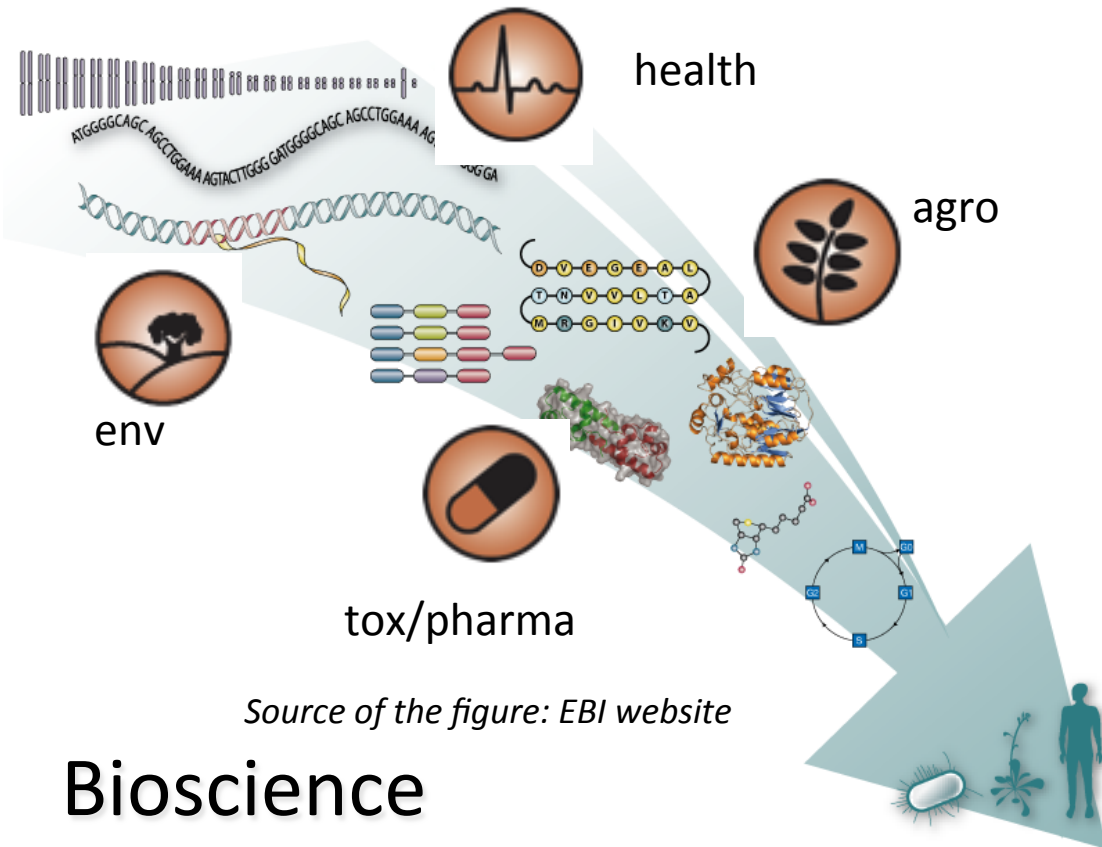
OntoMaton

Risa


isatoowl

- Related projects & main points

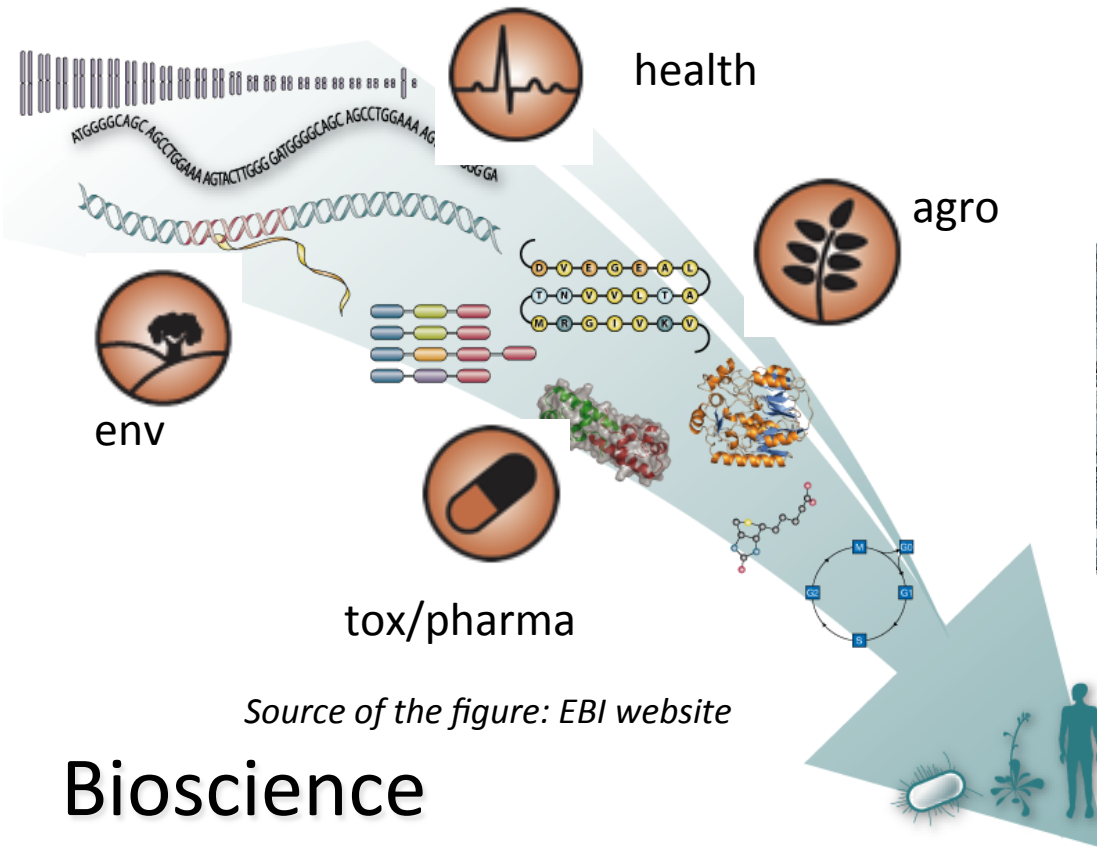
Setting the scene



Source of the figure: EBI website

Bioscience
is multi-domain...

Setting the scene

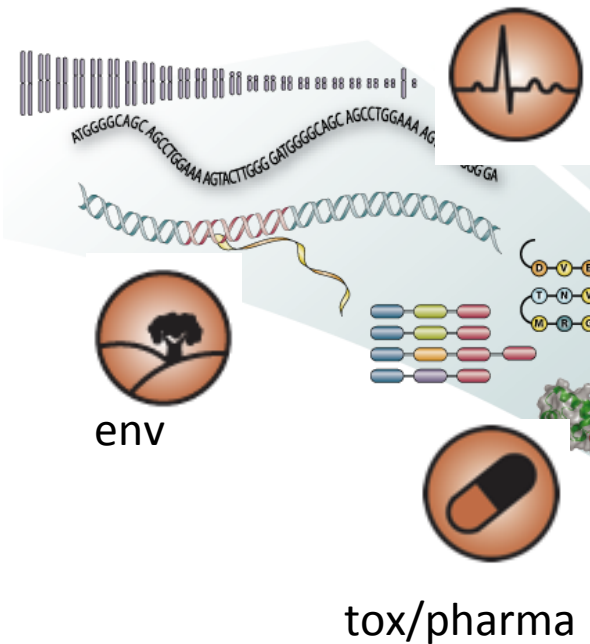


Bioscience
is multi-domain...



Petabytes of data

Setting the scene



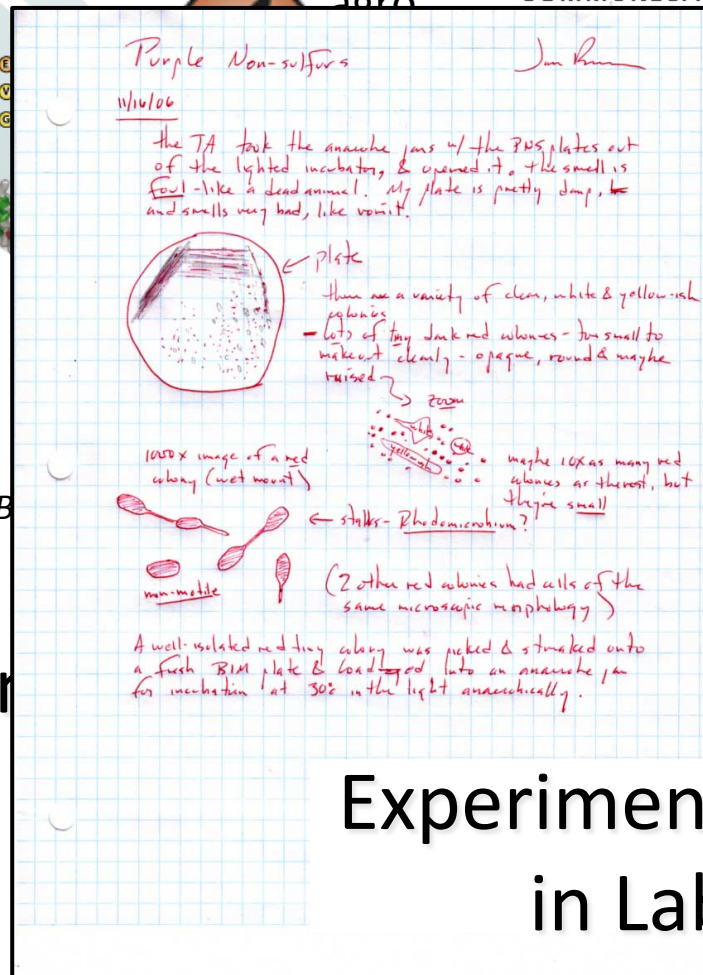
health

env

tox/pharma

Source of the figure: EB

Bioscience
is multi-domain



Experimental metadata
in Lab books

COMMUNICATIONS



Petabytes of data



investigation study assay

- Assist in the **annotation** and **management** of experimental data at source
- Deal with data from **high-throughput studies** using one or a combination of **omics** and **other technologies**
- Empower users to uptake community-defined **checklists** and **ontologies**
- Facilitate **data sharing**, **reuse**, **comparison** and **reproducibility** of experiments, **submission** to international public repositories

The  **isa** ecosystem

isatab 

 **isatools**
isa-tools.org

 **isacommons**
isacommons.org

The isa ecosystem

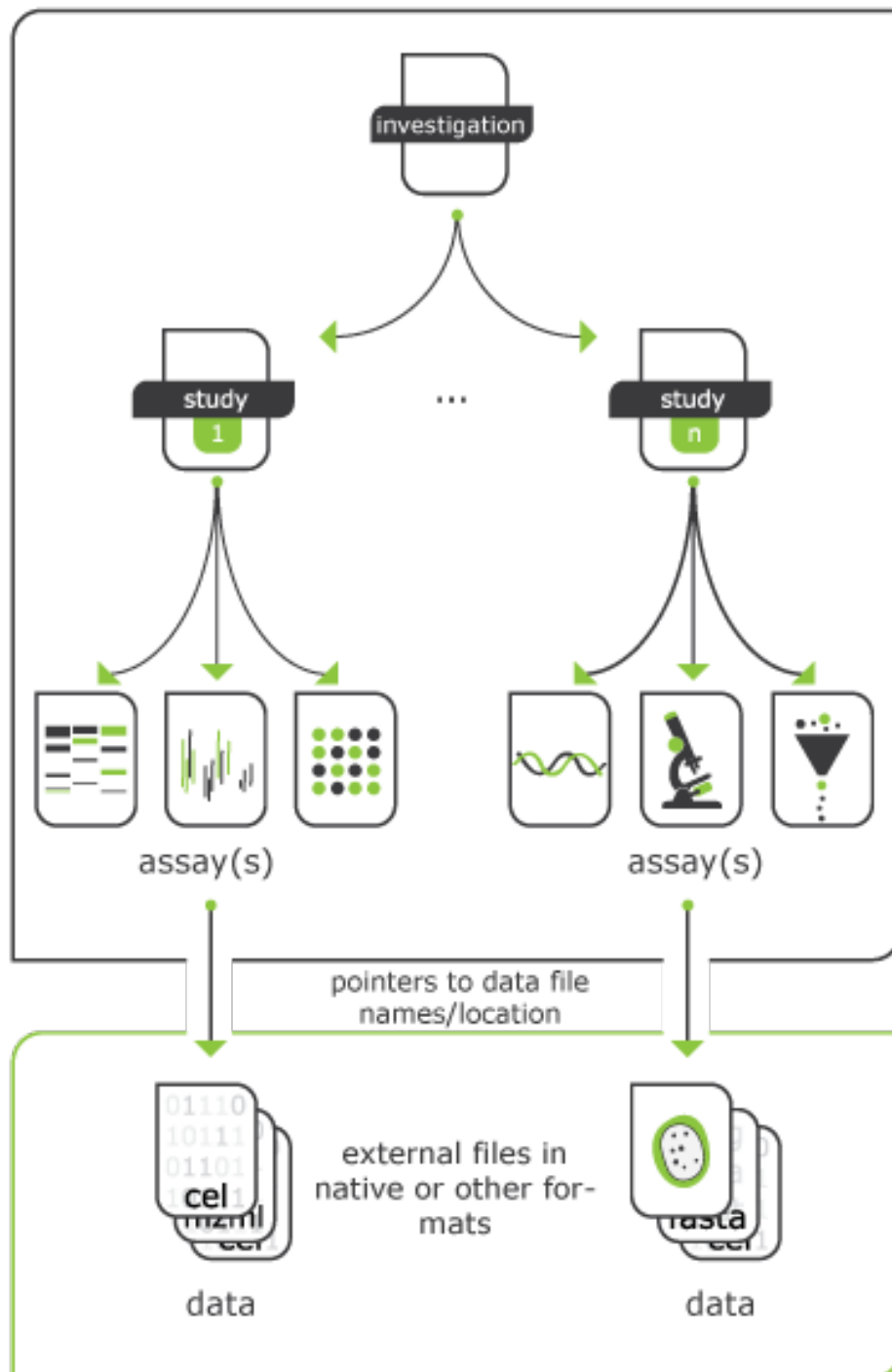
isatab^{'''}



ISA software suite: supporting standards-compliant
experimental annotation and enabling curation at the
community level
Rocca-Serra et al, 2010
Bioinformatics



Towards interoperable bioscience data
Sansone et al, 2012
Nature Genetics



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)

General purpose & flexible format
Domain agnostic
Captures metadata in omics experiments and traditional experiments (e.g. clinical chemistry and histology)



faahKO dataset

- Available in BioConductor
- Subset of the original data on **global metabolite profiling**

14332

Biochemistry **2004**, 43, 14332–14339

Assignment of Endogenous Substrates to Enzymes by Global Metabolite Profiling[†]

Alan Saghatelian, Sunia A. Trauger, Elizabeth J. Want, Edward G. Hawkins, Gary Siuzdak, and Benjamin F. Cravatt*

The Skaggs Institute for Chemical Biology and Departments of Cell Biology and Chemistry, The Scripps Research Institute, 10550 North Torrey Pines Road, La Jolla, California 92037

Received September 11, 2004; Revised Manuscript Received October 1, 2004

ABSTRACT: Enzymes regulate biological processes through the conversion of specific substrates to products. Therefore, of fundamental interest for every enzyme is the elucidation of its natural substrates. Here, we describe a general strategy for identifying endogenous substrates of enzymes by untargeted liquid chromatography-mass spectrometry (LC/MS) analysis of tissue metabolomes from wild-type and enzyme

Saghatelian et al.
Biochemistry. 2004

- LC/MS peaks from the spinal cords of **6 wild-type** and **6 FAAH** (fatty acid amide hydrolase) **knockout mice**

- # faahKO investigation

file study view utilities options help

isatab[™] overview

- ✓ Global metabolite profiling of faah(-/-) mice
 - ✓ s_faahko.txt
 - a_metabolite.txt

studydefinition

study description

Study Identifier	Global metabolite profiling of faah(-/-) mice
Study Title	Global metabolite profiling of faah(-/-) mice
Study Description	Enzymes regulate biological processes through the conversion of specific substrates to products. Therefore, of fundamental interest for every enzyme is the elucidation of its natural substrates.
Study Submission Date	16/11/2004 oct 14
Study Public Release Date	16/11/2004 oct 14

STUDY ASSAYS

+
add new assay(s)

VIEW ✕

metabolite profiling
mass spectrometry
Agilent 1100 LC-MSD SL
a_metabolite.txt

faahKO study

- Subjects studied: source(s), sampling methodology, characteristics
- treatments/manipulations performed to prepare the specimens

	● Source Name	● Characteristics[NEWT:Organism LC]	● Characteristics[Genotype]	● Characteristics[targeted gene]
1	Saghantelian_1	NEWT:Mus musculus (Mouse)	fatty acid amide hydrolase gene knock out	MGI:fatty acid amide hydrolase gene
2	Saghantelian_2	NEWT:Mus musculus (Mouse)	fatty acid amide hydrolase gene knock out	MGI:fatty acid amide hydrolase gene
3	Saghantelian_3	NEWT:Mus musculus (Mouse)	fatty acid amide hydrolase gene knock out	MGI:fatty acid amide hydrolase gene
4	Saghantelian_4	NEWT:Mus musculus (Mouse)	fatty acid amide hydrolase gene knock out	MGI:fatty acid amide hydrolase gene
5	Saghantelian_5	NEWT:Mus musculus (Mouse)	fatty acid amide hydrolase gene knock out	MGI:fatty acid amide hydrolase gene
6	Saghantelian_6	NEWT:Mus musculus (Mouse)	fatty acid amide hydrolase gene knock out	MGI:fatty acid amide hydrolase gene
7	Saghantelian_7	NEWT:Mus musculus (Mouse)	wild type	
8	Saghantelian_8	NEWT:Mus musculus (Mouse)	wild type	
9	Saghantelian_9	NEWT:Mus musculus (Mouse)	wild type	
10	Saghantelian_10	NEWT:Mus musculus (Mouse)	wild type	
11	Saghantelian_11	NEWT:Mus musculus (Mouse)	wild type	
12	Saghantelian_12	NEWT:Mus musculus (Mouse)	wild type	

NEWT UniProt Taxonomy Database

Mouse Genome Informatics

- **Subjects studied:** source(s), sampling methodology, characteristics
- **treatments/manipulations** performed to prepare the specimens

12 Mouse Adult Gross Anatomy Sample Definition

e]	● Protocol REF	● Sample Name	● Characteristics[tissue]	● Factor Value[Genotype]
gene	sample collection	KO1	MA:spinal cord	fatty acid amide hydrolase gene knock
gene	sample collection	KO2	MA:spinal cord	fatty acid amide hydrolase gene knock
gene	sample collection	KO3	MA:spinal cord	fatty acid amide hydrolase gene knock
gene	sample collection	KO4	MA:spinal cord	fatty acid amide hydrolase gene knock
gene	sample collection	KO5	MA:spinal cord	fatty acid amide hydrolase gene knock
gene	sample collection	KO6	MA:spinal cord	fatty acid amide hydrolase gene knock
	sample collection	WT1	MA:spinal cord	wild type
	sample collection	WT2	MA:spinal cord	wild type
	sample collection	WT3	MA:spinal cord	wild type
	sample collection	WT4	MA:spinal cord	wild type
	sample collection	WT5	MA:spinal cord	wild type
	sample collection	WT6	MA:spinal cord	wild type

- measurement type, e.g. metabolite profiling
- technology, e.g. mass spectrometry

faahKO assay

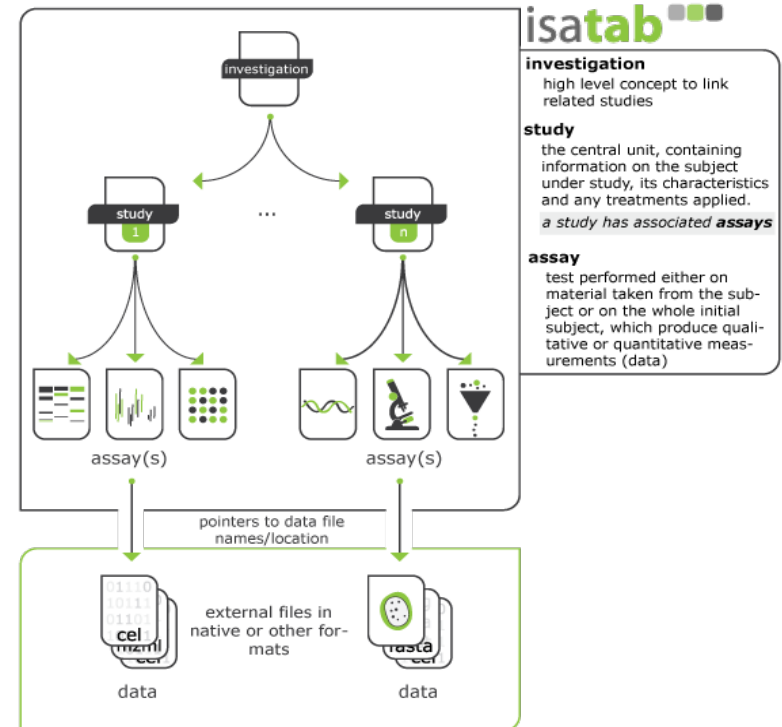
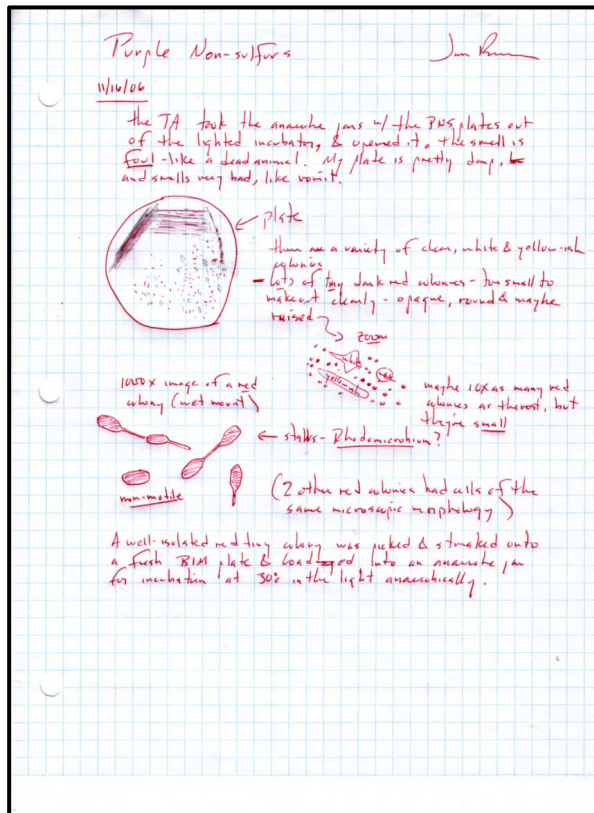
	● Sample Name	● Protocol REF	● Extract Name	● Protocol REF	● Parameter Value[instrument]	● Parameter Value[ion sou...
1	KO1	extraction	KO1_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
2	KO2	extraction	KO2extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
3	KO3	extraction	KO3_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
4	KO4	extraction	KO4_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
5	KO5	extraction	KO5_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
6	KO6	extraction	KO6_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
7	WT1	extraction	WT1_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
8	WT2	extraction	WT2_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
9	WT3	extraction	WT3_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
10	WT4	extraction	WT4_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
11	WT5	extraction	WT5_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization
12	WT6	extraction	WT6_extract	mass spectrometry	Agilent 1100 LC-MSD SL	MS:electrospray ionization

Assay measuring **metabolite profiling** using **mass spectrometry**

● Parameter Value[ionization mode]	● MS Assay Name	● Raw Spectral Data File	● Factor Value[Genotype]
positive mode	lc-ms-1	./cdf/KO/ko15.CDF	fatty acid amide hydrolase gene knock...
positive mode	lc-ms-2	./cdf/KO/ko16.CDF	fatty acid amide hydrolase gene knock...
positive mode	lc-ms-3	./cdf/KO/ko18.CDF	fatty acid amide hydrolase gene knock...
positive mode	lc-ms-4	./cdf/KO/ko19.CDF	fatty acid amide hydrolase gene knock...
positive mode	lc-ms-5	./cdf/KO/ko21.CDF	fatty acid amide hydrolase gene knock...
positive mode	lc-ms-6	./cdf/KO/ko22.CDF	fatty acid amide hydrolase gene knock...
positive mode	lc-ms-7	./cdf/WT/wt15.CDF	wild type
positive mode	lc-ms-8	./cdf/WT/wt16.CDF	wild type
positive mode	lc-ms-9	./cdf/WT/wt18.CDF	wild type
positive mode	lc-ms-10	./cdf/WT/wt19.CDF	wild type
positive mode	lc-ms-11	./cdf/WT/wt21.CDF	wild type
positive mode	lc-ms-12	./cdf/WT/wt22.CDF	wild type

isatab'''

isatab





isatab



experimentalist



OntoMaton

isatab



Report and edit the description of the investigation using Google Spreadsheets.

Use Google Spreadsheets in combination with ISA-Tab templates (created through importing the Excel file from the ISAconfigurator) and **OntoMaton** (for ontology search and tagging support) to report an investigation.



experimentalist



OntoMaton

Ontology Search and Tagging in Google Spreadsheets

- collaborative annotation
- distributed groups of users
- version control & history

The screenshot displays the ISAcreeator-Google web application interface. At the top, the browser address bar shows the URL: <https://docs.google.com/spreadsheet/ccc?key=0A15WvYyk0zzmdDNLeEcXWHZJX042d50taXJPNXpJMHc#gid=4>. The application header includes the text "ISAcreeator-Google" and a "Share" button. Below the header, a menu bar lists "File", "Edit", "View", "Insert", "Format", "Data", "Tools", "Help", and "OntoMaton". The main content area shows a Google Spreadsheet with columns C, D, and E. In column D, rows 12 through 16 contain the text "biome", "coast", "sea", "water", and "metagenon" respectively. An "OntoMaton" dialog box is open in the center, featuring the logo and the text "Select the cells in the spreadsheet you wish to tag with ontology terms, then click the 'tag' button below. Results will appear shortly." Below this text is a green "Tag" button. The dialog box also displays "Results - choose replacement(s) for free text" with a list of terms: "biome", "coast", "Environment Ontology", "sea", "water", and "metagenome". A "Replace" button is visible next to "coast (Environment Ontology version 45418)". The bottom of the screen shows a tab bar with "i_investigation.txt", "s_sample.txt", "a_assay.txt", "Terms", and "Restrictions". A "Count: 5" indicator is in the bottom right corner.

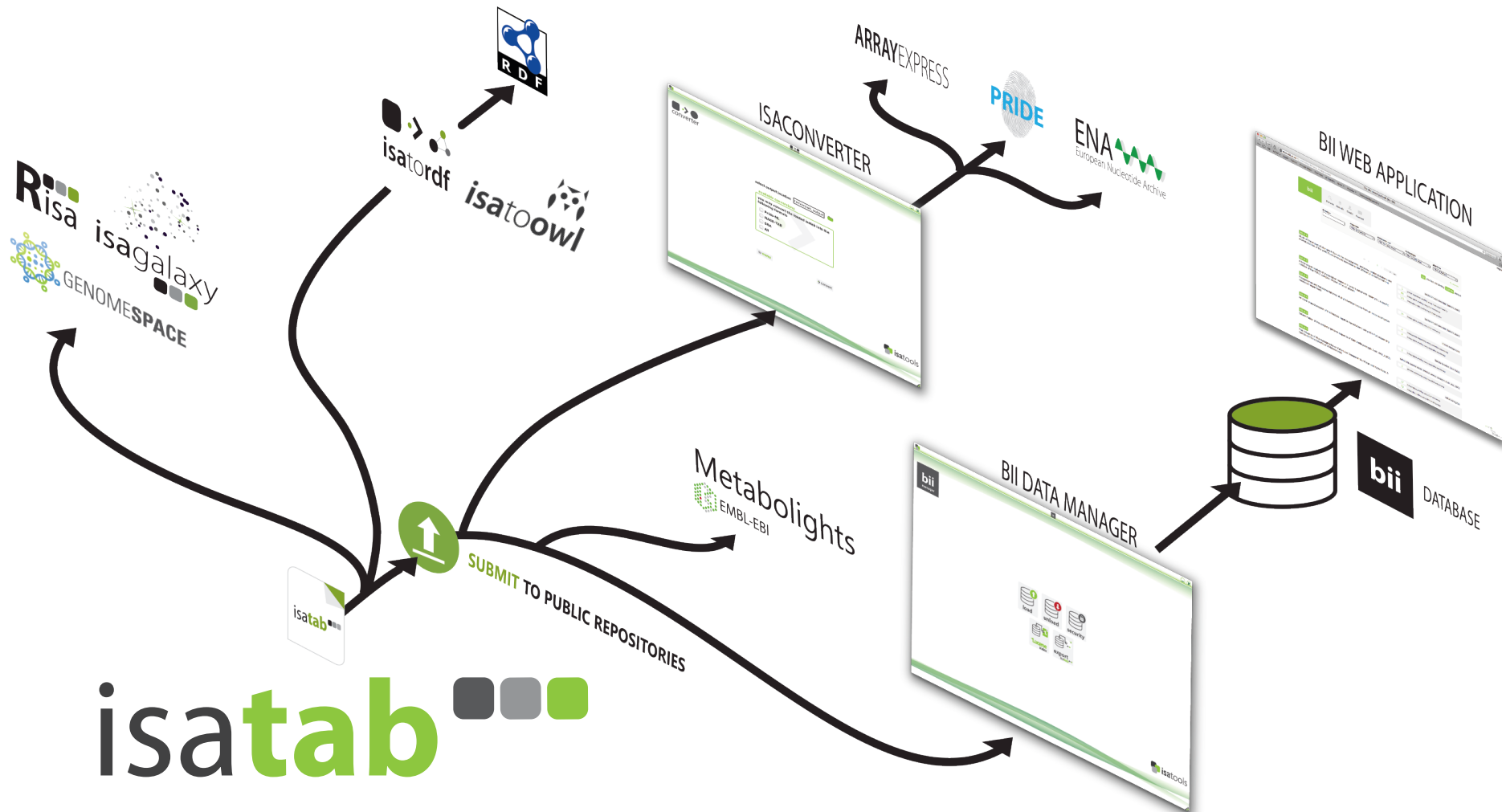


isatab[™]

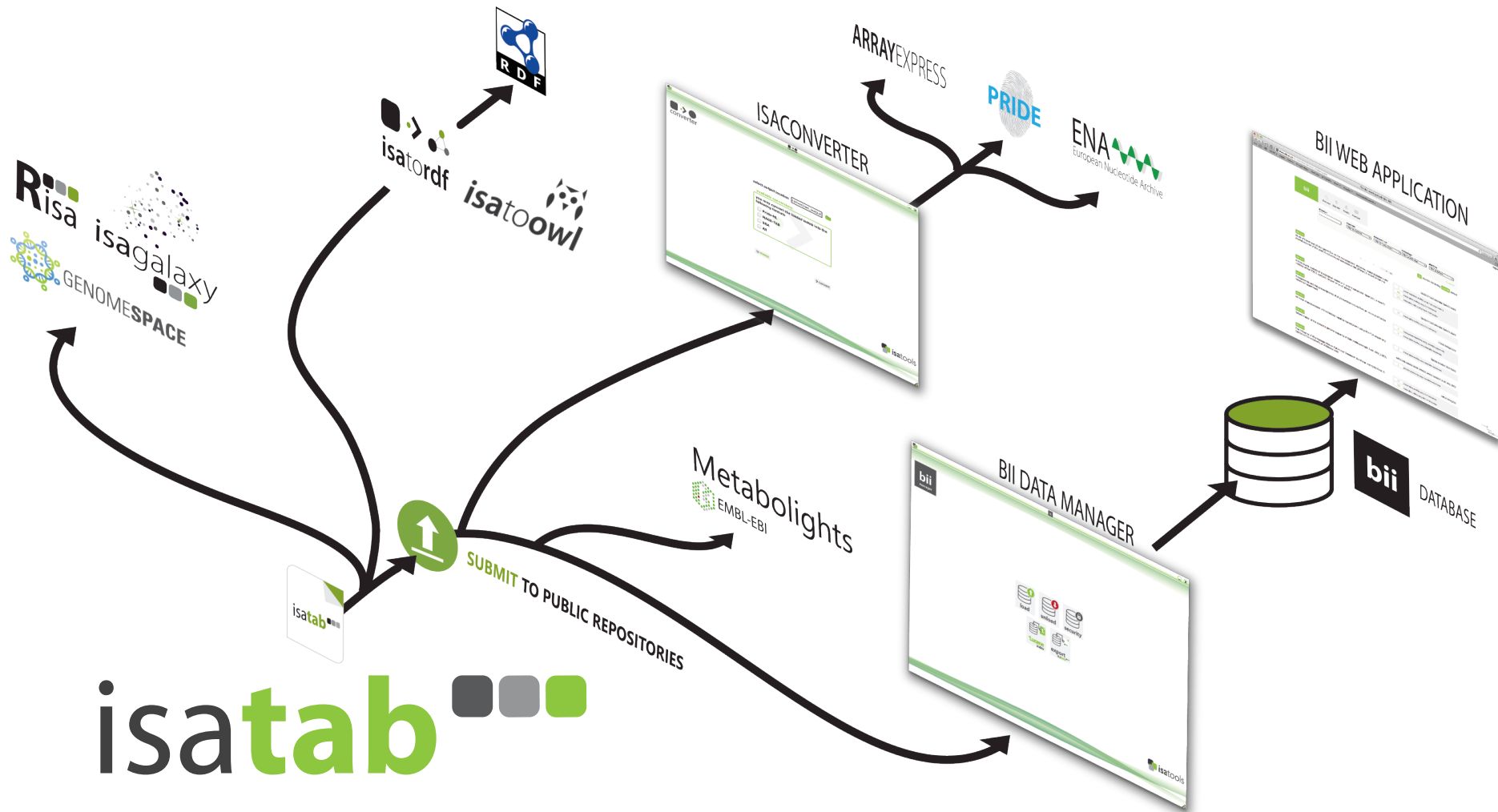


Create templates detailing the steps to be reported for different investigations, complying to community standards (listed at [biosharing](http://www.biosharing.org)), e.g. configuring fields to be (i) ontology terms, (ii) text (with/without regular expression testing), (iii) numbers etc.

From the **ISA-Tab** we can perform analysis, convert to RDF/OWL and other formats for submission/sharing to local/remote repositories,



From the **ISA-Tab** we can perform analysis, convert to RDF/OWL and other formats for submission/sharing to local/remote repositories,



+ Visualisation Methods



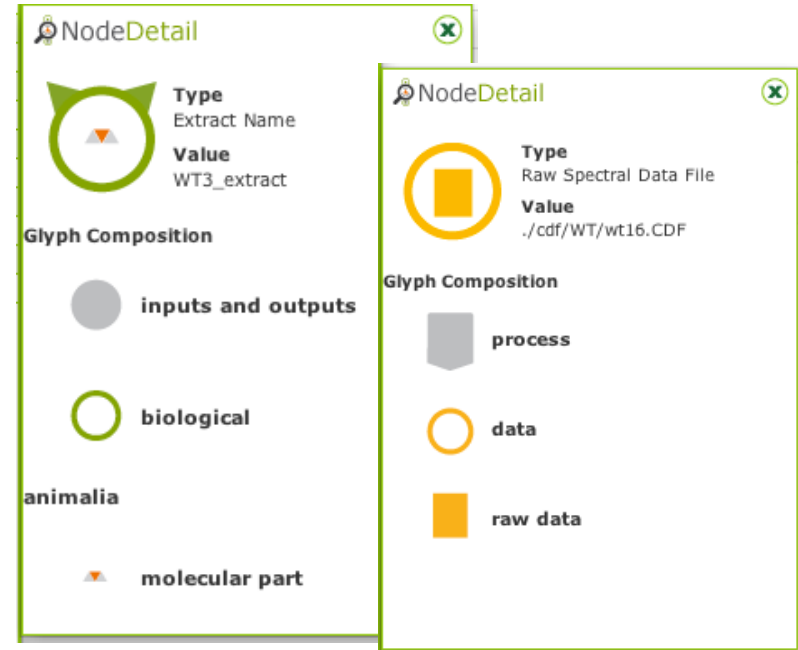
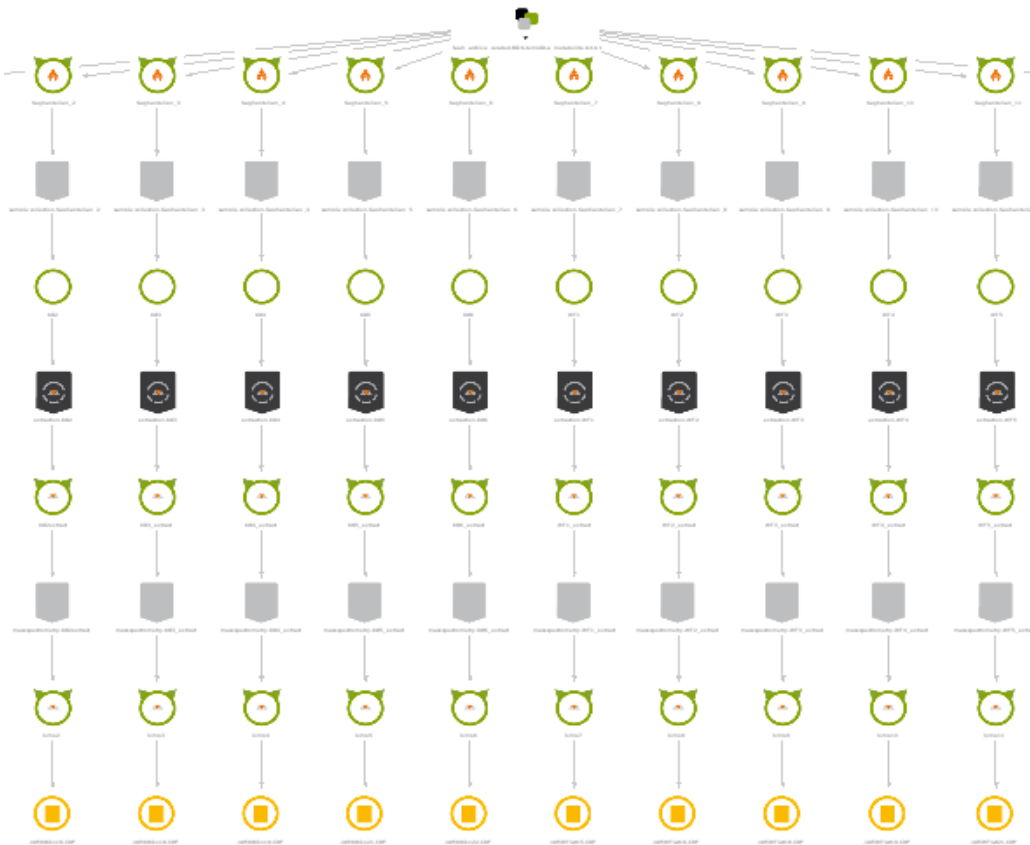
fatty acid amide hydrolase gene knock out (6 samples)



I type (6 samples)

faahKO Groups

faahKO Workflow



IEEE TRANSACTIONS ON
**VISUALIZATION AND
 COMPUTER GRAPHICS**
 A publication of the IEEE Computer Society

Maguire E, Rocca-Serra P, Sansone SA,
 Davies J and Chen M.

**Taxonomy-based Glyph Design -- with a
 Case Study on Visualizing Workflows of
 Biological Experiments,**

*IEEE Transactions on Visualization and
 Computer Graphics, volume 18, 2012 (in
 press)*



- R package available in BioConductor 2.11
<http://bioconductor.org/packages/release/bioc/html/Risa.html>
- ISAtab class
- Read ISAtab files into ISAtab objects and save ISAtab files
- Build xcmsSet (xcms package) objects from mass spectrometry assays
- Augment the ISAtab dataset after analysis
-  **github** SOCIAL CODING source & issues tracking

<https://github.com/ISA-tools/Risa>

GITHUB.COM/ISA-TOOLS



- faahKO package v. 2.12 contains ISAtab files describing the experiment

```
faahkoISA = readISAtab(find.package("faahKO"))  
assay.filename <- faahkoISA["assay.names"][[1]]  
xset = processAssayXcmsSet(faahkoISA, assay.filename)
```

...

```
updateAssayMetadata(faahkoISA, assay.filename, "Derived Spectral  
Data File", "faahkoDSDF.txt" )
```

- MTBLS2 processing and analysis using Risa, xcms and CAMERA BioConductor packages



Metabolights – an open access general-purpose repository for metabolomics studies and associated meta-data

Haug et al, 2012

Nucleic Acids Research

ISA syntax & Underlying Material/Data workflows



Input Material or
Data Node

Output Material or
Data Node

*Characteristics[...]
Factor Value[...]*

*Characteristics[...]
Factor Value[...]*

Protocol REF

Parameter Value [...]

fields

Sample Name
Protocol REF
Extract Name
Protocol REF
Labeled Extract Name
Label
Protocol REF
Parameter Value[instrument]
Parameter Value[ion source]
Parameter Value[detector]
Parameter Value[analyzer]
MS Assay Name
Raw Spectral Data File
Protocol REF
Normalization Name
Data Transformation Name
Derived Spectral Data File
Protocol REF
Metabolite Assignment File
Factors



- Make the **semantics** of ISAtab explicit, including materials & data entities & processes
- **Exploit** the semantic **annotations** available in ISAtab datasets
- Augment ISA syntax with new elements (e.g. groups), facilitating the understanding & querying of experimental design
- Facilitate data integration & knowledge discovery/reasoning

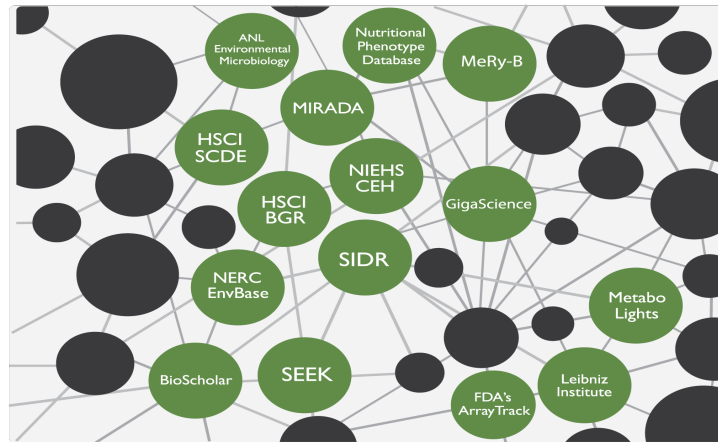
ISAtab datasets as linked data

- Connect to the growing Linked Data universe

RDF = Resource Description Framework, OWL = Web Ontology Language

- Collaborations with Toxbank ( isatordf)

& W3C Health Care & Life Sciences Interest Group
(HCLSIG)



<subject, predicate, object>

<lipoprotein> <participates_in> <inflammatory response>

<PRO:212342352> <BFO_0000056> <GO:0006954>

isatab



ISAtab dataset
Parser



ISAtab Graph
Analysis



ISA Mapping
Parser



isaToowl



Study Factor	independent variable specification	http://purl.obolibrary.org/obo/OBI_0000736	denotes	http://purl.obolibrary.org/obo/IAO_0000219	investigate
Study Factor Name	written name	http://purl.obolibrary.org/obo/IAO_0000599	denotes	http://purl.obolibrary.org/obo/IAO_0000219	independent
Study Design Type	study design(http://purl.obolibrary.org/obo/OBI_0500000)	http://purl.obolibrary.org/obo/OBI_0500000			
Study Assay	analyze assay	http://purl.obolibrary.org/obo/OBI_0000443	achieves plan objective		assay measurement
Study Assay Measurement Type	analyze measurement objective	http://purl.obolibrary.org/obo/OBI_0000437	denotes	http://purl.obolibrary.org/obo/IAO_0000219	assay
Study Assay Technology Type	planned process	http://purl.obolibrary.org/obo/OBI_0000245	is part of	http://purl.obolibrary.org/obo/IAO_0000219	
Study Assay Technology Platform	organization	http://purl.obolibrary.org/obo/OBI_0000245	has role	http://purl.obolibrary.org/obo/IAO_0000087	manufacture
Study Assay File	information content entity	http://purl.obolibrary.org/obo/IAO_0000030			
Study Assay File Name	written name	http://purl.obolibrary.org/obo/IAO_0000599	denotes	http://purl.obolibrary.org/obo/IAO_0000219	information
Study Protocol	protocol	http://purl.obolibrary.org/obo/OBI_0000022			
Study Protocol Name	written name	http://purl.obolibrary.org/obo/IAO_0000599	denotes	http://purl.obolibrary.org/obo/IAO_0000219	protocol
Study Protocol Type	objective specification	http://purl.obolibrary.org/obo/IAO_0000005	denotes	http://purl.obolibrary.org/obo/IAO_0000219	protocol
Study Protocol Description	textual entity	http://purl.obolibrary.org/obo/IAO_0000030	denotes	http://purl.obolibrary.org/obo/IAO_0000219	protocol
Study Protocol URI	written name	http://purl.obolibrary.org/obo/IAO_0000599	denotes	http://purl.obolibrary.org/obo/IAO_0000219	protocol
Study Protocol Version	version number	http://purl.obolibrary.org/obo/IAO_0000129	denotes	http://purl.obolibrary.org/obo/IAO_0000219	protocol
Study Protocol Parameter	controlled variable specification	http://purl.obolibrary.org/obo/OBI_0000785	denotes	http://purl.obolibrary.org/obo/IAO_0000219	protocol
Study Protocol Parameters Name	written name	http://purl.obolibrary.org/obo/IAO_0000599	denotes	http://purl.obolibrary.org/obo/IAO_0000219	controlled
Source	material entity	http://purl.obolibrary.org/obo/IAO_0000040			
Source Name	written name	http://purl.obolibrary.org/obo/IAO_0000599	denotes	http://purl.obolibrary.org/obo/IAO_0000219	material entity(http://purl.obolibrary.org/obo/IAO_0000040)
(Sample Name)(Label Extract)	processed material	http://purl.obolibrary.org/obo/OBI_0000047			
(Sample Name)(Extract Name)(Label Extract Name)	written name	http://purl.obolibrary.org/obo/IAO_0000599	denotes	http://purl.obolibrary.org/obo/IAO_0000219	processed
Source Name	written name	http://purl.obolibrary.org/obo/IAO_0000090	denotes	http://purl.obolibrary.org/obo/IAO_0000219	entity(http://purl.obolibrary.org/obo/IAO_0000040)
(Sample Name)(Label Extract)	processed material	http://purl.obolibrary.org/obo/OBI_0000047			
(Sample Name)(Extract Name)(Label Extract Name)	written name	http://purl.obolibrary.org/obo/IAO_0000090	denotes	http://purl.obolibrary.org/obo/IAO_0000219	processed



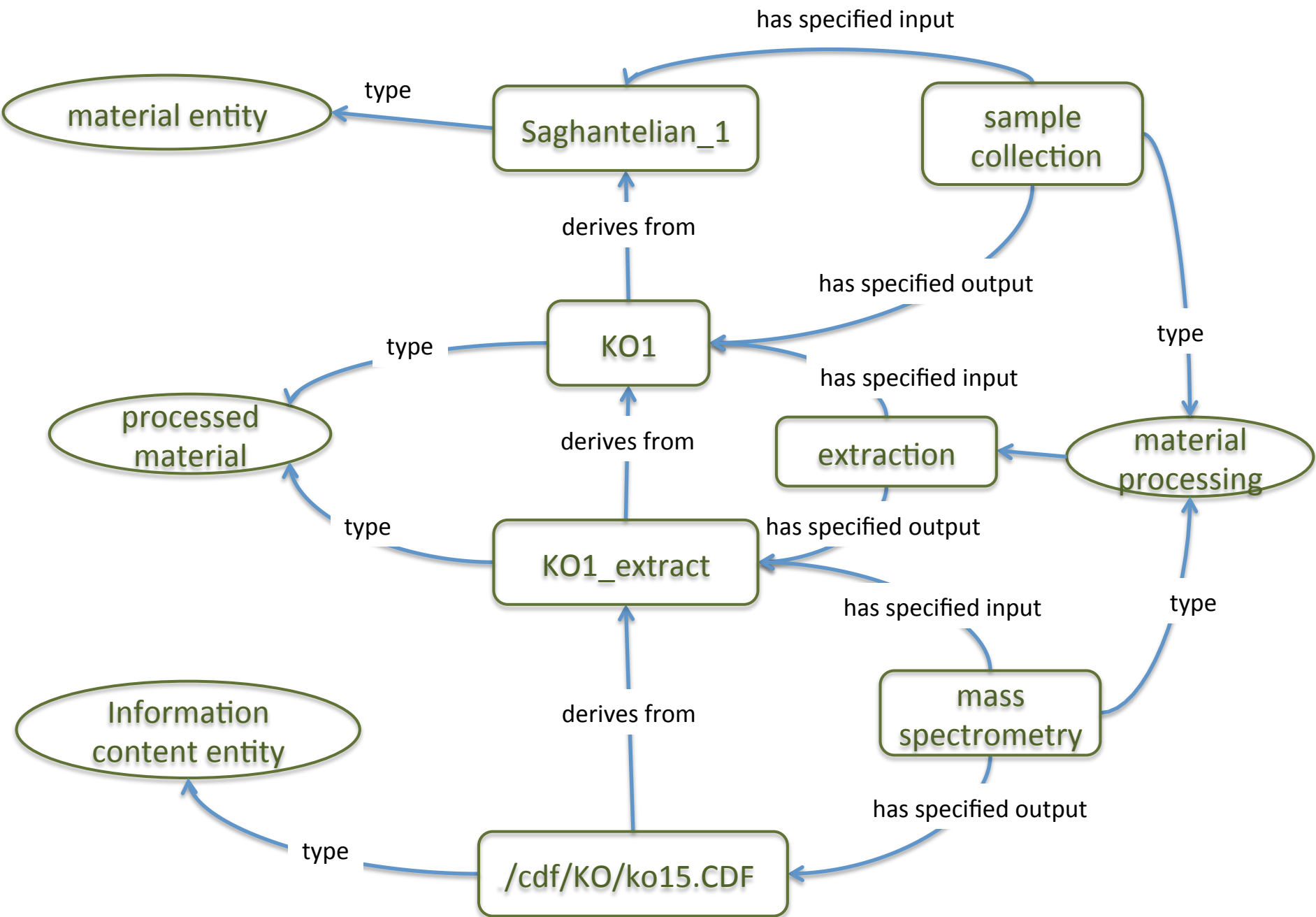
OntoMaton



OntoMaton

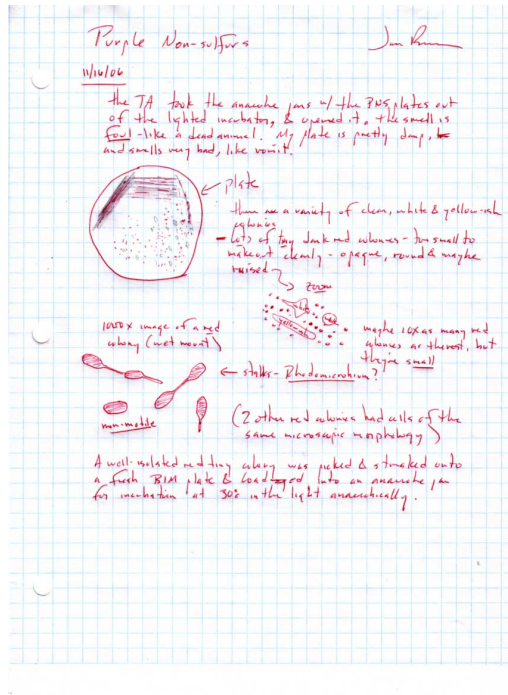
ISA-OBO-mapping

Study Factor	independent variable specification	http://purl.obolibrary.org/obo/OBI_0000750	denotes
Study Factor Name	written name	http://purl.obolibrary.org/obo/IAO_0000590	denotes
Study Design Type	study design(http://purl.obolibrary.org/obo/OBI_0500000)	http://purl.obolibrary.org/obo/OBI_0500000	
Study Assay	analyte assay	http://purl.obolibrary.org/obo/OBI_0000443	achives plan object
Study Assay Measurement Type	analyte measurement objective	http://purl.obolibrary.org/obo/OBI_0000437	denotes
Study Assay Technology Type	planned process		is part of
Study Assay Technology Platform	organization	http://purl.obolibrary.org/obo/OBI_0000245	has role
Study Assay File	information content entity	http://purl.obolibrary.org/obo/IAO_0000030	
Study Assay File Name	written name	http://purl.obolibrary.org/obo/IAO_0000590	denotes
Study Protocol	protocol	http://purl.obolibrary.org/obo/OBI_0000272	
Study Protocol Name	written name	http://purl.obolibrary.org/obo/IAO_0000590	denotes
Study Protocol Type	objective specification	http://purl.obolibrary.org/obo/IAO_0000005	denotes
Study Protocol Description	textual entity	http://purl.obolibrary.org/obo/IAO_0000300	denotes
Study Protocol URI	written name	http://purl.obolibrary.org/obo/IAO_0000590	denotes
Study Protocol Version	version number	http://purl.obolibrary.org/obo/IAO_00000129	denotes
Study Protocol Parameter	controlled variable specification	http://purl.obolibrary.org/obo/OBI_0000785	denotes
Study Protocol Parameters Name	written name	http://purl.obolibrary.org/obo/IAO_0000590	denotes
Source	material entity	http://purl.obolibrary.org/obo/BFO_0000040	
Source Name	written name	http://purl.obolibrary.org/obo/IAO_0000590	denotes
{Sample Extract Labeled Extract}	processed material	http://purl.obolibrary.org/obo/OBI_0000047	
{Sample Name Extract Name Labeled Extract Name}	written name	http://purl.obolibrary.org/obo/IAO_0000590	denotes
Characterization	quality	http://purl.obolibrary.org/obo/BFO_0000010	

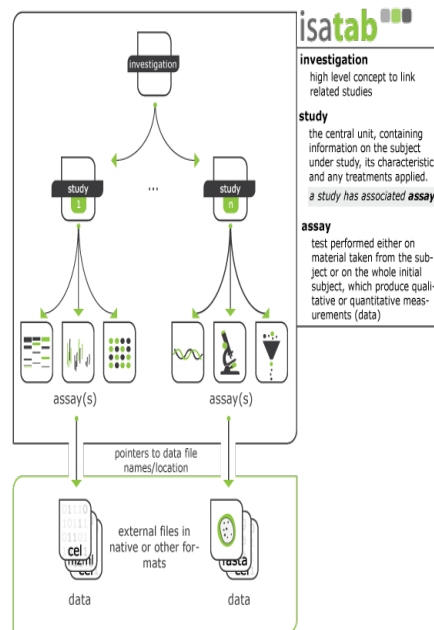


Increasing level of structure...

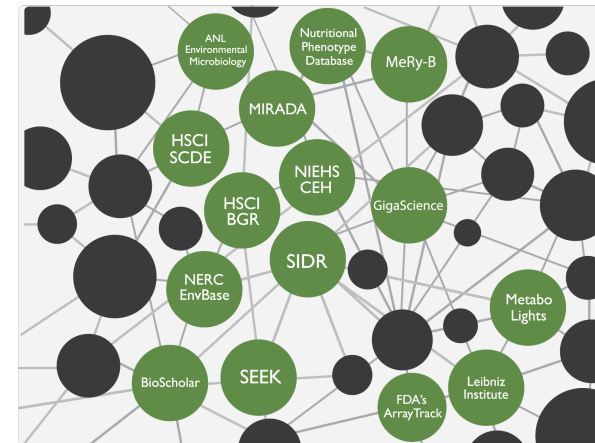
...different target audiences



Notes in Lab books
(information for humans)



Spreadsheets & Tables
(ISAtab metadata)



Facts as RDF statements
(information for machines)

biosharing.org

STANDARDS

FORMATS



TERMINOLOGIES



BioPortal
OBO

CHECKLISTS



mibbi
equator

A catalogue of reporting standards (minimum reporting guidelines, exchange formats and terminologies) and organizations that develop these.

DATABASES



BioDBcore

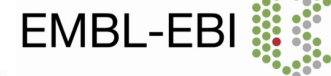
A catalogue of databases, described according to the BioDBcore guidelines, along with the standards used within them; compiled in collaboration with 2012 NAR Database.



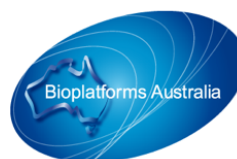
core organization in the



UK Node



Janssen Research
& Development, LLC



The Novartis Institutes
for BioMedical Research

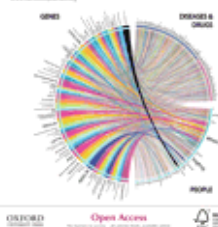


Implementation at Harvard



Nucleic Acids Research

VOLUME 40, SUPPLEMENT 1, JANUARY 1, 2012
www.nar.oxfordjournals.org



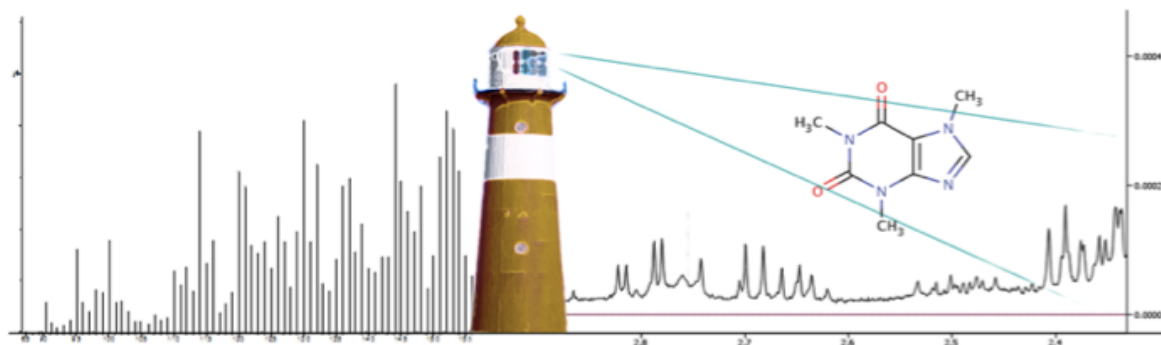
The Stem Cell Discovery Engine: an integrated repository and analysis system for cancer stem cell comparisons

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<http://discovery.hsci.harvard.edu/>

Implementation at the EBI

<http://www.ebi.ac.uk/metabolights>



MetaboLights: a database for metabolomics experiments and derived information

MetaboLights is a database for Metabolomics experiments and derived information. The database is cross-species, cross-technique and covers metabolite structures and their reference spectra as well as their biological roles, locations and concentrations, and experimental data from metabolic experiments. [About MetaboLights.](#)



Metabolights – an open access general-purpose repository for metabolomics studies and associated meta-data

Haug et al, 2012

Nucleic Acids Research

The isa ecosystem

isatab^{isa}



coreisateam



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