Metadata

Introduction to Data Management Practices course

NBIS DM Team

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https://nbisweden.github.io/module-metadata-dm-practices/index.html

CC BY

What is the problem?

“Someone unfamiliar with your project should be able to look at your computer files and understand in detail what you did and why.”

“Your primary collaborator is yourself six months from now, and your past self don’t answer e-mails.”

Metadata

The data about the data (or anything really)

“One person’s metadata, is another person’s data”

Metadata

- Describe data at different levels
  - e.g. a whole study vs the samples

Examples

- Creators
- File types and formats of the data
- Licence for re-use of the data
- Methodology for data collection
- Analytical and procedural information
- Sources of samples
- Sample treatment
- Geolocation(s) of samples

What problems do you see with the descriptions of these samples?

	animal ID	date	mouse line	strain	age
1	800793	2018-01-06	Alk3	BALB/cJ	10
2	804396	2019-01-07	Vegfr	C57BL/6	6
3	805431	2018-01-12	Vegfr	C57BL/6	P9
4	805992	2019-01-13	Vegfr	C57BL/6	P1
5	808935	2020-01-14	Alk3	BALB/cJ	12
6	810875	2019-01-16	alk6	C57BL/6	E1
7	812308	2018-01-19	Alk3	BALB/cJ	12
8	814334	2019-01-19	Vegfr	C57BL/6	P9
9	816649	2018-01-20	Vegfr	C57BL/6	P1

samples_metadata_lesson.csv

Problems

- Date formats
- Different terms for the same information
- Misspelled terms
- Not clear what a data point means
- Not clear what unit

Stringency

- Descriptions must be understandable over time - *not only for you*
- FAIR principles → also for computers
- Consistency
  - Date formats
  - Units
  - Terms

How much metadata?

- What is necessary for you to do your particular analysis
- What is necessary for someone to understand the data
- All the metadata you have

- *“How can I make this dataset as useful as possible for others?”*

Terms

“A biologist would rather share a toothbrush with another biologist than share a gene name”

- Consistency and stringency

- **Controlled vocabularies**
- **Ontologies**
- Thesauruses (Thesauri)
- Taxonomies

NBIS NATIONAL BIOINFORMATICS INFRASTRUCTURE SWEDEN

SciLifeLab

How many terms for *Breast Cancer* can you think of?

MeSH synonyms

Breast Neoplasm
Neoplasm, Breast
Breast Tumors
Breast Tumor
Tumor, Breast
Tumors, Breast
Neoplasms, Breast
Breast Cancer
Cancer, Breast
Mammary Cancer
Cancer, Mammary
Cancers, Mammary
Mammary Cancers
Malignant Neoplasm of Breast
Breast Malignant Neoplasm
Breast Malignant Neoplasms
Malignant Tumor of Breast
Breast Malignant Tumor
Breast Malignant Tumors
Cancer of Breast
Cancer of the Breast
Mammary Carcinoma, Human
Carcinoma, Human Mammary
Carcinomas, Human Mammary
Human Mammary Carcinomas
Mammary Carcinomas, Human
Human Mammary Carcinoma
Mammary Neoplasms, Human
Human Mammary Neoplasm
Human Mammary Neoplasms
Neoplasm, Human Mammary
Neoplasms, Human Mammary
Mammary Neoplasm, Human
Breast Carcinoma
Breast Carcinomas
Carcinoma, Breast
Carcinomas, Breast

Controlled vocabulary

- List of terms to describe some domain of knowledge
- Only one term per phenomenon
- Term definition
- List synonyms
- Each term has a unique identifier

Medical Subject Headings - MeSH

Breast Neoplasms

Definition: Tumors or cancer of the human BREAST

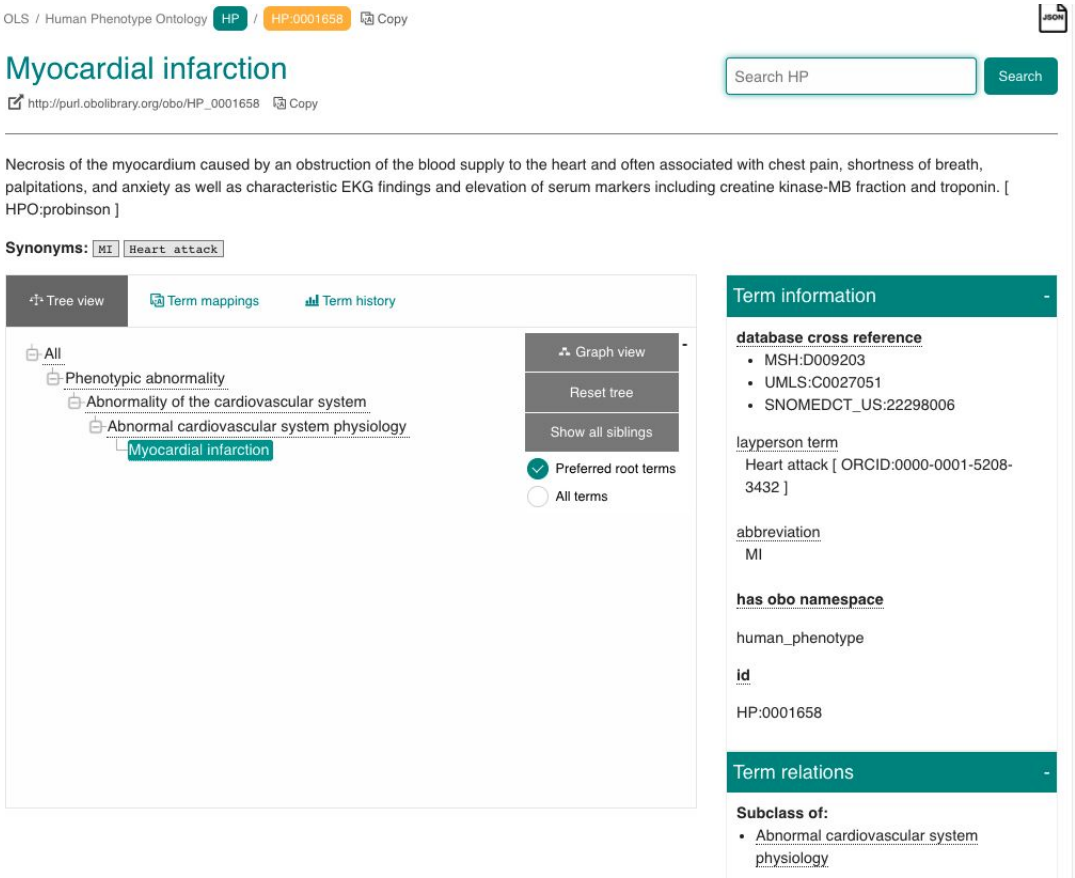
Synonyms: Breast Tumors, Breast Tumor, Breast Cancer, …

MeSH Unique ID: D001943

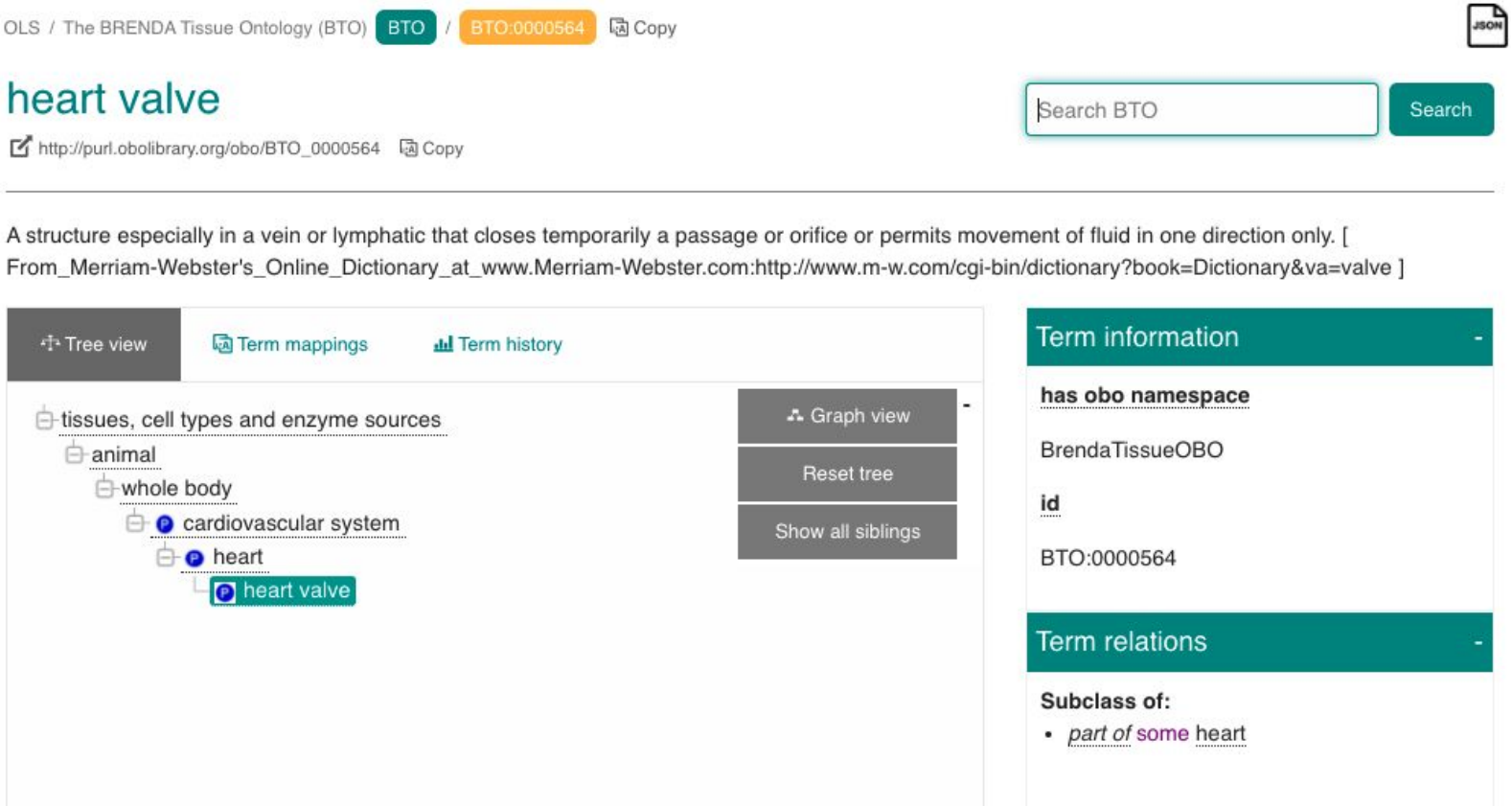
Ontology

- A controlled vocabulary
- Captures term relationships, e.g.
  - *is a*
  - *part of*
  - *contained in*
  - *produced by*
- Hierarchy / Tree
  - A term can be present at several places in the hierarchy

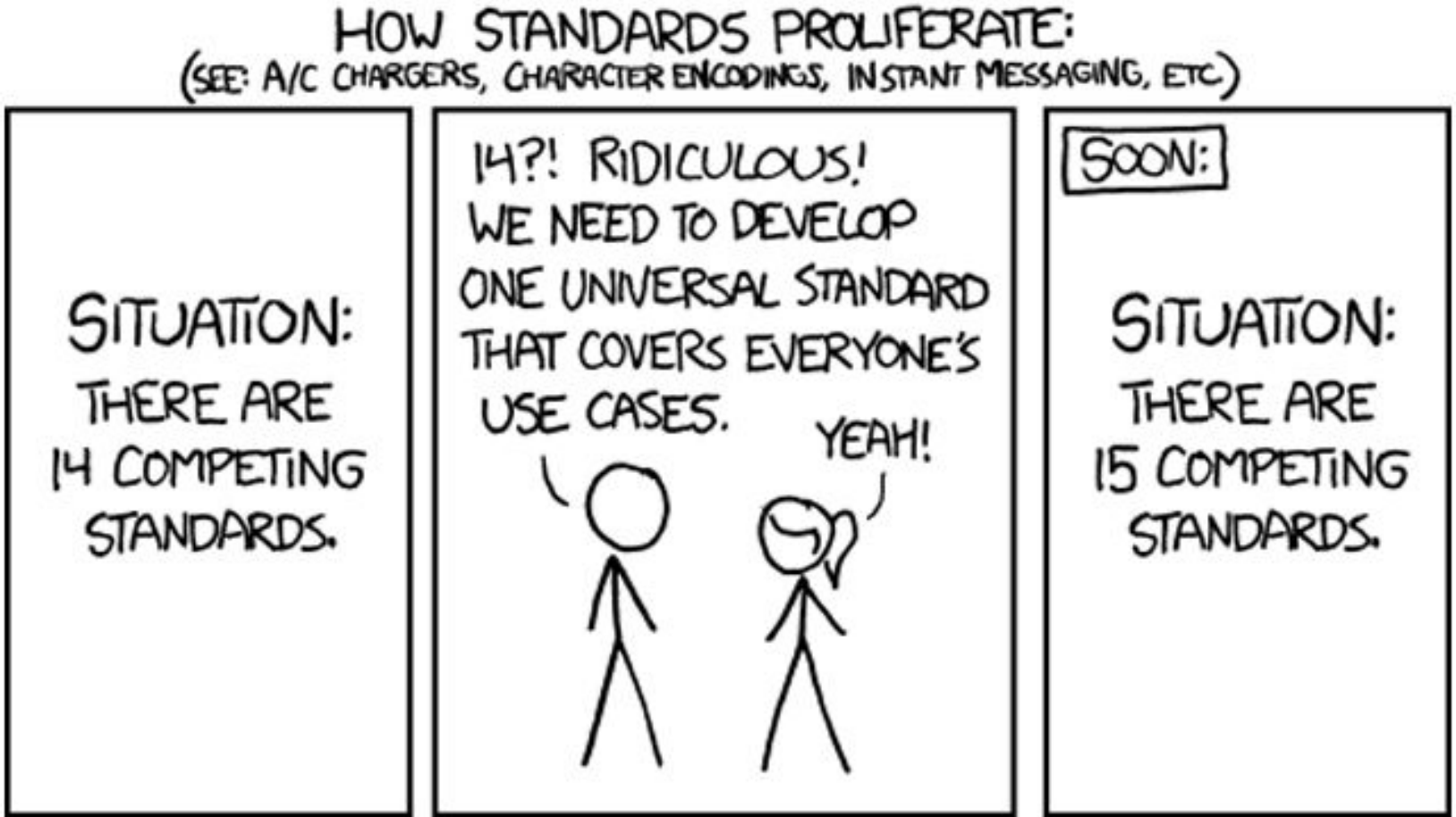
Human Phenotype Ontology



Brenda Tissue Ontology



A universal standard



Making your own?

- At what point does it make sense to use something that exists?
  - Number of terms
  - Nature of terms
  - Relationships of terms
  - Terms management
    - Definitions
- FAIRness
  - Unique identifiers
  - Home brew vocabularies makes it harder to achieve machine readability

Metadata standards

- Collections of metadata **elements** of relevance for a particular purpose
- Elements
  - Mandatory, Recommended, or Optional
  - Defined input value type
    - Free text, data, geographical position, numerical values, ontology terms
  - Can itself be an ontology term
- Stricter → potentially increased FAIRness
- Generic to Specific

Generic - Dublin Core

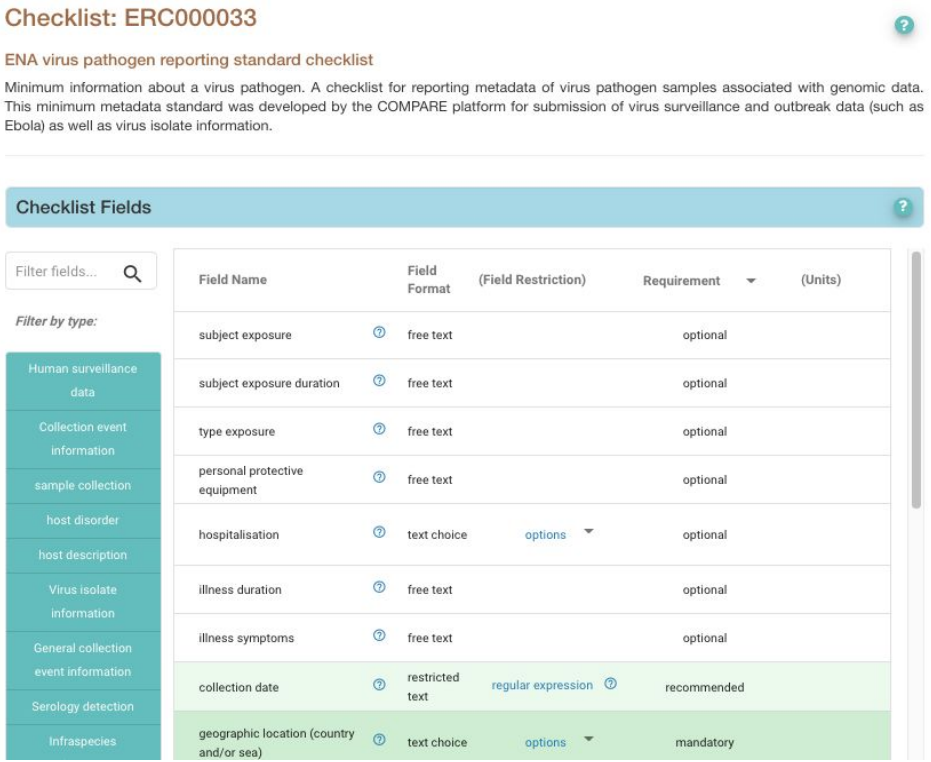
- Describing digital and physical resources
- 15 elements

Term Name: creator	
URI:	http://purl.org/dc/elements/1.1/creator
Label:	Creator
Definition:	An entity primarily responsible for making the resource.
Comment:	Examples of a Creator include a person, an organization, or a service. Typically, the name of a Creator should be used to indicate the entity.
Term Name: date	
URI:	http://purl.org/dc/elements/1.1/date
Label:	Date
Definition:	A point or period of time associated with an event in the lifecycle of the resource.
Comment:	Date may be used to express temporal information at any level of granularity. Recommended best practice is to use an encoding scheme, such as the W3CDTF profile of ISO 8601 [W3CDTF].
References:	[W3CDTF] http://www.w3.org/TR/NOTE-datetime
Term Name: description	
URI:	http://purl.org/dc/elements/1.1/description
Label:	Description
Definition:	An account of the resource.
Comment:	Description may include but is not limited to: an abstract, a table of contents, a graphical representation, or a free-text account of the resource.
Term Name: format	
URI:	http://purl.org/dc/elements/1.1/format
Label:	Format
Definition:	The file format, physical medium, or dimensions of the resource.
Comment:	Examples of dimensions include size and duration. Recommended best practice is to use a controlled vocabulary such as the list of Internet Media Types [MIME].
References:	[MIME] http://www.iana.org/assignments/media-types/

https://www.dublincore.org/specifications/dublin-core/dces/

Specific - an ENA checklist

- *ENA virus pathogen reporting standard checklist*
- Reporting metadata of virus pathogen samples associated with genomic data
- 35 elements - 9 mandatory and 15 recommended



Checklist: ERC000033

ENA virus pathogen reporting standard checklist

Minimum information about a virus pathogen. A checklist for reporting metadata of virus pathogen samples associated with genomic data. This minimum metadata standard was developed by the COMPARE platform for submission of virus surveillance and outbreak data (such as Ebola) as well as virus isolate information.

Checklist Fields

Filter fields...

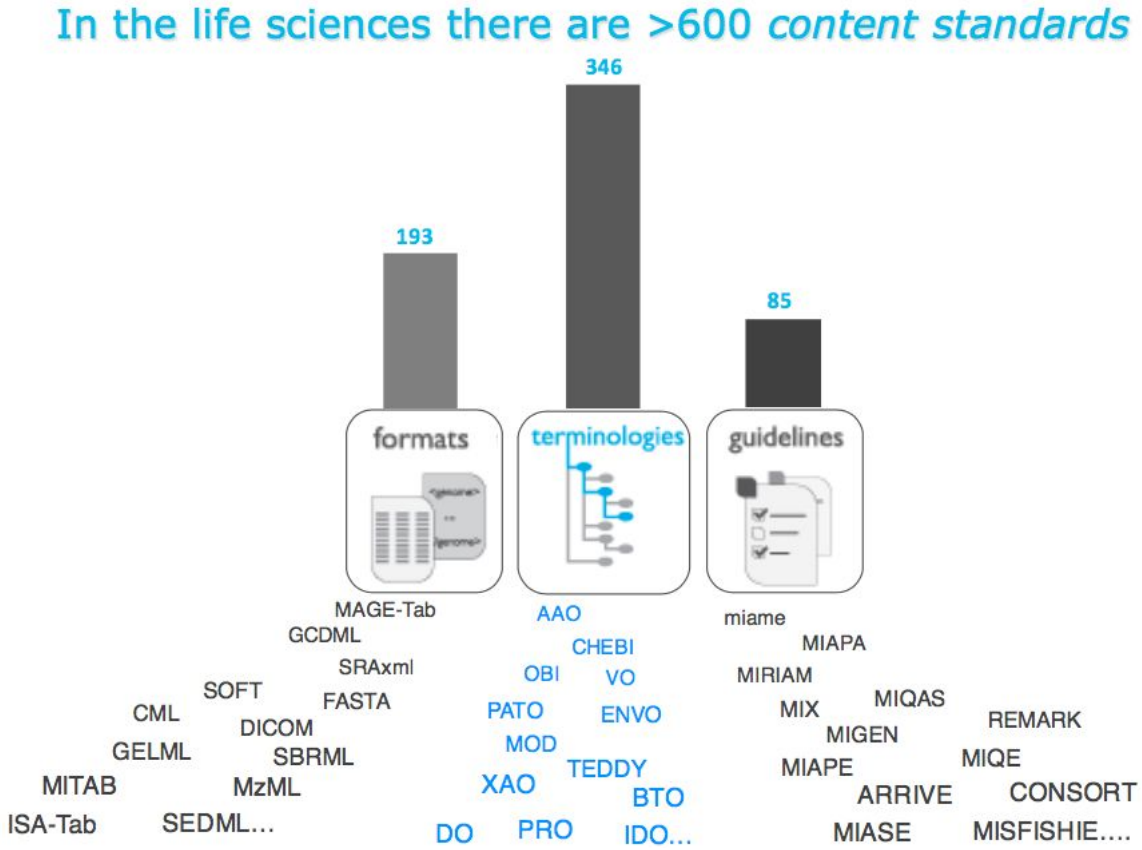
Filter by type:

- Human surveillance data
- Collection event information
- sample collection
- host disorder
- host description
- Virus isolate information
- General collection event information
- Serology detection
- Infraspecies

Field Name	Field Format	(Field Restriction)	Requirement	(Units)
subject exposure	free text		optional	
subject exposure duration	free text		optional	
type exposure	free text		optional	
personal protective equipment	free text		optional	
hospitalisation	text choice	options	optional	
illness duration	free text		optional	
illness symptoms	free text		optional	
collection date	restricted text	regular expression	recommended	
geographic location (country and/or sea)	text choice	options	mandatory	

https://www.ebi.ac.uk/ena/browser/view/ERC000033

How do I know what to use?



Data dictionary

- Your own metadata standard
- Document what type of information is supposed to be entered for the metadata fields
- Name, units, allowed values, definitions, ...

Exercise:
Start a data dictionary

Start a Data dictionary

1. Open **samples_metadata_lesson.csv**
2. Create a new **data_dictionary** file
3. Add headings to **data_dictionary**
   - Current variable name
   - ENA variable name
   - Measurement unit
   - Allowed values
   - Definition
   - Description

3.

	A	B	C	D	E	F
1	Current variable name	ENA Variable name	Measurement unit	Allowed values	Definition	Description
2	animal ID					
3	date					
4	mouse line					
5	strain					
6	age					
7	developmental stage					
8	sex					
9	organism part					
10	genotype					
11	experiment type					
12	experiment reference					
13	researcher					

2. data_dictionary

4.

1. samples_metadata_lesson.csv

	A	B	C	D	E	F	G	H	I	J	K	L
1	animal ID	date	mouse line	strain	age	developmental stage	sex	organism part	genotype	experiment type	experiment reference	researcher
2	800793	2018-01-06	Alk3	BALB/cJ	10	adult	F		wt	behaviour	Jan0618_B	Kim
3	804396	2019-01-07	Vegfr	C57BL/6	6	adult	mael	lung	wild type genotype	sequencing assay	up_201_2	Sam
4	805431	2018-01-12	Vegfr	C57BL/6	P9	pup	female	lung	wild type genotype	IHC	Jan1218_IHC	Sam
5	805992	2019-01-13	Vegfr	C57BL/6	P10	pup	male	lung	wild type genotype	IHC	Jan1319_IHC	Sam
6	808935	2020-01-14	Alk3	BALB/cJ	12	adult	M		wt	behaviour	Jan1420_B	Kim
7	810875	2019-01-16	alk6	C57BL/6	E16	embryo	N/A	brain	KO	culture	Jan1619_C	Jo
8	812308	2018-01-19	Alk3	BALB/cJ	12	adult	F		wt	behaviour	Jan1918_B	Kim
9	814334	2019-01-19	Vegfr	C57BL/6	P9	pup	mael	lung	wild type genotype	IHC	Jan1919_IHC	Sam
10	816649	2018-01-20	Vegfr	C57BL/6	P10	pup	female	lung	wild type genotype	IHC	Jan2018_IHC	Sam
11	819947	2019-01-24	vegfr	C57BL/6	6	adult	male	lung	wild type genotype	sequencing assay	up_432_1	Alex
12	820421	2019-01-31	Vegfr	C57BL/6	P9	pup	female	lung	wild type genotype	IHC	Jan3119_IHC	Sam
13	821756	2018-02-04	vegfr	C57BL/6	P9	pup	male	lung	wild type genotype	IHC	Feb0418_IHC	Alex
14	877817	2019-04-13	vegfr	C57BL/6	6	adult	male	lung	wild type genotype	sequencing assay	up_432_2	Alex
15	821844	2002-07-18	Vegfr	C57BL/6	P10	pup	female	lung	wild type genotype	IHC	Feb0718_IHC	Sam
16	826176	2019-02-14	Vegfr	C57BL/6	P10	pup	male	lung	wild type genotype	IHC	Feb1419_IHC	Sam
17	832626	2020-02-16	Vegfr	C57BL/6	P9	pup	Male	lung	wild type genotype	IHC	Feb1620_IHC	Sam
18	834217	2020-02-18	Alk3	BALB/cJ	4	adult	male	lung	Vegfr2 Y949F/Y949F	sequencing assay	up_235_1	Kim

4. Copy headings from **samples_metadata_lesson.csv** to **rows** in **data_dictionary**

- Add some definitions
- Add some units

Data dictionary - start

	A	B	C	D	E	F
1	**Current variable name**	**ENA Variable n**	**Measurement**	**Allowed values**	**Definition**	**Description**
2	animal ID					
3	date			format: YYYY-MM-DD, >=proj_start_date & <=today	Date of experiment ???	
4	mouse line					
5	strain				The mouse strain of the animal	
6	age		days (?)		Age of animal	
7	developmental stage					
8	sex			male, female, unknown	Sex of the animal	
9	organism part					
10	genotype					
11	experiment type					
12	experiment reference					
13	researcher					
14						

Plan ahead

- Use standards of deposition databases were you plan to publish your data
- Helps with selecting elements
- Makes data submission much easier

Exercise:

Look up an ENA checklist to improve the data dictionary

Improve data dictionary

1. Go to https://www.ebi.ac.uk/ena/browser/checklists to see the available checklists
2. Scroll down the listing until you find the **ERC000011 ENA default sample checklist**

3. Go through the data dictionary and find suitable field names in the ENA default sample checklist for those fields. Add them to the ENA Variable name column of your data dictionary file.

Improve data dictionary

Checklist: ERC000011

ENA default sample checklist

Minimum information required for the sample

Checklist Fields

Filter fields...

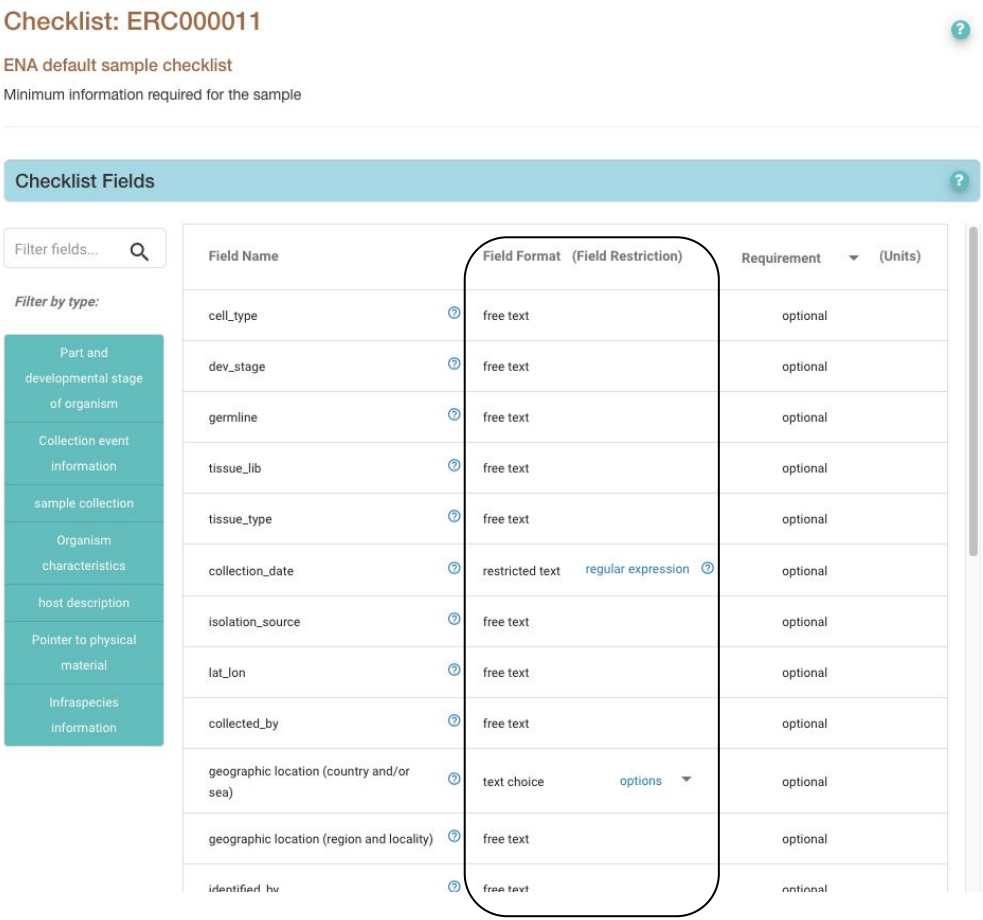
Filter by type:

- Part and developmental stage of organism
- Collection event information
- sample collection
- Organism characteristics
- host description
- Pointer to physical material
- Infraspecies information

Field Name	Field Format	(Field Restriction)	Requirement	(Units)
bio_material	free text		optional	
culture_collection	free text		optional	
specimen_voucher	free text		optional	
cultivar	free text		optional	
ecotype	free text		optional	
isolate	free text		optional	
sub_species	free text		optional	
variety	free text	name or identifier of a genetically or otherwise modified strain from which sample was obtained, derived from a parental strain (which should be annotated in the strain field; sub_strain from which sample was obtained	optional	
sub_strain			optional	
cell_line			optional	
serotype	free text		optional	

	A	B	C	D	E	F
1	**Current variable name**	**ENA Variable n**	**Measurement**	**Allowed values**	**Definition**	**Description**
2	animal ID					
3	date			format: YYYY-MM-DD, >=proj_start_date & <=today	Date of experiment ???	
4	mouse line	**sub_strain**				
5	strain	**strain**			The mouse strain of the animal	
6	age		days (?)		Age of animal	
7	developmental stage	**dev_stage**				
8	sex	**sex**		male, female, unknown	Sex of the animal	
9	organism part	**tissue_type**				
10	genotype					
11	experiment type					
12	experiment reference					
13	researcher					
14						

Finding ontologies



- This standard is very liberal when it comes the allowed values for the different fields
- *We can do better!*
- Use ontology terms
  - Improves FAIRness
  - But which ontologies…?

Finding ontologies

- Tools
  - FAIRsharing.org
  - EBI Ontology Tooling page
    - Zooma - map free text to ontology terms
    - Ontology Lookup Service - OLS

- Not an exact science… There is no perfect way...
- Sometimes hard
- Trial and error

FAIRsharing.org

FAIRsharing.org
standards, databases, policies

Standards | Databases | Policies | Collections | Add/Claim Content | Stats | Log in or Register

A curated, informative and educational resource on data and metadata *standards*, inter-related to *databases* and data *policies*.

HOW CAN WE HELP?

We guide consumers to discover, select and use these resources with confidence, and producers to make their resource more discoverable, more widely adopted and cited.

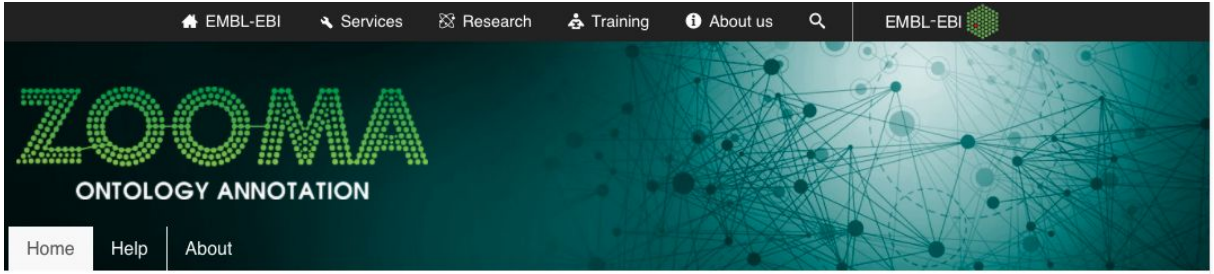
Societies, unions and community alliances

Raise awareness around standards, databases, repositories and data policies, as well as mobilise your community to take action to promote the registration, use and citation of key resources...
[read more]

Researchers | Developers & Curators | Journal Publishers | Librarians & Trainers | Societies & Alliances | Funders

Find | Discover | Learn

Zooma



Query

Use the text box to find possible ontology mappings for free text terms in the ZOOMA repository of curated annotation knowledge. You can add one term (e.g. 'Homo sapiens') per line. If you also have a type for your term (e.g. 'organism'), put this after the term, separated by a tab. If you are new to ZOOMA, take a look at our getting started guide.

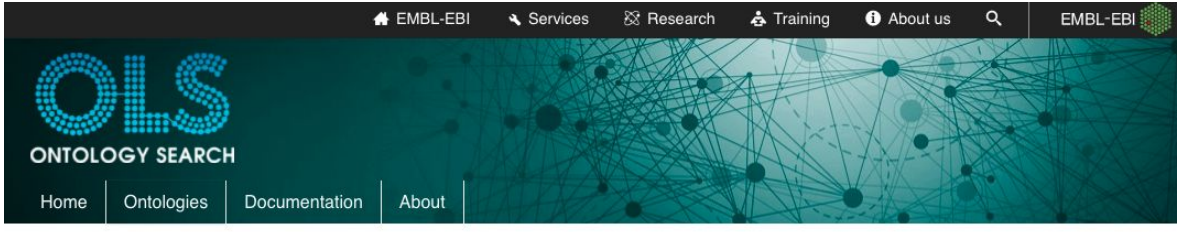
Show me some examples...

```
Bright nuclei
Agammaglobulinemia 2  phenotype
Reduction in IR-induced 53BP1 foci in HeLa  cell
Impaired cell migration with increased protrusive activity  phenotype
C57Black/6  strain
nuclei stay close together
Retinal cone dystrophy 3B  disease
segregation problems/chromatin bridges/lagging chromosomes/multiple DNA masses
Segawa syndrome autosomal recessive  phenotype
BRCA1  gene
Deafness, autosomal dominant 17  phenotype
cooked broccoli  compound
```

Datasources

ZOOMA maps text to ontology terms based on curated mappings from selected datasources (more preferred), and by searching ontologies directly (less preferred). Here, you can select which curated datasources to use, optionally ranked in order of preference. You can also select

OLS



Welcome to the EMBL-EBI Ontology Lookup Service

Search OLS...

Search

Examples: diabetes, GO:0098743

Looking for a particular ontology?

About OLS

The Ontology Lookup Service (OLS) is a repository for biomedical ontologies that aims to provide a single point of access to the latest ontology versions. You can browse the ontologies through the website as well as programmatically via the OLS API. OLS is developed and maintained by the Samples, Phenotypes and Ontologies Team (SPOT) at EMBL-EBI.

Related Tools

In addition to OLS the SPOT team also provides the OxO, Zooma and Webulous services. OxO provides cross-ontology mappings between terms from different ontologies. Zooma is a service to assist in mapping data to ontologies in OLS and Webulous is a tool for building ontologies from spreadsheets.

Report an Issue

For feedback, enquiries or suggestion about OLS or to request a new ontology please use our GitHub issue tracker. For announcements relating to OLS, such as new releases and new features sign up to the OLS announce mailing list

Data Content

Updated 18 Feb 2021 07:58

- 260 ontologies
- 6,466,998 terms
- 31,530 properties
- 497,537 individuals

Tweets by @EBIOLS

EBISPOT OLS
@EBIOLS

A number of our users have custom installations of OLS, OxO and Zooma. @NicoMatentzoglu has created a page where you can you tell us about your custom EBI Ontology Tools installation and your use case:
github.com/EBISPOT/ontoto…

EBISPOT/ontot…
Configuration to …
github.com

Exercise:
Find suitable ontologies for your data

Finding ontologies and terms

Try finding and deciding on suitable ontologies and terms to use for the data file

- **strain**, using OLS
- **dev_stage**, using Zooma
- **tissue_type**, using FAIRsharing.org

Update data dictionary

	A	B	C	D	E	F
1	**Current variable name**	**ENA Variable n**	**Measurement**	**Allowed values**	**Definition**	**Description**
2	animal ID					
3	date			format: YYYY-MM-DD, >=proj_start_date & <=today	Date of experiment ???	
4	mouse line	sub_strain				
5	strain	strain		**NCIT ontology: C56BL/6 Mouse (NCIT:C14424), BALB/cJ Mouse (NCIT:C14657)**	The mouse strain of the animal	
6	age		days (?)		Age of animal	
7	developmental stage	dev_stage		**BTO ontology: pup (BTO:0004377), adult (BTO:0001043), embryo (BTO:0000379)**		
8	sex	sex		male, female, unknown	Sex of the animal	
9	organism part	tissue_type		**MA ontology: lung (MA:0000415), brain (MA:0000168)**		
10	genotype					
11	experiment type					
12	experiment reference					
13	researcher					

Summary

- Information about data is called **metadata**
- Good metadata is a necessity for understanding the data - FAIRness
- Try to be **consistent** when describing data
- Use **controlled vocabularies** and **ontologies** when specifying metadata
- **Metadata standards** - generic and domain specific
- Use **data dictionaries** to document standards for your data
- There are tools to help you decide on ontologies and terms to use