



Metadata

Introduction to Data Management Practices course

NBIS DM Team

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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



Metadata in the Data Life Cycle





Using metadata to perform analysis



FAIR principles



Box 2 | The FAIR Guiding Principles

To be Findable:

- F1. (meta)data are assigned a globally unique and persistent identifier
- F2. data are described with rich metadata defined by R1 below)
- F3. metadata clearly and explicitly include the identifier of the data it describes
- F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:

- A1 (meta)data are retrievable by their identifier using a standardized communications protocol
- A1.1 the protocol is open, free, and universally implementable
- A1.2 the protocol allows for an authentication and authorization procedure, where necessary
- A2. metadata are accessible, even when the data are no longer available

To be Interoperable:

- 11. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- 12. (meta)data use vocabularies that follow FAIR principles
- 13. (meta)data include qualified references to other (meta)data

To be Reusable:

- R1. meta(data) are richly described with a plurality of accurate and relevant attributes
- R1.1. (meta)data are released with a clear and accessible data usage license
- R1.2. (meta)data are associated with detailed provenance
- R1.3. (meta)data meet domain-relevant community standards





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

	A	В	С	D	E
1	sample id =	patient id 🔻	sex ₹	date =	geographic location
2	PE300_COVseq_OAS-1	OAS-1	female	31 March	Italy, Turin, Nizza Mille
3	PE150_COVseq_OAS-1	OAS-1	Female	32 March	Italy, Turin, Nizza Mille
4	NEBNext_OAS-1	OAS-1	female	33 March	Italy, Turin, Nizza Mille
5	PE300_COVseq_OAS-10	OAS-10	male	2020-03-31	Italy, Turin, Turin
6	PE150_COVseq_OAS-10	OAS-10	male	2020-03-31	Italy, Turin, Turin
7	NEBNext_OAS-10	OAS-10	male	2020-03-31	Italy, Turin, Turin
8	PE300_COVseq_OAS-11	OAS-11	male	2020-03-31	Italy, Turin, Piemonte
9	PE150_COVseq_OAS-11	OAS-11	Male	2020-03-31	Italy, Turin, Piemonte
10	NERNOV+ OAS-11	ΛΛ ς_11	Mala	プ ロプロ_03_31	Italy Turin Diamonta

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





How many different medical conditions do you think this list of terms describes?

Bloodstream Infection, Circulatory Failure, Toxic Shock Syndrome, Pyemia, Circulatory Collapse, Blood Poisoning, Endotoxin Shock, Pyohemia, Hypovolemic Shock, Septicemia, Sepsis-associated hypotension, Pyaemia



Solution



Sepsis	Shock	Septic shock
Blood Poisoning	Circulatory Collapse	Endotoxin Shock
Bloodstream Infection	Circulatory Failure	Sepsis-associated hypotension
Pyaemia	Hypovolemic Shock	Toxic Shock Syndrome
Pyemia		
Pyohemia		
Septicemia		



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 Sepsis

Definition: Systemic inflammatory response syndrome with a proven or suspected infectious etiology.

Synonyms: Blood Poisoning, Bloodstream Infection, Pyaemia, Pyemia, ...

MeSH Unique ID: D018805



Ontology

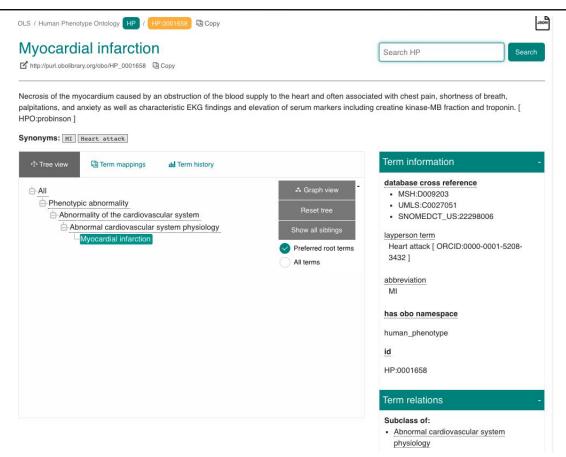


- A controlled vocabulary
- Captures term relationships, e.g.
 - is a
 - part of
 - contained in
 - produced by
- Hierarchy / Tree
 - A term can be present at several places in the hierarchy



Human Phenotype Ontology

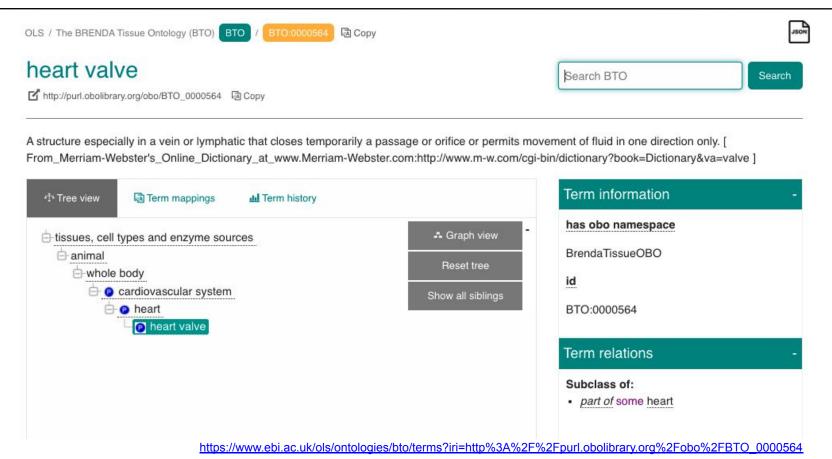






Brenda Tissue Ontology







A universal standard



HOW STANDARDS PROLIFERATE: (SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC.)

SITUATION: THERE ARE 14 COMPETING STANDARDS.



500N:

SITUATION: THERE ARE 15 COMPETING STANDARDS.

https://xkcd.com/927/

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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

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: des	ription
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: forn	nat
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/

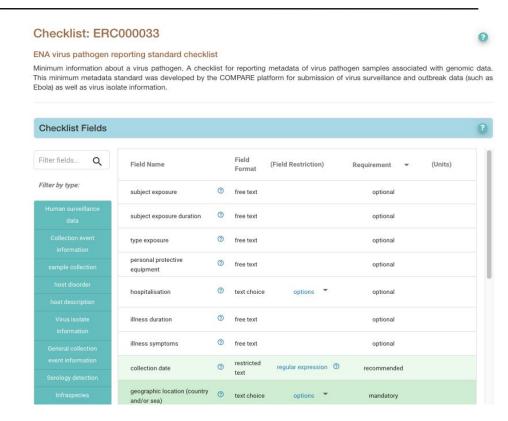
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Specific - an ENA checklist



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

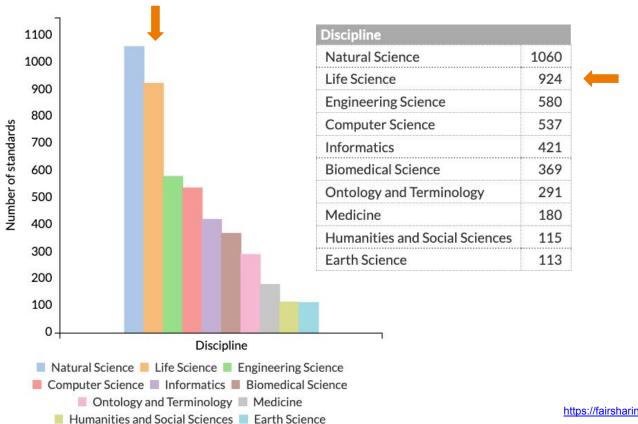


https://www.ebi.ac.uk/ena/browser/view/ERC000033



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, ...



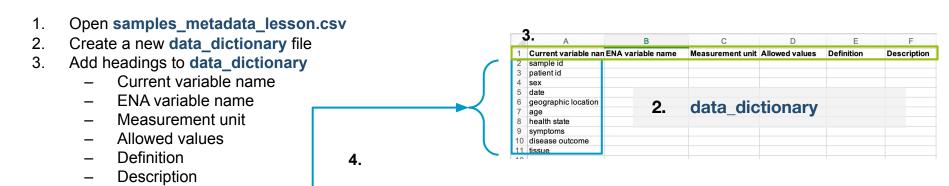


Exercise: Start a data dictionary



Start a Data dictionary





4	A	В	С	D	E	F G	Н	1	J
1	sample id	patient id	sex	date	geographic location	age health state symptoms		disease outcome tissue	
2	PE300_COVseq_OAS-1	UAS-T	remare	31 Warch	italy, Turin, Nizza Millelonu	48 III	iever, sore inroat	dead	ıaryngopnarynx
3	PE150_COVseq_OAS-1	OAS-1	Female	32 March	Italy, Turin, Nizza Millefonti	48 ill	fever, sore throat	dead	laryngopharynx
4	NEBNext_OAS-1	OAS-1	female	33 March	Italy, Turin, Nizza Millefonti	48 ill	fever, sore throat	dead	laryngopharynx
5	PE300_COVseq_OAS-10	OAS-10	male	2020-03-31	Italy, Turin, Turin	35	N/A		lung
6	PE150_COVseq_OAS-10	OAS-10	male	2020-03-31	Italy, Turin, Turin	35	N/A		lung
7	NEBNext_OAS-10	OAS-10	male	2020-03-31	Italy, Turin, Turin	35	N/A		lung
8	PE300_COVseq_OAS-11	OAS-11	male	2020-03-31	Italy, Turin, Piemonte	59 healthy	N/A	healthy	nasopharynx
9	PE150_COVseq_OAS-11	OAS-11	Male	2020-03-31	Italy, Turin, Piemonte	59 healthy	N/A	healthy	nasopharynx
10	NEBNext_OAS-11	OAS-11	Male		Italy, Turin, Piemonte	59 healthy	N/A	healthy	nasopharynx
11	PE300_COVseq_OAS-12	OAS-12	female	2020-003	mples metada	tahea acc	son csv	healthy	nasopharynx
12	PE150_COVseq_OAS-12	OAS-12	female	2020-03-31	Italy, Turin, Turi n	60 he althy	N/A	healthy	nasopharynx
13	NEBNext_OAS-12	OAS-12	female	2020-03-31	Italy, Turin, Turin	60 healthy	N/A	healthy	nasopharynx
14	PE300_COVseq_OAS-13	OAS-13	female	31/3/2020	Italy, Turin, Torino	83 ill	fatigue, loss of taste	dead	laryngopharynx
15	PE150_COVseq_OAS-13	OAS-13	female	31/3/2020	Italy, Turin, Torino	83 ill	fatigue, loss of taste	dead	laryngopharynx
16	NEBNext_OAS-13	OAS-13	female	31/3/2020	Italy, Turin, Torino	83 ill	fatigue, loss of taste	dead	laryngopharynx
17	PE300_COVseq_OAS-14	OAS-14	Male	4/1/2020	Italy, Turin, Campidoglio	21 ill	fever	dead	laryngopharynx
18	PE150_COVseq_OAS-14	OAS-14	M	4/1/2021	Italy, Turin, Campidoglio	21 ill	fever	dead	laryngopharynx
19	NEBNext_OAS-14	OAS-14	M	4/1/2022	Italy, Turin, Campidoglio	21 ill	fever	dead	laryngopharynx

- 4. Copy headings from samples_metadata_lesson.csv to rows in data_dictionary
 - Add some definitions
- Add some units
- Add some allowed value definitions



Data dictionary - start



	A B C		D	E	F	
1	Current variable nan	ENA variable name	Measurement unit	Allowed values	Definition	Description
2	sample id					-
3	patient id					
4	sex			male, female, unknown	Sex of individual	
5	date			format: YYYY-MM-DD, >=proj_start_date & <=today	Date of sampling	
6	location					
7	age		years		Age of the individual at	
8	health state				Health state of individual at	
9	symptoms			fever, sore throat, fatigue, loss of taste, not applicable	Symptoms experienced in connection with illness	
10	disease outcome			healthy, dead	Final outcome of disease	
11	tissue			-	Tissue sampled	
12						



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



- Go to https://www.ebi.ac.uk/ena/browser/checklists to see the available checklists
- 2. Scroll down the listing until you find the ERC000033 ENA virus pathogen reporting standard 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.
 - a. Are all mandatory fields present, or will you need to add fields?
 - b. Are there fields that need to be split into more fields?
 - c. Are there controlled vocabularies you should adhere to?



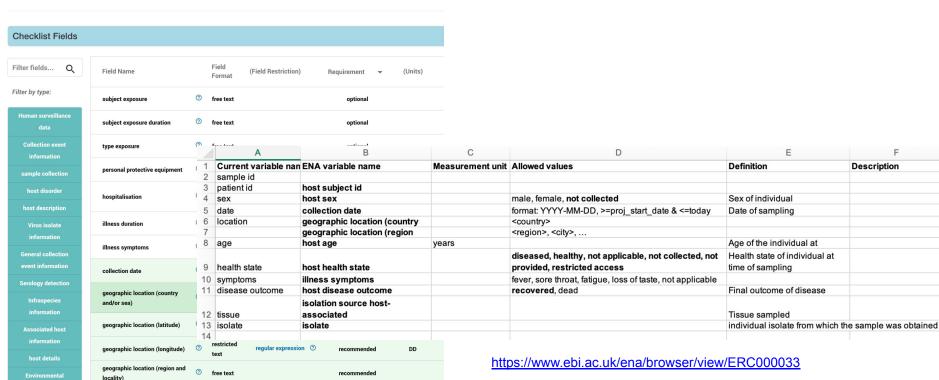
Improve data dictionary



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 minimum metadata standard was developed by the COMPARE platform for submission of virus surveillance and outbreak data (such as Ebo well as virus isolate information.





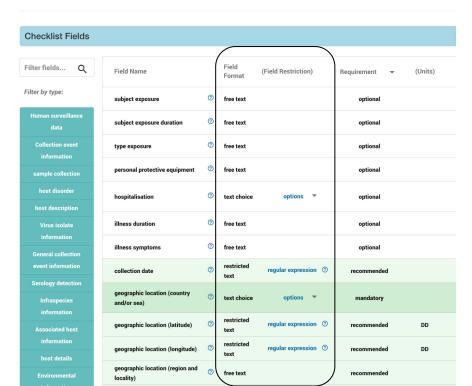
Finding ontologies



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 minimum metadata standard was developed by the COMPARE platform for submission of virus surveillance and outbreak data (such as Ebo well as virus isolate information.



- This standard is liberal when it comes the allowed values for the different fields
- We can do better!

- Use ontology terms
 - Improves FAIRness
 - But which ontologies…?

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



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





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
Fi	nd	Disc	cover	Lea	rn

https://fairsharing.org/



Zooma





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About ZOOMA

What's this? 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 Senawa cyndrome autocomal recessive nhanotyna

Zooma is a tool for mapping free text annotations to ontology term based on a curated repository of annotation knowledge.

Where mappings are not found in the curated respository one or more ontologies can be selected from the Ontology Lookup Service to increase coverage. For example if you want to map GWAS annotations select the GWAS datasource and a common disease ontology such as EFO or DOID to maximise coverage when terms have no curated mappings.

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.

Annotate

Clear

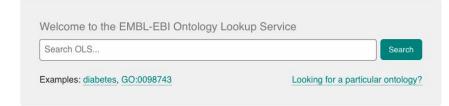
https://www.ebi.ac.uk/training/online/courses/cellular-microscopy-phenotype-ontology-quick-tour/annotating-data-with-cmpo/ CC BY 4.0



OLS







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.

Nelated 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.

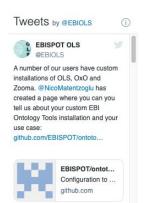
A Report an Issue

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

Jul Data Content

Updated 18 Feb 2021 07:58

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



https://www.ebi.ac.uk/ols/





Exercise: Find suitable ontologies for your data



Finding ontologies and terms SciLifeLab



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

- illness symptoms, using OLS
- isolation source host-associated, using FAIRsharing.org



Update data dictionary



	Α	В	С	D	E	F
1	Current variable nan	ENA variable name	Measurement unit	Allowed values	Definition	Description
2	sample id					
3	patient id	host subject id				
4	sex	host sex		male, female, not collected	Sex of individual	
5	date	collection date		format: YYYY-MM-DD, >=proj_start_date & <=today	Date of sampling	
6	location	geographic location (country and/or sea)		<country></country>		
7		geographic location (region and locality)		<region>, <city>,</city></region>		
8	age	host age	years		Age of the individual at	
9	health state	host health state		diseased, healthy, not applicable, not collected, not provided, restricted access	Health state of individual at time of sampling	
10	symptoms	illness symptoms		NCIT ontology: Fever (NCIT:C3038), Sore Throat (NCIT:C50747), Fatigue (NCIT:C3036), Ageusia (NCIT:C116374), not applicable		
11	disease outcome	host disease outcome		recovered, dead	Final outcome of disease	
12	tissue	isolation source host-associated		FMA ontology: Laryngopharynx (FMA:54880), Nasopharynx (FMA:54878), Lung (FMA:7195)	Tissue sampled	
13	experiment type					
14 15	isolate	isolate			individual isolate from which the sample was obtained	



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