

# Metadata

*Introduction to Data Management Practices course*

NBIS DM Team

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



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*“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.”*

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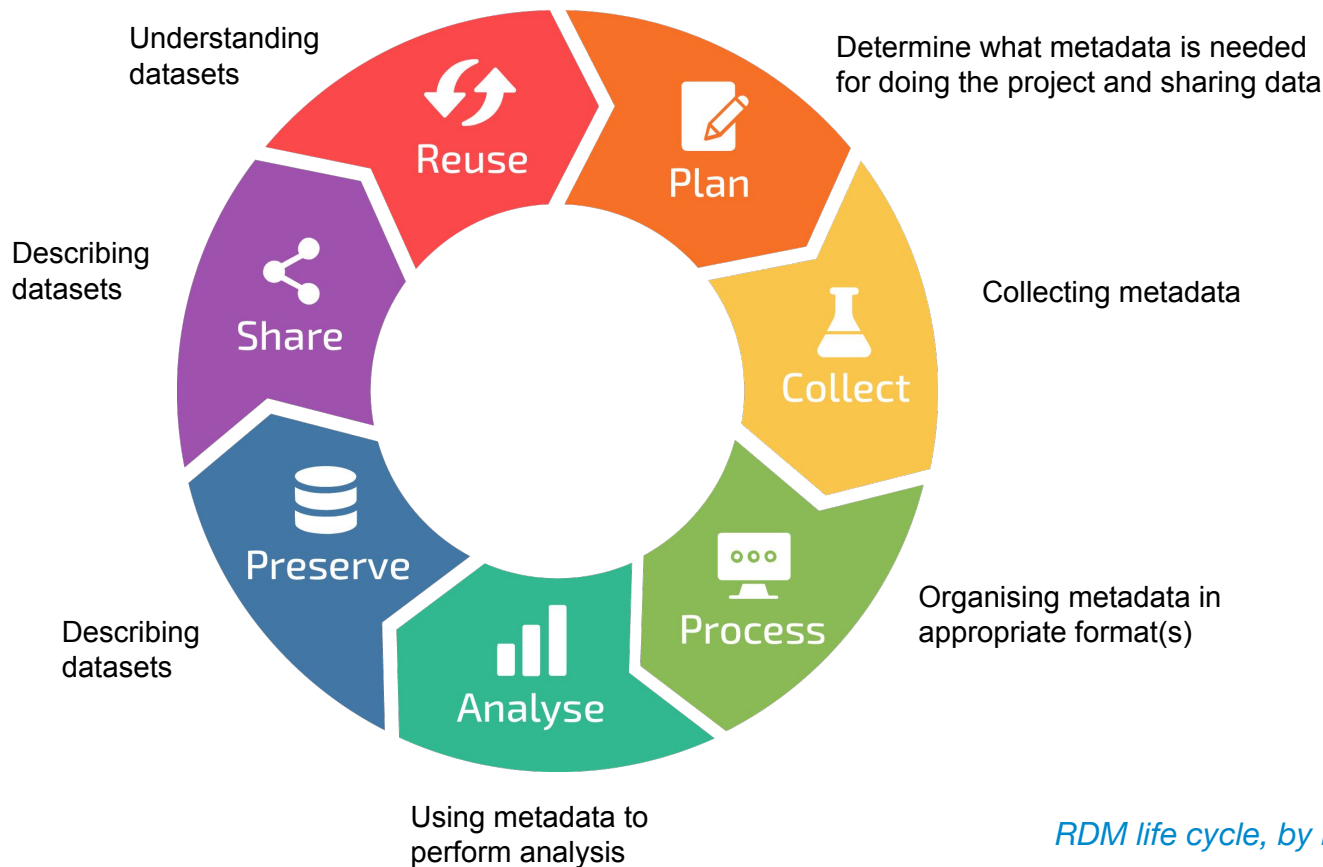
The data about the data (or anything really)

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

- 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



## 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:

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (meta)data use vocabularies that follow FAIR principles
- I3. (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	B	C	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	NEBNext_OAS-11	OAS-11	Male	2020-03-31	Italy, Turin, Piemonte

[samples\\_metadata\\_lesson.csv](#)

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



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

- 
- 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?”*

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

- Consistency and stringency
- **Controlled vocabularies**
- **Ontologies**
- Thesauruses (Thesauri)
- Taxonomies

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**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*

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

- 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

- 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

OLS / Human Phenotype Ontology **HP** / **HP:0001658** 






## Myocardial infarction




 [http://purl.obolibrary.org/obo/HP\\_0001658](http://purl.obolibrary.org/obo/HP_0001658)  Copy

Necrosis of the myocardium caused by an obstruction of the blood supply to the heart and often associated with chest pain, shortness of breath, palpitations, and anxiety as well as characteristic EKG findings and elevation of serum markers including creatine kinase-MB fraction and troponin. [ HPO:probinson ]

Synonyms: **MI**

 Tree view
 Term mappings
 Term history

- All
- Phenotypic abnormality
  - Abnormality of the cardiovascular system
    - Abnormal cardiovascular system physiology
      - Myocardial infarction

 Graph view

Reset tree

Show all siblings

Preferred root terms  
 All terms

### Term information

#### database cross reference

- MSH:D009203
- UMLS:C0027051
- SNOMEDCT\_US:22298006

#### layperson term

Heart attack [ ORCID:0000-0001-5208-3432 ]

#### abbreviation

MI

#### has obo namespace

human\_phenotype

#### id

HP:0001658

### Term relations

#### Subclass of:

- [Abnormal cardiovascular system physiology](#)



OLS / The BRENDA Tissue Ontology (BTO) **BTO** / **BTO:0000564**  Copy






## heart valve




 [http://purl.obolibrary.org/obo/BTO\\_0000564](http://purl.obolibrary.org/obo/BTO_0000564)  Copy

A structure especially in a vein or lymphatic that closes temporarily a passage or orifice or permits movement of fluid in one direction only. [ From\_Merriam-Webster's\_Online\_Dictionary\_at\_www.Merriam-Webster.com:http://www.m-w.com/cgi-bin/dictionary?book=Dictionary&va=valve ]

 Tree view
 Term mappings
 Term history

- └ tissues, cell types and enzyme sources
  - └ animal
    - └ whole body
      - └ cardiovascular system
        - └ heart
          - └ heart valve

 Graph view

Reset tree

Show all siblings

### Term information

**has obo namespace**

BrendaTissueOBO

**id**

BTO:0000564

### Term relations

**Subclass of:**

- *part of some* heart

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

SITUATION:  
THERE ARE  
14 COMPETING  
STANDARDS.

14?! RIDICULOUS!  
WE NEED TO DEVELOP  
ONE UNIVERSAL STANDARD  
THAT COVERS EVERYONE'S  
USE CASES.



SOON:

SITUATION:  
THERE ARE  
15 COMPETING  
STANDARDS.

<https://xkcd.com/927/>

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- 
- 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

- 
- 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

- Describing digital and physical resources
- 15 elements

<b>Term Name: creator</b>	
URI:	<a href="http://purl.org/dc/elements/1.1/creator">http://purl.org/dc/elements/1.1/creator</a>
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.
<b>Term Name: date</b>	
URI:	<a href="http://purl.org/dc/elements/1.1/date">http://purl.org/dc/elements/1.1/date</a>
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] <a href="http://www.w3.org/TR/NOTE-datetime">http://www.w3.org/TR/NOTE-datetime</a>
<b>Term Name: description</b>	
URI:	<a href="http://purl.org/dc/elements/1.1/description">http://purl.org/dc/elements/1.1/description</a>
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.
<b>Term Name: format</b>	
URI:	<a href="http://purl.org/dc/elements/1.1/format">http://purl.org/dc/elements/1.1/format</a>
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] <a href="http://www.iana.org/assignments/media-types/">http://www.iana.org/assignments/media-types/</a>

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

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- *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.

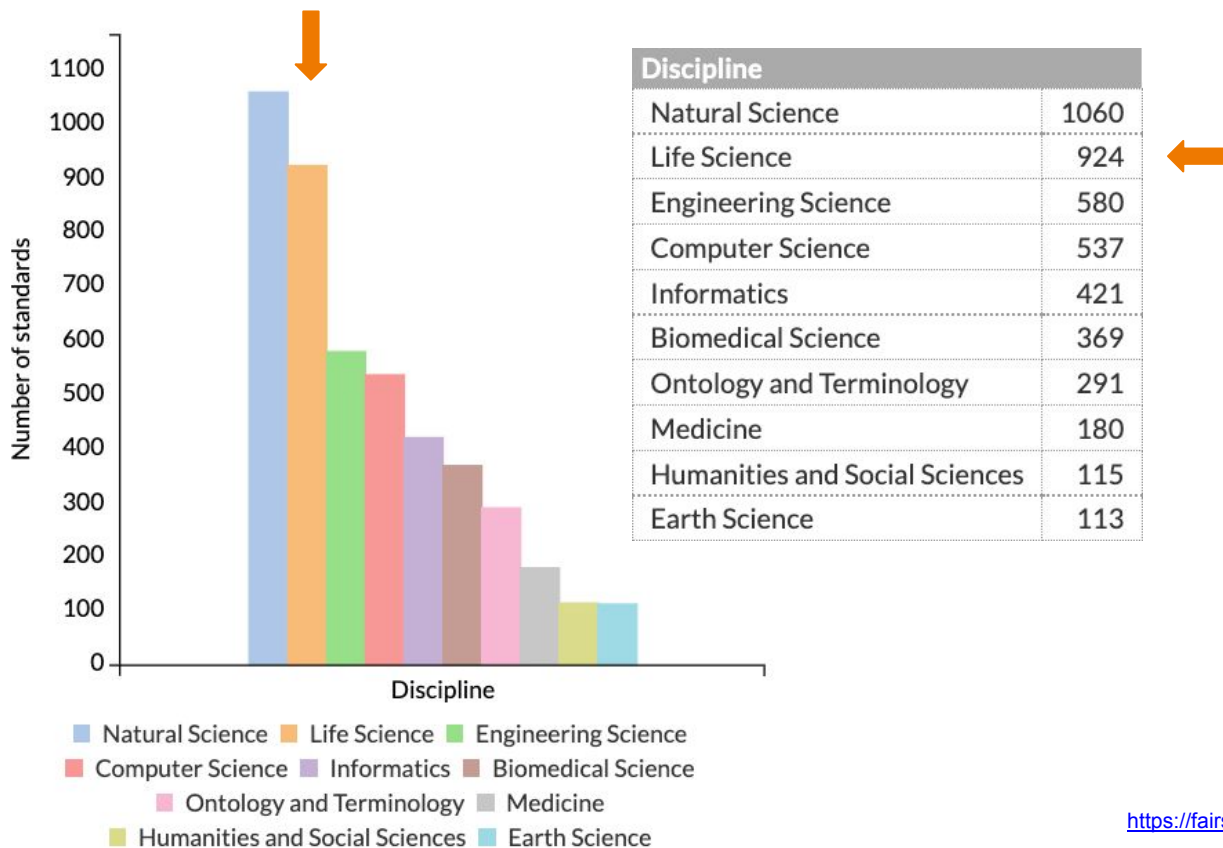
#### Checklist Fields

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	



- 
- 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**

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	sample id					
3	patient id					
4	sex					
5	date					
6	geographic location					
7	age					
8	health state					
9	symptoms					
10	disease outcome					
11	tissue					

2. `data_dictionary`

4.

1. `samples_metadata_lesson.csv`

	A	B	C	D	E	F	G	H	I	J
1	sample id	patient id	sex	date	geographic location	age	health state	symptoms	disease outcome	tissue
2	PE300_COVseq_OAS-1	OAS-1	female	31 March	Italy, Turin, Nizza Millefonti	48	ill	fever, sore throat	dead	laryngopharynx
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	2020-03-31	Italy, Turin, Piemonte	59	healthy	N/A	healthy	nasopharynx
11	PE300_COVseq_OAS-12	OAS-12	female	2020-03-31	Italy, Turin, Turin	60	healthy	N/A	healthy	nasopharynx
12	PE150_COVseq_OAS-12	OAS-12	female	2020-03-31	Italy, Turin, Turin	60	healthy	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

	A	B	C	D	E	F
1	<b>Current variable name</b>	<b>ENA variable name</b>	<b>Measurement unit</b>	<b>Allowed values</b>	<b>Definition</b>	<b>Description</b>
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						

- 
- 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**

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 **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?

## Checklist: ERC000033

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#### Checklist 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

Intraspecies information

Associated host information

host details

Environmental information

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	1 sample id 2 patient id	3 host subject id		
hospitalisation	4 sex 5 date	6 collection date		
illness duration	6 location	7 geographic location (country) 8 geographic location (region)		
illness symptoms	8 age	9 host age	years	
collection date	9 health state	10 host health state		
geographic location (country and/or sea)	10 symptoms 11 disease outcome	11 illness symptoms 12 host disease outcome		
geographic location (latitude)	12 tissue 13 isolate	13 isolation source host-associated 14 isolate		
geographic location (longitude)	restricted text	regular expression	recommended	DD
geographic location (region and locality)	free text		recommended	

A	B	C	D	E	F
<b>Current variable name</b>	<b>ENA variable name</b>	<b>Measurement unit</b>	<b>Allowed values</b>	<b>Definition</b>	<b>Description</b>
sample id	host subject id				
patient id	host sex		male, female, <b>not collected</b>	Sex of individual	
sex	collection date		format: YYYY-MM-DD, >=proj_start_date & <=today	Date of sampling	
date	geographic location (country)		<country>		
location	geographic location (region)		<region>, <city>, ...		
age	host age	years		Age of the individual at time of sampling	
health state	host health state		<b>diseased, healthy, not applicable, not collected, not provided, restricted access</b>	Health state of individual at time of sampling	
symptoms	illness symptoms		fever, sore throat, fatigue, loss of taste, not applicable		
disease outcome	host disease outcome		<b>recovered, dead</b>	Final outcome of disease	
tissue	isolation source host-associated			Tissue sampled	
isolate	isolate			individual isolate from which the sample was obtained	

## Checklist: ERC000033

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Checklist Fields					
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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		
geographic location (latitude)	restricted text	regular expression	recommended	DD	
geographic location (longitude)	restricted text	regular expression	recommended	DD	
geographic location (region and locality)	free text		recommended		

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



- Tools
  - [FAIRsharing.org](https://fairsharing.org)
  - [EBI Ontology Tooling page](#)
    - [Ontology Lookup Service - OLS](#)
    - [Zooma](#) - map free text to ontology terms
- Not an exact science... There is no perfect way...
- Sometimes hard
- Trial and error



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

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.

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Identify and cite the standards, databases or repositories that exist for your discipline when creating a data management plan, releasing data or submitting a manuscript to a journal...

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Welcome to the EMBL-EBI Ontology Lookup Service



Examples: [diabetes](#), [GO:0098743](#)

[Looking for a particular ontology?](#)

### Data Content

Updated 18 Feb 2021

07:58

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

### 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](#)

### Tweets by [@EBIOLS](#)

**EBISPOT OLS**  
[@EBIOLS](#)

🐦

A number of our users have custom installations of OLS, OxO and Zooma. [@NicoMatentzogl](#) 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...](https://github.com/EBISPOT/ontoto...)

**EBISPOT/ontoto...**  
Configuration to ...  
[github.com](#)

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

# ZOOMA

## ONTOLOGY ANNOTATION

Home | Explore | Help | 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 syndrome autosomal recessive phenotype

Annotate Clear

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 repository 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](#).

 [Configure Datasources](#)

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

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<https://www.ebi.ac.uk/spot/zooma/>

**Exercise:**  
**Find suitable ontologies for your data**

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](https://fairsharing.org)

	A	B	C	D	E	F
1	<b>Current variable name</b>	<b>ENA variable name</b>	<b>Measurement unit</b>	<b>Allowed values</b>	<b>Definition</b>	<b>Description</b>
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>		
7		geographic location (region and locality)		<region>, <city>, ...		
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		<b>NCIT ontology:</b> <b>Fever (NCIT:C3038), Sore Throat (NCIT:C50747), Fatigue (NCIT:C3036), Ageusia (NCIT:C116374), not applicable</b>		
11	disease outcome	host disease outcome		recovered, dead	Final outcome of disease	
12	tissue	isolation source host-associated		<b>FMA ontology:</b> <b>Laryngopharynx (FMA:54880), Nasopharynx (FMA:54878), Lung (FMA:7195)</b>	Tissue sampled	
13	experiment type					
14	isolate	isolate			individual isolate from which the sample was obtained	
15						

- 
- 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