

# 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.”*

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

# 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
Pyæmia	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**  Copy



## 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** **Heart attack**

 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

Search


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.



- 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>

- *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... 

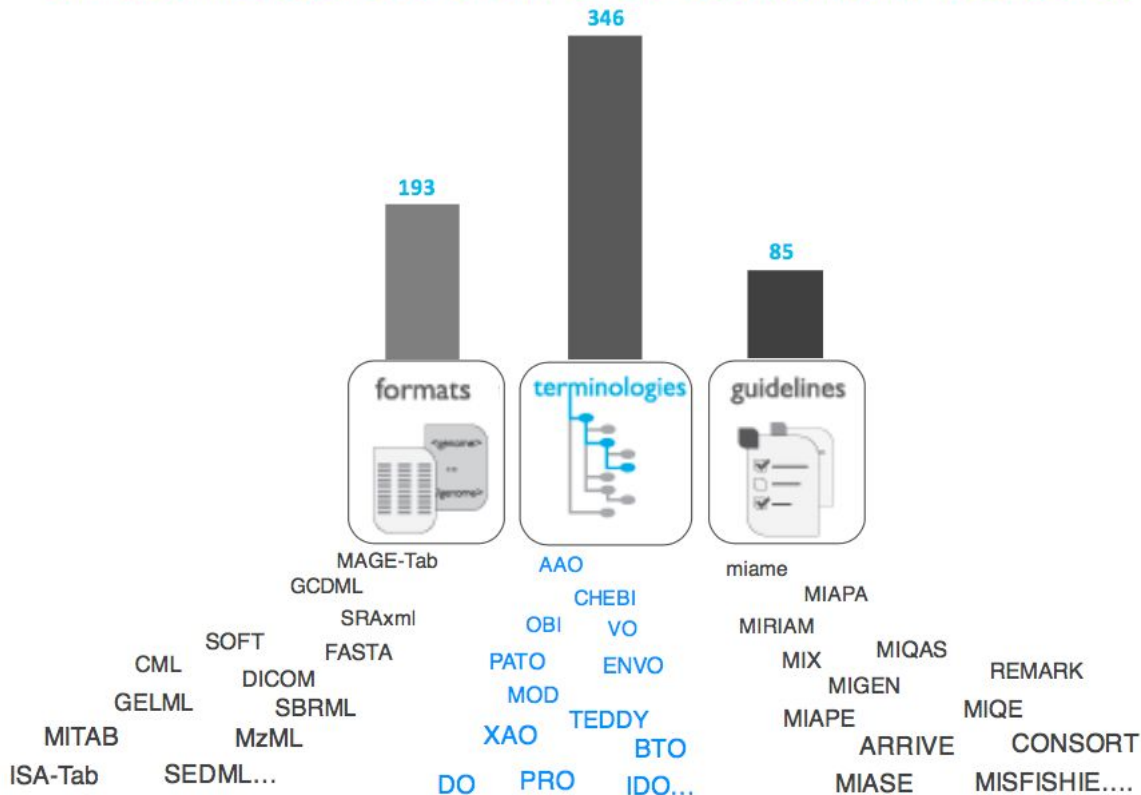
Filter by type:

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	

# How do I know what to use?

In the life sciences there are **>600 content standards**



- 
- 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

4.

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](#)

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

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	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



	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

### 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.

#### 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

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				
personal protective equipment				
hospitalisation				
illness duration				
illness symptoms				
collection date				
geographic location (country and/or sea)				
geographic location (latitude)				
geographic location (longitude)				
geographic location (region and locality)				

A	B	C	D	E	F
1 Current variable name	2 ENA variable name	3 Measurement unit	4 Allowed values	5 Definition	6 Description
1 sample id	2 patient id				
3 sex	4 host sex		male, female, <b>not collected</b>	Sex of individual	
5 date	6 collection date		format: YYYY-MM-DD, >=proj_start_date & <=today	Date of sampling	
7 location	8 geographic location (country)		<country>		
7 location	8 geographic location (region)		<region>, <city>, ...		
8 age	9 host age	years		Age of the individual at	
9 health state	10 host health state		<b>diseased, healthy, not applicable, not provided, restricted access</b>	Health state of individual at	
10 symptoms	11 illness symptoms		fever, sore throat, fatigue, loss of taste, not applicable	Final outcome of disease	
11 disease outcome	12 isolation source host-associated		<b>recovered, dead</b>		
12 tissue	13 isolate			Tissue sampled	
13 isolate	14 isolate			individual isolate from which the sample was obtained	
14					
geographic location (longitude)	restricted text	regular expression	recommended	DD	
geographic location (region and locality)	free text		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 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... 	Field Name	Field Format (Field Restriction)	Requirement	(Units)
Filter by type:				
Human surveillance data	subject exposure	free text	optional	
Collection event information	subject exposure duration	free text	optional	
sample collection	type exposure	free text	optional	
host disorder	personal protective equipment	free text	optional	
host description	hospitalisation	text choice <a href="#">options</a>	optional	
Virus isolate information	illness duration	free text	optional	
General collection event information	illness symptoms	free text	optional	
Serology detection	collection date	restricted text <a href="#">regular expression</a>	recommended	
Infraspecies information	geographic location (country and/or sea)	text choice <a href="#">options</a>	mandatory	
Associated host information	geographic location (latitude)	restricted text <a href="#">regular expression</a>	recommended	DD
host details	geographic location (longitude)	restricted text <a href="#">regular expression</a>	recommended	DD
Environmental information	geographic location (region and locality)	free text	recommended	

- 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...?

- Tools
  - [FAIRsharing.org](https://fairsharing.org)
  - [EBI Ontology Tooling page](https://eutils.ebi.ac.uk/ontology/tooling/)
    - [Zooma](https://zooma.ebi.ac.uk/) - map free text to ontology terms
    - [Ontology Lookup Service - OLS](https://ontology.ebi.ac.uk/ols/)
- 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*.**

## 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



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ONTOLOGY ANNOTATION

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## Query

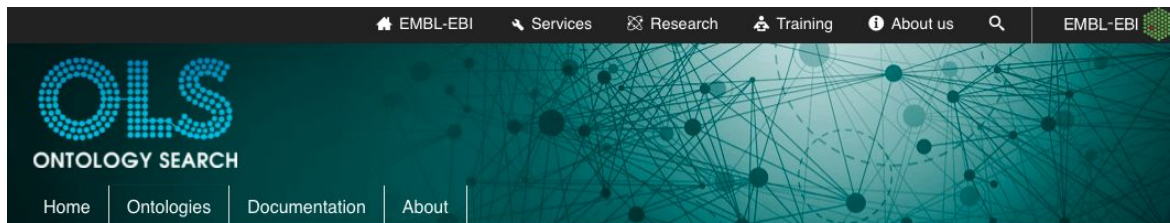
Use the text box to find possible ontology mappings for free text terms in the ZOOMA repository of curated annotation knowledge. You can add one term (e.g. 'Homo sapiens') per line. If you also have a type for your term (e.g. 'organism'), put this after the term, separated by a tab. If you are new to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



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 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://github.com)

---

# **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
-

	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						

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- 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