How to use LexMapr

For people who have little to no experience with command line

and

For macOS and Linux users only

Note: this tutorial shows you how to use LexMapr through the command-line, but a web application is currently in development

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Open up your terminal

macOs:

cmd + space to open spotlight search

type terminal

hit return

Linux:

ctrl + alt + t

Terminal tutorial

The terminal opens in your Home (also known as ~) directory

Type the following command into your terminal:

ls

This will print out all the sub-directories and files in your home directory

Terminal tutorial

You can change terminal directories with the cd command:

cd Desktop	Navigate to	your Desktop	subdirectory
------------	-------------	--------------	--------------

1s View the contents of your Desktop

cd .. Navigate to the parent directory

1s View the contents of your Home again

If you ever get lost, you can return Home with $cd \sim$

Do you have Conda?

In your terminal, type:

conda -V

If you have Conda, the terminal will tell you your Conda version number

If you do not have Conda, the terminal will tell you the conda command was not found

Install Conda

Go to https://docs.conda.io/en/latest/miniconda.html

Install the appropriate 64-bit bash installer for Python 3.7

In your terminal, navigate to the folder containing the installer

Assuming this was the Downloads folder:

cd ~

cd Downloads

Install Conda

In this folder, we run the installer through a terminal command macOS:

bash Miniconda3-latest-MacOSX-x86_64.sh

Linux:

bash Miniconda3-latest-Linux-x86_64.sh

Follow the prompts to completion

Bioconda

Bioconda is a channel that allows users to easily install various bioinformatic packages, including LexMapr

Run the following terminal commands to set up Bioconda:

```
conda config --add channels default
conda config --add channels bioconda
conda config --add channels conda-forge
```

RUN THESE COMMANDS IN ORDER

Install LexMapr into a Conda environment

Enter the following command from any directory:

conda create -n LexMapr python=3.6 lexmapr

Follow the prompts to completion

This creates a Conda environment called "LexMapr", that contains a Bioconda installation of LexMapr

Whenever you want to run LexMapr, all you have to do is:

Start the terminal

Activate your LexMapr Conda environment:

conda activate LexMapr

Run LexMapr commands

lexmapr --help

LexMapr input files

LexMapr takes input csv files with the following format:

SampleId,Sample

- 1, Chicken Breast
- 2,Baked Potato
- 3, Canned Corn
- 4, Frozen Yogurt
- 5,Apple Pie

LexMapr input files

Open up Microsoft Excel, Apple Numbers or LibreOffice Calc Create a spreadsheet like so:

	Α	В
1	SampleId	Sample
2	1	Chicken Breast
3	2	Baked Potato
4	3	Canned Corn
5	4	Frozen Yogurt
6	5	Apple Pie

Save as "small_simple.csv"

In the terminal, cd to the folder containing small_simple.csv

With the LexMapr Conda environment activated, try:

lexmapr small_simple.csv

Taking a while?

The first run will be slow

LexMapr caches a lookup table on the first run

LexMapr uses this table to make subsequent runs much faster

Output:

```
Sample_Id
                Sample_Desc
                                Cleaned_Sample
                                                Matched_Components
                                chicken breast
small_simple1
               Chicken Breast
                                                ['breast:uberon_0000310']
small_simple2
                Baked Potato
                                baked potato
                                                []
small_simple3
               Canned Corn
                                canned corn
small_simple4
               Frozen Yogurt
                                                ['frozen:pato_0001985']
                                frozen yogurt
small_simple5
                                                []
               Apple Pie
                                apple pie
```

You can specify an "output" tsv file for your results to be written to

Saves your results

tsv files can be opened in Excel, Numbers or Calc for easier viewing

✓

Try:

lexmapr small_simple.csv -o small_simple_output.tsv

small_simple_output.tsv was created in the directory

Open it up in Excel, Numbers or Calc for easy viewing of your output, separated into columns

A problem

Output:

```
Sample_Id
               Sample_Desc
                              Cleaned_Sample
                                             Matched_Components
                              chicken breast
small_simple1
               Chicken Breast
                                             ['breast:uberon_0000310']
small_simple2
               Baked Potato
                              baked potato
                                             []
small_simple3
              Canned Corn
                              canned corn
                                             ['frozen:pato_0001985']
small_simple4
               Frozen Yogurt
                              frozen yogurt
small_simple5
              Apple Pie
                              apple pie
```

Missing matches

Mapping samples against online ontologies

Unless told otherwise, LexMapr maps samples against a highly limited collection of pre-defined resources → missed matches

You should instead map samples against terms of your own choosing

You can do this by supplying LexMapr with a config file

Config files

When running LexMapr, use a config file that specifies the online ontology terms you want to map your samples against

e.g., we could create a config file that tells LexMapr to map against terms belonging to the Food ontology "Foodon", and use it whenever we run LexMapr on a collection of food samples

Config files can specify terms from:

Entire ontologies

Subsets of ontologies

Multiple ontologies

You re-use config files for multiple runs, or create new config files when you want to switch things up, but you can only provide one config file each time you run LexMapr

Config file format

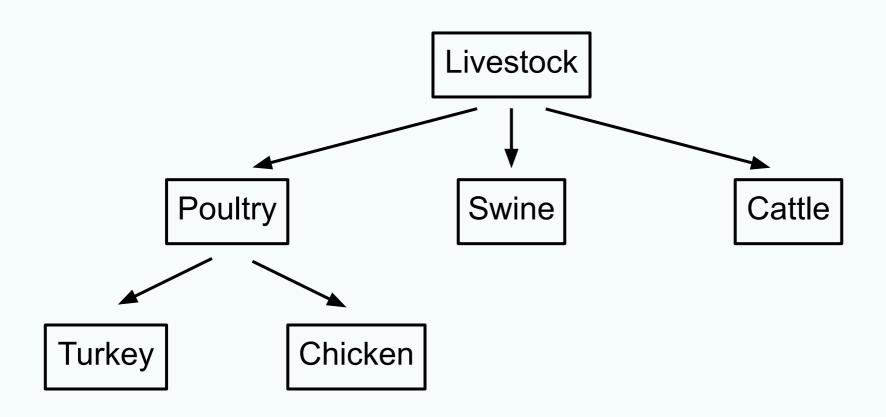
```
[
     {"ONTOLOGY_IRI_1":"ROOT_IRI_1"},
     {"ONTOLOGY_IRI_2":"ROOT_IRI_2"},
     ...,
```

Config file format

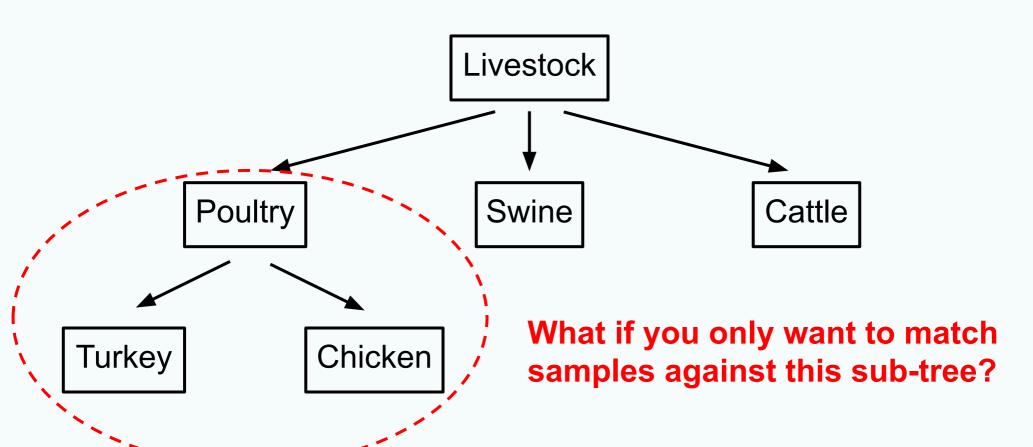
IRI of ontology you want to map your samples against

```
e.g., "http://purl.obolibrary.org/obo/foodon.owl"
```

Ontology refresher



Ontology refresher



Config file format

```
{"ONTOLOGY_IRI_1":"ROOT_IRI_1"},
{"ONTOLOGY_IRI_2":"ROOT_IRI_2"},
...,
```

IRI of the "top" of the sub-tree, within the specified ontology e.g., the IRI for "poultry or game bird" within FOODON:

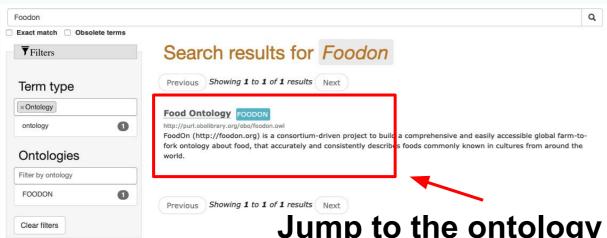
"http://purl.obolibrary.org/obo/FOODON 03411563"

We're going to map our small_simple.csv file against everything under "plant food product" in FOODON

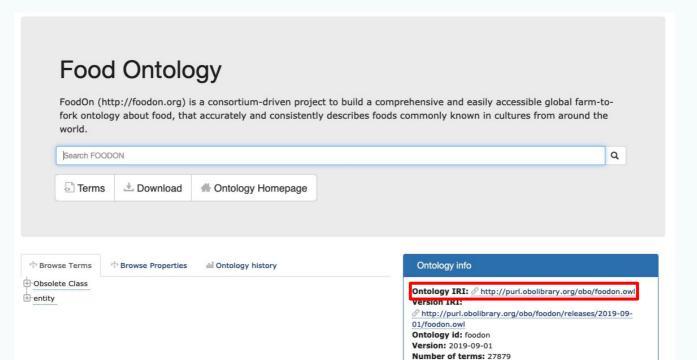
We need IRI values

Go to https://www.ebi.ac.uk/ols/ontologies

Search up "foodon"



Under the box titled "Ontology info" on the Foodon ontology page, note the Ontology IRI:

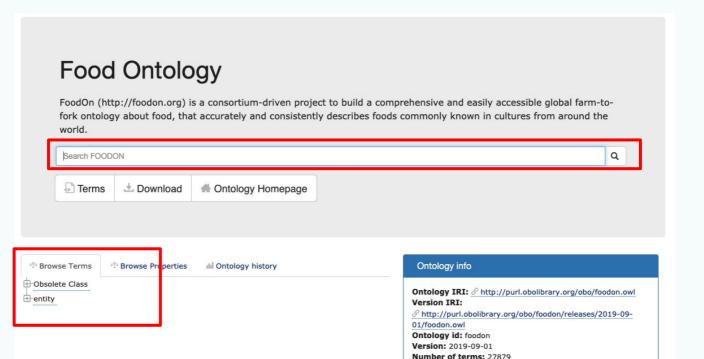


Under the box titled "Ontology info" on the Foodon ontology page, note the Ontology IRI:

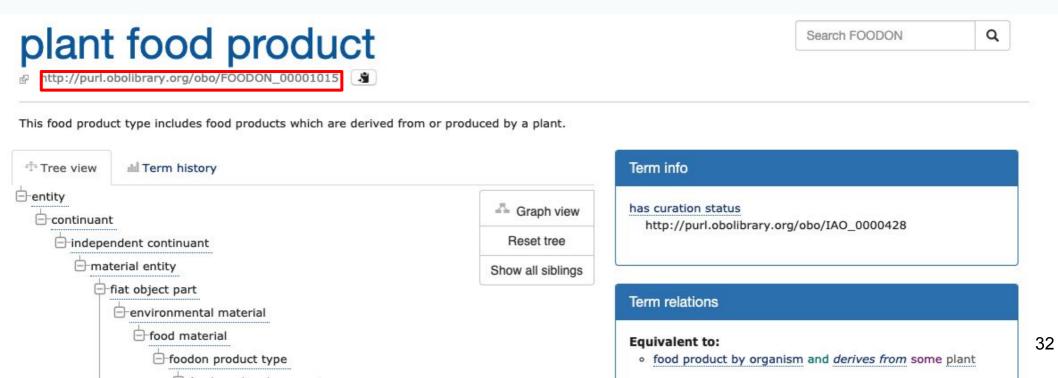
http://purl.obolibrary.org/obo/foodon.owl

This is your **ONTOLOGY_IRI**

You can then use the "browse terms" tab, or the search bar, to locate the OLS page for "plant food product"



The IRI for "plant food product" is under the title of its OLS page:



The IRI for "plant food product" is under the title of its OLS page:

http://purl.obolibrary.org/obo/FOODON_00001015

This is your **ROOT_IRI**

Open a text editor, and write the following:

```
[
{"http://purl.obolibrary.org/obo/foodon.owl": "http://purl.obolibrary.org/obo/F00D0N_00001015"}
]
```

Save the file as small_simple_config.json, in the same folder as small_simple.csv

Notice that we're using the IRI values we just searched for

So you now have a config file that tells LexMapr to map samples against everything under "plant food product" in Foodon

Note for macOs users:

TextEdit may not allow you to save JSON files

You can use another text editor, or google for an online JSON editor

Mapping samples against online ontologies

In terminal:

Navigate to the folder with small_simple.csv and small simple config.json

With your LexMapr conda environment activated, try:

```
lexmapr small_simple.csv -c small_simple_config.json -o small_simple_output.tsv
```

This may take a while, as lexmapr creates a lookup table for each config file (to speed up subsequent runs)

Mapping samples against online ontologies

Output:

```
Sample Id
               Sample Desc
                               Cleaned Sample
                                               Matched Components
               Chicken Breast
                               chicken breast
small simple1
                                               ['breast:uberon 0000310']
small simple2
               Baked Potato
                               baked potato
                                               ['potato (whole, baked):foodon_03302196']
               Canned Corn
                               canned corn
                                               ['corn (canned):foodon_03302665']
small simple3
small simple4
               Frozen Yogurt
                               frozen yogurt
                                               ['frozen:pato 0001985']
small_simple5
               Apple Pie
                               apple pie
                                               ['apple pie:foodon 00002475']
```

That's better!

But small simple1 and small simple4 could be better.

Fetch the IRI values for "meat food product" and "dairy food product" under Foodon the same way, and extend your config file:

```
[
{"http://purl.obolibrary.org/obo/foodon.owl": "http://purl.obolibrary.org/obo/F00D0N_00001015"},
{"http://purl.obolibrary.org/obo/foodon.owl": "http://purl.obolibrary.org/obo/F00D0N_00001006"},
{"http://purl.obolibrary.org/obo/foodon.owl": "http://purl.obolibrary.org/obo/F00D0N_00001256"}
]
```

Note the commas

Save the file

Your config file now tells LexMapr to map samples against everything under "plant food product", "meat food product" and "dairy food product" in Foodon

Mapping samples against online ontologies

Run:

```
lexmapr small_simple.csv -c small_simple_config.json -o small_simple_output.tsv --no-cache
```

The --no-cache flag is needed whenever you update a config file, so LexMapr can update the corresponding lookup table

Output:

```
Sample Id
                Sample Desc
                                Cleaned Sample
                                                Matched Components
                                chicken breast
small_simple1
                Chicken Breast
                                                ['chicken breast:foodon 00002703']
                Baked Potato
small_simple2
                                                ['potato (whole, baked):foodon_03302196']
                                baked potato
small_simple3
               Canned Corn
                                canned corn
                                                ['corn (canned):foodon_03302665']
small simple4
                                                ['frozen yogurt:foodon_03307445']
                Frozen Yogurt
                                frozen yogurt
                                                ['apple pie:foodon 00002475']
small simple5
               Apple Pie
                                apple pie
```

Perfect

Third-party classification schemes

Try:

```
lexmapr small simple.csv -c small simple config.json -o small simple output.tsv -b
```

The -b flag classifies all samples into broad categories:

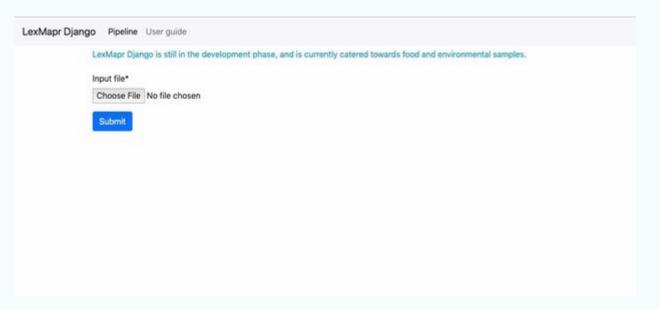
```
Sample Id
               Sample Desc
                              Cleaned Sample
                                             Matched Components
                                                                Third Party Classification
small_simple1
                                            ['chicken breast:foodon_00002703'] ['chicken']
               Chicken Breast chicken breast
small_simple2
                                             ['potato (whole, baked):foodon_03302196']
               Baked Potato
                              baked potato
                                                                                          ['root/underground (tubers)']
small_simple3
                                             ['corn (canned):foodon 03302665'] ['seeded vegetables (other)']
               Canned Corn
                              canned corn
small simple4
               Frozen Yogurt
                              frozen vogurt
                                             ['frozen yogurt:foodon 03307445'] ['dairy']
small simple5
                                             ['apple pie:foodon 00002475'] ['pome fruit']
               Apple Pie
                              apple pie
```

The categories were selected by a third-party, and follow their highly specific classification scheme, which is geared towards food

In the future, LexMapr will allow you to introduce classification schemes of your own

LexMapr Django

https://watson.bccdc.med.ubc.ca/lexmapr/



Django-powered web interface, that allows you to run LexMapr from your browser

LexMapr Django

Not as powerful as the command-line tool yet

Built-in config file specialized for food and environment samples

Cannot specify your own config file

Highly specific third-party classification scheme always used

Will become more powerful in the future