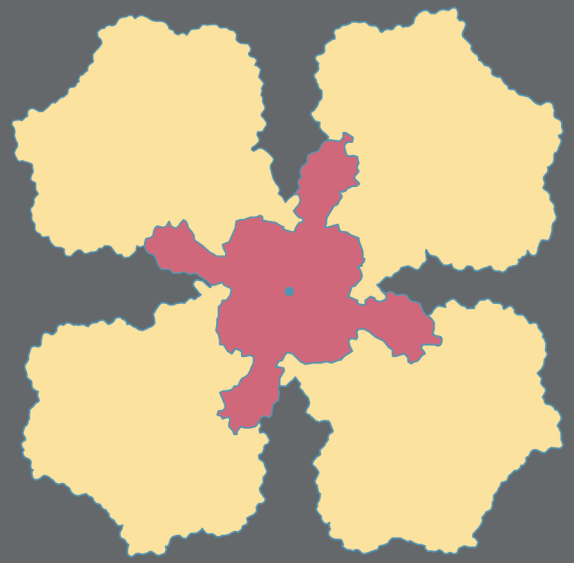
ComMap Manual

Brief Introduction

ComMap is a software for protein complexes structural mapping for cross-linking mass spectrometry (CXMS). The cross-linking peptides is identified from LC-MS/MS data by other identification software, such as pLink2, SpotLink et. al. ComMap can be used for both targeted protein complex analysis and large-scale protein-structure mapping analysis.



Icon explanation:
Complex structure of
Acetohydroxyacid Synthase

The configuration

Hardware configuration

CPU: Intel or AMD processor with 64-bit support; 2.3 GHz or faster processor with at least 8 cores is recommended

RAM: 16GB or higher is recommended

ROM: 5G or higher is recommended

OS: Windows

Other: Internet access for online mode

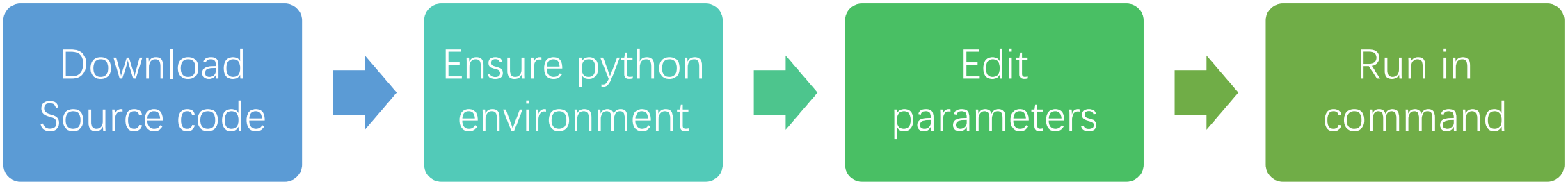
Runtime configuration

OS: Windows

Runtime: python 3.8

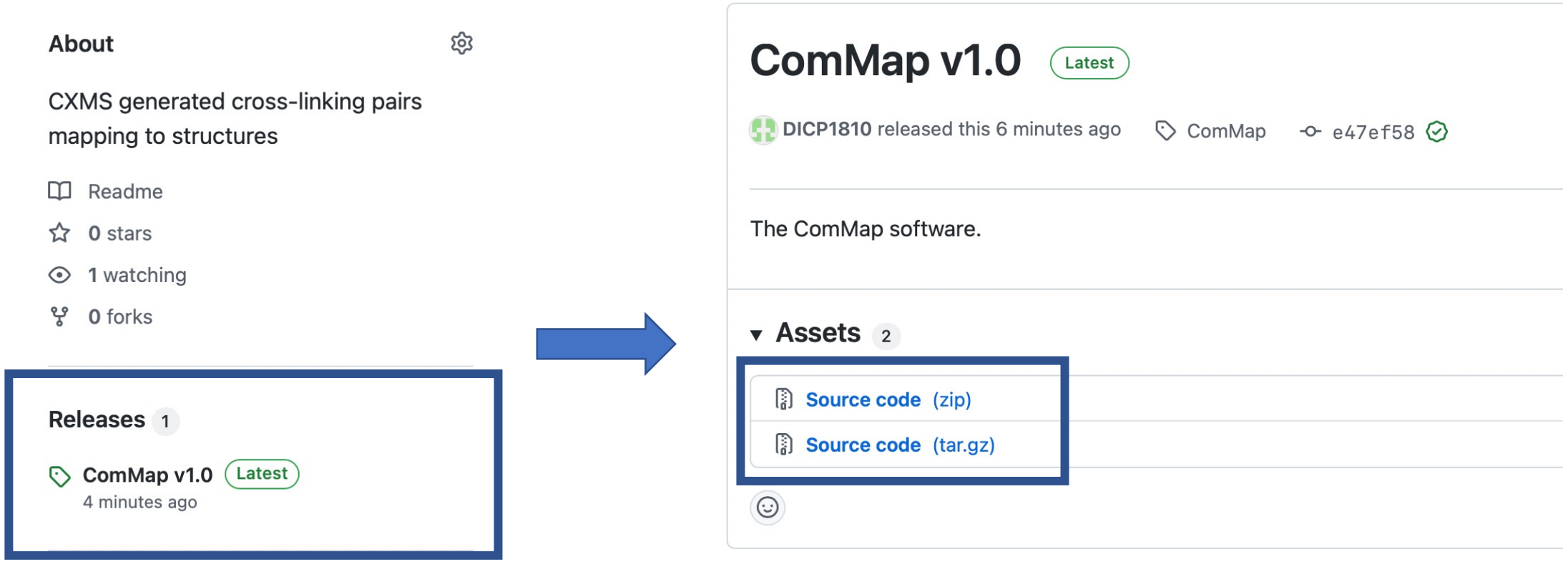
External runtime library: numpy, pandas

How to run ComMap?



Download
Source code

Download ComMap source code on GitHub.
Unzip the code in suitable folder. (C drive is not recommended.)



Ensure python environment

If you are new to python:

Please download and install Anaconda3-2021.05-Windows-x86_64.exe from Anaconda.

Else:

Please ensure python version 3.8 with installed numpy and pandas.


```
Python 3.8.8 (default, Apr 13 2021, 15:08:03) [MSC v.1916 64 bit (AMD64)]
Type 'copyright', 'credits' or 'license' for more information
IPython 7.22.0 -- An enhanced Interactive Python. Type '?' for help.

In [1]: import numpy

In [2]: numpy.__version__
Out[2]: '1.20.1'

In [3]: import pandas

In [4]: pandas.__version__
Out[4]: '1.2.4'
```

Edit parameters

Please copy Configuration.commap file from source code to your project folder.
Then open and edit it with any text editor.
(such as Windows Notepad or Visual Studio Code)

```
################
###   Basic  ###
################

# fasta file for identifying cross-links (absolute path)
A3_PATH_FASTA =

# calculation type (1 for on-line mode, 0 for off-line mode)
C60_CALCULATION_TYPE =

# (ONLY FOR OFF-LINE MODE) protein structure map (absolute path)
C60_TYPE0_PROTEIN_STRUCTURE_MAP =

# PDB structure files (default location: "Data" folder in the source code) (absolute path)
C60_PDB_STRUCTURE_PATH =

# result output folder (absolute path)
E1_PATH_EXPORT =

# input cross-linking result type (0 for generic TAB delimited format; 1 fpr SpotLink format; 2 for pLink2 cross-link format; 3 for pLink2 loop-link forma
C61_INPUT_LINK_RESULT_TYPE =

# input cross-linking result file (absolute path)
C61_INPUT_LINK_RESULT_FILE =

################
### Advanced ###
################


# (ONLY FOR ON-LINE MODE) max protein structure query times
C62_MAX_DOWNLOAD_TRY_TIME = 3

# the arm length of chosen cross-linker (in angstrom)
C65_LINKER_ARM_LENGTH = 11.4

```

Run in command

Run ComMap with command:
python COMMAP_LOCATION COMMAP_FILE_LOCATION

COMMAP_LOCATION
The location of ComMap.py file.
If you are unfamiliar with command operation, please filled with the absolute path of this file.

COMMAP_FILE_LOCATION
The location of .commap file modified in the previous step.
If you are unfamiliar with command operation, please filled with the absolute path of this file.

```
[ComMap] Copyright © 2021. All rights reserved.
2022-04-25 14:43:40.833374

[ComMap] ComMap whole workflow.
2022-04-25 14:43:40.839376
[ComMap] Start to read fasta file and cross-link result file.
2022-04-25 14:43:40.840374
[ComMap] Start to download Uniprot information.
2022-04-25 14:43:40.897374
[ComMap] End downloading Uniprot information.
2022-04-25 14:43:40.898374
[ComMap] Start to download Protein Data Bank information.
2022-04-25 14:43:40.898374
[ComMap] End downloading Protein Data Bank information.
2022-04-25 14:43:40.917373
[ComMap] Start sequence alignment.
2022-04-25 14:43:40.917373
[ComMap] End sequence alignment.
2022-04-25 14:43:49.399178
[ComMap] Start structure distance calculation.
2022-04-25 14:43:49.399178
[ComMap] End structure distance calculation.
2022-04-25 14:43:54.607179
[ComMap] Organize and output.
2022-04-25 14:43:54.607179
[ComMap] Start quality control.
2022-04-25 14:43:54.624180

[ComMap] Finished!
2022-04-25 14:43:54.631180
```

Q & A

- Which format of protein structure files does ComMap support?

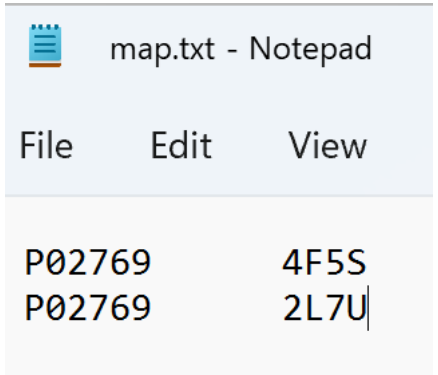
  mmCIF is a flexible and extensible tag-value format for representing macromolecular structural data. The set of mmCIF tags, which determine the classes of information present in a given mmCIF format file, are defined in an mmCIF dictionary. The structure of the dictionary is in turn defined by a ddl. The standard mmCIF dictionary - now stable since being ratified by the IUCr in 1997 - was pioneered by Paula M. Fitzgerald, Helen Berman, Phil Bourne, Brian McMahon, Keith Watenpaugh, and John Westbrook. However, work is still ongoing fine-tuning dictionary extensions. More information on mmCIF can be found at the mmCIF Resource pages at the RCSB.

- What is the difference between on-line mode and off-line mode?

  The online mode will obtain protein structure information from the Protein Data Bank database, and the offline mode will obtain protein structure information from the protein structure folder provided by the user.

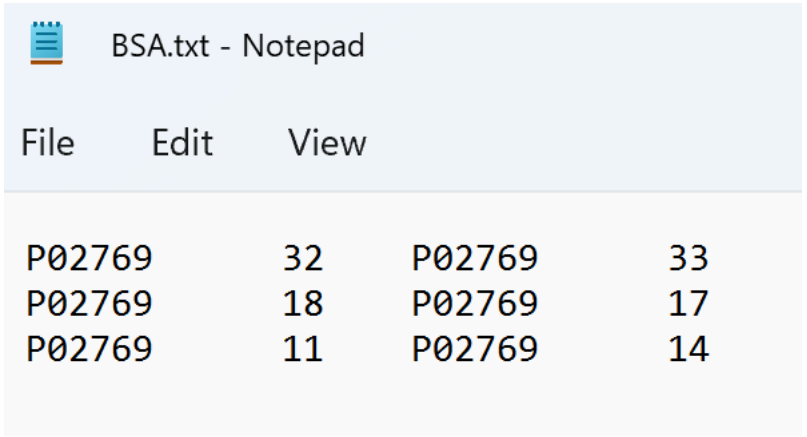
Q & A

- What is the protein structure map file looks like in the off-line mode?



The first column in the file stores the name of the protein, and the second column stores the name of the protein structure file. (Tab delimited)
Please make sure protein names match with the name in fasta file and the name of the protein structure file exists in the structure folder.

- What is the generic TAB delimited format looks like?



The first and third columns of the file store the names of interacting proteins, and the second and fourth columns represent the sites of interacting proteins. (Tab delimited)

Please make sure protein names match with the name in fasta file and the cross-linking sites match with sequence in the input fasta file.

Q & A

- What is the input SpotLink file looks like?

Please select the SpotLink-generated file with the name result_filtered.csv as input.

- What is the input pLink2 file looks like?

Please select the pLink2-generated file with the name filtered_cross-linked_spectra.csv or filtered_loop-linked_spectra.csv as input.

- What is the meaning of each parameter in the .commap file ?

The meaning of the parameters is explained in detail in the comments of the .commap file in the source code

- What do the files output by ComMap contain?

ComMap generated three main files as outputs, including a comprehensive file saved all PPI and structural distance information, and a categorized file of PPIs based on its structure, and a score file contained the ComMap score for PPI-structure. The categorized file offered pymol scripts for each protein structure for visualization.

Q & A

- ValueError: numpy.ndarray size changed, may indicate binary incompatibility. Expected 88 from C header, got 80 from PyObject

  Please try pip install --upgrade numpy or pip uninstall numpy pip install numpy

Thanks!