

Puerto Rico - IDeA Networks of Biomedical Research Excellence



## Python3 Part 3 – Crash Course in Python3 for Future STEM Coders

Judith S. Rodriguez-Martinez, MSc, PhD

Penn State University – University Park Campus jzr5814@psu.edu



**PennState** 

the Life Sciences









- The following material is the result of PR-INBRE research and curriculum development effort to provide a set of educational materials for research training and curriculum changes in biology programs across the island to support PR-INBRE efforts to establish a Community of Practice in Bioinformatics that offers a fruitful environment to increase computational and bioinformatics skills among traditional researchers and students (undergraduate and graduate) in the island. They have been developed as a part of the NIH funded project "Puerto Rico IDeA Network Biomedical Research Excellence (PRINBRE)" (Award Number 5P20GM103475).
- Unless otherwise specified, all the information contained within is Copyrighted © by University of Puerto Rico. Permission is granted for use, modify, and reproduce these materials for research and teaching purposes. A copy of the modified material should be sent to help@hpcf.upr.edu.
- Most recent versions of these presentations can be found at <a href="http://inbre.hpcf.upr.edu/">http://inbre.hpcf.upr.edu/</a>.







#### Competencies

June 2, 2025 - Record and write simple and common **Python scripts to deal with Bioinformatic needs for biological data analyses** using a Jupyter Notebook

June 3, 2025 — Exploit datatypes that can record objects, as well as, reason logical statements

Today – create your own dataset using Python





#### **Objectives**

- Create a dataset
- Open and Read data of different file formats using either a for loop or a Python Library
  - TXT File
  - CSV File
- Write to different file formats
  - TXT File
  - CSV File
- Import a Python Library to your code
- Using Panda Library, create a **Pandas DataFrame** with columns and **export the DataFrame as a CSV File**







#### **Objectives**

- Continue to use Google Colab as an environment to practice and learn common Python lines of code.
- Create a new file using the function open()
- Write information to a file using the write() function
- Using for Loops analyze lines of a file
  - **import** python libraries





#### **Target Audience**

• This training is addressed to beginners, highly motivated (eager to learn what is needed in order to be competitive without the tendency to self-limit when learning computational skills by saying that is difficult) wanting to become familiar with the Python programming language and become the Script Master of their bioinformatic analysis.







#### The importance of Python

- R is great; however, you'll eventually run into the Python language
- No matter your field, python will be a necessity (chemistry, biology, engineering, ecology, mathematics, etc)
- Knowing Python gives you an edge when job searching and navigating graduate research
- The majority bioinformatic tools are python-based and will lead you to understand under the hood code in order to successfully execute said program's purpose.





## Lesson 3.0.0 Create Files





Indicate with 'w' that you want to write to this file



[21] with open('first\_file.txt', 'w') as f:

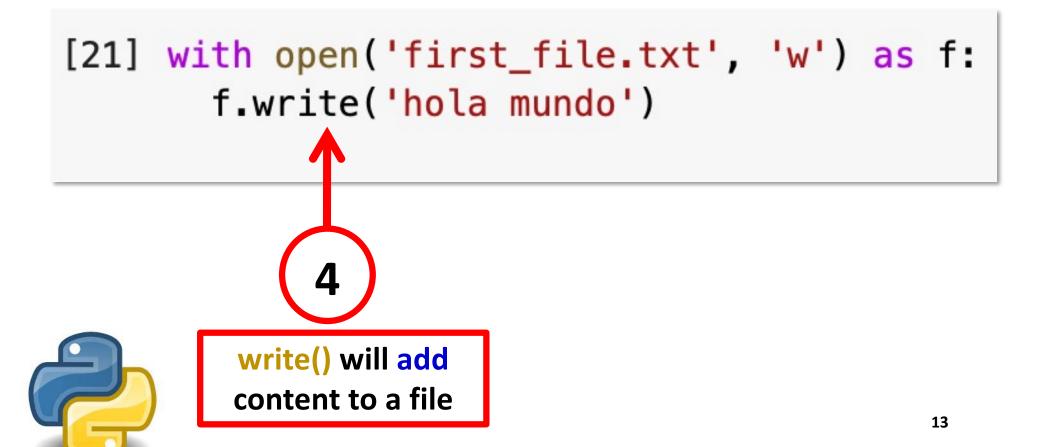


Assign a variable to this new file



```
[21] with open('first_file.txt', 'w') as f:
```





```
[21] with open('first_file.txt', 'w') as f:
    f.write('hola mundo')
```



Use write() to write 'hola mundo' to your new file called f

#### Success! Check out your first file!









# Exercise 3.0.0 Create a file with gene names found in a List



#### input is a list

```
[28] crtam_genes_list = ['CRTAM_HUMAN','CRTAM_MOUSE','CADM1_HUMAN']
    print(crtam_genes_list)
```



#### input is a list

```
[28] crtam_genes_list = ['CRTAM_HUMAN', 'CRTAM_MOUSE', 'CADM1_HUMAN']
    print(crtam_genes_list)

['CRTAM_HUMAN', 'CRTAM_MOUSE', 'CADM1_HUMAN']
```



#### output the following txt file





#### input is a list

```
[31] crtam_genes_list = ['CRTAM_HUMAN', 'CRTAM_MOUSE', 'CADM1_HUMAN']
    print(crtam_genes_list)

['CRTAM_HUMAN', 'CRTAM_MOUSE', 'CADM1_HUMAN']
```

#### **Answer**





#### input is a list

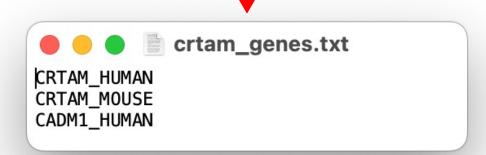
```
[31] crtam_genes_list = ['CRTAM_HUMAN', 'CRTAM_MOUSE', 'CADM1_HUMAN']
    print(crtam_genes_list)

['CRTAM_HUMAN', 'CRTAM_MOUSE', 'CADM1_HUMAN']
```

#### **Answer**

Tip: Use '\n' to indicate a new line





#### input is a list

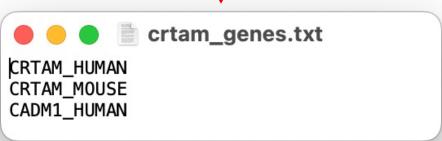
```
[31] crtam_genes_list = ['CRTAM_HUMAN', 'CRTAM_MOUSE', 'CADM1_HUMAN']
    print(crtam_genes_list)

['CRTAM_HUMAN', 'CRTAM_MOUSE', 'CADM1_HUMAN']

[32] with open('crtam_genes.txt', 'w') as f:
    for gene in crtam_genes_list:
        f.write(gene)
        f.write('\n')
```











## Lesson 3.1.0 Reading in your newly created files







## Lesson 3.1.1 Read in the lines of a file using a For Loop



```
crtam_genes_file = open('crtam_genes.txt','r')
Use open()
function
```



crtam\_genes\_file = open('crtam\_genes.txt','r')

Identify your
file of
interest





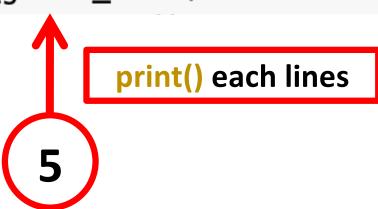




Use a for loop to loop through the lines in a file



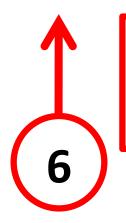
```
crtam_genes_file = open('crtam_genes.txt','r')
for crtam_genes_line in crtam_genes_file:
    print(crtam_genes_line)
```







```
crtam_genes_file = open('crtam_genes.txt','r')
for crtam_genes_line in crtam_genes_file:
    print(crtam_genes_line)
crtam_genes_file.close()
```



close() a file is
important to
prevent xyz



```
0
```

```
crtam_genes_file = open('crtam_genes.txt','r')
for crtam_genes_line in crtam_genes_file:
    print(crtam_genes_line)
crtam_genes_file.close()
```

CRTAM\_HUMAN

CRTAM\_MOUSE

CADM1\_HUMAN



## How many lines are being printed out?



```
crtam_genes_file = open('crtam_genes.txt','r')
for crtam_genes_line in crtam_genes_file:
    print(crtam_genes_line)
crtam_genes_file.close()
```

CRTAM\_HUMAN

CRTAM\_MOUSE

CADM1\_HUMAN



## How many lines are being printed out?

```
crtam_genes_file = open('crtam_genes.txt','r')
 for crtam_genes_line in crtam_genes_file:
   print(crtam_genes_line)
 crtam_genes_file.close()
OCRTAM_HUMAN
2 CRTAM_MOUSE
3
4 CADM1_HUMAN
```



#### Remove these blank lines using strip()

```
crtam_genes_file = open('crtam_genes.txt','r')
 for crtam_genes_line in crtam_genes_file:
   print(crtam_genes_line)
 crtam_genes_file.close()
OCRTAM_HUMAN
2 CRTAM_MOUSE
3
4 CADM1_HUMAN
```



#### Remove these blank lines using strip()







# Lesson 3.1.2 Read in the lines of a file using a While Loop



#### Read in your file using a while loop

crtam\_genes\_file = open('crtam\_genes.txt','r')

Use open()
function



#### Read in your file using a while loop

crtam\_genes\_file = open('crtam\_genes.txt','r')
crtam\_genes\_lines = crtam\_genes\_file.readline()

## Using readline() function will allow you to while loop the lines of a file



crtam\_genes\_file = open('crtam\_genes.txt','r')
crtam\_genes\_lines = crtam\_genes\_file.readline()
while crtam\_genes\_lines:

Perform while loop through lines of this file

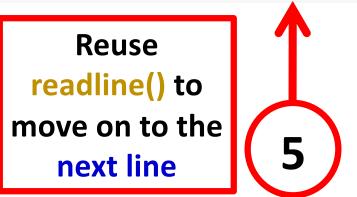




```
crtam_genes_file = open('crtam_genes.txt','r')
crtam_genes_lines = crtam_genes_file.readline()
while crtam_genes_lines:
  print(<u>crtam_genes_lines</u>.strip('\n'))
              Strip and print
                 each line
```



crtam\_genes\_file = open('crtam\_genes.txt','r')
crtam\_genes\_lines = crtam\_genes\_file.readline()
while crtam\_genes\_lines:
 print(crtam\_genes\_lines.strip('\n'))
 crtam\_genes\_lines = crtam\_genes\_file.readline()





```
crtam_genes_file = open('crtam_genes.txt','r')
crtam_genes_lines = crtam_genes_file.readline()
while crtam_genes_lines:
    print(crtam_genes_lines.strip('\n'))
    crtam_genes_lines = crtam_genes_file.readline()
crtam_genes_file.close()
```





```
crtam_genes_file = open('crtam_genes.txt','r')
crtam_genes_lines = crtam_genes_file.readline()
while crtam_genes_lines:
    print(crtam_genes_lines.strip('\n'))
    crtam_genes_lines = crtam_genes_file.readline()
crtam_genes_file.close()
OCRTAM_HUMAN
1CRTAM_MOUSE
2CADM1_HUMAN
```







## Lesson 3.2.0 Manipulate files the Panda way







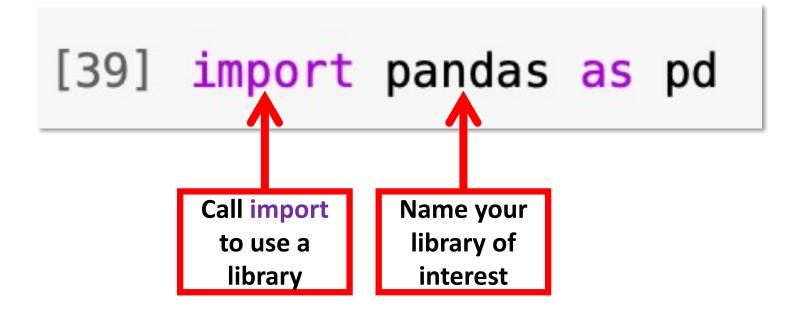
# Lesson 3.2.1 Import the Panda Library



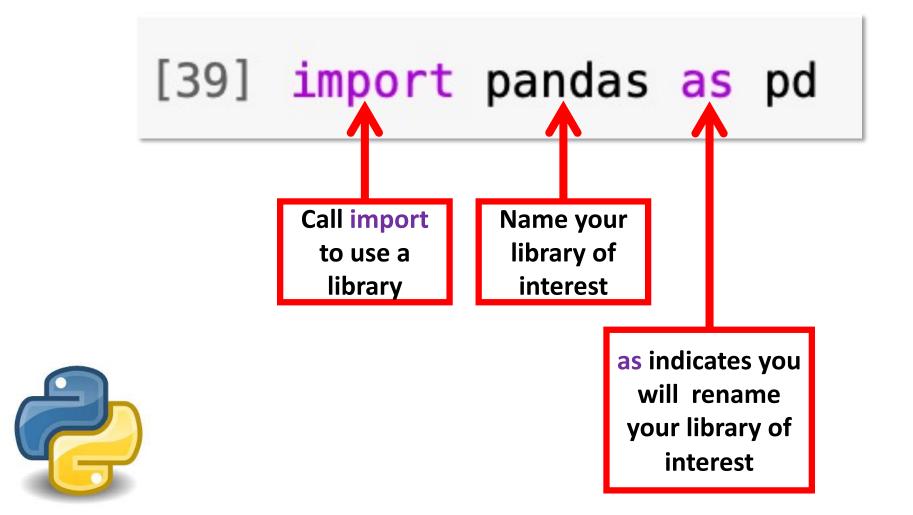
```
[39] import pandas as pd

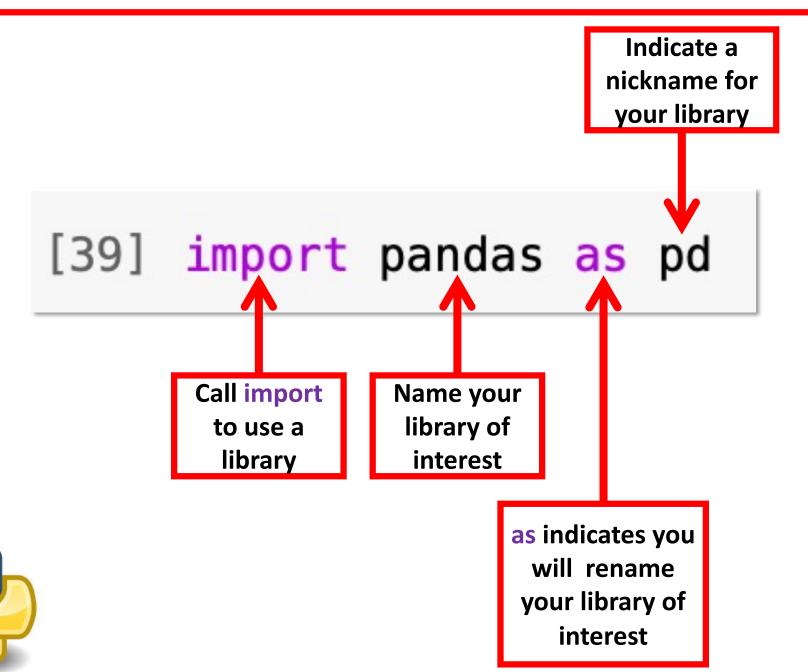
Call import to use a library
```















# Lesson 3.2.2 Read in a CSV file using Panda Library







# Lesson 3.2.2a Reading in a CSV file with a header using Panda Library





gene, length CRTAM\_HUMAN, 393 CRTAM\_MOUSE, 781 CADM1\_HUMAN, 442



```
crtam_with_header.csv

gene, length
CRTAM_HUMAN, 393
CRTAM_MOUSE, 781
CADM1_HUMAN, 442
```

```
[66] pd.read_csv('crtam_with_header.csv',header=0,delimiter=',')
```



```
crtam_with_header.csv

gene, length
CRTAM_HUMAN, 393
CRTAM_MOUSE, 781
CADM1_HUMAN, 442
```

```
[66] pd.read_csv('crtam_with_header.csv',header=0,delimiter=',')
```

Call pandas library by its nickname



```
crtam_with_header.csv

gene, length
CRTAM_HUMAN, 393
CRTAM_MOUSE, 781
CADM1_HUMAN, 442
```



```
gene, length
CRTAM_HUMAN, 393
CRTAM_MOUSE, 781
CADM1_HUMAN, 442
```

```
[66] pd.read_csv('crtam_with_header.csv',header=0,delimiter=',')
```

Name your file of interest



```
gene, length
CRTAM_HUMAN, 393
CRTAM_MOUSE, 781
CADM1_HUMAN, 442
```

```
[66] pd.read_csv('crtam_with_header.csv',header=0,delimiter=',')
```

Indicate that there is a header exist

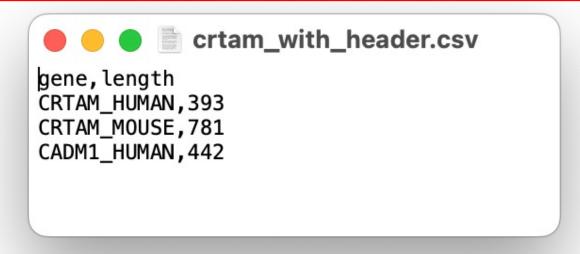


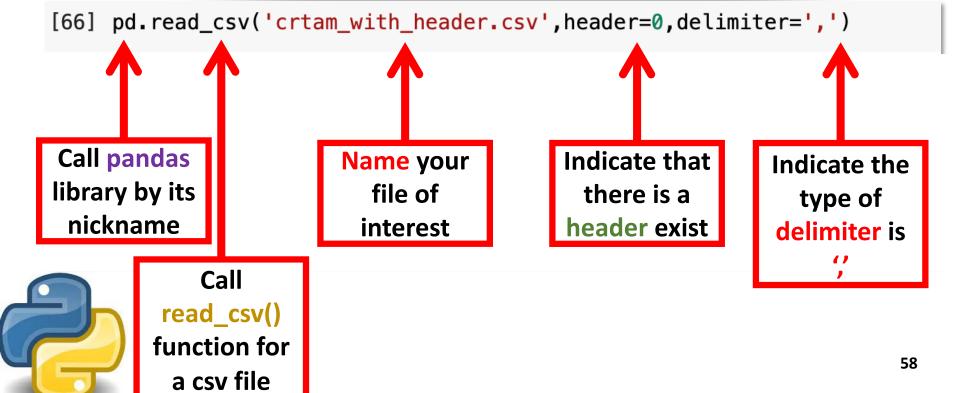
```
gene, ength
CRTAM_HUMAN, 893
CRTAM_MOUSE, 781
CADM1_HUMAN, 142
```

```
[66] pd.read_csv('crtam_with_header.csv',header=0,delimiter=',')
```

Indicate the type of delimiter is







```
crtam_with_header.csv

gene,length
CRTAM_HUMAN,393
CRTAM_MOUSE,781
CADM1_HUMAN,442
```

```
[66] pd.read_csv('crtam_with_header.csv',header=0,delimiter=',')

gene length header

0 CRTAM_HUMAN 393

1 CRTAM_MOUSE 781

2 CADM1_HUMAN 442
```

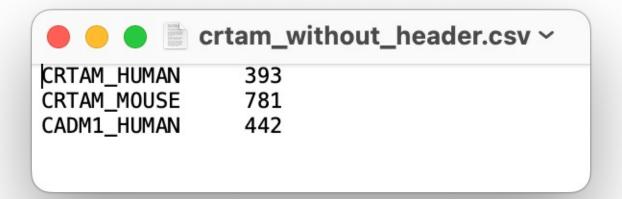






# Lesson 3.2.2b Reading in a CSV file with no header using Panda Library



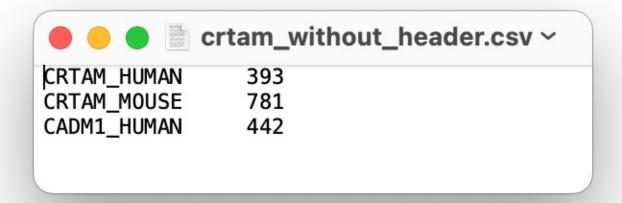


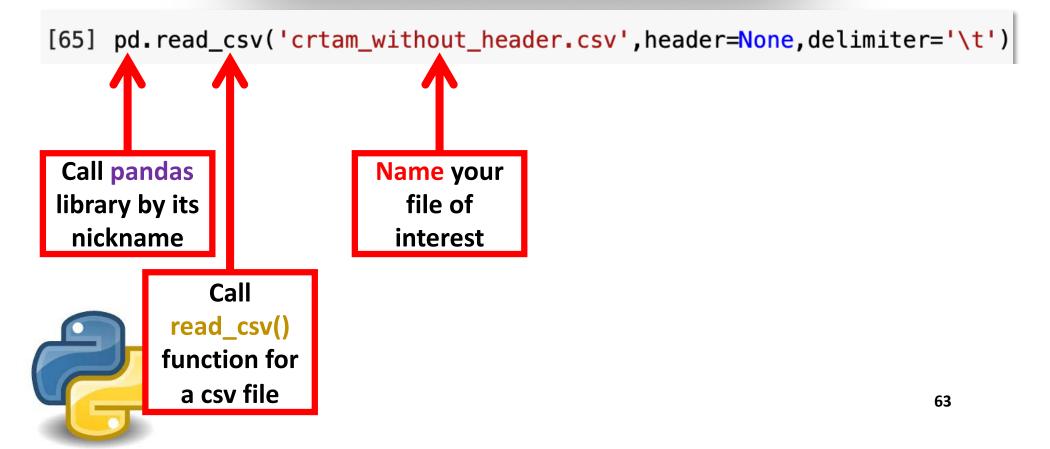


```
CRTAM_HUMAN 393
CRTAM_MOUSE 781
CADM1_HUMAN 442
```

```
[65] pd.read_csv('crtam_without_header.csv',header=None,delimiter='\t')
```







```
CRTAM_HUMAN 393
CRTAM_MOUSE 781
CADM1_HUMAN 442
```

```
[65] pd.read_csv('crtam_without_header.csv',header=None,delimiter='\t')
```

Indicate that there is no header exist

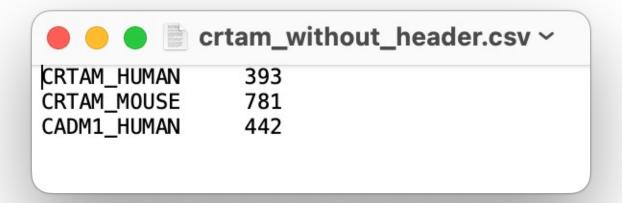


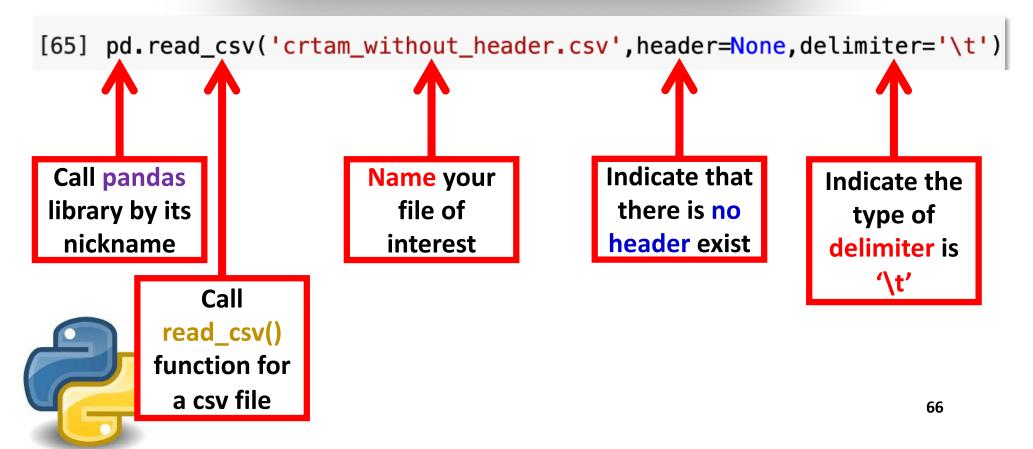
```
CRTAM_HUMAN 393
CRTAM_MOUSE 781
CADM1_HUMAN 442
```

```
[65] pd.read_csv('crtam_without_header.csv',header=None,delimiter='\t')
```

```
Indicate the type of delimiter is '\t'
```







```
CRTAM_HUMAN 393
CRTAM_MOUSE 781
CADM1_HUMAN 442
```

```
pd.read_csv('crtam_without_header.csv',header=None,delimiter='\t')

0 1 header

0 CRTAM_HUMAN 393

1 CRTAM_MOUSE 781

2 CADM1_HUMAN 442
```







### Lesson 3.2.3 Create a DataFrame and export a new CSV file using Panda Library



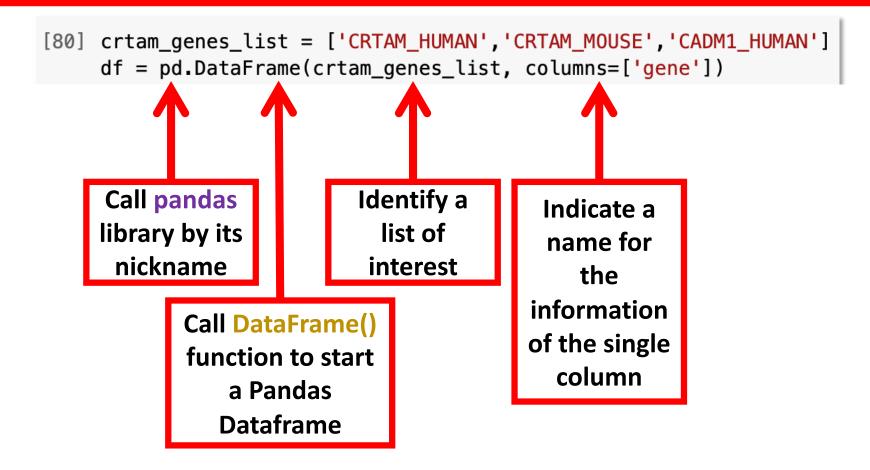


# Lesson 3.2.3a Create a Panda DataFrame from a single List



[80] crtam\_genes\_list = ['CRTAM\_HUMAN','CRTAM\_MOUSE','CADM1\_HUMAN']









```
[80] crtam_genes_list = ['CRTAM_HUMAN','CRTAM_MOUSE','CADM1_HUMAN']
    df = pd.DataFrame(crtam_genes_list, columns=['gene'])
    df
                gene
       CRTAM_HUMAN
       CRTAM_MOUSE
       CADM1_HUMAN
   index
```







# Lesson 3.2.3b Create a Panda DataFrame from multiple Lists



```
[81] crtam_human_list = ['CRTAM_HUMAN',393,'human']
    crtam_mouse_list = ['CRTAM_MOUSE',781,'mouse']
    cadm1_human_list = ['CADM1_HUMAN',442,'human']
```



Call pandas library by its nickname

Call DataFrame()
function to start
a Pandas
Dataframe



**List of Lists** 







```
[81] crtam_human_list = ['CRTAM_HUMAN',393,'human']
    crtam_mouse_list = ['CRTAM_MOUSE',781,'mouse']
    cadm1 human list = ['CADM1 HUMAN',442,'human']
    df = pd.DataFrame([crtam_human_list,crtam_mouse_list,cadm1_human_list],
                       columns=['gene','length','organisms'])
    df
                      length organisms
        CRTAM HUMAN
                         393
                                  human
        CRTAM MOUSE
                         781
                                  mouse
        CADM1_HUMAN
                         442
                                  human
```





```
[81] crtam_human_list = ['CRTAM_HUMAN',393,'human']
    crtam mouse list = ['CRTAM MOUSE',781,'mouse']
    cadm1 human list = ['CADM1 HUMAN',442,'human']
    df = pd.DataFrame([crtam human list,crtam mouse list,cadm1 human list],
                      columns=['gene','length','organisms'])
    df
                                                 column names
                gene length organisms
       CRTAM_HUMAN
                         393
                                  human
        CRTAM MOUSE
                         781
                                  mouse
     2 CADM1_HUMAN
                         442
                                  human
```



```
[81] crtam_human_list = ['CRTAM_HUMAN',393,'human']
    crtam mouse list = ['CRTAM MOUSE',781,'mouse']
    cadm1 human list = ['CADM1 HUMAN',442,'human']
    df = pd.DataFrame([crtam human list,crtam mouse list,cadm1 human list],
                      columns=['gene','length','organisms'])
    df
                      length organisms
                                                 crtam_human_list
        CRTAM_HUMAN
                         393
                                  human
        CRTAM MOUSE
                         781
                                  mouse
     2 CADM1_HUMAN
                         442
                                  human
```



```
[81] crtam_human_list = ['CRTAM_HUMAN',393,'human']
    crtam mouse list = ['CRTAM MOUSE',781,'mouse']
    cadm1 human list = ['CADM1 HUMAN',442,'human']
    df = pd.DataFrame([crtam human list,crtam mouse list,cadm1 human list],
                      columns=['gene','length','organisms'])
    df
                      length organisms
        CRTAM HUMAN
                         393
                                  human
        CRTAM_MOUSE
                                                  crtam_mouse_list
                         781
                                  mouse
       CADM1_HUMAN
                         442
                                  human
```



```
[81] crtam_human_list = ['CRTAM_HUMAN',393,'human']
    crtam mouse list = ['CRTAM MOUSE',781,'mouse']
    cadm1 human list = ['CADM1 HUMAN',442,'human']
    df = pd.DataFrame([crtam human list,crtam mouse list,cadm1 human list],
                      columns=['gene','length','organisms'])
    df
                      length organisms
       CRTAM_HUMAN
                         393
                                  human
        CRTAM MOUSE
                         781
                                  mouse
                                                 cadm1_human_list
       CADM1_HUMAN
                         442
                                  human
```







## Lesson 3.2.3c Create a Pandas DataFrame from a Nested Dictionary























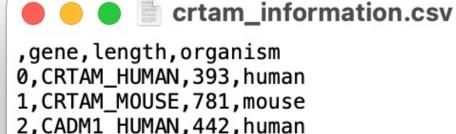


## Lesson 3.2.4 Export a Panda DataFrame as a CSV File



|   |             | •   | •     |
|---|-------------|-----|-------|
| 0 | CRTAM_HUMAN | 393 | human |
| 1 | CRTAM_MOUSE | 781 | mouse |
| 2 | CADM1_HUMAN | 442 | human |

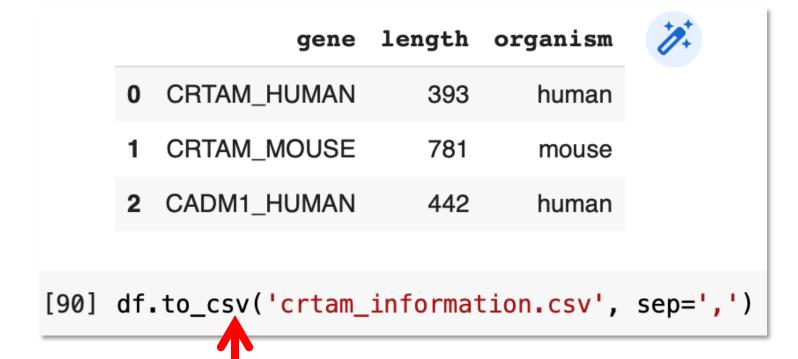






|  |           |      | •     | gene | len | gth | org | anism | 7 |  |
|--|-----------|------|-------|------|-----|-----|-----|-------|---|--|
|  | 0         | CRTA | M_HU  | MAN  |     | 393 |     | human | 1 |  |
|  | 1         | CRTA | AM_MC | USE  |     | 781 |     | mouse | • |  |
|  | 2         | CADI | M1_HU | MAN  |     | 442 |     | human | 1 |  |
|  |           |      |       |      |     |     |     |       |   |  |
| [90] df.to_csv('crtam_information.csv', sep=',') |           |      |       |      |     |     |     |       |   |  |
|  |           |      |       |      |     |     |     |       |   |  |
| Call variable                                    |           |      |       |      |     |     |     |       |   |  |
| of   | of your   |      |       |      |     |     |     |       |   |  |
| dat  | dataframe |      |       |      |     |     |     |       |   |  |







Call to\_csv()
function to start
a Pandas
Dataframe

|      |     | gene                          | length   | organism  | <b>**</b> |
|------|-----|-------------------------------|----------|-----------|-----------|
|      | 0   | CRTAM_HUMAN                   | 393      | human     |           |
|      | 1   | CRTAM_MOUSE                   | 781      | mouse     |           |
|      | 2   | CADM1_HUMAN                   | 442      | human     |           |
|      |     |                               |          |           |           |
| [90] | df. | to_csv(' <mark>crtam</mark> _ | informat | ion.csv', | sep=',')  |
|      |     |                               |          |           |           |

Name your file of interest

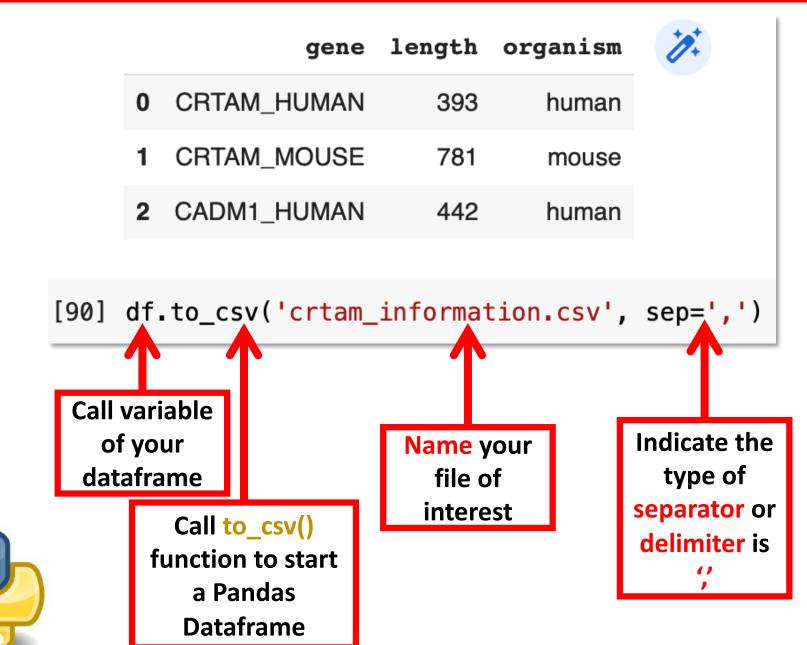


|   | gene        | length | organism |
|---|-------------|--------|----------|
| 0 | CRTAM_HUMAN | 393    | human    |
| 1 | CRTAM_MOUSE | 781    | mouse    |
| 2 | CADM1_HUMAN | 442    | human    |

[90] df.to\_csv('crtam\_information.csv', sep=',')

Indicate the type of separator or delimiter is





#### Check out your new CSV file!



,gene,length,organism
0,CRTAM\_HUMAN,393,human
1,CRTAM\_MOUSE,781,mouse
2,CADM1\_HUMAN,442,human













## Proficiency assessment Show off your new skills!

- 1. Read in the Fasta File called crtam.faa
- 2. Choose at least 3 of the following options below to create a dataframe with your columns of interest.
  - Gene\_names
  - Length in amino acid
  - Length in it's DNA sequence
  - Total RSNNEETS
  - Total KAH
  - Total PGLRLRLLL
- 3. Export a file to import into Excel

