



University of Puerto Rico

Puerto Rico - IDeA Networks of Biomedical Research Excellence



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



Ph.D. Candidate
Penn State University – University Park Campus
jzr5814@psu.edu











- 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).
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Competencies

June 2, 2024 - Record and write simple and common **Python scripts to deal with Bioinformatic needs for biological data analyses** using a Jupyter Notebook

June 3, 2024 — 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



file

Identify the name of your new file

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



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

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

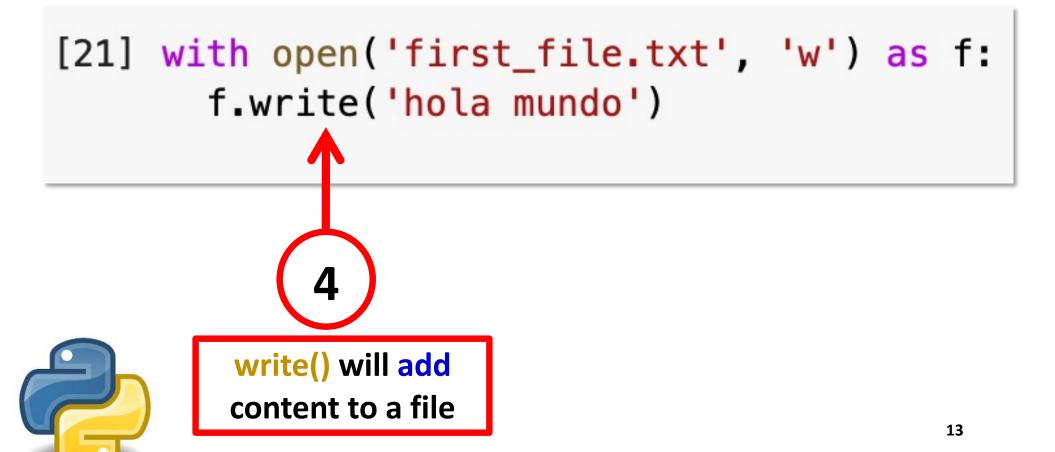


Assign a variable to this new file

3

```
[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

14

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)
```



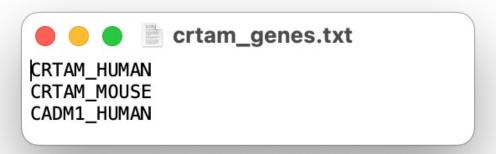
input is a list

```
[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





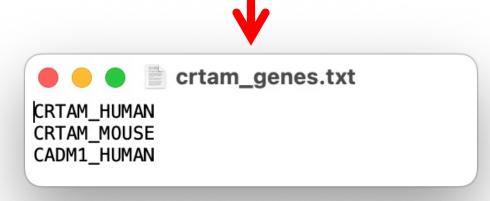
input is a list

```
[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

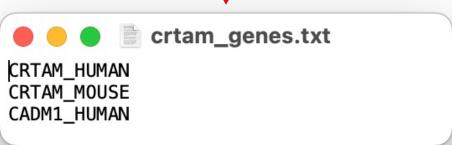
```
[31] crtam_genes_list = ['CRTAM_HUMAN', 'CRTAM_MOUSE', 'CADM1_HUMAN']
    print(crtam_genes_list)

['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



crtam_genes_file = open('crtam_genes.txt','r')

Indicate that you want to read the file

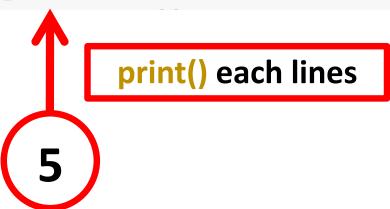


```
crtam_genes_file = open('crtam_genes.txt','r')
for crtam_genes_line in crtam_genes_file:

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

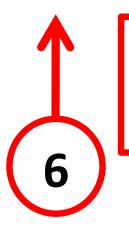


crtam_genes_file = open('crtam_genes.txt','r')
for crtam_genes_line in crtam_genes_file:
 print(crtam_genes_line)





```
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



```
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
2CRTAM MOUSE
3
4CADM1_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
2CRTAM 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





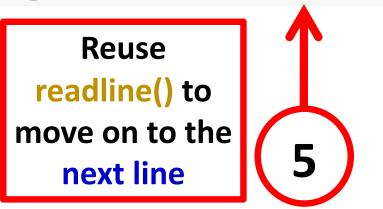
```
crtam_genes_file = open('crtam_genes.txt','r')
crtam_genes_lines = crtam_genes_file.readline()
while crtam_genes_lines:
  print(crtam_genes_lines.strip('\n'))
```

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





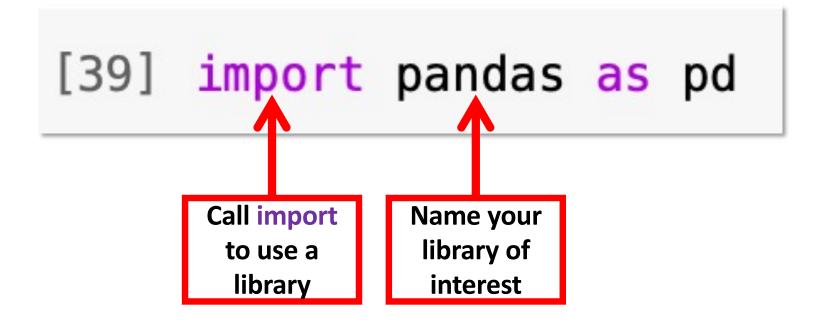


Lesson 3.2.1 Import the Panda Library

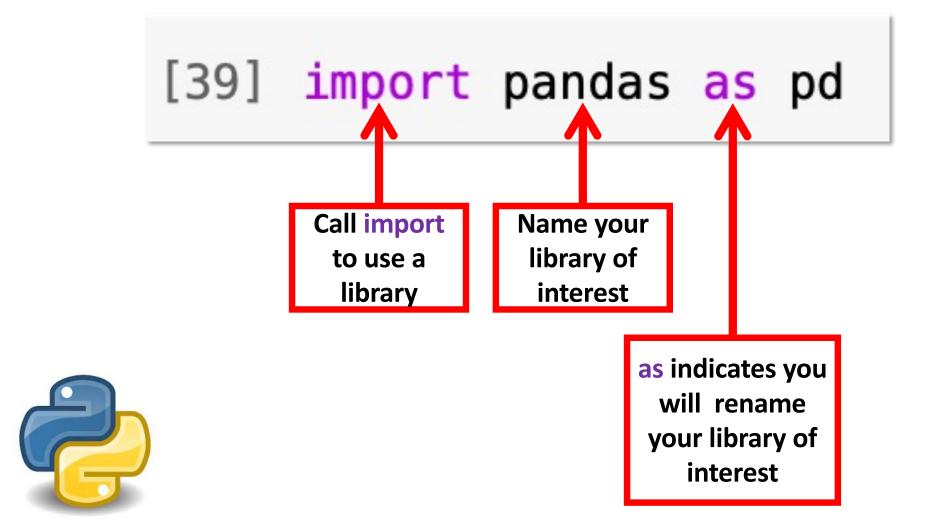


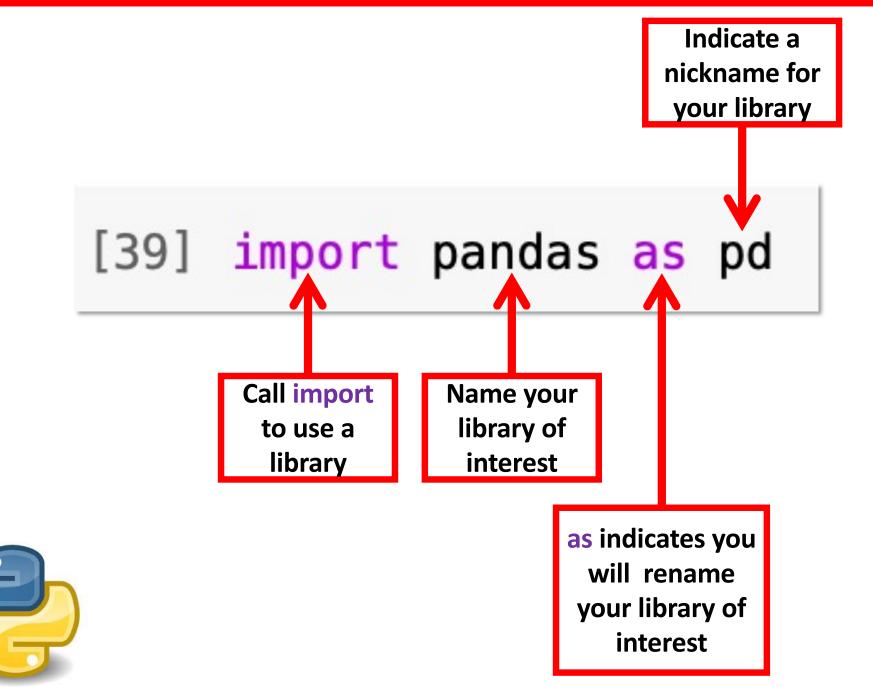
















Lesson 3.2.2 Read in a CSV file using Panda Library

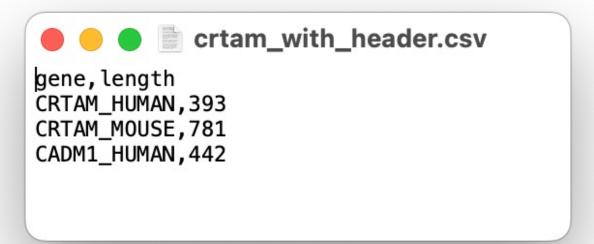






Lesson 3.2.2a Reading in a CSV file with a header using Panda Library







```
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
```



```
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=',')

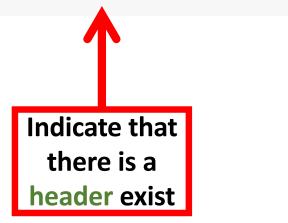
Name your
file of
```

interest



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

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



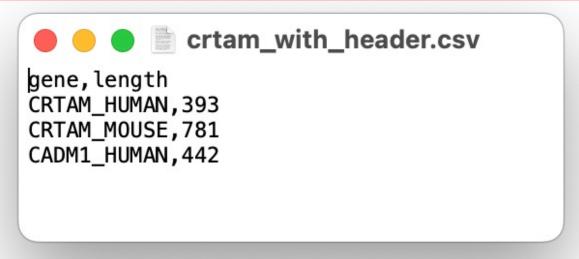


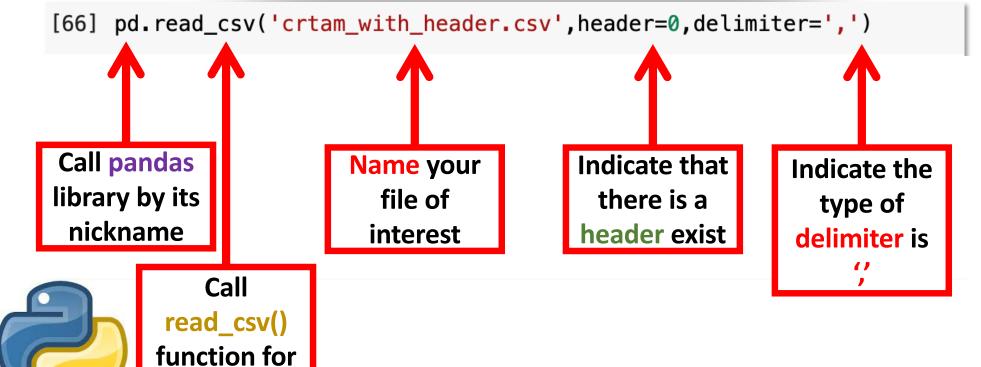
```
gene, ength
CRTAM_HUMAN, 893
CRTAM_MOUSE, 781
CADM1_HUMAN, 142
```

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

```
Indicate the type of delimiter is
```







a csv file

```
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
```

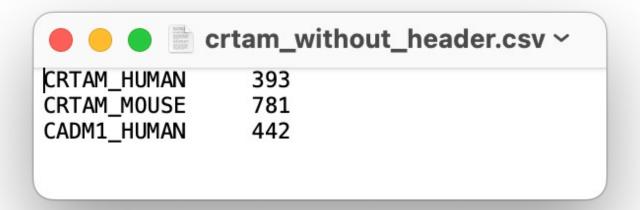






Lesson 3.2.2b Reading in a CSV file with no header using Panda Library



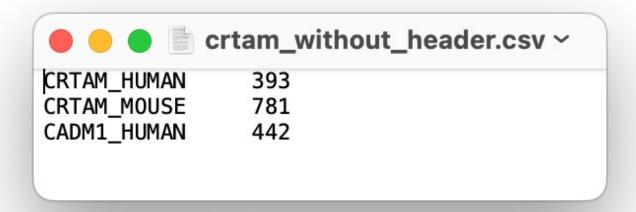




```
CRTAM_HUMAN 393
CRTAM_MOUSE 781
CADM1_HUMAN 442
```

```
[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

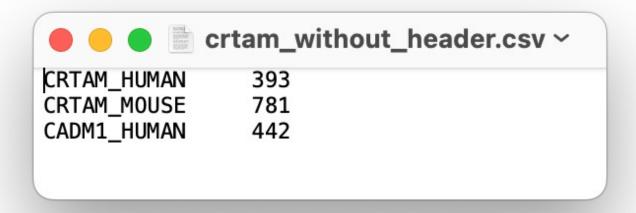


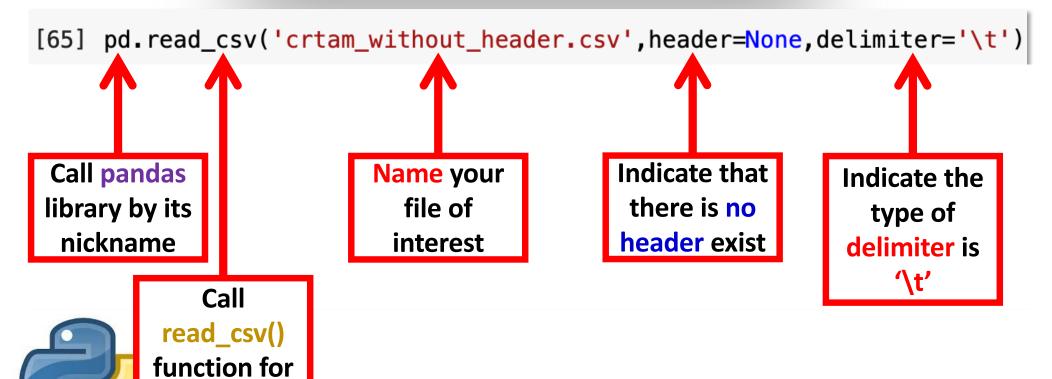
```
CRTAM_HUMAN 393
CRTAM_MOUSE 781
CADM1_HUMAN 442
```

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

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







a csv file

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

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

```
0 1 header
```

- O 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



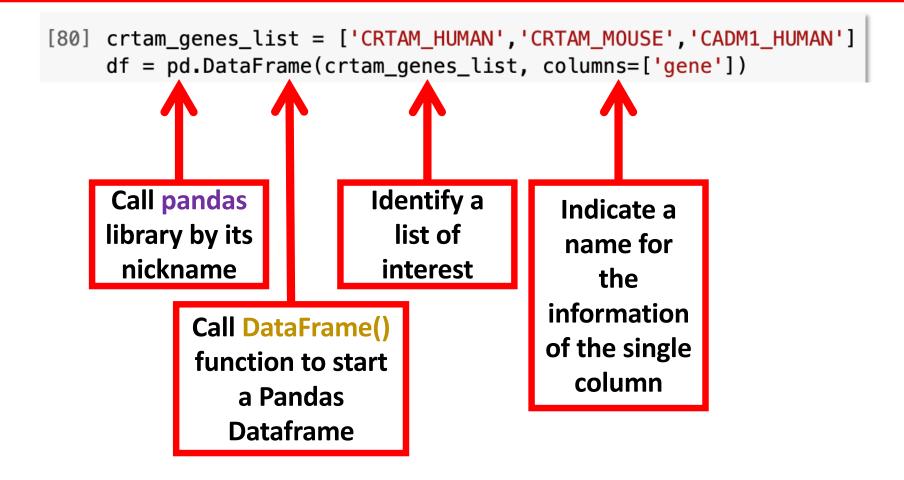


Lesson 3.2.3a Create a Panda DataFrame from a single List



```
[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







	gene	length	organisms
0	CRTAM_HUMAN	393	human
1	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
                                                 column names
                      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_list
        CRTAM MOUSE
                         781
                                  mouse
     2 CADM1 HUMAN
                                  human
                         442
```



```
[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



```
[89] crtam_dictionary = {'CRTAM_HUMAN':{'length':393,'organism':'human'},
                         'CRTAM_MOUSE':{'length':781,'organism':'mouse'},
                         'CADM1_HUMAN':{'length':442,'organism':'human'}}
    df = pd.DataFrame(crtam_dictionary).T.reset_index().rename(columns={'index':'gene'})
    df
```

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









```
crtam_information.csv
,gene,length,organism
0, CRTAM_HUMAN, 393, human
1, CRTAM_MOUSE, 781, mouse
2,CADM1_HUMAN,442,human
```

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

```
[90] df.to_csv('crtam_information.csv', sep=',')
```

Call variable of your dataframe



	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=',')



Call to_csv()
function to start
a Pandas
Dataframe

0 CRTAM_HUMAN 393 human1 CRTAM_MOUSE 781 mouse
1 CRTAM MOUSE 781 mouse
2 CADM1_HUMAN 442 human

[90] df.to_csv('crtam_information.csv', sep=',')

Name your file of interest

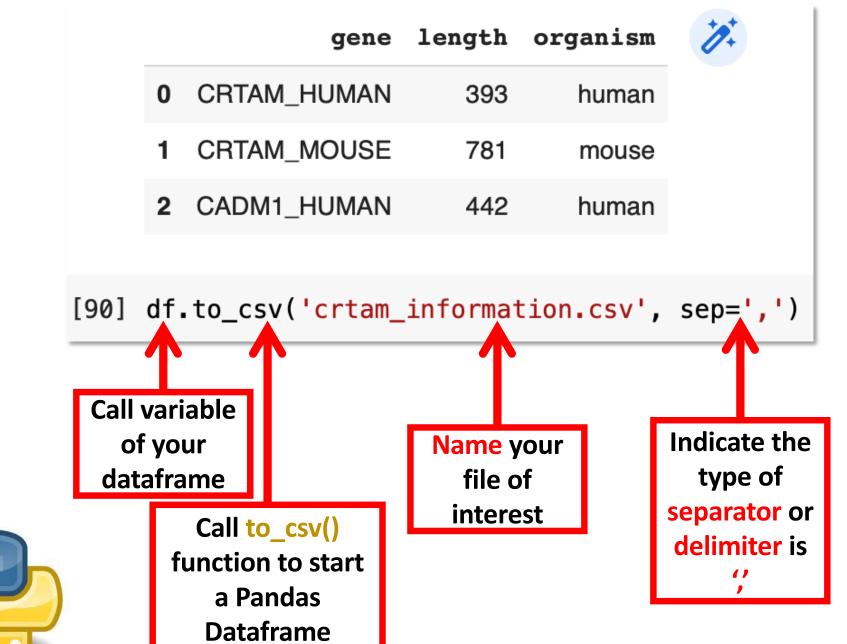


	gene	length	organism
0	CRTAM_HUMAN	393	human
1	CRTAM_MOUSE	781	mouse
2	CADM1_HUMAN	442	human

[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 PGLRLRLLLL
- 3. Export a file to import into Excel

