

#### Setting up the computational environment

Module 2B - Centre for Drug Discovery, University of Buea



### What is GitHub primarily used for?

<u> </u>	0	0	0	
	Video hosting	Social networking	Code hosting and version	
			control	



# How does GitHub help in open source projects?

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It sells the open-source software.	It offers a platform for collaborative development	It provides financial support for all open-source projects.

#### What is your GitHub user name?



## In what order will you start your data science journey?

1st Write my first python notebook with Google Colab
 2nd Create a GitHub account
 3rd Install Visual Studio Code
 4th Install Conda
 5th Install Docker



## Which system is more convenient for data science

```
1st Linux (Ubuntu)

2nd MacOSX

3rd Windows
```

### Which software tool scares you the most?



#### What does API stand for?

Ο	0	0	0	
Application	Applied	Advanced	Alien	
Programming	Protocol	Performance	Pancake	
Interface	Input	Index	Invasion	



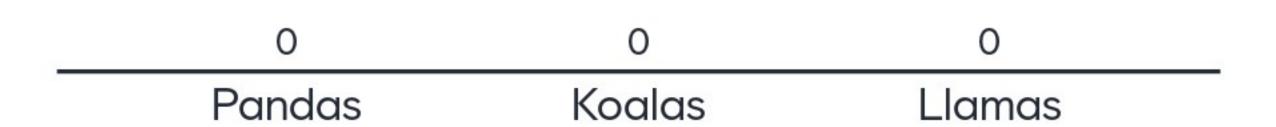
#### Command line interface is useful for...

	С	Ο		0		0	
Acces	ss and	Send API	Aut	tomate	Ві	rowse	
ope	erate	queries	rep	etitive	fc	olders	
ren	note		t	asks	cor	ntaining	
comp	outers				pie	ctures	

#### Why do we prefer Python?

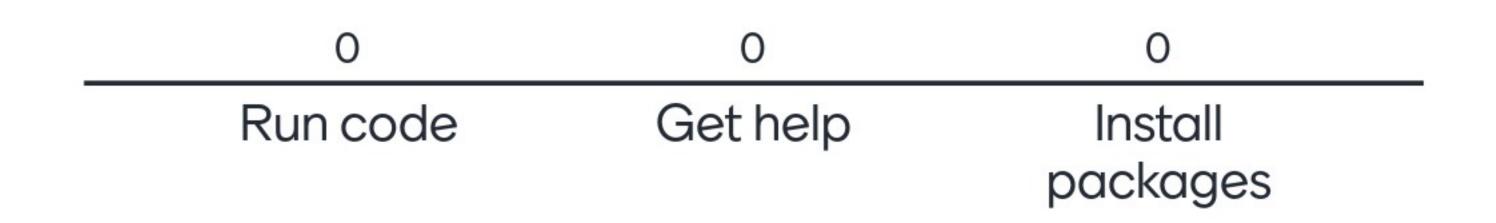


### What Python package will we use to deal with data tables?





### In Python, the 'pip' is used to...



### Which Python packages are more relevant to your research?

```
1st RDKit
```

2nd Pandas

3rd Matplotlib

4th Seaborn

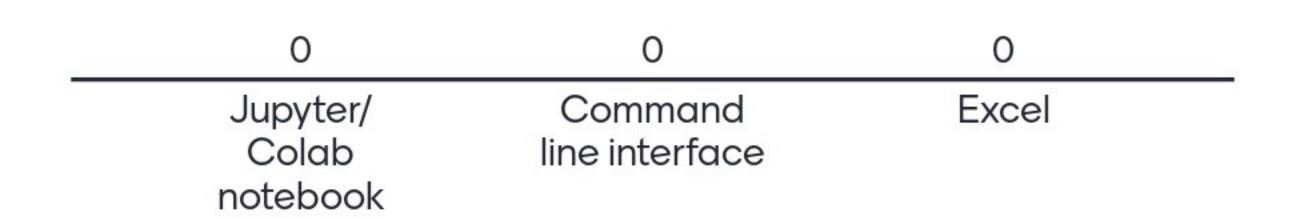
5th Scikit-Learn

6th PyTorch

#### RDKit can be used to...



## In an exploratory phase of a project, including plots and quick calculations, I will use...



### When working with conda, typically...

Ο	0	0	
One project	One	l will install	
will have one	computer will	my packages	
environment	have one	in the 'base'	
	environment	environment	



#### colab.research.google.com

My first Google Colab notebook!