Antibase Cytoscape Networking

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1 Introduction

The goal of these set of scripts is to go through your mass spec data (in mzXML file format) and see if any Antibase compounds or their adducts are present in your sample. This will be visualized in a custom cytoscape network and you can see which scans in your mzXML hypothetically maps to an Antibase compound. If you have any questions, you can contact me at **rnguyen2018@berkeley.edu**. If it is after May 2018, then contact me at **ryan.nguyen@yale.edu**.

2 Download Instructions

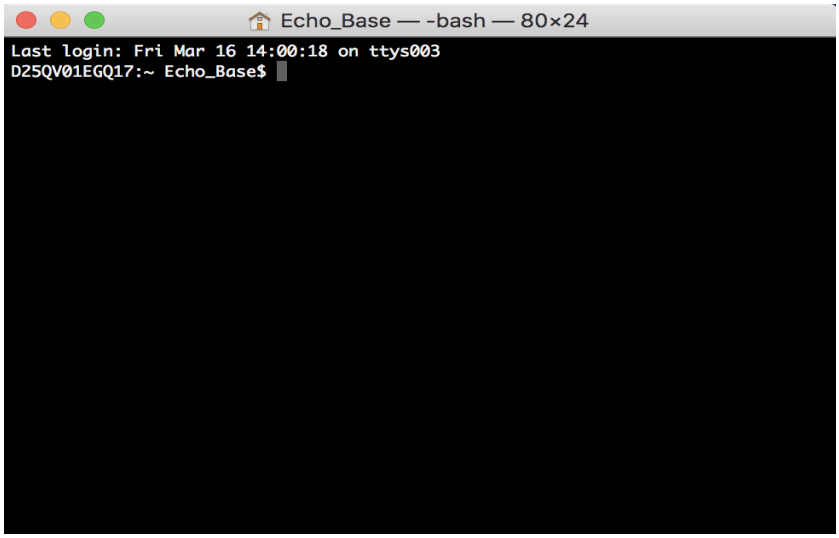
In order to use these scripts, you will need a couple of things (links to download are listed as well):

- Python 3: https://www.python.org/downloads/release/python-360/
- Git: https://git-scm.com/downloads

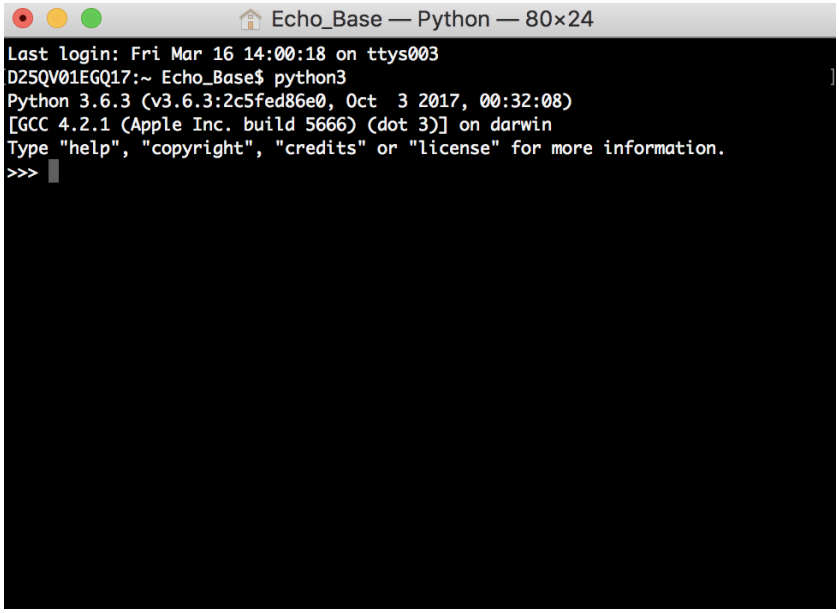
Pick the download that works for your system (MacOS or Windows). Both of these are already downloaded onto the Mac in the microscope room. If these downloaded onto your computer successfully, you should be able to open them up on terminal (Mac) or Command Prompt (Windows).

2.1 Making sure Python works on Mac

For Mac users, click on the magnifying glass in the upper right hand corner of your screen and type in "Terminal". Click on that. It should look something like this.



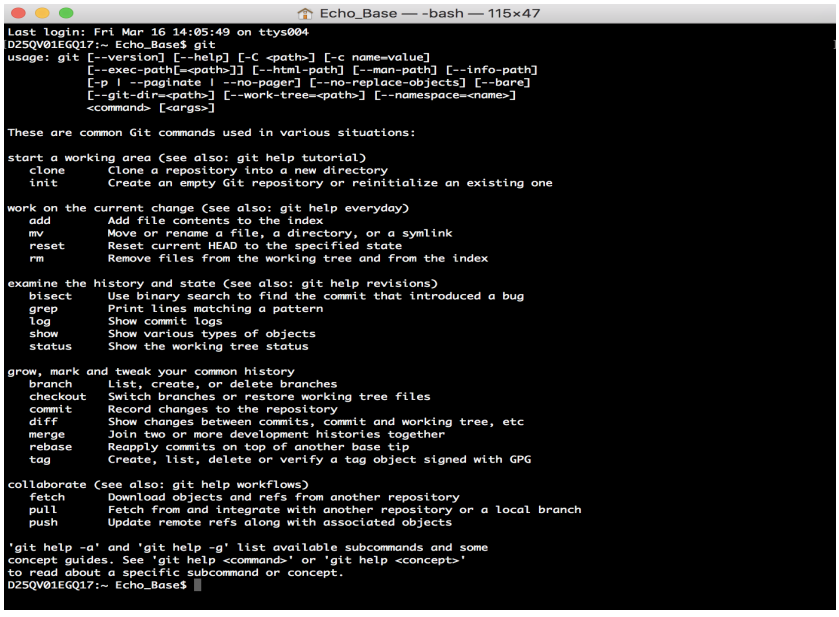
If you type in **python3**, you should get this on your screen.



Hooray! It works. Now, press Ctrl-D to quit python.

2.2 Making Sure Git works on your Mac

To make sure that git works, type in **git** into your Terminal. You should see this on your screen:



Hooray! It works.

2.3 Downloading the scripts

So this step is to put a folder on your desktop where all the scripts will be stored. To do this, open up your Terminal and type in this line by line:

cd ~/Desktop (make sure there is a space between **cd** and the following statement)
mkdir antiBase
cd antiBase

DO NOT EXIT YOUR TERMINAL. On your desktop, there should now be a folder called **antiBase**. Now, type in this:

git init
git clone https://github.com/Traxlab/antibase.git

If no errors popped up, then you have downloaded it correctly. Congrats!

3 Running the Scripts

Okay, open up the antiBase folder on your desktop and make sure there are no mzXML files in there. Once you've done that, put your mzXML file of interest into the folder. You are now ready to run the scripts.
NOTE: If you plan to use the MS-Dial output as your source, please make sure that it is a csv file and that the filename starts with "avg". Before running, make sure there are no other MS-DIAL csv files in the folder.
Open terminal and run these lines of code:

cd Desktop/antiBase
python3 antibaseComp.py

DO NOT EXIT TERMINAL. This will take about 5-6 minutes to run, and you will know when it's done when it prints out the amount of seconds it took to run. Your Json file with all of your data has now been made! To vizualize this, run this line of code:

python3 -m http.server

You might be asked to allow Python to run a server. Say allow. Then, open Google Chrome and search

localhost:8000

You might need to scroll around the webpage a little to find it, but your visualization will be there. On any given network, you will see the chemical formula for the antibase compound and its molecular weight. Connected to that will be a node(s) that contains its scan number in your mzXML, the m/z value of that scan, and what adduct it can map to. To stop the visualization, simply go to your Terminal and press Ctrl-C.
If you would like to view this again item at a later time, all you have to do is this :

cd Desktop/antiBase
python3 -m http.server

Then navigate again to **localhost:8000**

4 Example Output