

In this notebook I will illustrate how to remote login to Emu and convert all the .raw files to .mzXML

```
In [1]: pwd
```

```
Out[1]: u'/home/srlab/Documents/rhonda'
```

To ssh into ipython notebook on Emu:

- 1) I opened a Git Bash terminal locally and entered `ssh -N -L localhost:8000:localhost:7000 srlab@128.95.149.26` to login into Emu linux machine
- 2) I was prompted for the password and entered it
- 3) Terminal is active but it won't return any command prompt. You have created a tunnel into Emu

To start ipython on Emu

- 4) Open a new Git Bash terminal, but keep the first one open.
- 5) Enter `ssh srlab@128.95.149.26`
- 6) Input password
- 7) Enter `ipython notebook --no-browser --port=7000`

Now you are remotely logged into Emu and have started ipython without the browser.

- 8) Open a browser locally and enter `localhost:8000`
- 9) This will open Jupyter in your browser on the Emu machine. It will prompt you for the token which you can find in the second Git Bash terminal you opened.

```
In [2]: cd /home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016  
/home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016
```

In [3]:

```
ls
```

20161205_Blank_05.raw*
20161205_Blank_06.raw*
20161205_Blank_07.raw*
20161205_Blank_08.raw*
20161205_Blank_09.raw*
20161205_Blank_10A.raw*
20161205_Blank_11A.raw*
20161205_Blank_12A.raw*
20161205_PRTC+BSA_01.raw*
20161205_PRTC+BSA_02.raw*
20161205_PRTC+BSA_03.raw*
20161205_PRTC+BSA_04.raw*
20161205_PRTC+BSA_05.raw*
20161205_PRTC+BSA_06.raw*
20161205_PRTC+BSA_07.raw*
20161205_PRTC+BSA_08.raw*
20161205_PRTC+BSA_09.raw*
20161205_PRTC+BSA_10.raw*
20161205_PRTC+BSA_11.raw*
20161205_Sample_11A.raw*
20161205_Sample_11.raw*
20161205_Sample_12A.raw*
20161205_Sample_12.raw*
20161205_Sample_16A.raw*
20161205_Sample_16.raw*
20161205_Sample_19A.raw*
20161205_Sample_19.raw*
20161205_Sample_1A.raw*
20161205_Sample_1.raw*
20161205_Sample_20A.raw*
20161205_Sample_20.raw*
20161205_Sample_24A.raw*
20161205_Sample_24.raw*
20161205_Sample_27A.raw*
20161205_Sample_27.raw*
20161205_Sample_28_161205200228.raw*
20161205_Sample_28A.raw*
20161205_Sample_28.raw*
20161205_Sample_32A.raw*
20161205_Sample_32.raw*
20161205_Sample_35A.raw*
20161205_Sample_35.raw*
20161205_Sample_36A.raw*

```
20161205_Sample_36.raw*
20161205_Sample_3A.raw*
20161205_Sample_3.raw*
20161205_Sample_40A.raw*
20161205_Sample_40.raw*
20161205_Sample_43A.raw*
20161205_Sample_43.raw*
20161205_Sample_44A.raw*
20161205_Sample_44.raw*
20161205_Sample_48A.raw*
20161205_Sample_48.raw*
20161205_Sample_4A.raw*
20161205_Sample_4.raw*
20161205_Sample_51A.raw*
20161205_Sample_51.raw*
20161205_Sample_52A.raw*
20161205_Sample_52.raw*
20161205_Sample_56A.raw*
20161205_Sample_56.raw*
20161205_Sample_8A.raw*
20161205_Sample_8.raw*
blank9_method1.PNG*
blank9_method2.PNG*
blank9_method3.PNG*
blank9_sampleinfo.PNG*
md5.txt*
pressure.PNG*
PRTC8_method1.PNG*
PRTC8_method2.PNG*
PRTC8_sampleinfo.PNG*
PRTCplusBSA myco April 2016.sky*
PRTCplusBSA oyster seed Dec 2016.sky*
PRTCplusBSA oyster seed Dec 2016.skyd*
PRTCplusBSA oyster seed Dec 2016.sky.view*
sample16A_method1.PNG*
sample16A_method2.PNG*
sample40_sampleinfo.PNG*
```

```
In [4]: cd /home/shared/ReAdW
```

```
/home/shared/ReAdW
```

```
In [9]: !WINEPREFIX=~/.wine32 wine ReAdW.2016010.msfilereader.exe \  
        ~/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/20161205_Sample_1.raw \  
        ~/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/20161205_Sample_1.mzXML  
  
=Application tried to create a window, but no driver could be loaded.  
Make sure that your X server is running and that $DISPLAY is set correctly.  
err:systray:initialize_systray Could not create tray window  
fixme:thread:GetThreadPreferredUILanguages 52, 0x32fafc, 0x32fc74 0x32fb04  
fixme:heap:HeapSetInformation (nil) 1 (nil) 0  
ReAdW 2016.1.0(build Jun 21 2016 11:13:06)  
Xcalibur interface initialized (5).  
(Thermo lib opened file /home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/201612  
05_Sample_1.raw)  
file version is 66, interface version is 2.0 or greater  
file should contain scan numbers 1 through 109165  
(got computer name: emu)  
Error opening output file /home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/2016  
1205_Sample_1.mzXML  
unable to open /home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/20161205_Sample  
_1.mzXML
```

```
In [6]: cd /home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016  
  
/home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016
```

In [7]:

```
ls
```

20161205_Blank_05.raw*
20161205_Blank_06.raw*
20161205_Blank_07.raw*
20161205_Blank_08.raw*
20161205_Blank_09.raw*
20161205_Blank_10A.raw*
20161205_Blank_11A.raw*
20161205_Blank_12A.raw*
20161205_PRTC+BSA_01.raw*
20161205_PRTC+BSA_02.raw*
20161205_PRTC+BSA_03.raw*
20161205_PRTC+BSA_04.raw*
20161205_PRTC+BSA_05.raw*
20161205_PRTC+BSA_06.raw*
20161205_PRTC+BSA_07.raw*
20161205_PRTC+BSA_08.raw*
20161205_PRTC+BSA_09.raw*
20161205_PRTC+BSA_10.raw*
20161205_PRTC+BSA_11.raw*
20161205_Sample_11A.raw*
20161205_Sample_11.raw*
20161205_Sample_12A.raw*
20161205_Sample_12.raw*
20161205_Sample_16A.raw*
20161205_Sample_16.raw*
20161205_Sample_19A.raw*
20161205_Sample_19.raw*
20161205_Sample_1A.raw*
20161205_Sample_1.raw*
20161205_Sample_20A.raw*
20161205_Sample_20.raw*
20161205_Sample_24A.raw*
20161205_Sample_24.raw*
20161205_Sample_27A.raw*
20161205_Sample_27.raw*
20161205_Sample_28_161205200228.raw*
20161205_Sample_28A.raw*
20161205_Sample_28.raw*
20161205_Sample_32A.raw*
20161205_Sample_32.raw*
20161205_Sample_35A.raw*
20161205_Sample_35.raw*
20161205_Sample_36A.raw*

20161205_Sample_36.raw*
20161205_Sample_3A.raw*
20161205_Sample_3.raw*
20161205_Sample_40A.raw*
20161205_Sample_40.raw*
20161205_Sample_43A.raw*
20161205_Sample_43.raw*
20161205_Sample_44A.raw*
20161205_Sample_44.raw*
20161205_Sample_48A.raw*
20161205_Sample_48.raw*
20161205_Sample_4A.raw*
20161205_Sample_4.raw*
20161205_Sample_51A.raw*
20161205_Sample_51.raw*
20161205_Sample_52A.raw*
20161205_Sample_52.raw*
20161205_Sample_56A.raw*
20161205_Sample_56.raw*
20161205_Sample_8A.raw*
20161205_Sample_8.raw*
blank9_method1.PNG*
blank9_method2.PNG*
blank9_method3.PNG*
blank9_sampleinfo.PNG*
md5.txt*
pressure.PNG*
PRTC8_method1.PNG*
PRTC8_method2.PNG*
PRTC8_sampleinfo.PNG*
PRTCplusBSA myco April 2016.sky*
PRTCplusBSA oyster seed Dec 2016.sky*
PRTCplusBSA oyster seed Dec 2016.skyd*
PRTCplusBSA oyster seed Dec 2016.sky.view*
sample16A_method1.PNG*
sample16A_method2.PNG*
sample40_sampleinfo.PNG*

In [27]: `cd /home/shared/ReAdW`

`/home/shared/ReAdW`

```
In [3]: !WINEPREFIX=~/.wine32 wine ReAdW.2016010.msfilereader.exe \  
        ~/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/20161205_Sample_1.raw \  
        ~/Documents/rhonda/20161205_Sample_1.mzXML
```

```
=Application tried to create a window, but no driver could be loaded.  
Make sure that your X server is running and that $DISPLAY is set correctly.  
err:systray:initialize_systray Could not create tray window  
fixme:thread:GetThreadPreferredUILanguages 52, 0x32fafc, 0x32fc74 0x32fb04  
fixme:heap:HeapSetInformation (nil) 1 (nil) 0  
ReAdW 2016.1.0(build Jun 21 2016 11:13:06)  
Xcalibur interface initialized (5).  
(Thermo lib opened file /home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/201612  
05_Sample_1.raw)  
file version is 66, interface version is 2.0 or greater  
file should contain scan numbers 1 through 109165  
(got computer name: emu)  
Calculating sha1-sum of mzXML  
--done (mzXML sha1):9428790b3482b2d7b1390e292f51402d58b3a782
```

```
In [5]: !WINEPREFIX=~/.wine32 wine ReAdW.2016010.msfilereader.exe \  
        ~/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/*.raw \  
        ~/Documents/rhonda/*.mzXML
```

```
=Application tried to create a window, but no driver could be loaded.  
Make sure that your X server is running and that $DISPLAY is set correctly.  
err:systray:initialize_systray Could not create tray window  
fixme:thread:GetThreadPreferredUILanguages 52, 0x32fafc, 0x32fc74 0x32fb04  
fixme:heap:HeapSetInformation (nil) 1 (nil) 0  
ReAdW 2016.1.0(build Jun 21 2016 11:13:06)  
Xcalibur interface initialized (5).  
(Thermo lib opened file /home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/201612  
05_Blank_05.raw)  
file version is 66, interface version is 2.0 or greater  
file should contain scan numbers 1 through 6344  
(got computer name: emu)  
Error opening output file /home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/2016  
1205_Blank_06.raw  
unable to open /home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/20161205_Blank_  
06.raw
```

```
In [34]: cd ~/Documents/rhonda2016oyster/trochophora/C_gigas_Proteome2016  
/home/srlab/Documents/rhonda2016oyster/trochophora/C_gigas_Proteome2016
```

```
In [35]: !find . -name "20161205_Sample_***.raw"
```

./20161205_Sample_16.raw
./20161205_Sample_27.raw
./20161205_Sample_28.raw
./20161205_Sample_28_161205200228.raw
./20161205_Sample_36.raw
./20161205_Sample_40.raw
./20161205_Sample_52.raw
./20161205_Sample_4.raw
./20161205_Sample_12.raw
./20161205_Sample_24.raw
./20161205_Sample_32.raw
./20161205_Sample_35.raw
./20161205_Sample_43.raw
./20161205_Sample_51.raw
./20161205_Sample_1.raw
./20161205_Sample_20.raw
./20161205_Sample_48.raw
./20161205_Sample_56.raw
./20161205_Sample_3.raw
./20161205_Sample_11.raw
./20161205_Sample_44.raw
./20161205_Sample_19.raw
./20161205_Sample_8.raw
./20161205_Sample_3A.raw
./20161205_Sample_4A.raw
./20161205_Sample_16A.raw
./20161205_Sample_35A.raw
./20161205_Sample_36A.raw
./20161205_Sample_52A.raw
./20161205_Sample_8A.raw
./20161205_Sample_11A.raw
./20161205_Sample_12A.raw
./20161205_Sample_19A.raw
./20161205_Sample_20A.raw
./20161205_Sample_24A.raw
./20161205_Sample_27A.raw
./20161205_Sample_28A.raw
./20161205_Sample_32A.raw
./20161205_Sample_40A.raw
./20161205_Sample_48A.raw
./20161205_Sample_51A.raw
./20161205_Sample_56A.raw
./20161205_Sample_1A.raw

```
./20161205_Sample_43A.raw  
./20161205_Sample_44A.raw
```

```
In [ ]: /home/shared/ReAdW/WINEPREFIX=~/.wine32 wine ReAdW.2016010.msfilereader.exe \  
~/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/20161205_Sample_1.raw \  
~/Documents/rhonda/20161205_Sample_1.mzXML
```

In bash window to convert all of the files at once I entered:

```
`for file in ~/Documents/rhonda2016oyster/trochophora/C_gigas_proteome2016/20161205Sample*.raw  
do  
  
no_path=${file##*/}  
  
no_ext=${no_path%.raw}  
  
WINEPREFIX=~/.wine32 wine ReAdW.2016010.msfilereader.exe "file " /Documents/rhonda/ "no_ext".mzXML  
  
done`
```

```
In [36]: !curl http://gigaton.sigenae.org/ngspipelines/data/dcc6581978/analysis/f78867df95/contigs.fasta.transdec
```

% Total		% Received		% Xferd		Average Speed		Time	Time	Time	Current
						Dload	Upload	Total	Spent	Left	Speed
100	11.7M	100	11.7M	0	0	3265k	0	0:00:03	0:00:03	--:--:--	3264k

```
In [38]: !gzip -d ~/Documents/rhonda/contigs.fasta.transdecoder.pep.gz
```

```
In [39]: !head contigs.fasta.transdecoder.pep
```

```
>CHOYP_043R.1.5|m.16874 CHOYP_043R.1.5|g.16874 ORF CHOYP_043R.1.5|g.16874 CHOYP_043R.1.5|m.16874 typ
e:internal len:199 (-) CHOYP_043R.1.5:1-594(-)
TPSGTPSGTPSVTPTPSGTPSVTPTPSGSTPSGTPSVTPTPSGTPSGTPSVTPT
PSGTPSVTPTPSVPTPSGTPSVTPTPSGTPSVTPTPSGTPSGTPSVTPTPSGTP
SGTPSVTPTPSVTPTPSGTPSVTSTPSAPTSGTPSGTPSVTPTPSGTPSGTPS
VTPTPSGTPSVTPTPSG
>CHOYP_043R.5.5|m.64252 CHOYP_043R.5.5|g.64252 ORF CHOYP_043R.5.5|g.64252 CHOYP_043R.5.5|m.64252 typ
e:internal len:821 (+) CHOYP_043R.5.5:2-2461(+)
SRPTPSVTPTPSGTPSVTPTPSVSTPSGTPSVTPTPSGSPSVTPTPSGSPSGTPS
ATPTPSGTPSGTTPSGSTPSATITTTISTPSTTVCSYVDIGPEQAIDVSLRSPSEDPDAP
IENILQTNSVYKPKKEPTYDENVVVKIISQDTPILRVSFVTNVRADTVGLEYLTDYKQKI
ITQNNETVEFVFAAGIITDNFTINIRSDSAEQPEISNLKIRACYKPVIGQPSTTTNPSI
```

```
In [40]: !curl http://comet-ms.sourceforge.net/parameters/parameters_201601/comet.params.high-low \
> ~/Documents/rhonda/Pcomet.params.high-low
```

% Total	% Received	% Xferd	Average Speed	Time	Time	Time	Current
			Dload Upload	Total	Spent	Left	Speed
100 8761	100 8761	0 0	24112 0	--:--:--	--:--:--	--:--:--	24134

```
In [41]: !head ~/Documents/rhonda/Pcomet.params.high-low
```

```
# comet_version 2016.01 rev. 0
# Comet MS/MS search engine parameters file.
# Everything following the '#' symbol is treated as a comment.

database_name = /some/path/db.fasta
decoy_search = 0 # 0=no (default), 1=concatenated search, 2=separate search

num_threads = 0 # 0=poll CPU to set num threads; else specify num threads direc
tly (max 64)

#
```

```
In [1]: cd ~/Documents/rhonda
```

```
/home/srlab/Documents/rhonda
```

```
In [5]: !curl https://raw.githubusercontent.com/ElIior2/Fish-546-Bioinformatics/master/analyses/DDA_2016/contam.  
> contam.bovin
```

% Total		% Received		% Xferd		Average Speed		Time	Time	Time	Current
						Dload	Upload	Total	Spent	Left	Speed
100	4032	100	4032	0	0	8388	0	--:--:--	--:--:--	--:--:--	8400

```
In [3]: !curl https://raw.githubusercontent.com/ElIior2/Fish-546-Bioinformatics/master/analyses/DDA_2016/contam.  
> contam.human
```

% Total		% Received		% Xferd		Average Speed		Time	Time	Time	Current
						Dload	Upload	Total	Spent	Left	Speed
100	26621	100	26621	0	0	37095	0	--:--:--	--:--:--	--:--:--	37076

```
In [4]: !curl https://github.com/ElIior2/Fish-546-Bioinformatics/blob/master/analyses/DDA_2016/contam.other \  
> contam.other
```

% Total		% Received		% Xferd		Average Speed		Time	Time	Time	Current
						Dload	Upload	Total	Spent	Left	Speed
100	70845	0	70845	0	0	83417	0	--:--:--	--:--:--	--:--:--	83347

In [12]:

```
ls
```