

### 1. Ongoing assignment (10 minutes)

There will be 3 ongoing (student final project gene specific) assignments. Check the Github C3 folder. It will be made available few days after the class. The ongoing assignments are setup to help students solve the final project.

### 2. ChemSketch (15 minutes)

Find a molecule (ex. Aspirin, Imatinib etc.) of your interest (related to your gene for final project) in PubChem. Extract the compound Canonical SMILES or InChi ID and use ChemSketch to view the molecule. Also make sure you know how to create a figure (png/jpeg etc.) of the compound and insert it in a presentation (pptx file). This task will be helpful for the final project presentation preparation.

ChemSketch is a freeware for Windows and can be downloaded from here

<https://www.acdlabs.com/resources/freeware/chemsketch/>

### 3. RStudio (30 minutes)

1. Create two vectors of length 100.  $x$  &  $y$  are numbers from 1 to 100 and to this add a little bit of noise. Set a seed (please use 100 as seed) for getting the same result before generating the noise vector. Hint: we can use random numbers for mimicking noise
2. calculate mean, median and sd for  $x$  and  $y$
3. Explore  $x$  and  $y$  using histogram
4. Plot  $x$  and  $y$
5. Build a suitable model based on step d
6. Look at the model parameters
7. Plot the predicted model,  $\hat{y}$ , along with the  $x$  and  $y$

### 4. Preparation for Edirect (45 minutes)

- a. Make sure you can log into SLURM cluster. Check your email from Administrator for the IP address or hostname for the SLURM cluster.
- b. Review of Linux important commands  
[https://github.com/hoodcollege/BIFX550\\_Spring2020/blob/master/C2/4-SR-Linuxtutorial.pdf](https://github.com/hoodcollege/BIFX550_Spring2020/blob/master/C2/4-SR-Linuxtutorial.pdf)
- c. Shell Programming by example. We will examine a shell script that accomplishes the following tasks. The folder was made available during the class.
  - i. How to count the number of unresolved genomic positions in a chromosome (say Chromosome 22)?
  - ii. Demonstrate how easy to answer this question using SHELL programming

### 5. Break (5 minutes)

### 6. E-Direct (45 minutes)

Motivation for e-direct tool. Compare Edirect with PubMed

(we are going to work on edirect and NCBI pubmed; open a browser tab and SLURM login window and put them side-by-side)

- a. **PubMed:** Go to PubMed
- b. **PubMed:** search for the keyword **opsin gene conversion**

- i. clear all the filters (if any from previous searches)
- c. **Edirect:** run the following command  
`esearch -db pubmed -query "opsin gene conversion"`  
 Look for the counts and compare them with the websearch
- d. **PubMed:** Look for related articles  
 Find Related Data → Choose DB: PubMed and option "similar articles"  
 Note the count (hits)
- e. **Edirect:** run the following command to convince they are producing the same results  
`esearch -db pubmed -query "opsin gene conversion" | elink -related`
- f. **PubMed:** Add a filter word **tetrachromacy**
- g. **PubMed** PubMed → Advanced → Choose the previous query and add additional queries like filtering. You can accomplish using the following way. In the filter box, choose "Text Word" and enter **tetrachromacy** and search
- h. **PubMed:** Note the count
- i. **Edirect:**  
`esearch -db pubmed -query "opsin gene conversion" | esearch -db pubmed -query "opsin gene conversion" | elink -related | efilter -query "tetrachromacy"`
- j. **PubMed:** Change the output format as "Abstract"
- k. **Edirect:** You can accomplish all the PubMed query steps using this one line code:

`esearch -db pubmed -query "opsin gene conversion" | esearch -db pubmed -query "opsin gene conversion" | elink -related | efilter -query "tetrachromacy" | efetch -format abstract`

Replace a query that is relevant for your gene and repeat the Edirect exercise.