

### 1. ChemSketch (15 minutes)

Find a molecule of interest in PubChem use Canonical SMILES or InChi ID and use ChemSketch to see the molecule.

### 2. 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,  $y_{\text{hat}}$ , along with the  $x$  and  $y$

### 3. Preparation for Edirect (30 minutes)

- a. Make sure you can log into SLURM cluster (IP: 144.175.88.21)
- b. Linux important commands (15 minutes)  
[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. Why Shell programming:
  - i. How to count the number of unresolved genome positions in a chromosome (say Chromosome 22)?
  - ii. Demonstrate how easy to answer this question using SHELL programming

### 4. Break (5 minutes)

### 5. E-Direct (30 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: clear all the filters
- b. PubMed: search for the keyword **opsin gene conversion**
- 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 --> 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.