1. Lab 1 Report Template

**Lab Report for Lab 1: Chemoinformatics**

**Name: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

**Date: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

**Objective:**

**Data and Results**:

1. First five simple plots (Steps **1B - 1F**)
2. Plot of LogP vs PSA colored by QED **(2D)**
3. Plot of LogP vs PSA colored by \_\_\_\_\_\_\_\_\_ **(Module 3)**
4. Plot of \_\_\_\_ vs \_\_\_\_\_ colored by \_\_\_\_ **(Module 4)**

**Discussion:**

1. What are the Lipinski rules?
2. Write code for filtering by drugs that pass all of the Lipinski rules (Hint: this can be done with an if statement and a for loop. See slide 14)
3. Now that you’ve done some basic coding, suggest a research question that you could ask of the DrugBank dataset. You do not need to write the code, but what hypothesis could you formulate, and then test within the data, using python?