Assignment-1

You will use Google Colab to accomplish the following tasks. Give edit permissions to your GoogleColab link and submit in this form. You need to be logged in to submit the form.

Topics: Introduction to Python, Pandas, Numpy, Seaborn plotting library.

- Download the QM9 dataset from this link - https://raw.githubusercontent.com/OpenDrugAI/AttentiveFP/master/data/qm9.csv
- Use pandas to load the above dataset into a data frame
- Filter the data point that does not contain Sulphur and Chlorine atoms on the above data frame
- Extract Atomization energies from the above data frame as a NumPy array. Convert atomization energy units to Hartrees (relation: 1HF = 627.5 kcal/mol)
- On the filtered data:
    - Make a scatter plot for “Number of atoms” vs “Atomization energy in Hartrees” of the molecules (Reference: https://seaborn.pydata.org/generated/seaborn.scatterplot.html)
    - Make a histplot of the Atomization energies in Hartrees.