Challenge 2

LCVC Module 2 – 2021/2022

Access the Google Colab Notebook at:

https://colab.research.google.com/drive/1XxBEBzwkdWio_yd-MbUAjU6SzqnZU7nx?usp=sharing

1. Defining the Monte Carlo Driver

    a. Define the energy function with the TorchANI energy function component

    b. Define the RotamerMutator

    c. Define a Callback to print the accepted structure every step

    d. Define the thermostat

    e. Define the simulation Monte Carlo Driver

2. Running the simulation

    a. Load "mol1.pdb". Export the first "frame" of the simulation to a file.

    b. Run the simulation.

    c. Visualize the results in PyMOL.