

# Practical examples 2

LCVC Module 2 – 2021/2022

Access the Google Colab Notebook at:

[https://colab.research.google.com/drive/16nVvIa0W2inXEzzgTIRc38aqML\\_GFSnB?usp=sharing](https://colab.research.google.com/drive/16nVvIa0W2inXEzzgTIRc38aqML_GFSnB?usp=sharing)

## 1) Loading an energy function

- a. Create an empty energy function in ProtoSyn.jl
- b. Add the TorchANI energy function component
- c. Measure the “mol1.pdb” energy, according to the TorchANI ML model.
- d. Visualize the current pose in PyMOL. Copy the current pose to a new pose2. Rotate the phi dihedral on residue 48 of pose2 to be 50°.
- e. Measure the pose2 energy (after rotation), according to the TorchANI ML model. Visualize both poses in PyMOL (before and after the rotation).
- f. Add the ProtoSyn.Peptides.Calculators.Caterpillar default energy function component to the current energy function and re-evaluate both poses. Adjust the relative weights for the individual components if necessary.