

Practical examples 1

LCVC Module 2 – 2021/2022

Access the Google Colab Notebook at:

<https://colab.research.google.com/drive/1NybwMgKclglw8SAHvH9IsOhgoXhjAV1A?usp=sharing>

1) Load “mol1.pdb” in PyMOL.

- Visualize the structure in various modes: “stick”, “cartoon”, “spheres” and “surface”.
- Visualize the structure in two simultaneous modes: “stick” and “cartoon”.
- Select residue 48 by ID, colour its carbon atoms with a different colour.
- Select all ARG residues my name, colour all of their atoms with a different colour.
- Employ the “measure” function to calculate the distance between two atoms.
- Employ the “measure” function to calculate the phi dihedral angle in residue 48.

2) Setting a backbone dihedral

- Load “mol1.pdb” in ProtoSyn
- Measure the phi dihedral in Residue #48.
- Rotate the phi dihedral in Residue #48 to be 85°.
- Measure the phi dihedral in Residue #48 after rotation.
- Export the rotated structure to a file and visualize in PyMOL.
- Employ the “measure” function (on PyMOL) to calculate the phi dihedral angle in residue 48.

3) Rotating a sidechain dihedral

- Load “mol1.pdb” in ProtoSyn (again)
- Rotate the chi1 dihedral in Residue #48 by +10°.
- Export the rotated structure to a file and visualize in PyMOL in comparison with the original structure.
- On ProtoSyn, generate a trajectory of structures by rotating the chi1 dihedral in Residue #48 by +10° 35 times.
- Export the generated trajectory and visualize in PyMOL.