Practical examples 1

Ex.1) Load “mol1.pdb” in PyMOL. Visualize the structure in “stick” mode. How many aminoacids has the molecule? Identify and measure the *phi* dihedral on the second aminoacid.

Ex.2) Load “mol1.pdb” as a Molecule (in the Python code). Rotate the *phi* dihedral on the second aminoacid by + 360°, in 10° steps/intervals, appending each new conformation as a new frame to export to “mol2.pdb”.

Ex.3) Rotate the *phi* dihedral on the second aminoacid by +X°, where X is a random number between 50° and 150°. Export the changed structure to “mol2.pdb” and visualize in PyMOL. Create a function to measure the current value of a dihedral, given its third atom, based on the internal coordinates. Measure the current value of the *phi* dihedral (after adding a random rotation) and compare with the measured value in PyMOL.

Ex.4) Rotate the *phi* dihedral on the second aminoacid to a specific value of -65°.

Ex.5) Rotate the *chi-4* dihedral on the second aminoacid to a specific value of 90°.

Laboratório de Visualização e Computação Científica

Module 2 – Computational Design of Peptides

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