Challenge 2

Ex.1) Create a Monte Carlo simulation that runs for 500 steps. Export the current conformation every 10 steps. Each step, the simulation should:

1. Save the current conformation as a backup
2. Choose a random aminoacid from the Molecule
3. Sample a random Rotamer from the Rotamer Library (based on the current *phi* and *psi* angles)
4. Apply the sampled rotamer to the chosen aminoacid
5. Measure the energy of the new conformation
6. Choose whether to keep the new conformation or reload the backup, based on the Metropolis algorithm. As described below, accept the new conformation if.

$$e_{n+1} < e_n \quad \text{or} \quad rand() < e^{-\frac{e_{n+1}-e_n}{T}}$$

Note: e_{n+1} is the energy of the new conformation; e_n is the energy of the backup structure; T is the temperature of the system. For this exercise, use T = 0.5;

Laboratório de Visualização e Computação Científica

Module 2 – Computational Design of Peptides

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