Report

LCVC Module 2 – 2021/2022

The following topics are criteria for evaluation of the final report for Module 2.

The report should be delivered as a .DOCX/.PDF file either via the e-learning or via e-mail to jose.manuel.pereira@ua.pt. The report should not exceed 10 pages. Other than that, the format of the text is free to the student's discretion. The following topics should be covered in the text report (although not in a question-answer format), with the given weights in the final grade shown. Any additional files (such as code workbooks, images, videos, etc) can be attached to the final report.

8/20 Introduction

- Why is protein design important?
- What are the advantages of computational assisted protein design?
- What software's will be used for the manipulation and visualization of molecular systems in this report?
- What is the simulation algorithm employed?
- How is the system's energy evaluated? What are some other options for evaluating the system's energy, and what differentiates them?

10/20 Simulation (see below)

- Showcase the code (for example, in workbook format). Don't forget to add comments.
- Showcase results (using images, videos, gifs, etc …). A great deal of emphasis will be given on the evaluation of the quality of the presented materials: images & videos should be high-resolution and explicitly show the emphasis of the visualization. Use colours, transparency, labels, depth cues, etc to add information and quality.

2/20 Conclusion

- What were some of the obstacles felt during this work? How did you overcome them?
- Did you learn anything new?
- What are the prospects of protein design? Explain some of the most interesting future use cases to you.

For this report, the following challenge needs to be simulated. The student should showcase the code and the requested visualizations in the final report (or as annexes).

1. Perform a mutation (to any aminoacid you'd like, other than Proline – PRO/P) on any residue you'd like. Showcase the mutation performed. (2/10)
2. Set-up and run a Monte Carlo simulation to find the best rotamer for the newly mutated aminoacid. Use the Dunbrack 2011 rotamer library. The Monte-Carlo simulation should run for 100 steps, using a constant temperature of 0.01. Evaluate each conformation attempt in the Monte Carlo with an energy function using TorchANI as the single energy function component. (4/10)
    a. Print and visualize (i.e.: show) each frame of the simulation, using a Callback, highlighting the conformational changes being made. (1/10)
3. How did the system's energy change during the simulation? (1/10)
4. Perform the same simulation, on the same residue, but applying different initial mutations (i.e.: mutate to different target aminoacids). Are there any noticeable differences both in energy and structure? (2/10)