



Workshop: De novo design of proteins using Rosetta and Alphafold 2

Thursday 23. 6. 2022, from 9:00 to 17:00

Large Lecture Hall, National Institute of Chemistry, Hajdrihova 19, Ljubljana, Slovenia

Protein design is of great technological importance and can solve many biomedically relevant challenges. Examples include new therapeutic agents (COVID-19 inhibitors, COVID-19 vaccines, flu inhibitors), nanomaterials (cages, layers, fibers) and sensors.

The workshop is set up as a “crash course” in protein design, highlighting what is possible with current technology. Participants will learn how to **build a four-helix bundle protein from scratch** (i.e. using only mathematics). At the end of the workshop, they will obtain a sequence for the protein that folds into the designed structure. The basics of Rosetta, parametric backbone design, design of loops and design of side chains will be introduced. Alphafold 2 and its uses will also be presented.

The workshop will be led by dr. Ajasja Ljubetič, a Marie Skłodowska-Curie Fellow that has trained in the Baker lab (Seattle, USA), one of the most famous protein design labs in the world.

Start	Length	End	Program
09:00	1:30	10:30	Introduction to protein design, PyRosetta and RosettaXML
10:30	0:30	11:00	Coffee Break
11:00	1:30	12:30	Parametric design of backbones
12:30	1:00	13:30	Lunch
13:30	1:30	15:00	Residue selectors, loop design, layer design, minimisation
15:00	0:30	15:30	Coffee Break
15:30	1:30	17:00	Design of side chains, pack rotamers, filtering with Alphafold2

Target audience: The workshop is intended for undergraduate and graduate students as well as postdocs and young scientist **interested in protein design**. Participants should know the basics of protein structure (what is an alpha helix, what are backbone and sidechains). The basics of Python (how to import modules and execute commands) is also recommended.

Prerequisites: Participants need to **bring their own laptop**. Google Colab will be used as the computational environment so only a browser is needed. Participants will also need a Google account.

Application: Applications are free of charge and accepted until **13. 6. 2022**. Coffee breaks with a light snack are included, however lunch is not included. Participation will be limited to 25 persons who will be notified of acceptance in a separate e-mail by 15. 6. Apply using the link below:

<https://tinyurl.com/RosettaCrashCourse>

Organizers: Ajasja Ljubetič, Eva Rajh, Tadej Satler
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