KEMIJSKI INŠTITUT

Workshop:
De novo design of proteins using Rosetta and deep learning methods

Wednesday 13. 3. 2024, 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 is predicted to fold into the designed structure. The basics of Rosetta, parametric backbone design, design of loops and design of side chains will be introduced. The latest deep learning methods (Alphafold2, ProteinMPNN and RFDiffusion) will 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 helical bundles with PyRosetta
12:30	1:00	13:30	Lunch
13:30	1:30	15:00	Design of sidechains using ProteinMPNN and AlphaFold2
15:00	0:30	15:30	Coffee Break
15:30	1:30	17:00	Designing proteins using RoseTTAFold Diffusion

Target audience: The workshop is intended for undergraduate and graduate students as well as postdocs and young scientists **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 in a Jupyter Notebook) are also needed.

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 **25. 2. 2024**. Coffee breaks with a light snack are included, however lunch is not included. Participation will be limited to 40 attendees who will be notified of acceptance in a separate e-mail by 1. 2. 2024.
Apply using the link below:

http://tinyurl.com/RosettaCrashCourse2

Organizers: Ajasja Ljubetič, Eva Rajh, Tadej Satler
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