Title: Data-driven Methodology for Predicting, Explaining, and Understanding of RNA and Small Molecule Ligand Binding (NCN/OPUS)

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Project description:

RNA molecules are central to virtually all cellular processes — from storing and transmitting genetic information to catalysing biochemical reactions and regulating gene expression. Many RNA molecules, including bacterial ribosomes and riboswitches, are established or emerging targets for small-molecule drugs. At the same time, computational methods for predicting how small molecules interact with RNA lag far behind analogous tools for protein targets — a critical bottleneck in RNA-targeted drug discovery.

Aim:

The project aims to develop DeepLeaRNA, a novel general-purpose computational methodology for predicting, explaining, and designing small-molecule ligands that bind to RNA. The approach integrates machine learning, deep learning, and Explainable AI (XAI) with carefully curated structural and biological data. It builds directly on the group's prior work: the AnnapuRNA scoring function for RNA–ligand structure prediction and fingeRNAt, a tool for detecting and classifying noncovalent interactions in RNA–ligand complexes.

Requirements:

- Master's degree in bioinformatics, computational biology, biochemistry, chemistry, computer science, or a related field
- Hands-on experience in at least one of the following: Python programming, machine learning, cheminformatics, or structural bioinformatics
- Familiarity with RNA biology, structural biology, molecular biology, organic chemistry, medicinal chemistry, or drug design will be an advantage
- Knowledge of deep learning frameworks (e.g. PyTorch, TensorFlow) will be an advantage
- Written and spoken fluency in English
- Willingness to learn, take on new challenges, and work both independently and collaboratively
- Analytical thinking and good interpersonal skills

Number of positions available: 1

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