Title: Data-driven methodology for predicting, explaining and understanding of RNA and small molecule ligand binding.

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Laboratory: Laboratory of Bioinformatics and Protein Engineering
www: https://shorturl.at/Is6cO

Project description:

Ribonucleic acid (RNA) molecules are pivotal in various biological processes, including transmitting genetic information, responding to cellular signals, and catalyzing chemical reactions. These functions make RNA an attractive target for novel drug development. However, the computational methods available for predicting RNA-ligand interactions are less advanced compared to those for protein-ligand interactions, limiting the potential for RNA-targeted therapies. To address this gap, our project aims to develop DeepLeaRNA, an advanced computational framework designed to predict and analyze RNA-ligand interactions.

Aim:

The primary objective of DeepLeaRNA is to create a comprehensive methodology that enhances our understanding of how small molecules bind to RNA. By leveraging advanced machine learning techniques and a coarse-grained representation of interacting partners, DeepLeaRNA aims to provide more accurate and interpretable predictions. This framework will significantly contribute to the rational design of new drugs targeting RNA.

Requirements:

- Master's degree in chemistry, biology, physics, computer science or a related field
- Knowledge in at least one of the following disciplines: bioinformatics, cheminformatics, organic chemistry, molecular biology, structural biology, algorithms and data structures, machine learning.
- Desired experience in programming (python), algorithm design, computer data processing
- Desired experience in software for visualisation and processing of biological (e.g. proteins) and/or chemical structures, methods related to computer support of drug design (e.g. molecular docking) or simulations (e.g. molecular dynamics)
- Written and spoken fluency in English
- Willingness to learn and take new challenges, ability to work independently, analytical thinking
- Good interpersonal skills and a collaborative attitude

Number of positions available: 1

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