



Master project 2021-2022

Personal Information

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Project

Structural bioinformatics

Project Title:

Development of strategy for finding RNA ligands

Keywords:

Computational Chemistry, Molecular Modeling, Targeting RNA, Drug Design

Summary:

Targeting RNA is a new frontier in drug design, but a new molecular-level understanding of how to design agents for this is a critical need. RNA molecules are inherently flexible and, therefore, traditional rigid computational docking strategies are unsuited for the task. Therefore, strategies based on RNA conformational sampling studies followed by docking to the most populated states seem promising methodologies to develop.

Expected skills::

Biochemistry with programming skills or knowledge

Possibility of funding::

Yes

Possible continuity with PhD: :

To be discussed

Comments:

Initial duration: 6-8 months
