Mention M2 -BI

In Silico Drug Design

INTERNSHIP SUBJECT
Academic Year 2021/2022

Name of the Laboratory Manager:

Laboratory: Computational structural biology group
Precise address of the Laboratory : 845 Sherbrooke St W, Montreal, Quebec H3A 0G4, Canada
Name of the host team leader and name of the team: Jerôme Waldispuhl

Name of Internship Leader(s): Jerôme Waldispuhl
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Specialty of the internship : Research
Is this topic a first step towards a thesis: no
Indicate by a few key words, the scientific orientation of the subject:
Neural Network , RNA-ligand complex, docking ,Computer science

Title: "analysis of simplified model of ligand-RNA complex in neural network training"

Project Summary (15 lines):

Ribonucleic acids (RNA) are one class of biological target with a handful of known druggable compounds capable of binding to it. We estimate that up to 70% of our genome codes for RNAs and only a very small fraction of drugs actively target those RNAs. But the design of such compounds remains arduous. The current traditional physic based toolkit at our disposal struggles to identify compounds capable of binding specifically to RNA. With the recent breakthrough in neural networks , the computational structural biology group has been able to develop a model that can accurately predict RNA-ligand complexes. However, this kind of model is very complex and has multiple hidden layers that make it impossible to analyze and determine key features in ligand-RNA complexes. The main point of the internship is to develop a variational auto-encoder with a simplified model of the ligand-RNA complex. Thus , we will reduce the degree of complexity of our model. We hope that it will make our model simple enough to be interpretable.