M2 internship on modelling mRNA-lipid adducts

Workplace: CiTCoM, Université Paris Cité, Paris, France
Keywords: computational chemistry, molecular modelling software, protein-RNA complex, RNA modifications, bioinformatics
Occupation: Research training

Context

The internship will be conducted in the **STAV** (Structure and Translation of Viral RNAs) team of CiTCoM (UMR CNRS 8038, Université Paris Cité UPC), a multidisciplinary unit with expertise in molecular modelling, biochemistry, organic chemistry, structural biology, and microbiology. One of the team research axes is dedicated to RNA functional modifications from experimental to computational point of view. As shown by the recent pandemic, messenger RNA (mRNA), a promising tool in vaccine and therapeutic development, is reliant on intact mRNA delivery into target cells. In this context, the interaction and the formation of mRNA-lipid adduct can be crucial as well as the impact of the environment properties. Therefore, a better understanding of these aspects can have significant implications for the design and development of future mRNA-based biopharmaceuticals. From experimental point of view, our team has been studying mRNA structure in relation to vaccines. From the computational point of view, in the last years we have tackled other RNA modifications by using a large variety of approaches including molecular dynamics simulations and quantum mechanics/molecular mechanics calculations that there will be applied in this context. The project will be conducted in close collaboration with our experimental colleagues in the team who are expert in biochemistry and biology, as well as our collaborators at UPCité.

Position and assignments

The M2 internship is related to the study the formation of mRNA lipid adduct to understand the specificity of the reaction, and drive the design of modified lipids that would not react with mRNA. To study the reactivity, preliminary QM/MM calculations will be conducted. Statistical and bioinformatics analyses will be performed by using standard tools and by developing new scripts.

The M2 internship should be considered as an initiation into theoretical and computational methods spanning from simple QM calculations to standard and advanced all-atom molecular dynamics simulations using a variety of molecular modelling software and visualisation tools. Moreover, the intern will have the opportunity to learn about bash script coding, python, Matlab, High Performance Computing and to perform bibliographic research.

The internship will start at the beginning of the second semester of 2026/2027 M2 courses (January/February 2027).

Application

Please send your CV and a cover letter (one page) to **elisa.frezza@u-pariscite.fr** using “RNA modifications M2 internship - mRNA-lipid adducts” as subject.