

A Post-Doc position in structural biocomputing/molecular modelling available @ IGBMC, Strasbourg and TBI-INSa, Toulouse

A Post-Doc position is available in molecular modelling (biocomputing) within the framework of an ANR-funded project between the **Institut de Génétique et de Biologie Moléculaire et Cellulaire (IGBMC)** in **Strasbourg France** and the **Toulouse Biotechnology Institute (TBI)** in **Toulouse France**.

The IGBMC is affiliated with INSERM, the CNRS and the University of Strasbourg. It carries out interdisciplinary research in structural, molecular and cellular biology: <https://www.igbmc.fr/> The TBI is affiliated with INSA, the CNRS and INRAE, and carries out research in catalysis and enzyme engineering, systemic and synthetic biology, fermentation, process engineering and eco-design: <https://www.toulouse-biotechnology-institute.fr/>

Job description

The successful candidate will be a key member of the ANR-funded research project **PyoClick** that aims to investigate and design non-ribosomal peptide synthases (NRPS) involved in the bioproduction of new-to-nature peptides for biomedical applications.

The candidate will be in charge of conducting molecular modelling studies to get a better understanding of molecular determinants involved in the function and substrate recognition of the targeted enzyme. The project will also aim at redesigning the enzyme to achieve the desired catalytic reaction and drive experimental construction of enzyme mutant libraries. This work will be carried out in close interaction with our experimental collaborators in charge of enzyme engineering and evaluation tasks.

We are looking for a highly motivated scientist who has a sound understanding of protein modelling and protein-ligand interactions. He/She should have research expertise/training in a number of areas of computational biology, including protein modelling, molecular docking, molecular dynamics simulations and computational protein design. Experience in sequence analysis and familiarity with emerging design tools based on AI would be a plus. Knowledge of the Linux operating system is expected. She/He will apply a range of molecular modeling and bioinformatics techniques (sequence analysis, protein structure prediction, molecular docking, molecular dynamics simulations, free energy prediction ...) to decipher essential structural and dynamical determinants of NRPS enzyme function and engineering.

The perspective post-doc will have the opportunity to work in a diverse and rich multidisciplinary environment, surrounded by both computational and experimental experts in the fields of enzyme catalysis, design and engineering. The successful candidate should enjoy teamwork and have very good communication skills. Good English skills are required and notions of French would be a plus. He/She will be a key player in this collaboration between the IGBMC and TBI laboratories.

Qualifications

- PhD in Molecular Modelling, Structural bioinformatics, Biophysics or related field.
- Essential skills required include protein modelling, biomolecular simulation, and bioinformatics methods and techniques.
- Strong communication and organizational skills and willingness to work in a team-oriented environment.
- Good English skills are required and notions of French would be a plus.

The position is available starting from January 1st, 2026 and for a duration of 12 months (with possible renewal).

Applicants should send a detailed curriculum vitae, a letter of intent explaining their motivations for the position, and contact details of at least two references. Send your applications to:

Roland Stote: rstote@igbmc.fr
Jérémy Esque: esque@insa-toulouse.fr