



Nantes Université recrute

Pour son laboratoire US2B – Site de la Lombarderie - Nantes

A Post Doctoral Researcher to optimize Rac1 inhibitors

Nantes University is a public institution of higher education and research which proposes a **model of university which is unique in France**, uniting a university, a university hospital (CHU de Nantes), a technological research institute (IRT Jules Verne), a national research organisation (Inserm) and the grandes écoles (Centrale Nantes, Ecole des Beaux-Arts Nantes Saint-Nazaire, Ecole d'Architecture de Nantes).

These organisations are combining their strengths **to develop the excellence of Nantes'research** and offer **new training opportunities** in all areas of knowledge.

Sustainable and open to the World, Nantes University ensures the quality of the study and working conditions offered to its students and staff, in order to encourage their development on all its campuses in Nantes, Saint-Nazaire and La Roche-sur-Yon.

Work context

The Biological Sciences and Biotechnologies unit (US2B) is an academic laboratory developing basic research in **biochemistry** and **biology** resulting from the merger of two laboratories with, on the one hand, the 5 teams of the UFIP (Functionality and Protein Engineering Unit, UMR CNRS 6286) and on the other hand, the LBPV host team (Laboratory of Plant Biology and Pathology, EA 1157).

Through in-vitro, in-vivo and in-silico approaches, the laboratory conducts research centered on the themes of the regulation of protein functions and the bioregulation of biological activities. In particular, the research will aim to respond to fundamental and applied issues in the fields of structural biology (understanding of the sequence-structure-function relationship), molecular engineering, glycosciences, control of the integrity of genomes, epigenetic regulations of genome expression (from chromatin to translation), biological interactions (microalgae-bacteria, plant-bacteria, plant-plant, etc.) and biological adaptation to the environment (see team projects).

The unit is under the supervision of INSB, CNRS and Nantes University.

Assignments

The post-doctoral contract is supported by the ANR ORBIT project. This program aims at the molecular study of the Rac1 protein and members of the Rac family. The objectives of the *in silico* study of these complexes will be (i) the optimization of ligands of interest already identified, (ii) the implementation of *in silico* protocols for protein-ligand interaction energy calculations, (iii) the proposal of chemical evolution paths of promising molecules for experimental synthesis, (iv) the validation of the specificity of the innovative molecules for the target with respect to other proteins of the family.

Main activities

The candidate will need to possess or learn the following know-how and knowledge:

- Chemoinformatics training, including the use of the rdkit library (<https://rdkit.org>)
- Virtual screening and optimization of Rac1-specific small chemical entities
- Small and large scale libraries of chemical derivatives
- Decomposition of interaction analysis using Free Energy analysis, including MM-GB/PBSA
- Keep up to date with publications in the domain, but also possess excellent scientific writing skills.

Applicant's profile

- Versant: Fonction publique d'Etat
- Type of recruitment : Post-doctoral Contract, 12 months
- Scientific integrity, autonomy and rigor
- Workplace : Nantes
- Formation/ qualification : PhD, with a demonstrated knowledge of molecular modelling and/or virtual screening

Required skills and knowledge

General, theoretical or disciplinary knowledge:

The candidate shall possess a demonstrated training in structural bioinformatics and chemoinformatics with a particular focus on virtual screening and analysis. Partial profile will be considered, training shall be provided if required.

Operational skills:

Writing scientific articles
Molecular Modelling and Molecular Dynamics Modelling
Virtual screening protocols and analysis
Effective GNU/Linux knowledge
Shell and Python programming
Knowledge of AMBER modelling suite and rdkit are required

Know-how :

Scientific rigor and integrity
Team work
Scientific curiosity

Our strengths

- *45 days of annual vacation*
- *Working time 37h15*

Tips for Candidates:

Please consult the laboratory web site and our publications prior sending us full resumé, recommendations and applications. Do not hesitate to contact us prior to full application, by mail.

Deadline for applications: May 4th, 2023

Date of the recruitment committee: May 11th, 2023

Starting date: June 1st, 2023

Contact : all applications must be sent to: stephane.teletchea@univ-nantes.fr and pole-st-recrutement@univ-nantes.fr in CC and must include a resume, a cover letter and recommendation if available.