

PhD fellowship in molecular modeling and machine learning

> Entity/Service: Institute of Chemistry of Nice (ICN, UMR 7272 CNRS - UniCA)

- **Recruitment type: contract employee (1y renewable temporary contract, CDD)**
- **Category : A**
- **Working hours: full-time**
- **Location: Parc Valrose, 28 Avenue Valrose, 06000 Nice**
- **Job advertisement reference : 2026-ICN06**

The challenge

Do you have experience in machine learning and molecular simulation ?
We're looking for our future PhD student !

Join us at Université Côte d'Azur, recognized since 2016 for its scientific and educational excellence, to create a responsible and innovative university to serve as a model for the 21st century.

Within ICN, the ChemSenSim group (<https://lab.chemsensim.fr/>) develops interdisciplinary research projects on the molecular basis of chemical senses (smell and taste). Understanding the chemical ecology of an animal requires in-depth knowledge of the odors it perceives and their effects. Using computational approaches, this project aims to decode the function of insect odorant receptors. By doing so, we can identify new semiochemical compounds that manipulate insect behavior and develop more effective biocontrol methods

Your missions

This PhD project aims to elucidate the molecular mechanisms underlying pheromone detection by odorant receptors, which belong to the ion channel family, and identify new active compounds using molecular simulations. Two complementary strategies will be employed: structure-based virtual screening (docking simulations + molecular dynamics) and ligand-based virtual screening (machine learning models). We have recently demonstrated the feasibility of identifying new bioactive molecules via ML techniques [1,2] and structure-based approaches [3] and that MD simulations can capture receptor dynamics relevant to binding event [4]. Predicted ligands will be evaluated experimentally by research partners (iEES Versailles, IBS Grenoble).

Related references:

- [1] G. Caballero-Vidal et al. Sci. Rep. 2020, 1655.
- [2] Caballero-Vidal et al. Cell. Mol. Life Sci., 2021, 78, 6593-6603
- [3] Comte et al. Int. J. Biol. Sci. 2025, 21(5), 2101-2117.
- [4] Pacalon et al. Nat. Commun. 2023, 14, 8182.

This job is for you if

- you possess a master degree in computational chemistry, bioinformatics, or a related field
- you have mastered molecular modeling techniques, machine learning algorithms, and programming languages like Python
- you are highly collaborative, with excellent communication skills and a passion for interdisciplinary research
- you like tackling complex problems, working at the interface of biology, chemistry, and computer science, and publishing your results in top-tier journals

Your professional background

The candidate should hold a master's degree in chemistry, physics or biology and should have experience of molecular modelling techniques. A good knowledge of scientific computing in a Linux environment and programming skills will be highly appreciated.

Doctoral research will take place at the Institut de Chimie de Nice (UMR 7272 CNRS-UniCA) within the ChemSenSim group. The candidate will benefit from an established national and international collaboration framework.

It is essential that the candidate has skills in:

- Molecular simulation and virtual screening (molecular dynamics, docking, ...)
- Machine learning
- Data analysis

The candidate should also have:

- Good interpersonal and writing skills
- Adaptability
- Excellent command of English

Compensation and benefits

- Contractual remuneration (excluding variable compensation): ~2300 € gross per month
- Vacation: 45 days annual leave
- Partial coverage of supplementary medical insurance fees
- Access to CROUS university restaurants and cafeterias at special rates
- Tickets for entertainment and outings at preferential rates

The work environment

The Valrose Campus in Nice is a vibrant scientific hub nestled in a beautiful park, home to the Institute of Chemistry of Nice (ICN) and a hotspot for interdisciplinary research in chemistry, biology, mathematics and physics.

The little extras : Free parking, Wooded park, Sports complex/Library access,

How to apply

Interested in this ad? Don't hesitate! Apply now by email to: sebastien.fiorucci@univ-cotedazur.fr

For any questions regarding the research project, candidates can contact sebastien.fiorucci@univ-cotedazur.fr

Your application should include a CV and cover letter, which we will read carefully.

Recruitment calendar:



UNIVERSITÉ CÔTE D'AZUR

Open to Europe and to the world, Université Côte d'Azur coordinates higher-education and research activities in the Côte d'Azur region and has created an environment where education, research and innovation meet the highest standards. While engaged in a deep and ongoing transformation of its role and organization, Université Côte d'Azur is also a dynamic leader in the local region known for its exceptional quality of life between sea and mountains. In this context, Université Côte d'Azur is recognized for its excellence and is committed to human-centered values, socially engaged, and ethically responsible.

> Key figures

36 116 Students

21 Component education institutions including 8 Graduate Schools and 6 associate components

60 Laboratories and research

5432 Permanent employees

including 1,809 faculty, 1,347 administrative staff plus around 2,276 lecturers and fellow researchers at CNRS, INSERM, OCA, Inria, INRAE, etc.

> Values



WHY JOIN US ?

> A socially committed university

- Disability support
- Gender equality
- Quality of life at work
- Scientific ethics and integrity
- Prevention of discriminations
- Eco-responsible campuses

> Our benefits

- Numerous skills development programs: training and advice on careers and mobility
- Up to 2 days of telework per week, subject to the needs of the service
- 45 days of annual leave per year (full-time)
- Sustainable mobility allowance (for cycling, carpooling)
- Partial reimbursement of public transport costs
- Partial coverage of supplementary medical insurance
- Sporting activities, cultural events and social clubs
- Staff cafeteria
- Full range of French social benefits
- Parenting support



[10 good reasons to join us](#)

> Current job opportunities

- All our job offers are available on the web [Working at Université Côte d'Azur](#)
- All our positions are open to people with disabilities