



## Postdoctoral Researcher, 18 months, Computational Enzyme Design and Enzyme Mechanism Elucidation, Ecole Polytechnique and IFPEN



### Position Overview:

We are seeking a highly motivated and talented postdoctoral researcher to join our BioFUMAC interdisciplinary consortium to work on computational enzyme design and enzyme mechanism elucidation for 18 months, starting preferably in spring 2025 and at the latest in September, at Ecole Polytechnique (Palaiseau, France) and IFPEN (Rueil-Malmaison, France).

The BioFUMAC project has been selected by the French National Research Agency (ANR) in the context of Priority Research Programmes and Equipments (PEPR) B-BEST "Biomass, biotechnologies and sustainable technologies for chemistry and fuels", part of the "France 2030" investment plan. It has a five-years duration and involves six partners (INSA/TBI, INRAE/TWB, IFPEN, CEA-Genoscope, Ecole polytechnique, Université de Toulouse) with a wide range of specialities. The goal of the project is to establish a new, bio-sourced pathway to acrylic acid, a high-tonnage chemical building block for polymers, resins, coatings, sealants, and adhesives. There is no industrial process for producing bio-based acrylic acid yet. Our strategy is to obtain fumaric acid by fungal production, then convert it to acrylic acid with a newly designed decarboxylase incorporated in bacteria.

The contribution of the postdoctoral researcher is positioned at the early stage of the BioFUMAC project and focuses on the elucidation of the reaction mechanism of a decarboxylase, its engineering and optimization for the conversion of fumaric acid to acrylic acid. The successful candidate will engage in cutting-edge research at the intersection of computational biology, bioinformatics, and enzymology. This position offers an exciting opportunity to contribute to groundbreaking work that will advance our understanding of enzyme catalysis and enable the design of innovative biocatalysts, preparing for an oil-free future. We offer a rewarding and challenging job in an international environment characterized by collegial respect and responsibility.

### Qualifications:

- Ph.D. in computational/theoretical chemistry/biology, or structural bioinformatics, no more than 3 years ago.
- Proficiency in molecular modeling software and other relevant computational/programming tools.
- Good knowledge of quantum chemistry.
- Familiarity with machine learning methods applied to protein structure prediction and design.
- Experience in enzyme engineering and mechanistic studies.
- Excellent communication skills, both written and oral.
- Ability to work independently and as part of a collaborative, interdisciplinary team.

### Application Instructions:

Interested candidates should submit the following documents to Thomas Gaillard ([thomas.gaillard@polytechnique.edu](mailto:thomas.gaillard@polytechnique.edu)) and Étienne Jourdier ([etienne.jourdier@ifpen.fr](mailto:etienne.jourdier@ifpen.fr)) by March 1, 2025:

- A cover letter outlining their research interests and how their background aligns with the position.
- A detailed curriculum vitae (CV).
- Contact information for at least two references.

We are committed to fostering an inclusive and supportive research environment and encourage applications from candidates of diverse backgrounds.