18-Month Postdoctoral Position in AI/ML-driven Structural Bioinformatics/Biocomputing for Enzyme-Materials Systems - TBI-INSA, CNRS, INRAE, Toulouse, France

A Post-Doctoral position is available in **AI/ML-driven structural bioinformatics and enzyme–material interaction prediction** at **Toulouse Biotechnology Institute** (TBI) located on the grounds of INSA-Toulouse, France. The laboratory (https://www.toulouse-biotechnology-institute.fr/en/) is affiliated to the French National Research Institute for Agriculture, Food and Environment (INRAE, UMR INSA-INRAE 792) and the French National Centre for Scientific Research (CNRS, UMR INSA-CNRS 5504).

Scientific context

The transition toward sustainable, bio-based industries requires the development of more efficient and robust catalytic systems for biomass valorization. In this context, hybrid catalysis, combining chemo- and biocatalysts in a single process, represents a promising strategy for next-generation biorefineries. However, its deployment remains limited by the instability of enzymes and the lack of rational strategies to design efficient catalytic systems.

The **PEPR B-BEST** "**CALIBRATE"** project addresses this challenge by developing a systematic and predictive framework for enzyme immobilization and hybrid catalysis. It focuses on the design of catalytic biocomposites, combining enzymes with advanced materials, metal–organic frameworks (MOFs), enabling improved stability, recyclability, and catalytic performance.

The project brings together complementary expertise from leading academic partners, including Centrale Lille (UCCS), CEA Genoscope, Université Paris-Saclay / ILV, IRCELYON and TBI, covering enzyme discovery, materials science, high-throughput experimentation, AI and computational modeling.

This position offers a unique opportunity to work at the interface of AI, structural bioinformatics, and biocatalysis, contributing to the development of next-generation predictive tools for enzyme–material systems.

Position

The postdoctoral researcher will play a key role in this interdisciplinary project. He/she will develop and apply advanced computational approaches combining AI/ML, structural bioinformatics, and molecular modeling to analyze, model, and predict enzyme–MOF interactions and catalytic performance.

More specifically, the successful candidate will:

- Develop and apply computational pipelines to analyze structural and physicochemical features of enzymes;
- Analyze and integrate large-scale datasets combining enzyme, material, and experimental descriptors;
- Implement machine learning models to predict enzyme immobilization efficiency, activity, and stability;
- Contribute to the development of predictive tools for selecting optimal enzyme–support combinations;
- Work closely with experimental partners to guide validation, interpret results and iteratively improve models.

The project involves close collaboration with researchers in enzymology, materials science, AI, and biotechnology, within a highly interdisciplinary environment.

This recruitment will be carried out as a **18-month** fixed-term contract, funded by INSA Toulouse, with an expected start date **between June and early September 2026**. The position may be extended for an additional 12 months.

Candidate profile
Applicants should hold a PhD in computational biology, structural bioinformatics or machine learning applied to biomolecules.

The ideal candidate should have:

- A background in structural bioinformatics, with experience in protein 3D modelling and sequence analysis;
- Experience in machine learning and data analysis;
- Programming skills in Python;
- Experience in handling and integrating heterogeneous datasets
- Communication and organizational skills, and a clear motivation to work in a collaborative, interdisciplinary, and team-oriented environment.

We welcome candidates with diverse backgrounds at the interface of computational biology, structural bioinformatics, AI/machine learning, and molecular modelling, including applicants with a primary background in AI/ML who are motivated to deepen their expertise in structural biology and biomolecular systems.

Application
Applicants should send as soon as possible a detailed curriculum vitae, a letter of intent explaining their motivations for the position, and contact details of at least two references to:
Sophie Barbe (sophie.barbe@insa-toulouse.fr) and **David Camilo Corrales Munoz** (corrales@insa-toulouse.fr)