

18-Month Postdoctoral Position in AI/ML Structural Bioinformatics (Biocomputing) - TBI-INSA, CNRS, INRAE, Toulouse, France

A Post-Doctoral position is available in AI/ML Structural Bioinformatics (Biocomputing) 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 climate emergency calls for a transition from fossil-based economies toward sustainable, bio-based systems. In this context, lignocellulosic biomass (LCB) represents one of the most abundant renewable carbon resources available for building a circular bioeconomy. However, LCB is intrinsically recalcitrant and requires the coordinated action of multiple enzymes to be efficiently deconstructed. In nature, microbial systems achieve this through optimized enzyme synergies, where enzymes act in close proximity and in a coordinated manner. Understanding and reproducing these synergistic effects remain a major scientific and technological bottleneck.

The **PEPR B-BEST “Nanomachines”** project aims to address this challenge through a unique combination of large-scale enzyme discovery, high-throughput experimental screening, high-content product profiling, and AI-based modeling, analysis and prediction. It brings together complementary expertise from several leading academic and applied research partners, including Toulouse Biotechnology Institute (TBI), CEA Genoscope, Aix-Marseille Université / AFMB, INRAE BBF Marseille, and IFP Energies nouvelles (IFPEN). Together, these efforts aim to generate new knowledge on enzyme activity and cooperation, and to enable the rational design of optimized multi-enzyme systems.

This postdoctoral position offers the opportunity to work at the frontier of AI-driven biology, tackling fundamental questions with strong impact on biotechnology and sustainable chemistry.

Position

The postdoctoral researcher will play a key role in this interdisciplinary project. He/she will be responsible for developing and applying computational approaches combining AI (machine/deep learning) and structural bioinformatics to analyze and predict enzyme synergies involved in lignocellulosic biomass deconstruction.

More specifically, the successful candidate will:

- analyze and integrate heterogeneous datasets including enzyme sequences, 3D structures, functional annotations, and experimental product profiles;
- develop ML-based predictive approaches to identify enzyme combinations with enhanced synergy and/or controlled product formation;
- investigate sequence–structure–function relationships underlying enzyme cooperation;
- contribute to biodiversity mining and the identification of novel candidate enzyme combinations;
- interact closely with experimental partners to guide validation and iterative improvement of predictive models.

The project will involve close collaboration with researchers in enzymology, structural biology, bioinformatics, AI, and biotechnology, within a highly stimulating interdisciplinary environment.

This recruitment will be carried out as an **18-month** fixed-term contract, funded by INSA Toulouse. The position should ideally **start between June and early September 2026**.

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;
- 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 backgrounds at the interface of computational biology, structural bioinformatics and AI/machine learning, 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)