

# André Lanrezac

Bioinformatician | Scientific Developer

📧 <https://lanzac.github.io>

📍 Paris, France

🔗 [github.com/lanzac](https://github.com/lanzac)

✉ [a.lanrezac@gmail.com](mailto:a.lanrezac@gmail.com)

## Education

**Ph.D. in Bioinformatics** - Université Paris Cité

2023

**B.S. in Biology ⇒ M.S. in Bioinformatics** - Sorbonne Université, Paris

2019

## Experience

**Research Assistant ⇒ Research engineer**

Nov 2019 - June 2024

Laboratoire de Biochimie Théorique, IBPC · CNRS, Paris

Supervised by Dr. Marc Baaden

- Lead author of a review article on interactive molecular simulations (IMS) [1]
- Extended and optimized the molecular-visualization software UnityMol (Unity, C#) and the BioSpring engine (C++) to simulate protein insertion into implicit membranes (analytical model), including real-time interaction and monitoring of simulation data [2,3,5]
- Developed UNILIPID, a multiscale methodology to describe lipid–protein interactions in simple, bilayer or curved implicit membranes, with parameterization reproducing experimental hydrophobicity scales [3]
- Implemented CI/CD pipelines (GitHub Actions, Docker) to facilitate maintenance and open-source distribution of the interactive suite

**Bioinformatics Drug Design Intern**

Feb 2019 - June 2019

Bioinformatics & Biophysics Research Team, IMPMC · Sorbonne université, Paris

Supervised by Dr. Dirk Stratmann

- Developed an automated protocol coupling REMD (GROMACS) and molecular docking (AutoDock4/Vina) for docking cyclic peptides into allosteric protein pockets
- Implemented and validated the workflow on a crystallographic model system (streptavidin–cyclic ligand), including conformational sampling, clustering, large-scale docking and RMSD/energy analysis
- Designed and evaluated allosteric cyclic peptides targeting caspase-3, integrating REMD, docking and preliminary receptor-flexibility tests (HADDOCK)

**Bioinformatics Structural Analysis Intern**

July 2018

Atelier de bioinformatique (ABI), ISYEB · Sorbonne université, Paris

Supervised by Dr. Mathilde Carpentier

- Continued development of YAKUSA, a fast protein structural similarity search tool based on shared high-scoring structural pairs (SHSPs)
- Re-implemented Bellman's algorithm (Python) to compute the longest path through shared motifs and optimize similarity search
- Developed heuristic algorithms to accelerate structural alignment and improve matching speed

## Skills

### Programming

Python, C++, C# (Unity), Bash

### Bioinformatics

VMD, GROMACS, AutoDock, HADDOCK, Chimera

### Web & Data Viz

Django (PostgreSQL), Plotly, HTML, CSS, Bootstrap 5

### Software Engineering & CI/CD

Git, GitHub Actions, Docker, pytest

### Languages

French (native), English (proficient), Mandarin (beginner)

## Publications

- 1 André Lanrezac, Nicolas Férey, and Marc Baaden. "Wielding the power of interactive molecular simulations". WIREs Computational Molecular Science (July 2022). DOI:10.1002/wcms.1594.
- 2 André Lanrezac et al. "Fast and Interactive Positioning of Proteins within Membranes". Algorithms (Nov. 2022). DOI:10.3390/a15110415.
- 3 André Lanrezac and Marc Baaden. "UNILIPID, a Methodology for Energetically Accurate Prediction of Protein Insertion into Implicit Membranes of Arbitrary Shape". Membranes (Mar. 2023). DOI:10.3390/membranes13030362.
- 4 André Lanrezac, Nicolas Férey, and Marc Baaden. "Interactive Molecular Dynamics". Reference Module in Chemistry, Molecular Sciences and Chemical Engineering. Elsevier, 2023. DOI:10.1016/B978-0-12-821978-2.00115-X.
- 5 Laurent B, Lanrezac A, Santuz H, Férey N, Delalande O, Baaden M. "BioSpring: An elastic network framework for interactive exploration of macromolecular mechanics". Protein Science (April 2025). DOI:10.1002/pro.70130/

## Personal projects

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**OpenNutriLab** Open-source web application for nutrition

**Jan 2025 - Present**

🔗 [github.com/lanzac/OpenNutriLab](https://github.com/lanzac/OpenNutriLab)

- Developing an open-source web application using Python/Django that leverages public databases (OpenFoodFacts and Ciqual / ANSES) to analyze food products and their nutritional composition. The project is intended as a public-service decision-support tool for nutrition; it is in an early stage but actively developed.

**Development environment:** Python 3.13 & Django | Docker / DevContainer, Uvicorn | PostgreSQL | Bootstrap 5, Node.js & npm, Webpack | pytest, pyright | uv