André Lanrezac

Bioinformatician | Scientific Developer
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Education

Ph.D. in Bioinformatics - Université Paris Cité **2023**
B.S. in Biology ⇛ M.S. in Bioinformatics - Sorbonne Université, Paris **2019**

Experience

Research Assistant ⇛ Reseach 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, Ferey 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/