

André Lanrezac

Bioinformatician | Scientific Developer

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Education

Ph.D. in Bioinformatics – Université Paris Cité

2023

Supervised by Dr Marc Baaden

B.S. in Biology & M.S. in Bioinformatics – Sorbonne Université, Paris

2019

Experience

Research Assistant & Research engineer

Nov 2021 - June 2024

Laboratory of Theoretical Biochemistry, IBPC · CNRS , Paris

- Lead author of a review article on interactive molecular simulations (IMS) [1], summarizing decades of work by the scientific community
- Enhanced the molecular visualization software UnityMol (Unity, C#) and the molecular engine BioSpring (C++) for real-time experiments on protein insertion into an analytical membrane [2, 3]
- Developed UNILIPID, a method and specialized bioinformatic Python tool for adapting implicit lipid-protein membrane parameters across all-atom and coarse-grained models, enabling interactive simulations with curved membrane geometries [3]
- Participated in the maintenance and release process of BioSpring by building a CI/CD pipeline (GitHub Actions, Docker) to automate releases, resolve multi-year dependency issues, and enhance software accessibility

Bioinformatics Drug Design Intern

Feb 2019 - June 2019

Bioinformatics Research Team, ISYEB · Sorbonne université , Paris

- Developed a workflow combining Autodock with REMD simulations in GROMACS to assess binding affinity and stability of cyclic peptides, comparing results with HADDOCK to optimize peptide designs
- Manually designed cyclic peptides using UCSF-Chimera to optimize sequences and structures for targeted protein pockets, ensuring high binding affinity and stability

Bioinformatics Structural Analysis Intern

July 2018

Bioinformatics Research Team, ISYEB · Sorbonne université , Paris

- Optimized a protein similarity search by re-implementing Bellman's algorithm (Python) to find the longest path through shared motifs, and developing heuristic algorithms for faster matching

Skills

Programming: Python, C++, C#, Bash, C, HTML, CSS

Softwares & Frameworks: Django, React, Unity, CMake, SQL

DevOps: Git, CI/CD (GitHub Actions), Docker

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.