André Lanrezac

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Bioinformatician | Scientific Developer
lanzac.github.io

Education

Université Paris Cité – Ph.D. in Bioinformatics 2023
Advisor: Dr Marc Baaden

Sorbonne Université, Paris – B.S. in Biology & M.S. in Bioinformatics 2019

Experience

Research Assistant & Reseach engineer 2019 – 2024
Laboratory of Theoretical Biochemistry, IBPC · CNRS , Paris

- Led the writing of the first detailed review article on interactive molecular simulations (IMS) [1] synthesizing decades of community research and published in a high-impact journal
- Enhanced a 3D molecular visualization interface (Unity, C#) for real-time interaction and visualization of protein-membrane insertion studies [2, 3]
- Standardized multi-threaded workflows (C++, C#) for real-time simulation control and monitoring, enabling seamless data exchange and live analysis of system state properties
- Developed specialized Python algorithms adapting all-atom implicit membrane models to coarse-grained Martini3, enabling interactive simulations with curved membrane geometries [3]
- Built a CI/CD pipeline (GitHub Actions, Docker) automating simulation engine releases, resolving multi-year dependency issues, and ensuring broader software accessibility

Bioinformatics Drug Design Intern Feb 2019 – June 2019
Bioinformatics and biophysics team, IMPMC · Sorbonne université , Paris

- Developed a workflow combining Autodock with REMD simulations in GROMACS (using a national supercomputer), and compared the results with HADDOCK
- Manual design of cyclic peptides with UCSF-Chimera

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: Python3, C++, C# , Bash, C, HTML, CSS
Technologies: Git, CI/CD (GitHub Actions), Docker, Unity, GDB, LLDB, CMake, MongoDB
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.