André Lanrezac

Bioinformatician | Scientific Developer
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Education

Ph.D. in Bioinformatics – Université Paris Cité **2023**
Supervised by Marc Baaden
B.S. in Biology & M.S. in Bioinformatics – Sorbonne Université, Paris **2019**

Experience

Research Assistant & Reseach engineer **Nov 2019 - 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, 5]
- Developed UNILIPID, a method and specialized bioinformatic Python tool for adapting lipid–protein interaction parameters, enabling the extension of implicit membrane representations from all-atom to coarse-grained models, and allowing 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
Supervised by Dirk Stratmann

- 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
Supervised by 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#, 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.

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/