André Lanrezac

Bioinformatician — Scientific Developer

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https://lanzac.github.io/

Skills

Programming languages: Python3, C++11, C#, Bash, C, Unix, HTML/CSS

Development tools: git, gdb, lldb, CMake, Unity, Docker, Pixlr E, Jekyll, MongoDB, Streamlit

Scientific software: VMD, PyMol, APBS, GROMACS, NAMD, HADDOCK, Desmos, AutoDock, Chimera, HADDOCK

OS: macOS, Linux

Communication: Apple/Microsoft office suites, Website design, Authorea, LaTeX

Languages: French (native), English (proficient)

Experience

Laboratory of Theoretical Biochemistry, CNRS — Paris

Research Assistant & Reseach engineer — *2019 – 2024*

- Lead author of an advanced review on interactive molecular simulations (IMS) [1]
- Development of a software suite integrating visualisation and molecular simulation with human interaction [2, 3]
- Exploratory research on MDverse web app for large-scale molecular simulation data analysis.

Institute of Mineralogy, Physics of Materials and Cosmochemistry, CNRS — Paris

Bioinformatics Drug Design Intern — *2019*

- Developed a cyclic peptide docking method by combining Autodock with REMD simulations in GROMACS, and compared the results with the HADDOCK docking tool.
- Manual design of cyclic peptides with UCSF-Chimera.

Institute of Systematics, Evolution and Biodiversity, CNRS — Paris

Bioinformatics Structural Analysis Intern — *2018*

- Contributed to developing a program for rapid protein structure similarity searches. (Python, C).

Projects

BioSpring *Developer • C++* — *2019 – Present*

Interactive simulation engine based on an extended elastic network model.

UnityMol *Developer • C#* — *2019 – Present*

Molecular viewer using Unity game engine.

MDDriver *Developer • C* — *2019 – Present*

Socket for data communication of molecular simulation software.

UNILIPID *Designer & Developer • Python3* — *2019 – Present*

UNiversal Implicit LIPId-protein Description. It is versatile implicit lipid-protein framework for modeling membrane interactions across multiple scales, offering support for complex membrane geometries, and advanced user features like real-time analysis.

NutoMetrics *Designer & Developer • Python3, MongoDB, Streamlit* — *2024 – Present*

Side project application that performs detailed nutritional analysis by inventorying food products and analyzing their nutrients. The app provides users with a scientific overview of their dietary intake and allows for experimental combinations of foods to optimize nutritional value.

Education

Université Paris Cité — Paris

Ph.D. in Bioinformatics — *2019 – 2023*

Advisor: Dr Marc Baaden

Sorbonne Université — Paris

B.S. in Biology & M.S. in Bioinformatics — *2014 – 2019*

Publications

[1] André Lanrezac, Nicolas Férey, and Marc Baaden. "Wielding the power of interactive molecular simulations". *WIREs Computational Molecular Science* 12.4 (July 2022).

[2] André Lanrezac et al. "Fast and Interactive Positioning of Proteins within Membranes". *Algorithms* 15.11 (Nov. 2022), p. 415.

[3] André Lanrezac and Marc Baaden. "UNILIPID, a Methodology for Energetically Accurate Prediction of Protein Insertion into Implicit Membranes of Arbitrary Shape". *Membranes* 13.3 (Mar. 2023), p. 362.

[4] André Lanrezac, Nicolas Férey, and Marc Baaden. "Interactive Molecular Dynamics". *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*. Elsevier, 2023, B978012821978200115X.