André Lanrezac

Bioinformatician | Scientific Developer

Education

Ph.D. in Bioinformatics - Chemistry Physics • Nov, 2019 — Apr, 2023

Laboratory of Theoretical Biochemistry - CNRS, France

"Interpretation of experimental data through interactive simulation and molecular visualization"

M.S. in Bioinformatics and Modelisation • 2017 — 2019

Sorbonne Université, Paris

Structural bioinformatics and modelisation

B.S. in Molecular and cellular biology • 2014 — 2017

Université Pierre et Marie Curie, Paris

Biology, Bioinformatics

Experience

Reseach engineer

Laboratory of Theoretical Biochemistry, CNRS, France • Sep, 2023 — Jun, 2024

- **Research**: MDverse web app for large-scale molecular simulation data analysis.
- **Development**: Molecular simulations software suite (Unity, C#, C++, Python, C)

Research Assistant

Laboratory of Theoretical Biochemistry, CNRS, France • Nov, 2019 — Apr, 2023

- 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] (Unity, C#, C++, Python, C)

Bioinformatics Drug Design Intern

Institute of Mineralogy, Physics of Materials and Cosmochemistry, Sorbonne Université - CNRS, France • 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.

Bioinformatics Structural Analysis Intern

Institute of Systematics, Evolution and Biodiversity, Sorbonne Université - CNRS, France • 2018

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

Skills

Languages : French (native), English (proficient)

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

Communication : Apple/Microsoft office suites, Website design (HTML/CSS), Authorea, $\LaTeX$

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

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

OS : macOS, Linux

Publications & scientific production

Publications:

[4] Lanrezac A, Férey N, Baaden M. "*Interactive Molecular Dynamics*" Reference Module in Chemistry, Molecular Sciences and Chemical Engineering (2023) DOI: 10.1016/B978-0-12-821978-2.00115-X

[3] Lanrezac A, Baaden M. "*UNILIPID, a Methodology for Energetically Accurate Prediction of Protein Insertion into Implicit Membranes of Arbitrary Shape*" Membranes (2023) DOI: 10.3390/membranes13030362

[2] Lanrezac A, Laurent B, Santuz H, Férey N, Baaden M. "*Fast and Interactive Positioning of Proteins within Membranes*" Algorithms (2022) DOI: 10.3390/a15110415

[1] Lanrezac A, Férey N, Baaden M. "*Wielding the power of interactive molecular simulations*" WIREs Comput Mol Sci (2021) DOI: 10.1002/wcms.1594

Poster:

(1) Lanrezac A, Férey N, Baaden M. "*Combining human interaction and empirical data using interactive elastic network models*" EMBO Workshop: Advances and Challenges in Biomolecular Simulations (2021)

Softwares & Tools

I pursued the development of BioSpring, UnityMol and MDDriver during my thesis, and they are currently my side project. These are projects developed by Marc Baaden's team at the Theoretical Biochemistry Laboratory.

- `BioSpring` : Interactive simulation engine based on an extended elastic network model
Developer • 2019 — 2024 • C++11

- `UnityMol` : Molecular viewer
Developer • 2019 — 2024 • C#

- `MDDriver` : Socket for data communication
Developer • 2019 — 2024 • C

- `LIPTUNE` : ***L**everaging **I**MPALA **P**arameterization **T**echnique **U**sing **N**ew **E**nergies* [4]. The tool tests 4 methods to calibrate each amino acid and obtain a set of hydrophobicity parameters to improve protein insertion with the IMPALA membrane analytical model. The approach can be used for any type of representation, from atomic to coarse-grained scales.
Designer & Developer • 2023 • Python3

- `AlimBDD` : 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.
Designer & Developer • 2024 — Now • Python3, MongoDB, Streamlit

Outside Interests

Sport : Climbing (boudering), badminton, cycling

Miscellaneous : Music (funk, new-disco, electronic, trip hop, classical), science (physics, astronomy), computer science (qualified in Google CodeJam 2022), coffee enthusiast, chess.

Social Links

- **Github**: https://github.com/lanzac
- **LinkedIn**: https://www.linkedin.com/in/andre-lanrezac
- **ResearchGate**: https://www.researchgate.net/profile/Andre-Lanrezac
- **Mail**: a.lanrezac@gmail.com

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