Jérôme **Rihon**

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PhD candidate in Molecular Modeling, Free and Open-Source Software enthusiast, toolmaker

About me

Currently a PhD candidate on the topic of modified nucleic acids by means of *in silico* research. I use computational chemistry to characterise nucleosides and perform simulations to understand their structural dynamics. I program to optimise research methodologies. Coming from a pharmaceutical background, I bring the best of both worlds.

I am interested in writing performant libraries for chem- and bioinformatics tools, targetting developers as my audience.
Open to academic and industry positions.

Professional and Education

PhD in Pharmaceutical Sciences
2020 - Present

Rega Institute for Medical Resarch, Catholic University of Leuven, Leuven
BE

- Thesis: *Molecular modeling tools to improve and expand computational research on synthetic nucleic acids* (Supervisors : prof.dr. E. Lescrinier, prof.dr. V.B. Pinheiro)
- Researching the fundamentals of (xenobiotic) nucleic acids through computational chemistry and molecular modeling
- Software development to facilitate computational research on nucleic acids
- Teaching assistant in the Biopharmaceutical Analysis practical courses

Keywords : Molecular Dynamics, Computational Chemistry, Python, Rust, Linux, Shell, Linear Algebra

Master of Drug Design and Development (*cum laude*)
2018 - 2020

Catholic University of Leuven, Leuven
BE

- Thesis: *Development of an allergophore to predict and analyse cross-reactivity in corticosteroid-mediated drug allergy* (Supervisor : prof.dr. E. Lescrinier)

Keywords : Molecular Dynamics, Linux, Shell, Molecular Docking

Bachelors of Pharmaceutical Sciences
2013 - 2018

Catholic University of Leuven, Leuven
BE

Projects

- **Ducque : the Mechanical Nucleic Acid Architect.** Build virtual 3D models of synthetic and natural nucleic acids. Used to design and predict duplex structures through a rigorous *in silico* methodology. Provides interface for users to implement custom chemistries. Written in Python3. Sole developer of the tool. jrihon/Ducque
- **Pucke.rs : A CLI tool to generate conformational landscapes for peptides, fivering and sixring systems.** Part of a full *in silico* pipeline to design and predict nucleic acid structures. Written in Rust. Sole developer of the tool. (Manuscript in submission)
- **Pucke.py : A library to generate conformational landscapes, calculate puckering coordinates and geometric properties.** Part of a full *in silico* pipeline to design and predict nucleic acid structures. Extends pucke.rs with additional functions. Backend in Rust, wrapped with Python3. Sole developer of the tool. (Manuscript in submission)
- **Mutineer : an extensible NeoVim tool to (un)comment in your desired programming language.** Simplify (un)commenting by a keystroke. jrihon/mutineer.lua
- **Solve Rosalind Bioinformatics problems in Rust.** Solved 20 problems to acquire Doctoral School course credits, on topics outside of my research. Rosalind Challenge

Competencies

Informatics

- Python (Software development, figures, scripting)
- Shell (Scripting, sysadmin)
- LaTeX (Manuscripts, presentations)
- Rust (Software development)
- Typst (PhD thesis, this CV)
- Lua (NeoVim plugins)

Languages

- Dutch (native)
- English
- French

Software knowledge

- **Operating System** : I main GNU/Linux on all machines, but am comfortable on Windows and MacOS.
- **Scientific Software** : ORCA for quantum mechanics applications, AMBER MD for atomistic simulations of biomolecular systems.
- **Graphic Design** : Proficient in InkScape for vectorised figures. Matplotlib for all generated graphs.
- **Dev. Environment** : NeoVim for programming and general text manipulation purposes. Tmux to keep track of multiple projects. Git for version control.

Other skills

Student Associations

- **LHC Plutonica** Secretary (2020-2021): Design template for annual magazine. Document and virtualise all activities.
- **LHC Plutonica** Treasurer (2019-2020): Doubled cashflow w.r.t. the previous fiscal year. Introduced online management of funds. Established LHC Plutonica as a factual association.
- **Hades** Vice President (2018-2019): Supportive role to the president of the association.
- **Farmaceutica** Faculty Bar Manager (2015-2017): Responsible for all bar events. Manage inventory, maintain communication with distributors. General upkeep.
- **Farmaceutica** Cantor (2016-2017): Head organiser and lead in all cantus events. Organised small events on student culture.

Teaching assignments

- **Teaching assistent**: Guide and supervise 3rd Bachelor Pharmaceutical Sciences students in the lab practicals of "Biopharmaceutical Analysis" (2020-Present, KU Leuven).
- **Supervisor** : Guide a master's student on the topic of nucleic acid *in silico* research (2022-2023, Rega Institute for Medical Research). Student continues as colleague PhD.
- **Tutor** : Tutor in Chemistry for students taking part in the medicine and dentistry entrance exam (2018-2020, Slaagsleutels in Leuven).

Publications

1. **Rihon J.**, Mattelaer C.-A., Montalvão R.W., Froeyen M., Pinheiro V.B. & Lescrinier E. (2024, Feb) "Structural insights into the morpholino nucleic acid/RNA duplex using the new XNA builder Ducque in a molecular modeling pipeline". *Nucleic Acids Research*. 10.1093/nar/gkae135

2. **Rihon J.**, Reynders S., Pinheiro V.B. & Lescrinier E. (Manuscript in submission) "The pucke.rs toolkit to facilitate sampling the conformational space of biomolecular monomers".

3. Schofield P., Taylor A.I., **Rihon J.**◆, Martinez C.D.P., Zinn S., Mattelaer C.-A., Jackson J., Dhaliwal G., Schepers G., Herdewijn P., Lescrinier E., Christ D. & Holliger P. (2023, Jul) "Characterization of an HNA aptamer suggests a non-canonical G-quadruplex motif". *Nucleic Acids Research*. 51 (15), 10.1093/nar/gkad592

4. Mattelaer C.-A., Mattelaer H.-P., **Rihon J.**, Froeyen M. & Lescrinier E. (2021, May) "Efficient and Accurate Potential Energy Surfaces of Puckering in Sugar-Modified Nucleosides". *Journal of Chemical Theory and Computation*. 17 (6), 10.1021/acs.jctc.1c00270

5. Xu Y., Groaz E., **Rihon J.**, Herdewijn P. & Lescrinier E. (2023, Jul) "Synthesis, antiviral activity, and computational study of β-d-xylofuranosyl nucleoside phosphonates". *European Journal of Medicinal Chemistry*. 10.1016/j.ejmech.2023.115379

6. Depuydt A.-S., **Rihon J.**◆, Cheneval O., Vanmeert M., Schroeder C.I., Craik D.J., Lescrinier E., Peigneur S. & Tytgat J. (2021, Jun) "Cyclic Peptides as T-Type Calcium Channel Blockers: Characterization and Molecular Mapping of the Binding Site". *ACS Pharmacology and Translational Science*. 4 (4), 10.1021/acsptsci.1c00079

7. **Rihon J.** (2022, Sep) "Synthetic biology in action: beyond standard metabolism". *European Molecular Biology Organization (EMBO)*. Download poster

◆ joint first-author