

Profile

I am a driven life scientist with a Master's degree in Biochemistry and Biotechnology from the University of Antwerp. I have expertise in molecular biology, bioinformatics, and statistical analysis. Currently, I am pursuing a PhD in computational drug discovery, in collaboration with Eurofins-VillaPharma at UCAM and under the supervision of Prof. Horacio Pérez-Sánchez. The main focus of my PhD is both the development and application of novel computational drug discovery techniques.

Education

UCAM Universidad Católica San Antonio de Murcia | Murcia, Spain **2021-Present**

PhD-student at BIO-HPC

- Scope: The discovery and optimization of ligands against protein targets using computational drug discovery techniques
- Key words: *in silico* drug design, molecular docking, virtual screening
- Thesis Director: Prof. Horacio Pérez-Sánchez

University of Antwerp | Antwerp, Belgium **2018-2021**

MSc Biochemistry and Biotechnology

- Major: Systems biology
- Minor: Research
- Key Modules: Datamining, Applied Bioinformatics, Protein technology and Proteomics, Medical Cell Biology, Gene and Genome technology
- Master Thesis (February – June 2021)
 - Title: *FEP viewer: a user-friendly webtool to display free energy perturbation calculations*
 - Summary: Development of an easy-to-use webtool which is able to orderly display previously performed free energy perturbation (FEP) calculations, as well as initiating new FEP calculations.
 - Promotor: Prof. Hans De Winter
 - Laboratory of Medicinal Chemistry (UAMC), University of Antwerp
- FELASA A,B,C accreditation

University of Antwerp | Antwerp, Belgium **2015-2019**

BSc Biochemistry and Biotechnology

- Key Modules: Bioinformatics, (Bio)Statistics, Organic Chemistry, Molecular Biology, Genetics, Cellular Biology, Immunology, Integrated Metabolism
- Internship associated with Bachelor Thesis (March-April 2019)
 - Title: *Systematic meta-analysis of resistance markers for Isoniazid of Mycobacterium tuberculosis*
 - Promotor: Prof. Kris Laukens, Supervisor: Emmanuel Rivière

- Adrem Datalab, University of Antwerp
- The results from this internship contributed to a published paper, which resulted in co-authorship: <https://doi.org/10.1016/j.cmi.2020.07.004>

Experience

Internships

Laboratory of Medicinal Chemistry (UAMC) | University of Antwerp

August 2020

Voluntary Internship

Development of a pharmacophore-based conformational sampling tool for small molecules under the supervision of Prof. Hans De Winter.

Biomina | University of Antwerp

July 2020

Voluntary Internship

Development of a Python script which is able to visualize molecular structures in the world Minecraft, a popular 3D game. After providing a SMILES-string as input, the script can build the corresponding molecule in the 3D environment of a Minecraft world as either a 2D or 3D molecular structure. This project was performed in association with Biomina, under the supervision of Prof. Kris Laukens.

Biomina | University of Antwerp

July 2019

Voluntary Internship

Development of several Python scripts in order to largely automate the workflow of utilizing their in-house developed TCRex tool. This webtool can be used to predict TCR-epitope binding for human T-cell receptors. This project was completed at Biomina, under the supervision of Prof. Kris Laukens.

Evonik | Antwerp, Belgium

July 2018

Student Job

Laboratory Assistant at the environmental lab of Evonik Antwerp.

Conferences

- Using consensus molecular docking for the discovery of Wee1 inhibitors in the context of cancer, II Symposium on Chemical and Physical Sciences for Young Researchers, 24/03/2022-25/03/2022, Universidad de Murcia
- Optimizing Consensus docking by incorporating predicted binding pose similarity: a Wee1 case study, I Simposio de Estudiantes Hispanohablantes de Bioinformática y Biología Computacional, 02/06/2022-03/06/2022, Online (SEH2Bioinfo)
- Optimizing consensus docking by incorporating predicted binding pose similarity: a Wee1 case study, VIII Jornadas de Investigacion y Doctorado, 24/06/2022, UCAM
- Visualizing the Impact of Chemical Substructures on Compound Activity for Improving the Drug Discovery Process, III Symposium on Chemical and Physical Sciences for Young Researchers, 15/06/2023-16/06/2023, Universidad de Murcia
 - Awarded a prize for the **best Flash presentation**
- Unpacking the Black Box: Understanding Machine Learning models to Aid the Drug Discovery Process, IX Jornadas de Investigacion y Doctorado, 23/06/2023, UCAM

- Visualizing Molecular Impact: Understanding the Role of Substructures in Drug Activity Prediction, II Congreso Estatal de Estudiantes de Biociencias (CEEBI), 18/07/2023-21/07/2023, Universidad de Granada
 - Also paired with an article in the Spanish magazine “Hidden Nature” (ISSN 2531-0402) titled “[Descodificando la caja negra: Mejorando y guiando el descubrimiento de fármacos usando inteligencia artificial e interpretabilidad de las subestructuras moleculares](#)”.

Publications

- J. Nelen, M. Carmena-Bargueño, C. Martínez-Cortés, A. Rodríguez-Martínez, J. M. Villalgordo-Soto, and H. Pérez-Sánchez, “ESSENCE-Dock: A Consensus-Based Approach to Enhance Virtual Screening Enrichment in Drug Discovery,” *J. Chem. Inf. Model.*, p. acs.jcim.3c01982, Feb. 2024, doi: 10.1021/acs.jcim.3c01982.
- G. Dakpa, K. J. S. Kumar, J. Nelen, H. Pérez-Sánchez, and S.-Y. Wang, “Antcin-B, a phytosterol-like compound from *Taiwanofungus camphoratus* inhibits SARS-CoV-2 3-chymotrypsin-like protease (3CLPro) activity in silico and in vitro,” *Sci Rep*, vol. 13, no. 1, p. 17106, Oct. 2023, doi: 10.1038/s41598-023-44476-x.
- E. Rivière, M. G. Whitfield, J. Nelen, T. H. Heupink, and A. Van Rie, “Identifying isoniazid resistance markers to guide inclusion of high-dose isoniazid in tuberculosis treatment regimens,” *Clinical Microbiology and Infection*, vol. 26, no. 10, pp. 1332–1337, Oct. 2020, doi: 10.1016/j.cmi.2020.07.004.

Additional Skills

- **Languages:** Dutch (Native), English (Fluent), Spanish (Novice), French (Notion)
- **Microsoft Office:** Proficient in Word, Excel and PowerPoint
- **Programming Languages:** Python (Advanced), R (Intermediate), Java (Intermediate), HTML (Intermediate), CSS (Intermediate), JavaScript (Intermediate), PHP (Novice)