Jochem Nelen

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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.

Teaching

Physics and Chemistry | Grado en Veterinaria | UCAM **Sep-Dec 2024**

Taught Physics and Chemistry to 1st-year Bachelor of Veterinary Sciences students (4.5 ECTS), delivering 60 hours of instruction, including theory lectures and supervised laboratory sessions, while also grading practical reports and providing feedback to students.

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

- Nelen J, Pérez-Sánchez H, De Winter H, Van Rompaey D. Matched pairs demonstrate robustness against inter-assay variability. Journal of Cheminformatics 2025;17:8. https://doi.org/10.1186/s13321-025-00956-y.
- Grzelczyk J, Pérez-Sánchez H, Nelen J, Carmena-Bargueño M, Gałązka-Czarnecka I, Budryn G, et al. Interaction of an anticancer oxygenated propenylbenzene derivatives with human topoisomerase II α and actin: molecular modeling and isothermal titration calorimetry studies. J Therm Anal Calorim 2024. https://doi.org/10.1007/s10973-024-13569-8.
- Rodríguez-Martínez A, Nelen J, Carmena-Bargueño M, Martínez-Cortés C, Luque I, Pérez-Sánchez H. Enhancing MD simulations: ASGARD's automated analysis for GROMACS. Journal of Biomolecular Structure and Dynamics 2024:1–13. https://doi.org/10.1080/07391102.2024.2349527.
- Nelen J, Carmena-Bargueño M, Martínez-Cortés C, Rodríguez-Martínez A, Villalgordo-Soto JM, Pérez-Sánchez H. ESSENCE-Dock: A Consensus-Based Approach to Enhance Virtual Screening Enrichment in Drug Discovery. J Chem Inf Model 2024;64:1605–14. https://doi.org/10.1021/acs.jcim.3c01982.
- Dakpa G, Kumar KJS, Nelen J, Pérez-Sánchez H, Wang S-Y. 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 2023;13:17106. https://doi.org/10.1038/s41598-023-44476-x.
- Rivière E, Whitfield MG, Nelen J, Heupink TH, Van Rie A. Identifying isoniazid resistance markers to guide inclusion of high-dose isoniazid in tuberculosis treatment regimens. Clinical Microbiology and Infection 2020;26:1332–7. https://doi.org/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)