Jochem Nelen

Computational Chemist

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PROFILE

Computational chemist specialised in virtual screening, structure-based drug discovery, and protein–ligand modelling. My current postdoctoral research at the University of Oxford, as part of the OpenBind consortium, focuses on protein–ligand binding prediction, benchmark development, and the curation of large-scale structural and affinity datasets. During my PhD, which I completed summa cum laude, I developed consensus-based virtual screening methods and applied them to hit identification and lead optimisation projects in collaboration with academic and industrial partners. My research interests include robust benchmarking, reproducible computational workflows, and the integration of physics-based and machine-learning approaches for drug discovery.

RESEARCH EXPERIENCE

Oxford Protein Informatics Group (OPIG), University of Oxford 2025 – Present
Postdoctoral Research Associate Oxford, UK

Work within the OpenBind consortium on computational methods for structure-based drug discovery, with a focus on protein–ligand binding prediction, data curation, benchmark design, and method evaluation:

- Curate and analyse protein–ligand structural and affinity datasets for benchmarking classical docking, virtual screening, and co-folding approaches.
- Contribute to benchmark design and model evaluation workflows, including AlphaFold3-based assessments and comparison with classical structure-based methods.
- Support the design and prioritisation of compounds for experimental testing in collaborative discovery projects.
- Collaborate with researchers developing next-generation co-folding methods, including OpenFold3-related work, to connect benchmarking and dataset design with model development needs.

BIO-HPC, UCAM Universidad Católica San Antonio de Murcia Oct. 2021 – Oct. 2025
Doctoral Researcher Murcia, Spain

- Developed and applied consensus-based virtual screening strategies as part of my PhD thesis in close collaboration with Eurofins-Villapharma.
- Developed ESSENCE-Dock, a consensus docking pipeline for improving virtual screening enrichment.
- Developed ConFiLiS, a consensus fingerprint screening method for ligand-based hit identification.
- Applied computational–experimental workflows to kinase inhibitor discovery, including WEE1, DDR1, and p38α projects.
- Published first-author research in peer-reviewed journals and contributed as co-inventor to a Spanish patent.

McCarthy Team, EMBL Grenoble Jun. 2024 – Jul. 2024
Visiting Research Intern Grenoble, France

- Investigated *T. gondii* CPSF4-YTH inhibition using crystallographic fragments as starting points.
- Built structure-guided pharmacophore models for fragment-informed virtual screening and explored fragment linking with DiffLinker to generate potential lead-like candidates.

UAMC, University of Antwerp Apr. 2024 – Jun. 2024
Visiting Research Intern Antwerp, Belgium

- Assessed inter-assay variability in ChEMBL bioactivity datasets using matched-pair analysis and custom curation pipelines.
- Worked in collaboration with Dries Van Rompaey at Drug Discovery Data Sciences, Janssen Pharmaceutica NV.

EDUCATION

UCAM Universidad Católica San Antonio de Murcia Oct. 2021 – Oct. 2025
PhD in Health Sciences Murcia, Spain
Thesis: *Enhancing Virtual Screening in Drug Discovery Through Consensus-Based Methods*. Director: Prof. Horacio Pérez-Sánchez.
Grade: Summa Cum Laude (Sobresaliente Cum Laude).

University of Antwerp Sep. 2018 – Sep. 2021
MSc Biochemistry and Biotechnology Antwerp, Belgium
Thesis: *FEP viewer: a user-friendly webtool to display free energy perturbation calculations*. Promotor: Prof. Hans De Winter.

University of Antwerp Sep. 2015 – Sep. 2019
BSc Biochemistry and Biotechnology Antwerp, Belgium
Thesis: *Systematic meta-analysis of resistance markers for Isoniazid of Mycobacterium tuberculosis*. Promotor: Prof. Kris Laukens.

PUBLICATIONS

- A. Rodríguez-Martínez, **J. Nelen**, M. Carmena-Bargueño, C. Martínez-Cortés, and H. Pérez-Sánchez. "STELLAR: A Fragment-Based Docking Workflow for Highly Flexible Long-Chain Biopolymers". In: *Journal of Chemical Information and Modeling* (Sept. 16, 2026). ASAP article. doi:10.1021/acs.jcim.6c00987.
- A. Rodríguez-Otero, M. Mussa-Juane, M. Paredes-Ramos, **J. Nelen**, A. Borrallo Rentero, H. Pérez-Sánchez, A. Gómez Tato, and J. M. López Vilariño. "Freshness flavour perception via quantum-inspired and quantum ligand-based virtual screening". In: *Scientific Reports* (Aug. 21, 2026). doi:10.1038/s41598-026-66827-0.
- **J. Nelen**, B. Sarkar, J. Jiménez-Bernad, A. C. Darragh, A. M. Hanna, N. B. Servant, M. Jahic, J. M. Villalgordo-Soto, G. I. Georg, and H. Pérez-Sánchez. "Wee1-targeting inhibitors: From virtual screening to lead discovery". In: *Bioorganic & Medicinal Chemistry* 138 (July 2026), p. 118645. doi:10.1016/j.bmc.2026.118645.
- **J. Nelen**, M. I. Goettert, M. Forster, L. Breuils, J. M. Villalgordo-Soto, S. A. Laufer, and H. Pérez-Sánchez. "Computational Discovery and Optimization of a Potent, Selective, and Drug-Like Scaffold for p38α Inhibition". In: *Drug Design, Development and Therapy* 20 (June 3, 2026), p. 585325. doi:10.2147/DDDT.S585325.
- F. Iesce, **J. Nelen**, A. Rodríguez-Martínez, C. Martínez-Cortés, C. Minnelli, G. Mobbili, A. Di Gregorio, C. Vignaroli, H. Pérez-Sánchez, and R. Galeazzi. "Discovery of Novel Molecular Scaffolds to Overcome Pseudomonas aeruginosa Aminoglycoside Resistance: Insights for a Consensus Scoring Rational Design Approach". In: *International Journal of Molecular Sciences* 27.6 (Mar. 13, 2026), p. 2642. doi:10.3390/ijms27062642.
- **J. Nelen**, L. Zhao, X. Song, L. Liu, Z. Tu, Z. Wang, K. Ding, and H. Pérez-Sánchez. "Enhancing Drug Repurposing with Consensus Docking: Discovery of Novel Discoidin Domain Receptor 1 Inhibitors". In: *ChemMedChem* 21.2 (Jan. 31, 2026), e202500747. doi:10.1002/cmdc.202500747.
- **J. Nelen**, V. Naponelli, J. M. Villalgordo-Soto, M. Falasca, and H. Pérez-Sánchez. "Targeting drug resistance in cancer: Dimethoxycurcumin as a functional antioxidant targeting ABCC3". In: *Antioxidants* 14.5 (2025), p. 599. doi:10.3390/antiox14050599.
- **J. Nelen**, H. Pérez-Sánchez, H. De Winter, and D. Van Rompaey. "Matched pairs demonstrate robustness against inter-assay variability". In: *Journal of Cheminformatics* 17 (2025), p. 8. doi:10.1186/s13321-025-00956-y.
- J. Grzelczyk, H. Pérez-Sánchez, **J. Nelen**, M. Carmena-Bargueño, I. Gałązka-Czarnecka, G. Budryn, D. Hernik, E. Brenna, and F. Boratyński. "Interaction of anticancer oxygenated propenylbenzene derivatives with human topoisomerase IIα and actin: molecular modeling and isothermal titration calorimetry studies". In: *Journal of Thermal Analysis and Calorimetry* (2024). doi:10.1007/s10973-024-13569-8.
- A. Rodríguez-Martínez, **J. Nelen**, M. Carmena-Bargueño, C. Martínez-Cortés, I. Luque, and H. Pérez-Sánchez. "Enhancing MD simulations: ASGARD's automated analysis for GROMACS". In: *Journal of Biomolecular Structure and Dynamics* (2024). doi:10.1080/07391102.2024.2349527.
- **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". In: *Journal of Chemical Information and Modeling* 64.5 (2024), pp. 1605–1614. doi:10.1021/acs.jcim.3c01982.
- G. Dakpa, K. 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 activity in silico and in vitro". In: *Scientific Reports* 13 (2023), p. 17106. 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". In: *Clinical Microbiology and Infection* 26.10 (2020), pp. 1332–1337. doi:10.1016/j.cmi.2020.07.004.

PREPRINTS

- **J. Nelen**, O. Khan, E. Adams, J. C. Aschenbrenner, W. Thompson, A. Ebrahim, E. Çapkin, C. Vallée, OpenBind Consortium, E. J. Shotton, E. J. Griffen, J. D. Chodera, C. M. Deane, F. von Delft, M. AlQuraishi, and F. Imrie. "The first OpenBind release: An open experimental structure–affinity dataset and benchmark for structure-based AI". In: *bioRxiv* (Aug. 28, 2026). doi:10.64898/2026.08.27.747600.

SELECTED CONFERENCE CONTRIBUTIONS

- Poster and flash presentation: *The first OpenBind release: An open experimental structure–affinity dataset and benchmark for structure-based AI*. 10th RSC-BMCS Fragment-based Drug Discovery Meeting (Fragments 2026), Churchill College, Cambridge, UK, Sep. 2026.
- Poster: *Leveraging consensus: A novel approach to molecular docking for improved enrichment of active compounds*. 1st SEBiBC Congress, Spanish Society for Bioinformatics and Computational Biology, Valencia, Spain, Oct. 2024.
- Poster: *ESSENCE-Dock: A unified framework for integrating docking methods and enhancing hit identification*. 24th European Symposium on QSAR, Barcelona, Spain, Sep. 2024.
- Oral communication: *Visualizing molecular impact: Understanding the role of substructures in drug activity prediction*. II Congreso Estatal de Estudiantes de Biociencias, University of Granada, Spain, Jul. 2023.
- Flash presentation: *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, University of Murcia, Spain, Jun. 2023. Awarded Best Flash Presentation.

TEACHING EXPERIENCE

UCAM Universidad Católica San Antonio de Murcia Sep. 2025 – Dec. 2025
Lecturer, Physics & Chemistry, Bachelor in Veterinary Sciences Murcia, Spain

- Delivered 60 hours of lectures and laboratory sessions in English for first-year veterinary students.