Uxía Veleiro

Ph.D. in Machine Learning and Bioinformatics

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EXPERIENCE

Postdoctoral Associate — *Abu Dhabi, UAE*

Integrative Computational Network Biology Lab @ MBZUAI — *Present*

- Recently joined the Prof. Natasa Przulj lab, a leading research group in multi-omics data fusion and network science applied to precision medicine and precision therapeutics.

Doctoral Researcher — *Pamplona, Spain*

CIMA University of Navarra — *February 2022 - March 2026*

- PhD thesis defended with *cum laude* distinction and international doctorate mention.
- *Research Topic*: Drug repurposing through deep learning on graphs.
- *Advisors*: Mikel Hernaez and Antonio Pineda-Lucena.
- *Supervision*: Supervised two theses (MSc, University of Zaragoza; Bachelor's, Public University of Navarre).
- *TA*: Sequence Analysis and Structural Bioinformatics, MSc in Computational Methods, University of Navarra (21/22, 22/23).
- *Attended and presented at*: international conferences; participated in summer schools (OxML'24, M2L'25).

Visiting Researcher — *Basel, Switzerland*

Basel University — *November 2024 - February 2025*

- *Advisor*: Ivan Dokmanić
- Evaluated the viability of hypergraph-based methods for patient phenotype prediction from RNA-Seq and WES data.
- Received a PhD mobility grant awarded by the Government of Navarre.

Internship — *Galicia, Spain*

MD.USE Innovative Solutions — *August & September, 2020*

- Worked on **SuPepMem**, an open-access database of molecular dynamics simulations of peptides in different membrane models.
- Implemented scripts to systematically analyze how antimicrobial peptides interact with membranes.

ML-PROJECTS LEAD

- **Drug Synergy prediction**. [2025 - Ongoing]
  Developing a novel drug synergy prediction model with a strong focus on generalization and explainability to uncover the mechanisms behind synergistic drug pairs.
- **Cancer subtype stratification from RNA-Seq clinical cohorts**. [2024 - Ongoing | Manuscript under preparation]
  Worked on methods for cancer subtype classification. Assessed the use of generative models to create synthetic patient data and implemented biologically driven dimensionality reduction strategies to address high-dimensional data challenges.
- **Towards a more inductive world for drug repurposing approaches**. [Nat.Mach.Intell., 2025; Oral ($\frac{6}{76}$) at AI4D3 NeurIPS 2023].
  Benchmarked drug-target interaction models and proposed practical design guidelines. Analyzed generalization properties comparing transductive vs. inductive approaches. Developed a novel biologically-driven subsampling technique for predicting unseen interactions. Collaborated with experimental biologists on planning wet-lab validation.
  In collaboration with Dr. Olivier Gevaert from Stanford University.
- **GENNIUS: an ultrafast drug–target interaction inference method based on graph neural networks**. [Bioinformatics, 2024]
  Designed an inductive model for drug-target interaction prediction with focus on generalization and prediction reliability.

SKILLS

Personal

Experienced in designing novel ML models for drug repurposing and patient-aware therapeutic discovery, with a focus on graph-based approaches.
Highly motivated, self-disciplined, and proactive.
Used to working in interdisciplinary research teams.

Programming Languages

Python, R, UNIX/Bash.

Technologies

Git/GitHub, Docker, Slurm, HPC Systems, W&B.

Software Developed (open-source)

GeNNius (GitHub); GraphEmb (GitHub)

Machine Learning

Graph Neural Networks, Autoencoders, Representation Learning, Logistic Regression, SVM, XGBoost.

Libraries

PyTorch, PyTorch Geometric, PyTorch Lightning, SciPy, Scikit-learn.

Chemical informatics

RDKit, ChEMBL, PubChem APIs.
Feature engineering: molecular fingerprints, chemical descriptors, protein sequence/structure features.

Languages

Spanish [native], Galician [native], English [TOEFL 102, 2023; CAE, 2019], German [intermediate], Portuguese [beginner]

PUBLICATIONS

- J. de la Fuente*, G. Serrano*, U. Veleiro*, M. Casals, L. Vera, M. Pizurica, A. Pineda-Lucena, I. Ochoa, S. Vicent, O. Gevaert, M. Hernaez, *Towards a more inductive world for drug repurposing approaches*.
  Nature Machine Intelligence (Feb 2025). https://doi.org/10.1038/s42256-025-00987-y
- U. Veleiro, J. de la Fuente, G. Serrano, M. Pizurica, M. Casals, A. Pineda-Lucena, S. Vicent, I. Ochoa, O. Gevaert, M. Hernaez, *GeNNius: An ultrafast drug-target interaction inference method based on graph neural networks*.
  Bioinformatics (Jan 2024). https://doi.org/10.1093/bioinformatics/btad774
- F. Suárez, M. Calvelo, G.F. Tolufashe, A. Muñoz, U. Veleiro, C. Porto, M. Bastos, A. Piñeiro, R. Garcia-Fandino, *SuPepMem: A database of innate immune system peptides and their cell membrane interactions*.
  Computational and Structural Biotechnology Journal (Jan 2022). https://doi.org/10.1016/j.csbj.2022.01.025
- P. F. Garrido, M. Calvelo, A. Blanco-González, U. Veleiro, F. Suárez, D. Conde, A. Cabezón, Á. Piñeiro, R. Garcia-Fandiño. *The Lord of the NanoRings: Cyclodextrins and the battle against SARS-CoV-2*.
  International Journal of Pharmaceutics (July 2020). https://doi.org/10.1016/j.ijpharm.2020.119689

EDUCATION

University of Navarra (UNAV) — *Pamplona, Spain*
Doctoral Program: Applied Medicine and Biomedicine — *February, 2022 - March, 2026*

- Attended several interdisciplinary courses, including scientific writing, communication, innovation, and technology transfer.

Mediterranean Machine Learning Summer School (M²L 2025) — *Split, Croatia*
Organized by: the AI Education Foundation — *8-12 September, 2025*

- Acceptance rate: 18%; received a travel grant.

Oxford Machine Learning Summer School (OxML 2024) — *Oxford, UK*
Organized by: AI for Global Goals — *11-14 July, 2024*

- *Track*: Representation Learning and Generative AI.

University of Zaragoza — *Zaragoza, Spain*
M.Sc. in Quantitative Biotechnology (60 ECTS) — *2020 - 2021*

- Master Thesis (30 ECTS): *BFT-3: Virtual Screening - Combining Experimental and Computational Tools.*
  Applied molecular docking and molecular dynamics to analyze protein-ligand interactions across two chemical libraries.

Ruprecht-Karls-Universität Heidelberg — *Heidelberg, Germany*
ERASMUS Scholarship — *2018 - 2019*

University of Santiago de Compostela (USC) — *Santiago de Compostela, Spain*
B.Sc. in Physics (240 ECTS) — *2015 - 2020*

- Bachelor Thesis: *Cyclodextrin as drug carrier for Ibuprofen using Molecular Dynamics simulations*

ORGANIZER/VOLUNTEERING

Organizer — *Pamplona, Spain*
PhD Day at CIMA — *2024-2026*

- Member of the organizing committee of the PhD Day @ Cima, event designed to foster community among PhD students.
- Fundraising, event organization, budget management, and chairing the event.

Organizer — *Madrid, Spain*
Madrid Meet Up - Learning on Graphs Conference — *2023*
https://logmeetupmadrid.github.io/

- Spanish branch of the Learning on Graphs conference. Organized in collaboration with Antonio G. Marqués (URJC).
- Created the event website, prepared the schedule, administered expenses, and coordinated attendee registrations.
- Hosted speakers from 13 academic institutions (7 in Spain, another 5 in the rest of Europe: UK, NL, DE, NO) and 2 from private sector companies, as well as 3 plenary speakers from the Universities of Oxford (UK), TUM (DE) and Basel (CH).

SELECTED CONFERENCES

ISMB/ECCB 2025 — *Liverpool, UK*
Talk - Towards a more inductive world for drug repurposing approaches — *20-24 July 2025*

Mining and Learning with Graphs Workshop (MLG) @ ECML PKDD 2023 — *Turin, Italy*
Flashtalk and Poster - GeNNius — *22 September 2023*

ISMB/ECCB 2023 — *Lyon, France*
Poster - GeNNius — *23-27 July 2023*