



CRBM external seminar

Thursday July 2nd at Salle Marcel Dorée (CRBM) 11:00 am

Contact: andrey.kajava@crbm.cnrs.fr

Machine Learning and Structure-Based Approaches for the Discovery of Biomarkers and Bioactive Compounds

Dr. Alan Talevi

Universidad Nacional de La Plata (UNLP) & Argentine National Council of Scientific Research (CONICET), La Plata, ARGENTINA



Dr. Alan Talevi is Full Professor at the Faculty of Exact Sciences, Universidad Nacional de La Plata (UNLP), Principal Researcher at CONICET, and Director of the Laboratory for Research and Development of Bioactive Compounds (LIDeB). His research focuses on computer-aided drug discovery, chemoinformatics, and the application of machine learning to the identification of novel bioactive compounds and therapeutic targets. He has contributed extensively to the development of ligand- and structure-based virtual screening strategies, drug repurposing approaches, and predictive models for pharmacological activity. His work integrates computational and experimental validation pipelines, with applications spanning neglected and rare diseases. He has authored over 100 peer-reviewed publications and multiple book chapters in the field of computational drug discovery and has led numerous national and international research collaborations. His recent work emphasizes data-centric machine learning strategies and the integration of chemical, biological, and phenotypic data to improve predictive performance and translational impact.

Abstract: The identification of reliable biomarkers and bioactive compounds remains a central challenge in biomedical research, particularly in complex and data-scarce scenarios. In this context, machine learning and structure-based approaches have emerged as powerful and complementary tools to explore chemical and biological spaces efficiently. This talk will present recent advances in the integration of supervised and unsupervised machine learning techniques with ligand- and structure-based virtual screening strategies. Emphasis will be placed on data-centric approaches, the impact of training data quality on model performance, and the use of predictive models to identify biologically relevant patterns and candidate molecules.

Recent publications:

Pérez-Mauad N, Alberca LN, Schoijet AC, Vilchez Larrea SC, Barrionuevo EM, Muraca G, Sülsen V, Alba-Soto CD, Alonso GD, Talevi A. Application of Data-Centric Supervised Machine Learning to Predict Phenotypic Activity Against Clinically Relevant Stages of *Trypanosoma cruzi*. *Pharmaceutics*. 2025 ;17(12):1513.

Talevi A, Alberca LN, Bellera CL. Tackling the issue of confined chemical space with AI-based de novo drug design and molecular optimization. *Expert Opin Drug Discov.* ;2025, 20(11):1405-1418.

Prada Gori DN, Barrionuevo EM, Alberca LN, Sbaraglini ML, Llanos MA, Giovannuzzi S, Carta F, Marchetto MI, Supuran CT, Alba Soto CD, Gavernet L, Talevi A. Discovery of *Trypanosoma cruzi* Carbonic Anhydrase Inhibitors by a Combination of Ligand- and Structure-Based Virtual Screening. *J Chem Inf Model*. 2025;65(10):4980-4993.