

Patrícia Sobral

PhD student | Cheminformatics & computational drug discovery



Patrícia Sobral is a PhD student in Sustainable Chemistry at NOVA FCT. Her work brings together cheminformatics, machine learning and medicinal chemistry to support the discovery of small molecules for cancer immunotherapy. She works across LAQV-REQUIMTE and UCIBIO and collaborates with Stematters through the CAR T-Matters project.

Her doctoral research explores small-molecule modulation of targets relevant to CAR T-cell therapy. These include the glyco-immune checkpoints Siglec-7 and Siglec-9, the PD-1/PD-L1 immune checkpoint axis, and inflammatory pathways involving IL-1R1 and IL-6.

Patrícia develops computational workflows that begin with the collection, curation and analysis of chemical and biological data. She represents compounds with molecular descriptors and fingerprints, builds quantitative structure-activity relationship (QSAR) models, and evaluates their predictive performance and applicability domains. She then integrates model predictions with virtual screening and structure-based methods, including molecular docking, to select compounds for experimental follow-up.

This work involves multidisciplinary collaboration with synthetic chemists and experimental teams. Candidate molecules are prioritized for synthesis and testing, allowing computational hypotheses to be assessed against laboratory results. Her research aims to make the search for immunomodulatory small molecules more focused and evidence-driven.

Scientific background

She holds a BSc in Applied Chemistry from NOVA FCT and an MSc in Pharmaceutical and Therapeutic Chemistry from the Faculty of Pharmacy, University of Lisbon. Her MSc research at Hovione compared portable NMR with gas chromatography for in-process control. Before starting her PhD, she worked as an analytical chemist and later as a senior analytical chemist at Recipharm. She has been involved in glycoimmunology and cheminformatics research at NOVA FCT since 2022.