Dr. Carlos Simões and Dr. João Carvalho
Second Symposium on Computational Chemistry, 11 December 2026, Brussels

From binding pocket to business docket

Computer-assisted drug discovery (CADD) at **VIB Discovery Sciences (VDS)** began with simple docking studies on targets emerging from VIB laboratories and has evolved into a translational capability supporting programs now advanced by spinouts including **Augustine Therapeutics, Tanai Therapeutics, and TRIM Therapeutics**. What started with a few docking runs has grown into large-scale virtual screening of make-on-demand chemical spaces containing trillions of compounds, executed through **Nextflow pipelines** on VIB's commodity compute infrastructure.

In this presentation, we will "open the box" on two main fronts. First, we will introduce key components of the platform. We will offer a brief account on how we explore structure-based *in silico* screening on curated libraries of in-stock chemistry and on a collection of *synthons* translating into an ultra-vast, virtually accessible compound space. **VDS-Dexter** is a versatile Nextflow pipeline that calculates and predicts more than 70 developability and liability descriptors and is routinely used to prepare our screening decks. **VDS-MolSim** serves as a flexible system for 2D and 3D similarity-based virtual screening. We will discuss the modular architecture of these workflows and how student and academic projects contributed to developing, benchmarking, and deploying them as "push-button", open-source alternatives to commercial software. We will also highlight the assembly and continuous monitoring of virtual libraries that combine vendor catalogues with differentiated chemistry, efforts that have directly shaped the physical compound collection hosted by the **VIB Screening Core**.

Second, we will describe our work with the **VIB Data Core** to deploy these pipelines and expand access across the VIB community, and more recently with an external partner to port them to **a cloud infrastructure** hosted by VIB.

Finally, we invite discussion on how such computational workflows can be sustainably maintained and shared within the **Belgian computational chemistry community**. We envisage a concrete two-way model for open discussion: the community gains privileged access to these workflows, and methods developed by the community can in turn be evaluated for integration, all sustained by a non-profit cost-recovery structure. We warmly welcome ideas, discussion and collaboration.

https://www.linkedin.com/in/carlosjvsimoes/
https://www.linkedin.com/in/jfcarv/

Dr. Carlos Simões and Dr. João Carvalho
Second Symposium on Computational Chemistry, 11 December 2026, Brussels

Curriculum vitae of Dr. Carlos Simões



Carlos Simões is Senior Scientist in Translational Research at VIB Discovery Sciences in Leuven, where he leads computer-assisted drug discovery (CADD). He directs the CADD team's work on neuroscience and oncology programmes, runs virtual screening campaigns across ultra-large chemical libraries, and is steering VIB's cheminformatics pipelines into the cloud. He is also involved in CADD activities performed for TRIM Therapeutics, a VIB spinout.
Carlos trained as a pharmacist and earned his PharmD and PhD at the University of Coimbra, carrying out his doctoral research at the University of Leeds. His virtual screening work on amyloid inhibitors produced experimentally confirmed hits and became the scientific foundation of BSIM Therapeutics, the spin-out he co-founded after a brief postdoctoral involvement in PRACE – the Partnership for Advanced Computing in Europe. During ten years as CTO/COO, he combined molecular modeling and machine learning with the business side of drug discovery. That included CRO partnerships, DMPK studies, and two patent families he took from provisional filing to grant in the US and Europe.

Curriculum vitae of Dr. João Carvalho



João Carvalho is Drug Discovery Director at Tanai Therapeutics in Belgium, with a background in medicinal chemistry and computational drug discovery. His experience spans academic research at PhD and postdoctoral level, the industry at Charles River, and translational drug discovery at VIB Discovery Sciences. His work integrates computational approaches, including CADD and virtual screening, with medicinal chemistry and experimental data to support small-molecule drug discovery programs. He has a particular interest in the practical application of computational tools to compound design, prioritization and decision-making throughout the drug discovery process.

https://www.linkedin.com/in/carlosjvsimoes/
https://www.linkedin.com/in/jfcarv/