Use of ML/AI Methods for Drug Discovery: "It's All About You" – Dr. Sandro Boland

Over the past decades, *in silico* methods have become a cornerstone in the discovery and optimization of new drug candidates. With the rapid evolution of machine learning (ML) and artificial intelligence (AI), these approaches have moved firmly into the spotlight. Today, they play a crucial role in predicting protein structures, generating novel chemical matter, and estimating chemical and biological properties.

In this presentation, we will share insights from our experience at CISTIM/CD3 in applying ML/AI methods within real-world drug discovery projects. While the progress in the field has been remarkable, challenges remain. Publicly available datasets and pre-trained models often introduce pitfalls, limiting the robustness and reliability of predictions.

We will highlight how integrating in-house data, project-specific considerations, and proprietary chemistry helps to overcome these hurdles. This tailored approach not only improves the performance of ML/AI models but also ensures that the results truly meet the needs of end users. Ultimately, the key to success in AI-driven drug discovery lies in making the technology work for you.

Curriculum vitae of Dr. Sandro Boland

Sandro Boland obtained his PhD in Sciences (Chemistry) from Université de Namur (1999–2004), where he specialized in structure-based drug design and crystallography. He began his industry career at Devgen (2004–2008) as Senior Scientist, applying a broad range of drug design methodologies to support medicinal chemistry programs. He then moved to Silicos NV (2008–2009), focusing on computer-aided drug design (CADD), virtual screening, and hit-to-lead optimization.

At Amakem NV, he established and implemented a CADD platform, first as Senior Scientist (2010–2011) and later as Platform Project Manager (2011–2016). In this role, he drove multiple discovery and development projects, including a Phase II clinical compound, and contributed extensively to intellectual property, with 12 patents and 5 peer-reviewed publications.

Since 2016, Sandro has been part of CISTIM, a non-profit research institute bridging academic biomedical research and industry needs. He served as Lead Chemist in Medicinal Chemistry (2016–2024) before taking on his current role as Head of CADD & ML/AI (2024–present), where he leads the integration of computational and AI-driven methods into drug discovery projects.