Insights from Alumni in Industry 2025
- Program -

Last updated: February 25, 2025

March 25, 2025
Conference & Common Room, Mathematikon 5th floor

Overview

	Welcoming Remarks by the Organizers	
13:30–14:15	**Jan Wenzel** Sanofi	Advancing Drug Safety: Computational Toxicology Models in Pharmaceutical Research
14:15–15:00	**Eva-Maria Didden** Johnson&Johnson	A journey from Statistics at LMU (Munich) to Rare Disease Epidemiology at Johnson&Johnson (Basel), via HGS MathComp (Heidelberg) and other waypoints
15:00–15:30	**Coffee**	
15:30-16:15	**Markus Blatt** Dr. Markus Blatt - HPC-Simulation-Software & Services	A Journey in Open-Source from SciComp education to a professional Service Provider
16:15-17:00	**Maximilian Scheurer** Covestro	Quantum Computing for Quantum Chemistry
17:00–open end	**Get-Together**	

Abstracts

Advancing Drug Safety: Computational Toxicology Models in Pharmaceutical Research

Jan Wenzel

Sanofi, R&D, Preclinical Safety – Digital Toxicology, Frankfurt am Main, Germany

Computational toxicology is an interdisciplinary field that combines computer science, chemistry, and toxicology to predict and assess the potential toxicity of chemicals using predictive computational methods. In all phases of the R&D process, such predictive models are key enablers to support the investigation and development of new safe pharmaceutical molecules. The accurate prediction of absorption, distribution, metabolism, excretion, and toxicity (ADME-Tox) properties, for example, is an efficient task in early discovery helping to identify molecules with an appropriate and safe profile of interest. At development or market stages, support via computational methods is also provided, e.g., towards identification and classification of reactive impurities. Deep neural nets (DNNs) emerged as transformative technology to analyze large datasets and to predict ADME-Tox properties and even drug adverse effects. For special toxicities driven by chemical reactivity or photo effects, applying quantum chemistry methods allows a deeper analysis of the mechanisms behind those effects.

In this talk, I will showcase different examples of actual applications of computational toxicity models in different phases of drug life cycles. This includes a fully industrialized approach to generate, apply, and visually interpret different types of DNNs to model ADME-Tox data. Finally, I will introduce a computational quantum chemistry approach to assess the reactivity of genotoxic nitrosamine impurities, demonstrating the usage of computational methods for marketing products.