

safescimet course 4.5 - In silico ADME and Predictive Toxicology

(11–15 May 2020, Paris, France)

A unique opportunity to broaden your knowledge of drug discovery and development with special emphasis on drug safety.

safescimet offers an outstanding faculty of academic and industry experts and an interactive programme, including case studies from the pharmaceutical industry providing a broad understanding of the latest developments in safety sciences.

In silico ADME and Predictive Toxicology

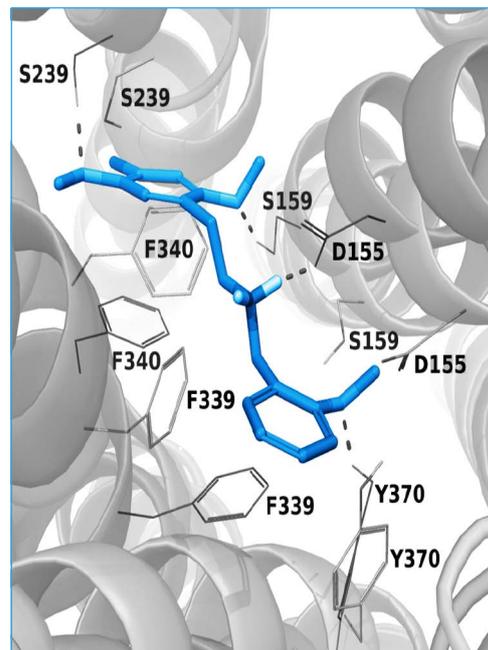
This course will provide the participants with a comprehensive overview of in silico methods in drug discovery and development as well as where they can be used and what their strengths and limitations are. Additionally, students will get hands-on experience with several predictive in silico methods, e.g. web-based tools to predict simple ADME/Tox endpoints and purpose-developed software to predict more complex ADME/Tox endpoints.

Key Subjects

- Computational tools used in drug discovery and development, with focus on ADME/Tox
- Critical analysis of experimental data
- Prediction of absorption and distribution
- Phase I and II metabolism – the Cytochrome P450 enzymes
- Prediction of metabolism,
- Prediction of site of metabolism
- Prediction of toxicity (e.g. genotoxicity, phospholipidosis, hERG etc)
- Genomic effects on metabolism and toxicity
- Different QSAR systems available analysis

Learning Outcomes

- Gain comprehensive overview of up-to-date in silico methods used in drug discovery and development
- Explore and understand the diversity of large datasets
- Critically analyse experimental data
- Use web-based tools to predict simple ADME/Tox endpoints like drug-likeness, solubility, absorption, genotoxicity, phospholipidosis etc.
- Use purpose-developed computational tools for prediction of complex ADME/Tox endpoints like prediction of metabolism and site of metabolism
- Understand the principles of the most commonly used types of predictive methods



Course Organisers



Prof Olivier Taboureau
Computational Modeling Protein-Ligand
Interactions (CMPLI), Université de Paris, France



Dr Alexander Amberg
D&R DSAR / Preclinical Safety Frankfurt,
Sanofi-Aventis Deutschland GmbH, Germany

Participant Feedback

Excellent to do case studies to learn.



[Link to apply to this course](#)

Deadline for registration 01 May 2020