safescimet course 4.5 - In silico ADME and Predictive Toxicology

Key Questions Addressed

- The drug discovery and development process – with special 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 – classification
- Prediction of metabolism – site of metabolism
- Prediction of toxicity (e.g. genotoxicity, phospholipidosis, hERG etc.)
- Genomic effects on metabolism and toxicity
- Different QSAR systems available

Feedback from the Previous Course

"Excellent to do case studies to learn."

safescimet Executive Office
University of Konstanz, Universitätsstraße 10, Box 622, 78457 Konstanz, Germany - Phone +49 7531 88 3518/3171
To contact us or to register to our courses visit safescimet@uni-konstanz.de or http://ssm.afww.uni-konstanz.de/safescimetcourses

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About safescimet

safescimet is a unique pan-European network of academia and pharmaceutical industry, which have joined forces to establish a comprehensive modular education and training in Safety Sciences for medicines. The programme covers all aspects of safety in drug development, in order to fulfill the needs of drug safety scientists in the pharmaceutical industry, regulatory authorities and academia. The aim of the programme is to bridge crucial gaps in the education and training of scientists evaluating the safety of drug candidates and new medicines and to ensure that European drug safety scientists are at the forefront of their field.

The course In silico ADME and Predictive Toxicology and the other single courses of the safescimet programme provide new opportunities for Continuous Professional Development (CPD) and are part of European Master for Advanced Safety Sciences for Medicines degree at the University of Konstanz. The individual courses are clustered within five separate domains. Each domain deals with one or more specialised topics and contains from two to six single courses. Please visit www.safescimet.eu for details of the full course programme and confirmation of course dates.

Course Objectives

In silico methods, defined as experiments and compound testing performed via computer simulation, have become an important tool in drug discovery and in the development of medicines. Predictive in silico methods are getting considerably more reliable, they cover a broader spectrum of predictive endpoints and are getting easier to use also for non-specialists. Reliable predictive models may replace costly experiments and thereby contribute to a cost-reduction of the drug discovery and development process. 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 Covered by the Course

- 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

Target Audience

safescimet courses are open to all scientists and students from industry, academia and regulatory authorities, who need a broad comprehensive understanding of the drug development process with particular emphasis on safety. The applicant will normally possess an MSc degree in a Life Science discipline or equivalent. In addition, applicants are expected to have an at least one year working experience in a related discipline.

Why Join the Course

The on-site training of the course during the first week consists of five days with lectures, practical exercises, group work and discussions. This setup offers an intense and broad training with leading experts in their field and ample opportunities for lecturer-student interactions. The balance of academic, industry and regulatory teachers provides knowledge directly available to drug safety assessment, including dataset discussions from real case studies.

Learning Outcomes

On successful completion of the course, participants should have an integrated hands-on experience with in silico methods for prediction of various ADME/Tox relevant end-points. More specifically, participants will be able to

- 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 method

Course Programme

The first week of the course consists of five days lectures, practical exercises, group work and discussions, provided by specialists from academia, pharmaceutical industry and regulatory authorities with diverse backgrounds on drug safety aspects.

On-site Training

Day 1	Introduction; Data, databases and dataset selection
Day 2	Statistics; Absorption
Day 3	Metabolism
Day 4	Toxicology
Day 5	Future trends; Exam

Individual Home Assignments

After the week of on-site training, students will receive an individual 38 hours home assignment consisting of written questions and a case study. These individual assignments are to be completed through a frequent exchange with the safescimet teachers using distance learning approach. Written individual assignments are to be completed and submitted via Moodle within 6 weeks after the on-site training and will then be approved by the course leader.

Course Credits

Participants attending the on-site training week only, without completing the exam and/or the home assignment, will be given a certificate of attendance confirming completion of a Continuing Professional Development (CPD) course.

In order to receive the full 3 ECTS credits for a successfully completed course, participants need to pass the written exam of the on-site training week as well as to have successfully completed the home assignment.

Syllabus

The syllabus contains lecture hand outs, list of abbreviations and list of reading materials and will be provided by the course leaders 14 days prior to the course. The information and the material for the individual home assignment will be provided during the first week of the course.

Assessment

The assessment is based on a 2-hour written examination on the last day of the first course week and on the evaluation of the home assignment.

Type	- The purpose of the examination is to test that the examinee has acquired a broad knowledge and comprehension of the course subjects during the lectures. - The percentage of items on the test devoted to a particular topic will roughly correspond to the emphasis given on the topic during the course. - Experimental Design: 25% - Pre-clinical: 50% - Clinical: 5% - Translational: 20%
Assessors	Course leaders
Exam aids	All written exam aids are allowed, especially the provided material: lecture hand outs, list of abbreviations and case studies.

Contact Person

Prof Olivier Taboureau
Computational Modeling of Protein Ligand Interactions (CMPLI) – INSERM U1133, CNRS UMR 8251, Université de Paris, France
e-mail olivier.taboureau@u-paris.fr

Course Leaders

Prof Olivier Taboureau - CMPLI – INSERM U1133, CNRS UMR 8251, Université de Paris, France / e-mail olivier.taboureau@u-paris.fr
Dr Alexander Amberg - D&R DSAR / Preclinical Safety Frankfurt, Sanofi-Aventis Deutschland GmbH, Germany

Practical Information

Course credits	3 ECTS credits
Level	Master's level (second cycle higher education)
Location	University Paris Diderot, 35 rue Helene Brion, Bâtiment Lamarck A, 75013 Paris, France
Teaching methods	Lectures, case reports, demonstrations and home assignments.
Student workload	- Preparation: 12 hours - Course: 38 hours - Assignment: 38 hours - Examination: 2 hours - Total: 90 hours
Course fee	Please visit on www.safescimet.eu **Fees** and **How to apply** for more information.
Course capacity	20 participants
Language	- The official language of the course is English. - No simultaneous translations will be provided.
Course notes	Complete course notes, except for the textbook, will be available for all the participants.
Course accreditation	- safescimet courses meet the criteria for Continuous Professional Development (CPD) diplomas, and are part of Master programme Advanced Safety for Medicines. - When registering for one or several "Stand Alone"courses of our programme, this course provides CPD credits for your individual CPD portfolio. Each course is credited with 38 contact hours. - The course setup is already consistent with the requirements of the Bologna process. The full Master programme is undergoing evaluation for being accredited and certified as a regular postgraduate MSc degree at the University of Constance/Germany.

Accommodation

Appart'City hotel, Quality Suites Bercy Bibliothèque, Ibis style Paris Tolbiac, Hotel Mercure Paris Bercy, Ibis Hotel (The cheapest but a little further away)

Transport

The course will be located in the Lamarck A building of the Paris Diderot University (35 rue Hélène Brion), close to the François Mitterand national library:

- From Charles de Gaulle airport, take the RER B until Saint Michel - Notre Dame. Then take the RER C (direction Saint Martin d'estampes, dourdan, juvisy) and stop at the station Bibliothèque François Mitterand). We are at 5 min walk from there.
- From Orly airport, you can take a bus that will bring you to the RER C (station Pont de Rungis). Take the RER C to the direction Pontoise, Saint-Quentin en Yvelines and stop at the station Bibliothèque François Mitterand.
- If you take the train, you can reach the Station Bibliothèque François Mitterand with the metro line 14.

Registration

To apply please visit www.safescimet.eu. Your application needs your registration on www.safescimet.eu.

Cancellation

For our cancellation policy please visit **How to Apply/Terms and Conditions** on www.safescimet.eu.