In silico Methods – Computational Alternatives to Animal Testing

As introduced in the 3R principle (Replace, Reduce, Refine) by Russell & Burch, alternatives to animal testing are of utmost interest and significance. However, besides the great progresses regarding *in vitro* toxicology screening and human-on-a-chip platforms, the importance and potential of *in silico* methods to contribute valuably to the reduction of lab animal usage are scarcely visible and unknown. Here, we aim at presenting **the diversity and range of applications of** *in silico* methods by experts during a seminar with subsequent networking possibilities. In addition, we will offer an interactive workshop to generate ideas for bridging the communication gap and further the implementation of the 3R.

We are looking forward to welcoming you at our Seminar and Workshop at August 17th & 18th in Berlin!

Your Organization Team Dr. Annemarie Lang, Prof. Andrea Volkamer, Laura Behm & Prof. Frank Buttgereit







Seminar – Network Event Thursday 17th of August 4:00 – 7:00 pm Charité Campus Mitte, DRFZ/MPI Seminar room I

16:00 Welcome

Dr. Annemarie Lang & Prof. Frank Buttgereit

- 16:05 Introduction to the 3R principle Prof. Marlon Schneider (Bf3R, Berlin)
- 16:20 From female hormonal cycle to arthritis Computational systems biology in action Prof. Susanna Röblitz (ZIB, FU-Berlin)
- 16:55 Computational bone tissue engineering: *in vitro*,
 in vivo ... in silico Prof. Liesbet Geris (University of Liège, KU Leuven, Belgium)
- 17:30 Coffee Break
- 17:45 *In silico* **Toxicity Prediction for Risk Assessment** *Prof. Andrea Volkamer* (*Charité, BB3R, Berlin*)
- 18:20 **eTOX:** *In silico* **prediction of toxicities** *Dr. Joerg Wichard (Bayer AG, Berlin)*
- 18:55 Discussion and Closing
- 19:30 Network Dinner

Grand Bar (Oranienburger Straße 33); at one's own expense

Meet the Speakers/Experts

Prof. Marlon Schneider

German Center for the Protection of Laboratory Animals (Bf3R) German Federal Institute for Risk Assessment (BfR), Berlin



Marlon Schneider studied veterinary medicine and got his PhD from the LMU Munich. After working at the Gene Center (LMU Munich) for several years as well as receiving a habilitation in Genetics and Biotechnology (2010) and Physiology (2016), he is currently the Head of Unit ZEBET-Alternative Methods to Animal Experiments at the German Center for the Protection of Laboratory Animals (Bf3R), Federal Institute for Risk Assessment (BfR).

Prof. Susanna Röblitz



Computational Systems Biology, Zuse Institute Berlin (ZIB)

Susanna Röblitz got her doctoral degree in Mathematics from Freie Universität Berlin and worked several years as postdoctoral researcher at ZIB where she has been the Head of the research group Computational Systems Biology since 2010. She has been assistant professor at FU Berlin since 2015. Computational Systems Biology aims at the construction and analysis of predictive mathematical models for the description of complex interactions in biological systems.

Prof. Liesbet Geris

Biomechanics Research Unit, University of Liège, Belgium Prometheus, skeletal tissue engineering, KU Leuven, Belgium Biomechanics Section, KU Leuven, Belgium



Liesbet Geris research focusses on the multi-scale and multi-physics modeling of biological processes. Liesbet is scientific coordinator of a musculoskeletal Tissue Engineering platform (50+ researchers). She has edited several books on computational modeling and tissue engineering. Together with her team and clinical collaborators, she uses these models to investigate the etiology of non-healing fractures, to design *in silico* potential cell-based treatment strategies and to optimize manufacturing processes of these tissue engineering constructs. She is the current executive director of the Virtual Physiological Human Institute (VPH).

Prof. Andrea Volkamer

In-silico Toxicology Group, Institute of Physiology, Charité Universitätsmedizin Berlin



Andrea Volkamer received her Master degree in Bioinformatics from Saarland University in 2007. In 2013, she defended her PhD thesis with focus on computational druggability predictions. After a short ProExzellezia PostDoc period, she joint BioMedX Innovation Center in Heidelberg as a PostDoc researcher, where she has been working on tools to assist the development of selective kinase inhibitors. Since July 2016, Andrea Volkamer has been an assistant professor at the Charité Berlin with the focus on *in-silico* toxicology predictions.

Dr. Joerg Wichard

Predictive Toxicology, Bayer AG, Berlin



Joerg Wichard joined the Computational Chemistry Department at Schering AG from 2004-2006 as postdoctoral researcher. From 2006-2010 he was a research scientist in the Computational Chemistry and Drug Design Group at FMP (Institute of Molecular Pharmacology) in Berlin. In 2010 he joined the Genetic Toxicology Department at Bayer AG in Berlin where he is mainly responsible for the application of in silico tools in toxicology and for the implementation of toxicological databases. In addition, he was involved in several work packages of the eTOX project.

RETHINK 3R - Workshop

Friday 18th of August 9.00 am – 5:00 pm Charité Campus Mitte, RFL, Seminar room

Interactive Design Thinking Workshop with experts, interested researchers and PhD-students on the challenges to implement *in silico* methods to promote the 3R. Design Thinking is a systematic approach to problem solving. It combines creativity with analytical methods from engineering, design, arts, social sciences, and business, to exploit the intrinsic innovative potential of multi-disciplinary teams. The Design Thinking process helps to **identify key questions**, **perform research with a focus on gaining empathy for the users**, **and design a serious and realistic solution**. Important aspects of the process are interdisciplinary teamwork, "thinking outside the box", a flexible work environment, visualization and empathy.

<u>Schedule</u>

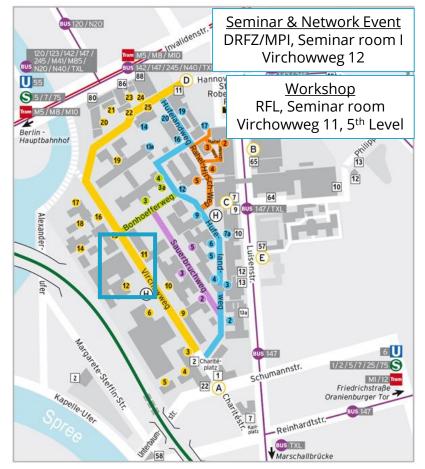
- 09:00 Welcome & Introduction
- 09:20 Understanding the challenge
- 09:50 Coffee Break
- 10:00 Understanding the customer needs
- 11:15 Synthesizing & Problem statement
- 12:00 Lunch Break
- 13:00 Problem statement II
- 13:30 Ideas & Prototypes of solutions
- 14:30 Break
- 14:45 Testing prototypes in the teams
- 16:00 Presentation & Discussion
- 17:00 Closure

Coaches: Annemarie Lang & Laura Behm





Charité Campus Mitte



Registration Please register under the following link:

http://t1p.de/Rethink3R

If you have further questions, please do not hesitate to contact us:

Annemarie.lang@charite.de & Andrea.volkamer@charite.de

