

# QSP modeling in R

ACoP10 Workshop: Using R and the IntiQuan R tools to support efficient QSP modeling, simulation and parameter estimation

ACoP10 - Thursday, October 24, 2019, 13:30-17:30

## Workshop Description

IntiQuan is running a full-day hands-on workshop on QSP modeling, simulation, parameter estimation and enhanced QSP modeling with variability. The presented IntiQuan tools to perform QSP modeling are implemented and fully embedded in the open-source and freely available R environment. The major topics covered are:

- QSP modeling in R – description of models and simulation
- Reuse of models from model databases – import of SBML models to R
- Introduction to a realistic QSP modeling example
- Robust parameter estimation based on sensitivity equations and multi-start optimization in R
- Analyzing models, informing modeling decisions, using profile likelihood

After the workshop, the participants will have learned to write their own mechanistic QSP models, simulate models, graphically explore their data, and perform parameter estimation using the functionality provided by IQR Tools.

The workshop is designed as a hands-on tutorial. Each topic will first be presented on slides and will be illustrated based on realistic examples. Between topics, the participants will have the chance to implement and reproduce the different modeling steps on their own resorting on a provided example model that is suitable for the workshop. IntiQuan personnel will be around at all time to support the participants.

Participants are supposed to bring their laptops. Ideally, R and IQR Tools should be installed before the workshop. Participants will receive installation instructions before the workshop and are encouraged to contact the presenters for support to setup IQR Tools on their system.

Basic knowledge of writing scripts in R is of advantage.

Contact: For more information, regarding the workshop, please contact IntiQuan ([info@intiquan.com](mailto:info@intiquan.com)).

## Registration

Cost will be 350\$ for industry, and 200\$ for academia/government/non-profit. The fees include workshop material and coffee breaks.

## Program

Time	Topic	Presenter
13:30 – 13:45	Welcome and introduction	Daniel Kaschek
13:45 – 15:45	Set-up and simulation of mechanistic QSP models Linking models and data. Model-supported data exploration. Parameter estimation and multi-start optimization	
15:45 – 16:00	Coffee break	
16:00 – 17:30	Uncertainty analysis using the profile likelihood method Hands-on session	

## Presenters

### [Daniel Kaschek, PhD, Principal Consultant at IntiQuan GmbH](#)

Daniel Kaschek is an experienced modeler working in the field of Quantitative Systems Pharmacology and Systems Biology since 2008. Over the past years, he has actively worked on the developed of novel mathematical and statistical approaches to data analysis and parameter estimation in ordinary differential equations with applications in Quantitative Systems Pharmacology and Systems Biology. He is an enthusiast R package developer, authoring several open-source packages on Data pre-processing and dynamic modeling.

### [Henning Schmidt, PhD, IntiQuan GmbH](#)

Henning Schmidt is an expert in Model-Informed Drug Development with over fourteen years of industry experience. He has been supporting projects from target validation in the early phases of drug discovery to study design for post-marketing commitments. During the last years, he has provided decision-making support to drug discovery and development teams in various therapeutic areas, including oncology, dermatology, immunology, respiratory, bone and muscle wasting diseases. This has led to several go/no-go decisions on the progression of novel drugs through their development cycle and successful registrations. Henning received undergraduate education at Darmstadt University, Germany and SUPELEC in Paris, France. He obtained his PhD in Control Theory and Systems Biology at

the Royal Institute of Technology in Stockholm, Sweden. He has worked for Fraunhofer Chalmers Research Center (Gothenburg, Sweden) and Novartis Pharma AG (Basel, Switzerland) prior to founding IntiQuan in 2015.