

USP Workshop on
Computer Modeling – In vitro and In vivo Studies
October 23–25, 2017
USP Meetings Center, Rockville, MD USA

Final Agenda

DAY ONE: Monday, October 23, 2017

8:00 – 8:30 a.m.	Registration & Coffee
8:30 a.m.	Welcome
8:30 – 9:00 a.m.	USP Revision Process John Mauger, Ph.D., <i>USP General Chapters-Dosage Forms Expert Committee, Professor, Pharmaceutical Chemistry, University of Utah</i>
9:00 – 9:30 a.m.	Bridging In silico with In vivo for Better Drug Development Alan Parr, Ph.D., <i>USP Compounding Expert Committee, Managing Member, BioCeutics, LLC</i>
9:30 – 10:00 a.m.	Modeling and Measurement Uncertainty Jane Weitzel, <i>USP General Chapters-Statistics Expert Committee, Independent Consultant</i>
10:00 – 10:30 a.m.	Morning Break
10:30 – 11:00 a.m.	Applications of Modeling in Quantitative Biopharmaceutics to Bridge Formulation and Clinical Performance David Good, Ph.D., <i>Senior Research Investigator, Bristol-Meyers Squibb</i>
11:00 – 11:30 a.m.	Predicting Product Performance: Integrated In vitro Dissolution and In vivo Absorption Modeling David C. Sperry, Ph.D., <i>Research Advisor, Eli Lilly & Company</i>
11:30 a.m. – 12:00 p.m.	Q&A
12:00 – 1:00 p.m.	Lunch
1:00 – 1:30 p.m.	Dissolving a Drug In vitro and In vivo via In silico – A Case Study Hu Wang, Ph.D., <i>USP Expert Panel Member-Use of Enzymes in the Dissolution Testing of Gelatin Capsules, Senior Scientist, Merck & Co.</i>
1:30 – 2:00 p.m.	Translating In vitro Data to In vivo Predictions – Is PBPK Modeling the Missing Link? Edmund Kostewicz, Ph.D., <i>Senior Scientist, Goethe University, Germany</i>
2:00 – 2:30 p.m.	Afternoon Break

- 2:30 – 3:00 p.m. **Mechanistic Oral Absorption & PBPK Modelling to Understand Formulation Behavior & Preclinical Pharmacokinetics**
Devendra Pade, Ph.D., *Senior Research Scientist, Simcyp Limited (a Certara Company), Blades Enterprise Center, Sheffield, UK*
- 3:00 – 3:30 p.m. **Prediction of Formulation Bioperformance and Bioequivalence by Incorporating Dissolution Data in PBPK Models**
Amitava Mitra, Ph.D., *Clinical Development, Sandoz, Inc.*
- 3:30 – 4:00 p.m. **Q&A**
- 4:00 – 5:00 p.m. **Networking Reception**

DAY TWO: Tuesday, October 24, 2017

- 8:00 – 8:30 a.m. **Registration & Coffee**
- 8:30 – 9:00 a.m. **Oral IVIVC Simulation**
James E. Polli, Ph.D., *Professor, University of Maryland School of Pharmacy*
- 9:00 – 9:30 a.m. **Clinical Relevant Product Specifications: Understanding In vitro and In vivo Data Using In silico Approaches**
Raimar Löbenberg, Ph.D., *USP BDSHM and NBDS - General Chapters Joint Subcommittee, Professor, Pharmacy & Pharmaceutical Studies, University of Alberta, Canada*
- 9:30 – 10:00 a.m. **In vitro Evaluation of Dissolution and PBPK Modeling to Understand the Impact of Absorption of High Dose Low Solubility Drugs from the Lower Intestine**
Maria Vertzoni, Ph.D., *Faculty of Pharmacy, University of Athens, Greece*
- 10:00 – 10:30 a.m. **Morning Break**
- 10:30 – 11:00 a.m. **Comparison Between Mechanistic Dissolution Modeling and Experimental Observations of Dissolution of Pharmaceuticals**
Susan Ewing, *Senior Scientist, Biopharmaceutics Group, Pfizer, Inc.*
- 11:00 – 11:30 a.m. **In silico Simulations of Intrinsic Dissolution**
Humberto Ferraz, Ph.D., *Professor, Department of Pharmacy, University of Sao Paulo, Brazil*
- 11:30 a.m. – 12:00 p.m. **Q&A**
- 12:00 – 12:50 p.m. **Lunch**
- 12:50 – 1:00 p.m. **Workshop Evaluation**

- 1:00 – 1:30 p.m.** **Simulation and Comparison of Hydrodynamics in Compendial Dissolution Apparatuses Using Computational Fluid Dynamics (CFD)**
Deirdre M. D’Arcy, Ph.D., *Assistant Professor, Trinity College of Dublin, School of Pharmacy and Pharmaceutical Studies*
- 1:30 – 2:00 p.m.** **A Case for Bioequivalence Knowledge Creation**
Ene Ette, MBA, Ph.D., *President, Anoxis Corporation*
- 2:00 – 2:30 p.m.** **Physiologically Base Pharmacokinetic and Absorption Modeling and Simulation – Cases Studies**
Xinyuan (Susie) Zhang, Ph.D., *Pharmacologist, CDER, U.S. Food and Drug Administration*
- 2:30 – 3:00 p.m.** **Afternoon Break**
- 3:00 – 3:30 p.m.** **Development of a Multivariate Model for Simulation of Cascade Impactor Data**
Dennis Sandell, Ph.D., *Director, S5 Consulting*
- 3:30 – 4:00 p.m.** **Predicting Deposition and Absorption Rate for Orally Inhaled Products Based on Dissolution Data and a PK Simulation Model**
Guenther Hochhaus, Ph.D., *Professor, Pharmaceutics, University of Florida*
- 4:00 – 4:30 p.m.** **Combining in vitro Mouth-Throat Deposition Measurements, Cascade Impactor Data and Computational Fluid Dynamics (CFD) Simulations**
Herbert Wachtel, Ph.D., *Senior Principal Scientist, Boehringer Ingelheim, Germany*
- 4:30 – 5:00 p.m.** **Q&A**

DAY THREE: Wednesday, October 25, 2017

- 8:00 – 8:30 a.m.** **Registration & Coffee**
- 8:30 – 9:00 a.m.** **In Silico Modeling and Simulations to Support Development and Bioequivalence Assessment of Generic Drug Product**
Jasmina Novakovic, Ph.D., *Scientific Leader, Apotex Inc.*
- 9:00 – 9:30 a.m.** **Using In silico Simulation to Aid Development of an In-vivo Assay for Vaccine Potency Assessment**
Ryan Yamagata, *USP Bioassay General Chapter Expert Panel, Principal Statistician, GSK*
- 9:30 – 10:00 a.m.** **Challenges in Physiologically Based Pharmacokinetic Modeling for the Prediction of In vivo Performance After Oral Administration**
Nikoletta Fotaki, Ph.D., *Reader (Assoc/Full Professor) in Pharmaceutics, Department of Pharmacy and Pharmacology, University of Bath*
- 10:00 – 10:30 a.m.** **Morning Break**

- 10:30 – 11:00 a.m.** **Population-Based PBPK and IVIV_E of Dissolution and Precipitation: Current Status and What Next?**
David Turner, Ph.D., *Principal Scientist, Simcyp Limited (a Certara Company)*
- 11:00 – 11:30 a.m.** **Advances and Challenges of Modeling and Simulation Studies in Regulatory Submissions**
Maziar Kakhi, Ph.D., *Staff Fellow, U.S. Food & Drug Administration*
- 11:30 a.m. – 12:00 p.m.** **Computer Modeling and Biphasic Dissolution**
Jim Mullin, *Principal Scientist, Simulations-Plus, Inc.*
- 12:00 – 12:30 p.m.** **Q&A**
- 12:30 – 12:35 p.m.** **Workshop Report / Closing Remarks**
Margareth Marques, Ph.D., *USP Principal Scientific Liaison, General Chapters*
- 12:35 p.m.** **Workshop Concludes**
Boxed Lunches will be available