



Program

10th Swiss Course on Medicinal Chemistry Leysin, October 14 to 19, 2012

Sunday, October 14, 2012

from 16:00 on	Check-in	
18:00 – 20:00	<i>Welcome reception, Dinner</i>	
20:00 – 20:15	Welcome	Prof. Beat Ernst, Univ. of Basel Dr. Gerhard Müller, Mercachem
	This week's program	Dr. Gerhard Müller, Mercachem
20:15 – 21:00	Lecture: Medicinal Chemistry: The Only Constant is Change	Prof. Beat Ernst, Univ. of Basel
	Introduction to Tutorials	



Monday, October 15, 2012: General Topics

Morning (Chair: Gerhard Müller)

08:30 – 09.15	Lecture: Nuclear Hormone Receptors as Drug Targets	Prof. Pedro Hermkens, Univ. of Nijmegen
09:15 – 10:00	Lecture: Rules and filters and their impact on success in chemical biology and drug discovery, part 1	Dr. Christopher Lipinski, Melior Discovery
10:00 – 10:30	<i>Coffee break</i>	
10:30 – 11:15	Lecture: Rules and filters and their impact on success in chemical biology and drug discovery, part 2	Dr. Christopher Lipinski, Melior Discovery
11:15 – 12:15	Lecture: Developing a Lead	Dr. Andrew Mortlock, AstraZeneca
12.15 – 13:30	<i>Lunch</i>	

Tutorials

15:00 – 15:30	<i>Coffee</i>	
15:30 – 18:00	Tutorials	
	T1: Physicochemical Parameters Relevant for Drug Absorption	Dr. Robert Taylor and Dr. Darren Matthews, Sirius Analytical Inc.
	T2: Fragment-based Lead Generation	Dr. Mark Whittaker and Dr. Michael Mazanetz, Evotec
	T3: Developing a Lead	Dr. Andrew Mortlock, AstraZeneca
	T4: Structure-Based Lead Optimisation: Molecular Modeling	Dr. Tien Luu, Accelrys
	T5: IP in Drug Discovery	Dr. Frank Schager, Actelion
	T6: The NMR Toolbox for Medicinal Chemists	Dr. Christoph Rademacher, MPI Berlin
	T7: Retrosynthesis	Dr. Ruben Leenders and Dr. Johan Veerman, Mercachem

Afternoon / Evening (Chair: Hugo Kubinyi)

18:15 – 19:00	Lecture: Fragment-based Drug Discovery	Prof. Beat Ernst, Univ. of Basel
19:00 – 20:30	<i>Dinner</i>	
20:30 – 21:15	Case History: Target Structure and Physical Property-Based Design Approaches Applied to Cancer Drug Discovery	Dr. Alan D. Brown, Pfizer



Tuesday, October 16, 2012: Off-Target Optimization

Morning (Chair: Karl-Heinz Altmann)

08:30 – 09.15	Lecture: Privileged Structures	Dr. Gerhard Müller, Mercachem
09:15 – 10:00	Lecture: Early ADMET: Compound Profiling and Optimization in Drug Discovery	Dr. Manfred Kansy, Hoffmann-La Roche
10:00 – 10:30	<i>Coffee break</i>	
10:30 – 11:15	Lecture: Experimental ADME: Major DMPK Properties to Assess During Lead Optimization	Dr. Christoph Funk, Hoffmann-La Roche
11:15 – 12:15	Lecture: Drug Metabolism	Prof. Hugo Kubinyi, University of Heidelberg
12:15	<i>Lunch package (only when weather is nice)</i>	
12:15 – 15:00	<i>With cable car to „La Berneuse“, enjoy the great view, ev. walk downhill to Leysin (approx. 1 ½ h)</i>	

Tutorials

15:00 – 15:30	<i>Coffee</i>	
15:30 – 18:00	Tutorials	
	T1: Physicochemical Parameters Relevant for Drug Absorption	Dr. Robert Taylor and Dr. Darren Matthews, Sirius Analytical Inc.
	T2: Fragment-based Lead Generation	Dr. Mark Whittaker and Dr. Michael Mazanetz, Evotec
	T3: Developing a Lead	Dr. Andrew Mortlock, AstraZeneca
	T4: Structure-Based Lead Optimisation: Molecular Modeling	Dr. Tien Luu, Accelrys
	T5: IP in Drug Discovery	Dr. Frank Schager, Actelion
	T6: The NMR Toolbox for Medicinal Chemists	Dr. Christoph Rademacher, MPI Berlin
	T7: Retrosynthesis	Dr. Ruben Leenders and Dr. Johan Veerman, Mercachem

Afternoon / Evening (Chair: Gerd Folkers)

17:30 – 18:30	Lecture: Epigenetics	Dr. Robert A. Copeland, Epizyme
19:00 – 20:30	<i>Dinner</i>	
20:30 – 21:30	Lecture: Natural Product-based Drugs	Prof. Karl-Heinz Altmann, ETHZ



Wednesday, October 17, 2012: Hit to Lead to Candidate

Morning (Chair: Hugo Kubinyi)

08:30 – 09.15	Lecture: Proteases as Drug Targets	Dr. Richard Sedrani, Novartis
09:15 – 10:00	Case History: FXa Inhibitors as Anticoagulant Drugs	Dr. Susanne Röhrig, Bayer Health Care
10:00 – 10:30	<i>Coffee break</i>	
10:30 – 11:15	Lecture: Structure Based Design on G Protein-Coupled Receptors	Dr. Jonathan Mason, Heptares
11:15 – 12:15	Lecture: Kinetics and Thermodynamics of Binding	Dr. Dave Swinney, Institute for Rare and Neglected Diseases Drug Discovery
12.15 – 13:30	<i>Lunch</i>	

Afternoon (Chair: Christoph Rademacher) / **Evening**

14:00 – 15:00	Lecture: Structure-Based Drug Design: Applications and Limitations	Dr. Alexander Alex, Alexander Alex Consulting
15:00 – 16:00	Lecture: GPCRs as Drug Targets	Dr. Rogier Buijsman, NTRC

16:30 – 17:30	<i>Bus ride to Bex</i>	
18:00 – 20:00	<i>Visit of the salt mines</i>	
20:00 – 22:00	<i>Dinner underground</i>	
22:30 – 23:30	<i>Bus ride back to Leysin</i>	



Thursday, October 18, 2012:

Morning (Chair: Andrew Mortlock)

08:30 – 09.15	Lecture: Prodrugs and Soft Drugs	Prof. Hugo Kubinyi, University of Heidelberg
09:15 – 10:00	Case History: A new treatment option for multidrug resistant tuberculosis: Discovery of bedaquiline (TMC207)	Dr. Kristof van Emelen, Janssen
10:00 – 10:30	<i>Coffee break</i>	
10:30 – 11:15	Lecture: Biochemical Profiling in Early Drug Discovery	Dr. Doris Hafenbradl, Biofocus-Galapagos
11:15 – 12:15	Lecture: Bioisosterism	Dr. Nicholas A. Meanwell, BMS
12.15 – 13:30	<i>Lunch</i>	

Tutorials

15:00 – 15:30	<i>Coffee</i>	
15:30 – 18:00	Tutorials	
	T1: Physicochemical Parameters Relevant for Drug Absorption	Dr. Robert Taylor and Dr. Darren Matthews, Sirius Analytical Inc.
	T2: Fragment-based Lead Generation	Dr. Mark Whittaker and Dr. Michael Mazanetz, Evotec
	T3: Developing a Lead	Dr. Andrew Mortlock, AstraZeneca
	T5: IP in Drug Discovery	Dr. Frank Schager, Actelion
	T6: The NMR Toolbox for Medicinal Chemists	Dr. Christoph Rademacher, MPI Berlin
	T7: Retrosynthesis	Dr. Ruben Leenders and Dr. Johan Veerman, Mercachem

Afternoon (Chair: Beat Ernst) / **Evening**

17:30 – 18:30	Lecture: Protein-Protein Interactions	Dr. Daniel Obrecht, Polyphor
19:30 – 22:00	<i>Course Dinner (raclette or fondue)</i>	



Friday, October 19, 2012: Early development

Morning (Chair: Daniel Obrecht)

08:30 – 09:15	Lecture: Kinases as Drug Targets	Dr. Gerhard Müller, Mercachem
09:15 – 10:00	Lecture: Personalized Medicine	Dr. Joseph Walsh, Siemens
10:00 – 10:30	<i>Coffee break</i>	
10:30 – 11:15	Lecture: In vivo Efficacy Models	Dr. Cathleen Lutz, Jackson Laboratories
11:15 – 12:00	Panel Discussion: Innovation in the Pharma Industry	Prof. Beat Ernst, Univ. of Basel, Dr. Gerhard Müller, Mercachem
12:00 – 12:10	Final Remarks	Prof. Beat Ernst, Univ. of Basel, Dr. Gerhard Müller, Mercachem
12:10 – 13:30	<i>Lunch</i>	
<i>Departure</i>		

