



Main May 24 - 30, 2009 - Certosa di Pontignano, Siena (Italy)

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Each workshop topic will be considered in terms of individual tasks and their inter-relationships within the discovery cycle. The major topics will be the following: ligand/structure based drug design, in silico ADME - Tox and metabolism, design and screening of virtual libraries, molecular modelling methodologies, cheminformatics/bioinformatics and synthetic feasibility. These topics will be covered by lectures in the mornings.

The goal of the afternoon working sessions is to create, using case studies, an environment that is similar to what happens inside pharmaceutical companies today. The participants will be divided into teams which will be led and coordinated by tutors who are research group leaders in their companies and Universities. Each team will work through a different drug design case, emulating a real research team. The team's work will be focused on rational design and will include writing reports, project status reviews, and planning events of real-life research teams, as well as in-depth work with appropriate modelling software.

Preliminary Program

SUNDAY 24

17.00-19.00: registration
 20.00: dinner
 21.00 : welcome
 21.10-22.00: **Garland Marshall** (Washington University, USA): "The premise of Preorganisation: The Devil's in the Details"

MONDAY 25

Chairman: Hugo Kubinyi
 09.00-09.50: **Andrew Leach** (GSK, UK): "Practical Applications of Computational Chemistry in Drug Discovery"
 10.00-10.50: **Michele Parrinello** (ETH, Switzerland): " Large Scale Motions in Proteins"
 11.00-11.20: coffee break

Chairman: Garland Marshall
 11.30-12.20: **Teresa Carlomagno** (EMBL Heidelberg, Germany): " Visualizing the Intermolecular Interactions Network in Protein/Ligand Complexes by INPHARMA"
 12.30-13.00: **Anna Tsantili-Kakoulidou** (University of Athens, Greece): Immobilised Artificial Membrane Chromatography as a Friendly Technique for the Estimation of Drug Permeability and Drug-Membrane Interactions"
 13.10: lunch
 14.30-18.00: case study
 16.30-17.00: coffee break
 20.00: dinner
 21:00-22:00: Wine tasting in Certosa

TUESDAY 26

Chairman: Andrew Leach
 09.00-09.50: **Tudor I. Oprea** (University of New Mexico, USA): "From Digital to Experimental Reactivity: the Characterisation of a Novel Estrogen Receptor"
 10.00-10.50: **William L. Jorgensen** (University of Yale, USA): "Efficient Drug Lead Optimisation Guided by Free-Energy Calculations"
 11.00-11.20: coffee break

Chairman: Johann Gasteiger
 11.30-12.20: **Gabriele Cruciani** (University of Perugia, Italy): Seeking the Soft Spots"
 12.30-13.00: **Antonio Macchiarulo** (University of Perugia, Italy): "Voyages into the Chemical Space of Human Metabolome and Beyond"
 13.10: lunch
 14.30-18.00: case study
 16.30-17.00: coffee break
 20.00: dinner
 21.00-22.00: after dinner

WEDNESDAY 27

Chairman: Gabriele Cruciani
 09.00-09.50 **Charles L. Brooks III** (University of Michigan, USA): "Modeling and Docking to Flexible Receptors from Kinases to Class A GPRC:s"
 10.00-10.50: **Klaus-Jürgen Schleifer** (BASF, Germany): "Modelling Support for Agricultural Research"
 11.00-11.20: coffee break

Chairman: Tudor I. Oprea
 11.30-12.20: **Alexander Tropsha** (UNC Chapel Hill, USA): "Best Practices fo Developing Predictive QSAR Models"
 12.30-13.00: **Luciana Marinelli** (University of Napoli, Italy): "Computational Approaches in Drug Design: "Hands-on" Experience on Integrin Receptors"
 13.10: lunch
 14.30-20.00: free afternoon
 20.00: Dinner in Siena (Piazza del Campo)

**THURSDAY 28**

Chairman: Wolfram Altenhofen

09.00-09.50: **Hugues-Olivier Bertrand** (Accelrys): "High-Potency Olfactory Receptor Agonists Discovered by Virtual High-Throughput Screening: Molecular Probes for Receptor Structure and Olfactory Function"10.00-10.50: **Johann Gasteiger** (Molecular Networks, Germany): "Representation of Chemical Structures for the Drug Design Process"

11.00-11.20: coffee break

Chairman: Gerhard F. Ecker

11.30-12.20: **Thierry Langer** (Prestwick Chemicals, France): "SOSA and Parallel Pharmacophore-Based Virtual Screening"12.30-13.10: **Jürgen Borkak** (Fraunhofer Institute of Toxicology and Experimental Medicine, Germany): "Liver Enriched Transcription Factors in Primary and Secondary Liver Malignancies"

13.30: lunch

14.30-18.00: case study

16.30-17.00: coffee break

20.00: dinner

21.00-22.00: after dinner

**FRIDAY 29**

Chairman: Maurizio Botta

09.00-09.50: **Hugo Kubinyi** (Germany): "Chemogenomics in Drug Discovery"10.00-10.50: **Wolfram Altenhofen** (Chemical Computing Group, Germany): "Detection, Analysis and Visualisation of Relevant Scaffolds in Medicinal Chemistry Project Data"

11.00-11.20: coffee break

Chairman: Hugues-Olivier Bertrand

11.30-12.20: **Marco Mor** (University of Parma, Italy): "Computer-Aided Design and Optimisation of Carbamate-Based Inhibitors of FAAH"12.30-13.20: **Ferran Sanz** (Barcelona Biomedical Research Park, Spain): "Integrative Approaches in Pharmacoinformatics"

13.30: lunch

14.30-18.00: case study

16.30-17.00: coffee break

20.00: Social dinner

SATURDAY 30

Chairman: Thierry Langer

09.00-09.50: **Wolfgang Sippl** (University of Halle, Germany): "Comparative Modelling and Virtual Screening in the Drug Discovery Process"10.00-10.50: **Maurizio Recanatini** (University of Bologna, Italy): "Modeling the hERG K+ Channel: Where are we?"

11.00-11.20: coffee break

Chairman: Charles L. Brooks III

11.30-12.20: **Gerhard F. Ecker** (University of Wien, Austria): "Machine Learning Algorithms and Drug Design-Use Your Brain"12.30-13.20: **Eric Ennifar** (University of Strasbourg, France): "A Structure-Based Approach for Targeting the HIV-1 Genomic RNA Dimerisation Initiation Site"

13.30: farewell lunch