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Sponsors

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

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 teams 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, Swizerland): " 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** (Univeristy 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 Fexible 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 Borlak** (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 Dsign 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: Therry 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