VIII EWDD
Eighth European Workshop in Drug Design
May, 22nd - 28th, 2011 - Certosa di Pontignano, Siena (Italy)
www.unisi.it/EWDD

Programme

SUNDAY 22

17.00-19.00: registration
20.00: dinner
21.00: welcome (Prof. Maurizio Botta, Università di Siena – Italy)

MONDAY 23

Chairman: Hugo Kubinyi

09.00-09.50: Richard D. Cramer, Tripos - USA: “Topomer Cornucopia: An Overview”
10.00-10.50: Gabriele Cruciani, Università di Perugia – Italy: “High-throughput, fully automated, specific MetID. A revolution for Drug Discovery”
11.00-11.20: coffee break

Chairman: Federico Gago

11.30-12.20: Christian Ottmann, Max-Planck Institut – Germany: "Structural view on small molecule modulation of Protein-Protein Interactions"
13.00: lunch
14.30-15.00 Andrea Altieri, Asinex Ltd – Russia: “Incorporating Medchem Expertise into Compound Library Design”
15.00-18.30: case study
16.30-17.00: coffee break
20.00: dinner
21.00: wine tasting

TUESDAY 24

Chairman: Thierry Langer

09.00-09.50: William Jorgensen, Yale University - USA: “Efficient Drug Lead Optimization Guided by Free-Energy Calculations”
10.00-10.50: Andrea Cavalli, Università di Bologna and Istituto Italiano di Tecnologia, Genova – Italy: “Protein-ligand binding free energy and kinetics”
11.00-11.20: coffee break

Chairman: Andrea Cavalli
11.30-12.20: **Thierry Langer, Prestwick Chemical - France:** “Pharmacophore-based Parallel in Silico Screening: An Interesting Concept for Efficient Activity Profiling in Drug Discovery”

12.30-13.00: **Daniel Cappel, Schrödinger GmbH - Germany:** “Methodological advancements to improve the accuracy of induced-fit docking”

13.00: Lunch

15.00-15.20: **Kundan Ingale, VLIFE Sciences Ltd. - India:** “Novel Target based and Ligand based lead optimization methods: VLIFE GQSAR, VLIFE SCOPE and SATREA”

15.30-18.30: Case study

16.30-17.00: Coffee break

20.00: Dinner in Piazza del Campo

**Wednesday 25**

Chairman: William Jorgensen

09.00-09.50: **Gerhard F. Ecker, University of Wien - Austria:** “Predicting off-target effects - linear versus non-linear approaches”

10.00-10.50: **Daniel Rauh, Max-Planck Institut - Germany:** “Targeting Protein Kinases in Chemical Oncology Research”

11.00-11.20: Coffee break

Chairman: Richard Cramer

11.30-12.20: **Klaus-Jürgen Schleifer, BASF SE - Germany:** “Design of Active Ingredients for Crop Protection”

12.30-13.20: **Federico Gago, University of Alcala - Spain:** “Structure-activity relationships from drug-receptor complexes using the comparative binding energy (COMBINE) method”

13.30: Lunch

15.00-15.20: **Piero Altoè, E4 Computer Engineering Spa - Italy:** “E4 Computer Engineering: the IT company with a penchant for science”

15.30-18.30: Case study

16.30-17.00: Coffee break

20.00: Dinner

**Thursday 26**

Chairman: Tudor I. Oprea

09.00-09.50: **Hanoch Senderowitz, Bar-Ilan University - Israel:** “CFTR: Structure, function, genetics and drugability”

10.00-10.50: **Wolfgang Sippl, University of Halle - Germany:** “Combining virtual and biological screening for efficient lead structure generation”

11.00-11.20: Coffee break

Chairman: Katherine L. Seley-Radtke

11.30-12.20: **Tudor I. Oprea, The University of New Mexico/Sunset Molecular Discovery LLC - USA:** “Computer Aided Drug Repurposing”

12.30-13.00: **Antti Poso, University of Eastern Finland - Finland:** “Analyzing drug-receptor interactions”

13.00: Lunch

Chairman: Wolfgang Sippl
14.30-15.00: **Simon Cross, Molecular Discovery - UK:** “Finding pharmacophores: from features to fields”
15.00-15.20: **Silvia Pileri, GE Healthcare Europe GmbH - Italy:** “Integrated use of biophysical techniques in profiling inhibitor selectivity for PARP-family members”
15.30-18.30: coffee break
16.30-17.00: coffee break
20.00: social dinner

**FRIDAY 27**

Chairman: Simon Cross

09.00-09.50: **Alexander Tropsha, University of North Carolina at Chapel Hill - USA:** “Current Trends in the Development and Use of Predictive QSAR Models”
10.00-10.50: **Didier Rognan, CNRS, University of Strasbourg - France:** “Massive ligand profiling by parallel protein-ligand based pharmacophore searches”
11.00-11.20: coffee break

Chairman: Gerhard F. Ecker

11.30-12.20: **Katherine L. Seley-Radtke, University of Maryland - USA:** “Flexibility. A New Paradigm for Nucleoside Drug Design”
12.30-13.00: **Giulio Rastelli, Università di Modena e Reggio Emilia - Italy:** “Validation of free energy-based scoring functions in virtual screening”
13.00: lunch
15.00-17.00: case study: results presentation
17.00-17.20: coffee break
17.30-19.00: **FIVE-MINUTES POSTER PRESENTATIONS**
20.00: dinner

**SATURDAY 28**

Chairman: Alexander Tropsha

09.00-09.50: **Hugo Kubinyi - Germany:** "Drug Metabolism"

**GRANTS ASSIGNMENT - SHORT TALK SELECTED AMONG ATTENDEES**
10.00-10.50: **Stefano Alcaro, Università “Magna Graecia”, Catanzaro - Italy:** “The DNA G-quadruplex fold as an attractive targeting structure against cancer”
10.20-10.40: **Ivan Dimitrov, Medical University of Sofia - Bulgaria:** “Allertop – a Bioinformatics Tool for Allergenicity Prediction”
10.40-11.00: **Jens Pilger, Max-Planck Institut, Göttingen - Germany:** “NMR-based pharmacophore mapping”
11.00-11.20: **Rino Raggio, Università di Roma ‘La Sapienza’ - Italy: 2011:** “The 3-D QSAR is Alive! The 3D-QSAR Server (www.3d-qsar.com)”
11.20-11.40: **Renxiao Wang, Chinese Academy of Sciences - China:** “Automatic Tailoring and Transplanting: A Practical Method that Makes Virtual Screening More Useful”
12.00: farewell lunch