IX EWDD

Ninth European Workshop in Drug Design

May, 19th-25th – Certosa di Pontignano, Siena, Italy

www3.unisi.it/EWDD

Sunday 19th

17.00-19.00  Registration
20.00        Dinner
21.00        Welcome - Prof. Maurizio Botta, University of Siena
21.10-22.00  PL1 – Arthur J. Olson – Scripps Research Institute, USA -
             “Interacting with Proteins interactions”

Monday 20th

Session 1 –

09.00-09.50  PL2 – Andrea Cavalli – University of Bologna, Italy - “Protein-ligand binding investigated via molecular dynamics simulations: the case study of a transition-state analog inhibitor binding to the PNP enzyme.”
10.00-10.50  PL3 – Iwan De Esche – University of Amsterdam, Netherland - “Fragment-Based Lead Discovery: Small has become big in Drug Design”
11.00-11.20  Caffee Break

Session 2 –

11.30-12.20  PL4 – Stefan Knapp – University of Oxford, UK - “Modulating transcription by selective targeting protein interactions mediated by epigenetic effector domains”
12.30-13.00  OC1 – Gabriele Cruciani.University of Perugia- “Lipidomics or Randomomics?”
13.00        Lunch

Session 3 –
14.30-15.00 OC2 – Sandro Cosconati -"DiSTABiF", Second University of Naples, Italy – “Protein Flexibility in High-Throughput Docking: From Theory to Practical Applications”

15.00-18.30 Case Study

16.30-17.00 Coffee Break

20.00 Dinner

21.00 Wine Tasting

Tuesday 21st

Session 1 -

09.00-09.50 PL5 – Christian Ottmann – Max-Planck Institute, Germany- ”Modulation of 14-3-3 PPIs by small-molecules”

10.00-10.50 PL6 — Francesco Gervasio – University College London, UK - “Conformational changes and allosteric control of protein kinases”

11.00-11.20 Coffee Break

Session 2 -

11.30-12.20 PL7 Daniel Rauh – Max-Planck Institute, Germany - “Targeting protein kinases with covalent inhibitors”

12.30-13.00 OC3 – Arnout Voet “ Computational methods in the discovery of small molecule protein-protein interaction inhibitors.”

13.00 Lunch

Session 3 -

15.00-15.20 OC4 – Matt Geballe-OpenEye- “SZMAP: Using a semi-continuum solvent approach to guide Structure-Based Drug Design”

15.30-18.30 Case Study

16.30-17.00 Coffee Break

20.00 Social Dinner

Wednesday 22nd

Session 1 -
09.00-09.30  PL8 – Teresa Carlomagno – EMBL, Germany - “Structural mechanisms of drugs studied by INPHARMA-NMR: methodology and applications”

10.00-10.50  PL9 – Michele Parrinello – ETH, Zurich, Switzerland- “Molecular dynamics simulation of nucleation and growth of crystals from solution”

11.00-11.20  Coffee Break

Session 2 -

11.30-12.20  PL10-William Jorgensen – “Yale University, USA - Application of Computational Methods to Accelerate Drug Discovery”

12.30-13.20  PL11 – Gerhard F. Ecker – University of Vienna, Austria-“Exploiting Open Data - A new era in pharmacoinformatics”

13.30  Lunch

Session 3 -

15.00-15.20  OC5 – Markus Lill – Purdue University, USA- “Efficient incorporation of protein flexibility and dynamics in protein-ligand docking”

15.30-18.30  Case Study

16.30-17.00  Coffee Break

20.00  Dinner

Thursday 23th

Session 1

09.00-09.50  PL12 – Simon Cross-University of Perugia, Italy- “FLAPdock and WaterFLAP: mixing MIFs with classical energetics”

10.00-10.50  PL13 – Thierry Langer – Prestwick Chemical, France-“Advanced Feature-based Pharmacophore Models: Efficient Tools for Ligand Optimization and Profiling”

11.00-11.20  Coffee Break

Session 2 -

12.30-13.00 OC6 – Maciej Purwin- Universidad CEU San Pablo University, Spain and University of Bialystok, Poland- “Click synthesis of dual CK2 and HDAC1 inhibitors: a new strategy to design antitumor agents”

13.00 Lunch

**Session 3 -**

14.30-15.00 OC7 – Andrea Brancale – Cardiff University, UK - “Haptic-driven molecular modelling: a critical assessment”

15.30-18.30 Case Study

16.30-17.00 Coffee Break

20.00 Social Dinner

**Friday 24th**

**Session 1 -**

09.00-09.50 PL15 – Wolfgang Sippl – University of Halle, Germany- “Docking and Virtual Screening for Epigenetics Targets”

10.00-10.50 PL16 – Beatriz Pascual-Teresa Fernandez – Universidad San Pablo CEU Madrid, Spain - “Gaining selectivity within the gelatinase subfamily: new and potent MMP2 inhibitors”

11.00-11.20 Coffee Break

**Session 2 -**

11.30-12.20 PL17 – Ugo Kubinyi – Weisenheim am Sand, Germany - “Solving Problems in Lead Optimization”

12.30-13.00 OC8 – Jonathan Mason – Heptares Therapeutics, UK- “The New Wave in GPCRs: Using structure-based drug design to deliver selective drug candidates and water network energetics for druggability, potency & kinetics”

13.00 Lunch

15.30-17.00 Case Study

17.00-17.20 Coffee Break

**Session 3 – Poster Presentations**

*Poster presentations selected from the committee*
17.30-19.00  FIFTEEN MINUTES POSTER PRESENTATION

20.00  Dinner

Saturday 25th

09.00-09.50  PL18 – Hanoch Senderowitz – Bar-Ilan University, “What could be learnt on the structure, dynamics and energetics of the ABC transporter CFTR from atomistic simulations”

10.00-10.20  OC9-Masha Niv- The Hebrew University- “Taste and promiscuity: what we learn from bitter taste receptors and their ligands”

10.20-10.40  OC10– Daniel Cappel - Schrodinger Inc, USA – “Boosting virtual screening enrichments using data fusion: Coalescing 2D fingerprints, shape, and docking”

10.40-11.00  OC11- Alessio Lodola- Università di Parma- “Design and Optimization of Covalent Inhibitors of N-Acetylthanolamine Acid Amidase (NAAA), a Novel Target for the Treatment of Inflammatory States”

11.00-11.20  OC12- Sun Choi-Ewha Womans University-“Molecular modeling studies of the agonism of adenosine receptor using the multiple receptor conformation and network analysis”

11.20-11.40  OC13

12.00  Farewell Lunch

Case Studies:

1- Multifaceted role of computational chemist in drug discovery: from screening library design to lead optimization
2- Identification and In Silico Design of Ligands for the Adenosine A2A Receptor Using Advanced Pharmacophore Models and Accurate Virtual Screening
3- In silico drug discovery unveiled through molecular interactions
4- Looking at Molecular Modelling with an OpenEye: Computational Drug Discovery with Shape & Electrostatics