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."***

10.00-10.5 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 - "***Madulating 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 Caffee 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, Zuirich, 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 -

11.30-12.20 PL14 – Alexander Tropsha – University of North Carolina, USA- "***Best Practices and New Applications of QSAR Modeling"***

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 Optimation of Covalent Inhibitors of N-Acetylethanolamine Acid Amidase (NAAA), a Novel Target for the Treatment of Inflamatory 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