XII EWDD Programme

Sunday, May 19th

Sala Affresco – Certosa di Pontignano

17.00-19.30: *Registration and posters' billsticking*

20.00: Dinner

Sala Bracci – Certosa di Pontignano

21.15: ***Welcome:*** **Maurizio Botta - University of Siena, Siena, Italy**

21.30–22.30: **Yvan Guindon – IRCM, Canada:** *Free Radicals from Bad to Good: Novel Lead Molecules Targeting Pancreatic Cancer*

22:30: Cantucci & Vinsanto, Grappa

Monday, May 20th

Sala Bracci – Certosa di Pontignano

Chairman: Vittorio Limongelli

09.00-09.40: **Nigel Richards - Cardiff University, Cardiff, United Kingdom**: *Asparagine Biosynthesis and Anti-Cancer Drug Discovery*

09.40-10.20: **Wolfgang Sippl - Martin Luther Universität Halle Wittenberg, Halle Wittenberg, Germany**: *Structure based design of histone deacetylase inhibitors: lessons learned from computational studies and X-ray crystallography*

10.20-10.40: **Piero Procacci - University of Florence, Florence, Italy**: *SAMPL6 challenge: LogP blind predictions using a non equilibrium (alchemical) work (NEW) approach*

10.40-11.00: **Marcel Bermudez - Freie Universität Berlin, Berlin, Germany**: *Interference with binding pocket closure as a blueprint for biased GPCR ligands*

11.00-11.20: *Coffee Break*

Chairman: Tiziano Tuccinardi

11.20-12.00: **William Jorgensen - Yale University, New Haven, USA**: *Computer-Guided Efficient Discovery of Potent Enzyme Inhibitors*

12.00-12.40: **Andrea Cavalli - University of Bologna, Bologna, Italy:** *Dynamic docking to investigate thermodynamics and kinetics of drug-target*

12.40-13.00: **Dan Cannon - Schrödinger GmbH, Mannheim, Germany:** *Performing Hit Identification and Lead Optimization at Very Large Scale*

13.00-14.30: *Lunch*

14.30-15.10: **Gerhard Ecker – University of Vienna, Vienna, Austria:** *In silico Toxicology - from prediction of transporter interaction profiles to toxicological read across and beyond*

Sala Caratelli, Focolare, Palio, Veranda – Certosa di Pontignano

15.10-16.30: *Start Case Studies Session 1:* ***BiKi, Funnel Metadynamics, OpenEye*** *and* ***Schrödinger***

16.30-17.00: Coffee Break

17.00-18.40: *End Case Studies session*

20.00: *Dinner in Certosa di Pontignano*

21.30/after dinner: Social event

Tuesday, May 21st

Sala Bracci – Certosa di Pontignano

Chairman: Mattia Mori

09.00-09.40: **Kenneth Merz - Michigan State University, East Lansing, USA**: *Exploration of Molecular Recognition Processes Using Machine Learning*

09.40-10.20: **Alessio Ciulli - University of Dundee, Dundee, United Kingdom**: *Targeted Protein Degradation with Small Molecules: How PROTACs work*

10.20-10.40: **Barbara Füzi - University of Vienna, Vienna, Austria:** *Predicting drug pathways through drug interactome reconstruction*

10.40-11.00: *Coffee Break*

Chairman: Dieter Schinzer

11.00-11.40: **ChemMedChem Lecture: Antti Poso - University of Eastern Finland, Finland:** *Virtual screening: from docking to molecular dynamics and quantum mechanics. Role of solvation effects and pKa in ligand-receptor interactions.*

11.40-12.20: **Thierry Langer - University of Vienna, Vienna, Austria:** *Towards Next Generation Pharmacophore models: Concepts and Applications*

12.20-12.40: **Gunther Stahl – OpenEye Scientific Software Ltd., Cologne, Germany:** *REAL-ly large-scale Virtual Screening - Traversing Enormous Regions of Chemical Space with the GPU and CPU*

12.40-14.10: *Lunch*

Sala Caratelli, Focolare, Palio, Veranda – Certosa di Pontignano

14.10-15.30: *Strat Case Studies Session 1:* ***BiKi, Funnel Metadynamics, OpenEye*** *and* ***Schrödinger***

15.30-16.00: Coffee Break

16.00-17.40: End Case Studies session

20.00: *Social Dinner*

Wednesday, May 22nd

Sala Bracci – Certosa di Pontignano

Chairman: Maria Letizia Barreca

09.00-09.40: **Christian Ottmann – Eindhoven University, Eindhoven, Netherlands***: Stabilization of 14-3-3 Protein-Protein Interactions*

09.40-10.20: **Stefano Forli - Scripps Research, La Jolla, USA**: *AutoDock Reactive Docking: HTVS of covalent binders for in silico proteomics*

10.20-10.40: **Andrea Rizzi - Sloan Kettering Institute, New York, USA:** *The SAMPL6 SAMPLing challenge: Assessing reliability and efficiency of binding free energy calculations*

10.40-11.00: **Anna Tomberg - AstraZeneca Gothenburg, Gothenburg, Sweden**: *Teaching Chemical Intuition to Computers for Regioselectivity Prediction*

11.00-11.20: *Coffee Break*

Chairman: Gabriele Cruciani

11.20-12.00: **Gianni De Fabritiis - Universitat Pompeu Fabra, Barcelona, Spain:** *PlayMolecule: A computational environment for structural biology and drug design*

12.00-12.30: **Graziano Seghezzi - Sofinnova, France:** *Who are the venture capitalists?*

12.30-13.00: **Garegin A. Papoian - University of Maryland, USA:** *Physical Principles behind Epigenetic Regulation of Nucleosomes and Chromatin*
13.00-14.30: *Lunch*
14.30-15.10: **Hanoch Senderowitz - Bar-Ilan University, Israel:** *The structure and dynamics of the wild-type and mutant ABC transported CFTR as gleaned from MD simulations*
Sala Caratelli, Palio, Veranda – Certosa di Pontignano
15.10-16.30: *Strat Case Studies Session 2:* ***BioSolveIT, Inte:Ligand*** *and* ***MolDiscovery***
16.30-17.00: Coffee Break
17.00-18.40: End Case Studies session
20.00: Dinner
21.30/after dinner: Social event

Thursday, May 23rd
Sala Bracci – Certosa di Pontignano
Chairman: Hugo Kubinyi
09.00-09.40: **Gabriele Cruciani - University of Perugia, Perugia, Italy**:
09.40-10.20: **Zoe Cournia - Academy of Athens, Athens, Greece:** *Exploiting allostery for computer-aided drug design of oncogenes*
10.20-10.40: **Orazio Nicolotti - University of Bari, Bari, Italy:** *A multi-fingerprint similarity search algorithm for protein drug target identification*
10.40-11.00: *Coffee Break*
Chairman: Francesca Spyrakis
11.00-11.40: **Modesto Orozco - IRB Barcelona, Barcelona, Spain**: *The importance of dynamics to understand pathology and drug binding*
11.40-12.20: **Gerhard Wolber - Freie Universität Berlin, Berlin, Germany:** *New insights from dynamic 3D macromolecule-ligand interaction patterns*
12.20-12.40: **Marcus Gastreich - BioSolveIT, Germany:** *Picking "Accessibles" from Vast Chemical Space: Lessons Learned*
12.40-14.10: *Lunch*
14.10-14.50: **Hugo Kubinyi - BASF SE and University of Heidelberg, Germany:** *ADME/ToxProblems? Rescue Your Drug*
Sala Caratelli, Palio, Veranda – Certosa di Pontignano
14.50-16.00: *Start Case Studies Session 2:* ***BioSolveIT, Inte:Ligand*** *and* ***MolDiscovery***
16.00-16.30: Coffee Break
16.30-18.20: End Case Studies session
20.00: Gala Dinner in Certosa

Friday, May 24th
Sala Bracci – Certosa di Pontignano
Chairman: Alessio Lodola
09.00-09.40: **Alexander Tropsha - University of North Carolina, USA:** *Application of Text Mining*

and Artificial Intelligence Approaches to Drug Discovery and Repurposing

09.40-10.20: **Jan Wenzel - Sanofi-Aventis Deutschland, Germany:** *Predictive Deep Neural Network Models for ADME-Tox Properties: Learning from Large and Small Data Sets*

10.20-10.40: **Jissy Kuriappan - Istituto Italiano di Tecnologia, Genova, Italy:** *Targeting Alpha Isoform Specificity in Human Topoisomerase II*

10.40-11.00: **Fernando Durães - University of Porto, Porto, Portugal:** *Design and synthesis of thioxanthones as potential bacterial efflux pump inhibitors*

11.00-11.20: *Coffee Break*

11.20-12.00: **Chris De Graaf - Sosei Heptares, United Kingdom:** *Allegory, Impossible Object, Chiaroscuro: Structure-Based Drug Design Across the GPCRome*

12.00-12.40: *Shotgun poster presentation presentations and prizegiving*

12.40-13.00: *Farewell*

13.00: *Lunch*