IFOM
FIRC INSTITUTE OF MOLECULAR ONCOLOGY

Società Chimica Italiana

UNIVERSITÀ DEGLI STUDI DI MILANO

5th CDDD Meeting
COMPUTATIONALLY DRIVEN DRUG DISCOVERY
November 16-17, 2017 | IFOM, Milan - Italy

Program

Thursday, 16 November 2017

08:30	09:30	REGISTRATION
09:30	09:40	*Welcome & Introduction*
Session 1: Molecular Dynamics of Complex Systems		
09:40	10:20	**Keynote - Role of Molecular Dynamics and Related Methods in Drug Discovery** **Andrea Cavalli** - *University of Bologna, Italian Institute of Technology, Genoa, IT*
10:20	10:40	***Computational modelling of pyruvate dehydrogenase functional mechanism and inhibitors design*** **Jacopo Sgrignani** - *Institute for Research in Biomedicine, Bellinzona, CH*
10:40	11:00	***A Comprehensive Description of the Homo and Heterodimerization Mechanism of the Chemokine Receptors CCR5 and CXCR4*** **Daniele Di Marino** - *Department of Informatics, USI, Lugano, CH*
11:00	11:20	***Differential modulation of αvβ3 dynamics upon RGD-ligands*** **Antonella Paladino** - *Institute of Chemistry of Molecular Recognition, Milan, IT*
11:20	11:50	*Coffee break*
11:50	12:10	***Assessing Equilibrium Properties of Intrinsically Disordered Proteins through Enhanced Sampling Simulations*** **Mattia Bernetti** - *Department of Pharmacy and Biotechnology, Bologna University, IT*
12:10	12:30	***Tuning the molecular mechanism of Hsp70 via a new allosteric network*** **Silvia Rinaldi** - *ICRM-CNR, Milan,IT*
12:30	12:50	***Investigating the interaction of peptidomimetic ligands with e-cadherin using NMR and computational studies*** **Monica Civera** - *Department of Chemistry, University of Milan, IT*
13:00	14:00	*Lunch buffet*
Session 2: Biophysics and Computational		
14:00	14:40	**Keynote - Lipidomics in pharmaceutical research and drug design** **Gabriele Cruciani**, *University of Perugia, IT*
14:40	15:00	***Integrating Molecular Dynamics and Molecular Interaction Fields in virtual screening: the case of casein kinase 1d*** **Francesca Spyrakis** - *University of Turin, IT*
15:00	15:20	***Insights into Binding Functions of Immune Checkpoint Inhibitors: Microscale Thermophoresis Study of PD-1/PD-L1 and -L2 Interactions.*** **Daniela Dolciami** - *University of Perugia, IT*
15:20	15:40	***Selectivity of bitter taste GPCR receptors*** **Antonella Di Pizio** - *The Hebrew University of Jerusalem,IL*
15:40	16:00	***MetaQSAR as a source of data for accurately predicting UGT-mediated metabolism*** **Angelica Mazzolari** - *University of Milan, IT*
16:00	16:30	*Coffee break*
16:30	16:50	***Application of standard and enhanced sampling approaches on non-canonical structures of DNA and RNA*** **Federica Moraca** - *University "Magna Graecia", Catanzaro, IT*

16:50	17:10	***Molecular modelling studies of the endocannabinoid membrane enzymes*** **Laura Scalvini** - *University of Parma, IT*
17:10	17:30	***PepSuMD: an innovative approach to simulate peptide-protein recognition events by Supervised Molecular Dynamics.*** **Mattia Sturlese** - *University of Padova, IT*
17:30	17:50	***Towards an automated protocol for free energy paths calculations in protein ligand binding/unbinding*** **Claudio Peri** - *Italian Institute for Technology, Genoa, IT*
17:50	18:10	***Computational strategies in discovering Novel p38α MAPK inhibitors*** **Andrea Astolfi** - *University of Perugia, IT*
18:10	19:30	Poster Session - *Drinks & snacks*
19:30	21:00	*Social event (dinner buffet) at Barrio Alto Via Serio 14 (only for registered participants)*

Friday, 17 November 2017

Session 3: Drug Discovery

09:00	09:40	**Keynote - CADD Applied to FBDD: from Fragment Screening to Lead Optimisation** **Gianni Chessari** - *Astex Therapeutics, Cambridge, UK*
09:40	10:00	***Integrated CADD Methods for Drug Discovery at Nuevolution*** **Loris Moretti** - *Nuevolution, Copenhagen, DK*
10:00	10:20	***The MuTaLig Chemotheca virtual platform as tool for rapid identification of multi-targeting agents*** **Stefano Alcaro** - *University "Magna Graecia", Catanzaro, IT*
10:20	10:40	***Novel DrugLike Tangible Chemical Space: collection of robust reactions, library enumeration and profiling with application in drug discovery*** **Candida Manelfi** - *Dompé Farmaceutici Research Center, Naples, IT*
10:40	11:00	***Lead optimization: calculating relative binding free energies with FEP+*** **Davide Branduardi** - *Schrödinger Inc., Cambridge, UK*
11:00	11:20	***Computational Design of Novel Strategies to Fight Breast Cancer*** **Angelo Spinello** - *CNR-IOM and SISSA, Trieste, IT*
11:20	11:40	*Coffee break*
11:40	12:00	***Optimizing Proteins and Ligands for Computerized Drug Discovery*** **Alberto Cuzzolin** - *Acellera, Barcelona, ES*
12:00	12:20	***Structure-Based Virtual Screening of novel SMO antagonists: a ligand repurposing approach*** **Giorgio Amendola** - *University of Campania "Luigi Vanvitelli", Naples, IT*
12:20	12:40	***Recognition of good and poor substrates by the poly-specific transporter AcrB*** **Ivana Malvacio** - *Department of Physics, University of Cagliari, IT*
12:40	13:00	***Towards the identification of HMGB1 inhibitors: structural and functional studies*** **Federica De Leo** - *Vita-Salute San Raffaele University, Milan, IT*
13:00	14:00	*Lunch buffet (area catering)*

Session 4: Computational Genomics

14:00	14:40	**Keynote - Chromatin 3D architecture and cancer genomics** **Francesco Ferrari** - *IFOM, Milan, IT*
14:40	15:00	***Novel approaches for the identification of kinase rearrangements in tumors as new therapeutic targets*** **Roberta Bosotti** - *Nerviano Medical Sciences, IT*
15:00	15:20	***ADPredict: ADP-ribosylation site prediction based on physicochemical and structural descriptors*** **Matteo Lo Monte** - *Institute of Protein Biochemistry (IBP) CNR, Naples, IT*
15:20	15:40	***The endocytic protein Epsin3 drives EMT and cancer stem cell expansion in breast cancer*** **Irene Schiano Lomoriello** - *IFOM, Milan, IT*
15:40	16:00	***What's important here? Interactive filtering and exploration of chemical patent data with KNIME*** **Gregory Landrum** - *KNIME AG, Zurich, CH*
16:00	16:10	*Closing Remarks*