6th CDDD Meeting
COMPUTATIONALLY DRIVEN DRUG DISCOVERY

March 28-29, 2019, Università Cattolica del Sacro Cuore, Rome, Italy

Meeting Program

Thursday, 28 March 2019		
8.30	9:30	REGISTRATION
9:30	10:00	Welcome and Introduction **Antonio DiCarlo** – CECAM-IT-SIMUL Node director **Roberto Di Santo** – Vice-Presidente della Divisione di Chimica Farmaceutica della SCI
Session 1: Big Data and Machine Learning		
10:00	10:40	Keynote – Genomics and bioinformatics approaches for the identification of novel oncological target **Roberta Bosotti** – Nerviano Medical Sciences, IT
10:40	11:00	Improved exploration of structure (sequence)-activity relationships via advanced search & visual analytics **Ismail Ijjaali** – Perkin Elmer, IT
11:00	11:20	MetaQSAR database and ligand-based methods for metabolism prediction **Angelica Mazzolari** – University of Milan, IT
11:20	11:50	*Coffee break*
11:50	12:10	The multi-target drug discovery paradigm implemented in the Net4Science academic spin-off **Antonio Lupia** – University Magna Graecia of Catanzaro, IT
12:10	12:30	A free accessible web platform for protein drug target prediction **Orazio Nicolotti** – University of Bari, IT
12:30	12:50	In quest of new treatments for immune-related diseases: virtual screening and machine learning applications targeting AhR **Daniela Dolciami** – University of Perugia, IT
12:50	14:00	*Lunch buffet*
Session 2: Kinetics and Residence Time in Drug Discovery		
14:00	14:40	Keynote - Molecular dynamics-based approaches for the prediction of binding kinetics and protein ligand complex stability **Giovanni Bottegoni** – University of Birmingham, UK
14:40	15:00	From activity to mechanism: understanding interaction of small molecules with P-glycoprotein through enhanced sampling molecular dynamics **Stefano Guglielmo** – University of Turin, IT
15:00	15:20	Targeting alpha isoform specificity in human Topoisomerase II **Jissy Akkarapattiakal Kuriappan** – IIT Genova, IT
15:20	15:40	From dynamical protein ligand binding/unbinding to free energy: a unifying computational framework **Sergio Decherchi** – IIT Genova, IT
15:40	16:00	Automated molecular dynamics simulations to assess ligand-target complex stability in drug discovery **Loris Moretti** – Nuevolution A/S, Copenhagen, DK
16:00	16:30	*Coffee break*
16:30	16:50	A hydrophobic tunnel explains the binding of hallucinogenic amphetamines in the 5-HT2A receptor **Icaro A. Simon** – University of Copenhagen – DK

16:50	17:10	Molecular dynamics for pharmacogenetic: the multiple sclerosis case study **Francesca Cavaliere** – University of Parma, IT
17:10	17:30	Fragment-based screening by supervised molecular dynamics (SuMD): Bcl-XL as a case study **Mattia Sturlese** – University of Padua, IT
17:30	17:50	On the usage of novel hydrophobic molecular fields for CADD **Alessandro Deplano** – Pharmacelera, ES
17:50	18:10	Investigating and disrupting the interaction between hemoglobin and MRSA hemophores: *in silico* approaches to design novel antimicrobials **Eleonora Gianquinto** – University of Turin, IT
18:10	19:30	*Poster Session*

Friday, 29 March 2019

Session 3: Cryptic and allosteric pocket identification and related computational methods		
9:00	9:40	Keynote – The BioGPS pocketome database: application in pharmaceutical research **Gabriele Cruciani** – University of Perugia, IT
9:40	10:00	The variability of backbone geometry as a novel and powerful tool for protein structure quality assessment **Luigi Vitagliano** – Institute of Biostructures and Bioimaging - CNR (Naples), IT
10:00	10:20	Allosteric targeting of aromatase enzyme as a novel strategy for the development of next-generation inhibitors **Angelo Spinello** – SISSA, IT
10:20	10:40	Why propargylamine drugs vary in efficiency for inactivation of MAO **Livia Basile** – University of Catania, IT
10:40	11:00	Investigation of Nuclear Receptor structural variability **Giulia D'Arrigo** – University of Turin, IT
11:00	11:20	*Coffee break*
11:20	11:40	Drugging the undruggable: the prion protein as a case study of aggregating proteins **Mariangela Agamennone** – D'Annunzio University of Chieti-Pescara
11:40	12:00	A computational approach to estimate absolute and hydration free energies in atomistic simulations **Dorothea Gobbo** – IIT Genova, IT
12:00	12:20	Efficient and accurate modelling of conformational transitions in proteins: the case of c-Src kinase **Marco D'Abramo** – Sapienza University of Rome, IT
12:20	12:40	First-of-its-kind STARD3 inhibitor identified through pharmacophore-driven consensus docking **Giulio Poli** – University of Pisa, IT
12:40	13:00	Combining reaction-based enumeration, free energy perturbation and active learning in hit-to-lead campaigns: the case of CDK2 **Davide Branduardi** – Schrödinger Inc
13:00	14:00	*Lunch buffet*
Session 4: Innovative Approaches in Drug Discovery		
14:00	14:40	Keynote - Towards next generation pharmacophores: concepts and applications **Thierry Langer** – University of Vienna, AT
14:40	15:00	Drug design and synthesis of PDZ1 targeting NHERF1 inhibitors as anticancer agents **Antonio Coluccia** – Sapienza University of Rome, IT
15:00	15:20	Virtual screening of novel inhibitors of NEK6 kinase with antitumor activity **Benedetta Righino** – Università Cattolica del Sacro Cuore, IT
15:20	15:40	Identification of small molecule inhibitors of the Aurora-A/TPX2 complex **Giulia Guarguaglini** – CNR Rome, IT
15:40	16:00	Computational chemistry tool for disentangling the details of the mechanism of action of platinum anticancer drugs **Fortuna Ponte** – University of Calabria, IT
16:00	16:10	*Closing Remarks*