eChemInfo EURO 2018 Program

Training and Innovation Course in Drug Design

Mon, 16. Jul. 2018 - 09:00 to Fri, 20. Jul. 2018 - 15:00
Department of Pharmaceutical Sciences
Via L. Mangiagalli, 25 / 20133 Milano
University of Milan, Italy

MONDAY, 16 July		
TIME	TITLE	SPEAKER
08.30	Registration Open	
09.00	Welcome and Introduction to Workshop Concept	
09.15	Key Note: Malaria Drug Discovery Methods	Nicoletta Basilico, University of Milan
10:15	Introduction of Speakers and Case Studies	
12.00	Lunch	
13:00	From Library Preparation to Ligand-based and Structure-based Virtual Screening	Alessandro Pedretti, University of Milan
14:00	Homology Modelling	Ivano Eberini, University of Milan
15:00	Tutorials or Group Work on Case Studies	
17:00	Poster Session I	
18:30	End of Workday	

TUESDAY, 17 July		
TIME	TITLE	SPEAKER
09.00	Shape-based methods in lead discovery and lead hopping	Paul Hawkins, OpenEye
10.00	Prepare to Be Squonked - Moving from Individual Tools to Complete Workflows	Tim Dudgeon, Informatic Matters / Anthony Bradley, University of Oxford
11.00	Key Note: Novel Approaches to Drug Design and Development: Case Studies in Molecular Structure, Computation, Ligand-Receptor Interaction and Modelling	Rosella Ombrato, Angelini
12:00	Tutorials	
13:00	Lunch	
15:00	Group Work on Case Studies	
18:30	End of Working Day	

WEDNESDAY, 18 July		
TIME	TITLE	SPEAKER
09:00	Recent Computational Trends in Exploring G Protein-Coupled Receptor (GPCR) Ligand Recognition Pathways	Stefano Moro, University of Padova
10.00	Key Note: Design of cyclopeptidic drugs	Laura Belvisi / Monica Civera, University of Milan
11.00	Molecular dynamic stimulations for drug design and discovery	Alessandro Contini, University of Milan
12.00	Tutorials	
13.00	Lunch	
14.00	Tutorials or Group Work on Case Studies	
17.00	Poster Session II	
18.30	Social Reception	

THURSDAY, 19 July		
TIME	TITLE	SPEAKER
09.00	Key Note: Aspects of industrial drug design	Roman Affentranger, Roche
10.00	Pitfalls in docking calculations	Thomas Exner, Douglas Connect
11.00	Chem- and Bioinformatics for drug design and tox modelling	Andreas Bender & Lewis Mervin, Cambridge
12.00	Tutorials	
13:00	Lunch	
14:00	Group Work on Case Studies	
17:30	Social Event	

FRIDAY, 20 July		
TIME	TITLE	SPEAKER
09:00	Off-target-based toxicologic effects by SPILLO-PBSS	Alessandro Di Domizio, University of Milan
10:00	Quantum mechanics in the hit-to-lead phase	Adam Pecina, ITT Genoa
11:00	Tutorials	
13:00	Lunch	
14:00	Group presentations of case studies results	
14:45	Awarding of workshop certifications	
15:00	End of workshop	