

MONDAY, 16 July		
TIME	TITLE	SPEAKER
08:30	Registration Open	
09:00	Welcome and Introduction to Workshop Concept	
09:15	Key Note: Fighting Neglected Tropical Diseases (NTDs): novel approaches against Leishmania infections	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, 18 July		
TIME	TITLE	SPEAKER
09:00	Shape-based methods in lead discovery and lead hopping	Paul Hawkins, OpenEye
10:00	Prepare and run docking calculations	Thomas Exner, Douglas Connect
11:00	Prepare to Be Squonked - Moving from Individual Tools to Complete Workflows	Tim Dudgeon, Informatic Matters / Anthony Bradley, University of Oxford
12:00	Tutorials	
13:00	Lunch	
15:00	Group Work on Case Studies	
18:30	End of Working Day	

WEDNESDAY, 19 July		
TIME	TITLE	SPEAKER
09:00	Key Note: 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, 20 July		
TIME	TITLE	SPEAKER
09.00	Off-target-based toxicologic effects by SPILLO-PBSS	Alessandro Di Domizio, University of Milan
10.00	Chem- and Bioinformatics for drug design and tox modelling	Andreas Bender & Lewis Mervin, Cambridge
11.00	Tutorials	
13:00	Lunch	
14:00	Group Work on Case Studies	
17:30	Social Event	

FRIDAY, 21 July		
TIME	TITLE	SPEAKER
09:00	Quantum mechanics in the hit-to-lead phase	Adam Pecina, IIT Genova
10:00	Key Note: Aspects of industrial drug design	TBA
11:00	Group presentations of case studies results	
13:00	Lunch	
14:00	Group presentations of case studies results	
14:45	Awarding of workshop certifications	
15:00	End of workshop	