	Day 1 **07/09/22**	**Day 2** **08/09/22**	**Day 3** **09/09/22**	**Day 4** **10/09/22**
9.00-10.00		**Computational protein model generation: AlphaFold e RoseTTAFold** *Anna Marabotti*	**Biophysical studies of protein-ligand adducts** *Luigi Scietti*	**Role of molecular dynamics in drug discovery** *Alessandra Magistrato*
10.00-11.00		**Introduction on structure- and ligand-based drug design** *Maria Letizia Barreca*	**Sample preparation and MX data collection for fragment and ligand screening** *Manfred Weiss*	**Innovative small molecule degraders affecting protein folding** *Andrea Astolfi*
11.00-11.15		Coffee break	Coffee break	Coffee break
11.15-12.15		**Protein-inorganic ligand interactions** *Adriana Pietropaolo*	**Fragment-based drug design** *Mattia Sturlese*	**Advanced MD-based methods for fragment-protein studies: Supervised Molecular Dynamics** *Mattia Sturlese*
12.15-13.15		**Principles of small molecules docking** *Angelo Spinello*	**Fitting ligands into MX/CryoEM electron density** *Rob Nicholls*	**TES-1025: a case study for structural validation of protein-ligand interactions** *Michele Cianci*
13.15-14.15	Registration	lunch	lunch	Discussion and closing remarks
14.15-15.00	**We all need models …** *Silvia Onesti*	PRACTICALS **Practical approach to docking** *Giuseppe Felice Mangiatordi*	PRACTICALS **Coot and Phenix tools for ligand finding** *Rob Nicholls*	
15.00-15.45	**The role of MX in protein-ligand interaction study** *Roberto Steiner*			
15.45-16.15	Coffee break	Coffee break	Coffee break	
16.15-17.00	**Kinetics and thermodynamic of protein–ligand binding** *Menico Rizzi*	PRACTICALS **Quality assessment of protein-ligand docking** *Giuseppe Felice Mangiatordi*	PRACTICALS **Preparing a CIF file for ligand molecules** *Belviso Benny Danilo*	
17.00-17.45	**The role of SAXS and Cryo-EM in protein-ligand interaction study** Federico Forneris	Question Time	Question Time	