

	<b>Day 1</b> <b>07/09/22</b>	<b>Day 2</b> <b>08/09/22</b>	<b>Day 3</b> <b>09/09/22</b>	<b>Day 4</b> <b>10/09/22</b>
9.00-10.00		<b>Computational protein model generation: AlphaFold e RoseTTAFold</b> <i>Anna Marabotti</i>	<b>Biophysical studies of protein-ligand adducts</b> <i>Luigi Scietti</i>	<b>Role of molecular dynamics in drug discovery</b> <i>Alessandra Magistrato</i>
10.00-11.00		<b>Principles and applications of ligand- and structure-based drug design</b> <i>Maria Letizia Barreca</i>	<b>Crystallographic fragment-screening at the HZB: workflow, tools and procedures</b> <i>Manfred Weiss</i>	<b>Innovative small molecule degraders affecting protein folding</b> <i>Andrea Astolfi</i>
11.00-11.15		Coffee break	Coffee break	Coffee break
11.15-12.15		<b>Protein-inorganic ligand interactions</b> <i>Adriana Pietropaolo</i>	<b>Fragment-based drug design</b> <i>Mattia Sturlese</i>	<b>Advanced MD-based methods for fragment-protein studies: Supervised Molecular Dynamics</b> <i>Mattia Sturlese</i>
12.15-13.15		<b>Principles of small molecules docking</b> <i>Angelo Spinello</i>	<b>Fitting ligands into MX/CryoEM electron density</b> <i>Rob Nicholls</i>	<b>TES-1025: a case study for structural validation of protein-ligand interactions</b> <i>Michele Cianci</i>
13.15-14.15	Registration	lunch	lunch	Discussion and closing remarks
14.15-15.00	<b>We all need models ...</b> <i>Silvia Onesti</i>	<b>PRACTICALS Practical approach to docking</b> <i>Giuseppe Felice Mangiatordi</i>	<b>PRACTICALS Coot and CCP4 tools for ligand finding</b> <i>Rob Nicholls</i>	
15.00-15.45	<b>The role of MX in protein-ligand interaction study</b> <i>Roberto Steiner</i>			
15.45-16.15	Coffee break	Coffee break	Coffee break	
16.15-17.00	<b>Kinetics and thermodynamic of protein-ligand binding</b> <i>Menico Rizzi</i>	<b>PRACTICALS Quality assessment of protein-ligand docking</b> <i>Giuseppe Felice Mangiatordi</i>	<b>PRACTICALS Preparing a CIF file for ligand molecules</b> <i>Belviso Benny Danilo</i>	
17.00-17.45	<b>The role of SAXS and Cryo-EM in protein-ligand interaction study</b> <i>Federico Forneris</i>	Question Time	Question Time	