Program

DAY1 – Monday 6 June 2016

9:00 – 12:30 Auditorium

- 9:00-10:30 *Modeling and visualizing protein interactions: from chemical ligands to cellular environments* (Arthur J. Olson, The Scripps Research Institute, La Jolla, CA, USA)
- 10:30 -11:00 Coffee break
- 11:00 – 12:30 Role, relevance and limitations of homology modeling in biomolecular sciences (Allegra Via, Università La Sapienza, Rome, Italy)

12:45 – 14:00 Lunch

14:30 – 18:30 Computer room

- Tutorial: Building structural models by homology (Allegra Via, Domenico Raimondo)

DAY2 – Tuesday 7 June 2016

9:00 – 12:30 Auditorium

- 9:00 – 10:30 Computational methods to detect druggable sites on pharmaceutical targets (Anne-Claude Camproux, Université Paris-Diderot, Paris, France)
- 10:30 – 11:00 Coffee break
- 11:00 – 12: 30 Computational modeling of protein-protein interactions (Alexandre Bonvin, Utrecht University, Utrecht, the Netherlands)

12:45 – 14:00 Lunch

14:00 – 18:30 Computer room

- Tutorial: PockDrug-server, a web server for druggability prediction: use and applications (Anne-Claude Camproux, Hiba Abi Hussein)

DAY3 – Wednesday 8 June 2016

9:00 – 13:00 Computer room

- Tutorial: Docking and virtual Screening with the AutoDock Suite (Arthur J. Olson, Stefano Forli)

13:15 – 14:15 Lunch

14:30 – 1900 Computer room

- Tutorial: Protein-protein docking with HADDOCK (Alexandre Bonvin, Anna Vangone)

DAY4 – Thursday 9 June 2016

9:00 – 12:30 Computer room

- 9:00-10:30 Simulating macromolecular recognition through diffusional Brownian dynamics (Neil Bruce, Heidelberg Institute for Theoretical Studies, Heidelberg, Germany)
- 10:30 – 11:00 Coffee break
- 11:00 – 12:30 Tutorial: webSDA (Neil Bruce)

12:45 – 14:00 Lunch

14:00 – 16:00 Computer room

- Poster Session

19:30 – 24:00 Social dinner (to be confirmed)

DAY5 – Friday 10 June 2016

9:00 – 12:30 Auditorium

- 9:00 – 10:30 Role of enhanced-sampling methods in drug discovery (Walter Rocchia, Italian Institute of Technology, Genoa, Italy)
- 10:30 – 11:00 Coffee break
- 11:00 – 12:30 Not only affinity: enhanced sampling methods to study biological processes other than binding (Fabio Pietrucci, Université Pierre et Marie Curie – Sorbonne Universités, Paris, France)
- 12:30 -12:45 Concluding remarks

12:45 – 14:00 Lunch

14:00 Departure