

Role of MD in drug discovery

September 29, 2025 - October 1, 2025
Location: Montelino, Bettona (PG, Umbria) Italy

Monday, September 29, 2025

12:00 to 13:30	Registration & Finger lunch
13:30 to 13:45	Welcome: Gabriele Cruciani & Andrea Cavalli
13:45 to 14:15	Inaugural: Modesto Orozco
14:15 to 14:45	Lecture 1 - Giorgio Colombo: Structures, dynamics, complexes, and functions: from classic computation to artificial intelligence
14:45 to 15:15	Lecture 2 - Laura Scalvini: Computational insights into the mechanism of action of nitrile-containing bioactive compounds
15:15 to 16:00	Coffee break
16:00 to 16:30	Lecture 3 - James Gebbie-Rayet: BioSimDR: Data tools and UK national infrastructure for biomolecular simulation
16:30 to 17:00	Lecture 4 - Sofia Oliveira: How can nonequilibrium simulations help understand drug resistance and allostery in proteins?
17:00 to 17:30	Lecture 5 - Silvia Gervasoni: Integrating molecular dynamics and quantum calculations into open databases for drug discovery
17:30 to 18:00	Discussion
18:30 to 21:00	Networking & aperitif



Tuesday, September 30, 2025

09:00 to 09:30	Lecture 6 - Francesca Spyraakis: Multiscale modelling and machine learning to interfere with NLRP3 inflammasome activation
09:30 to 10:00	Lecture 7 - Yasaman Karami: ComPASS: decoding communication pathways within protein-nucleic acid complexes
10:00 to 10:45	Coffee break
10:45 to 11:15	Lecture 8 - Mattia Bernetti: Dissecting the RAD51-BRC4 conformational landscape through integrative simulations and experimental
11:15 to 11:45	Lecture 9 - Claudio Soares: Glycan shielding in Proteins responsible for Host Attachment and Viral Entry: MD approaches to inform protein design
11:45 to 12:15	Discussion
12:30 to 14:30	Lunch
14:30 to 15:00	Lecture 10 - Giulia Palermo
15:00 to 15:30	Lecture 11 - Alessia Ghidini: Binding free energy calculations with path collective variables
15:30 to 16:15	Coffee break
16:15 to 16:45	Lecture 12 - Andrew Emerson: Molecular dynamics workflows for absolute binding free energy prediction in drug candidate selection
16:45 to 17:15	Lecture 13 - Benoit Roux: Predicting the potency of covalent kinase inhibitors from computations
17:15 to 18:00	Discussion
19:00 to 23:00	Workshop dinner



Wednesday, October 1, 2025

09:00 to 09:30	Lecture 14 - Jas Kalayan: Absolute entropies from molecular dynamics simulations with the multiscale cell correlation (MCC) method
09:30 to 10:00	Lecture 15 - Giovanni Bottegoni: Molecular dynamics as a versatile tool in an integrated hit identification and optimization platform
10:00 to 10:30	Lecture 16 - Adam Hospital: Open MD data for drug discovery: systems of pharmaceutical interest in the European repository for biosimulation data (MDDDB)
10:30 to 11:15	Coffee break
11:15 to 11:45	Lecture 17 - Paraskevi Gkeka: The long road to drug discovery: From unbiased MD, to binding site identification, binding affinity calculations and autoencoders for collective variable identification
11:45 to 12:15	Lecture 18 - Francesco Musiani: Precision medicine in cancer: drug repurposing strategies targeting DNA polymerase ϵ for cancer therapy
12:15 to 12:45	Discussion
12:45 to 13:00	Closing Remarks: Erik Lindahl

** All meals in the programme are provided by MDDB.*



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