Role of MD in drug discovery

September 29, 2025 - October 1, 2025
Montelino, Bettona (PG, Umbria) Italy
Registration deadline: July 15, 2025

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**

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Tuesday, September 30, 2025

09:00 to 09:30	**Lecture 6** - Francesca Spyrakis: 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**

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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 (MDDB)
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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