ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

DIPARTIMENTO
DI FARMACIA
E BIOTECNOLOGIE

AVVISO DI SEMINARIO

Il giorno **16 maggio 2025**
alle ore **11:00**

Dr. Massimiliano Bonomi,

Head of Computational Structural Biology Unit - Institut Pasteur (France)
(ospite di Prof. Matteo Masetti)

terrà un seminario in lingua inglese dal titolo:

Structural and dynamic biology with integrative approaches

Area tematica:
Drug discovery and development;
Integrative structural biology

in presenza:
Aula Magna U.E.1, Navile, via della Beverara 123/1, Bologna

e in streaming:
https://teams.microsoft.com/l/meetup-join/19%3aN09c0NIyEssBnF7ObCyDOQwkgDWm1qdd9f7F2nJV9fw1%40thread.tacv2/1631519544944?context=%7b%22Tid%22%3a%22e99647dc-1b08-454a-bf8c-699181b389ab%22%2c%22Oid%22%3a%225a941351-ef41-4aa4-8771-fa50a6d62ca1%22%7d

Colleghi e studenti sono cordialmente invitati

ABSTRACT

Understanding the molecular mechanisms by which biological systems carry out their functions is often essential for the rational targeting of associated diseases. In many cases, determining the threedimensional (3D) structure of these systems provides valuable insights. However, it is often the interplay between structural and dynamical properties that determines the behavior of complex systems. While both experimental and computational methods are invaluable for studying protein structure and dynamics, the limitations of each individual technique can hinder their capabilities [1].

Here, I present our lab's work on developing integrative computational-experimental approaches that

combine experimental data with molecular dynamics (MD) simulations to determine accurate protein

structural ensembles of biological systems [2,3]. I will showcase the capabilities of these methods through various applications to systems of significant interest. First, I will demonstrate how accurate protein structural ensembles can be obtained from 3D cryo-electron microscopy maps using our recently developed EMMIVox approach [4]. Then, I will highlight how we characterize the structural and dynamic properties of the CyaA toxin by integrating coarse-grained MD simulations with Hydrogen/Deuterium eXchange Mass Spectrometry (HDX-MS), Small-Angle X-ray Scattering (SAXS), and 2D single-particle cryo-EM data.

Finally, I will show how structural information provided by Artificial Intelligence approaches, such as

AlphaFold, can be synergistically combined with low-resolution experimental data to generate accurate models of protein complexes.

References:

[1] M. Bonomi, G. T. Heller, C. Camilloni, M. Vendruscolo. Curr. Opin. Struct. Biol. 42 (2017) 106
[2] M. Bonomi, C. Camilloni, A. Cavalli, M. Vendruscolo. Sci. Adv. 2 (2016) e1501177
[3] P. Cossio, G. Hummer. J. Struct. Biol. 184 (2013) 427
[4] S. E. Hoff, F. E. Thomasen, K. Lindorff-Larsen, M. Bonomi. PLoS Comput. Biol. 20 (2024) e1012180.

BIOGRAPHICAL SKETCHES

Max Bonomi is the head of the Computational Structural Biology Lab at Institut Pasteur (Paris, France) and a research director at CNRS. He obtained his PhD in 2010 at ETH Zurich, where he worked in the group of Prof. Michele Parrinello. He completed his first postdoc in the Sali lab at the University of California, San Francisco, and his second postdoc in the Vendruscolo lab at the University of Cambridge. Since late 2018, Max Bonomi has held a tenured position at Institut Pasteur. His work focuses on the development and application of integrative approaches that combine molecular simulations, artificial intelligence, and experimental data to characterize the structural and dynamic properties of biological systems. Max Bonomi is also an active developer of open-source software, which has become state-of-the-art in the computational structural biology community, and is involved in the dissemination of best practices and the training of the younger generation of scientists.