



Mercoledì 17 luglio 2024 alle ore 11:30 presso l'aula L1

il Dr. Toni Giorgino

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terrà il seminario dal titolo:

## Molecules to Models: Biomolecular Dynamics through Large-Scale Simulations

This seminar explores the integration of large-scale molecular dynamics (MD) simulations with statistical techniques to model biomolecular behaviors. Statistical learning encodes data extracted from noisy domains (e.g., real or simulated observations) into models, thus condensing information and enabling predictions. We'll discuss the application of methods rooted in statistics and AI demonstrating their use to bridge timescales, model physico-chemical determinants, rationalize genotype-phenotype relationships, and support drug discovery.

*La presenza della S. V. sarà molto gradita*

*Stefano Corni*

*Il Direttore del Dipartimento*  
*Stefano Mammi*