

BioFrontiers - Biology Seminar

November 14, 2025; 3:00 PM

Life Sciences Building - A117

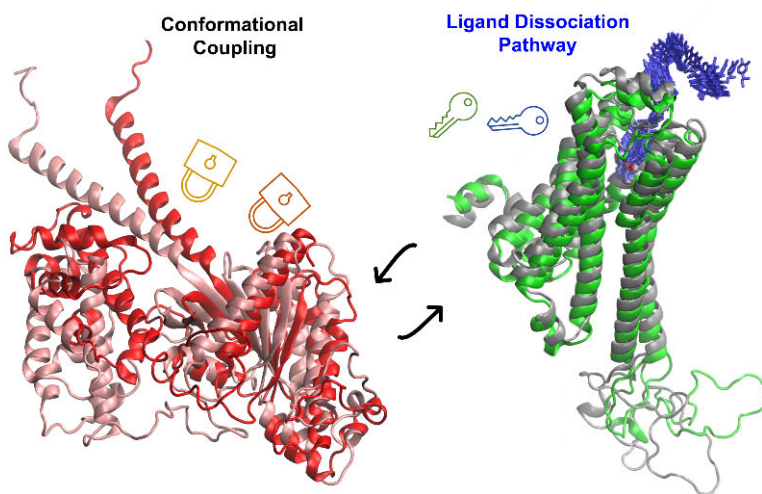


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Multiscale simulations in biological systems

Computational simulations based on physics-based models provide powerful tools for understanding complex biological systems across multiple spatial and temporal scales. At the quantum mechanical level, simulations reveal the electronic structures and reaction mechanisms of biomolecules. Atomistic molecular dynamics simulations extend this understanding to larger systems, capturing the conformational dynamics and interactions of proteins, lipids, and nucleic acids in realistic environments. Coarse-grained models further expand the accessible system size and timescale, allowing investigation of mesoscale organization and emergent collective behavior. Integrating these methods enables the construction of multiscale frameworks that connect atomic-level mechanisms with cellular-scale functions. In particular, atomistic simulations play a central role in bridging the gap between molecular and cellular models, offering critical insights into how local molecular events drive global biological phenomena. This presentation will highlight recent advances and applications of multiscale simulations in elucidating the mechanisms of biological systems.



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