CNR-IBF
Istituto di Biofisica

Seminari di Istituto

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Institute for Research in Biomedicine - Barcelona

Streamed on Teams

3 December 2026
h 11:00 – 12:00

The seminar will be held in English

Unlocking GPCR Drug Discovery with Molecular Dynamics

G protein-coupled receptors (GPCRs) represent the largest family of drug targets in the human genome, yet our structural understanding of them has long been limited to static snapshots. Molecular dynamics (MD) simulations bridge this gap by capturing the full conformational landscape of these receptors, revealing alternative binding conformations and cryptic pockets invisible to crystallography and cryo-EM, and showing how ligands and membrane environments shape receptor behaviour. Here, we demonstrate how large-scale MD simulations expand the druggable pocket space of GPCRs, opening new avenues for drug discovery.