TOR VERGATA
UNIVERSITÀ DEGLI STUDI DI ROMA

Dipartimento di Scienze e Tecnologie Chimiche

AVVISO DI SEMINARIO

Il giorno 18/04/2023 alle ore 14:30

nell'aula Gismondi

Il Prof. ***GIOVANNI BUSSI***

Scuola Internazionale Superiore di Studi Avanzati – Trieste
Molecular and Statistical Biophysics Group

terrà un seminario dal titolo

"Dissecting RNA dynamics by combining molecular simulations and solution experiments"

Proponente: Prof. Lorenzo Stella

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Dissecting RNA dynamics by combining molecular simulations and solution experiments

Giovanni Bussi

Conformational dynamics is crucial for ribonucleic acid (RNA) function. A range of techniques, including nuclear magnetic resonance (NMR), small-angle X-ray scattering, chemical probing, and denaturation experiments can be used to probe RNA dynamics at different time and space resolutions [1]. Their combination with accurate atomistic molecular dynamics (MD) simulations paves the way for quantitative and detailed studies of RNA dynamics. In this talk, I will show how our group uses data obtained with the mentioned techniques to refine ensembles and force fields for RNA systems [2,3]. In addition, I will discuss how MD simulations can be used to investigate the mechanism underlying chemical probing experiments [4].

[1] Bernetti and Bussi, COSB (2023) https://doi.org/10.1016/j.sbi.2022.102503
[2] Bernetti, Hall, and Bussi, NAR (2021) https://doi.org/10.1093/nar/gkab459
[3] Piomponi, Fröhlking, Bernetti, and Bussi, ACS (2022) https://doi.org/10.1021/acscentsci.2c00565
[4] Calonaci, Bernetti, Jones, Sattler, and Bussi, submitted (2023) https://arxiv.org/abs/2209.12640