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MUR PNRR National Center for Gene Therapy and Drugs based on RNA Technology

Spoke 6: RNA drug development

veRNAdì

A webinar series about RNA

to share projects and competences, increase networking, discuss issues and new ideas, and disseminate results

Every last Friday of the month

https://rb.gy/y40y6

10th veRNAdì: Friday 29 November 2024, 15:00

Molecular dynamics simulations for understanding RNA biology and design of RNA therapeutics

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RNA is a fundamental and versatile molecule in biology, capable of storing genetic information, catalyzing chemical reactions and regulating diverse cellular processes such as DNA transcription and protein synthesis. Consequently, RNA molecules are emerging as an important tool and target in precision medicine. All-atom molecular dynamics (MD) simulations are a powerful tool for dissecting the molecular mechanisms driving RNA biology at atomistic resolution and can thus importantly complement and enhance experimental findings. Additionally, they facilitate the design of novel RNA-targeting and/or RNA-based drugs against various human diseases, including cancer and neurodegeneration. Here, we will present an overview on how MD simulations, coupled with enhanced sampling techniques and quantum mechanical calculations, can illuminate the molecular processes involved in RNA maturation (e.g. splicing), posttranscriptional RNA modifications or RNA-membrane association, and can assist in RNA structure refinement. Finally, we will illustrate how MD simulations can guide the design of novel RNA-targeting small molecules, focusing on RNA-splicing modulating drugs.