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Analyzing causality of molecular interactions: A case study of molecular dynamics simulation of protein-RNA system

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In this study, we investigate the interactions and analyze associative behaviour at the interface between protein and RNA. In this study, we have combined molecular dynamics simulation and information theoretic measures, such as transfer entropy to investigate the driving forces at the interface of complex biomolecular systems. The modular architecture of binding site may greatly simplify the design of new molecular systems interactions and provides a feasible view of how these interactions evolve. Combining complex information theoretic measures and free-energy calculations, we show that identification of the dominant contributions to the free energy of complex interactions can guide experiments aimed at the design of protein interaction inhibitors and provide a stepping-stone to important applications such as interface redesign.

Biography

Hiqmet Kamberaj has completed his PhD in 2005 from Manchester Metropolitan University and Post-doctoral studies from University of Minnesota, Arizona State University and National Institute of Nanotechnology at University of Edmonton. He is an Associate Professor at International Balkan University and the Acting Dean of the Faculty of Engineering. He has published around 20 papers in reputed journals and has been serving as an Editorial Board Member and Ad-Hoc Reviewer of repute.

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