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Showcasing research from the group of Dr Padmesh Anjukandi at the [theochemistry@IITPKD](mailto:theochemistry@IITPKD) laboratory, Indian Institute of Technology Palakkad.

Multifaceted folding-unfolding landscape of the TrpZip2  $\beta$ -hairpin and the role of external sub-piconewton mechanical tensions

Investigating the influence of sub-piconewton forces on folding-unfolding of proteins is crucial due to the biological forces. TrpZip2  $\beta$ -hairpin experiences an uneven local force due to the divergent solvations owing to their thermal motion. Metadynamics simulations on both unbiased and biased hairpins reveal Janus folding pathways. While the unbiased case exhibited a two-state model, the biased case projected a downhill free energy surface due to various trapped intermediates.

Image acknowledgement: Subodh Vijayan, IIT Palakkad.

As featured in:



See Padmesh Anjukandi *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 11093.