Steered molecular dynamics and single molecule atomic force microscopy to explore the mechanical response of talin

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Talin is cytoplasmic protein connecting integrin receptors to actomyosin network. This linkage is essential for cell anchoring and spreading and naturally also for development. Talin acts as a hub for molecular interactions in focal adhesions and the interactions between talin and binding partners are regulated by mechanical signals. We study the mechanical response of talin by steered molecular dynamics. Both constant force and constant velocity simulations in explicit water have been found useful to explore the molecular features of talin. We have found talin rod subdomains to differ from each other in terms of their mechanical stability. Importantly, we have been able to compare and validate the results by using experimental data obtained with single-molecule atomic force microscopy. Destabilizing point mutations applied on talin rod have been found to cause significant changes in cell spreading, migration and cellular traction force. Our recent studies focus on mechanically weakened talin forms, intermediates of protein unfolding and engineering of unfolding-resistant talin forms.

Recent Publications


Biography

Vesa P Hytönen is a Head of the Protein Dynamics research group in Faculty of Medicine and Life Sciences at the University of Tampere, Tampere, Finland. After graduating PhD from the University of Jyväskylä, Jyväskylä, Finland at 2005, he conducted Postdoctoral training at ETH Zurich, Switzerland during 2005–2007. He then continued as a Postdoctoral researcher at the University of Tampere and established independent research group at 2010. He is currently working as Associate Professor at the University of Tampere. His research interests are mechanobiology, protein engineering and vaccine research and he has authored more than 100 scientific articles.