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Mechanical properties of NRR domain from human Notch 1 studied by single molecule AFM force spectroscopy and steered molecular dynamics ASHIM DEY, Department of Physics, Kansas State University, Manhattan, KS, JIANHAN CHEN, HUI LI, ANNA ZOLKIEWSKA, HUI-CHUAN WU, MICHAL ZOLKIEWSKI, Department of Biochemistry, Kansas State University, Manhattan, KS, ROBERT SZOSZKIEWICZ, Department of Physics, Kansas State University, Manhattan, KS — For proteins in living cells, forces are present from macroscopic to single molecule levels. Single molecule atomic force microscopy in force extension (FX-AFM) mode measures forces at which proteins undergo major conformational transitions with $\sim$ 10 pN force sensitivity (FX-AFM). Here, we present the results of the FX-AFM experiments on a construct comprising the NRR domain from human Notch 1. It is believed that understanding the mechanical properties of Notch at the single molecule level can help to understand its role in triggering some breast cancers. The experimental results on our Notch construct revealed several conformational transitions of this molecule under force. These results were confronted with the steered molecular dynamics simulations based on a simplified Go model. These results opened a path for further investigations of Notch constructs at various physiologically relevant conditions.

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