Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for Compressive-Force Induced Activation of Apo-Calmodulin in Protein Signaling

Susovan Roy Chowdhury, Sunidhi Jaiswal, H. Peter Lu*

Department of Chemistry, Center for Photochemical Sciences, Bowling Green State University, Bowling Green, Ohio 43403, United States

AFM tip and tip force constant calibration

We have used Cr-Au coated AFM Probe (Micromash HQ:CSC38/Cr-Au). There are three cantilevers A, B, C. with force constant 0.09nN/nm, 0.03nN/nm and 0.05nN/nm. We typically used the cantilever B with 0.03nN/nm force constant. We have calibrated the cantilever force constant in our experiments by using Thermal K provided for Agilent AFM. Thermal K calculates an AFM probe spring constant by describing the motion of the cantilever as a harmonic oscillator through the use of the equipartition theorem from fundamental thermodynamic theory. The curvature for the Cr-Au coated tip has less than 35 nm of radius.

Cartoon scheme of the AFM experiment

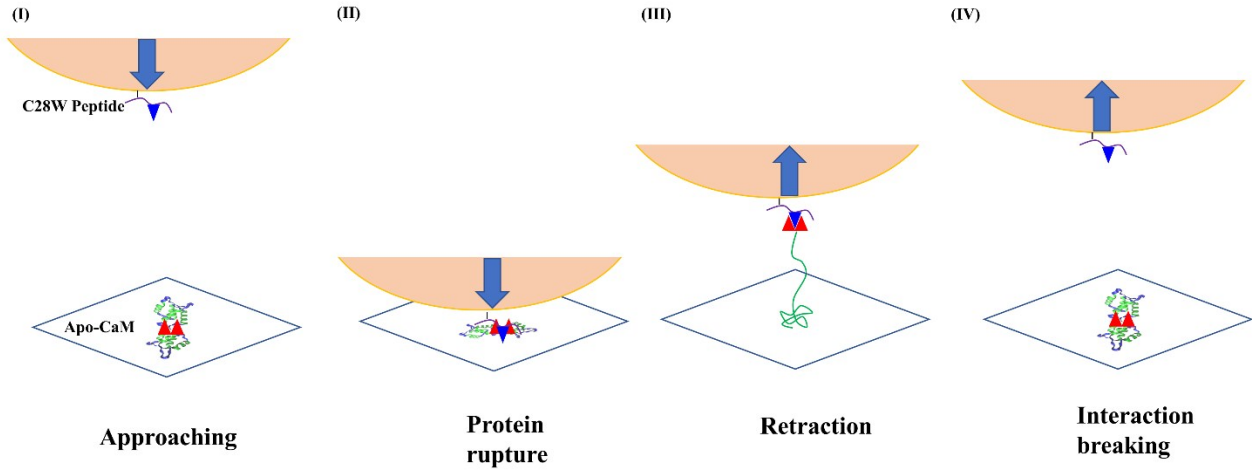

Fig. S1 The AFM experiment scheme. (I) C28W peptide covered AFM tip approaches the surface with tethered Apo-CaM molecules. The binding domain is hidden as the structure is compact in nature (II) After loading of threshold amount of compressive force by the AFM tip, the protein gets ruptured as a result the binding domain gets exposed, which trigger the binding between the peptide and ruptured Apo-CaM molecule. (III) As the AFM tip is retracted from the surface we see the negative force loading on the AFM tip due to the interaction between peptide and the protein molecule. (IV) Once the force exceeds the interaction threshold force, the interaction gets broken, hence the force drop on the retraction part of the force curve.