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Single Molecule Dynamics Reveals the Role of Flexibility in Bio-molecular Recognition

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With combined single molecule study of flexible protein binding with an energy landscape inspired microscopic model, we found strong evidences of a new paradigm that bio-molecular recognition is determined by flexibilities in addition to structures. The single-molecule study show conformational fluctuations of the protein complex that involves bound and loosely bound states, which can be quantitatively explained in our model as a result of cooperative binding. Theoretical predictions on the key residues are consistent with mutational experiments. The combined study provides a test ground for fundamental mechanisms and insights for future explorations on recognition with large conformational changes.