Abstract Submitted
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Coarse-grained Molecular Dynamics Simulation of Calmodulin-target Interactions[1] PENGZHI ZHANG, Department of Physics, University of Houston, QIAN WANG, Sealy Center for Structural Biology and Molecular Biophysics, University of Texas Medical Branch, SWARNENDU TRIPATHI, MARGARET CHEUNG, Department of Physics, University of Houston — Calmodulin (CaM) is a ubiquitous small protein playing an important role in Ca^{2+} signaling in eukaryotic cells, which can bind and regulate hundreds of target enzymes in the presence of Ca^{2+}. Although the binding process is known to be diffusion controlled, however, due to the flexibility of CaM, methodology that provides molecular insights on target binding and recognition. In this study, Brownian dynamics simulations were used to mimic the process Ca^{2+}-bound CaM binds with two target peptides: CaMKI and CaMKII. Using an experimentally-analogous criterion of number of contacts between targets and a specific residue of CaM to define the encounter complexes and to calculate the association rates, we are able to reveal the molecular reason why CaM-CaMKI has twice the rate of CaM-CaMKII while the numbers of amino acids are similar.

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