Abstract Submitted
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The effect of macromolecular crowding, ionic strength and calcium binding on calmodulin dynamics[1] QIAN WANG, KAO-CHEN LIANG, University of Houston, NEAL WAXHAM, University of Texas Health Science Center-Houston, MARGARET CHEUNG, University of Houston — The flexibility in the structure of calmodulin (CaM) allows its binding to over 300 target proteins in the cell. To investigate the structure-function relationship of CaM in response to the changing intracellular environment, we use a combined method of computer simulation and experiments based on circular dichroism (CD). The conformation, helicity and EF hand orientation of CaM are analyzed computationally to address the effect of macromolecular crowding, ionic strength and calcium binding in the experiments. We applied a unique solution of charges computed from QM/MM to accurately represent the charge distribution in the transition from apo-CaM to holo-CaM. Computationally, we found that a high level of macromolecular crowding, in addition to calcium binding and ionic strength, can impact the conformation, helicity and the EF hand orientation of CaM. Our result may provide unique insight into understanding the promiscuous behavior of calmodulin in target selection inside cells.

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