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Understanding Binding Peptide Design Using a Synthesis of Residue Physicality and Energetic Frustration LENAYA FLOWERS, Department of Physics, University of Houston, SWARNENDU TRIPATHI, MARGARET CHEUNG, Department of Physics, University of Houston and Center for Theoretical Biological Physics, Rice University — The ubiquitous nature of Calmodulin (CaM) allows it to bind to numerous peptides, thus altering the function of a protein complex. Variations in CaMs function are a product of the numerous binding targets (BT) and their significant biological pathways. Given that CaM is a well-studied protein, we have found that certain amino acids in CaMs sequence play an important role in the event of protein binding. 36 CaM binding targets were analyzed to find sequential, physical commonalities. Using the *Frustrometer* (frustrometer.tk), we obtained z-scores (a numerical value for level of frustration) for each amino acids in a given binding target sequence. From those results, we were able to identify which residues show a highly favorable energetic change after binding and those that do not. We have found charged residues show the most prominent change when bound to CaM, these amino acids may provide a critical role in the overall design and function of a CaM-BT complex.

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