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**Amino Acid Propensities for  $\alpha$  to  $\beta$  Secondary Structural Conversion** NORMA PEA FLORES, CAMILA UZCATEGUI, PREM CHAPAGAIN, BERNARD GERSTMAN, Florida International University — Numerous proteins undergo an alpha-helix to beta-sheet conversion, which can then lead to the formation of toxic amyloid fibrils. The resulting fibrous protein aggregation is associated with the pathology of many debilitating illnesses and neurodegenerative disorders, such as type II diabetes, Alzheimer's disease, and Parkinson's disease. Many factors determine the preference that an amino acid has to assume an  $\alpha$ -helix versus  $\beta$ -strand secondary structure. We use Replica Exchange Molecular Dynamics computer simulations to study the amino acids that make up the small, engineered protein cc $\beta$  that undergoes similar structural transitions as amyloid proteins. We examine the propensities for the various pairs of amino acids in cc $\beta$  to form specific secondary structures as a function of temperature.

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