

Abstract Submitted
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Quantifying Stability-Flexibility Relationships in Proteins¹ DONALD JACOBS, JEREMY HULES, SHELLEY GREEN, California State University, Northridge, DENNIS LIVESAY, California State Polytechnic University, Pomona — Given a 3D protein structure, thermodynamic properties are calculated using a Distance Constraint Model¹ (DCM) within a mean-field treatment in practical computational times. Using a 3 free parameter free-energy decomposition scheme in terms of distinct interaction types, non-additivity of component entropies are accounted for by using network rigidity. Over a diverse set of proteins, the essential features of heat capacity agree well with differential scanning calorimetry measurements². Landau free energy curves are obtained as a function of a global flexibility order parameter, and used as a reaction coordinate. Comparing the rigidity transition to the thermodynamic transition state allows compactness of the transition state to be inferred. Correlation in flexibility between backbone residues gives insight into folding pathways and allosteric effects in the native state. ¹D.J. Jacobs, et. al., Phys. Rev. E 68:061109 (2003) ² D.R. Livesay, et. al., FEBS Lett. 576:468-476 (2004)

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Donald Jacobs
California State University, Northridge

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