

Abstract Submitted  
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**Reliability Study of Normal Mode Analysis on the BPTI Protein**

RACHEL BAARDA, DANIEL COX, University of California, Davis — Normal mode analysis (NMA) is a method of treating a system as a collection of spring-connected masses, with the spring constants determined by the forces acting on the system. This technique is widely used in analyzing proteins to ascertain large-scale correlated movements which may be important to the proteins function, as well as mechanical properties such as stiffness. We wish to apply NMA to an engineered protein mesh formed by a regular lattice of fibrillar proteins as a measure of its mechanical strength and stability. In order to determine the reliability of such measurements, we use the same parameters to perform NMA on the well-studied protein Bovine Pancreatic Trypsin Inhibitor (BPTI). We use two force models: (1) a full molecular dynamics force field, which parametrizes forces between all atom types; and (2) an anisotropic network model, which couples proximal central carbon atoms to a harmonic potential. These two models are applied to both all-atom and coarse-grained representations of the protein. We obtain the frequency spectrum and root-mean-square fluctuation per residue and compare these data across models, and to simulated and experimental literature values.

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