

CBIMMS Invited Seminar
Co-Sponsored by the Chemistry Department

“Exploring the Molecular Basis of Elasticity”

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ABSTRACT

Elastin is a cross-linked protein in the extracellular matrix that provides elasticity for many tissues. Since native elastin is large and insoluble, many studies have focused on elastin-based peptides with VPGVG repeats in an effort to elucidate the structure-function relationship for elastin. We have been using molecular dynamics simulation to investigate the molecular basis of elastin's conformational properties and associated elasticity as well as the reason for its inverse temperature transition. The hydrophobic domain of elastin, as explored through VPGVG repeats, is best described as a compact amorphous structure with distorted β -strands, fluctuating turns, buried hydrophobic residues, and main-chain polar atoms that form hydrogen bonds with water. Water plays a critical role in determining elastin's conformational behavior, making it extremely dynamic in its relaxed state and providing an important source for elasticity. We have also performed single-molecule 'pulling' simulations to characterize the molecular basis of elasticity. Again, water plays an important role in determining its elastomeric properties and ability to respond to force. We have also investigated some of the effects of sequence changes on elastin's conformational behavior and introduced elastin turns into globular proteins, leading to increased kinetic stability above room temperature.