MINIMUM STRUCTURE NECESSARY FOR PROTEIN DYNAMICAL TRANSITION

YUNFEN HE, ANDREA G. MARKELZ , *University at Buffalo, SUNY, Buffalo, NY 14260, USA*.

The biomolecular dynamical transition is a rapid increase in the temperature dependent average atomic mean square displacement at around 200 K. The increase in structural flexibility coincides with the onset of function in some systems. Among the possible origins of the effect are: thermally activated small scale diffusive motions, or an intrinsic transition in the biological water adjacent to the biomolecule . While the effect is often measured using neutron quasi-elastic scattering, terahertz dielectric response is also sensitive to the rapid change in flexibility of the system. This sensitivity arises from either the relaxational loss from picosecond diffusive motions, or low frequency structural vibrational mode absorption. Recently we found the dynamical transition is still present for hen egg white lysozyme denatured in 6 M guanidine hydrochloride, indicating tertiary structure is not necessary for the effect. Here we explore the minimum amount of structure required for the transition and how the transition depends on side chain composition. Measurements on polyalanine as a function of chain length show that the dynamical transition does not occur for peptide length shorter than 5. However, the transition is observed for 5 mer and higher. Structural and simulation studies indicate that the 5 mer transiently occupies structured form [1,2]. These results suggest that A) thermally activated side chain motion is not sufficient for the dynamical transition and B) secondary structure is necessary for the dynamical transition. Secondary structure possibly induces sufficient ordering in the adjacent water to result in a fragile to strong glass transition resulting in increased protein flexibility [3].

1. KAH Wildman et al. Solid State Nucl. Magn. Reson. 24 (2003) 94-109. 2. Yuguang Mu,et al. Proteins 58, (2005) 45-52. 3. S.-H. Chen et al. PNAS (2006) 9012-9016.