# Joint Keck Center / John P. McGovern Lectureship

## The Two Aspects Of The Protein Folding Problem

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For more than six decades Dr. Scheraga has pioneered the theory and experimental investigation of protein architecture and dynamics. Starting at Duke and Harvard in the 1940s, Dr. Scheraga has investigated the interactions that (a) dictate the folding of a polypeptide chain in water into the three-dimensional structure of a native protein and (b) determine the reactivity of such a protein molecule (e.g., as an enzyme) with other small and large molecules.

The first aspect to the theory of folding is to compute the thermodynamically stable native structure, and the second aspect is to compute the folding pathways from the unfolded to the folded native form. The evolution of physics-based computational methodology from an all-atom representation of the polypeptide chain to a united-residue representation of the chain will be discussed. With parallel processing, thousands of folding pathways can nowadays be explored, and folding scenarios and kinetic and thermodynamic characteristics can be predicted, as demonstrated with staphylococcal protein A. The results of recent computations, and the methods leading to them will be discussed.

**DATE:** Wednesday, October 19, 2005

**TIME:** 4:00PM – 5:30PM

**PLACE:** Onstead Auditorium, 3rd floor,

**Mitchell Basic Sciences Research Building (BSRB),**

**Room K3.8013, 6767 Bertner Ave., Houston, TX 77030**

Parking is available in the McGovern Commons (adjacent)

Refreshments are provided following the talk in the outdoor courtyard of the McGovern Commons

For information contact Mrs. Hilary Wriggers at 713.500.2429

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