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Computational spectroscopy of myoglobin and five mutants

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Abstract

Globular proteins contain cavities/voids thought to play specific roles in controlling protein function. Elongated cavities provide migration channels, from the protein's exterior to its interior, for the transport of ions and Small molecules to the active center of a protein or enzyme. Using Monte Carlo methods and molecular dynamics on fully atomistic protein/water models, a new computational methodology is described that is able to characterize a protein's dynamic structure by following the time evolution spectrum of cavity and channel sizes. To demonstrate its utility, the new computational methodology is applied to wild type myoglobin and five of its mutants. Experimentally, it is known that mutant ligand---binding kinetics are slower relative to the wild type. Although the five mutants differ by only one amino acid (tryptophan exchange for another amino acid), the mutant's computed cavity and channel size distributions reveal significant differences relative to wild type myoglobin. Computer visualization of the channels leading to the heme center indicates restricted ligand access for the mutants consistent with existing experimental observations. The new methodology provides a quantitative measure of the extent of structural misfolding in the mutants and could become a valuable computational tool for the structural characterization of proteins and enzymes.

Biography

Professor Isaac C. Sanchez holds the William J. Murray Chair in the College of Engineering at the University of Texas. He was elected to the National Academy of Engineering in 1997 and is a charter member of the Texas Academy of Medicine, Engineering, and Science. He has been a member of the UT Chemical Engineering Department since 1988; he also spent 3 years in industrial laboratories (Xerox and Alcoa) and 10 years at the US National Institute of Science & Technology. He has been very active in US graduate and post-doctoral education issues by serving since 1997 on a NRC/NAS Advisory Panel for all post- and pre-doctoral programs administered by the NRC; this includes Ford Foundation Fellowships that are designed to increase the diversity of the nation's college and university faculties. Currently, he is the Graduate Student Advisor to 175 UT Chemical Engineering graduate students.