

Thursday 15th December 2011

10:00am - Room 531

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### *The use of molecular modeling to study enzymic actions*

Abstract:

This talk will illustrate how advanced molecular modeling techniques can be combined with experimental findings to increase our understanding of protein function and regulation. The use of different molecular modeling techniques to study enzymic function, ranging from the dynamic conformational preference of a short peptide inhibitor, to the unusual synergistic allostery in the tetramer of an important enzyme from *Mycobacterium tuberculosis*, the pathogen responsible for tuberculosis, will be discussed.

