

# **5<sup>th</sup> Annual Joint Bioinformatics Workshop**

**July 19, 2005**  
2229 Seamans Center  
University of Iowa

by

**Lei Yang**  
Iowa State University

## ***Motion Analysis of HIV-1 Protease by Anisotropic Network Model and Principle Component Analysis***

### ***ABSTRACT***

Protein functions are to a great extent related to the conformational changes of protein structures. The analysis and characterization of the collective motions of proteins are very important for predicting and understanding protein functions. The HIV-1 protease is an ideal test system to study the relation between protein functions and structures due to the abundance of available crystallography structures and its relative small size. In this study, the normal modes of HIV-1 protease are obtained by the Anisotropic Network Model (ANM). On the other hand, the principle deformation modes are extracted by Principle Component Analysis (PCA). The two motion spaces are then compared by computing the overlap between each ANM mode and each principle component. A significant high overlap between the third slowest mode and the first principle component is found, indicating that most functions of this protein are realized by a specific mode. Further study of the principle mode may help us understanding how this protein functions in detail.