# John P. McGovern Lectureship in Biomedical Computing and Imaging

## Towards a Dynamical Understanding of Biomolecules: Ligand Flexibility and Protein Function


**Francisco Javier Luque Garriga**

Professor
Departament de Chemical Physics
University of Barcelona
Barcelona, Spain



Predicting interactions between small molecules and their targets is crucial to understand the molecular basis of biological processes. In particular, knowledge of the fine structural features that mediate ligand-receptor binding is fundamental in drug discovery. Often, this information does not suffice to establish the relationship between structure and function, and a comprehensive understanding of the biological process cannot be gained without resorting to a dynamical description of molecules. This point will be discussed in two different topics. First, the identification of the bioactive conformation of ligands, which is a key aspect in molecular recognition, to optimize the potency of bioactive molecules and to increase the accuracy of structure-based drug design methods. Quantifying the relative energy of the bioactive conformation, nevertheless, is a challenging issue as noted by recent studies focused on this subject. Second, the implication of dynamical changes in protein function, which will be illustrated from the analysis of local and global conformational fluctuations in the truncated hemoglobin N from *M. tuberculosis*, which seems to contribute to the survival of the bacillus under nitrosative stress.


**Date:** Wednesday, October 15, 2008
**Time:** 4:00PM
**Place:** GSBS Library (BSRB S3.8351)
Mitchell Basic Sciences Research Building
6767 Bertner, Houston, Texas 77030

For information contact: Yukiko.Bryson@uth.tmc.edu

The University of Texas
School of Health Information Sciences at Houston
*A part of The University of Texas Health Science Center at Houston*

deus ex biomachina
biomachina.org