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Title of the Lecture: The Challenges of Conformational Plasticity in Drug Design

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Title: Simulation of Electron Spectra for Nucleoside Antibiotics

Abstract
Theoretical electron spectroscopy, such as ionization potentials, provides a useful quantum mechanical diagnostic for the oxidative potentials of a molecule. Ionization spectra closely link quantum mechanical molecular orbital theory to spectroscopic measurements, such as electron momentum spectroscopy (EMS), synchrotron sourced photoelectron spectroscopy (PES) and X-ray photoemission spectroscopy (XPS), etc. Recent experimental measurements using synchrotron sources have made significant progresses in gas phase for larger bio-molecules. However, to accurately predict/simulate electron spectra for even small bio-molecules, using practical and less computationally demanding models, still presents challenges in theoretical spectroscopy. In this presentation, recent progresses targeting electron spectroscopy of a number of nucleoside antibiotics,

such as anti AIDS drug, 3'-azido-3'-deoxythymidine (zidovudine or AZT), 1-(β-D-ribofuranosyl)-2-pyrimidone (zebularine or zeb) and 1-(β-D-ribofuranosyl)-5-methyl-2-pyrimidinone (d5) etc, will be presented. Preliminary results from a joint synchrotron sourced experimental and theoretical XPS study for small dipeptides will also be presented.

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Title: Theoretical Spectroscopy in Biochemistry: Probing In-situ Microscopic Structure

Abstract
Atomistic structure is the key for understanding the functionality of many biologically relevant systems in their natural chemical environment. Very often, non-covalent interactions such as hydrogen bonds and pi-electron interactions play a crucial role as structural driving forces.

In such situations, quantum mechanical and hybrid classical-quantum simulations can be combined with ab-initio spectroscopy calculations to gain valuable insight into molecular structure on the atomistic level. The spectroscopic signatures of relatively small geometric rearrangements are often much more significant than the energetic changes. We elucidate the predictive power of theoretical spectroscopy via QM/MM molecular dynamics simulations on the example of the rhodopsin chromophore in its dark and batho states.

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TITLE:
Dynamics-based alignment of enzymatic functional families: a novel scheme for comparing large-scale movements in proteins with same or different fold

ABSTRACT:
The biological function of several proteins and enzymes is assisted by large scale conformational changes that are excited in thermal equilibrium. In terms of the traditional logical cascade, sequence -> structure -> function, it is expected that the functional movements of a protein are influenced by the structural architecture. Proteins with similar structures are known to sustain similar large-scale movements; yet it has recently emerged that similar functional movements are shared by proteins with different architecture or topology.

This observation parallels the known paradigm that (i) proteins with similar primary sequences usually attain a similar fold but also that (ii) the same fold is adopted by non-homologous proteins. The sophisticated interplay between sequence and structure has now been extensively characterized thanks to the availability of sequence and structural alignment methods. By analogy, the availability of quantitative methods for comparing the functional-oriented dynamics in proteins (possibly of different structure) would allow to take to a new level the investigation of the structure/function relationship.

We report on a first attempt in this direction by discussing a pairwise alignment scheme that identifies groups of amino acids that undergo similar concerted movements in proteins. The alignment method is based on a coarse-grained elastic network model (BGM) and requires as input the sole proteins' native structures. No prior detection of structure and sequence correspondence is used. The scheme is first used to perform a dynamics-based alignment (and grouping) of a data

set of >70 representative enzymes covering the main functional and structural classes. Finally we discuss an application where the method is used to identify the putative nucleic-acids-binding regions of proteins having non-canonical OB-fold domains.

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