

4th International Conference on **Nanotek & Expo**

December 01-03, 2014 DoubleTree by Hilton Hotel San Francisco Airport, USA

Structural bioinformatics of proteins combined with computational protein biophysics: Implications for nanotechnology exemplified by G protein-coupled receptors

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It has long become evident that bioinformatics of genes and proteins, and biophysical understanding of the mechanisms underlying biomolecular function are very incomplete without one another. Thus, our previous studies have shown that significant insights could be gained in interpreting DNA microarray data within non-statistical, physical criteria-based approaches. More, the “leader gene” approach based on analysis of protein and gene interactions, developed in Prof. Nicolini’s team, allowed to identifying key genes involved in the given biological process, adding further insights into microarray data. On the other hand, our biophysical studies on the role of electrostatics in protein functioning showed that bioinformatics extension of the results, via homologous proteins, was strongly beneficial for understanding protein functioning, especially for its nanotechnological optimization. This report focuses on G Protein-Coupled Receptors (GPCR), especially the most common drug targets like adrenoreceptors and also light-sensitive proteins with enormous nanotechnology potential like octopus rhodopsin. For such proteins, the key property is their dynamics, especially the parts of the protein conformational space available to them, and how that available space is affected by drug binding or a quantum of light. We describe the combined use of molecular dynamics and structural bioinformatics analysis in exploration of the GPCR conformational space, and show insights into their function and its further optimization. Such insights are unavailable without the combination of biophysics and bioinformatics that could be properly termed “physical bioinformatics”.

Biography

Victor Sivozhelezov, PhD, is a Leading Scientist, Institute of Cell Biophysics and Russian Academy of Sciences. After obtaining a MS in Chemistry in 1985 at Department of Chemistry, Moscow State University, he joined the same Scientific Computational Center as a Research Associate, and since then was holding tenure positions with the Russian Academy of Sciences, as Junior Researcher (1987), Researcher (1992), Senior Researcher (1998), and Leading Researcher (2008 until now). He was also improving his qualification both as a researcher and in the English language. Since 1994 until now, he was systematically holding Postdoctoral fellowships and doubly-affiliated Visiting Scientist positions at Chair of Biophysics, later Biophysics and Nanobiotechnologies Laboratories, University of Genoa, Italy and Fondazione EL.B.A. – Nicolini, Pradalunga Bergamo, Italy. His research interests range from molecular recognition, and structure/function relations of proteins and DNA to bioinformatics.