Institute of Biosciences and Applications

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The Institute of Biosciences and Applications (***IBA***), one of five institutes of NCSR "Demokritos", is currently an internationally competitive institute focusing in Biomedical and Biotechnological research staffed by 23 permanent researchers. The three major scientific programs operating at the IBA are: 1) "Regulation of Cellular Function/Age-Related Diseases"; 2) "Model Systems for the Study of Cellular Function"; and 3) "Structural and Computational Biology". Extensive collaborations link the three different programs, and, furthermore, collaborations with the other institutes of the Centre strengthen the impact of research performed in areas related to the development of markers for diagnostic and therapeutic purposes, and innovative high throughput screening for the development of new pharmaceutical reagents. Research performed by faculty members is in concert with today's thrust in biomedical applications and focuses on diseases most commonly affecting patients, such as atherosclerosis, cancer, diabetes, Alzheimer's disease, cell senescence, intervertebral disc degeneration, and addiction to narcotics. Additional studies address the development of screening systems for malaria mosquito vector odorants, the development of novel analgesics for combating chronic pain as well as other pharmaceuticals using high throughput approaches. Targeted drug development based on protein structure and molecular modeling is also practiced. Fungal systems are studied as models of structure and function of cell surface transporter systems and membrane trafficking. Moreover, computational approaches and bioinformatics examine the evolution and functional significance of different genomic domains.

In Silico (Computer-Aided) Modeling of Protein Structure using Molecular Dynamics Simulations

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Knowledge of the detailed 3D-structure of biological macromolecules (e.g. proteins) is essential for a full understanding of their function. However, experimental determination of their structure is not always possible. Structural bioinformatics techniques, such as *in silico* (computer-aided) molecular modeling and molecular dynamics simulations, offer a very powerful alternative tool towards this goal. In the presentation, I will talk about the conformational preferences of an important class of amino-acid (building blocks of proteins) repeats, as revealed by applying such bioinformatics techniques.

"Snapshots" from the recent activities of "Theoretical Biology / Computational Genomics Group"

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Our activities include:

- Study of the functional asymmetry between the two complementary strands of the DNA molecule, by means of the deviations from the so-called "Chargaff's second parity rule". In other words, the quantities: A-T/A+T and G-C/G+C are examined both locally and for whole prokaryotic genomes. Application of this approach may drive to a better understanding of the mechanisms of genomic functions/features like: DNA replication, RNA transcription, mutational dynamics, neighbor preferences in the genomic composition, etc

- Study of the large-scale structure of the eukaryotic genome by means of the examination of the size-distribution of the distances between: coding exons, transposable elements (repeats), conserved [between species] but not protein-coding sequence stretches, and other functional genomic localizations. A frequent occurrence of the so-called “power-law” size distribution is observed. This result is corroborated by the finding (in most of these cases) of fractality, which is measured by means of standard statistical methods: entropic approaches, box-counting method etc. These results are compatible with recent experimental findings that the chromatin organization at nuclear (whole genome) scale presents clear indications of fractality and self-similarity.