

Special Issue on Protein Nanotechnology for Biophysical and Biomedical Studies - Introduction

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In the post-genomic era, the structural and functional proteomics come to the forefront and this requires novel approaches for the fast and successful proteins characterization. Advanced biophysical studies are required in order to understand protein-protein interaction, lying at the base of our understanding of all life processes and of major challenges of the century - cancer and degenerative diseases. Biomedical investigations brings the accumulated knowledge towards the future application in medicine and pharmaceutical science.

This Special Issue concerns advanced biophysical and biomedical methods based on nanotechnology. Among them, Langmuir-Blodgett (LB) nanotemplates for protein crystallography opens the new avenue for structural proteomics, allowing successful crystallization and 3D structure determination of protein, difficult to crystallize with other methods (including membrane proteins) resulting in better diffraction quality and radiation stability of protein crystals in comparison with classical vapor diffusion method. Indeed, LB nanotemplate crystallization has significantly improve the resolution of the diffraction data of L-Asparaginase from *Rhodospirillum rubrum*, the enzyme that can be potentially used for combined chemical and enzymatic therapy of malignant blood disorders and therefore for new anticancer drug development. Radiation stability of protein crystals, obtained by classical and LB nanotemplate method was studied by means of Molecular Dynamics and Monte Carlo simulations, confirming the exceptional quality of LB grown crystals. Molecular dynamics and Monte Carlo simulations reveal the role of various crystallization techniques as well as the role of bound water in the protein conformational plasticity, thermal and radiation stability of protein crystals. This is especially important since always more intense X-ray radiation sources are now used for protein 3D structure determination (such as last generation of synchrotrons and X-ray free electron lasers, XFELs). Next, Anodic Porous Alumina (APA) nanotemplate micro-porous array was created for the optimal protein confinement. While fluorescence study shows the protein incorporation into the pore, Raman spectroscopy confirmed that no significant changes in the protein structure are caused by confinement. Suggested approach could find potential application in the protein microarray development both for diagnostic and for protein-protein interaction studies, with further developments concentrated on the label-free protein-protein interaction study on APA array. Finally, Insulin dynamomics, consisting in bioinformatics and molecular dynamics simulation of LB and classical insulin structure with and without insulin receptor, appeared to have profound implications for drug design and endocrinology. The slight differences in conformation and dynamics may explain why LB-insulin is more stable when binds to its receptor (lower free energy) and this could be useful when designing new drugs and pharmaceuticals.