MS12-P8 Molecular Dynamics and Monte Carlo Simulation for Protein Nanocrystallography.

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In the molecular dynamics (MD) method there is a polyatomic molecular system in which all atoms are interacting like material points, and behavior of the atoms is described by the equations of classical mechanics. This allows simulations of the system of the order of 106 atoms in the time range up to 1 microsecond. Despite of some limitations such approximation may describe the dynamics of macromolecules at the atomic level. However, this method does not consider the chemical reactions and the formation or breaking of chemical bonds. For these purposes there are approaches which combine classical and quantum mechanics simulations. The behavior of each atom can be described as Newton's equation of motion. In the present communication, we describe how MD can be applied for studying Langmuir-Blodgett (LB)-based protein crystals. Using MD analysis, we show how LB-based crystals and space ones can be compared with classically grown crystals. From our simulations LB crystals follow the trends of microgravity crystals, i.e. higher resolution, lower content of water, lower B-factor and higher number of reflections. Development of new approach using MD and Monte Carlo simulation allowing proper estimation of Radiation Damage (RD) occurring to the protein structure. Since RD represents a major problem in all advanced methods of 3D atomic structure determination (SR, XFELs, Cryo-EM), this goal is of high impact in evaluation of the resulting structures. The object of this research also is to solve the protein 3D atomic structure using Monte Carlo integration of high-quality diffraction intensities from which experimental phases could be determined. Monte Carlo simulation and MD can therefore play a major role in protein nanocrystallography and structural nanoproteomics.

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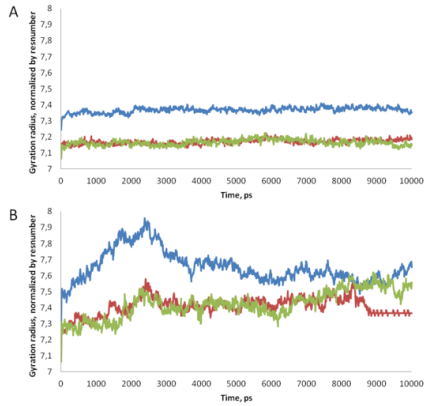

Figure 1. Normalized gyration radius of proteins crystallized by different techniques at 300 K (A) and 500 K (B). Blue line is classically (Hanging Drop) crystallized proteins, red is LB and green is space grown crystals.

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