

**International Journal of Biomedicine | June 2019 - Volume 9, Issue Suppl\_1:  
Abstracts From the Second Russian International Conference "Cryo-electron  
microscopy 2019: achievements and prospects"**

**POSTER ABSTRACT PRESENTATIONS**

**SESSION TITLE: COMPLEX AND EMERGING TECHNIQUES IN STRUCTURAL BIOLOGY**

DOI: 10.21103/IJBM.9.Suppl\_1.P43

**Abstract P-43: Approximating Protein Alpha-Helices with Cylinders for Free  
Electron Lasers Diffraction Experiments**

Grigory A. Armeev<sup>1</sup>, Mikhail A. Lozhnikov<sup>2</sup>, Valery N. Novoseletsky<sup>1</sup>, Aleksandr V. Kudriavtsev<sup>1</sup>,  
Alexey K. Shaytan<sup>1</sup>, Georgy M. Kobelkov<sup>2</sup>, Konstantin V. Shaitan<sup>1</sup>

*<sup>1</sup>Faculty of Biology, Lomonosov Moscow State University*

*<sup>2</sup>Faculty of Mathematics and Mechanics, Lomonosov Moscow State University*

**Background:** Free electron lasers open up new exciting possibilities for protein structure studies. Extremely high brilliance allows obtaining diffractograms from microcrystals, single particles (such as viruses) and, theoretically, even protein molecules. However, the analysis of these kind of data is significantly hampered by a small number of scattered photons, as well as the random orientation of the particles in the X-ray beam. For this reason, it is necessary to develop new approaches to the analysis of experimental data from such experiments. Here, we paid attention to the possibility of coarsening protein alpha helices models to simplify such analysis.

**Methods:** To calculate the diffractograms from electron density maps of protein alpha helices and model cylinders, we used the Condor software. Model experiments were carried out under conditions similar to those in setup for measuring diffraction from single particles in the European XFEL (6A wavelength, 500 nm focus, the distance to the detector - 70 cm and 10 cm for a wide angle, the detector is 20x20 cm). The electron density maps of protein alpha helices were calculated using the Chimera software (1 A resolution). Model electron density of cylinders was further smoothed with the Gaussian filter with a 3 A core.

**Results:** The obtained scattering patterns of model cylinders on small-angles are very similar to the scattering patterns of alpha-helices, which changes upon going to large scattering angles. The amino acid composition of alpha helices affects the character of diffraction patterns, which can be accounted for by selecting the effective radius of the model cylinders.

**Conclusion:** We have shown that protein alpha-helices can be described by cylindrical models with an effective radius, depending on the amino acid composition. These results can be used in the future to build simple geometric models that satisfy the experimental diffractograms for coarse interpretation of protein structures.

**Key Words:** X-ray laser • diffraction pattern • alpha-helices

**Sources of Funding:** This work was supported by the Russian Foundation for Basic Research No. 18-02-40010.

International Journal of Biomedicine. 2019;9 Suppl 1: S36. doi: 10.21103/IJBM.9.Suppl\_1.P43

©2019 International Medical Research and Development Corporation