Molecular Dynamics Simulation of Metal Sulfides Bacterial Processing

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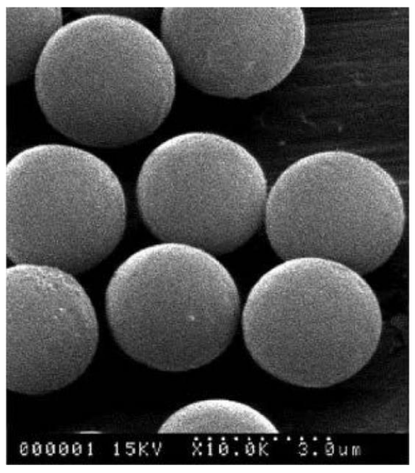
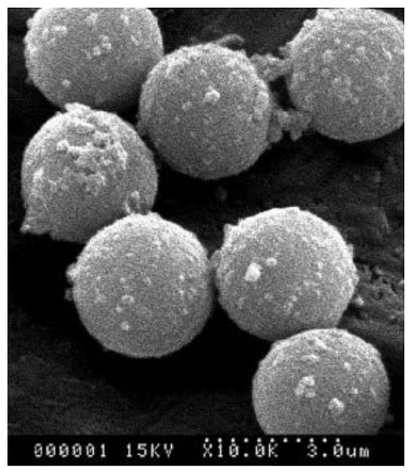
Introduction

The gool of this work is theoretically substantiate study of molecular mechanisms formation of metal sulfide nanoparticles by bacterial analysis using the bacteria Bacillus subtilis 168 [1]; it is actively used for the diagnosis and in vivo of various bioprocesses, as well as for targeted therapy of tumor.

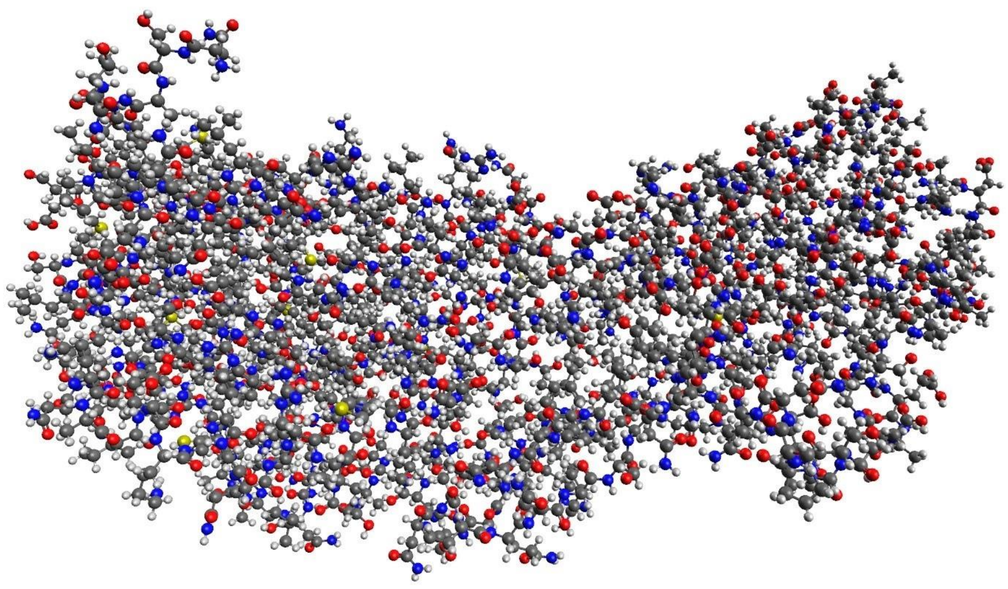


Initial amino-containing polyglycidylmethacrylate microspheres [1]



Amino-containing polyglycidylmethacrylate microspheres after ZnS immobilization in them [1]

The main characteristic of Bacillus subtilis 168 bacteria for production of zinc sulfide nanoparticles by biosynthesis [1] is that the only one protein involved in the bacterial processing is flagellin. Flagellin is present in bacteria flagella. This protein is able to create a hollow cylindrical structure due to its unique mobility characteristics.



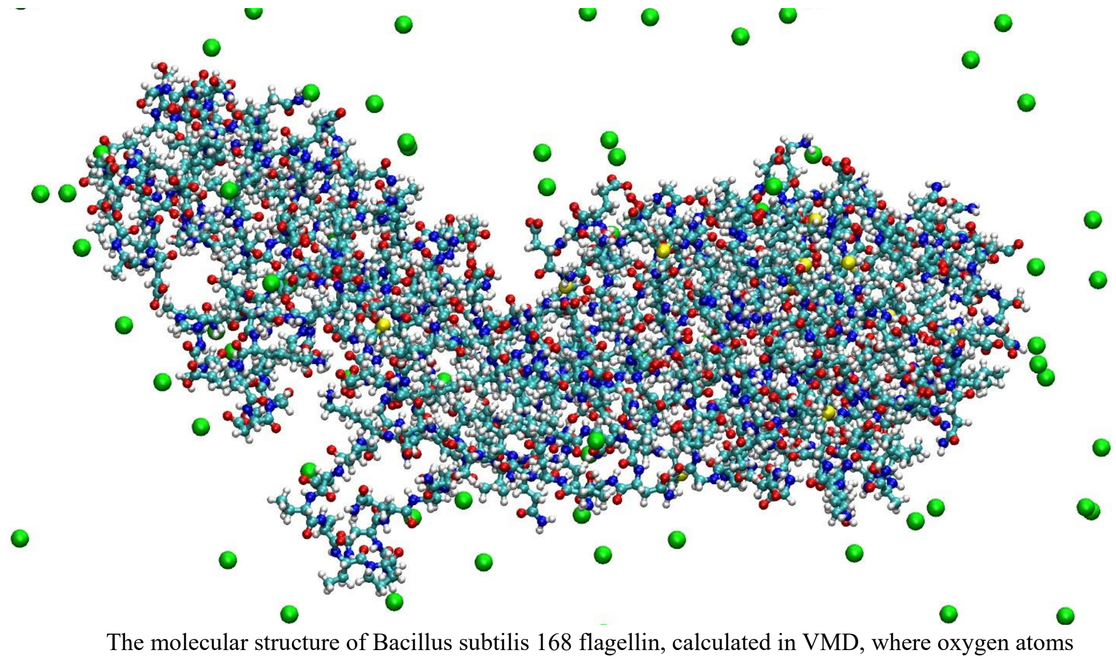
The molecular structure of the flagellin Bacillus subtilis 168, calculated in Avogadro, where oxygen atoms are marked in red, nitrogen in blue, carbon in dark gray, and hydrogen in gray;

Materials & Methods

The behavior of flagellin in aqueous solutions of salts used in the synthesis of zinc sulfide nanoparticles was studied using molecular dynamics methods. The amino acid sequence of flagellin 6GOW is taken from the international protein database RCSB PDB [2].

Based on the analysis of the average radius of inertia, the dynamics of flagellin molecules is studied. The calculations were performed using the GROMACS software package using the force fields AMBER99SB-ILDN protein, nuclear AMBER94 (Lindorff-Larsen et al., Proteins 78, 1950-58, 2010) [3] and a three-point TIP3P solvate.

As a result, a solvated electroneutral system consisting of protein and ions was obtained.

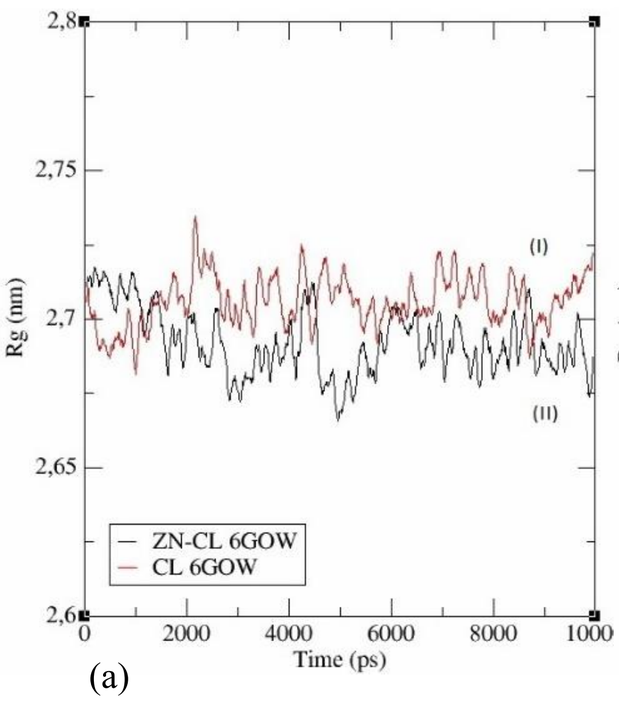


The molecular structure of Bacillus subtilis 168 flagellin, calculated in VMD, where oxygen atoms are marked in red, nitrogen atoms in blue, carbon atoms in blue, hydrogen atoms in white, and zinc ions in green;

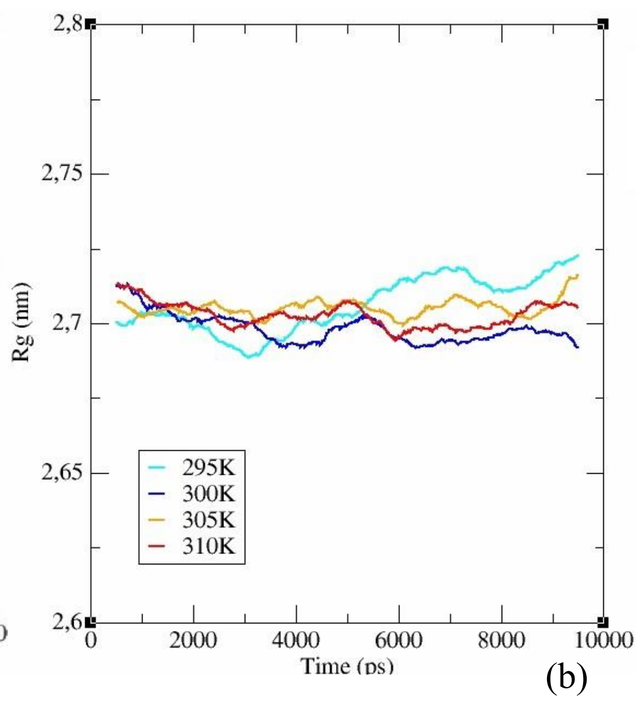
Results

It was found that in a solution containing chlorine and zinc ions, the average radius of inertia gradually decreased (in the graph in Fig. (a), the radius of inertia of the protein in the presence of zinc ions is indicated in black, without zinc ions - in red).

As a result of studying the trajectory of the flagellin molecule, it was noticed that in the presence of zinc ions, the radius of inertia of flagellin decreased. This indicates that there is an electrostatic interaction between zinc ions and flagellin amino acids, as a result of which the mobility of molecules decreases and zinc sulfide nanoparticles are formed. In addition, the frequency of hydrogen bonds between protein molecules and zinc ions increases over time, as shown in graph (c).

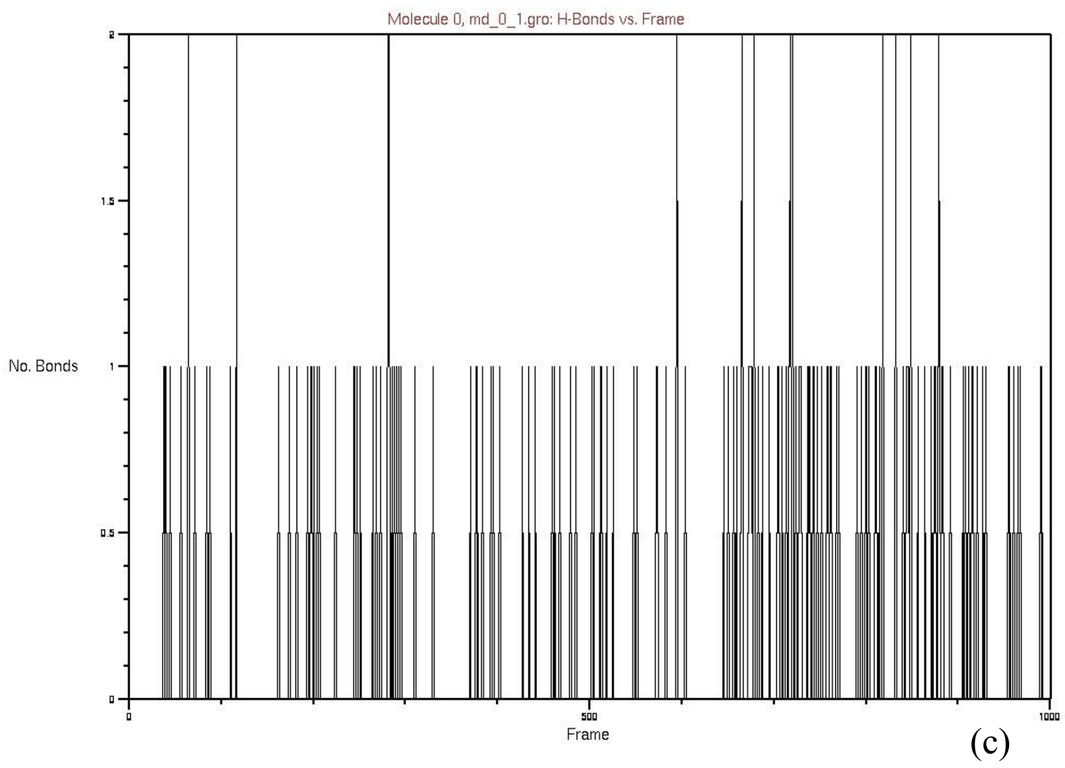


(a)



(b)

The dependence of the radius of inertia of the protein in a solution of zinc (Zn) and chlorine (Cl) ions on temperature was also studied. It follows from graph (b) that flagellin sought to occupy a more compact structure at T = 300K.



(c)

Concussions

Thus, according to the results of molecular modeling, it can be concluded that in the presence of zinc ions, the degree of complexation of the flagellin molecule increases significantly, which contributes to the formation of metal nanoparticles, and this process occurs most effectively at 300K (26.8 °C) — a temperature close to room temperature, when all biological processes are most active. An increase in the number of hydrogen bonds with a decrease in the radius of inertia confirms the electrostatic mechanisms of complexation in the case of flagellin amino acids and zinc ions.

References

1. Zhuravliova O.A., Voeikova T.A., Bulushova N.V., Debabov V.G., Khaddazh M.K., Bakhtina A.V., Gritskova I.A., Ismagulova T.T., Shaitan K.V., Gusev S.A., Lupanova T.N. Bacterial synthesis of cadmium and zinc sulfide nanoparticles: characteristics and prospects of application // Molecular Genetics, Microbiology and Virology. 2018. V. 33. № 4. p. 233-240.
2. RCSB Protein Data Bank: https://www.rcsb.org/3d-view/6GOW doi 10.2210/pdb6GOW/pdb
3. K. Lindorff-Larsen, S. Piana, K. Palmo, P. Maragakis, J. L. Klepeis, R. O. Dror, D. E. Shaw Improved side-chain torsion potentials for the Amber ff99SB protein force field // Proteins: Structure, Function, and Bioinformatics. 2010 Volume 78, Issue 8, P.1950-1958