Nanochemistry and biotechnology

Some general aspects of molecular recognition: protein-DNA complexes.

A.V. Shestopalova^{1,2}, M.Yu. Zhytnikova¹

¹Biophysical Department, O. Ya. Usikov Institute for Radiophysics and Electronics, Natl. Acad. of Sci. of Ukraine, Acad. Proskury Street, 12, Kharkiv, 61085, Ukraine.

²Department of Molecular and Medical Biophysics, V.N. Karazin Kharkiv National University, Svobody sq., 4, Kharkiv, 61077, Ukraine. E-mail: <u>a shestopalova@mail.ru</u>

Development of nanotechnologies requires understanding of fundamental principles of miniaturization, or compaction, and specificity that are realized in natural nanosystems. Protein-nucleic complexes, in particular, nucleosomes are remarkable examples of nanosystems formed in living cells. The molecular recognition is the key concept in the building of such «nanoscale assembly lines». Here we overview the general principles of molecular recognition on the level of biopolymer complexation.

Both nucleic acids and protein molecules possess a number of intrinsic characteristics that make them excellent candidates for the assembly of dynamic nanostructures and nanodevices. Their properties, for example, the self-assembly of complementary DNA strands or site-specific molecular recognition among interacting biopolymers have enabled nanotechnologists to create a molecular world «from the bottom up» using biologically based starting materials.

One of the unresolved problems is to understand the nature of molecular recognition, in particular, the specific mechanisms of protein-DNA recognition: how does such large and diverse number of DNA-binding proteins recognize their specific binding sites? The detailed analysis of crystallographic structures of the free DNA fragments, the protein-DNA complexes and the nucleosomal DNA [1-3] allows us to determine the influence of DNA conformation variability on the physical characteristics of the DNA double helix and their sequence specificity, which can be considered as factors important for protein-DNA recognition.

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2. *Zhitnikova M.Yu., Boryskina O.P., Shestopalova A.V.* Sequence-specific transitions of the torsion angle gamma change the polar-hydrophobic profile of the DNA grooves: implication for indirect protein-DNA recognition // J Biomol Struct Dyn. - 2014. - **32**. - N 10. - P.1670-1685.

3. Zhitnikova M.Yu., Boryskina O.P., Shestopalova A.V. Nucleosome as an example of a nanosystem formation: structural dynamics of nucleosomal DNA, P.95-128 /

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