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Self-similarity of biopolymer backbones in the ribosome

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ABSTRACT

Self-similar properties of the biopolymer backbones in the ribosome are investigated in terms of the fractal dimension. We especially estimate the chain fractal and capacity dimensions of the ribosomal RNAs and proteins, which are constituents of the ribosome. The fractal dimensions of both biopolymers are compared with that of the self-avoiding walk, which is a typical model of a polymer without interaction between monomers. We demonstrate that the fractality found in the ribosomal RNAs is pertinent to explain their structural characteristics: local helix formation and long-range tertiary interaction forming three-dimensional structures. The fractal dimension of the ribosomal protein supports the existence of the long and extended domain, which is hardly seen in the globular protein. The self-similarity also upholds the fact that the ribosomal proteins function primarily to stabilize the structure of the ribosome by both the long-extended domain of the protein penetrating into the inside of the RNA, and the globular domain interacting with the RNA on the exterior of it. These results partially, if not whole, unravel the structural characteristics of the biopolymers in the ribosome.

1. Introduction

The prokaryotic ribosome [1] is a macromolecule of size about 250 Å in diameter, and sediments at 70S, where the unit "S" is the measure of the sedimentation rate. It is mainly composed of two subunits: the 30S and 50S subunits. The 30S subunit, in turn, contains the 16S ribosomal RNA (rRNA) in addition to about 20 ribosomal proteins (r-proteins); whereas the 50S subunit consists of two rRNAs, the 5S and 23S rRNAs, together with about 30 r-proteins. While the 5S rRNA consists of about 120 nucleotides, the 16S and 23S rRNAs are composed of approximately 1500 and 3000 nucleotides respectively, each of which is made up of one of four different bases (denoted as A, C, G, and U) and sugar-phosphate backbones. The r-protein is a polypeptide chain that is made up of residues of 20 different amino acids linked by peptide bonds.

The ribosome, a large RNA–protein complex molecule, catalyzes protein synthesis in all organisms. In contrast to most cellular machines, a series of experiments verifies that the rRNAs, rather than the r-proteins, are the active participants in protein synthesis as a ribozyme [2–7]. Moreover, the structure of the ribosome showed the central importance of rRNA in all aspects of ribosome function: the 16S rRNA plays a main role in decoding mRNA, and the 23S rRNA catalyzes peptide bond formation [8].

The two subunits are the largest asymmetric molecules that have been resolved so far at the atomic level by the x-ray crystallography. The 2.4 Å resolution of the 50S subunit from the *Haloarcula marismortuii* [3,4] and the 3.05 Å resolution of the 30S subunit from the *Thermus thermophilus* [5,6] uncover the first detail structure of both subunits. In addition, the 3.5 Å resolution of the intact 70S from the *Escherichia coli* [9] reveals the features of the inter-subunit bridges. These results provide not only the high-resolution structure of the rRNAs and r-proteins, but also the first detail pictures of how the rRNAs and r-protein components are interacted to form the ribosome.

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The structure of a biopolymer is important since it is widely believed that the structure dictates its biological function. Due to considerable advances in the structural conformation of the ribosome, it is possible to investigate quantitative characteristics of the ribosome, especially from the statistical physics perspective. One quantitative approach toward the understanding of the structure of the ribosome is the self-similar property via the fractal dimension. It, particularly, may help to get the insight of the local and global structures of biopolymers in the ribosome. Note that due to the finite-size effect, there are both upper and lower size limits beyond which the biopolymers are no longer fractal.

The self-similar properties of the globular proteins have been studied extensively in terms of the chain fractal dimension [10–16]. The chain fractal dimension of a globular protein is conventionally estimated by two different approaches. The first method is based on the scaling exponent of the contour length, which is proportional to the number of monomers with respect to the end-to-end length [11]. The second method is based on the length of a line segment along the chain measured with a scale of the number of monomers in the segment [10,13]. Although these two methods are essentially the same, we believe that the latter is easier to implement than the former. Using the latter, called the internal line segment method, it was found that the chain fractal dimension of the globular proteins depended on the coarseness of the scale m, which is nothing but the number of residues included in a straight line segment. From this, it was argued that folding mechanism of the local and global backbones could be separately characterized by the different chain fractal dimensions. Besides these methods, the fractal dimension of the globular proteins is estimated from the method of the radius of gyration for the protein compactness [14,16].

In this paper, we investigate the self-similar characteristics of the rRNAs and r-proteins using the conventional methods for estimating the fractal dimensions. It is known that the main functional role of r-proteins is to shape and stabilize the ribosome by interacting with the rRNA even deep inside of it [4,6]. This is in contrast to the case of the globular proteins, each of which independently plays a role of an enzyme. From this, we can infer that the conformational feature of the r-proteins may differ from that of globular proteins. The fractal dimension analysis may not only unravel the intrinsic structural characteristics of the biopolymers in the ribosome but disclose the structural difference between the globular and ribosomal proteins in conjunction with its biological function.

From the notion that the rRNA and r-proteins are long chains of nucleotides or amino acids with multiple interactions between them, we focus on two different types of the fractal dimensions: the chain fractal dimension [12] and the capacity dimension [17]. The former takes into account the fact that a linear polymer can be described by successive "walks" between monomers along the chain; while the latter considers only the geometrical configurations of the backbone without reflecting the ordering of the monomers along the chain. We estimate the fractal dimensions of both 16S and 23S rRNAs, together with about 20 and 30 r-proteins in the 30S and 50S subunits, respectively. The structural details of the molecules are deposited in the Protein Data Bank (PDB) [18].

This paper is organized as follows. In Section 2, we describe methods for estimating the fractal dimensions and their feasibility. This section is followed by results of the estimates and their biological implications; the last section is devoted to the summary and conclusion.

2. Methods for estimating fractal dimensions

2.1. The chain fractal dimension

A chain fractal dimension D_c of a biopolymer chain is conventionally defined, in terms of the root mean square of the end-to-end distance R, as

$$R \propto N^{1/D_c} \propto N^{\nu}, \tag{1}$$

where N is the number of monomers along the chain, and ν is the Flory exponent. It is known that, in three dimension, $D_c = 2$ for the Gaussian walk (or Θ solvent), and $D_c = 5/3$ for the self-avoiding walk (SAW), which includes the excluded volume effect [19]. Note that since the SAW does not take into account any attractive force, the deviation from $D_c = 5/3$ is expected when there are interactions between monomers which are far apart along the chain but close in space [12]. Thus, more realistic polymers are likely to have chain fractal dimensions different from that of the SAW.

The chain fractal dimension of a biopolymer is also often estimated by the internal line segment method [10,13]. It is based on the scaling behavior of the segmental length $L(m)$ of the backbone which is defined as the sum of stepwise connections of straight lines measured for different interval of m monomers. That is,

$$L(m) = \ell(m) + \frac{k}{m+1}\langle \ell(m) \rangle, \tag{2}$$

where k ($k < m$) is the number of monomers left unconnected, and the second term on the right-hand side of Eq. (2) is a correction term which takes into account the contribution from the monomers left unconnected. $\langle \ell(m) \rangle$ is the mean length of the $\ell(m)$, and it is the average value of the end-to-end distance of m monomers. $\ell(m)$ is, in turn, defined as

$$\ell(m) = \sum_{i=0}^{N/m-1} |\vec{x}_{(i+1)m} - \vec{x}_{im}|, \tag{3}$$