USING THE IDEAS OF FRACTAL GEOMETRY TO DESCRIBE SOME STRUCTURAL PROPERTIES OF MYOSIN

Adriana Isvoran*

Abstract

The aim of this paper is to illustrate how we can use the ideas of the fractal geometry to describe some structural properties of myosin. The fractal dimension of the chain B backbone of myosin has been determined. It is 1.12 ± 0.012 for m<100. The spectral analysis was also used to determine the value for the spectral coefficient, –0.268 ± 0.04, and it reflects fractal aspects of the chain B of myosin structure.

Key words: myosin, fractal dimension, correlation dimension, fractal aspects.

1. Introduction

Proteins are heteropolymers with a variable composition of twenty different amino acids. The amino acid sequence dictates the three-dimensional structure of the protein because the varied composition and nature of their side groups result in a range of possible interactions within the protein. These interactions determine the final structure of protein. So, proteins have an intrinsic selfsimilarity in the compactness and the packing of their structure. This is a simple form of fractal behavior but it has important consequences for the morphology of the protein and for the thermodynamics of protein folding [1]. Deterministic chaos has also fractal properties. Several results have been reported on the existence of deterministic chaos in the biological function of the proteins, for example: enzyme catalysis (chymotrypsin [2,3], sea hare myoglobin [4], human lysozyme [5]), and antigen-antibody interactions [6,7]). There are also in the specific literature a few examples that reveal fractal aspects of proteins structures [8-11]. The aim of this paper is to illustrate the fractal aspects of myosin structure. Myosin is a muscle protein involved in the muscle contraction. The molecular mechanism of the muscle contraction is not completely determined and

* West University of Timisoara, Department of Physics, Blvd. V. Pirvan no. 4, 1900-Timisoara, e-mail: adriana@physics.uvt.ro

the detection of fractal aspects in the muscle proteins structures could help us to better understand this mechanism. Myosin has eight polypeptidic chains: A, B, C, D, E, F, G, and H. The chains A, C, E, and G form the motor domain of protein and the chains B, D, F and H form the essential light domain. Here I analyze only the fractal aspects of the B chain.

2. Method

The fractal dimension of a curve may be defined by measuring the length, *L,* with rulers of fixed length, ε. The length L is a function of ε and is given by

$$L(\varepsilon) = N(\varepsilon)\varepsilon \qquad (1)$$

where $N(\varepsilon)$ is the number of steps of length ε that are needed to cover the curve. In general

$$N(\varepsilon) \sim \varepsilon^{-D} \qquad (2)$$

and

$$L \sim \varepsilon^{1-D} \qquad (3)$$

where D is the fractal dimension of the curve [1].

In the previous studies, the length L of the protein backbone was measured by a stepwise connection of straight lines between C^{α} atoms of the protein backbone. The length was measured for different intervals of *m* residues and the fractal dimension of the backbone was obtained from the slope of a *log(L)* versus *log(m)* plot. For a large number of protein structures, this log-log plot was bilinear with a slope –0.38 for m<10 and one of –0.65 for m>10 [8]. The fractal dimensions are than 1.38 for m<10 and 1.65 for m>10. This approach is rather incorrect because line segments between C^{α} atoms are not fixed-length increments. Instead, one must use the root mean squared length of the segment. In this case the slope of the curve is no longer 1-D, but $\frac{1}{D} - 1$ [1].

Fractal aspects are always expressed by a power law behavior. This type of behavior emerges from a complex system when there is a luck of characteristic scale [12], i.e. the physical observable is of the form

$$f(bx) = b^{\beta} f(x) \qquad (4)$$

The solution of such an equation is assumed to be a power law with the exponent β, $1/f^{\beta}$. The spectral coefficient β can be obtain using the SA method [14]. Because any given time-series or spatial-series may exhibits a variety of autocorrelation structures, the exponent β ranges in the $0<\beta<2$ interval. If $\beta=2$ we obtain the power spectral density of white noise and if $\beta=1$ we have the power spectral density of pink-noise. The deviation of β from unity reveals fractality [13]. The long-range correlation is present if $0<\beta<1$ [14].

3. Results and discussions

The backbone of the chain B of myosin is presented in the figure 1 and the determination of the fractal dimension of its backbone is presented in the figure 2. We notice that in this diagram there are two linear regions. For the first region, m<100, the slope is –0.467 ± 0.022 and the fractal dimension is 1.12 ± 0.012. These results are in good agreement with other results presented in the literature. Two differences appear between the data presented in the literature and the results of this study:

i) the first linear region corresponds to m<100 in this study and in the literature the first region is reported for m<10;

ii) the second linear region corresponds to m>100, its slope is 7.08 ± 0.011. This value for the slope reveals a negative fractal dimension and it has not significance.

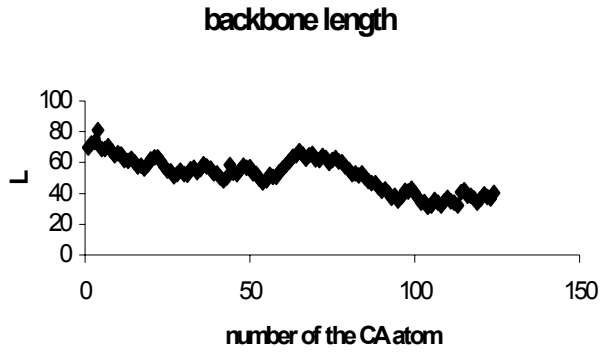

Fig. 1. The backbone of the chain B of myosin

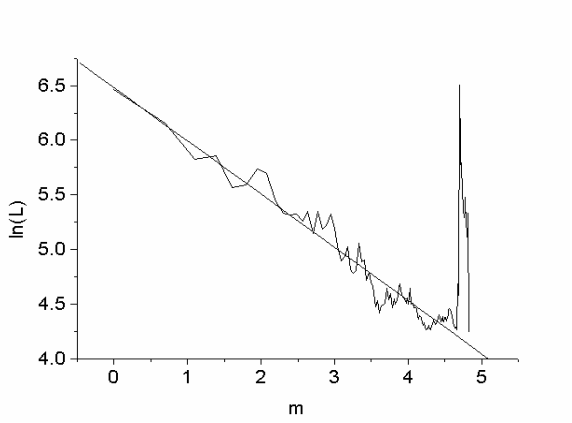

Fig. 2. The determination of the fractal dimension of the chain B of myosin

I explain these disagreements by underlying that myosin is a fibrillar protein, it contains two domains and every domain has four chains. The folding of a fibrillar protein could be different from a globular one, so it is possible that the local folding and the global folding have the same mechanism in this case. It is possible that the second linear region in the diagram to be connected to the interactions between the chains and/or the domains.

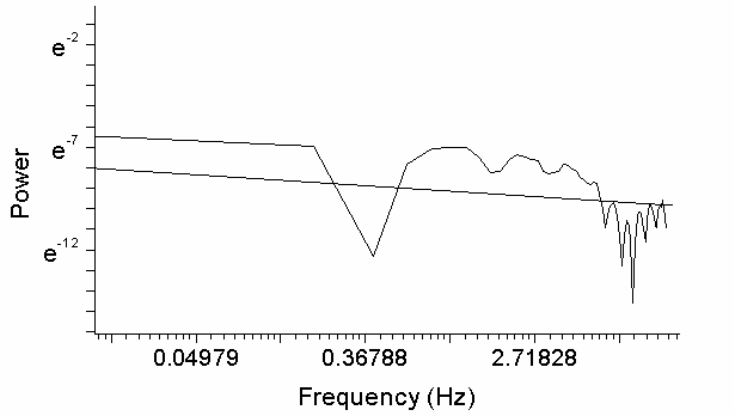

Fig.3. The determination of the spectral coefficient

The determination of the spectral coefficient is presented in the figure 3. Its value is –0.268 ± 0.04 and it reflects fractal aspects.

The results presented here reflect fractal aspects of the chain B of myosin structure. Taking into account the other results presented in the literature revealing fractal aspects of proteins structures and dynamics, I may make the hypothesis that it is possible to apply the ideas of the fractal geometry to study the structure and the dynamics of proteins. The obtained results can be useful for explaining a lot of molecular mechanisms involving protein dynamics. Any new result in this field open the possibility to certify the hypothesis.

Bibliography

1. **Dewey G. T.,** *Fractals in molecular biophysics*, Oxford University Press, New York, (1997)

2. **Havsteen B. H.,** *A new principle of enzyme catalysis: coupled vibrations facilitate conformational changes*, Journal of Theoretical Biology, **140**, 101-127 (1989)
3. **Havsteen B. H.,** *A stochastic attractor participates in chymotrypsin catalysis. A new facet of enzyme catalysis,* Journal of Theoretical Biology, **151**, 557-571 (1991)
4. **Isvoran Adriana,_Morariu V.V.,** *Comparison of the behavior of sea hare mioglobin when it forms two different complexes*, Chaos Solitons&Fractals, vol **12**, 1041- 1045, (2001)
5. **Isvoran Adriana, Negreanu-Maior A., Morariu V. V**., *Attractor control in the changes of molecular vibrations of the human lysozyme upon substrate binding*, International Journal of Chaos Theory and Applications**, 4,** 13-22 (1999)
6. **Havsteen B. H.,** *Attractor control of the binding of digoxine to a specific antibody*, Journal of Theoretical Biology, **189,** 367-376 (1997)
7. **Havsteen B. H**., *An esterolytic antibody with vibrational properties of a catalytic H chain and non-catalytic L chain*, Journal of Theoretical Biology, 196, 337-387 (1999)
8. **Wang C. X., Huang F. H.,** *Fractal study of tertiary structure of proteins*, Physical Revue A, **41**, 7043-7048 (1990)
9. **Isvoran Adriana, Licz A., Unipan Laura, Morariu V. V.,** *Determination of the fractal dimension of the lysozyme backbone for three different organisms*, Chaos Solitons&Fractals, **12**, 757-760 (2001)
10. **Isvoran Adriana,, A. Licz, V.V. Morariu**, *Determination of the fractal dimension of Ascarys Lumbricoides Trypsin Inhibitor*, Revue Roumaine de Chimie, **48** (8), 51-53, 2001
11. **Isvoran Adriana,** *Using the fractal concepts to describe the structural properties of adenylat kinase*, Chaos, Solitons&Fractals, in press, 2003
12. **Shen T. Y.,** et al., *Statistical analysis of the fractal gating motion on the enzyme acetylcholinesterase,* Physical Review E., **63**, 0419021-0419026 (2001)
13. **Szendro P., Vincze G., Szasz A.,** *Pink-noise behavior of biosystems*, Eur. Biophys. J., **30**, 227-231 (2001)

Morariu V. V., Coza A., *Quarter power scaling in dynamics: experimental evidence from cell biology and cognitive psychology*, Fluctuations and Noise Letters (2001)