The measure of the fractal dimension of proteins by NMR

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Introduction

Linear polymers share with disordered proteins the property of not having a definite secondary structure, and that only statistical properties can be used to describe their behavior. It was recently shown that NMR can be used to determine the fractal dimension of the chain, a quantity which has been widely used to study polymers. In the present work we explore how this notion can be useful the the study of ordered and disordered proteins.

IB5 is a 70 amino-acid, proline-rich salivary protein binding selectively polyphenols. We want to investigate the details of this interaction but the protein presents very small chemical shift spreading, and no NOE contacts, so the classical route cannot be taken. Thus, the fractal dimension was studied to extract some information.

Results

We have found that urea denatured peptides display a fractal dimension of 1.72, characteristic of an extended random chain, while ß-amyloid peptides, also unstructured, display a fractal dimension close to 2.2, indicating a much more compact organization. The fractal dimension for structured globular proteins is 2.56, close to the 3.0 maximum value, and characteristic of a chain nearly filling the available space. When applied to a family of polyproline peptides, a fractal dimension of 1.4 is observed, indicating that this series of peptides are structured in polyproline II secondary structure and diffuse as rigid rods.

As for IB5, its fractal dimension is about 2.0, a characteristic value of a random-walk polymer. Although it is composed of 40% prolines, the protein presents a very different pattern from the polyproline series.

Conclusion

The fractal dimension seems to be a very accurate value to characterise untructured proteins. Our goal now is to gather as many data as possible (such as relaxation data, SAXS, EPR…) to be able to study completely those proteins.

References

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