

Computational biophysics

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Github: <https://github.com/giacThePhantom/mathematical-modelling-in-biology>

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Chapter 1

Introduction and proteins

1.1 Introduction

Biomolecular modelling has seen a recent increase in its use in the recent years, with a field still destined to expand. Most of this models take a top-down approach, starting from the macroscopic rather than to build simulation from the fundamental and quantistic concepts. Examples of systems studied through biomolecular modelling are:

- Channels.
- Photosynthetic systems.
- Viruses.
- DNA/RNA interactions.
- Inorganic systems.

Through biomolecular modelling it is possible to obtain:

- Molecular rationale for biological processes like proteins' function or its misfolding.
- A prediction of properties of macromolecular structures and architectures.
- A quantitative evaluation of molecular driving forces.
- A comparative assessment of molecular affinities through the binding free energy.

1.2 Proteins

Proteins have different functions within a cell:

- Give structure.
- Catalytic.
- Provide exchange of materials.
- Movement.
- Code for messages.
- Storage.
- Transport ions.
- Act as toxins.

Proteins are a polymer of amino-acids and occupy a space-scale of $10nm$. The amino-acids are in the range of $1nm$. They are built through a polymerization reaction as chain of amino-acids coded through a degenerate code of RNA nucleotides. Three bases of RNA code for an amino-acid.

1.2.1 Amino-acids

Amino-acids are the monomers of a protein. They have a general structure with an amino and a carboxyl terminal group for all of them. They are distinguished by a residue on the α -carbon which gives them different chemical and physical properties.

1.2.2 Structure

There are four level of a protein structure.

- Primary structure: the amino-acid sequence.
- Secondary structure: here α -helices and β -sheet can be distinguished.
- Tertiary structure: the spatial, 3D dynamic configuration of a protein which arise during protein folding.
- Quaternary structure: the interaction of multiple correctly-folded proteins.

Chapter 2

Proteins' geometry

Chapter 3

Force fields

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Foundations of statistical mechanics

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