Ab initio Protein Structure Prediction

Abstract for the Expert Session in Trends in Bioinformatics on February 2nd, 2016

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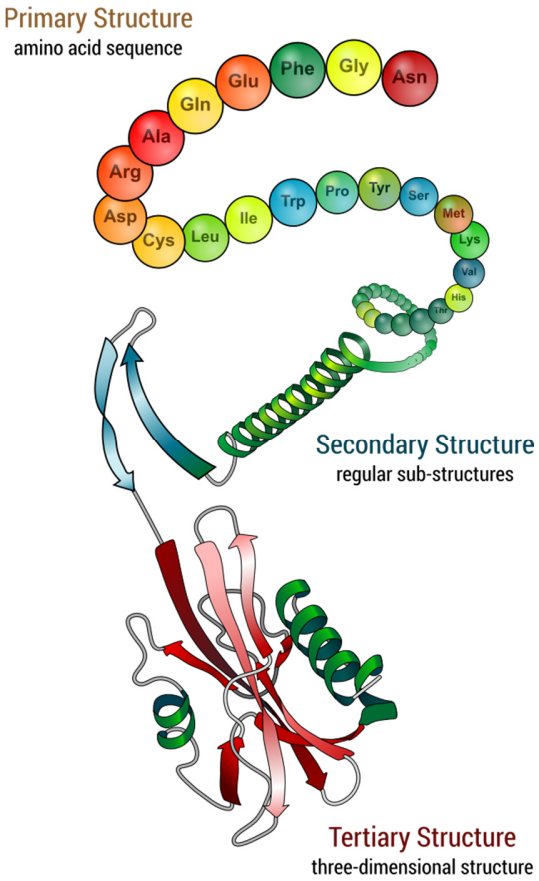
Proteins are not only an essential nutrient without which we could not grow muscles, they also are responsible for **basic processes in our bodies** such as the immune system. In a manner of speaking, they are the **building blocks of life**.

Proteins consist of **amino acids**, forming a chain called **primary structure**. Interactions between **residues** of different amino acids define how the protein finally folds into its **tertiary structure**, which in turn determines behavior and **functionality**.

Drugs can be designed to evoke therapeutic effects by adapting directly to their target protein, if the exact structure is known. A number of **experimental methods** already exist to detect the tertiary structure. However, they are not generally applicable, often expensive, and time-consuming, therefore posing a **major obstacle** for progress in drug design and further medical fields.

Inferring the tertiary structure from the easily accessible amino acid sequence through **computational methods** would be a favorable alternative but also embodies one of the **biggest unsolved problems** in science.[1]

Leading[2] ***ab initio* algorithms** create possible structures using a Monte Carlo mechanism, which involves random structural changes and substitutions. Solutions are scored based on their **stability**, where the most stable structures best approximate the native structure.



In our expert session we will explain the chemical interactions in protein structures in more detail and have a small "**hands-on session**" in protein folding. After that, we will lead over to imaging methods and to the exploration of two state-of-the-art *ab initio* algorithms, namely **QUARK** and **I-TASSER**. We will provide you with an overview of their current capabilities, as well as pending challenges and future chances in the field.

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[1] Editorial: **So much more to know**. *Science* 2005, **309**:78-102.

[2] According to **CASP11** (Critical Assessment of Techniques for Protein Structure Prediction, 2014).