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INGLES INSTRUMENTAL

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What Is Bioinformatics?

Bioinformatics is the field of science in which biology, computer science, and information technology merge to form a single discipline. The ultimate goal of the field is to enable the discovery of new biological insights as well as to create a global perspective from which unifying principles in biology can be discerned. At the beginning of the "genomic revolution", a bioinformatics concern was the creation and maintenance of a database to store biological information, such as nucleotide and amino acid sequences. Development of this type of database involved not only design issues but the development of complex interfaces whereby researchers could both access existing data as well as submit new or revised data.

Ultimately, however, all of this information must be combined to form a comprehensive picture of normal cellular activities so that researchers may study how these activities are altered in different disease states. Therefore, the field of bioinformatics has evolved such that the most pressing task now involves the analysis and interpretation of various types of data, including nucleotide and amino acid sequences, protein domains, and protein structures. The actual process of analyzing and interpreting data is referred to as **computational biology**. Important sub-disciplines within bioinformatics and computational biology include:

- the development and implementation of tools that enable efficient access to, and use and management of, various types of information
- the development of new algorithms (mathematical formulas) and statistics with which to assess relationships among members of large data sets, such as methods to
  locate a gene within a sequence, predict protein structure and/or function, and cluster protein sequences into families of related sequences

Why Is Bioinformatics So Important?

The rationale for applying computational approaches to facilitate the understanding of various biological processes includes:

- a more global perspective in experimental design

- the ability to capitalize on the emerging technology of **database-mining** - the process by which testable hypotheses are generated regarding the function or structure of a gene or protein of interest by identifying similar sequences in better characterized organisms

Protein Modeling

The process of evolution has resulted in the production of DNA sequences that encode proteins with specific functions. In the absence of a protein structure that has been determined by X-ray crystallography or nuclear magnetic resonance (NMR) spectroscopy, researchers can try to predict the three-dimensional structure using **protein or molecular modeling**. This method uses experimentally determined protein structures **(templates)** to predict the structure of another protein that has a similar amino acid sequence **(target)**.

Although molecular modeling may not be as accurate at determining a protein's structure as experimental methods, it is still extremely helpful in proposing and testing various biological hypotheses. Molecular modeling also provides a starting point for researchers wishing to confirm a structure through X-ray crystallography and NMR spectroscopy. Because the different genome projects are producing more sequences and because novel protein folds and families are being determined, protein modeling will become an increasingly important tool for scientists working to understand normal and disease-related processes in living organisms.

The Four Steps of Protein Modeling

- Identify the proteins with known three-dimensional structures that are related to the target sequence

- Align the related three-dimensional structures with the target sequence and determine those structures that will be used as templates

- Construct a model for the target sequence based on its alignment with the template structure(s)

- Evaluate the model against a variety of criteria to determine if it is satisfactory

FONTE: http://www.ncbi.nlm.nih.gov/About/primer/bioinformatics.html