

Bioinformatics in biomedical research: From data analysis to drug discovery.

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Introduction

Under such a circumstance, the structural bioinformatics was emerging naturally as the times required. In this review, three main strategies developed in structural bioinformatics, i.e., pure energetic approach, heuristic approach, and homology modeling approach, as well as their underlying principles, are briefly introduced. Meanwhile, a series of demonstrations are presented to show how the structural bioinformatics has been applied to timely derive the 3D structures of some functionally important proteins, helping to understand their action mechanisms and stimulating the course of drug discovery. Also, the limitation of these approaches and the future challenges of structural bioinformatics are briefly addressed [1].

Decades of costly failures in translating drug candidates from preclinical disease models to human therapeutic use warrant reconsideration of the priority placed on animal models in biomedical research. Following an international workshop attended by experts from academia, government institutions, research funding bodies, and the corporate and Non-Governmental Organisation (NGO) sectors, in this consensus report, we analyse, as case studies, five disease areas with major unmet needs for new treatments. In view of the scientifically driven transition towards a human pathways-based paradigm in toxicology, a similar paradigm shift appears to be justified in biomedical research. There is a pressing need for an approach that strategically implements advanced, human biology-based models and tools to understand disease pathways at multiple biological scales. We present recommendations to help achieve this [2].

Data mining of available biomedical data and information has greatly boosted target discovery in the ‘omics’ era. Target discovery is the key step in the biomarker and drug discovery pipeline to diagnose and fight human diseases. In biomedical science, the ‘target’ is a broad concept ranging from molecular entities (such as genes, proteins and miRNAs) to biological phenomena (such as molecular functions, pathways and phenotypes). Within the context of biomedical science, data mining refers to a bioinformatics approach that combines biological concepts with computer tools or statistical methods that are mainly used to discover, select and prioritize targets. In response to the huge demand of data mining for target discovery in the ‘omics’ era, this review explicates various

data mining approaches and their applications to target discovery with emphasis on text and microarray data analysis. Two emerging data mining approaches, chemogenomic data mining and proteomic data mining, are briefly introduced. Also discussed are the limitations of various data mining approaches found in the level of database integration, the quality of data annotation, sample heterogeneity and the performance of analytical and mining tools. Tentative strategies of integrating different data sources for target discovery, such as integrated text mining with high-throughput data analysis and integrated mining with pathway databases, are introduced [3, 4].

It is estimated that when the Human Genome Project's DNA sequencing phase reaches its peak steady-state, the production rate will be approximately 70 to 80 “new” genes each day, every day. This estimate is based on genomic sequencing and not Expressed Sequence Tags (ESTs) or full-length cDNA sequencing. The challenge to research scientists is to identify these “genes” to some level of detail and determine which are of potential value, and to exploit that information as quickly as possible. This is a daunting task even with powerful computer and information systems; however, without a sophisticated informatics infrastructure it is impossible [5].

Conclusion

The application of translational approaches (e.g. from bench to bench and back) is gaining momentum in the pharmaceutical industry. By utilizing the rapidly increasing volume of data at all phases of drug discovery, translational bioinformatics is poised to address some of the key challenges faced by the industry. Indeed, computational analysis of clinical data and patient records has informed decision-making in multiple aspects of drug discovery and development. Here, we review key examples of translational bioinformatics approaches to emphasize its potential to enhance the quality of drug discovery pipelines, reduce attrition rates and, ultimately, lead to more effective treatments.

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