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Journal of Proteomics &Bioinformatics

Perspective

Application of *In Silico* Method to Predict Biological Behavior of Proteins

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DESCRIPTION

Bioinformatics also called as *in silico* biology is a rapidly growing field involving the theory and application of computational approaches to model, predict and explain biological function at the molecular level. *In silico* refers to the computation of pharmacological hypotheses using methods such as databases, data analysis tools, data mining, homology models, machine learning, quantitative structure-activity *in-silico* techniques have been introduced to characterize protein properties and structures. Computational bioinformatics tools and servers are used to predict the physicochemical properties, structure, stability, MHC class I binding properties and ligand-receptor interactions of the chimeric protein. Generally, it means any biological experiment performed on a computer or by computer simulation. *In silico* screening uses virtual screening tools to predict the behavior of different compounds. This is achieved by modeling the interactions between chemical molecules and their biological targets. *In silico* evaluation uses practical computer models to rapidly predict a chemical's potential toxicity without the need for animal testing. New Approach Methods (NAM) or non-animal approaches, are getting better and better as computing power, scientific knowledge, and information about chemicals improving rapidly. Tools for *in-silico* analysis of proteins and whole proteomes are important in the growing field of proteomics for optimal use of accumulated data. To use this data for healthcare and drug development, first we need to understand the structure of the proteome across species (mainly humans). Nucleic acid sequencing, protein sequencing, protein tertiary structure, genomic analysis, and proteomic analysis is a useful resource for the analysis, characterization, and classification of protein sequences. Most proteomics tools perform structural analysis and prediction, region-specific detection, alignment, comprehensive database for data mining, 2D PAGE analysis or protein modeling. Continuous progress in proteome research has led to this influx of protein sequences from a wide range species that creating challenges in the field of bioinformatics. Genome sequencing is developing faster and it has led to an equally rapid increase in predicted protein sequences. All the type of protein sequences need to be stored in a comprehensive, non-redundant protein sequence database. It is very important to assemble and analyses them to represent a solid basis for further comparisons and investigations in particular, the human sequence including mice and other model organisms as well. In efforts to better understand health and disease in-silico proteome analysis is an important tool. Most of the predicted proteins sequences have no specific functional characteristics. The challenge is to provide statistical and comparative data analysis of these sequences and structural and other information as an important step towards an integrated analysis of organisms. The whole proteome plays an important role in comparisons between species and also between peoples with different health conditions. To fully use the potential of vast amount of data collected from databases, tools like in-silico proteome analysis are required. Sequence databases are main comprehensive source of information about nucleotide sequences and proteins, and are therefore of particular importance for various research fields. In nucleotide sequence databases, data on nucleic acid sequences results from the genome sequencing projects, and also from smaller sequencing where it is stored. Protein sequence databases store information about proteins. Every week, new discoveries are made that link one or more genetic diseases to detect specific genes. To take these trends into account, the protein sequence database SWISS-PROT is gradually enhanced by numbers addition of features that are specifically intended for researchers working on the basis of human genetic diseases as well as the polymorphisms. The proteome, the set of proteins expressed by a genome, cell, tissue, or organism at a given time, poses great analytical challenges, but also great advantages. Several prediction algorithms and tools have been developed over the past two decades to predict protein and peptide aggregation. These in-silico tools help predict aggregation propensity and amyloidogenicity and identify aggregation-prone regions. It helps in protein identification and characterization, DNA sequence to amino acid sequence conversion, similarity search, pattern and profile search, post-translational modification prediction, primary structure analysis, secondary and tertiary structure prediction, and transmembrane region detection. *In silico* screening can be used in any field that relies on biological research, such as drug development, food toxicity research, and cosmetic development. *In silico* screening tools allow scientist to identify potentially active molecules against specific targets and vice versa.

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Received: 08-Dec-2022, Manuscript No. JPB-22-20678; **Editor assigned:** 12-Dec-2022, PreQC No. JPB-22-20678 (PQ); **Reviewed:** 26-Dec-2022, QC No. JPB-22-20678; **Revised:** 02-Jan-2023, Manuscript No. JPB-22-20678 (R); **Published:** 09-Jan-2023, DOI: 10.35248/ 0974-276X.23.15.621

Citation: Tuzun N (2023) Application of *In Silico* Method to Predict Biological Behavior of Proteins. J Proteomics Bioinform.15:621