

Bioinformatics Approaches in Food Sciences

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Abstract

Food plays an important role in regulating the various processes within the body. With the continued progression of the “omics” era, bioinformatics curates and interprets biological data by computational means and therefore it has seen widespread integration across every discipline of life sciences including food sciences. Bioinformatics can be used for efficiently access to all genomics, proteomics and metabolomics data discovered so far and to make available this data to every individual group industry or company so as to increase quality, taste and nutritional value of food that is to be produced. Here, we have discussed the role of bioinformatics and some approaches in food sciences.

Keywords: Food; Bioinformatics; Genomics; Proteomics; Omics; Allergen; Bioactive; Database

Introduction

Food science is the combination of engineering, biological and physical sciences to study the nature of foods, causes of deterioration, principles underlying food processing and improvement of food quality. In many of these processes, bioinformatics can play an important role. The use of modern science would enable to combat difficult situations such as food scarcity, nutritional quality and food deterioration. The various success stories of application of bioinformatics approaches in different biological fields lead to its use in food sciences. Bioinformatics helps in management of biological data so that gathered biological information can be applied extensively in biotechnology. The field is expanding at an alarming rate and becoming a much essential tool for research [1].

Bioinformatics is an interdisciplinary field and has been established as an important scientific discipline. It brings a paradigm shift in various disciplines including comparative genomics, molecular medicine, molecular evolution, drug discovery, microbial genome applications and biotechnology [2]. Many bioinformatics approaches have recognised potential for a significant contribution in food sciences, but this field has been lesser appreciated. Here, in this article, we highlighted the bioinformatics approaches that can be applied in food and nutrition sciences to advance and expand research.

Bioinformatics plays an important role in predicting and assessing the desired and undesired effects of microorganisms on food, genomics and proteomics study to meet the requirements food production, food processing, improving the quality and nutritive value of food sources and many others. In addition, bioinformatics approaches can also be used in producing the good quality of the crop including high yield and disease resistant. There are also variety of databases that contain data on food, their constituents, nutritive value, chemistry and biology.

Food taste

Scientists found out the molecular and genetic details of the taste receptors. These include:

- **Sour:** For sour taste, an ion channel identical to degenerin-1 is found to be the receptor [3].
- **Bitter:** A family of ~50 G protein-coupled receptors (GPCRs) has been identified in human taste cells [4].
- **Umami:** For umami, mGluR4 which is a ‘splice variant’ of brain glutamate receptor has been identified in rat taste cells [5].
- **Sweet:** G protein coupled receptor; Tas1r3 has been identified as a sweetness receptor [6].
- **Salt:** The epithelial ion channel, ENaC is responsible for over 80% of salt taste transduction [7].

These taste receptors can be used to discover the next generation of taste modifiers for foods. New developments in computational algorithms and software with the available known structures of these receptors have made possible the molecular modeling and simulations. Such simulations will make possible to develop more intense tasting compounds as food additives. These also help in understanding the basis of taste persistence, antagonism and complementation. Bioinformatics sequence similarity algorithms have been used to determine homology between sweet taste receptors and brain glutamate receptors as well as in the identification of sour taste sensors in mammals [8].

Food flavour

Lactic acid plays an essential role in flavour formation in dairy products. Study of the genetic sequences of lactic acid bacteria revealed the flavour forming potential. The flavour profiles of many food products are not due to single compounds but due to the presence and interactions of many different molecules. Bioinformatics plays an important role in linking various flavour compounds for new product development based on insight knowledge, preferences and needs of the consumer [9].

Food quality and safety

There is a growing appreciation for bioinformatics in the area of food quality and safety. As the genome sequencing projects are now focusing on the food borne pathogens and innovative ways which will help in determining the source of the food borne illnesses [10]. In future, molecular markers may help in identification of the occurrence of spoilage and pathogenic bacteria and prediction of thermal preservation stress resistance. Bioinformatics experts have developed a tool for detecting and identifying bacterial food pathogens. This tool has been developed by FDA (Food and Drug Administration) for molecular characterization of bacterial food borne pathogens using microarrays [11].

Allergen detection

Bioinformatics can be used for food allergen related studies. Most of the allergens have same sequence and structural similarity. Therefore, homology studies and structural bioinformatics can be used in detecting the possible allergenicity and cross reactivity of proteins. This method encourages the WHO to incorporate sequences similarity search as a feature of the rules for evaluating allergenicity for genetically modified foods [12]. There are few databases that are dedicated to the food allergens such as AllerMatch [13], Informall FARRP Allergen database and SDAP [14].

Bioactive peptides

Bioactive peptides of food are the peptides that are present within the food and have exerted biological activities such as antioxidative, antihypertensive, mineral-binding, opiate-like, antimicrobial, immuno-, and cytomodulating activity. Bioinformatics recently divulged in the discovery of bioactive peptides [15]. One of the approaches for discovery of bioactive peptides is use of protein sequences from UniProtKB, SwissProt and TrEMBL. The occurrence frequency of bioactive peptides crypt in primary structures of food proteins and is calculated by a/N where "a" stands for the number of peptides exhibiting bioactivity of particular type present in sequence and "N" stands for the total number of amino acids residues present within the proteins. This approach reduces the time which was being required earlier to screen for bioactive peptides using classical approaches. It prompts the discovery of new and credible forerunners of known bioactive peptides. Few software's are also developed that are used to generate profiles for *in silico* peptides and have resulted due to the stimulation of proteolytic specificities of various enzymes [16].

Metabolic pathway construction

Microbial metabolism has been used for fermented foods. Fermentation of food can be improved by understanding microbial metabolism. It has advantage in ability of desirable microbes to convert substrates (usually carbohydrates) to organic tailor-made compounds contributing to the flavour, structure, texture, stability and safety of the food product. Use of modern genomic and bioinformatic approaches, expands the availability of tools to understand and control microbial metabolism. The integration of information on metabolic pathways available in the literature and databases with the genomic sequences of bacteria and stoichiometric models may describe cellular processes and link genotype and phenotype. As the knowledge increases, metabolic reconstruction models will become more important in studying the dynamic response of cells to external stimuli [17].

Food processing

Food products are processed to increase storage stability and safety. But lack of knowledge of composition and structural complexity of input material (biological materials like living organisms, generally microbes) and response of these materials on processing parameters bring out large array of errors. With the help of bioinformatics, knowledge of organisms for food processing can be acquired and the process may become optimized with lesser chances of error. The biological knowledge with functional genomics, proteomics and metabolomics is providing precisely the knowledge necessary to readdress food processing using bimolecular activities rather than simply with biomaterial properties. In future, the structure function properties of living organisms will increasingly dictate the design of new foods and new food processes [18].

Crop improvement

Sustainable agricultural production is an urgent issue in response to global climate change and population increase. One solution to increase plant yield is by designing plants based on a molecular understanding of gene function and on the regulatory networks involved in stress tolerance, development and growth. This can be achieved by using bioinformatics approaches like comparative genomics. Comparative genomics grasp the biological properties of each species that accelerate gene discovery and functional analyses of genes. Various tools and databases allow the best use of genomic resources including resource integration [19].

Theobroma cacao (cocoa) is used as a raw material for chocolate. To recognise a seed of higher quality and good flavour, DNA fingerprinting is implemented. This allows to select some genotypes that have a high probability of having the qualitative characteristics of that *T. cacao* type. About 300 molecular markers have already been mapped and permit the identification of numerous QTL mainly for agronomical characteristics. With the emerging new molecular tools from genomics, the challenge will be the implementation of these technologies in order to facilitate and improve the qualitative characteristics through gene discovery for further genetic modification [20].

Microbial informatics

Bioinformatics plays an increasing role in predicting and assessing the desired and undesired effects of microorganisms on food. Sequence-based prediction of microbial functionality with access to databases that integrate data from genomics, systems biology, phenotypes and 'biomarkers' for functionality in specific taxa will help in predicting the effects of microorganisms on food. Using microbial bioinformatics, biomass yield can be optimized that can improve the food production. For this, the genome sequence of the organism and metabolic models have been made for many microbes including several of food-relevant microorganisms. Complete genome-scale metabolic models together with algorithms such as flux balance analysis allow the *in silico* simulation of growth of the organism under the metabolic restrictions provided by the substrate availability in the medium. These growth simulations can then be used to optimize medium composition to better fit the organism requirement [21].

Databases in food sciences

FoodDB: FoodDB is the comprehensive resource on food constituents, chemistry and biology. It provides information on both macronutrients

and micronutrients including many of the constituents that give colour, flavour, texture, taste and aroma to the food. It is available online at <http://foodb.ca/>. Each chemical entry contains more than 100 separate data fields covering detailed biochemical, compositional and physiological information. The data are obtained from the literature and it includes data on the compound's description, nomenclature, chemical class, information on its structure, its physicochemical data, its food source(s), its colour, taste, aroma, physiological effect, presumptive health effects and concentrations in various foods.

EuroFIR-BASIS: It uniquely combines food composition and biological activity for bioactive compounds in plant-based foods. It is available only at <http://www.eurofir.org/>. The database covers multiple compound classes and 330 major food plants and their edible parts with data sourced from quality-assessed, peer-reviewed literature. The database will be a valuable resource for risk authorities, food regulatory and advisory bodies, epidemiologists and researchers interested in diet and health relationships and product developers within the food industry [22].

FoodWiki database: It is the repository for food and nutritional information in a consensus style. It utilizes the immense amount of data that is possible and easily managed by bioinformatics strategies and protocols. Such resources will advance and develop food and nutritional sciences with a view to improving the quality and nutritive value of food sources. This centralised, comprehensive food and nutrition database is crucial to the progression of bioinformatics in this area [23].

Foodomics database: It is a database for food molecular profiles. It released 28 of the USDA National Nutrient Databases for Standard Reference (SR28) and contains data for up to 150 food molecules. Nutrition Facts Labels (NFLs) on branded food reflect current nutrient information but usually contain less than 15 nutrients. The integration of current NFLs and SR28 is needed to obtain foodomic profiles of a person's (or animal's) dietary intake and therefore precision medicine for each person can be implemented. In this way, right food molecules are given in the right amount, at the right time, and to the right person having part precision medicine [24].

Conclusion

Like other branches of life sciences, food science is also becoming a much data enriched discipline. High throughput "omics" technologies generate large amount of data that require curation and analyses. For this, integration and implementation of bioinformatics is suitable to achieve this end. The latest technological advances in genomics, transcriptomics, proteomics and metabolomics combined with suitable software and tools provides the opportunity to explore and decipher composition of food, their micro constituents, nutritive value, chemistry and biology of food. To efficiently handle huge amounts of data that are generated from various projects, makes bioinformatics an important area in the food industry.

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Conflict of Interest

The authors confirm that they have no conflict of interest.

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