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Computational Prediction of Bioavailability and Bioactivity of Functional Food Components

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ABSTRACT: Computational methods have revolutionized the research of functional food by allowing the prediction of bioavailability and bioactivity of bioactive food compounds in a few seconds. The chapter emphasizes the use of advanced computational methods such as quantitative structure–activity relationship (QSAR) modeling, molecular docking, molecular dynamics simulation, absorption, distribution, metabolism, excretion (ADMET) prediction, physiologically based pharmacokinetic (PBPK) modeling, and artificial intelligence (AI) for the rapid assessment of functional food ingredients. All these techniques help in rapid identification of potential bioactive molecules with better pharmacokinetic properties and therapeutic potential with reduced time and cost of experimentation. AI-based applications in disease prevention, gut microbiome modulation, precision nutrition using machine learning, deep learning, network pharmacology, and multi-omics integration are also discussed. Topics such as data standardization, experimental validation, regulatory aspects, and explainable AI are also covered. In summary, computational prediction offers a comprehensive framework for creating evidence-based functional foods and nutraceuticals, enabling personalized nutrition and driving future advancements in healthcare and nutrition through data-driven innovation.

1. INTRODUCTION

Functional foods are natural or processed foods with biologically active components that can give health benefits that extend beyond their nutritional benefits. These foods contain abundant bioactive compounds, such as polyphenols, flavonoids, carotenoids, alkaloids, dietary fibers, bioactive peptides, phytosterols, omega-3 fatty acids, probiotics, prebiotics and other phytochemicals, which exert their preventive and therapeutic effects on chronic diseases by various molecular mechanisms (1). The positive effects of these compounds rely on both their inherent biological activity as well as their bioavailability, meaning the percentage of a compound that reaches the tissues in its active form after ingestion, absorption, distribution and metabolic processes (2). These compounds exhibit bioactivity by binding to specific molecular targets, influencing the regulation of signaling pathways, altering gene expression, decreasing oxidative stress, limiting inflammation and enhancing physiological functions related to human health (3). Although the functional food components have been more identified, the traditional experimental evaluation of their bioavailability and biological efficacy are generally expensive, labor intensive and time-consuming, which is a huge bottleneck in functional food research and product development (4). The use of computational prediction has thus become an essential tool for the discovery and assessment of bioactive food components, which includes a combination of cheminformatics, bioinformatics, molecular modeling, artificial intelligence and systems biology (5).The use of modern computational methods, such as quantitative structure–activity relationship (QSAR) modeling, molecular docking, molecular dynamics simulations, absorption, distribution, metabolism, excretion, and toxicity (ADMET) prediction, physiologically based pharmacokinetic modeling, and machine learning algorithms, can result in a rapid estimation of pharmacokinetic behavior, target interactions, metabolic stability, and biological functions before experimental validation (6). These methods enable more effective identification of more promising functional food components with lower expenditure of research, more accurate predictions, and analyses based on data. (7) In addition, deep learning, multi-omics integration, and explainable artificial intelligence are revolutionizing precision nutrition by allowing the prediction of individual responses to dietary bioactive compounds derived from genetic, metabolic, and microbiome differences (8). Hence, computational prediction has now emerged as a valuable tool in modern functional food science, assisting the selection of ingredients, rational formulation of food products, disease prevention strategies, and development of next-generation nutraceuticals. This chapter offers a detailed survey of the computational methods for predicting bioavailability and bioactivity of functional food components, their current applications, technological advancements in this field and the potential future applications of the use of artificial intelligence in precision nutrition and functional food research (9).

2. FUNCTIONAL FOOD BIOACTIVE COMPONENTS

Functional food bioactive components can be classified in a wide variety of naturally occurring groups that provide physiological benefits other than nutritional and are important in disease prevention and health promotion (10). The bioactive substances can be structurally classified as being phytochemicals, bioactive peptides, proteins, polysaccharides, dietary fibers, probiotics, postbiotics, and marine- or microorganism-derived metabolites (11). The phytochemicals found in plants such as polyphenols, flavonoids, phenolic acids, carotenoids, glucosinolates, alkaloids, lignans and terpenoids have been widely studied for their antioxidant, anti-inflammatory, antimicrobial, anticancer properties, as well as for their cardioprotective and neuroprotective properties (12). Bioactive peptides and proteins are products of the natural process of digestion and enzymatic hydrolysis in the process of food preparation, which possess antihypertensive, antioxidant, immunomodulatory, antimicrobial, and antidiabetic effects by interacting with specific molecular targets and signaling pathways (13). Cereals, fruits, vegetables, mushrooms, seaweeds, and legumes as sources of polysaccharides and dietary fibers can support the health of the gut by promoting intestinal function, regulating glucose and lipid metabolism, inducing satiety, and protecting the gut microbiota, all of which help reduce the likelihood of metabolic and gastrointestinal disorders (14). Probiotics, which are beneficial, live microorganisms (Lactobacillus and Bifidobacterium species), can alter the microbial balance, to increase immune responses, to strengthen intestinal barrier integrity, and to produce bioactive metabolites that contribute to the health of the host (15). Recently, a new generation of probiotics termed postbiotics has gained a lot of attention, as microbial metabolites, enzymes, peptides, short-chain fatty acids, cell wall fragments, and extracellular polysaccharides released during the fermentation of probiotics have also been found to have many health benefits and are more stable and safe for use (16). Moreover, marine and microbial bioactives such as omega-3 fatty acids, marine peptides, carotenoids, sulfated polysaccharides, fungal metabolites, and bacterial secondary metabolites are important sources of novel bioactive substances with antioxidant, anti-inflammatory, antiviral, anticancer, and cardiometabolic protective properties (17). The structural diversity and multifunctional biological activities of these bioactive components are remarkable, and thus they have emerged as promising candidates for computational screening and prediction

studies where they could be assessed for their bioavailability, target interactions, and therapeutic potential efficiently before experimentation and clinical validation (18).

3. BIOAVAILABILITY OF FUNCTIONAL FOOD COMPONENTS

Bioavailability is one of the most important properties to consider when evaluating the biological activity of functional food ingredients since the absorbed fraction of the bioactive compound can be metabolized and exert beneficial physiological effects (15). Functional food bioactives are liberated from food matrix following gastrointestinal digestion, during which mechanical digestion, gastric acid, digestive enzymes, bile salts and interactions with other dietary components can affect their stability and absorption (16). In the small intestine, the absorption is accomplished by passive diffusion, facilitated diffusion, active transport or endocytosis depending on the molecular size, polarity, lipophilicity, solubility and chemical structure of the compound. Several dietary bioactives are taken up and effluxed from the intestine through intestinal transport proteins, such as peptide transporters, glucose transporters, and ATP-binding cassette transporters, which influence their systemic availability (16). Many compounds are extensively metabolized to change their chemical structure and biological activity through phase I and phase II metabolic reactions, such as oxidation, hydrolysis, glucuronidation, sulfation and methylation, within the intestinal epithelium and liver prior to systemic uptake (17). Numerous factors affect the overall bioavailability of functional food components such as food processing methods, formulation, particle size, solubility, interactions with other nutrients, composition of gut microbiota, age, genetic variability, health status and individual metabolic capacity (17). The pharmacokinetic principles which involve absorption, distribution, metabolism and excretion (ADME) of food-derived bioactive compounds in humans have been integrated in computational prediction methods and provide a comprehensive understanding of the fate of these compounds in the human body. To estimate bioavailability and biological performance prior to laboratory testing, advanced in silico techniques integrate molecular descriptors, ADMET prediction, quantitative structure–activity relationship (QSAR) models, molecular docking, and artificial intelligence algorithms. These computational strategies can be used to quickly screen functional food components, identify promising candidates for further testing with enhanced pharmacokinetic properties and predict potential molecular targets, and thus decrease the amount of experiments and shorten the time to evidence-based functional food and nutraceuticals (18), as shown in Figure 1.

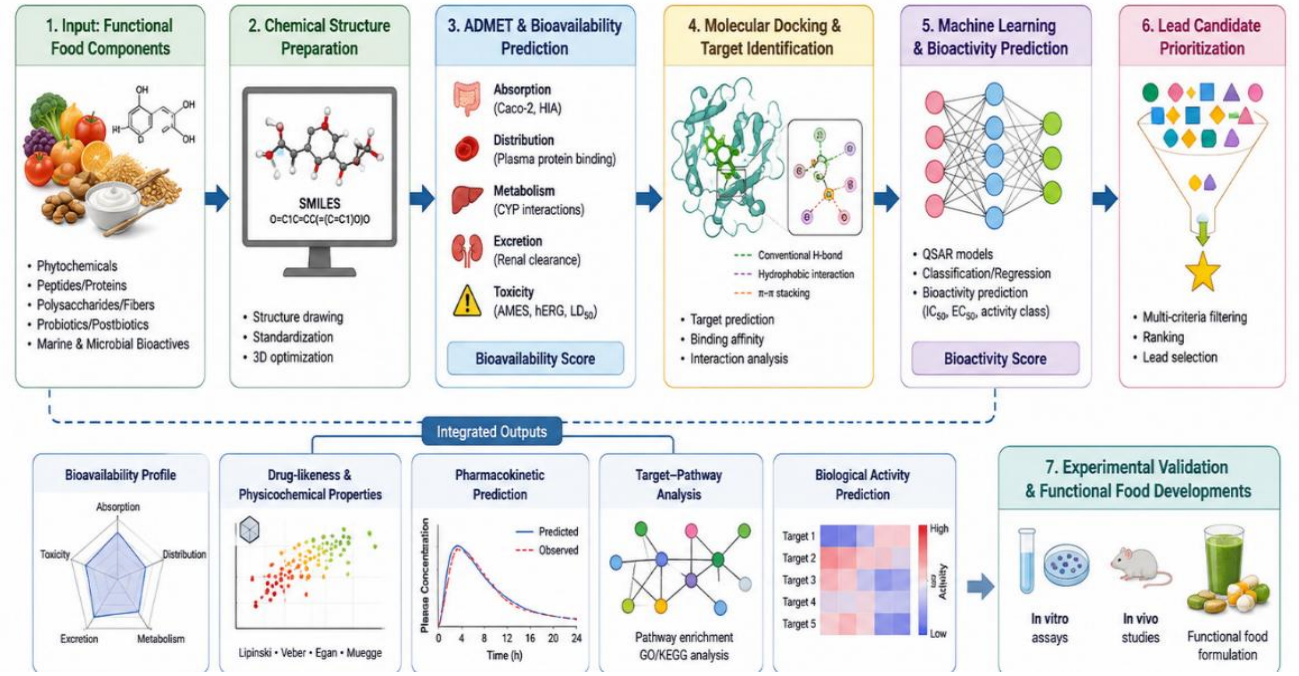

Figure 1. Computational Workflow for Predicting Bioavailability and Bioactivity of Functional Food Components

4. COMPUTATIONAL APPROACHES FOR BIOAVAILABILITY PREDICTION

The computational methods have become invaluable tools for predicting the bioavailability of functional food components since it allows a rapid, low cost, and high-throughput evaluation of its pharmacokinetic and biological properties prior to experimental validation (18). One of such procedures is Quantitative Structure–Activity Relationship (QSAR) modeling, which is based on the establishment of mathematical relationships between the chemical structure of bioactive compounds and their biological or pharmacokinetic properties, and by using molecular descriptors the researchers can predict absorption, permeability, solubility and biological activity (18). The recent developments in machine learning (ML) and deep learning (DL) have greatly enhanced the performance of predictions, with the use of algorithms like random forest, support vector machine, gradient boosting, convolutional neural network, and graph neural network, by making use of larger and more complex chemical and biological datasets. These models recognize the nonlinear relationship between molecular features and biological responses and enable efficient screening of large libraries of food-derived compounds (19). Prediction of Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) is another vital computational approach that helps estimate the absorption and distribution, metabolism, excretion and toxicity profile of bioactive molecules and to evaluate their pharmacokinetic behaviour and safety. Early ADMET assessment allows the exclusion of compounds with poor oral bioavailability or unfavorable toxicological characteristics, thus saving the cost and time of experimental studies (19). Physiologically Based Pharmacokinetic (PBPK) modeling further improves the prediction of bioavailability by combining some of the other physiological parameters, organ-specific blood flow, tissue distribution, metabolic pathways, and compound-specific characteristics to simulate the absorption, distribution, metabolism, and elimination of food bioactives under various bio-scenarios (20). The calculation of molecular descriptors and the effective engineering of features such as molecular weight, lipophilicity (LogP), hydrogen bond donors and acceptors, topological polar surface area, molecular flexibility, and structural fingerprints which are input into the predictive algorithms (20) are also important factors for the accurate computational prediction. Other databases and computational tools are also freely available, including PubChem, which is used for chemical information; ChEMBL, which holds structural data, as well as chemical and biological information; FooDB, which focuses on food bioactive compounds; DrugBank, which provides comprehensive chemical, biological, pharmacokinetic and structural data; UniProt, which offers a repository of protein sequences; BindingDB, which provides binding data; SwissADME, which provides ADME data; pkCSM, which offers comprehensive pharmacokinetic data; ADMETlab, which serves as an in-house, web-based, virtual laboratory for ADME; and the Protein Data Bank (PDB), which is a repository of protein structure, to support model development, virtual screening, molecular docking, and AI prediction of functional food bioactives (21). The ability to implement these computational strategies will allow for the identification of promising functional food compounds with additional biofortification features that provide more potential therapeutic benefits with less experimental analysis, thus accelerating the path towards evidence-based nutraceuticals and precision nutrition strategies (21).

Table 1. Computational Tools and Models for Predicting Bioavailability and Bioactivity of Functional Food Components

Computational Approach	Purpose	Representative Tools/Databases	Applications
QSAR Modeling	Predict structure–activity relationships	QSAR Toolbox, OCHEM	Bioactivity and permeability prediction
Machine Learning & Deep Learning	Predict pharmacokinetic and biological properties	DeepChem, TensorFlow, Scikit-learn	Bioavailability and activity prediction
ADMET Prediction	Assess absorption, distribution, metabolism, excretion, toxicity	SwissADME, pkCSM, ADMETlab	Drug-likeness and safety evaluation
PBPK Modeling	Simulate in vivo pharmacokinetics	GastroPlus, Simcyp, PK-Sim	Oral bioavailability and tissue distribution
Molecular Descriptor Analysis	Calculate physicochemical properties	PaDEL-Descriptor, Mordred, RDKit	Feature generation for predictive models

Public Databases	Chemical and biological information	PubChem, ChEMBL, FooDB, DrugBank, PDB	Virtual screening and computational modeling

5. COMPUTATIONAL PREDICTION OF BIOACTIVITY

The ability to predict bioactivity by computational techniques has now become an important tool in functional food research as it allows the identification of compounds that might be biologically active in the human body and the elucidation of their mechanisms of action before any experimental testing in the lab (21). Target identification and validation is the first step in this process, in which computational tools combine information from the genome, proteome, metabolome, and biochemistry to identify proteins, enzymes, receptors, transcription factors, and signaling molecules that have been implicated in a particular disease or physiological process. The selection of biologically relevant targets for functional food bioactives is possible with databases of experimentally validated targets and network-based algorithms (21). Molecular docking is one of the most popular in silico methods used for investigating binding affinity and interaction of food-derived compounds and biological macromolecules. Docking algorithms predict the orientation of the ligand, hydrogen bonding, hydrophobic interactions, electrostatic forces, and binding energies, thus prioritizing compounds that have high therapeutic potential (22). However, rigid docking models can be limited in their usefulness; molecular dynamics (MD) simulation can be useful in simulating the movement of molecules under physiological conditions to provide a dynamic representation of protein–ligand interactions. MD analysis is used to assess the structural stability, conformational flexibility, interactions with the solvent, and long-term binding behavior, thereby enhancing the docking prediction reliability (22). In recent years, network pharmacology has revolutionized the research of functional food, as the bioactive components of functional food are not only capable of acting on several molecular targets, but also on different interconnected signaling pathways. Understanding the whole therapeutic mechanisms of complex dietary compounds is achieved through protein–protein interaction networks, gene regulatory networks, pathway enrichment analyses and disease association studies (23). To gain a comprehensive view of the functional mechanisms of food, systems biology approaches combine transcriptomics, proteomics, metabolomics and microbiome data to address the impact of food on the biology of individual cells and organisms. Last but not least, the multi-target interaction analysis is used to assess the synergy between the multiple bioactive compounds and multiple disease-related targets simultaneously through molecular docking, network pharmacology, AI and systems biology. This combined approach is especially useful for complex diseases like cancer, diabetes, cardiovascular and neurodegenerative disorders, in which several signaling pathways must be modulated for therapeutic success. Thus, the computational bioactivity prediction has emerged as a key tool in the contemporary functional food research, streamlining the discovery, optimization, and elucidation of the mechanism of action of health-promoting food-derived bioactive compounds and lowering experimental costs and development time (24).

6. ARTIFICIAL INTELLIGENCE IN FUNCTIONAL FOOD RESEARCH

Artificial intelligence (AI) has transformed the landscape of functional food research by introducing powerful computational tools that can handle the vast amount of biological, chemical, nutritional, and clinical data available today, with unprecedented speed and accuracy (24). Random forest, support vector machine, gradient boosting, decision tree and ensemble learning methods are all popular machine learning (ML) algorithms used to predict bioavailability, bioactivity, toxicity, and therapeutic potential of functional food compounds using experimental data and molecular descriptors. These algorithms are able to uncover hidden relationships in complex biological data, and are better able to predict than traditional statistical algorithms (24). In recent years, deep learning (DL) methods, including convolutional neural networks (CNNs), recurrent neural networks (RNNs), graph neural networks (GNNs), and transformer-based neural networks, have significantly improved the prediction of bioactivity from molecular structures, sequences, and biological networks. Deep learning models achieve excellent prediction accuracy for compound–target interactions, pharmacokinetic properties and biological activity of food-derived bioactives (25). The disruptive power of emerging generative AI technologies is continuing to revolutionize compound discovery by designing new bioactive molecules, chemical structure optimization, predicting molecular properties and discovering new functional food ingredients, with increased biological activity and better pharmacokinetic profiles. These models decrease the amount of time and expense spent on traditional discovery pipelines (25). Moreover, the recent advent of Natural Language Processing (NLP) has made literature mining of millions of scientific literature, patents, clinical reports, and public records an invaluable tool for extracting scientific knowledge automatically. NLP can be used to automate the identification of bioactive compounds, disease

associations, molecular targets, and therapeutic mechanisms, which will promote evidence synthesis and knowledge discovery (26). While these impressive strides in AI have been made, the complexity of the models has also raised questions about the lack of transparency in how these predictions are made, leading to a demand for explainable artificial intelligence (XAI) that seeks to make the models more transparent by elucidating molecular features and biological factors underlying the model predictions. XAI improves scientific interpretability, regulatory confidence and clinical acceptance, and moves away from the "black-box" restrictions of traditional deep learning systems. Together, AI-powered computational technologies are revolutionizing functional food studies, supporting high-throughput screening, precision nutrition, personalized nutrition recommendations and the development of future generations of nutraceuticals, making AI a key element of modern computational food science (26).

7. APPLICATIONS IN DISEASE PREVENTION AND PRECISION NUTRITION

The functional food bioactive compounds, along with the sophisticated computational technologies, artificial intelligence have come into play as valuable tools for disease prevention and precision nutrition, as they allow identification of food molecules that could affect several biological pathways involved in chronic diseases (26). Computational prediction has identified polyphenols, flavonoids, omega-3 fatty acids, phytosterols, and bioactive peptides which can modulate lipid metabolism, decrease oxidative stress, inhibit inflammatory processes, enhance endothelial functions, and regulate blood pressure by targeting key molecular pathways involved in cardiovascular homeostasis in the context of cardiovascular diseases (26). Using artificial intelligence, such as screening, molecular docking and network pharmacology, the functional food components that reduce the insulin sensitivity, inhibit carbohydrate-digesting enzymes, regulate glucose transporters and inhibit lipid metabolism can more quickly be identified, which can help to reduce chronic inflammatory responses related to obesity and metabolic syndrome in diabetes and metabolic disorders (27). Moreover, computational tools are also being increasingly employed in cancer prevention to identify diet-derived phytochemicals that may modulate cell proliferation, apoptosis, angiogenesis, oxidative stress, immune response and multiple oncogenic signaling pathways to enable nutrition interventions for cancer prevention. (27) Likewise, many food bioactive compounds have therapeutic potential in neurodegenerative disorders, with computational studies showing that they interact with molecular targets identified in Alzheimer's and Parkinson's disease, oxidative stress, neuroinflammation, mitochondrial dysfunction, and protein aggregation, which results in neuroprotection and cognitive health (28).

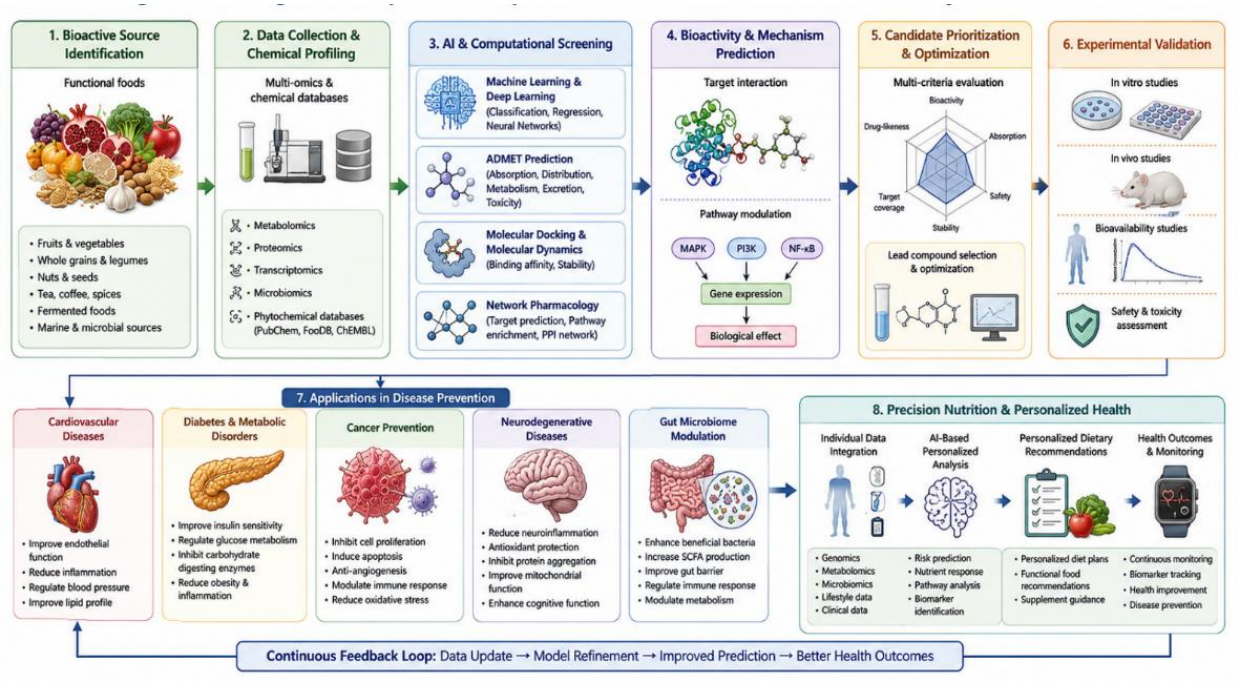

Figure 2. AI-Integrated Computational Pipeline for Functional Food Bioactive Discovery and Precision Nutrition

The other emerging application is gut microbiome modulation, and the computational tools developed to predict the interaction between food bioactives, probiotics, postbiotics, microbial metabolites and host metabolic pathways are supported by the sequencing of microbiome and metabolomics and systems biology. These analyses are useful for designing functional foods, the goal of which is to increase the diversity of the intestinal microbiota, improve barrier function, regulate immune function and metabolic health (28). The integration of these technologies (AI, multi-omics, molecular docking, ADMET prediction, network pharmacology and machine learning) is an AI-based computational pipeline to develop functional food bioactives for discovery, screening, optimization, and clinical translation as illustrated in Figure 2. These technologies can also be applied to the concept of 'precision nutrition,' 'precision health,' and combine genomic, transcriptomic, proteomic, metabolomic, microbiome and lifestyle information to inform individual responses to nutrition and the development of personalised nutrition strategies for disease prevention and health promotion. Therefore, AI-driven computational methods are revolutionizing functional food research, ranging from general nutrition claims to precision nutrition, resulting in better preventive nutrition care, and faster development of scientifically valid nutraceuticals and personalized nutrition interventions (29).

8. CHALLENGES AND FUTURE PERSPECTIVES

Despite the tremendous progress in the knowledge of functional food made by computational methods, some problems still exist. Poor data quality, varied experimental procedures, and poor standardization decreases predictive model accuracy and reproducibility. Computational integration of multi-omics data such as the genomics, transcriptomics, proteomics, metabolomics, and microbiome data is still a challenge. In silico predictions must be experimentally validated to ensure that the predictions are accurate before using the approach in a clinical setting. Guidelines are still being developed for the discovery of functional food using AI and there are a lack of internationally agreed guidelines. Moreover, the models require explainable artificial intelligence (XAI) to strengthen the transparency and trust in the models. The innovation of personalized functional foods is projected to gain momentum with future advancements in digital nutrition, precision health, and artificial intelligence (AI) in decision making.

9. CONCLUSION

The functional food research, which can be well evaluated by computational prediction, has revolutionized the research on bioactive compounds derived from food with regards to its efficiency in evaluating bioavailability, bioactivity, safety, and molecular mechanisms. Combining molecular modeling, ADMET prediction, machine learning, artificial intelligence and multi-omics has greatly sped up the identification of functional ingredients for disease prevention and precision nutrition. AI technologies for computational research lower research expenses, enhance prediction accuracy, and aid in evidence-based nutraceutical development. Explainable AI, high-quality biological data, strong experimental validation, and individual nutrition plans should be further investigated to enable the clinical translation and industrial use of the next-generation functional foods.

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Data Availability: No new data were generated or analyzed in this study.

Ethical Approval: Not applicable, as this study is based solely on published literature.

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