Natural Resources for Human Health
eISSN: 2583-1194

Original Research

Received 14 March 2026
Revised 18 April 2026
Accepted 16 May 2026

Natural Resources for Human Health 2026, Vol. 6 (3): 245–252

KEYWORDS:
Functional foods; Bioactive compounds; *In silico* drug discovery; Molecular docking; Molecular dynamics; Artificial intelligence; ADMET; Virtual screening; Precision medicine; Nutraceuticals.

In Silico Drug Discovery Using Functional Food Bioactive Compounds

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ABSTRACT: Functional foods produce bioactive compounds with several pharmacological properties and safety characteristics, which can be used as excellent candidates in the development of new therapeutic products. With the advent of new in silico drug discovery technologies, computational methods including artificial intelligence, molecular docking, virtual screening, molecular dynamics simulation, ADMET prediction, and others have significantly contributed to the identification, screening and optimization of these natural compounds. These techniques can be used to rapidly profile protein–ligand interaction, pharmacokinetic characteristics, and toxicity and can significantly reduce the time and expense required to the traditional drug discovery process. Moreover, the combination of machine learning, network pharmacology and multi-omics approaches has improved the discovery of targets and lead optimization in precision medicine. The therapeutic potential of bioactive compounds of functional foods has been reported against cancer, cardiovascular diseases, diabetes, neurodegenerative diseases, infectious and inflammatory diseases. Overall, computational approaches provide a rapid, robust platform to improve the functional food-based drug discovery process, and to develop safe, effective and personalized therapeutic agents.

1. INTRODUCTION TO *IN SILICO* DRUG DISCOVERY USING FUNCTIONAL FOOD BIOACTIVE COMPOUNDS

Foods with health promoting properties beyond their nutritive content, including biologically active constituents that can also contribute to health and prevent chronic disease are known as functional foods, and naturally occurring food products or bioactive compounds in foods that have a preventive or therapeutic effect are called nutraceuticals. The antioxidant, anti-inflammatory, antimicrobial, anticancer, cardioprotective, neuroprotective, and immunomodulatory properties of the bioactive compounds like polyphenols, flavonoids, alkaloids, terpenoids, carotenoids, phytosterols, peptides, dietary fibers and organosulfur compounds have attracted considerable attention. The compounds found in functional foods have been identified as valuable sources for the discovery of new therapeutic agents in the modern drug discovery programs because of their incredible diversity in structure, biological specificity and low toxicity of number of synthetic drugs (1,2). The research of novel pharmaceuticals has been transformed by recent developments in computational biology, bioinformatics, cheminformatics and artificial intelligence, which allow to identify, screen and optimize potential drug candidates prior to their experimental validation, in a fraction of time. The evaluation of binding affinity, molecular interactions, pharmacokinetic properties and toxicity profile of functional food bioactive compounds against disease-specific molecular targets was made possible using modern computational methods like molecular docking, virtual screening, pharmacophore modeling, molecular dynamics simulation, quantitative structure–activity relationship (QSAR) analysis, network pharmacology and absorption, distribution, metabolism, excretion, and toxicity (ADMET) prediction. These strategies significantly cut down on the resources needed for traditional drug development, such as time, cost, and failure rates, as well as improving the efficiency in identifying and optimizing leads (2,3). Furthermore, the screening of massive phytochemical libraries, protein structure archives, omic technologies, and the application of artificial intelligence algorithms have led to the identification of new bioactive compounds that have new therapeutic potential, opening the door to precision medicine and personalized nutrition plans (3,4). This chapter aims to summarize the basic concepts of functional food and nutraceuticals, biological therapeutic importance of food derived bioactives, Computational tools for target identification, molecular docking, molecular dynamics simulation, virtual screening and ADMET prediction, and emerging artificial intelligence based approaches to enable readers to get the comprehensive understanding of how in silico drug discovery using functional food bioactive compounds can help in the development of safe and effective therapeutic agents for prevention and management of human diseases from food based bioactives (4).

2. FUNCTIONAL FOOD BIOACTIVE COMPOUNDS AS POTENTIAL DRUG CANDIDATES

The remarkable chemical diversity, biological specificity, and potential to target multiple molecular targets associated with human diseases make functional food bioactive compounds an invaluable source of novel drug candidates. Among these, polyphenols and flavonoids like quercetin, kaempferol, catechins, resveratrol, curcumin, and epigallocatechin gallate (EGCG) have been well studied for several promising antioxidant, anti-inflammatory, anticancer, cardioprotective, antimicrobial, and neuroprotective activities. These compounds modulate important signaling pathways like NF-KB, MAPK, PI3K/Akt, and Nrf2, which play a role in disease prevention and therapeutic intervention (4,5). Another class of food-derived bioactive molecules of importance is the alkaloids and terpenoids, which have various pharmacological activities. Alkaloids like capsaicin and piperine have antimicrobial, analgesic, anticancer, and anti-inflammatory properties, and terpenoids such as limonene, lycopene, ginsenosides, and other essential oil constituents have been shown to have antioxidant, immunomodulatory, hepatoprotective, and chemopreventive properties, acting through various cellular targets (5,6). Also, milk, soybean, fish, cereal, legume, and other food-based peptides and proteins have been of great interest due to their antihypertensive, antioxidant, antimicrobial, immunomodulatory, antidiabetic, and cholesterol-lowering properties. These peptides can inhibit ACE (angiotensin-converting enzyme) and regulate inflammatory mediators, as well as maintain metabolic homeostasis, and therefore, have possible applications in developing drugs (6). Other classes of importance are carotenoids, phytosterols, and organosulfur compounds that have diverse biological mechanisms of action that are important for disease prevention. Carotenoids (such as β-carotene, lutein, astaxanthin, and lycopene) are highly antioxidant and photoprotective, and phytosterols have been shown to inhibit the absorption of cholesterol in the intestine and to help improve the health of the cardiovascular system. Oxidative stress, apoptosis, and epigenetic signaling are involved in the highly antimicrobial, anticancer, detoxifying, and anti-inflammatory properties of organosulfur compounds (OSCs) such as allicin, diallyl sulfide, and sulforaphane (6,7). The structure–activity relationships (SARs) of these molecules derived from food is a key determinant of their therapeutic properties, as the small changes in functional groups, stereochemistry, molecular size, polarity, glycosylation and hydrophobicity will significantly affect receptor binding, biological activity, pharmacokinetics and toxicity. Computational modeling, molecular

docking and QSAR analysis of these structural determinants can aid in the rational selection and optimization of functional food bioactive molecules as lead molecules for modern drug discovery (7).

3. COMPUTATIONAL APPROACHES IN FUNCTIONAL FOOD-BASED DRUG DISCOVERY

Computational techniques have been a prerequisite to systematically identify, evaluate and optimise bioactive compounds present in food sources against the molecular targets related to disease in drug discovery in the context of functional foods. Target identification and validation is the first step that involves the selection of proteins, enzymes, receptors, transcription factors or nucleic acids that are linked to disease pathogenesis, based on the biological evidence from genomics, proteomics, metabolomics and systems biology researches. The targets are validated, meaning that a modulation of their activity will lead to a desired therapeutic effect, without too many side effects (8,9). Once a suitable target is chosen, a ligand database is created to search for the chemical structures of bioactive molecules in functional foods that can be found in the publicly available chemical databases, like PubChem, ChEMBL, FooDB, DrugBank, and NPASS. These compounds are optimized structurally, energy minimized, stereochemically corrected, protonated and converted to formats for computational analysis (8,10). Virtual screening is then used to quickly screen thousands of compounds and select the ones that have the greatest potential to bind to a biological target.Structure-based virtual screening (SBVS) and ligand-based virtual screening (LBVS) based on chemical and biological properties of known active compounds are several screening strategies. These methods not only cut down on the amount of compounds to be tested in an experiment, but also increase the chances of finding a new molecule that can be used as a lead compound (9,10). Drug design strategies can be classified into two major categories: structure based drug design (SBDD) and ligand based drug design (LBDD). If the protein structure is not known, SBDD uses experimentally determined or computationally predicted structures to optimize the binding of the ligand to the protein active site, while LBDD leverages on pharmacophore modeling, QSAR analysis and similarity searching. Both techniques are complementary to each other in the fast tracking of lead optimization and specificity of the drug (9,11). The final step is typically a docking step that is performed via a molecular docking workflow, which involves the docking of the prepared ligands with the target protein in order to determine the binding orientation, the interaction patterns and the binding affinity. The docking analyses are followed by the visualisation of hydrogen bonding, hydrophobic, electrostatic contacts and the evaluation of the stability of protein–ligand complexes by molecular dynamics simulations. Together with the prediction of activity domain type, free energy calculations, these computational approaches provide a complete toolbox for identification of bioactive compounds found in foodstuffs of high therapeutic potential, thus significantly reducing the time, failure rate and cost of traditional drug discovery (11).

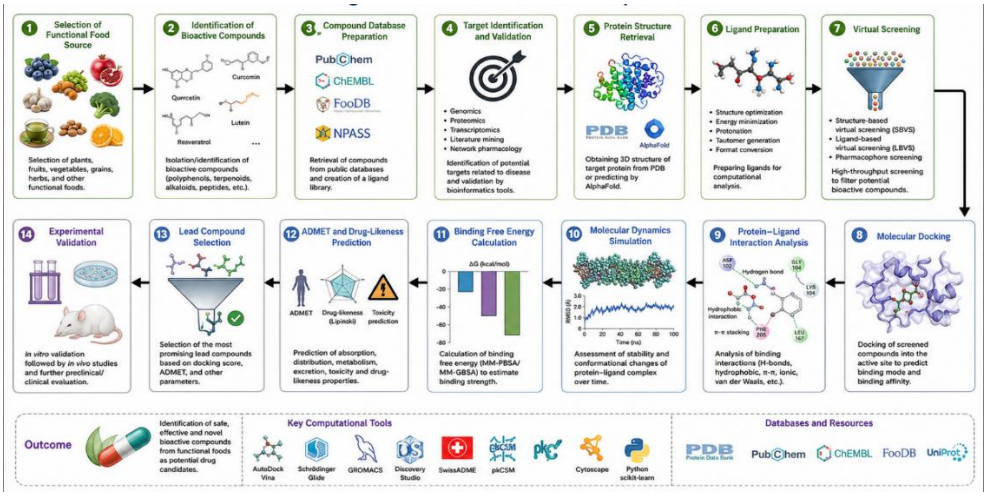

Figure 1. Comprehensive Workflow of *In Silico* Drug Discovery Using Functional Food Bioactive Compounds

4. MOLECULAR DOCKING, MOLECULAR DYNAMICS, AND BINDING INTERACTION ANALYSIS

The molecular docking, molecular dynamics (MD) simulation, and binding interaction analysis are basic computational tools that are a crucial part of functional food-based drug discovery, in which molecular interactions between bioactive compounds and biological targets are predicted. Molecular docking is a structure-based computational technique capable of predicting the preferred binding conformation and orientation of a molecule, or ligand, inside the active site of a target protein, as well as the

binding affinity. Protein and ligand preparation, the identification of the binding pocket, conformational sampling and scoring of the docked poses to find the best energetically docked complex. This is a useful method for screening large number of compounds obtained from the functional foods such as polyphenols, flavonoids, alkaloids, terpenoids and peptides that will help to identify promising lead compounds with high therapeutic potential in a short span of time (12, 13).Protein – ligand interaction analysis provides detailed information about the molecular mechanism of complex formation such as hydrogen bond, hydrophobic, van der Waals, π – π stacking, π – cation, electrostatic, salt bridge and water mediated contacts. Such interactions dictate the specificity, stability and biological activity of the interactions of a ligand and contribute to the identification of important amino acid residues that are involved in the target inhibition or activation. Visualization software such as Discovery Studio Visualizer, PyMOL, Chimera and LigPlot+ could be used to help understand these molecular interactions through interpretation. Interpretation with visualization software, such as Discovery Studio Visualiser, PyMOL, Chimera and LigPlot+ (12,14) are helpful for understanding these molecular interactions. The strength of the protein–ligand binding is quantified by binding affinity, which are empirical, knowledge based, force field-based algorithms, as well as machine learning harnessed algorithms. The lower scores obtained for the lower docking positions indicate better molecular interactions and thus better therapeutic potential, but the capacity of the docking score functions to take into account the molecular flexibility and the solvent effects is underestimated (13,15). To overcome the above-mentioned limitations the molecular dynamics (MD) simulation is used that involves simulation of structure stability and dynamics of a protein–ligand complex under physiological conditions. To measure conformational stability over time, the MD simulations yield the root mean square deviation (RMSD), root mean square fluctuation (RMSF), radius of gyration (Rg), solvent-accessible surface area (SASA), hydrogen bond occupancy, and principal component analysis (PCA) parameters (14,15). Finally, the conventional docking methods are not as accurate in estimating the binding free energy as free energy calculation methods such as Molecular Mechanics / Poisson–Boltzmann Surface Area (MM-PBSA), Molecular Mechanics / Generalized Born Surface Area (MM-GBSA), Free Energy Perturbation (FEP), and Thermodynamic Integration (TI). These techniques allow for the prioritization of highly stable lead compounds to be used for experimental validation, thus enhancing the efficiency, reliability and success of computational drug discovery with functional food bioactive compounds (12–15).

5. ADMET PREDICTION AND DRUG-LIKENESS EVALUATION

To successfully transform functional food-derived bioactives into therapeutic products, the biologic activity of the compounds is not the only criteria that must be met, but also the pharmacokinetic properties, safety, and drug-likeness of the compounds. Thus, Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) prediction has become an integral part of modern in silico drug discovery process to identify compounds with good pharmacological properties at an early stage in the development process and to eliminate those molecules that are likely to fail during the preclinical and clinical development of the drug. The partition coefficient (logP), molecular weight (≤500 Da), number of hydrogen bond donors (≤5) and number of hydrogen bond acceptors (≤10) are among the most accepted parameters used to assess the oral bioavailability of drug candidates according to the so-called Lipinski's Rule of Five. Topological polar surface area (TPSA), number of rotatable bonds, molecular flexibility, and water solubility are other parameters that can be used to predict oral absorption and drug-likeness (16,17). Computational pharmacokinetic prediction includes gastrointestinal absorption, intestinal permeability, penetration of the blood–brain barrier, plasma protein binding, metabolism by cytochrome P450 system, renal clearance and biological half-life.These forecasted results provide a method for determining bioactive compounds that are most likely to be accessible to the body and have the least pharmacokinetic restrictions, before expensive laboratory investigations (16,18). Through machine learning algorithms and predictive models validated with existing data, the comprehensive ADMET analysis evaluates the absorption, tissue distribution, metabolic stability, routes of excretion and potential toxicity of candidate molecules. New computational technologies like SwissADME, pkCSM, ADMETlab, ProTox-II, and admetSAR quickly predict hepatotoxicity, cardiotoxicity, mutagenicity, carcinogenicity, reproductive toxicity, and drug–drug interactions, enhancing the process of candidate selection (17,18). The toxicity prediction and safety assessment are especially critical for the functional food bioactive compounds as naturally occurring compounds can cause adverse biological effects at high concentrations or when exposure is prolonged. Prevents Attrition and helps identify compounds with acceptable therapeutic windows by conducting early toxicity screening. Lastly, lead optimization combines information on ADMET properties with molecular docking and/or molecular dynamics simulations and structure–activity relationship (SAR) analyses to modify the structure of the molecule for improved potency, selectivity, pharmacokinetic properties and safety, while reducing undesirable properties. This computational approach

is iterative and significantly faster in discovering drug candidates derived from functional foods that are clinically relevant, and more likely to be successfully validated in the lab and eventually put into therapeutic use (19).

Table 1. Major Computational Tools and Databases Used for Functional Food-Based Drug Discovery

Category	Representative Tools/Databases	Primary Application
Compound Databases	PubChem, ChEMBL, FooDB, NPASS	Retrieval of food-derived bioactive compounds
Protein Structure Databases	Protein Data Bank (PDB), AlphaFold Protein Structure Database	Three-dimensional protein structures for docking studies
Molecular Docking	AutoDock Vina, AutoDock4, Glide, GOLD	Prediction of protein–ligand binding poses and binding affinity
Virtual Screening	PyRx, DOCK, Glide HTVS	High-throughput screening of compound libraries
Molecular Dynamics Simulation	GROMACS, AMBER, NAMD, Desmond	Evaluation of protein–ligand stability and conformational dynamics
Pharmacophore Modeling	LigandScout, PharmaGist	Identification of pharmacophoric features and lead optimization
Drug-Likeness Prediction	SwissADME, MolSoft	Lipinski's Rule of Five, physicochemical properties, oral bioavailability
ADMET Prediction	pkCSM, ADMETlab 2.0, admetSAR, SwissADME	Prediction of absorption, distribution, metabolism, excretion, and toxicity
Toxicity Prediction	ProTox-II, VEGA QSAR, Toxtree	Prediction of hepatotoxicity, mutagenicity, carcinogenicity, and acute toxicity
Binding Free Energy	MM-PBSA, MM-GBSA, g_mmpbsa	Estimation of binding free energy and complex stability
Interaction Visualization	Discovery Studio Visualizer, PyMOL, UCSF Chimera, LigPlot+	Visualization of protein–ligand interactions
Network Pharmacology	Cytoscape, STRING, SwissTargetPrediction	Target identification and pathway analysis
QSAR Modeling	KNIME, PaDEL-Descriptor, QSAR Toolbox	Structure–activity relationship analysis and predictive modeling

6. ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN FUNCTIONAL FOOD DRUG DISCOVERY

AI and machine learning (ML) have revolutionized the functional food-based drug discovery process, enabling the processing of massive biological data, compound bioactivity predictions, and the identification of interesting therapeutic leads in a fast and efficient way. These computational technologies overcome many current limitations in the current drug discovery process, including cost reduction in experiments, speeding up the process of drug discovery and enhancing prediction accuracy. AI Virtual Screening is a powerful machine learning tool that is able to rapidly screen millions of natural food and nutraceuticals to discover the most promising candidates for binding to disease-associated targets. Not only can screening be improved with the use of AI but the use of molecular descriptors and protein structural data with physicochemical properties and docking scores can decrease the amount of false predictions of hits (20,21). Bioactivity Prediction using Machine Learning: Supervised learning and unsupervised learning algorithms include random forest, support vector machine, gradient boosting, k-nearest neighbors and artificial neural networks that form quantitative relationships between chemical structure and biological activity. These predictive models are able to predict the pharmacological activity, target specificity, toxicity and pharmacokinetic profile of compounds, as well as identifying bioactive compounds in functional foods, with high therapeutic potential and thus, without

the need for testing in the laboratory (20,22). In recent years, deep learning has revolutionized the field of lead optimization, with the use of multilayer neural networks, convolutional neural networks (CNNs), graph neural networks (GNNs), recurrent neural networks (RNNs), and transformer-based architectures for predicting molecular properties, optimizing chemical structures, generating novel compounds, and enhancing binding affinity.These techniques can then be adapted to learn about complex structural information contained in molecular graphs and biological data which can result in better drug-likeness prediction and rapid optimization of lead molecules (23). Further, network pharmacology and systems biology is now developed as powerful approach to comprehend the multi-target mechanisms of functional food bioactive components. Such approaches include the use of genomics, proteomics, metabolomics, transcriptomics, protein–protein interaction networks, signal transduction pathways and disease-associated genes, and can help uncover complex interactions in biology and multiple therapeutic targets in the disease process. Such systems analyses are particularly valuable when considering the therapeutic activity of many natural products which are multi-target compounds (22, 24). Despite their progress, a lot of AI models are still hard to comprehend and are not accepted in regulatory and clinical settings. Therefore, Explainable Artificial Intelligence (XAI) has emerged as a subfield with the goal of making the prediction understandable and identifying the molecular properties that influence the model's predictions. Explanatory AI helps to build trust in the computational drug discovery process, assists in biological interpretation, ensures regulatory compliance and rational design of safe and effective therapeutics from functional foods. Finally, the integration of AI, machine learning and deep learning, network pharmacology and explainable AI are expected to play a pivotal role in the evolution of precision nutrition, personalized medicine and next-generation functional food based drug discovery (24).

7. APPLICATIONS OF FUNCTIONAL FOOD BIOACTIVE COMPOUNDS IN DISEASE MANAGEMENT

Their effectiveness in regulating several molecular targets and biological pathways along with the extensive range of therapeutic benefits they have demonstrated in preventing and managing several chronic and infectious diseases makes the bioactive compounds of functional food appealing from therapeutic perspectives. Phytochemicals such as curcumin, resveratrol, epigallocatechin gallate (EGCG), quercetin and sulforaphane have been observed to show anti-tumour activity in cancer by modulating different signal transduction pathways including NF-κB, PI3K/Akt, MAPK and p53 pathways (24,25). Flavonoids, omega-3 fatty acids, phytosterols and polyphenols have been shown to have beneficial effects on endothelial function, oxidative stress, lowering cholesterol and regulating blood pressure in cardiovascular diseases, which results in a decreased risk of atherosclerosis and coronary artery disease (25,26). The functional food bioactives also have high significance in diabetes and metabolic disorders such as increased insulin sensitivity, decreased postprandial glucose, lipid metabolism regulation and inhibition of chronic inflammation via AMPK and PPAR signaling pathways (27). In addition, compounds like curcumin, luteolin, resveratrol and carotenoids have been shown to have neuroprotective activity in neurodegenerative diseases, which is mediated by their anti-neuroinflammatory, anti-oxidative and anti-protein aggregation activity against Alzheimer's and Parkinson's diseases. Other food-derived bioactive compounds including organosulfur compounds, flavonoids, bioactive peptides, have also strong antimicrobial and antiviral properties, and can be used to combat emerging infectious diseases; organosulfur compounds, flavonoids and bioactive peptides have potent properties to regulate cytokine production and immune responses in inflammatory and immune-mediated diseases. The combination of artificial intelligence and molecular docking, systems biology and multi-omics technologies has further advanced the identification of disease-specific targets and optimized functional food bioactive compounds to precision therapeutics, which paves the way for the development of safer, more effective and personalized treatment strategies (Figure 2) (28).

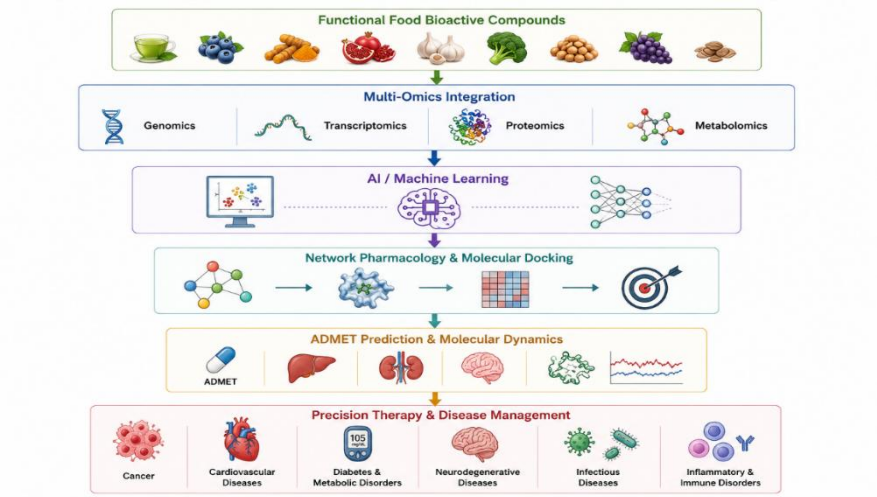

Figure 2. Workflow of Multi-Omics Integration and Machine Learning for Functional Food-Based Drug Discovery.

8. CHALLENGES, LIMITATIONS, AND FUTURE PERSPECTIVES

The computational drug discovery field has come a long way, but a number of challenges stand in the way of the transfer of the functional food bioactive compounds into clinically approved drugs. The variations in accuracy and reliability in predictions may be due to data quality, non-existence of databases, database incompleteness and algorithmic differences. Additionally, the amount of computational work needs to be validated with large-scale experimental and clinical data before being applied as therapy. While multi-omics, artificial intelligence and systems biology present more opportunities, they also pose challenges, including those of complexity, ethical considerations, regulatory compliance and model transparency. Predictive accuracy will continue to increase, lead optimization will be faster, and safe and effective functional food-based therapeutics that are personalized will be developed in the future due to advancements in precision nutrition, explainable AI, and high-performance computing.

9. CONCLUSION

In silico drug discovery is a potential tool to find and optimize bioactive compounds of functional foods that show therapeutic effects. Today, computational approaches like molecular docking, virtual screening, molecular dynamics simulation, ADMET prediction and artificial intelligence have greatly improved the efficiency, accuracy, and cost-effectiveness of drug discovery. These strategies enable the rapid identification of candidate compounds that can be used as prevention and treatment for cancer, cardiovascular diseases, diabetes, neurodegenerative diseases, infectious diseases or inflammation. The continued integration of computational biology, multi-omics technologies and precision nutrition will improve translational research and contribute to the development of new evidence-based and personalized functional food-based therapeutic strategies.

DISCLOSURE

The authors declare that there are no financial, commercial, or personal relationships that could have influenced the preparation or publication of this chapter. The content presented is based on an objective review and synthesis of the available scientific literature and is intended solely for academic and educational purposes. The authors have no conflicts of interest to disclose and received no specific funding from any public, commercial, or not-for-profit organization for the preparation of this work

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