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# AI-Assisted Discovery of Food-Derived Bioactive Compounds for Personalized Nutrition

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**ABSTRACT:** The antioxidant, anti-inflammatory, antimicrobial, and immunomodulatory properties of food-derived bioactive compounds have given rise to their role as important contributors to disease prevention and health promotion. However, traditional techniques for identification and validation of these compounds can be time-consuming and labour-intensive. Under the hood, the field has seen a massive transformation by artificial intelligence (AI), through the use of machine learning, deep learning, and predictive analysis, which have enabled fast screening, bioactivity prediction, molecular interaction analysis, and even personalised dietary recommendations. Advances in the integration of nutrigenomics, gut microbiome profiling, metabolomics, and other multi-omics technologies have further progressed precision nutrition by providing the ability to design dietary interventions based on an individual's genetic, metabolic, and physiological makeup. The application of AI computational methods can shorten the process of functional food ingredients identification and improve their safety, efficacy, and clinical relevance. Despite the challenges of data integration, explainable AI, and regulatory standards, the potential for personalized nutrition and preventive healthcare through AI technology is promising. Overall, the use of AI in the discovery of bioactive compounds from food is a paradigm shift in the field of developing evidence-based

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nutrition interventions to help reduce the prevalence of chronic diseases and improve overall human health.

## 1. INTRODUCTION

Bioactive compounds derived from food are naturally occurring substances found in fruits, vegetables, cereals, legumes, dairy products, marine foods, and fermented foods that have physiological effects in addition to their nutritional value. These compounds include polyphenols, flavonoids, carotenoids, bioactive peptides, dietary fibers, probiotics, omega-3 fatty acids, vitamins and phytosterols, and they have been the subjects of much research for their potential in regulating metabolic pathways, immune system responses, mitigating oxidative stress, and preventing chronic conditions like obesity, diabetes, cardiovascular disease, neurological disorders, and cancer (1). Traditional methods of compound identification and validation of bioactive compounds are time-consuming, costly, and labor-intensive, with a large number of experiments and clinical trials needed to identify and validate the compounds. This discovery process has been revolutionized by the emergence of novel technologies and tools within the field of artificial intelligence (AI), such as machine learning, deep learning, and predictive analytics, which allow for faster and more efficient analysis of large-scale food composition data, biological databases, and multiomics data to identify novel bioactive compounds with greater speed and accuracy (2). AI algorithms enable faster and more cost-effective identification of functional ingredients and prediction of biological activity, molecular interaction, bioavailability, toxicity, and therapeutic potential (3). In addition, the combination of genomics, transcriptomics, proteomics, metabolomics, and gut microbiome profiling with AI has also paved the way for personalized nutrition, where nutrition recommendations are customized based on the individual's genetic make-up, metabolic profile, gut microbiome, lifestyle, and health status (4). Precision nutrition techniques deliver a more personalized approach to nutrition, which helps optimize nutrition interventions, improve disease prevention strategies, and boost individual health outcomes (5). These recent advancements in wearable biosensors, digital health technologies, cloud computing, and explainable AI have further reinforced the application of AI in personalized nutrition, allowing for the continuous tracking of physiological responses and the generation of real-time personalized nutrition recommendations. In sum, the paradigm shift toward precision nutrition by using AI tools to identify bioactive food compounds is opening the door to future advances in evidence-based personalized nutrition, the development of next-generation functional foods with novel bioactive properties that can be harnessed for personalized healthcare, and the creation of food-based platforms for innovative, sustainable disease prevention.

## 2. FOOD-DERIVED BIOACTIVE COMPOUNDS

The bioactive compounds that are extracted from food of natural origin from plants and animals, which have physiological and therapeutic effects, besides their nutritional values, have significant importance, are called food-derived bioactive compounds. These compounds can be divided into several broad groups: polyphenols, flavonoids, carotenoids, alkaloids, organosulfur compounds, bioactive peptides, dietary fibers, probiotics and prebiotics, omega-3 fatty acids, phytosterols, vitamins and minerals, each of which exhibits different biological activities and mechanisms of action (7). Their food consists of fruits, vegetables, whole grains, legumes, nuts and seeds, herbs and spices, edible mushrooms, dairy foods, fish, marine algae, fermented foods, and medicinal plants. Recent research conducted on food chemistry and nutrigenomics identified bioactive compounds that exert different effects on oxidative stress, inflammation, immune responses, cellular signaling pathways, lipid and glucose metabolism, and gut microbiota composition that are associated with disease prevention and health promotion (8). The anti-inflammatory and anti-oxidant properties are high with polyphenols and flavonoids, anti-oxidants with carotenoids, and cardiovascular health benefits with flavonoids. Bioactive peptides have antihypertensive, antimicrobial, antioxidant, and immunomodulatory properties, and probiotics and prebiotics can be used to keep the balance between the microorganisms in the gut and promote the health of the intestines and the immune system (9). Similarly, omega-3 fatty acids are anti-inflammatory and have been shown to have a beneficial effect on the cardiovascular and neurological systems, and phytosterols have been demonstrated to reduce serum cholesterol levels. The regular consumption of these types of bioactive food has been linked to decreased risk of obesity, type 2 diabetes mellitus, cardiovascular diseases, neurodegenerative diseases, some cancers, and age-related metabolic abnormalities (10). Further, the discovery, characterization, and functional evaluation of bioactive molecules derived from food, enabled by the developments of artificial intelligence and multi-omics technologies, have identified new bioactive molecules with health-promoting properties and developed precision nutrition strategies using one's own genetic, metabolic, and microbiome profile. Therefore, food-derived bioactive compounds have become the central focus of the development of functional foods and nutraceuticals and have been scientifically proven to be used in personalised dietary interventions to seek longterm health benefits and prevent the occurrence of chronic diseases (12).

**Table 1.** Classification and Biological Activities of Major Food-Derived Bioactive Compounds

| Class of Bioactive Compound | Major Sources | Representative Compounds | Major Biological Activities |
|---|---|---|---|
| Polyphenols | Fruits, tea, cocoa, berries | Resveratrol, Catechins | Antioxidant, anti-inflammatory, cardioprotective |
| Flavonoids | Citrus fruits, onions, herbs | Quercetin, Kaempferol | Antioxidant, anticancer, neuroprotective |
| Carotenoids | Carrots, tomatoes, spinach | β-Carotene, Lycopene, Lutein | Antioxidant, eye health, immune support |
| Bioactive Peptides | Milk, soy, fish, eggs | Casein peptides, Lactoferrin | Antihypertensive, antimicrobial, antioxidant |
| Dietary Fibers | Whole grains, legumes, fruits | β-Glucan, Inulin | Gut health, cholesterol reduction, glycemic control |
| Probiotics & Prebiotics | Yogurt, kefir, fermented foods | *Lactobacillus*, *Bifidobacterium* | Gut microbiota modulation, immune enhancement |
| Omega-3 Fatty Acids | Fish, flaxseed, chia | EPA, DHA, ALA | Anti-inflammatory, cardiovascular, and brain health |
| Phytosterols | Vegetable oils, nuts, seeds | β-Sitosterol, Campesterol | Cholesterol lowering, cardioprotective |
| Organosulfur Compounds | Garlic, onion, cruciferous vegetables | Allicin, Sulforaphane | Antimicrobial, anticancer, antioxidant |
| Vitamins & Minerals | Fruits, vegetables, dairy, seafood | Vitamin C, Vitamin D, Zinc | Immune support, metabolic regulation, antioxidant defense |

## 3. ARTIFICIAL INTELLIGENCE IN BIOACTIVE COMPOUND DISCOVERY

The use of artificial intelligence (AI) has transformed the discovery of food-derived bioactive compounds, allowing for quicker, more precise, and data-driven identification of compounds that could have health-promoting properties. While the traditional experimental screening methods are time-consuming, cumbersome, and expensive, AI uses computational power and large-scale food composition databases, libraries of chemicals, biological data, and multi-omics information to speed up the discovery pipeline (13). Machine learning (ML) algorithms process complex datasets to discover patterns and relationships between molecular structures and biological activities, to predict functional properties, classify bioactive compounds and prioritise interesting compounds for experimental testing (14). The use of deep learning (DL), a branch of machine learning using artificial neural networks, boosts predictive power by automatically recognizing complex features from large datasets, like metabolomics, genomics, proteomics, food images, and chemical structures. Advanced deep learning architectures such as convolutional neural networks (CNNs), recurrent neural networks (RNNs), graph neural networks (GNNs) and transformer-based models have shown excellent performance in the prediction of molecular properties, protein–ligand interaction analysis, virtual screening, and bioactivity prediction (15). The predictive analytics involves a combination of statistical modeling, AI algorithms, and big data analytics to predict the therapeutic potential, bioavailability, toxicity, stability, and metabolic pathway of food-derived compounds prior to laboratory testing, which can help decrease development costs and enhance research efficiency (16). AI-based predictive models also aid in molecular docking, quantitative structure–activity relationship (QSAR) analysis, ADMET prediction, and biomarker discovery, guiding the choice of compounds with optimal efficacy and safety. (17) Moreover, 24/7 enhancements of predictive models through the combination of AI and cloud computing, explainable AI (XAI), and multi-omics technologies boost the interpretability of computational decisions, thereby increasing the trust in AI-supported nutritional research. Thus, AI has emerged as an essential enabler for discovering, characterizing, and optimizing bioactive compounds from food, aiding in the creation of next-generation precise nutrition approaches and strategies, precision nutrition, and functional foods and nutraceuticals designed to optimize individual health (18).

## 4. AI-ASSISTED SCREENING AND BIOACTIVITY PREDICTION

Artificial Intelligence (AI) has improved the efficiency of screening bioactive compounds found in foodstuffs by combining computational tools that can identify, evaluate and prioritize molecules for therapeutic potential in a swift and efficient way. Valuable information can be retrieved from large-scale food composition databases, metabolomic repositories, scientific literature, chemical libraries and biological datasets by using data mining techniques to find novel relationships between food compounds and human health outcomes (19). These multi-dimensional data is then used for machine learning algorithms to detect patterns and trends not previously known, predict biological activities and even suggest possible bioactive substances for testing. To complement this work, virtual screening can be used, by which thousands of natural compounds are screened against disease associated molecular targets computationally, which greatly reduce the time and cost of the laboratory screening (20). The virtual screening approach with the help of artificial intelligence (AI) resources involves the use of quantitative structure–activity relationship (QSAR) models, deep learning algorithms, and predictive analytics to prioritize compounds for further investigation via virtual screening by ranking them according to their potential for therapeutic activity. The computational discovery is further confirmed by molecular docking that simulates the interaction of the atoms of the bioactive compounds derived from food and the atoms of the target proteins and indicates the orientation of the molecule, the binding energy, the molecular stability and the mechanism of action (21).Recent developments in the use of the molecular docking approach combined with AI have enhanced the accuracy of prediction, automated ligand selection, optimized docking parameters, and identification of leads to be used in functional food studies. In addition, AI computational workflows are more and more combining with ADMET prediction, molecular dynamics simulation, network pharmacology and multi-omics analysis for the validation of candidate compounds and prediction of their pharmacokinetic properties prior to experimental testing (22). These computational methods are combined and allow for meaningful reduction in the number of experiments required, and increase the chance of identification of highly effective bioactive molecules for precision nutrition and in the development of functional foods. For this reason, the screening and prediction of the bioactivity of compounds derived from food with the help of artificial intelligence has become an indispensable part of the modern nutritional science, enabling the identification of food bioactive compounds that can be useful in the prevention of diseases and precision healthcare, which is safe, efficient and individualized to the person (23).

**Table 2.** AI Tools and Computational Approaches for Bioactive Compound Discovery

| AI Tool/Approach | Primary Function | Applications in Bioactive Compound Discovery |
|---|---|---|
| Machine Learning (ML) | Pattern recognition and prediction | Bioactivity prediction, compound classification |
| Deep Learning (DL) | Feature extraction from complex datasets | Molecular property prediction, target identification |
| Data Mining | Extraction of biological knowledge | Discovery of bioactive compounds from food databases |
| Virtual Screening | High-throughput computational screening | Identification of potential lead compounds |
| Molecular Docking | Protein–ligand interaction analysis | Binding affinity and mechanism prediction |
| QSAR Modeling | Structure–activity relationship prediction | Biological activity estimation |

| | | |
|---|---|---|
| ADMET Prediction | Pharmacokinetic and toxicity assessment | Safety and efficacy evaluation |
| Molecular Dynamics Simulation | Stability and interaction analysis | Validation of docking results |
| Network Pharmacology | Multi-target interaction analysis | Mechanistic pathway identification |
| Explainable AI (XAI) | Model interpretation | Transparent and reliable AI-assisted decision-making |

## 5. AI-DRIVEN PERSONALIZED NUTRITION

AI has revolutionized personalised nutrition, bringing together genomic, metabolic, microbiome and lifestyle data to create personalised food recommendations that can help maximise health and prevent chronic conditions. Precision dietary interventions use inter-individual variability in genetics, metabolism, physiological responses and environment to develop a precision nutrition (24), which differs from nutritional recommendations that are based on the average population. Nutrigenomics is a nascent branch of science that studies the interaction between nutrients and genes with the goal of elucidating the role of dietary components in influencing gene expression, metabolic pathways and disease susceptibility. The use of AI algorithms to crunch large-scale genomic and transcriptomic information to uncover genetic polymorphisms linked to nutrient metabolism allows for the development of personalized diet recommendations, which can enhance metabolic health and lower the risk of disease (25). The gut microbiome has also become an important factor that determines individual nutrition as the gut's microflora plays a significant role in the regulation of immune responses, energy metabolism, nutrient absorption, and inflammation.Machine learning and deep learning models combine microbiome sequencing information with dietary intake and clinical data to determine how a patient will react to certain foods and to suggest targeted nutritional strategies based on the microbiome (26). Precision nutrition also integrates nutrigenomics, metabolomics, proteomics, microbiome analysis, wearable sensors and EHRs with AI-driven predictive models to provide real-time, evidence-based dietary advice based on an individual's physiological state and health goals (27). These computational methods enhance the adoption of a healthy lifestyle, maximize metabolic efficiency, lower the likelihood of obesity, diabetes, cardiovascular diseases, and other chronic conditions, as well as to enable proactive healthcare by real-time tracking and personalized nutritional recommendations. Furthermore, explainable artificial intelligence, cloud computing, and digital health technologies improve the transparency, scalability, and clinical adoption of personalized nutrition systems to integrate them into routine clinical practice. Overall, AI-driven personalized nutrition is a paradigm shift that is poised to revolutionize the way nutrition is prescribed in the future, bringing together food science, computational biology, and precision medicine to offer personalized nutritional interventions that have the greatest therapeutic potential and maximize long-term health benefits.

**Table 3.** AI Applications in Personalized Nutrition and Clinical Outcomes

| AI Application | Data Utilized | Clinical/Nutritional Outcome |
|---|---|---|
| Nutrigenomic Analysis | Genomic and transcriptomic data | Personalized nutrient recommendations and disease risk reduction |
| Gut Microbiome Profiling | Microbiome sequencing data | Improved gut health, digestion, and immune regulation |
| Precision Nutrition Modeling | Multi-omics, lifestyle, and clinical data | Individualized dietary interventions |
| Machine Learning Prediction | Food intake and metabolic biomarkers | Prediction of glycemic and metabolic responses |
| Deep Learning-Based Dietary Assessment | Food images and dietary records | Accurate nutrient intake estimation |

| | | |
|---|---|---|
| Wearable Sensor Analytics | Continuous glucose, activity, and physiological data | Real-time nutrition monitoring and adaptive dietary guidance |
| Clinical Decision Support Systems | Electronic health records and laboratory data | Personalized nutrition planning and disease management |
| AI Risk Prediction Models | Genomic, metabolic, and lifestyle information | Early identification of nutrition-related disease risk |
| Explainable AI (XAI) | Integrated health datasets | Transparent and clinically interpretable nutritional recommendations |
| Digital Health Platforms | Mobile applications and cloud-based health data | Long-term dietary adherence and personalized health management |

## 6. APPLICATIONS IN DISEASE PREVENTION *(200 WORDS)*

The field of AI-driven discovery of bioactive compounds from food has emerged as a significant area of interest in the prevention of chronic diseases using personalised nutrition interventions. AI can be used in metabolic disorders like obesity, type 2 diabetes, and metabolic syndrome to identify bioactive molecules that modulate glucose metabolism, insulin sensitivity, lipid homeostasis, and energy balance, which can help guide individualized dietary recommendations for improved metabolic health. In cardiovascular diseases, bioactive compounds such as polyphenols, Omega-3 fatty acids, phytosterols and bioactive peptides have been found to help decrease oxidative stress, inflammation, hypertension and dyslipidaemia, which all help to reduce cardiovascular disease risk. Predictive models using AI techniques help to identify the most suitable dietary components for a person, given their genetic and metabolic makeup. Computational methods are used in cancer prevention to identify phytochemicals with antioxidant, anti-inflammatory, antiproliferative, and apoptosis-inducing effects that could help in preventing the initiation and progression of tumors and complement other cancer prevention measures. Moreover, personalized nutrition, with the aid of AI, can improve healthy ageing by identifying those dietary bioactive compounds that can protect against cell damage due to oxidative stress, boost immune response and improve cognitive function and maintain musculoskeletal health. Adaptive nutritional interventions throughout life are further supported by continuous monitoring provided by wearable technology and digital health platforms. As a whole, AI-driven precision nutrition offers a scientific approach to tackling complex chronic diseases, enhancing quality of life, and ensuring long-term healthy aging by addressing them on an individual level.

## 7. CHALLENGES AND FUTURE PERSPECTIVES

While significant strides have been made in realizing AI-driven personalized nutrition, there are still hurdles to overcome. It is crucial that different data types, ranging from genome data, metabolomics data, microbiome data, clinical data, wearable data, to dietary data, are provided in a standardised format and with high-quality data to make accurate predictions. Model development is complicated by variability of food composition databases, and because of differences in biological responses per individual. The other key challenge is explainable artificial intelligence because it has the potential to make the field more understandable and trustworthy, for both the researchers, clinicians and consumers, regarding how AI can make nutrition suggestions.The other big challenge is to provide “explainable AI,” which will provide researchers, clinicians and consumers with a better understanding of how AI is making nutrition advice, and increase trust in computational decision making. The regulatory landscape needs to also adapt to issues of data privacy, cybersecurity, algorithm validation, ethical considerations and clinical safety, and facilitate innovation. Going forward, developing more multi-omics platforms for use on various platforms, simplifying the models, validating AI predictions using clinical studies, and enhancing real-time digital health applications will be prioritized. The advances will improve precision nutrition and pave the way for its integration in the mainstream of health care and preventive medicine.

## 8. CONCLUSION

AI has revolutionized food-based bioactive compound discovery and utilization, making the process quicker, more accurate, and personalized for nutrition. The combination of machine learning, deep learning, predictive analytics, nutrigenomics, and gut microbiome research has created a solid foundation for precision nutrition research geared towards the prevention of chronic diseases and overall wellness. While data integration, explainability and regulatory governance are still challenges to address, ongoing progress in computational technologies and multi-omics research should help to overcome these limitations. AI-driven personalized nutrition holds great potential for creating evidence-based nutrition strategies for life-long health and disease prevention.

## DECLARATIONS

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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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