The role of AI in shaping future functional foods: Targeted delivery, biosynthesis, and personalized nutrition

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The functional food industry is shifting from general fortification to precision nutrition. However, conventional methodologies face bottlenecks in bioactive discovery, manufacturing, and delivery. This perspective articulates how artificial intelligence (AI) serves as the central orchestrator to resolve these challenges. We present a roadmap where AI converges with biotechnology: First, AI-driven algorithms and synthetic biology enable the efficient discovery and microbial biosynthesis of high-purity bioactives, replacing traditional agriculture. Second, AI models decode individual metabolic responses, facilitating evidence-based personalized dietary interventions. Third, delivery systems are evolving into autonomous, stimuli-responsive nanosystems capable of closed-loop navigation and real-time feedback. By integrating these pillars, AI transforms functional foods from static supplements into dynamic, closed-loop therapeutic systems. This paradigm shift promises a new era of predictive, personalized, and precisely engineered intelligent nutrition.

Driven by global aging and chronic disease, functional foods are pivotal in preventive healthcare. However, realizing personalized nutrition requires overcoming challenges in bioactive identification, delivery, and manufacturing. This Perspective outlines how Artificial Intelligence (AI) serves as the central orchestrator, converging with multi-omics, nanotechnology, and synthetic biology to redefine the functional food lifecycle (Figure 1). We explore how AI-powered discovery and precision nutrition strategies are unearthing novel bioactives and enabling targeted delivery. The convergence of these innovations promises to redefine the boundaries of nutritional science, transforming functional foods into predictive, personalized, and precisely engineered therapeutic tools.

THE EVOLVING LANDSCAPE OF FUNCTIONAL FOODS: FROM BIOACTIVES TO AI-DRIVEN INNOVATION

Market growth and the shift to targeted health outcomes.

Functional foods, offering health benefits beyond basic nutrition, are increasingly vital in addressing global health challenges, including rising subhealth prevalence and population aging. The global market is projected to grow from $ 260.1 billion to $ 442.1 billion by 2036 at a CAGR of 5.5%, with China at 7.4%. These foods have evolved from single-nutrient fortification (e.g., vitamin D–calcium milk, fiber-enriched bread) toward complex formulations targeting specific health outcomes—such as disease prevention, fitness enhancement, and weight management—driven by their bioactive components. Future development will emphasize precision nutrition and personalization to meet diverse population needs.[1]

High-purity bioactives: defining the future market standard.

Innovation in functional ingredients is central to advancing future functional foods. A distinct market shift is occurring toward high-purity bioactives, particularly plant-derived compounds with well-defined structures and identified molecular targets, which facilitate precise nutritional control. Key examples include polymethoxyflavones (e.g., tangeretin) for metabolic modulation, prenylated phenolics like 8-prenylnaringenin for bone and nerve health, tetracyclic triterpenes (e.g., ginsenosides), and alkaloids targeting sleep and glycemic control. Despite their immense commercial potential and favorable safety profiles, the translation of these compounds into efficacious ingredients necessitates rigorous preclinical and clinical evaluation. A key hurdle in this process remains the suboptimal bioavailability observed in certain compounds, such as curcumin.

AI and big data: accelerating discovery and screening.

Rapid identification of key bioactive compounds remains a significant challenge. Advancements in AI technologies are accelerating discoveries. Procyanidin C1 from grape seed extract, functioning as a senolytic agent to increase healthspan and lifespan, was identified via screening ~1000 natural products using an integrated approach combining natural pharmacy screening, biochemistry, cell biology, and bioinformatics.[2] An AI-powered platform, AgeXtend, was developed to screen ~1.1 billion compounds and identified numerous potential geroprotectors. Additionally, the recently established Gene-encoded Natural Diverse Components Repository offers a big-data-driven framework to expedite functional ingredient discovery.

FROM DISCOVERY TO MANUFACTURING: REVOLUTION IN NEXT-GENERATION FUNCTIONAL FOOD PRODUCTION

As scientific understanding of nutrient bioactivity advances, nutritional supplementation is poised to evolve toward greater personalization, universalization, and intelligence. However, limited natural availability hinders scalable production.[3] Synthetic biology facilitates the sustainable microbial biosynthesis of complex plant natural products, effectively circumventing natural scarcity. However, the reconstruction of high-yielding cell factories remains constrained by critical bottlenecks, including incomplete pathway elucidation and insufficient catalytic efficiency of key enzymes.

AI and multi-omics: decoding pathways and redesigning enzymes.

Integrated omics approaches-particularly genomics, transcriptomics, and metabolomics-combined with AI-driven data analysis, are increasingly employed to deorphanize biosynthetic genes and reconstruct complete metabolic pathways. For instance, the complete biosynthetic pathway of paclitaxel was recently elucidated by integrating genomic mining with multi-omics analysis and heterologous screening. This breakthrough highlights the power of multidisciplinary strategies in decoding complex metabolic pathways.[4]

Beyond prediction, computational protein design is enabling *de novo* enzyme engineering with desired catalytic properties. Generative models like RFDiffusion allow tailored design of protein backbones with high catalytic efficiency.[5] This capability will pave the way for the *de novo* construction of optimized biosynthetic pathways, enabling the sustainable and scalable production of targeted plant natural products in engineered microbial systems.

Automated biofoundries: accelerating strain optimization and scientific innovation.

Upon the reconstruction of the synthetic pathways, functional validation and optimization within living systems present the next challenge. This

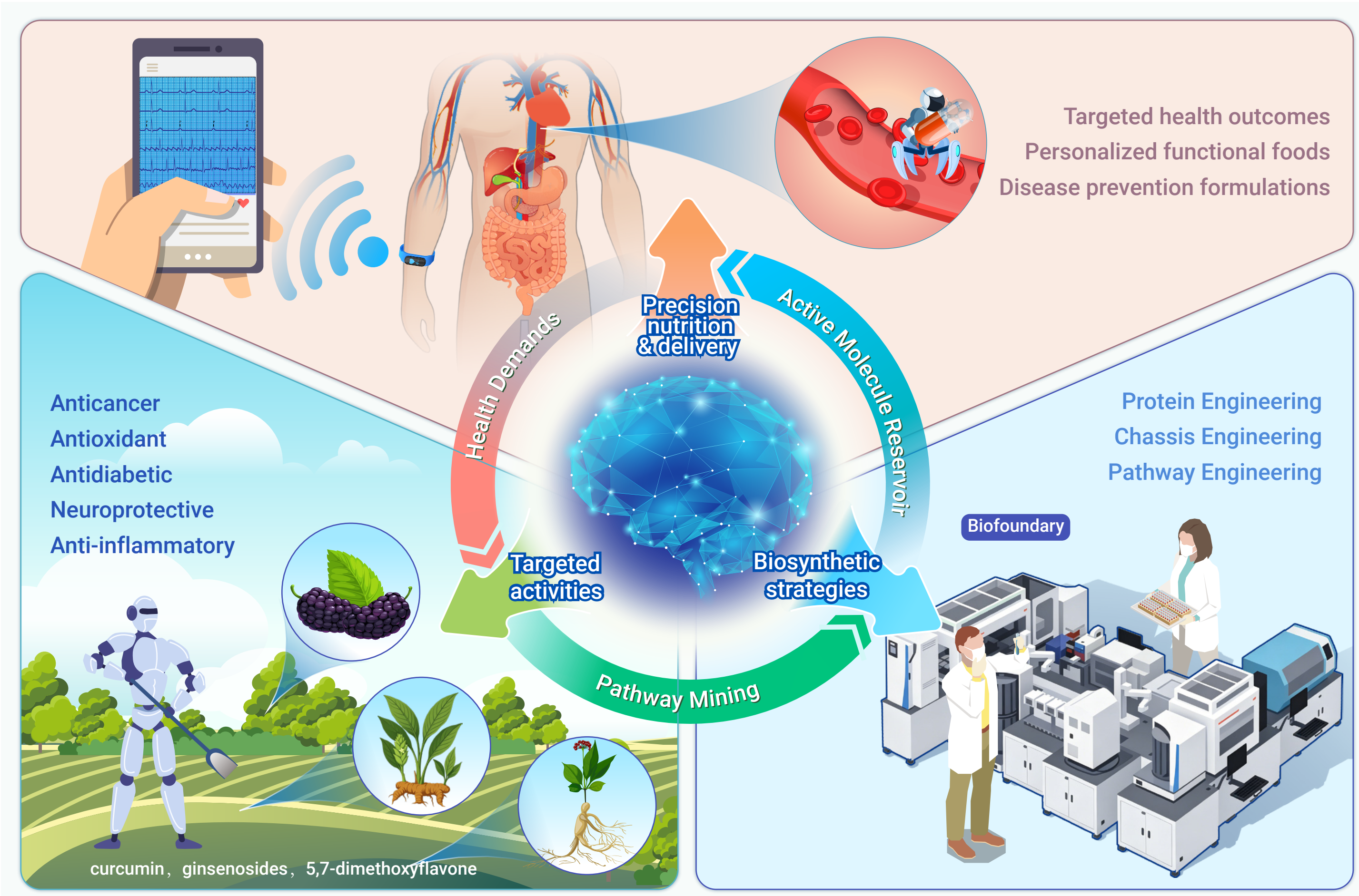

Figure 1. The AI-driven ecosystem of future functional foods This roadmap illustrates the paradigm shift toward intelligent nutrition. Artificial intelligence serves as the central orchestrator, integrating multi-omics and deep learning to discover high-purity bioactives. It converges with synthetic biology and automated biofoundries for sustainable microbial biosynthesis. Furthermore, AI enables smart, stimuli-responsive delivery systems that facilitate closed-loop navigation and real-time physiological feedback, thereby realizing precision and personalized health interventions.

process is inherently complex due to the interconnected nature of cellular metabolism, where imbalances in precursor supply, cofactor availability, toxic byproduct accumulation, or metabolic burden can severely compromise pathway efficiency and host viability. The synergy between AI-driven computational modeling of metabolic networks and automated biofoundries is revolutionizing strain engineering.

By integrating systems-level data to fine-tune gene expression and rebalance fluxes, AI algorithms guide robotic platforms in executing high-throughput DBTL cycles, thereby accelerating the optimization of biosynthetic pathways and host chassis for natural product synthesis. The potential of ML-driven automation is further demonstrated by the high-level production of naringenin. By leveraging a bottlenecking-and-debottlenecking strategy with ProEnsemble-mediated promoter optimization, researchers balanced pathway flux in *E. coli* through a rapid six-week evolution. As a result, the traditional role of scientists is undergoing a profound transformation. In the near future, staying at the forefront of synthetic biology will require more than expertise in molecular biology and wet-lab techniques. The most impactful researchers will be those who can seamlessly integrate knowledge across disciplines-mastering not only biology, but also robotics, data science, and AI/ML-to lead the next generation of bioengineering innovation.

THE CONVERGENCE OF AI AND PRECISION NUTRITION: CURRENT APPLICATIONS AND FUTURE TRAJECTORIES

The integration of AI into precision nutrition is rapidly evolving from theoretical promise to clinical utility, marking a transformative shift in the management of chronic diseases. While traditional dietary recommendations often adopt a "one-size-fits-all" approach, current advancements leverage machine learning (ML) algorithms to analyze high-dimensional datasets, including genomics, metabolomics, and continuous glucose monitoring.[6] Recent landmark trials, such as those utilizing random forest models to predict individualized postprandial glycemic responses based on microbiome composition, have demonstrated superior clinical outcomes compared to standard guidelines. Specific AI methodologies are now being tailored for nutritional research: for instance, deep learning architectures like convolutional neural networks (CNNs) are being applied to analyze complex food images for intake assessment, while natural language processing (NLP) extracts dietary patterns from unstructured electronic health records. Looking ahead, the field is moving toward reinforcement learning, where algorithms will function as intuitive coaches, continuously learning from a patient's daily habits and environmental cues to adjust dietary advice in real-time. To ensure robust translation into public health practice, future research must prioritize the development of explainable AI frameworks and validate these models within large-scale, diverse longitudinal cohorts to mitigate ethnic biases and enhance global applicability.[7]

TARGETED DELIVERY: AI-DRIVEN INNOVATION FOR FUTURE FUNCTIONAL FOODS

Functional foods offer great potential for chronic disease prevention and health promotion. However, their efficacy is limited by poor stability and low bioavailability of bioactive components. Conventional delivery systems suffer from nonspecific distribution, rapid GI clearance, and inefficient targeting. To address these challenges, targeted delivery systems are evolving toward intelligent, multifunctional platforms, with AI as a transformative driver.

Passive targeting: harnessing nanocarrier intrinsic properties.

Passive targeting exploits nanocarrier properties such as enhanced permeability and retention (EPR) effects and size-dependent tissue penetration. Food-compatible systems-including nanoparticles, liposomes, metal-organic frameworks (MOFs), exosomes, and nanogels-enable site-specific accumulation. For example, ZIF-8 nanoparticles enhance asiaticoside solubility and promote wound healing when integrated into hydrogels.[8] Pullulan-gliadin nanoparticles improved the delivery of astragaloside IV by overcoming poor solubility and rapid clearance.[9] AI optimizes such systems via machine learning, predicting optimal formulations by analyzing particle size and biocompatibility, thus reducing trial-and-error efforts. However, limited data on carrier-bioactive interactions hinder high-throughput AI screening, and *in vivo* safety models remain underdeveloped.

Active targeting: toward precision delivery via molecular recognition.

Active targeting uses ligand-receptor pairs (e.g., antibodies, peptides) or cell-mediated transport for precise delivery. AI accelerates ligand discovery through virtual screening, enabling personalized, peptide-based carriers for treatment like inflammatory bowel disease. A major challenge remains the lack of *in vivo* validation for AI-predicted ligands.

Stimuli-responsive systems: intelligent release through environmental cues.

Stimuli-responsive systems respond to endogenous (pH, enzymes, microbiota) or exogenous (light, ultrasound, magnetic fields) triggers, enabling site-specific release and minimizing off-target effects. Glutathione-responsive nanoplatforms co-assembled from artesunate prodrugs and icariin improved icariin solubility and exert potent antitumor effects via energy metabolism inhibition and tumor microenvironment remodeling in hepatocellular carcinoma.[10] AI models simulate physiological cues to optimize release kinetics, such as in glucose-responsive systems for diabetes. However, AI's ability to coordinate multi-stimuli responses needs improvement, and exogenous triggers face GI penetration barriers.

Intelligent nanorobots: the frontier of autonomous delivery.

Intelligent nanorobots represent the cutting-edge and future direction of targeted delivery for functional foods. These multifunctional systems, based on magnetic, DNA origami, or biomimetic designs, enable active navigation, prolonged target retention, and real-time response to physiological signals. By integrating data from wearable or *in vivo* sensors (e.g., glucose monitors), AI empowers these systems with decision-making capabilities for dynamic navigation and on-demand release.

Despite their immense potential, nanorobots face challenges including material safety, biocompatibility, and biodegradability. Oral administration may trigger immune responses, local inflammation, or tissue adhesion, with unclear long-term biosafety regarding organ accumulation and gut microbiota effects. More critically, AI-driven dynamic food systems lack specific regulatory approval pathways and unified safety assessment standards, representing a critical regulatory bottleneck for translation.

In summary, AI is driving a paradigm shift from passive to intelligent delivery in functional foods. Integrating multimodal targeting, sustainable biopolymers, and AI promises to overcome current bottlenecks, paving the way for precision nutrition.

CONCLUSION: TOWARD AN INTEGRATED ECOSYSTEM OF INTELLIGENT NUTRITION

In summary, we have outlined a transformative roadmap where AI serves as the linchpin in the functional food ecosystem. By integrating multi-omics, AI accelerates the discovery of high-purity bioactives and enables sustainable microbial biosynthesis through synthetic biology. Crucially, this perspective highlights AI's expanding role in precision nutrition, where algorithms decode complex dietary responses to tailor interventions. Furthermore, AI-driven smart delivery systems facilitate closed-loop interactions with the human body. While data standardization and regulatory frameworks remain challenges, embracing this holistic, AI-orchestrated approach is essential. It promises a future where functional foods evolve from static supplements into dynamic, personalized therapeutic systems, harmonizing human health with planetary sustainability.

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AUTHOR CONTRIBUTIONS

Jinping Wang: Investigation, manuscript preparation, figure preparation and visualization. Lingrong Wen: Investigation and manuscript preparation. Yaoguang Huang, Weiming Lai, Yongchuan Zhang, Dong-Hui Luo, Yile Li, and Jiawen Chen:Investigation. Bao Yang: Writing-review & editing, Supervision. Haijiao Wang: Writing – original draft, writing – review & editing, figure preparation and visualization, Supervision. All authors contributed to and approved the manuscript.

DECLARATION OF INTERESTS

The authors declare no competing interests.