Perspectives

Acupuncture and Herbal Medicine

AI-powered functional metabolomics: illuminating the dark matter of metabolism and transforming therapeutic discovery in traditional Chinese medicine

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Metabolites are chemical entities that are structurally changed during molecular metabolism and provide functional outcomes for the complete biochemistry of cells[1]. Metabolomics, the comprehensive study of small-molecule metabolites derived from cells, tissues, organisms, and bodily fluids, has emerged as a cutting-edge technique for biological discovery and medical innovations[2]. Beyond this, functional metabolomics is an advanced extension of metabolomics that moves beyond identifying static metabolic profiles to focusing on the biological functions of metabolites and their associated metabolic pathways[3]. While conventional metabolomics analysis is used to characterize differential metabolites, functional metabolomics approaches, such as the STORM strategy (Spatial Temporal Operative Real Metabolomics), adopts an innovative methodological framework by integrating multimodality omics techniques, mass spectrometry imaging, fluxomics, and biosynthetic biology to determine how these metabolites drive and regulate physiological and pathological phenotypic responses, which are related to biochemical functions and associated molecular mechanisms in metabolic reprogramming[4]. Despite its broad promise in metabolic discovery, this research field has long struggled with a profound challenge: the so-called "dark matter" of the metabolome in global metabolism[5], referring to the array of structurally uncharacterized, low-abundance, and functionally unknown metabolites that elude traditional detection and structural annotation methods. This gap has limited our understanding of the complete metabolic biochemistry and its central role in health, disease, and therapeutic interventions (Figure 1). Iterative artificial intelligence (AI) technologies, which are transformative data mining tools, are expected to reform the fundamental analytical capacity and real-world applicability of functional metabolomics in therapeutic medicine. By leveraging deep learning and integrative bioinformatic strategies, AI-powered functional metabolomics will revolutionize the ability to characterize unknown metabolites, decode their molecular roles in biological processes, and accelerate their translation into clinical applications[6]. This perspective article will explore the pivotal strategies of AI-powered functional metabolomics and propose the potential discoveries driving this biomedical revolution, from the deep expansion of metabolite profiling and functional annotation to the acceleration of disease biomarker discovery, therapeutic target identification, and drug development, including new horizons for translational application in traditional Chinese medicine (TCM)[7–8]. Ultimately, we attempt to highlight the potential impact and provide new insights that AI technologies bring to functional metabolomics, propelling the research niche into a new era of predictive diagnosis and innovative therapeutic medicine (Figure 2).

Deep measurement of the "dark matter" of systems metabolism facilitated by AI-powered functional metabolomics

One of the most profound challenges in functional metabolomics is the existence of "dark matter"[9], which represents the enormous fraction of metabolites that

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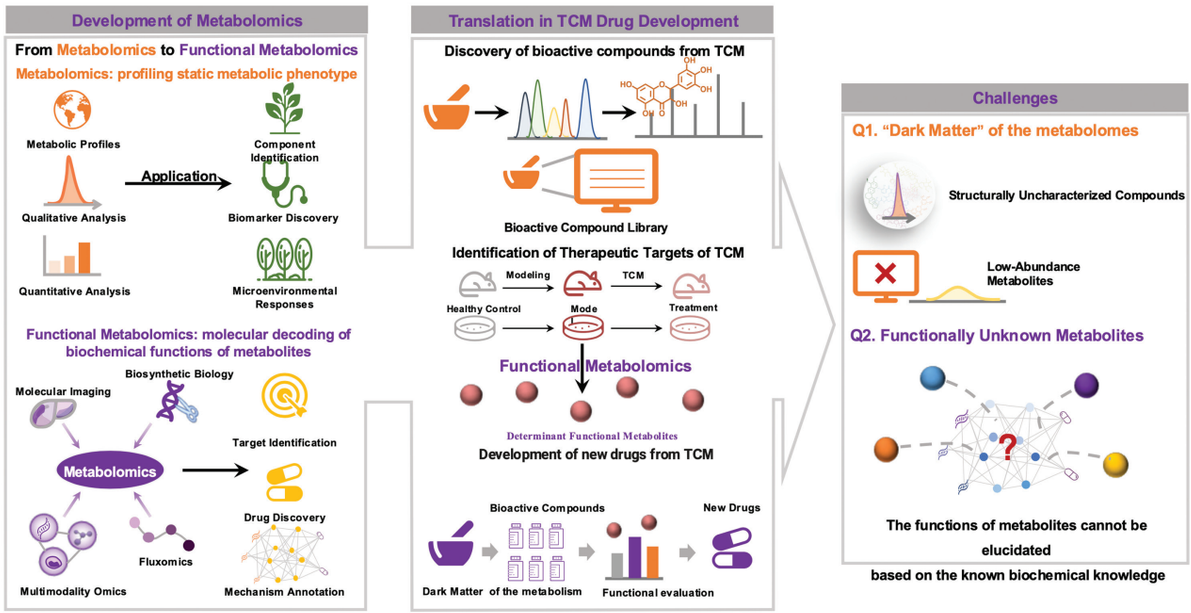


Figure 1. Translational applications and challenges of functional metabolomics. Metabolomics aims to capture static metabolic profiles of cells, tissues, and organisms. Beyond the capabilities of traditional metabolomics, functional metabolomics leverages an innovative methodological framework that integrates multimodal omics, mass spectrometry imaging, fluxomics, and synthetic biology to comprehensively decode biochemical functions and their associated regulatory mechanisms underlying the reprogramming of small-molecule metabolism. Functional metabolomics has been widely applied in TCM to screen bioactive compounds, identify system-level metabolic targets, and facilitate the discovery of new drugs based on bioactive compounds. Despite these advances, the development of functional metabolomics continues to face significant challenges, notably the so-called "dark matter" of the metabolome, referring to the large proportion of structurally uncharacterized, low-abundance, and functionally unknown metabolites that escape traditional detection and structural analysis methods. This limitation hampers a full understanding of metabolic biochemistry and its central role in health, disease, and therapeutic interventions. TCM: Traditional Chinese medicine.

remain structurally and functionally uncharacterized[10]. Conventional mass spectrometry and nuclear magnetic resonance (NMR) techniques often fail to detect low-abundance and structurally complex metabolites, particularly those with overlapping spectral signals or those present in dynamic and heterogeneous biological environments. AI-driven functional metabolomic strategies will dramatically expand the ability to profile metabolomes by pushing the boundaries between detection, annotation, and interpretation[11]. Currently, deep learning models trained on accessible spectral datasets can predict the structures and molecular properties of unknown metabolites, disentangle intricate overlapping signals, and annotate previously hidden metabolites with functional relevance. These algorithms can recognize subtle spectral patterns, reconstruct molecular structures, and infer physicochemical properties, enabling researchers to build comprehensive metabolome libraries covering both known and unknown metabolite entities[12]. For instance, AI-powered spectral deconvolution tools can resolve thousands of metabolites in a single biological sample, revealing key metabolic reactions, regulatory circuits, and chemical diversity previously inaccessible[13]. Deep learning techniques, such as convolutional neural networks (CNNs) and transformer models, further assist researchers in extracting key molecular features from complex metabolome data, facilitating the recognition of novel metabolite categories and their dynamic phenotypes under various stimulus conditions[14]. Collectively, these advancements can assist in deeply measuring the "dark matter" of metabolism, providing a complete understanding of the chemical landscape underlying biochemical systems and acquiring new metabolic discoveries in molecular regulation and disease mechanisms[15–16].

Functional decoding of small-molecule metabolites in biological systems driven by AI-powered functional metabolomics

Beyond cataloging metabolites, the central mission of functional metabolomics is to determine their functional roles in different biological processes and events, which is a key task in AI-powered functional metabolomics. This approach excels at integrating diverse omics datasets, including genomics, transcriptomics, proteomics, metabolomics, and fluxomics, to construct a complete systems-scale molecular map of metabolic modifications and modulations[17]. AI algorithms are uniquely capable of predicting metabolite–protein interactions, constructing dynamic metabolic networks, and analyzing condition-specific metabolic changes, enabling research to move beyond mere molecular correlation toward causation[18]. For example, graph-based neural networks and Bayesian inference models can predict how metabolites interact with enzymes, receptors, and signaling proteins, thereby revealing the molecular mechanisms by which metabolites drive cellular signaling, stress responses, development, and disease progression[19]. Furthermore, deep learning tools can analyze longitudinal datasets to identify metabolic modifications associated with environmental stimuli, genetic variation, or disease states, uncovering causal relationships that provide a mechanistic understanding[20]. Integrative AI platforms can model the interplay between metabolic pathways and regulatory

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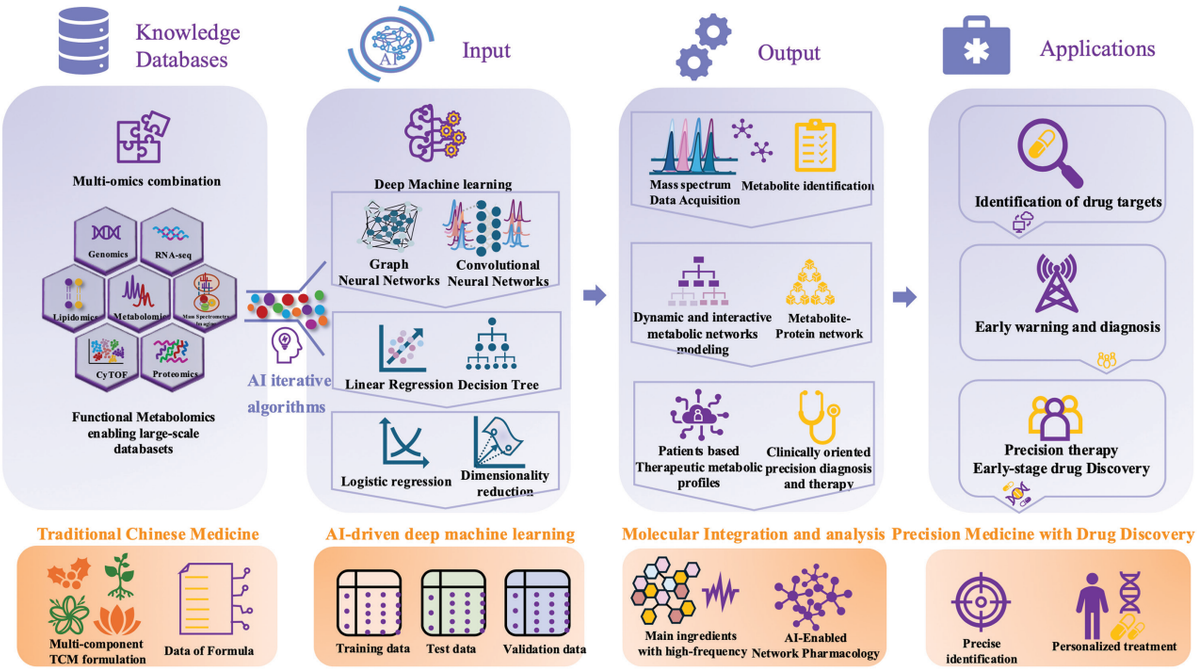


Figure 2. AI-powered functional metabolomics strategies transform research paradigms in precision medicine and traditional Chinese medicine. Functional metabolomics has been proposed to advance the deep integration of multimodal omics data, including transcriptomics, metabolomics, proteomics, lipidomics, genomics, single-cell omics, and spatial metabolomics, and iterative AI algorithms must be fully integrated into functional metabolomics to address critical research challenges in future translation. First, AI-powered molecular spectral analysis enables accurate prediction of the chemical structures and molecular properties of unknown metabolites, resolves complex overlapping signals, and annotates previously undetectable small-molecule metabolites with functional relevance. Second, these approaches allow the simultaneous resolution of thousands of metabolites, proteins, and lipids from a single biological sample, thereby facilitating the characterization of key metabolic reactions, regulatory circuits, and dynamic metabolic networks. Furthermore, AI-powered functional metabolomics can integrate large-scale clinical datasets to interpret clinically derived metabolic atlases, thereby promoting the precise treatment of complex diseases. In the context of translational therapeutic discovery in TCM, AI-powered functional metabolomics supports the integration, modeling, training, testing, and validation of multidimensional data related to TCM formulas for treating various complex diseases. This approach enables the effective identification of potential bioactive compounds from TCM formulas and relevant drug targets through the molecular decoding of regulatory and interactive networks among functional metabolites, target proteins, and therapeutic compounds. Consequently, this advances the discovery of new drugs derived from TCM and enables clinically oriented precision therapies. AI: Artificial intelligence; TCM: Traditional Chinese medicine.

circuits, thereby providing insights into metabolic flux, energy homeostasis, and cellular adaptation[21]. By constructing metabolic networks under various conditions, researchers can predict how perturbations in functional metabolism, such as disease progression, drug treatment, and genetic modifications, substantially affect metabolic outcomes, which will further guide experimental validation and therapeutic interventions[22]. Collectively, this systems-level approach will transform functional metabolomics from descriptive cataloging to predictive, mechanistic, and therapeutic science, enabling researchers to identify key functional regulatory metabolites, uncover hidden metabolic pathways, and design targeted interventions for the treatment of complex diseases[23–24].

Accelerating translational applications of AI-powered functional metabolomics in disease diagnosis and drug discovery

The integration of AI with functional metabolomics will dramatically accelerate the translation of basic discoveries into clinical applications, particularly in disease diagnosis, classification, and drug discovery. By mining large-scale clinical metabolomics data, AI can assist in identifying robust diagnostic and prognostic biomarkers with high specificity, validating them across populations, and controlling confounders such as age, sex, and comorbidities[25]. Machine learning classifiers such as random forests and support vector machines can readily distinguish disease states based on metabolic profiles, enabling early detection and personalized risk assessment[26–27]. AI technologies can also predict and prioritize metabolite-protein targets for drug discovery, screen virtual libraries for drug-like metabolites, and anticipate potential toxicities early in the research pipeline[28–30]. Deep machine learning models can be used to analyze molecular docking and binding affinities, guiding the selection of candidate compounds with optimal therapeutic properties. Furthermore, AI technologies can enable precision medicine practice by stratifying patients based on their functional metabolic profiles and guiding personalized diagnostic and therapeutic decisions[31–32]. For example, metabolic phenotyping can identify patient subgroups with distinct disease progression and treatment responses, facilitating tailored interventions and improving clinical outcomes[33–34]. AI-driven platforms integrate functional metabolomics with electronic health records, genomic data, and clinical phenotypes to provide comprehensive decision-making support to clinicians[35]. This integrated approach is transforming metabolite discoveries into actionable clinical tools by validating new drug targets for novel disease

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therapeutics. By shortening the timeline from discovery to translation, AI-powered functional metabolomics can revolutionize the landscape of biomarker development, target identification, and drug discovery, offering new applicable models for precision diagnostics and personalized treatments of complex diseases.

Expanding new-horizon translation of AI-powered functional metabolomics in TCM innovations

TCM is a rich but complex source of valuable therapeutic compounds, offering multicomponent herbal formulations with pharmacological potential for treating a wide spectrum of chronic and multifactorial diseases. However, the compositional complexity and pharmacological variability of TCM ingredients have historically created substantial barriers to modern drug development and the expansion of their therapeutic potential. AI-powered functional metabolomics will accelerate new drug discovery from TCM by integrating advanced computational tools with high-throughput metabolite profiling[3]. Deep learning algorithms enable the identification and characterization of bioactive compounds from a variety of TCM formulas by analyzing large-scale metabolomics data to identify novel metabolic signatures, predict functional compounds, and link these compounds to specific therapeutic outcomes[3,36–38]. AI-driven functional metabolomic approaches facilitate the precise mapping of compound–disease and compound–target interactions, supporting the selection of candidate compounds with high druggability and multi-target potential, which is a key principle in TCM's holistic treatment philosophy[39–40]. Network pharmacology powered by AI and functional metabolomics systematically reveals how TCM compounds interact at the molecular level, clarifying the synergistic and antagonistic effects that influence therapeutic efficacy[40]. The integration of AI with multiomics data, including genomics, transcriptomics, and spatial metabolomics, will fully support the stratification of patients and provide optimal TCM prescriptions based on individual metabolic profiles, representing a key step toward precision in TCM[41–42]. AI platforms also enable rapid screening and optimization of TCM-derived compounds for favorable pharmacokinetics and minimal toxicity, expediting preclinical evaluation and reducing resource consumption[39,43]. In summary, the combination of AI and functional metabolomics will transform TCM-based drug discovery by unraveling complex molecular mechanisms, validating multi-target efficacy, and supporting evidence-based therapeutic interventions for complex diseases in clinical practice, thus bridging the gap between ancient TCM formulas and modern precision Chinese medicine.

New insights and future impact of AI-powered functional metabolomics

The integration of AI with functional metabolomics is catalyzing a paradigm shift in biology and medicine, transforming a data-rich but mechanism-poor field into a predictive engine for discovery and clinical innovation. As AI continues to advance, this field will uncover new classes of functional metabolites, reveal hidden metabolic pathways, and enable highly targeted interventions for many complex diseases[4,44]. The long-term impact is profound, as AI-powered functional metabolomics promises to accelerate disease diagnosis, drug target identification, and drug discovery by redefining our understanding of human metabolism and establishing systemic metabolism as a central axis in health, disease, and innovative therapy. By integrating multi-omics data, modeling dynamic biological networks, and characterizing metabolic responses, iterative AI technologies can provide a novel framework for precision medicine, enabling researchers and clinicians to successfully monitor disease onset, progression, and therapeutic responses[13,45]. This approach can support the development of personalized diagnostics, targeted therapies, and evidence-based clinical decision-making to transform the precision medicine landscape. Furthermore, AI-powered functional metabolomics has opened new horizons in natural product discovery, microbiome research, and environmental health, enabling the expansion of the applicable scope of metabolomics beyond traditional boundaries[46–48]. The ability to deeply characterize the "dark matter" of metabolism, decode functional roles, and translate bench discoveries into clinical applications represents a new era of metabolomics discovery, ensuring long-term impact in precision medicine innovation.

In summary, AI-enabled functional metabolomics can propel this exploratory field into an actionable future, in which small-molecule metabolism is not only cataloged but also understood, predicted, and harnessed for transformative advances in disease pathogenesis, molecular diagnostics, and next-generation therapeutic discovery.

Conflict of interest statement

Zhaoxiang Bian and Aiping Lu are Editorial Board members of Acupuncture and Herbal Medicine. The article was subject to the journal's standard peer-review procedures, with peer review handled independently of these authors and their research group. The other authors have no conflicts of interest to disclose.

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Author contributions

Haitao Lu, Jiaxin Zhang, Jingjing Liu, and Yuan Tian wrote the manuscript. Jiaxin Zhang, Jingjing Liu, and Haitao Lu prepared the figures, and all authors contributed to the conception and development of the ideas and reviewed and approved the final manuscript.

Ethical approval of studies and informed consent

Not applicable.

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Data availability

All data generated or analyzed during this study are included in this published article.

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Declaration of generative AI in scientific writing

The authors wrote the article, and AI software assisted in slightly improving the grammar. The author reviewed, verified, and edited the scientific content and remains responsible for the final manuscript.

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