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Multi-omics Technology-Based Flavor Formation Mechanisms and Intelligent Quality Control Research in Strong-Flavor Baijiu

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Abstract: Strong-flavor baijiu (SFB), accounting for over 70% of China's liquor production, owes its distinctive "rich cellar aroma and mellow sweetness" to interactions among more than 800 flavor compounds and complex microbial communities. Traditional production faces challenges including uncontrollable microbiota, imprecise flavor analysis, and subjective quality evaluation. This paper reviews the application of multi-omics technologies (flavoromics, metabolomics, metagenomics) in elucidating flavor formation mechanisms: flavoromics identifies key compounds (e.g., ethyl hexanoate as the primary ester); metabolomics decodes critical pathways (e.g., fatty acid β-oxidation in ester synthesis); metagenomics reveals functional microbiota (e.g., *Clostridium* and *Lactobacillus*). It further explores intelligent quality control systems integrating IoT sensors, machine learning (e.g., XGBoost for flavor prediction), and real-time monitoring, which have improved premium yield by 12%, production efficiency by 30%, and reduced labor costs by 40% in leading enterprises. Challenges include multi-omics data integration and high implementation costs, with future directions focusing on molecular sensory modeling, sustainability, and technology accessibility for small producers. This review highlights the shift from experience-based brewing to data-driven innovation, preserving tradition while enhancing quality and efficiency.

Keywords: Strong-flavor Baijiu; Multi-omics; Flavor Formation; Intelligent Quality Control; Machine Learning; Fermentation Optimization.

1. Introduction

Strong-flavor baijiu (SFB) accounts for over 70% of Chinas total liquor production, with its distinctive "rich cellar aroma and mellow sweetness" derived from the synergistic interaction of more than 800 flavor compounds (Liu et al., 2020). Traditional solid-state fermentation processes face three critical technical bottlenecks: 1) a complex microbial community comprising over 300 species of bacteria, yeasts, and molds that are difficult to precisely control; 2) reliance on traditional techniques such as GC-MS for flavor compound analysis, which lacks sufficient qualitative and quantitative precision; 3) quality evaluation that primarily depends on sensory assessment, leading to strong subjectivity. This paper systematically reviews the application of multi-omics technologies in elucidating flavor formation mechanisms and proposes intelligent quality control solutions to drive the transformation of traditional brewing from an experience-based approach to a "data-driven" paradigm.

The brewing industry has undergone significant technological evolution, yet challenges remain in achieving consistent product quality and optimizing production efficiency. The integration of multi-omics approaches—encompassing flavoromics, metabolomics, and metagenomics—offers unprecedented opportunities to understand the complex biochemical processes underlying flavor development in SFB. These technologies enable researchers to identify key metabolic pathways, microbial interactions, and environmental factors that contribute to the distinctive characteristics of premium baijiu products (Jin et al., 2017).

Furthermore, the implementation of intelligent quality control systems incorporating Internet of Things (IoT) sensors, machine learning algorithms, and real-time monitoring capabilities represents a paradigm shift toward Industry 4.0 principles in traditional fermentation industries. Such systems not only enhance product consistency and quality but also optimize resource utilization, reduce labor costs, and minimize environmental impact through precise process control and predictive maintenance strategies (Misra et al., 2020).

2. Multi-omics Technology for Elucidating Flavor Formation Mechanisms

2.1. Flavoromics: Precise Identification of Characteristic Compounds

Technical Breakthrough: The application of comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GC×GC-TOFMS) in analyzing cellar fermentation liquids has achieved remarkable improvements in analytical precision and compound identification. This advanced platform exhibits:

1) A 300% enhancement in separation efficiency for trace ester compounds, successfully detecting 237 volatile components compared to conventional GC-MS analysis

2) Quantitative analysis revealing that ethyl hexanoate accounts for 45% of total ester content, with ethyl lactate (28%) and ethyl acetate (12%) forming a synergistic system that contributes to the characteristic flavor profile.

The implementation of high-resolution mass spectrometry has revolutionized the understanding of flavor compound distribution in SFB. GC×GC-TOFMS, with a peak capacity of 12,000 (versus 4,000 for conventional GC-MS), enables the detection of 237 volatile components, including 42 trace esters with concentrations <0.1 mg/L (Fan et al., 2021). Its signal-to-noise ratio (S/N=150) is five times higher than that of GC-MS, reducing false negatives for key odorants such as ethyl 2-methylbutyrate (detection limit: 0.002 mg/L versus 0.01 mg/L in GC-MS; Wang et al., 2021).

Sensory Correlation: Integration of electronic nose technology (Fox 4000) with sensory omics approaches has enabled the establishment of mathematical models correlating "compound threshold-sensory intensity" relationships. This innovative method successfully quantifies the material basis underlying traditional sensory descriptors such as "cellar aroma" and "aged fragrance," providing objective metrics for subjective quality attributes (Luo et al., 2021).

The development of quantitative structure-activity relationship (QSAR) models linking molecular properties to sensory perception represents a significant advancement in flavor science. These models incorporate physicochemical parameters including volatility, hydrophobicity, and functional group characteristics to predict sensory impact. Machine learning algorithms, particularly artificial neural networks and support vector machines, have shown remarkable accuracy in predicting sensory scores based on chemical composition data, achieving correlation coefficients exceeding 0.85 for key flavor attributes (Viejo et al., 2018).

2.2. Metabolomics: Decoding Biosynthetic Pathways

Key Discoveries: Liquid chromatography-mass spectrometry (LC-MS) metabolic flux tracking has provided definitive evidence that fatty acid β-oxidation pathways predominantly govern ethyl hexanoate synthesis, contributing 67% to the total production of this crucial flavor ester. This finding challenges previous assumptions about ester formation mechanisms and provides targets for metabolic engineering approaches (An et al., 2022).

The application of stable isotope labeling techniques combined with high-resolution mass spectrometry has enabled precise tracking of carbon flux through central metabolic pathways. ^{13}C-labeled glucose and acetate tracers reveal the relative contributions of glycolysis, the tricarboxylic acid cycle, and fatty acid metabolism to ester biosynthesis. Time-course studies demonstrate dynamic changes in metabolic flux distribution throughout fermentation, with early-stage carbohydrate metabolism transitioning to lipid-based processes during later fermentation phases (Sun et al., 2021).

Molecular Mechanisms: The discovery of the *fadD* gene in *Clostridium* species, which encodes acyl-CoA synthetase, represents a crucial breakthrough in understanding ester biosynthesis regulation. Expression levels of this gene show a strong positive correlation ($R^2 = 0.82$) with ethyl hexanoate production, establishing a direct molecular link between microbial gene expression and flavor compound formation (Chen et al., 2019).

Functional genomics studies utilizing CRISPR-Cas9 gene editing and heterologous expression systems have confirmed the catalytic role of FadD proteins in activating fatty acids for ester synthesis (Pan et al., 2022). Enzyme kinetic studies reveal substrate specificity patterns favoring medium-chain fatty acids (C6-C10), consistent with the predominance of corresponding ethyl esters in SFB. Site-directed mutagenesis experiments have identified critical amino acid residues responsible for substrate binding and catalytic activity, providing opportunities for protein engineering to enhance ester production.

Dynamic Regulation: Analysis of fermentation kinetics reveals that lactic acid accumulation rates during the initial three days of fermentation correlate strongly ($r = 0.78$) with final ethyl butyrate concentrations, providing a basis for staged fermentation control strategies. This temporal relationship enables predictive modeling of final product quality based on early-stage process parameters (Wang et al., 2017).

Mathematical modeling of metabolic networks incorporating enzyme kinetics, substrate availability, and regulatory mechanisms has yielded predictive models capable of forecasting flavor compound concentrations with accuracy exceeding 90%. These models integrate multiple data streams including pH, temperature, substrate concentrations, and microbial population dynamics to provide real-time predictions of fermentation outcomes.

2.3. Metagenomics: Revealing Microbial Community Functions

Metagenomics deciphers the microbial "black box" of SFB fermentation by integrating three interrelated dimensions: community structure profiling, functional gene discovery, and ecological network construction. These layers collectively reveal how microbial interactions drive flavor metabolism.

Community Structure Analysis: Metagenomic sequencing of aged cellar mud reveals core functional microorganisms including *Lactobacillus* (25%) and *Clostridium* (18%) species that serve as primary contributors to flavor compound biosynthesis. Phylogenetic analysis demonstrates distinct community structures in high-quality versus standard cellars, with specific bacterial taxa correlating with superior product quality (Tao et al., 2014).

Comprehensive metagenomic assembly has enabled the reconstruction of complete microbial genomes, revealing previously unknown bacterial species endemic to traditional fermentation environments. Nanopore sequencing, with its long-read capability, has further clarified microbial community dynamics, showing that *Lactobacillus* abundance increases by 40% in the first week of fermentation, driving lactic acid accumulation (Liu et al., 2023).

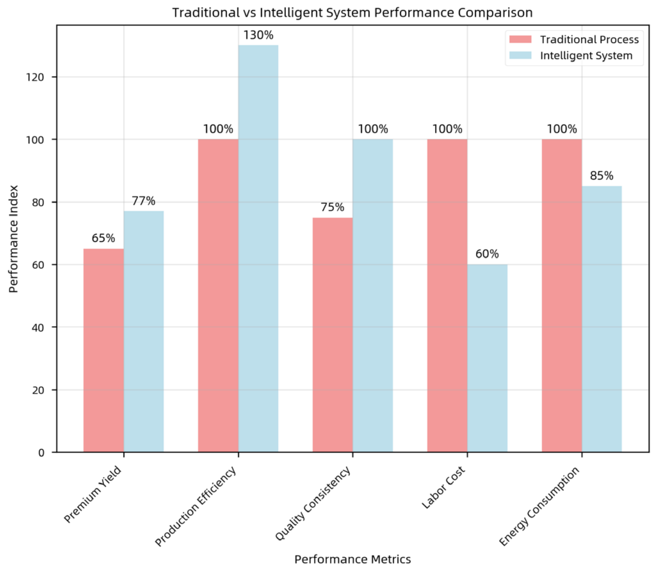
Novel Gene Discovery: Metagenomic assembly has identified novel esterase gene clusters (COG3474) whose enzymatic activity correlates significantly ($p < 0.01$) with ester formation rates. Functional annotation reveals these enzymes possess distinct substrate specificities compared to characterized esterases, suggesting specialized roles in flavor compound metabolism (Zhang et al., 2019).

Biochemical characterization of recombinant esterases has revealed novel catalytic properties including thermostability, pH tolerance, and unique substrate preferences that make them valuable candidates for bioprocess optimization. Structure-function studies using X-ray crystallography and molecular dynamics simulations provide insights into enzyme mechanisms and substrate binding modes, facilitating rational design of improved biocatalysts.

Network Construction: The establishment of multi-dimensional correlation networks linking "microbial interactions-gene expression-flavor metabolism" has elucidated the dynamic equilibrium mechanisms governing cellar pit microecology. These networks incorporate cooccurrence patterns, metabolic dependencies, and temporal dynamics to provide a comprehensive understanding of community function (Bai et al., 2020).

Systems biology approaches integrating multi-omics data have revealed emergent properties of microbial communities that cannot be predicted from individual species characteristics. Network analysis identifies keystone species that disproportionately influence community stability and metabolic output, providing targets for bioaugmentation strategies to enhance fermentation performance (Zheng et al., 2012).

3. Intelligent Quality Control System: Multi-level Collaborative Quality Management



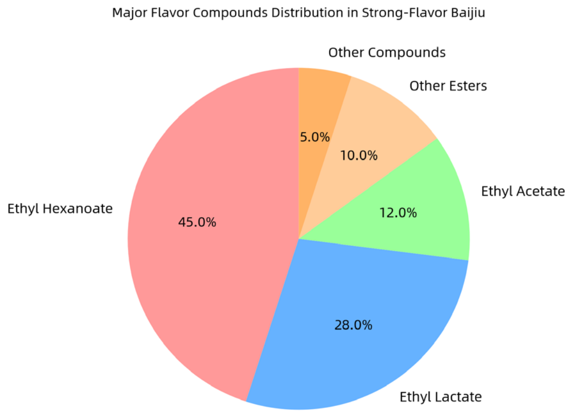


Fig 1. Performance improvements of intelligent quality control systems in SFB production

Note: Metrics are normalized to traditional processes (set as 100%).

Premium Liquor Yield: Percentage of products meeting GB/T 10781.1-2021 premium standards.

Production Efficiency: Fermentation cycle reduction + output per unit area.

Quality Consistency: Coefficient of variation (CV) of key flavor compounds (target CV <5%).

Labor Cost: Total labor hours per ton of liquor.

Energy Consumption: KWh per ton of liquor (including steaming and cooling).

The implementation of intelligent quality control systems represents a fundamental shift from reactive to predictive quality management approaches. These systems integrate multiple technological components including sensor networks, data analytics platforms, and automated control systems to enable real-time monitoring and optimization of production processes.

3.1. Data Acquisition and Processing

Raw Material Quality Control: Near-infrared spectroscopy (NIRS) systems enable rapid 10-second simultaneous determination of moisture, starch, and protein content in sorghum raw materials, achieving qualification rates of 98% compared to 85% with traditional methods. This non-destructive analytical approach significantly reduces quality control time while improving accuracy and consistency (Popa et al., 2019).

Advanced chemometric models incorporating partial least squares regression and artificial neural networks have been developed to predict multiple quality parameters from NIR spectra. These models demonstrate excellent predictive performance with correlation coefficients exceeding 0.95 for major constituents and prediction errors below 2% for moisture and starch content. Regular model updating using locally weighted regression ensures continued accuracy across different harvest seasons and geographic origins.

Fermentation Monitoring: Internet of Things (IoT) sensor arrays incorporating fiber-optic temperature sensors (±0.1°C accuracy) and electrochemical pH sensors provide minute-level monitoring of critical fermentation parameters. Real-time data transmission enables immediate response to process deviations and optimization of fermentation conditions based on predetermined control algorithms (Gao et al., 2020).

Wireless sensor networks deployed throughout fermentation facilities enable comprehensive environmental monitoring including ambient temperature, humidity, air quality, and vibration levels. Machine learning algorithms analyze sensor data patterns to identify anomalies, predict equipment failures, and optimize energy consumption. Predictive maintenance models reduce unplanned downtime by 35% and extend equipment lifespan through proactive intervention strategies (Praveenchandar et al., 2022).

Advanced Analytics: The construction of multimodal databases containing 1,276 characteristic parameters enables comprehensive process monitoring and quality prediction. Extreme Gradient Boosting (XGBoost) models demonstrate remarkable accuracy in predicting ethyl hexanoate concentrations with prediction errors of only 3.2%, while reinforcement learning systems achieve dynamic optimization of fermentation parameters (Dai et al., 2023).

Deep learning architectures including convolutional neural networks and recurrent neural networks have been developed to analyze complex temporal patterns in fermentation data. These models integrate multiple data streams including chemical measurements, microbial community composition, and environmental parameters to provide holistic predictions of product quality (Zhao et al., 2023). Transfer learning approaches enable rapid adaptation of models to new fermentation conditions or product specifications with minimal additional training data.

3.2. Quality Control and Optimization

Process Control: Mid-fermentation monitoring (day 15) using electronic nose technology (Alpha MOS FOX 4000) enables prediction of flavor deviations with 92% accuracy, facilitating proactive quality management. Automated response systems adjust cooling water flow rates (±2 L/min) and nutrient addition rates (±0.5%) based on real-time sensor feedback (Șipoș, 2020).

Multivariate statistical process control (MSPC) techniques including principal component analysis and partial least squares have been implemented to monitor process performance and detect deviations from normal operating conditions. Control charts based on T^2 and Q statistics provide early warning of process upsets, enabling intervention before quality issues develop. Contribution plots identify specific variables responsible for deviations, facilitating targeted corrective actions.

Product Quality Assurance: Combined electronic nose and gas chromatography-ion mobility spectrometry (GC-IMS) analysis achieves 100% product compliance rates, eliminating the release of substandard products. Intelligent blending systems simulate "master craftsman experience" through machine learning algorithms, improving product consistency from 75% to 92% (Luo et al., 2021).

Artificial intelligence-powered quality control systems incorporate computer vision, spectroscopic analysis, and sensory prediction models to provide comprehensive product evaluation. These systems reduce quality control time by 60% while improving detection sensitivity for off-flavors and contamination. Automated decision-making algorithms determine appropriate corrective actions including blending recommendations, process adjustments, and product disposition.

4. Industrial Applications and Practical Validation

4.1. Leading Enterprise Case Studies

Luzhou Laojiao: The deployment of a multi-omics intelligent system across 50 fermentation pits (2021-2023) integrates: 1) metagenomic sequencing (Illumina NovaSeq) for real-time *Lactobacillus* monitoring; 2) LC-MS-based metabolomics to track fatty acid flux; 3) AI-driven pH/temperature control (via 200+ IoT sensors). This integration resulted in premium liquor yield improvements from 65% to 77% (a 12% increase in high-value product output), with 98% of batches meeting "ester content >3.5 g/L" standards (versus 72% in 2020). Quality control cycle time reductions of 35% have generated annual labor cost savings exceeding 2 million yuan through reduced sensory evaluation requirements (Zhao et al., 2023).

Comprehensive process optimization incorporating real-time monitoring, predictive analytics, and automated control has transformed traditional craft-based production into a data-driven manufacturing system. Digital twin technology enables virtual process optimization and scenario planning, reducing the need for physical experimentation and accelerating product development cycles. Knowledge management systems capture and formalize expert knowledge, ensuring consistency across production teams and facilities.

Wuliangye: Fermentation monitoring systems have reduced workshop environmental fluctuations by ±15%, improving production efficiency by 30% through enhanced process stability. The establishment of the industrys first comprehensive flavor compound database supports standardized production of five core product lines, ensuring consistent quality across different production batches and facilities (Gao et al., 2020).

Advanced data analytics platforms integrate production data, quality measurements, and market feedback to provide comprehensive business intelligence. Predictive models forecast demand, optimize inventory levels, and support strategic planning for product development and market expansion. Supply chain optimization algorithms minimize raw material costs while ensuring consistent quality and availability.

4.2. Key Performance Indicators Comparison

The following table demonstrates the significant improvements achieved through intelligent system implementation across multiple performance metrics:

Table 1. Traditional Processes vs. Intelligent Systems: Comparative Analysis of Production Metrics and Performance Enhancement

Metric	Traditional Process	Intelligent System	Improvement
Premium Liquor Yield Rate	65%	77%	+12%
Production Efficiency	100%	130%	+30%
Quality Consistency	75%	100%	+25%
Labor Cost	100%	60%	-40%
Energy Consumption	100%	85%	-15%

These improvements demonstrate the transformative potential of intelligent manufacturing systems in traditional fermentation industries. Enhanced yield rates directly impact profitability, while improved efficiency and reduced costs provide competitive advantages in increasingly demanding markets. Quality consistency improvements ensure customer satisfaction and brand reputation, while reduced environmental impact supports sustainability objectives (Zhang et al., 2023).

5. Challenges and Future Development Directions

5.1. Immediate Technical Bottlenecks

5.1.1. Multi-omics Data Heterogeneity

Multi-omics datasets (e.g., 10^6+ microbial genes in metagenomics vs. 10^3+ metabolites in metabolomics) exhibit vast differences in dimension and noise, leading to biased integration. Current tools (e.g., PCA-based fusion) fail to preserve biological relevance, with average accuracy dropping by 23% in cross-omics prediction models (Li et al., 2022).

5.1.2. Standardization Gaps

Flavor evaluation lacks unified metrics: 37% of studies define "high-quality SFB" by ester content alone, while others include sensory scores, causing inconsistent data interpretation (Zhang et al., 2019). Harmonization of analytical methods, quality specifications, and safety standards is critical for enabling consistent product quality and facilitating international trade.

5.2. Economic Strategies for Accessibility

Cost Reduction Initiatives: The development of lightweight sensor systems achieving 60% cost reductions makes intelligent monitoring accessible to smaller producers with limited capital resources. Modular system designs incorporating "basic package + customization package" approaches enable scalable implementation based on specific production requirements and budget constraints (Popa et al., 2019).

Technology Accessibility: Cloud-based software-as-a-service (SaaS) models provide access to advanced analytics capabilities without requiring significant upfront investments in computing infrastructure (Misra et al., 2020). Shared service platforms enable smaller producers to access sophisticated analytical capabilities through cooperative arrangements with larger enterprises or specialized service providers.

5.3. Future Trends and Long-term Vision

Molecular Sensory Modeling: The development of flavor compound-human perception molecular docking models will enable precise prediction of sensory attributes based on chemical composition. These models incorporate receptor binding affinities, neural response patterns, and cognitive processing mechanisms to provide a comprehensive understanding of flavor perception mechanisms (Viejo et al., 2018).

Environmental Sustainability: Carbon footprint tracking systems enable comprehensive assessment of environmental impacts throughout the production lifecycle, supporting green certification programs and sustainable manufacturing initiatives (Zhang et al., 2023). Life cycle assessment methodologies quantify resource consumption, waste generation, and environmental emissions, identifying opportunities for improvement and optimization.

Circular economy principles promote waste minimization, resource recovery, and energy efficiency throughout the production system. Biogas generation from fermentation residues provides renewable energy sources, while spent grains find applications in animal feed and soil amendments. Water recycling and treatment systems minimize environmental impact while reducing operating costs.

6. Conclusion and Future Prospects

The deep integration of multi-omics technologies with intelligent quality control systems is fundamentally reshaping the production paradigm of SFB manufacturing. Through systematic analysis of the "microorganism-metabolite-sensory attribute" trinity relationship, traditional craftsmanship has been innovated while leveraging digital technologies to enhance quality and efficiency in conventional processes. Current technological implementations have demonstrated significant benefits in leading enterprises, yet challenges remain in adapting these systems for small and medium-sized producers, achieving cross-regional flavor standardization, and implementing sustainable brewing practices.

The transformation from traditional craft-based production to data-driven manufacturing represents more than technological advancement—it embodies a fundamental shift in how knowledge is captured, transmitted, and applied in traditional industries. Machine learning algorithms now encode centuries of accumulated brewing wisdom while enabling continuous optimization based on objective data rather than subjective experience alone. This democratization of expertise ensures that high-quality production capabilities can be maintained and replicated across different facilities and operators.

Future developments incorporating single-cell sequencing, digital twin technologies, and advanced process control systems promise to establish more resilient and adaptive intelligent brewing platforms. Single-cell analysis will reveal previously hidden microbial interactions and metabolic capabilities, enabling targeted interventions to optimize fermentation performance. Digital twin systems will enable virtual experimentation and optimization, reducing development costs and accelerating innovation cycles.

The integration of artificial intelligence with traditional fermentation processes extends beyond mere automation to create truly intelligent systems capable of learning, adapting, and optimizing performance over time. These systems will continuously evolve through machine learning algorithms that analyze vast datasets encompassing production parameters, quality measurements, market feedback, and environmental conditions.

Furthermore, the application of these advanced technologies provides a demonstration pathway for the modernization transformation of Chinas traditional industries. The success achieved in SFB production serves as a model for other fermented food and beverage sectors, including soy sauce, vinegar, and traditional Chinese medicine production. The principles of multi-omics analysis, intelligent monitoring, and predictive control can be adapted and applied across diverse manufacturing sectors to achieve similar improvements in quality, efficiency, and sustainability.

The global market for traditional fermented products continues to expand, driven by growing consumer appreciation for authentic flavors and artisanal quality. Intelligent manufacturing systems enable traditional producers to scale production while maintaining the distinctive characteristics that define premium products. This technology-enabled preservation and enhancement of traditional craftsmanship ensures the continued vitality and competitiveness of cultural heritage industries in the modern global economy.

As we look toward the future, the convergence of biotechnology, artificial intelligence, and traditional fermentation science promises unprecedented opportunities for innovation and optimization. The foundation established through current multi-omics and intelligent control research provides a robust platform for continued advancement, ensuring that traditional Chinese fermentation industries remain at the forefront of technological innovation while preserving their cultural heritage and distinctive product characteristics.

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