Standardizing Herbal Medicines with AI: Chemical Fingerprints, Bioactivity Profiles, Quality Markers, and Therapeutic Consistency

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ABSTRACT

Herbal medicine standardization remains a major challenge because botanical identity, plant part, production context, processing method, extraction conditions, multi-constituent chemistry, biological relevance, and safety awareness all influence product quality. Chemical fingerprints can support identity confirmation, compositional comparison, and batch-level quality assessment, but chemical similarity alone cannot establish therapeutic consistency. Bioactivity profiles can add biological meaning to analytical patterns, yet they require assay relevance, reproducibility, and cautious interpretation. This article develops an original AI-assisted conceptual model for herbal medicine standardization that connects botanical authentication, processing context, chemical fingerprinting, metabolomic profiling, marker compound quantification, bioactivity profiling, quality-marker selection, batch consistency, anomaly detection, safety-marker screening, validation gates, and therapeutic consistency boundaries. The proposed model positions artificial intelligence as a decision-support layer for feature selection, pattern recognition, batch classification, chemical–bioactivity alignment, candidate quality-marker prioritization, and uncertainty communication. It does not present AI outputs, chemical fingerprints, or bioactivity patterns as validated product standards or clinical equivalence claims. The main contribution is a structured conceptual framework that clarifies how analytical, biological, computational, and interpretive evidence can be integrated while preserving the distinction between standardization hypotheses, validated quality markers, therapeutic relevance, and regulatory interpretation.

Key Words: *Herbal medicines, Standardization, Artificial intelligence, Chemical fingerprints, Bioactivity profiles, Quality markers*

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INTRODUCTION

Herbal medicine standardization has become a central challenge in phytopharmaceutical research because complex preparations cannot be adequately represented by botanical naming or isolated chemical measurement alone. Contemporary standardization increasingly requires the integration of quality-marker logic, chemical fingerprint analysis, safety awareness, and quality-control practices that account for the multi-component nature of herbal materials and finished preparations [1-3].

Modern quality control has moved from narrow identification or single-compound testing toward multi-method analytical strategies that combine botanical, chemical, and quality-assurance information. This shift is important because each analytical method captures only part of the quality profile, and interpretation depends on the

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intended standardization claim, the herbal matrix, and the validation status of the method [4].

A core difficulty is that herbal medicines may vary because of botanical identity, plant part, geographic origin, cultivation or wild-harvest conditions, harvesting stage, storage, processing, preparation, and extraction. These variables can influence chemical composition and biological relevance, but they do not all carry the same evidentiary weight. A conceptual standardization model must therefore separate identity verification, compositional profiling, bioactivity interpretation, quality-marker selection, and therapeutic consistency assessment rather than treating them as interchangeable forms of evidence.

This article proposes an AI-assisted conceptual model for standardizing herbal medicines through chemical fingerprints, bioactivity profiles, quality markers, and therapeutic consistency boundaries. The model is designed as a structured decision-support framework: AI may assist feature selection, pattern recognition, batch classification, anomaly detection, and marker prioritization, but analytical validation, biological validation, expert interpretation, and regulatory evaluation remain necessary before any product-standard or therapeutic-consistency claim can be justified.

Herbal medicine standardization challenges

The first standardization challenge is botanical identity. DNA-based authentication studies have shown that herbal products may raise quality and fidelity concerns when declared identity does not match detected botanical content, and species identification across raw materials and finished products is therefore a necessary foundation for standardization [5, 6].

A second challenge is processing context. Herbal processing may alter chemical characteristics, preparation attributes, and interpretable quality features, meaning that processed and unprocessed materials should not be treated as equivalent unless the standardization evidence supports that interpretation [7].

A third challenge is the multi-constituent structure of herbal medicines. Marker compound quantification can be useful when the marker is traceable, measurable, specific, and relevant to quality, but single-marker standardization may be insufficient when the preparation contains multiple active, synergistic, inactive, or safety-relevant constituents. Chemical fingerprints and metabolomic profiles can broaden quality assessment, yet they still require interpretation in relation to botanical identity, processing, batch consistency, and biological relevance.

A fourth challenge is the growing use of computational classification in herbal quality control. Spectroscopic fingerprints combined with machine-learning models such as random forest or support vector machine regression have been applied to herbal quality assessment, showing how computational tools can assist pattern recognition while still depending on data quality, method suitability, and validation scope [8].

Chemical fingerprints and bioactivity profiles

Chemical fingerprints provide a structured representation of herbal composition across chromatographic, spectroscopic, or metabolomic data. Targeted and untargeted fingerprinting approaches can support identity assessment, sample comparison, and quality evaluation, but their standardization value depends on reproducible analytical workflows and cautious interpretation of chemical similarity [9].

Bioactivity profiling adds a biological layer to chemical fingerprinting by connecting observed chemical patterns with assay-relevant responses. For example, chromatographic fingerprinting combined with bioautography can distinguish herbal varieties while adding antioxidant activity information, and HPTLC metabolomics can reveal chemical variation relevant to quality-control interpretation [10]. Such approaches support chemical–bioactivity alignment, but they do not establish clinical benefit or therapeutic equivalence without further validation [11].

Metabolomic and functional profiling approaches can help interpret herbal medicines as chemically complex systems rather than as collections of isolated marker compounds. Functional metabolomics is particularly relevant to conceptual standardization because it can support hypotheses about how chemical features may relate to biological activity, while still requiring experimental confirmation before mechanistic or therapeutic claims are made [12].

Spectrum–effect and effect-constituent strategies provide a bridge between chemical fingerprints and bioactivity profiles. Spectrum–effect analysis can prioritize fingerprint features associated with antioxidant activity in a defined herbal formula context [13]. Similarly, bioassay-linked effect-constituent indexing can strengthen quality assessment by relating chemical constituents to a biological response, although such indices remain bounded by assay relevance and do not by themselves prove clinical consistency [14].

Table 1 summarises the roles and limitations of chemical fingerprints and bioactivity profiles in herbal medicine standardization.

Table 1. Chemical Fingerprints and Bioactivity Profiles in Herbal Medicine Standardization: Analytical Inputs, Biological Relevance, Batch-Consistency Value, Interpretation Limits, Validation Requirements, and AI-Assisted Integration Opportunities

Standardization evidence type	Core purpose	Typical input data	Standardization value	Main limitation	AI-assisted integration role	Validation requirement	Failure risk
Botanical identity-linked fingerprint	Confirm whether the chemical profile is consistent with the declared material	Authenticated reference material, chromatographic or spectroscopic profile, taxonomic metadata	Supports identity-aware quality assessment	Chemical similarity may mask species substitution or adulteration	Pattern recognition against authenticated reference sets	Botanical authentication plus analytical reproducibility	Accepting a chemically similar but botanically incorrect material
Plant part and processing fingerprint	Distinguish plant part, processed state, or preparation context	Plant part records, processing metadata, spectral or chromatographic data	Helps prevent inappropriate comparison across non-equivalent materials	Processing effects may be herb-specific and method-dependent	Classification of processing-related patterns	Processing documentation and orthogonal chemical confirmation	Treating processed and unprocessed materials as equivalent
Chromatographic fingerprint	Represent multi-constituent composition	HPLC, UHPLC, GC, HPTLC, or related chromatographic profiles	Supports batch comparison and compositional consistency assessment	Peak patterns do not automatically indicate biological relevance	Peak alignment, feature extraction, clustering, anomaly detection	Method specificity, precision, robustness, and reference comparison	Overinterpreting fingerprint similarity as therapeutic consistency
Spectroscopic fingerprint	Rapidly characterize global sample patterns	FTIR, NIR, Raman, NMR, or related spectra	Enables high-throughput screening and classification	Spectral patterns may be indirect and matrix-sensitive	Supervised or unsupervised classification	Calibration, transferability testing, and independent sample confirmation	Model drift, misclassification, or poor transfer across instruments
Metabolomic profile	Capture known and unknown chemical variation	Targeted or untargeted metabolomic features	Reveals broader chemical heterogeneity than selected markers alone	Feature annotation may be incomplete	Feature selection, clustering, pathway-oriented interpretation	Orthogonal confirmation and annotation-confidence reporting	Misannotating features or prioritizing unstable signals
Marker compound quantification	Measure defined constituents with traceable analytical methods	Calibrated marker assays, reference standards, validated quantification data	Provides measurable quality attributes	One marker may not represent complex herbal quality	Outlier detection and marker-panel prioritization	Calibration, accuracy, precision, linearity, and specificity	Reducing standardization to abundant but weakly relevant compounds
Bioactivity profile	Add biological relevance to chemical quality assessment	Validated assay outputs, response patterns, assay metadata	Helps distinguish chemical presence from biological relevance	In vitro response does not prove clinical benefit	Activity-pattern clustering and response classification	Assay reproducibility and biological relevance assessment	Treating assay activity as therapeutic proof
Chemical–bioactivity alignment	Identify candidate features associated with	Paired fingerprint and assay datasets	Supports candidate quality-marker prioritization	Correlation does not establish causality	Spectrum–effect modeling and multivariate association analysis	Confirmatory testing, fractionation, and mechanistic assessment	Selecting spurious feature–activity associations

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	biological responses						
Batch-consistency profile	Compare batches across chemical and biological dimensions	Fingerprints, marker levels, processing records, bioactivity profiles	Supports consistency hypotheses across batches	Consistency is conditional on defined inputs and acceptance logic	Batch clustering, anomaly detection, uncertainty flagging	Batch-level analytical and biological testing	False acceptance of inconsistent or unsafe batches
Safety-related profile	Detect safety-relevant chemical or biological concerns	Known toxic constituents, safety markers, toxicity-related assay data	Adds risk awareness to quality assessment	Safety relevance may require exposure and toxicological interpretation	Risk-feature prioritization and anomaly alerts	Toxicological confirmation and expert review	Missing low-abundance but high-risk constituents

Quality markers and therapeutic consistency

Quality markers should be understood as evidence-linked standardization elements rather than simply abundant or easily measurable compounds. Analytical strategies for quality-marker discovery emphasize that candidate markers require discovery, prioritization, and validation before they can support quality assessment, particularly when the intended claim involves identity, composition, safety, or biological relevance [15].

Data-driven quality evaluation can support quality-marker interpretation when the computational process remains tied to traceable evidence. Smart quality-evaluation strategies based on quality markers have been proposed to connect marker information with data mining and intelligence assessment [16]. Herb-specific marker systems also show that quality-marker logic should be adapted to the material, preparation, and intended quality attribute rather than imposed as a universal template [17].

Therapeutic consistency should be framed as a bounded hypothesis, not as a guaranteed clinical property. The quality-marker concept emphasizes that markers should reflect relevance, traceability, specificity, and measurability, which means a marker panel should be interpreted in relation to botanical identity, processing context, chemical profile, biological plausibility, and standardization purpose [18].

Safety markers are a necessary part of therapeutic consistency logic because a chemically consistent product can still be unsuitable if safety-relevant constituents or toxicity-linked patterns are not considered. Network toxicology-based toxicity quality-marker strategies support the inclusion of safety-related marker logic in herbal quality evaluation, but predicted toxicity relevance still requires confirmatory toxicological and exposure-based interpretation [19].

AI-assisted standardization logic

AI-assisted herbal standardization should be positioned as a decision-support process for integrating heterogeneous quality evidence. AI, bioinformatics, data fusion, and machine learning may assist herbal quality assessment by supporting feature selection, fingerprint classification, marker prioritization, batch clustering, and multimodal pattern recognition, but these outputs should not be treated as substitutes for analytical validation, biological validation, or expert interpretation [20–22].

In identity-oriented workflows, computational classification can help recognize materials rapidly when reference data are appropriate and the model is validated for the intended sample domain. A sequential decision-fusion pipeline using ATR-FTIR data for high-throughput species recognition illustrates how computational recognition may support authentication workflows, while remaining distinct from bioactivity or therapeutic validation [23].

In plant-material classification, machine learning can help distinguish herbal aerial parts and related material categories from spectral patterns. Such classification is useful for standardization only when the training data, preprocessing, model transferability, and independent validation are adequate for the intended quality-control setting [24].

The conceptual value of AI lies in connecting evidence layers that are often evaluated separately: botanical identity, plant part, processing context, chemical fingerprints, metabolomic features, marker compound quantities, bioactivity profiles, safety signals, and batch-level variation. In the proposed logic, AI generates ranked features, clusters, anomaly flags, or consistency hypotheses, while human experts and validated methods determine whether those outputs are analytically credible, biologically meaningful, and suitable for quality-standard interpretation.

Table 2 maps AI-assisted standardization functions for linking herbal identity, chemical fingerprints, bioactivity profiles, quality markers, and consistency assessment.

Table 2. AI-Assisted Standardization Logic for Herbal Medicines: Botanical Authentication, Chemical Fingerprint Learning, Bioactivity Pattern Recognition, Quality-Marker Prioritization, Batch Classification, Anomaly Detection, Safety Screening, and Consistency Assessment

AI-assisted function	Core standardization question	Required data	Computational output	Interpretation boundary	Validation need	Risk if misused	Model contribution
Botanical authentication support	Is the declared botanical identity plausible?	DNA, authenticated references, taxonomic metadata, spectral or chemical identity data	Identity-confidence class or anomaly flag	Identity confirmation does not prove quality, potency, or safety	Molecular or orthogonal authentication with expert taxonomic review	Accepting misidentified or adulterated material	Establishes the first gate of identity-aware standardization
Plant part verification	Is the correct plant part represented?	Plant part metadata, microscopic data, spectral fingerprints, chemical profiles	Plant-part classification or mismatch alert	Plant part classification does not establish therapeutic suitability	Reference-confirmed plant-part datasets and independent testing	Confusing pharmacologically distinct plant parts	Prevents inappropriate comparison across non-equivalent materials
Processing-context classification	Is the processing or preparation state consistent?	Processing records, preparation metadata, chemical or spectral profiles	Processing-state class or deviation flag	Processing class does not define clinical relevance by itself	Process documentation plus chemical confirmation	Treating processed and unprocessed materials as interchangeable	Links production context to analytical interpretation
Chemical fingerprint learning	What compositional pattern defines the sample or batch?	Chromatographic, spectroscopic, or metabolomic features	Feature map, cluster, or similarity pattern	Chemical similarity is not therapeutic equivalence	Method validation, alignment checks, and reference comparison	Overvaluing similarity metrics without biological support	Builds a structured chemical evidence layer
Bioactivity pattern recognition	Are biological response patterns consistent across samples?	Validated assay outputs, response profiles, assay metadata	Activity cluster or response-pattern class	Bioactivity does not prove clinical benefit	Assay reproducibility and biological relevance review	Treating in vitro activity as efficacy	Adds biological relevance while preserving boundaries
Chemical–bioactivity alignment	Which features are associated with biological responses?	Paired chemical fingerprint and bioactivity datasets	Candidate feature–activity association	Association does not prove causality	Confirmatory testing, fractionation, and mechanistic assessment	Selecting spurious correlations as markers	Supports evidence-aware quality-marker prioritization
Quality-marker prioritization	Which features should be considered candidate markers?	Chemical, biological, safety, processing, and traceability evidence	Ranked candidate marker panel	AI ranking is not validation	Analytical detectability, specificity, biological relevance, and expert review	Selecting abundant but irrelevant markers	Converts complex evidence into a reviewable marker hypothesis
Batch classification	Are batches comparable within defined evidence boundaries?	Fingerprints, marker quantities, process records, bioactivity profiles	Batch cluster, consistency class, or outlier flag	Batch class does not guarantee safety or therapeutic equivalence	Batch-level analytical and biological verification	False acceptance of inconsistent batches	Supports controlled batch-consistency assessment
Adulteration or anomaly detection	Does the sample deviate from expected identity or composition?	Reference datasets, chemical profiles, DNA data, spectral data	Anomaly alert or adulteration-risk flag	Anomaly flags are screening outputs	Orthogonal confirmatory testing	False reassurance or excessive false alarms	Adds surveillance logic to standardization

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Safety screening support	Are safety-relevant constituents or patterns present?	Toxicity markers, known risk compounds, safety-related assay data	Safety-warning feature or risk-prioritization output	Predicted safety concern is not clinical risk assessment	Toxicological testing and exposure interpretation	Missing low-level but high-risk constituents	Integrates safety into consistency logic
Therapeutic consistency hypothesis	Is the product plausibly consistent with a defined quality profile?	Identity, processing, chemistry, bioactivity, marker, safety, and batch evidence	Evidence-integrated consistency hypothesis	Hypothesis is not clinical equivalence	Analytical validation, biological validation, expert review, and regulatory interpretation	Presenting a conceptual output as validated equivalence	Defines the model's final interpretive boundary

Proposed conceptual model

The proposed model begins with an identity-and-context gate that separates botanical authentication, plant part verification, geographic or cultivation context, harvesting, storage, processing, preparation, and extraction conditions. This stage reflects the principle that advanced quality-control strategies for herbal medicines require integrated consideration of identity, production context, chemical evaluation, and quality interpretation rather than isolated testing [25].

The second stage is analytical characterization. Chemical fingerprints, metabolomic profiles, spectroscopic patterns, and marker compound quantification are treated as complementary evidence streams rather than interchangeable proof of quality. The relevance of analytical methods depends on the herbal matrix, the type of claim being made, and whether the method is suitable, reproducible, and validated for its intended purpose [26].

The third stage adds preparation-aware therapeutic consistency boundaries. Dosage and preparation context are essential because a standardized chemical profile does not automatically define exposure, use conditions, or therapeutic relevance. Herbal dosage standardisation scholarship supports the view that consistency claims must account for preparation and dosing logic rather than relying only on fingerprints or marker presence [27].

The fourth stage connects bioactivity profiles, chemical–bioactivity alignment, and candidate quality-marker selection. Effect-oriented quality-standard approaches show how constituent information can be related to biological response patterns, supporting consistency hypotheses when the assay, marker logic, and validation pathway are appropriate [28]. In the proposed model, such evidence is used to prioritize candidate markers, not to claim therapeutic equivalence.

The fifth stage establishes validation and interpretation gates. Quality-marker progress in herbal medicine shows that marker systems remain dependent on evidence strength, analytical detectability, biological relevance, safety interpretation, and quality-standard context [29]. Therefore, the model ends with analytical validation, biological validation, safety-marker review, expert interpretation, and regulatory interpretation boundaries before any quality-standard claim is considered.

Table 3 presents the proposed conceptual model for AI-assisted herbal medicine standardization.

Table 3. Proposed Conceptual Model for AI-Assisted Herbal Medicine Standardization: Botanical Identity, Processing Context, Chemical Fingerprints, Bioactivity Profiles, Quality Markers, Batch Consistency, Safety Markers, Therapeutic Consistency Boundaries, and Validation Gates

Model component	Core question	Required evidence	AI-assisted role	High-confidence signal	Caution signal	Validation gate	Standardization implication
Botanical identity	Is the declared species correct?	Voucher identity, DNA or orthogonal authentication, taxonomic records	Identity classification and mismatch detection	Agreement across authenticated evidence streams	Ambiguous taxonomy, mixed material, missing reference data	Botanical authentication	Standardization cannot proceed reliably without identity confidence
Plant part verification	Is the correct plant part used?	Plant part documentation, microscopy, chemical or spectral profile	Classification of plant-part patterns	Consistent plant-part evidence across batches	Undocumented substitution or mixed parts	Plant part confirmation	Prevents non-equivalent material comparison
Geographic and	Is source context documented	Source records, cultivation or wild-harvest metadata,	Source-pattern clustering	Stable context-linked profile	Unrecorded sourcing or	Source documentation review	Helps interpret chemical and batch variation

cultivation context	and interpretable?	environmental context		within defined boundaries	inconsistent provenance		
Harvesting and storage context	Could collection or storage affect quality?	Harvest records, storage conditions, stability indicators	Anomaly detection in time- or storage-sensitive profiles	Stable profile under documented conditions	Degradation, contamination, or undocumented storage	Stability and storage evaluation	Adds temporal and handling awareness to QC
Processing and preparation method	Is the processed state appropriate and reproducible?	Processing records, preparation method, process-sensitive chemical features	Processing-state classification	Documented process with consistent analytical signature	Inconsistent or undisclosed processing	Processing verification	Distinguishes comparable and non-comparable materials
Extraction context	Is the analytical or product extract comparable?	Solvent, extraction method, preparation parameters	Pattern comparison across extraction contexts	Reproducible extraction-dependent profile	Matrix or extraction bias	Method suitability check	Prevents comparing chemically non-equivalent extracts
Chemical fingerprint	What is the overall chemical pattern?	Chromatographic or spectroscopic profile	Feature extraction, alignment, clustering	Reproducible fingerprint across authenticated batches	Peak drift, matrix effects, unexplained outliers	Analytical validation	Supports compositional consistency but not therapeutic equivalence alone
Metabolomic profile	Which known and unknown features vary?	Targeted and untargeted metabolomic data	Feature ranking and multivariate profiling	Stable annotated features with reproducible variation patterns	Low-confidence annotation or unstable features	Annotation and orthogonal confirmation	Expands quality assessment beyond selected markers
Marker compound quantification	Are selected compounds measurable and consistent?	Validated quantitative assay and reference standards	Outlier detection and marker-panel monitoring	Reliable quantification with relevant marker rationale	Isolated abundance without biological or safety relevance	Quantitative method validation	Provides measurable quality attributes
Bioactivity profile	Are relevant biological responses observed consistently?	Assay outputs, response patterns, assay metadata	Activity-pattern recognition	Reproducible response in relevant validated assay	Non-specific or poorly controlled activity	Biological assay validation	Adds biological relevance without proving clinical benefit
Chemical–bioactivity alignment	Do chemical features align with bioactivity patterns?	Paired chemical and assay datasets	Spectrum–effect modeling and feature association	Reproducible feature–activity association	Correlation without confirmation	Confirmatory biological testing	Supports candidate quality-marker prioritization
Quality-marker panel	Which markers best represent quality evidence?	Traceability, specificity, detectability, biological relevance, safety relevance	Evidence weighting and marker ranking	Marker panel supported by chemistry, biology, and safety logic	Single-marker reductionism	Analytical and biological validation	Creates a defensible standardization hypothesis
Batch consistency	Are batches comparable within defined boundaries?	Batch fingerprints, marker levels, bioactivity profiles, process records	Batch clustering and consistency classification	Convergent chemical, biological, and process evidence	Similar chemistry but divergent bioactivity or safety signals	Batch-level testing	Supports consistency assessment, not equivalence claims
Safety-marker screening	Are safety-relevant signals controlled?	Known toxic constituents, safety assays, risk-related markers	Safety-feature prioritization and anomaly alerts	Absence or control of defined safety-relevant markers	Unknown risk markers or untested toxicity concerns	Toxicological review	Prevents quality claims that ignore safety consistency

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Therapeutic consistency boundary	What can be inferred about therapeutic consistency?	Integrated identity, chemistry, bioactivity, marker, safety, and validation evidence	Evidence integration and uncertainty communication	Convergent validated evidence across layers	Unsupported leap from fingerprint similarity to clinical equivalence	Expert and regulatory interpretation	Defines the boundary between a consistency hypothesis and validated standard

Figure 1 illustrates the proposed AI-assisted conceptual model for standardizing herbal medicines through chemical fingerprints, bioactivity profiles, quality markers, and therapeutic consistency boundaries.

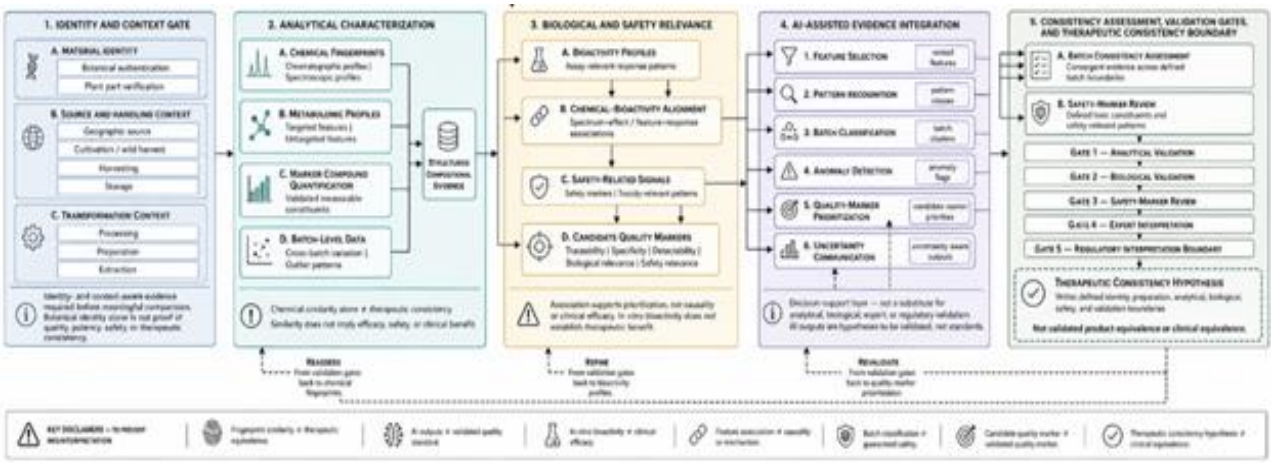

Figure 1. AI-Assisted Conceptual Model for Herbal Medicine Standardization

Alt-text description

A conceptual workflow diagram showing herbal medicine identity and processing context feeding into chemical fingerprinting, bioactivity profiling, quality-marker selection, AI-assisted pattern recognition, batch consistency assessment, safety screening, validation gates, and therapeutic consistency boundaries.

CONCLUSION

This article proposed an AI-assisted conceptual model for herbal medicine standardization that integrates botanical identity, plant part and processing context, chemical fingerprints, metabolomic profiles, marker compound quantification, bioactivity profiles, quality-marker selection, batch consistency, anomaly detection, safety-marker screening, validation gates, and therapeutic consistency boundaries. The model clarifies that AI can strengthen standardization only when used as an evidence-integration and decision-support layer, not as a replacement for rigorous analytical validation, biological relevance assessment, safety interpretation, expert review, or regulatory evaluation. By separating compositional similarity, bioactivity relevance, marker plausibility, batch consistency, and therapeutic consistency hypotheses, the model provides a structured framework for developing more transparent, evidence-aware, and cautious standardization logic for complex herbal medicines.

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