Predicting Chemical Change in Herbal Formulas: A Computational-to-Experimental Framework for Prospective Prioritization

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Abstract

Herbal preparations are chemically complex systems whose composition may vary across botanical sourcing, processing, decoction, herb–herb interactions, and post-preparation storage or exposure. Although modern analytical methods can characterize these changes, the number of constituents and possible variability conditions creates a large experimental search space and makes comprehensive testing impractical. This perspective proposes that computational approaches can provide a prospective prioritization layer that helps identify which compounds and chemical questions should receive targeted analytical attention.

A computational-to-experimental framework is presented in which predefined marker compounds are evaluated computationally, ranked before experimental analysis, subjected to a controlled variability condition, and compared with an analytical measure of observed chemical change. Post-preparation light exposure in a Jiang Huang (*Curcuma longa*) decoction is used as an illustrative proof-of-concept. Curcumin, demethoxycurcumin, and bisdemethoxycurcumin are selected as structurally related markers for comparative evaluation. Ground-state density functional theory and time-dependent density functional theory are proposed to generate structural, electronic, and excitation-related information from which a prospective ranking of relative light susceptibility can be developed. Thin-layer chromatography is positioned as an accessible initial readout for comparing normalized marker-band changes and broader fingerprint alterations between light-exposed and matched dark-control samples.

Directional agreement would support the feasibility of computational prioritization but would not establish definitive degradation mechanisms or complete representation of the herbal matrix. The proposed framework is intended to guide hypothesis-driven analytical investigation and could later be extended to additional variability sources, more complex herbal systems, and confirmatory methods such as high-performance liquid chromatography, liquid chromatography–mass spectrometry, and nuclear magnetic resonance spectroscopy.

Keywords: herbal chemical variability; computational chemistry; density functional theory; time-dependent density functional theory; curcuminoids; thin-layer chromatography; photostability; herbal decoctions

1. Introduction

Herbal preparations are chemically complex systems composed of multiple constituents rather than single isolated compounds. In multi-herb formulas, this complexity is further increased by differences in botanical materials, processing histories, extraction conditions, and interactions that occur when herbs are prepared together (Muyumba et al., 2021). The chemical composition associated with an herbal name or written formula is therefore not necessarily fixed. Differences introduced during sourcing, processing, preparation, and storage may alter the identity, abundance, and relative balance of detectable metabolites in the preparation ultimately analyzed or administered (Ji et al., 2024). Modern analytical platforms have substantially improved the ability to examine this complexity. Thin-layer chromatography (TLC), high-performance thin-layer chromatography, high-performance liquid chromatography, liquid chromatography–mass spectrometry, and nuclear magnetic resonance spectroscopy can provide chemical fingerprints, quantitative measurements, and structural information at different levels of analytical depth (Noviana et al., 2022).

Whole-profile fingerprinting can also provide a broader assessment of chemical consistency than measurement of a single selected marker. Nevertheless, interpretation remains dependent on the samples, conditions, and sources of variability chosen for investigation (Pei et al., 2023). The central challenge is therefore not the absence of capable analytical technologies, but the size of the experimental search space created by numerous constituents and multiple interacting sources of variability. Analytical methods can characterize selected samples and document differences between defined conditions, but they do not automatically determine which compounds, variability sources, or possible transformations should be investigated first (Ji et al., 2024). Comprehensive testing of every constituent under every relevant combination of sourcing, processing, preparation, interaction, and storage conditions is rarely practical. A complementary strategy is therefore needed to narrow the experimental question while retaining analytical chemistry as the essential means of determining whether chemical change has occurred.

Computational approaches may provide one such strategy. Depending on the research question, these methods can organize chemical information, identify patterns within datasets, simulate molecular interactions, calculate structural or electronic properties, and generate hypotheses that can subsequently be examined experimentally (Molski, 2025). Their proposed role in herbal-chemistry research is not to replace direct characterization or independently establish the composition of a complex preparation. Instead, computation may provide a prospective prioritization layer that helps identify which compounds or chemical questions warrant targeted analytical attention. Prospective prioritization differs from using computational results retrospectively to explain an experimental pattern after it has already been observed. Predictions and interpretation criteria should be defined before analytical findings are examined so that the experimental study can test whether computation provided useful guidance rather than merely a plausible post hoc explanation.

This perspective is guided by the following broad question: How can computational approaches be integrated with analytical chemistry to generate experimentally testable hypotheses for investigating chemical variability in herbal preparations? To address this question, the paper proposes a computational-to-experimental framework in which predefined marker compounds are evaluated computationally and ranked prospectively before a controlled variability condition is applied. The predicted ranking is then compared with an analytical measure of observed chemical change. The intended contribution is not a universal model capable of predicting every transformation within an herbal preparation. Rather, it is a structured process for reducing a broad characterization problem to a focused, transparent, and experimentally testable comparison.

A deliberately narrow proof-of-concept is used to illustrate the framework. Post-preparation light exposure was selected as the model variability source because light is a recognized stability factor that can be applied under defined conditions and evaluated against a matched dark control (Kim et al., 2019). Jiang Huang, the rhizome of *Curcuma longa*, serves as the initial single-herb model. Its major curcuminoids—curcumin, demethoxycurcumin, and bisdemethoxycurcumin—share a related conjugated scaffold while differing in methoxy substitution, providing a manageable system for comparative molecular ranking (Priyadarsini, 2014). Ground-state density functional theory (DFT) and time-dependent density functional theory (TD-DFT) are proposed to generate structural, electronic, and excitation-related information for the three markers. These outputs are used to create a prospective ranking of relative light susceptibility rather than to predict an exact degradation rate or mechanism (Ghosh & Sarkar, 2024).

Thin-layer chromatography is proposed as the initial analytical readout because it can compare authentic standards, light-exposed samples, and matched dark controls while also displaying broader changes in the chemical fingerprint. TLC is positioned as a first-line screening approach, with substantial or reproducible findings requiring stronger quantitative or structural confirmation (Kotra et al., 2019).

The model does not assume that isolated-molecule calculations will fully represent the behavior of curcuminoids within an aqueous herbal matrix. Solvation, pH, oxygen, aggregation, extraction efficiency, and interactions with co-extracted constituents may cause observed behavior to differ from the prospective molecular ranking (Jen et al., 2022).

Directional agreement between the computational ranking and the analytical response would therefore support the feasibility of computational prioritization, not establish a complete photochemical pathway. Disagreement would also remain informative by identifying limitations in the molecular model, experimental exposure, herbal matrix, or analytical sensitivity.

The novelty proposed here lies in integrating established components into a prospective, preparation-centered workflow. Computational analysis, controlled light exposure, turmeric chemistry, and TLC have each been investigated separately, but the framework connects them as a defined sequence in which prediction precedes experimental evaluation.

This paper first defines chemical variability and the resulting characterization gap. It then examines how computational approaches may support prospective prioritization, explains the rationale for each component of the Jiang Huang proof-of-concept, presents the integrated computational-to-experimental framework, and considers its broader implications, validation requirements, and future extension to additional variability sources and more complex herbal formulas.

2. Chemical Variability and the Characterization Gap

2.1 What Is Chemical Variability?

Chemical variability refers to differences in the identity, abundance, and relative balance of metabolites among raw herbs, decoctions, and finished herbal preparations. These differences may develop cumulatively across an herbal formula's lifecycle rather than arising solely from random analytical variation (Muyumba et al., 2021). As illustrated in Figure 1, chemical variability may be introduced across six stages: botanical identity; harvest and raw-material selection; processing; decoction preparation; herb–herb interactions; and storage or environmental exposure. The top-to-bottom arrangement emphasizes that each stage can influence the chemical composition carried forward into subsequent preparation, storage, and use (Ji et al., 2024).

The first stage is botanical identity, including plant species, geographic origin, and differences associated with the source material. Environmental growing conditions can influence secondary-metabolite biosynthesis before the herb is harvested (Ncube et al., 2012). The second stage is harvest and raw-material selection, including season, plant maturity, harvest timing, and the plant part selected. These factors affect the identity and abundance of constituents available for later processing and extraction (Moomin et al., 2023). The third stage is processing, including traditional *Pao Zhi* practices such as drying, steaming, and roasting. These procedures are chemically active and may alter constituent stability, solubility, extractability, or transformation before decoction occurs (Chen et al., 2018). The fourth stage involves decoction variables, including herb-to-water ratio, water properties, temperature, heating duration, extraction procedure, and filtration. Consequently, preparations made from the same named herb or formula may not be chemically equivalent when their decoction procedures are not standardized (Hlatshwayo et al., 2025).

The fifth stage involves herb–herb interactions during formula preparation. The chemistry of a combined decoction may differ from the simple sum of its individual herbs because co-extraction, complex formation, precipitation, pH-dependent effects, and altered dissolution can change which constituents remain detectable in the final preparation (Cheung et al., 2017). These interactions may modify both the identity and relative abundance of extracted compounds. Co-decoction should therefore be considered a chemically consequential process rather than merely the simultaneous extraction of independently behaving herbs (Jang et al., 2025). The sixth stage is storage and exposure, including light, oxygen, heat, humidity, time, and transportation

conditions. Chemical composition may continue to change after decoction even when the botanical material, processing method, and preparation procedure were initially standardized (Laher et al., 2013).

Together, the stages shown in Figure 1 produce a dynamic chemical composition in which metabolite identity, abundance, and relative balance may shift throughout preparation, storage, and use. The highlighted storage-and-exposure stage represents the present proof-of-concept focus while remaining one component of the broader variability lifecycle.

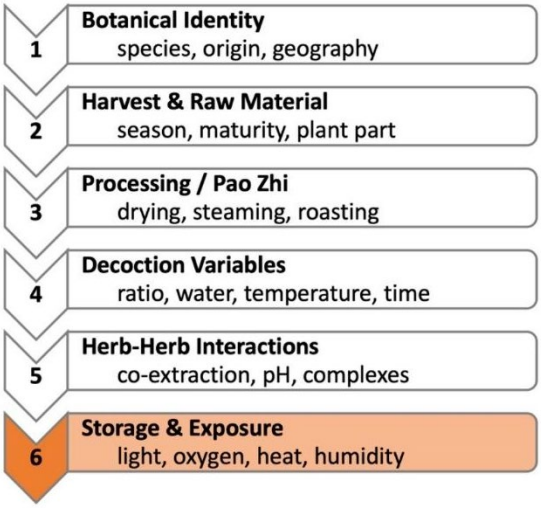

Figure 1. Lifecycle sources of chemical variability in herbal formulas. Six stages at which botanical identity, raw-material selection, processing, decoction conditions, herb–herb interactions, and post-preparation exposure may alter chemical composition. Storage and exposure are highlighted as the focus of the present proof-of-concept.

2.2 Why Does Chemical Variability Matter?

Chemical variability matters because the activity, safety, and quality of herbal formulas arise from chemically complex mixtures rather than from a single isolated constituent. Preparations carrying the same herbal or formula name may therefore differ chemically when their raw materials, processing histories, preparation procedures, or storage environments are not equivalent (Wang et al., 2023). Because chemical composition forms the basis of analytical characterization, uncontrolled variability directly affects the interpretation and reproducibility of experimental findings. It may become difficult to determine whether an observed chemical or biological difference reflects the intended formula or an uncontrolled sourcing, processing, preparation, or storage variable (Muyumba et al., 2021).

Variability also complicates standardization because confirmation of botanical identity or measurement of one selected marker compound does not necessarily establish equivalence across

the broader chemical profile. A single-marker assay may overlook coordinated changes among multiple constituents, shifts in the relative balance of related metabolites, or compounds formed during processing and storage (Noviana et al., 2022). Whole-profile fingerprinting and multivariate analysis can provide a broader assessment of chemical consistency than isolated-marker testing alone. However, the interpretation of these profiles still depends on adequately documenting and controlling the sources of variability affecting the samples being compared (Pei et al., 2023).

2.3 Why Current Analytical Characterization Remains Challenging

Modern analytical methods have substantially improved the detection, separation, quantification, and structural characterization of herbal constituents. TLC and HPTLC provide accessible chemical fingerprints, while HPLC, LC–MS, and NMR offer increasingly detailed quantitative and structural information (Muyumba et al., 2021). These techniques are indispensable and should remain central to herbal quality assessment and experimental validation. Fingerprinting approaches are particularly valuable because they capture broader compositional patterns that may not be represented by measuring a single marker compound (Noviana et al., 2022).

The central limitation is therefore not that current analytical technologies are ineffective, but that the number of constituents, variables, and possible transformations creates an exceptionally large experimental search space. Analytical measurements can describe the composition of a sample or document changes after they have occurred, but they do not automatically determine which compounds, conditions, or transformations should be investigated first (Ji et al., 2024). Exhaustively examining every constituent under every relevant combination of botanical origin, processing, preparation, interaction, and storage conditions is rarely practical. This challenge becomes greater in multi-herb formulas, where co-decoction may alter extraction, precipitation, dissolution, and constituent abundance in ways that cannot be inferred solely from analyses of the individual herbs (Jang et al., 2025).

The remaining characterization gap is therefore not the absence of powerful analytical tools, but the difficulty of deciding where experimental effort should be focused within a highly complex chemical system. Addressing this gap requires a complementary predictive strategy that can prioritize chemically relevant compounds, conditions, and testable molecular questions before extensive laboratory investigation, while retaining analytical chemistry as the essential means of validation (Noviana et al., 2022).

3. Computational Approaches for Prospective Prioritization

The characterization challenge identified in Section 2 is fundamentally a problem of prioritization: herbal preparations may contain numerous constituents affected by multiple sources of variability, yet every compound and condition cannot be investigated simultaneously. Computational approaches may help narrow this experimental search space by generating

testable hypotheses and identifying chemical questions that warrant targeted laboratory investigation (Molski, 2025).

In this context, computation is not intended to replace analytical characterization or independently establish what has occurred within an herbal preparation. Its proposed role is to provide a prospective layer of chemical reasoning that helps determine where experimental attention should be directed before analytical findings are known (Molski, 2025).

3.1 What Computational Approaches Can Contribute

Computational approaches examine chemical information at different scales and for different purposes. Some organize and compare large compound or analytical datasets, whereas others model molecular movement, interactions, electronic structure, or excitation-related behavior (Molski, 2025). These methods can contribute to herbal-chemistry research by screening potential marker compounds, identifying patterns within chemical fingerprints, estimating molecular properties, and evaluating possible interactions under defined conditions. Their practical value lies in reducing a broad chemical problem to a smaller number of experimentally testable priorities (Noviana et al., 2022).

A prospective computational strategy should generate predictions or ranking criteria before the corresponding experimental findings are interpreted. Defining those outputs in advance reduces the risk of selecting computational results retrospectively only because they appear to explain an observed analytical pattern (Molski, 2025). The relationship between computational and analytical methods should therefore remain complementary. Computational approaches can indicate which compounds, conditions, or responses may deserve focused investigation, while analytical measurements are required to determine whether the predicted behavior is observed in the herbal preparation (Molski, 2025).

3.2 Major Computational Approaches

Several computational approaches may contribute to the investigation of chemical variability in herbal preparations. As summarized in Table 1, they differ in their primary purpose, data requirements, modeled chemical scale, and principal limitations.

Table 1. Computational approaches relevant to prospective prioritization in herbal-chemistry research.

Computational approach	Primary contribution	Main requirement	Principal limitation
Cheminformatics and chemometrics	Organization, screening, and comparison of compound or fingerprint data	Curated chemical or analytical datasets	Conclusions depend on data quality and coverage (Noviana et al., 2022)
Machine learning and QSAR	Identification of predictive relationships across compounds or samples	Sufficiently large and standardized training datasets	Limited reliability when datasets are small, heterogeneous, or poorly standardized (Romano, 2019)
Molecular dynamics	Simulation of molecular movement, solvation, aggregation, and interactions	A defined molecular environment and substantial computational resources	Results depend on model assumptions and may become complex for multicomponent matrices (Jen et al., 2022)
Electronic-structure modeling	Evaluation of molecular geometry, energetics, electron distribution, reactivity, and excitation-related properties	A predefined and manageable set of molecular structures	Isolated-molecule models provide an incomplete representation of an herbal matrix (Molski, 2025)
Advanced hybrid or excited-state methods	Detailed investigation of solvent effects and photochemical pathways	Specialized expertise and high computational demand	Often disproportionate to the needs of an initial screening study (Gibbard, 2025)

Cheminformatics and chemometric methods are useful for organizing phytochemical information, screening compound collections, and comparing analytical fingerprints across multiple samples. Their usefulness depends on the availability, quality, and consistency of the chemical or analytical data included in the comparison (Noviana et al., 2022). Machine-learning and quantitative structure–activity relationship methods can identify predictive patterns across compounds or samples when appropriate training data are available. Their reliability is reduced when datasets are small, heterogeneous, poorly standardized, or insufficiently representative of the chemical question being investigated (Romano, 2019). Molecular dynamics simulates molecular movement and interactions over time within a defined environment. It can provide information about solvation, aggregation, and interactions among phytochemicals, although representing a multicomponent aqueous herbal matrix may introduce substantial computational and interpretive complexity (Jen et al., 2022).

Electronic-structure methods focus on the structural and electronic properties of individual molecules. They can provide interpretable information about optimized geometry, relative energetics, electron distribution, qualitative reactivity, and electronic excitation without requiring a large experimental training dataset (Molski, 2025). More advanced methods, including quantum mechanics/molecular mechanics models and excited-state molecular dynamics, can provide richer representations of solvent effects and photochemical pathways. Their methodological complexity and computational demands may nevertheless exceed what is required for an initial study intended primarily to prioritize compounds for experimental evaluation (Gibbard, 2025).

These computational approaches should not be viewed as mutually exclusive or arranged in a simple hierarchy. They address different questions and may become complementary as a research program progresses from small marker sets to complex matrices, larger compound libraries, and experimentally validated datasets (Molski, 2025).

3.3 Requirements for Prospective Computational Prioritization

The suitability of a computational approach depends on the chemical question it is expected to address. Method selection should consider the number and type of compounds, the amount and quality of available data, the condition being investigated, and the experimental outcome against which the prediction will be evaluated (Molski, 2025). The selected method should also generate outputs that are chemically interpretable and capable of being translated into a predefined experimental comparison. A computational result has limited practical value for prioritization when it cannot support a clear decision about which compound, condition, or response should receive laboratory attention (Molski, 2025).

The computational scale should correspond to the available evidence and the scope of the proposed study. Large-data methods are best supported when standardized training datasets exist, whereas molecule-centered approaches may be more practical when the investigation involves a small, predefined compound set (Romano, 2019). Model complexity should remain proportional

to the intended contribution of the study. An initial proof-of-concept designed to evaluate whether prospective prioritization is feasible does not require complete simulation of every constituent, solvent interaction, and reaction pathway within an herbal preparation (Gibbard, 2025).

Computational results must also be interpreted within the limitations of the modeled chemical environment. Predictions generated for isolated molecules or simplified solvent systems may differ from observations in aqueous herbal preparations because solvation, pH, oxygen, aggregation, and interactions with co-extracted constituents can alter molecular behavior (Jen et al., 2022). Finally, a prospective strategy requires an analytical endpoint capable of evaluating the type of outcome being predicted. The variability source, model system, marker compounds, computational method, and analytical readout must therefore be selected as connected components of one research question rather than as independent methodological decisions.

Section 4 applies these requirements to the proposed proof-of-concept and explains the rationale for selecting its variability source, herbal model, marker compounds, computational approach, and initial analytical readout.

4. Rationale for the Proof-of-Concept Model

To demonstrate how prospective computational prioritization could be applied to herbal chemical variability, the proposed framework requires a deliberately narrow and experimentally testable model. The variability source, herbal preparation, marker compounds, computational approach, and analytical readout must work together to generate a defined prediction that can subsequently be evaluated under controlled conditions.

The proof-of-concept therefore examines post-preparation light exposure in a Jiang Huang preparation using curcumin, demethoxycurcumin, and bisdemethoxycurcumin as comparative markers. Ground-state density functional theory and time-dependent density functional theory are proposed to generate a prospective susceptibility ranking, while thin-layer chromatography provides the initial analytical evaluation of directional agreement.

4.1 Selection of Post-Preparation Light Exposure

Storage and environmental exposure represent one of the six lifecycle stages identified in Figure 1 as potential sources of herbal chemical variability. Light was selected from this category because it is a recognized stability factor that can influence the chemical properties of finished herbal products during storage and handling (Kim et al., 2019). Light exposure also provides a controllable model stressor. Unlike uncontrolled room or window exposure, an experimental light condition can be defined and compared with a matched sample protected from light.

Published research demonstrates that curcumin-containing systems can undergo measurable chemical change following exposure to light. The magnitude and nature of that response may depend on wavelength, exposure dose, oxygen availability, solvent environment, and the

physical form of the sample (Appendino et al., 2022). Turmeric-derived materials also display light-associated changes in more chemically complex preparations. Fluorescent-light and white-light-emitting-diode exposure have been associated with changes in turmeric oleoresin color, fluorescence, and curcuminoid stability (Kim et al., 2025).

The major curcuminoids may not respond identically under the same conditions. Reported differences in the light-associated decomposition of curcumin, demethoxycurcumin, and bisdemethoxycurcumin provide a scientific basis for testing a relative susceptibility ranking rather than evaluating only whether curcumin changes (Price & Buescher, 1996). Most existing photostability evidence has been generated using purified compounds, solutions, pigments, extracts, or oleoresins rather than traditional aqueous decoctions. Applying light exposure to a Jiang Huang preparation therefore extends established chemical observations into a more preparation-specific proof-of-concept without assuming that the same response will necessarily occur in the herbal matrix.

Light is not presented as the only or most important source of herbal chemical variability. It serves as an experimentally manageable starting condition through which the feasibility of prospective computational prioritization can first be evaluated.

4.2 Selection of Jiang Huang and the Curcuminoid Markers

Jiang Huang, the rhizome of *Curcuma longa*, was selected because its principal curcuminoids are well characterized and widely used as analytical markers. Curcumin, demethoxycurcumin, and bisdemethoxycurcumin form a chemically related group that can be examined individually and comparatively (Priyadarsini, 2014). The three curcuminoids share a conjugated molecular scaffold but differ in the number of methoxy substituents present on their aromatic rings. These structural differences can influence electron distribution, intramolecular interactions, absorption behavior, stability, and chemical responsiveness (Priyadarsini, 2014).

Using all three markers provides more information than evaluating curcumin alone. Their structural similarity supports a controlled molecular comparison, while their differences permit construction of a relative ranking rather than a simple changed-versus-unchanged outcome.

Jiang Huang also offers a practical connection between traditional herbal preparation and modern phytochemical analysis. Its curcuminoids have been studied using chromatographic and spectroscopic methods, making them defensible marker compounds for an initial integrated framework (Kotra et al., 2019). The use of a single herb intentionally limits the complexity of the first model. Multi-herb formulas may introduce co-extraction, precipitation, complex formation, altered dissolution, and other interaction effects that could make it difficult to distinguish limitations of the computational prediction from effects of the formula matrix (Jang et al., 2025). Jiang Huang should therefore be understood as a controlled starting system for a framework ultimately intended for broader application to herbal formulas. Demonstrating feasibility in a

single-herb preparation provides a more interpretable foundation before progressing to herb combinations and multi-herb decoctions.

One important limitation is the low aqueous solubility of curcumin and related curcuminoids. Detectability in an aqueous preparation may consequently depend on extraction efficiency, sample concentration, and the sensitivity of the selected analytical method rather than only on chemical stability (Priyadarsini, 2014). The purpose of the model is not to characterize the complete Jiang Huang metabolome. It is to determine whether three predefined and structurally related markers can support a prospective comparison between predicted molecular susceptibility and observed chemical response.

4.3 Selection of Ground-State DFT and TD-DFT

The proof-of-concept involves three predefined molecular structures and does not rely on a large experimental training dataset. It also requires chemically interpretable outputs that can be connected to structural differences and light-related behavior.

Ground-state density functional theory is appropriate for establishing a consistent structural and electronic baseline for each curcuminoid. Geometry optimization and related calculations can provide comparative information about molecular structure, relative energetics, electron distribution, frontier molecular orbitals, and qualitative reactivity descriptors (Molski, 2025). These properties may help identify intrinsic differences among structurally related markers. They are interpreted as comparative indicators that may support prioritization rather than as direct measurements of photodegradation, degradation rate, or chromatographic band loss (Baira et al., 2022).

Since the selected variability source is light, the computational strategy must also address electronic excitation. Time-dependent density functional theory can estimate vertical excitation energies, approximate absorption wavelengths, oscillator strengths, and the orbital contributions associated with electronic transitions (Priyadarsini, 2009). These outputs create a more direct connection to the light-exposure question than ground-state descriptors alone. Predicted absorption behavior can be considered in relation to the spectral range of the selected light source when determining whether excitation is chemically plausible (Ghosh & Sarkar, 2024).

Ground-state DFT and TD-DFT therefore serve complementary functions within the model. Ground-state calculations provide structural and electronic context, whereas TD-DFT addresses absorption and excitation-related behavior more directly (Molski, 2025). The two methods are not expected to identify exact degradation products, complete reaction pathways, or quantitative degradation kinetics within the preparation. Those questions would require more advanced computational treatments together with analytical methods capable of stronger structural confirmation (Gibbard, 2025).

The surrounding chemical environment also remains a major limitation. Solvation, pH, oxygen, hydrogen bonding, aggregation, and interactions with co-extracted constituents may cause

molecules in an aqueous herbal preparation to behave differently from isolated compounds or simplified computational models (Jen et al., 2022). For these reasons, the computational output is defined as a prospective relative ranking rather than an exact prediction of experimental change. The selected methods are intended to prioritize the comparison and generate a testable hypothesis, not replace direct evaluation of the herbal preparation.

4.4 Selection of TLC as the Initial Analytical Readout

Thin-layer chromatography was selected because the initial research question concerns directional agreement between a prospective molecular ranking and observed changes in predefined markers. TLC permits authentic standards, control samples, and exposed samples to be compared on the same plate while also displaying the broader chemical fingerprint of the preparation.

TLC and HPTLC are established tools for botanical identification, fingerprint comparison, and curcuminoid marker analysis. Published turmeric methods demonstrate that curcuminoid bands can be separated and evaluated using silica-based stationary phases, appropriate mobile phases, ultraviolet visualization, and densitometric analysis when available (Kotra et al., 2019).

The method can reveal changes in parent-marker intensity, the appearance of additional bands, shifts in chromatographic patterns, and broader fingerprint perturbation. Standardized image analysis or densitometry can further reduce the subjectivity associated with visual comparison alone (Kushwaha et al., 2021).

TLC is also proportionate to the purpose of an initial proof-of-concept. The immediate objective is to determine whether a reproducible analytical pattern is detectable and whether the marker predicted to be most susceptible shows the greatest relative change.

The method is not being selected to identify unknown degradation products or establish complete mechanisms. TLC alone cannot provide the same level of quantification or structural confirmation available from HPLC, LC–MS, or NMR (Noviana et al., 2022).

Substantial and reproducible TLC findings would therefore provide a basis for prioritizing samples and compounds for confirmatory analysis. TLC is positioned as an accessible first-line screening approach rather than a complete analytical-validation platform.

The limited aqueous extraction of curcuminoids must nevertheless be considered when interpreting the results. Weak marker detection could reflect sample preparation or analytical sensitivity rather than either chemical stability or resistance to light-induced change.

Detailed decisions regarding sample concentration, control conditions, plate development, image acquisition, and normalization are part of the operational framework presented in Section 5. Their inclusion there preserves the distinction between why TLC was selected and how it would be applied.

4.5 Proof-of-Concept Question and Evaluation Logic

The selection of post-preparation light exposure, Jiang Huang, three comparative curcuminoid markers, DFT and TD-DFT, and TLC leads to the following proof-of-concept question:

Can ground-state DFT and TD-DFT generate a prospective ranking of curcumin, demethoxycurcumin, and bisdemethoxycurcumin that shows directional agreement with light-associated TLC changes in a Jiang Huang preparation?

The primary analytical outcome is the normalized change in each curcuminoid marker band relative to its matched dark control. Broader alteration of the TLC fingerprint is treated as a secondary outcome because whole-profile change does not directly establish which of the three selected markers was most responsive. The computational and analytical outcomes are compared through directional ranking rather than numerical equivalence. Calculated molecular properties and chromatographic band intensities represent different physical measurements and should not be interpreted as directly interchangeable values.

Directional agreement would support the feasibility of using computational prediction to prioritize compounds for targeted analytical evaluation. It would not prove that the calculations identified a complete degradation mechanism, nor would it establish that the same ranking applies across different preparation, matrix, storage, or light conditions. The contribution of the proof-of-concept therefore lies in the prospective integration of established components rather than in treating any individual component as novel. Section 5 describes how these selections are organized into a computational-to-experimental sequence and how the predicted ranking is evaluated against the observed analytical response.

5. Proposed Computational-to-Experimental Framework

5.1 Framework Overview

The proposed framework integrates prospective computational prediction with controlled experimental testing and analytical evaluation. As illustrated in Figure 2, the workflow progresses through three phases designed to determine whether calculated molecular properties can meaningfully prioritize compounds for targeted laboratory investigation.

The first phase selects and computationally evaluates predefined marker compounds to generate a prospective susceptibility ranking. The second phase subjects a standardized Jiang Huang decoction to controlled light exposure, and the third phase compares the predicted ranking with marker-band and fingerprint changes observed by thin-layer chromatography.

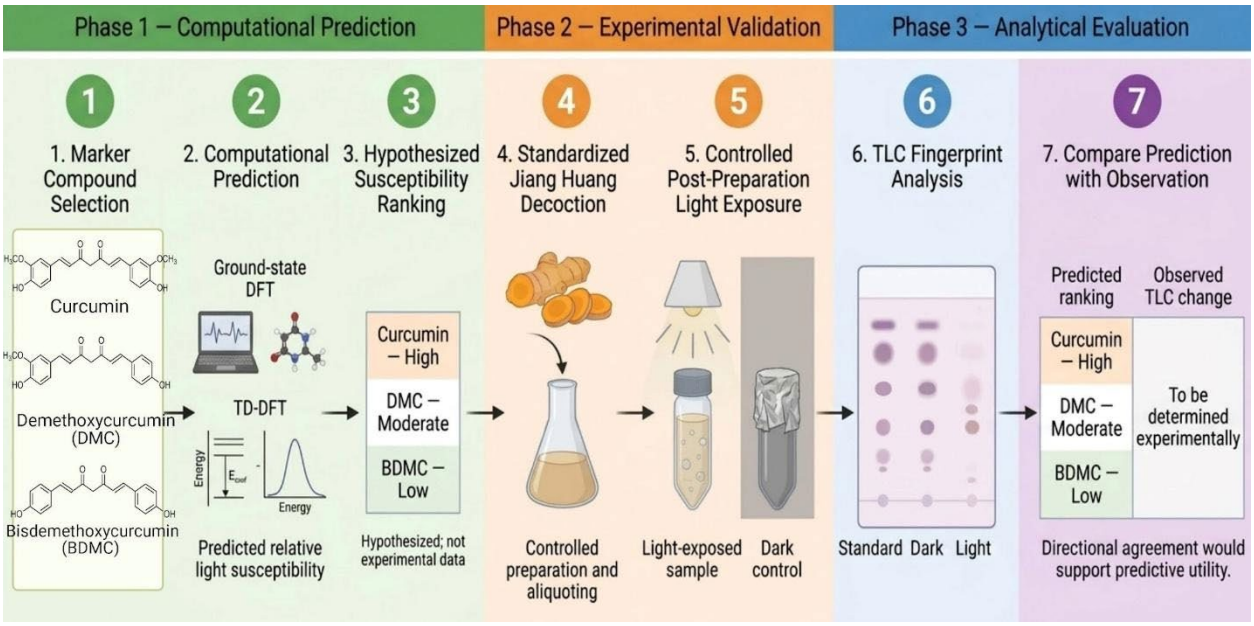

Figure 2. Proposed computational-to-experimental framework. Ground-state density functional theory (DFT) and time-dependent density functional theory (TD-DFT) generate a prospective susceptibility ranking for curcumin, demethoxycurcumin, and bisdemethoxycurcumin. The ranking is evaluated through standardized Jiang Huang decoction preparation, controlled light exposure, thin-layer chromatography (TLC) fingerprint analysis, and comparison of predicted and observed marker changes.

Recording the computational ranking before examining the analytical findings distinguishes the framework from a retrospective explanation developed after a chemical pattern is already known. Computation is therefore positioned as a hypothesis-generation and prioritization tool rather than as a post hoc interpretation of experimental results (Molski, 2025).

The framework does not assume that calculations performed on isolated molecules will reproduce every chemical process occurring within an aqueous herbal matrix. Instead, it tests whether a simplified molecular comparison can provide useful prospective direction for targeted analytical evaluation.

5.2 Computational Prediction and Prospective Ranking

The first phase of Figure 2 comprises marker selection, computational analysis, and generation of a prospective susceptibility ranking. Selected markers should be supported by the phytochemical literature, detectable using the intended analytical method, and sufficiently related in structure to permit meaningful comparison (Kotra et al., 2019). Curcumin, demethoxycurcumin, and bisdemethoxycurcumin provide a defined three-marker set rather than relying on curcumin alone to represent the broader curcuminoid profile. Their shared conjugated scaffold supports controlled structural comparison, while differences in methoxy substitution allow the outcome to be expressed as a relative ranking (Priyadarsini, 2014).

Ground-state DFT would first be used to optimize the molecular structure of each marker and calculate selected structural and electronic descriptors. These calculations provide a consistent molecular baseline and comparative information about intrinsic differences in molecular geometry, electron distribution, frontier orbitals, and qualitative reactivity (Molski, 2025). The ground-state outputs would be interpreted comparatively rather than as direct indicators of experimental degradation. A frontier-orbital energy, energy gap, or related reactivity descriptor cannot independently predict the percentage of marker-band loss observed by TLC (Baira et al., 2022).

TD-DFT would then be used to estimate vertical excitation energies, approximate absorption wavelengths, oscillator strengths, and the orbital character of relevant electronic transitions. These outputs allow predicted transitions to be compared with the wavelength range of the selected light source (Ghosh & Sarkar, 2024). Spectral overlap would indicate that molecular excitation is plausible under the proposed exposure conditions, but it would not independently establish that photochemical degradation will occur. The interpretation should therefore consider absorption wavelength, oscillator strength, excitation energy, transition character, and supporting ground-state information together (Priyadarsini, 2009).

The criteria used to derive the susceptibility ranking should be defined before the TLC findings are examined. If the calculated properties do not clearly distinguish two markers, the result should be reported as tied, partially ranked, or indeterminate rather than forced into an unsupported order. The final ranking and the rules used to generate it should be documented before experimental interpretation begins. This preserves the prospective purpose of the framework and reduces the risk of selectively emphasizing computational outputs because they agree with the observed TLC pattern.

5.3 Standardized Preparation and Controlled Light Exposure

The second phase of Figure 2 translates the prospective ranking into a controlled herbal experiment. Preparation conditions must be standardized because herb-to-water ratio, water properties, heating duration, temperature, extraction procedure, and filtration can alter which constituents enter the liquid phase and their relative abundance (Hlatshwayo et al., 2025). A single standardized Jiang Huang decoction should be divided into matched aliquots after preparation so that the light-exposed and dark-control samples begin with the same chemical profile. Replicate aliquots should be included when feasible to help distinguish reproducible chemical change from variation introduced during preparation, storage, or sample handling (Moomin et al., 2023).

The light-exposed aliquots should be maintained under a defined source for a predetermined period, while matched dark controls remain protected from light under otherwise equivalent conditions. The light source should be documented by type, wavelength range, exposure duration, and irradiance when measurable, and temperature should be monitored to distinguish light-associated effects from lamp-generated heating (Kim et al., 2019). Container type, storage

duration, sample volume, headspace, and environmental conditions should remain as similar as possible between the exposed and control groups. The primary difference between the two conditions should be the presence or absence of light exposure.

The lamp spectrum should be compared with the predicted absorption ranges before the experimental outcome is interpreted. Even when spectral overlap is present, solvation, pH, oxygen, aggregation, and interactions with co-extracted constituents may cause the Jiang Huang decoction to behave differently from isolated-molecule predictions (Jen et al., 2022). Curcuminoid detectability also requires consideration because curcumin and related compounds have limited aqueous solubility. Weak marker detection should not automatically be interpreted as degradation, and standardized concentration, drying, or reconstitution may be required before decoction samples are applied to the TLC plate (Kushwaha et al., 2021).

Any concentration or reconstitution procedure should be applied identically to light-exposed and dark-control aliquots. This ensures that observed differences are less likely to arise from inconsistent sample preparation before chromatography.

5.4 TLC Evaluation and Directional Agreement

The third phase of Figure 2 evaluates authentic curcuminoid standards, matched dark controls, and light-exposed samples under consistent TLC conditions. Authentic standards provide reference positions for the selected markers, while the control and exposed lanes permit direct comparison of marker-band and broader fingerprint changes. The primary analytical outcome is the normalized change in each curcuminoid marker-band intensity in the light-exposed sample relative to its matched dark control. Broader changes, including newly appearing bands, disappearing bands, or alterations in the overall chromatographic pattern, are treated as secondary fingerprint outcomes (Pei et al., 2023).

Application volume, sample concentration, plate type, mobile phase, development conditions, visualization method, and image-acquisition settings should remain consistent across samples. Standardized image analysis or densitometric measurement is preferable to unaided visual inspection because it reduces subjectivity when estimating relative band change (Pei et al., 2023). The normalized change for each marker should be calculated using the dark-control band as the reference condition. This comparison helps distinguish light-associated change from differences already present in the starting decoction or introduced during sample processing.

A minimum threshold for meaningful marker-band change should be established before comparing the computational and experimental rankings. Changes below that threshold or within measurement uncertainty should be classified as unchanged or tied rather than converted into an unsupported rank order. Computational and TLC outcomes should be compared through directional agreement rather than numerical equivalence. Calculated molecular properties and chromatographic band intensities represent different physical measurements, so computational

values should not be interpreted as direct predictions of a specific percentage of experimental band loss.

Within the proposed framework, complete agreement occurs when the observed order of change reproduces the full predicted three-marker ranking. Partial agreement occurs when the highest-ranked marker shows the greatest meaningful change but the remaining markers are tied or reversed. Absent agreement occurs when the marker predicted to be most susceptible does not show the greatest meaningful change. An indeterminate outcome should be reported when marker detection, measurement uncertainty, or insufficient differentiation prevents a defensible comparison.

These categories evaluate whether computation successfully prioritized the relative experimental response. They do not establish that the calculations identified the exact degradation pathway or that every observed TLC alteration resulted directly from photochemical degradation.

5.5 Framework Boundaries and Confirmatory Analysis

Directional agreement would provide preliminary support for the predictive utility of the framework, whereas disagreement could reveal limitations related to the molecular model, lamp spectrum, decoction matrix, marker extraction, or analytical sensitivity. Either outcome would therefore provide information about the feasibility and boundaries of prospective computational prioritization. Agreement should not be interpreted as proof that isolated-molecule calculations fully represent chemical behavior within the decoction. Environment-dependent excitation, solvation, aggregation, oxygen availability, and interactions among co-extracted compounds may alter the response of curcuminoids within the herbal matrix (Jen et al., 2022).

TLC can reveal relative marker-band changes and broader chromatographic perturbations, but it cannot independently establish the identity of an unknown product or the mechanism responsible for its formation. Even complete directional agreement would support framework feasibility rather than definitive confirmation of a photochemical pathway (Kotra et al., 2019). Samples showing substantial and reproducible changes should be prioritized for subsequent analysis using HPLC, LC–MS, or NMR. These methods can provide stronger separation, quantification, and structural identification than TLC alone (Noviana et al., 2022).

The proposed framework prospectively connects molecular prediction, standardized herbal preparation, controlled environmental exposure, and targeted analytical evaluation. Computation narrows the initial question, TLC provides a feasible first-line screen, and more resource-intensive analytical methods are reserved for compounds and samples supported by the strongest reproducible preliminary evidence.

6. Broader Implications and Future Directions

The broader implication of the proposed framework is a shift toward more explicitly hypothesis-driven investigation of herbal chemical variability. By generating priorities before

experimentation, computational approaches may help researchers focus limited analytical resources on compounds and conditions supported by a defined chemical rationale.

This framework is not intended to establish clinical equivalence, safety, efficacy, or universal stability classifications from computational predictions alone. Its immediate contribution is methodological: it provides a transparent process for deciding which chemical questions should be investigated first while preserving direct analytical measurement as the basis for determining what occurs in the preparation.

6.1 Extension Across Variability Sources and Herbal Systems

Post-preparation light exposure represents only one of the lifecycle sources of variability identified in Figure 1. Future applications could examine other storage conditions, processing methods, decoction variables, and raw-material factors, provided that each investigation is reduced to a defined and experimentally testable question (Ji et al., 2024). Preparation-related applications may examine changes in herb-to-water ratio, water properties, temperature, heating duration, extraction procedure, or filtration. These variables can alter which constituents enter the liquid phase and their relative abundance, making them appropriate targets for prospective prioritization before conducting extensive extraction comparisons (Hlatshwayo et al., 2025).

The framework could also progress from a single-herb Jiang Huang preparation to herb pairs and multi-herb formulas. Co-decoction may alter extraction, dissolution, precipitation, and constituent abundance in ways that cannot be predicted solely from analysis of the individual herbs (Jang et al., 2025). Expansion should occur gradually because increasing the number of herbs also increases the number of constituents, interactions, and possible explanations for an observed change. Beginning with well-characterized herb pairs or small formulas would preserve interpretability while testing whether the prioritization logic remains useful in more complex matrices.

The computational approach should evolve with the chemical question rather than remain fixed across all applications. Molecular dynamics may become useful when solvation, aggregation, or interactions among constituents are the primary focus because these processes are not fully represented by isolated-molecule electronic-structure calculations (Jen et al., 2022). Cheminformatics and chemometric methods could support the organization of larger compound libraries and comparison of analytical fingerprints across multiple preparations. Machine-learning approaches may become appropriate only after sufficiently large, standardized, and experimentally relevant datasets have been generated (Romano, 2019).

The different computational methods should therefore be viewed as complementary components of a developing research strategy rather than as competing replacements for one another. Electronic-structure modeling may guide small molecule-centered questions, while interaction-based and data-driven approaches may become more informative as matrix complexity and the experimental evidence base increase.

6.2 Strengthening Validation and Reproducibility

TLC provides a feasible first-line analytical evaluation for the proposed proof-of-concept, but future investigations should incorporate methods capable of stronger quantification and structural confirmation. HPLC can improve separation and quantitative comparison, while LC–MS and NMR can provide additional evidence concerning the identities of altered or newly appearing constituents (Noviana et al., 2022). Confirmatory analysis would be especially important when TLC reveals substantial marker loss, newly appearing bands, or disagreement with the predicted ranking. These findings could reflect chemical transformation, matrix interference, limited extraction, insufficient chromatographic resolution, or limitations in the computational model.

Future studies should also evaluate reproducibility across independently prepared decoctions rather than relying only on aliquots derived from one preparation. Repeating the exposure and analytical workflow across separate preparation batches would help determine whether an observed ranking is reproducible or dependent on one starting sample. Additional replication across TLC plates, exposure runs, operators, and analytical instruments would strengthen confidence in the framework. After the model has been refined within one laboratory, cross-laboratory evaluation could determine whether the prioritization process remains interpretable under different research settings.

Prospective decision rules should remain central as the framework develops. Computational-ranking criteria, procedures for handling conflicting descriptors, minimum analytical-change thresholds, and definitions of agreement should be documented before the corresponding experimental findings are interpreted. Both agreement and disagreement should be reported because each provides information about the framework's boundaries. Restricting publication or analysis to successful predictions would prevent meaningful evaluation of the conditions under which computational prioritization is or is not useful.

6.3 Toward a Scalable Prioritization Framework

Over time, the proposed workflow could develop into a structured system for recording paired computational predictions and experimental observations. Each record could include the herbal preparation, marker compounds, variability source, computational method, predicted ranking, analytical endpoint, observed response, and classification of agreement. Accumulating these records would create an evidence base for evaluating when prospective prioritization performs consistently and when matrix complexity, analytical sensitivity, or model assumptions limit its usefulness. Negative and indeterminate findings would be as important as successful rankings because they could reveal where additional modeling or stronger analytical methods are required.

A sufficiently standardized collection of prediction–observation records could later support larger-scale cheminformatic or machine-learning analysis. The usefulness of those approaches would depend on consistent documentation of preparation procedures, exposure conditions, computational outputs, analytical measurements, and unsuccessful as well as successful

predictions (Romano, 2019). Such a system could also improve transparency by making the basis for compound selection and experimental prioritization explicit. Rather than presenting computational results only after laboratory findings are known, the framework would preserve a record of what was predicted, how the prediction was derived, and how it performed when challenged experimentally.

The long-term value of the framework is therefore not limited to correctly predicting the relative response of three curcuminoids. Its broader purpose is to establish an iterative process through which computational hypotheses can be prospectively generated, experimentally evaluated, and refined as new evidence becomes available. This progression maintains the central boundary of the proposed approach: computational methods guide the allocation of experimental attention, but analytical chemistry remains necessary to characterize the composition and chemical changes of herbal preparations. The following section summarizes the proposed framework and its intended contribution to hypothesis-driven herbal chemistry research.

7. Conclusion

Chemical variability in herbal preparations can arise across botanical sourcing, raw-material selection, processing, decoction, herb–herb interactions, and post-preparation exposure. Although modern analytical methods can characterize complex chemical profiles, the number of constituents and variability conditions makes comprehensive testing difficult and creates a need for more deliberate experimental prioritization (Noviana et al., 2022). This perspective proposes that computational approaches can provide a prospective layer of chemical reasoning before extensive analytical investigation begins. Their purpose is not to determine what has occurred within an herbal preparation, but to identify compounds and chemical questions that warrant targeted experimental attention (Molski, 2025).

The proposed proof-of-concept applies this principle to controlled post-preparation light exposure in a Jiang Huang decoction. Curcumin, demethoxycurcumin, and bisdemethoxycurcumin provide a manageable marker set because they share a related conjugated scaffold while differing in structural features that may influence electronic and light-related behavior (Priyadarsini, 2014).

Ground-state density functional theory and time-dependent density functional theory are proposed to generate a prospective ranking of relative light susceptibility, while thin-layer chromatography provides an accessible initial evaluation of marker-band and broader fingerprint changes. Comparing the computational ranking with normalized changes in matched light-exposed and dark-control samples allows the predictive hypothesis to be evaluated without treating calculated molecular descriptors and chromatographic measurements as numerically equivalent (Ghosh & Sarkar, 2024). Directional agreement would provide preliminary support for the feasibility of computational prioritization, but it would not establish an exact degradation pathway, identify unknown transformation products, or demonstrate that isolated-molecule predictions fully represent the decoction matrix. Substantial or reproducible changes would

therefore require confirmation using methods capable of stronger quantification and structural characterization, such as HPLC, LC–MS, or NMR (Noviana et al., 2022).

The broader contribution of the framework lies in its sequence: define a focused chemical question, record a computational prediction before experimentation, apply a controlled variability condition, and evaluate the prediction analytically. By making prioritization explicit and prospective, this approach may support more transparent, efficient, and hypothesis-driven investigation of herbal chemical variability while maintaining analytical chemistry as the essential basis for experimental determination.

References

Appendino, G., Allegrini, P., de Combarieu, E., Novicelli, F., Ramaschi, G., & Sardone, N. (2022). Shedding light on curcumin stability. *Fitoterapia, 156*, 105084. https://doi.org/10.1016/j.fitote.2021.105084

Baira, K., Ounissi, A., Merouani, H., Alam, M., Ouddai, N., Erto, A., Yadav, K. K., Islam, S., Cheon, J.-K., Jeon, B.-H., & Benguerba, Y. (2022). Multitask quantum study of the curcumin-based complex physicochemical and biological properties. *International Journal of Molecular Sciences, 23*(5), 2832. https://doi.org/10.3390/ijms23052832

Chen, L.-L., Verpoorte, R., Yen, H.-R., Peng, W.-H., Cheng, Y.-C., Chao, J., & Pao, L.-H. (2018). Effects of processing adjuvants on traditional Chinese herbs. *Journal of Food and Drug Analysis, 26*(2 Suppl.), S96–S114. https://doi.org/10.1016/j.jfda.2018.02.004

Cheung, H. P., Wang, S. W., Ng, T. B., Zhang, Y. B., Lao, L. X., Zhang, Z. J., Tong, Y., Chung, F. W. S., & Sze, S. C. W. (2017). Comparison of chemical profiles and effectiveness between Erxian decoction and mixtures of decoctions of its individual herbs: A novel approach for identification of the standard chemicals. *Chinese Medicine, 12*, Article 1. https://doi.org/10.1186/s13020-016-0123-8

Ghosh, M., & Sarkar, N. (2024). Exploring the world of curcumin: Photophysics, photochemistry, and applications in nanoscience and biology. *ChemBioChem, 25*(23), e202400335. https://doi.org/10.1002/cbic.202400335

Gibbard, J. A. (2025). On the intrinsic stability of curcumin. *Physical Chemistry Chemical Physics, 27*(42), 22698–22709. https://doi.org/10.1039/D5CP02049B

Hlatshwayo, S., Thembane, N., Krishna, S. B. N., Gqaleni, N., & Ngcobo, M. (2025). Extraction and processing of bioactive phytoconstituents from widely used South African medicinal plants for the preparation of effective traditional herbal medicine products: A narrative review. *Plants, 14*(2), 206. https://doi.org/10.3390/plants14020206

Jang, D., Shin, S., Lee, S. M., Lee, S., Kim, C.-E., & Jung, J. (2025). Combined decoction selectively modifies chemical composition of traditional Asian medicine: A systematic analysis

on Palmijihwang-tang using theoretical additive model. *BMC Complementary Medicine and Therapies, 25*, 417. https://doi.org/10.1186/s12906-025-05153-w

Jen, M., Lee, S., Lee, G., Lee, D., & Pang, Y. (2022). Intramolecular charge transfer of curcumin and solvation dynamics of DMSO probed by time-resolved Raman spectroscopy. *International Journal of Molecular Sciences, 23*(3), 1727. https://doi.org/10.3390/ijms23031727

Ji, P., Yang, X., & Zhao, X. (2024). Application of metabolomics in quality control of traditional Chinese medicines: A review. *Frontiers in Plant Science, 15*, 1463666. https://doi.org/10.3389/fpls.2024.1463666

Kim, J.-H., Lee, K., Jerng, U. M., & Choi, G. (2019). Global comparison of stability testing parameters and testing methods for finished herbal products. *Evidence-Based Complementary and Alternative Medicine, 2019*, 7348929. https://doi.org/10.1155/2019/7348929

Kim, H., Oh, J., & Hong, J. (2025). Photodegradation of turmeric oleoresin under fluorescent light and white LED: Impacts on the chemical stability, bioactivity, and photosensitizing property of curcuminoids. *Molecules, 30*(15), 3187. https://doi.org/10.3390/molecules30153187

Kotra, V. S. R., Satyabanta, L., & Goswami, T. K. (2019). A critical review of analytical methods for determination of curcuminoids in turmeric. *Journal of Food Science and Technology, 56*(12), 5153–5166. https://doi.org/10.1007/s13197-019-03986-1

Kushwaha, P., Shukla, B., Dwivedi, J., & Saxena, S. (2021). Validated high-performance thin-layer chromatographic analysis of curcumin in the methanolic fraction of *Curcuma longa* L. rhizomes. *Future Journal of Pharmaceutical Sciences, 7*, 178. https://doi.org/10.1186/s43094-021-00330-3

Laher, F., Aremu, A. O., Van Staden, J., & Finnie, J. F. (2013). Evaluating the effect of storage on the biological activity and chemical composition of three South African medicinal plants. *South African Journal of Botany, 88*, 414–418. https://doi.org/10.1016/j.sajb.2013.09.003

Molski, M. (2025). Reactivity of curcumin: Theoretical insight from a systematic density functional theory-based review. *International Journal of Molecular Sciences, 26*(21), 10374. https://doi.org/10.3390/ijms262110374

Moomin, A., Russell, W. R., Knott, R. M., Scobbie, L., Mensah, K. B., Adu-Gyamfi, P. K. T., & Duthie, S. J. (2023). Season, storage and extraction method impact on the phytochemical profile of *Terminalia ivorensis*. *BMC Plant Biology, 23*, 162. https://doi.org/10.1186/s12870-023-04144-8

Muyumba, N. W., Mutombo, S. C., Sheridan, H., Nachtergael, A., & Duez, P. (2021). Quality control of herbal drugs and preparations: The methods of analysis, their relevance and applications. *Talanta Open, 4*, 100070. https://doi.org/10.1016/j.talo.2021.100070

Ncube, B., Finnie, J. F., & Van Staden, J. (2012). Quality from the field: The impact of environmental factors as quality determinants in medicinal plants. *South African Journal of Botany, 82*, 11–20. https://doi.org/10.1016/j.sajb.2012.05.009

Noviana, E., Indrayanto, G., & Rohman, A. (2022). Advances in fingerprint analysis for standardization and quality control of herbal medicines. *Frontiers in Pharmacology, 13*, 853023. https://doi.org/10.3389/fphar.2022.853023

Pei, W., Huang, Y., Qu, Y., Cui, X., Zhou, L., Yang, H., Zhao, M., Zhang, Z., He, F., & Zhou, H. (2023). A strategy for quality evaluation of complex herbal preparations based on multi-color scale and efficacy-oriented high-performance thin-layer chromatography characteristic fingerprint combined with chemometric method: Sanwujiao Pills as an example. *Heliyon, 9*(11), e22098. https://doi.org/10.1016/j.heliyon.2023.e22098

Price, L. C., & Buescher, R. W. (1996). Decomposition of turmeric curcuminoids as affected by light, solvent and oxygen. *Journal of Food Biochemistry, 20*(5), 125–133. https://doi.org/10.1111/j.1745-4514.1996.tb00577.x

Priyadarsini, K. I. (2009). Photophysics, photochemistry and photobiology of curcumin: Studies from organic solutions, bio-mimetics and living cells. *Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 10*(2), 81–95. https://doi.org/10.1016/j.jphotochemrev.2009.05.001

Priyadarsini, K. I. (2014). The chemistry of curcumin: From extraction to therapeutic agent. *Molecules, 19*(12), 20091–20112. https://doi.org/10.3390/molecules191220091

Romano, J. D., & Tatonetti, N. P. (2019). Informatics and computational methods in natural product drug discovery: A review and perspectives. *Frontiers in Genetics, 10*, 368. https://doi.org/10.3389/fgene.2019.00368

Wang, H., Chen, Y., Wang, L., Liu, Q., Yang, S., & Wang, C. (2023). Advancing herbal medicine: Enhancing product quality and safety through robust quality control practices. *Frontiers in Pharmacology, 14*, 1265178. https://doi.org/10.3389/fphar.2023.1265178